



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:05 AM GMT

PDB ID : 1W0D
Title : THE HIGH RESOLUTION STRUCTURE OF MYCOBACTERIUM TUBERCULOSIS LEUB (RV2995C)
Authors : Singh, R.K.; Kefala, G.; Janowski, R.; Mueller-Dieckmann, C.; Weiss, M.S.; (Tb), Tb Structural Genomics Consortium
Deposited on : 2004-06-03
Resolution : 1.65 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

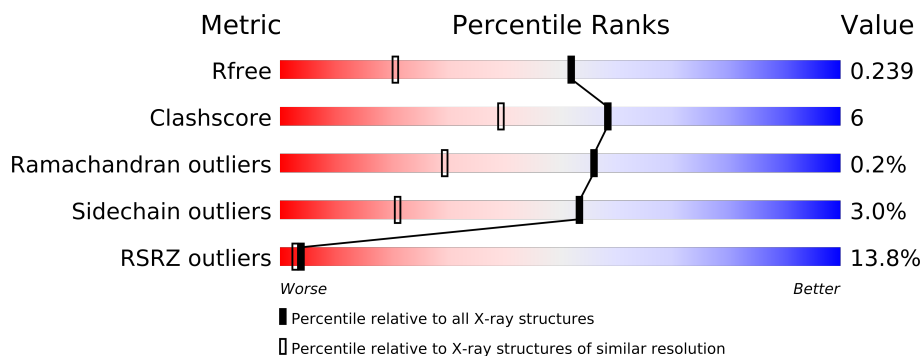
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



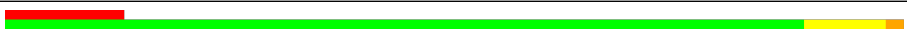
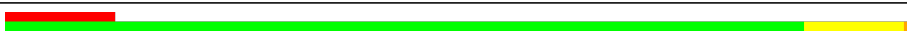
The reported resolution of this entry is 1.65 Å.

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}	66092	1404 (1.68-1.64)
Clashscore	79885	1001 (1.66-1.66)
Ramachandran outliers	78287	1581 (1.68-1.64)
Sidechain outliers	78261	1580 (1.68-1.64)
RSRZ outliers	66119	1404 (1.68-1.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	337	
1	B	337	
1	C	337	
1	D	337	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10609 atoms, of which 0 are hydrogen and 0 are deuterium.

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 3-ISOPROPYLMALATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	3	0
			2511	1568	461	475	7			
1	B	337	Total	C	N	O	S	0	1	0
			2500	1561	458	475	6			
1	C	337	Total	C	N	O	S	0	2	0
			2507	1565	461	475	6			
1	D	337	Total	C	N	O	S	0	2	0
			2507	1565	461	475	6			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

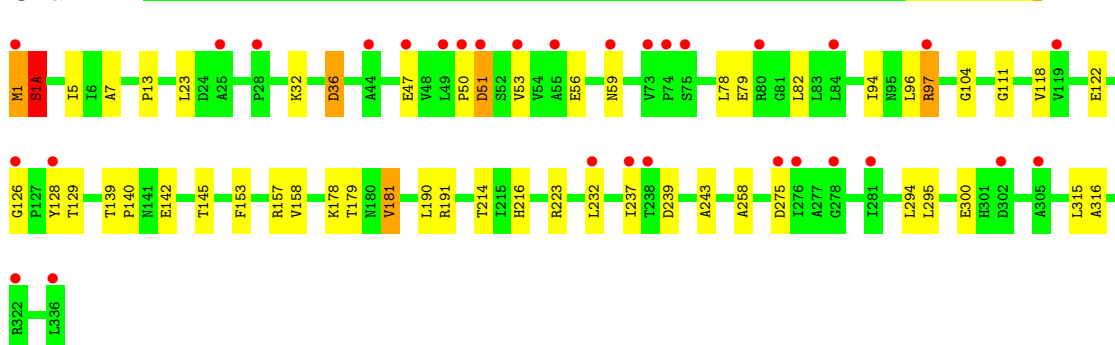
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	140	Total 140	O 140	0	0
3	B	87	Total 87	O 87	0	0
3	C	177	Total 177	O 177	0	0
3	D	175	Total 175	O 175	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

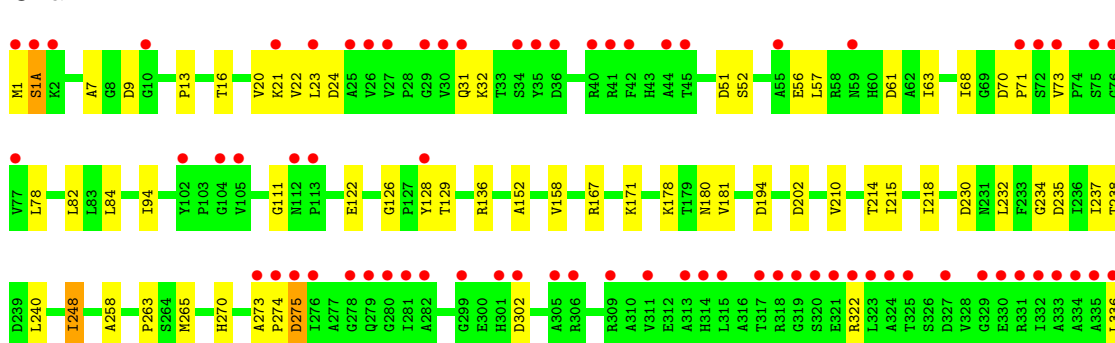
• Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE

Chain A:



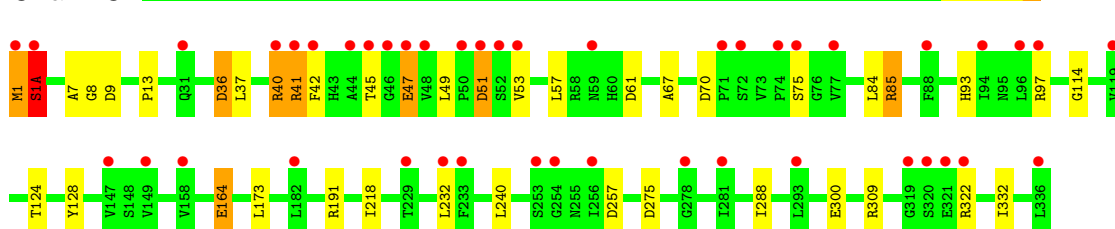
• Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE

Chain B:



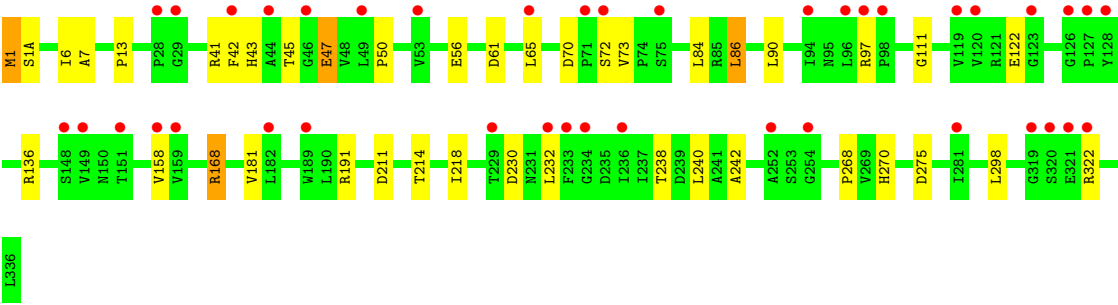
• Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE

Chain C:



• Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.47Å 97.06Å 181.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.65 29.91 – 1.65	Depositor EDS
% Data completeness (in resolution range)	93.1 (30.00-1.65) 93.1 (29.91-1.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.213 , 0.241 0.214 , 0.239	Depositor DCC
R_{free} test set	3127 reflections (2.05%)	DCC
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 25.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 155551 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10609	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.77	0/2567	0.96	6/3495 (0.2%)
1	B	0.70	0/2548	0.91	8/3471 (0.2%)
1	C	0.84	2/2559 (0.1%)	1.04	12/3485 (0.3%)
1	D	0.81	0/2559	1.00	6/3485 (0.2%)
All	All	0.78	2/10233 (0.0%)	0.98	32/13936 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	97[A]	ARG	CZ-NH1	5.41	1.40	1.33
1	C	97[B]	ARG	CZ-NH1	5.41	1.40	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	97[A]	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	C	97[B]	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	A	51	ASP	CB-CG-OD2	7.61	125.15	118.30
1	C	9	ASP	CB-CG-OD2	6.68	124.32	118.30
1	C	191	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	C	36	ASP	CB-CG-OD2	6.22	123.90	118.30
1	D	230	ASP	CB-CG-OD2	5.95	123.65	118.30
1	D	275	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	194	ASP	CB-CG-OD2	5.86	123.57	118.30
1	D	61	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	136	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	36	ASP	CB-CG-OD2	5.73	123.45	118.30
1	A	111	GLY	N-CA-C	5.70	127.34	113.10
1	C	61	ASP	CB-CG-OD2	5.69	123.42	118.30
1	D	70	ASP	CB-CG-OD2	5.69	123.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	275	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	9	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	230	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	173	LEU	CB-CG-CD2	-5.51	101.63	111.00
1	D	136	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	C	275	ASP	CB-CG-OD2	5.46	123.21	118.30
1	D	191	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	257	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	97[A]	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	A	97[B]	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	C	309	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	C	70	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	51	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	302	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	51	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	191	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2511	0	2518	48	0
1	B	2500	0	2504	46	0
1	C	2507	0	2513	25	0
1	D	2507	0	2513	29	0
2	D	5	0	0	0	0
3	A	140	0	0	2	0
3	B	87	0	0	0	1
3	C	177	0	0	4	1
3	D	175	0	0	2	0
All	All	10609	0	10048	125	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (125) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:168:ARG:HG2	1:D:168:ARG:HH11	1.30	0.95
1:D:218:ILE:HD11	1:D:240:LEU:HD11	1.52	0.91
1:A:181:VAL:HG13	1:B:128:TYR:CD1	2.13	0.84
1:A:243:ALA:CB	1:B:218:ILE:HD11	2.09	0.82
1:B:210:VAL:O	1:B:214:THR:HG23	1.83	0.79
1:D:122:GLU:HG2	1:D:158:VAL:HG21	1.67	0.77
1:B:52:SER:O	1:B:56:GLU:HG3	1.87	0.75
1:A:243:ALA:HB1	1:B:218:ILE:HD11	1.69	0.73
1:C:1:MET:O	1:C:1(A):SER:HB2	1.88	0.72
1:C:164:GLU:HG2	3:C:2096:HOH:O	1.89	0.72
1:A:79:GLU:OE2	1:B:180:ASN:ND2	2.24	0.70
1:A:181:VAL:CG1	1:B:128:TYR:CD1	2.75	0.69
1:D:45:THR:OG1	1:D:47:GLU:HG2	1.93	0.69
1:C:36:ASP:O	1:C:41:ARG:HB3	1.95	0.67
1:D:168:ARG:HG2	1:D:168:ARG:NH1	2.07	0.67
1:A:243:ALA:HB3	1:B:218:ILE:HD11	1.76	0.67
1:B:122:GLU:HG2	1:B:158:VAL:HG21	1.76	0.66
1:B:248:ILE:HD12	1:B:270:HIS:HA	1.78	0.66
1:A:126:GLY:O	1:A:129:THR:HG23	1.96	0.65
1:C:128:TYR:CD1	1:D:181:VAL:HG11	2.31	0.65
1:B:167:ARG:HA	1:B:171:LYS:HD3	1.78	0.65
1:C:41:ARG:O	1:C:45:THR:OG1	2.14	0.64
1:A:1:MET:O	1:A:1(A):SER:HB2	1.98	0.64
1:C:49:LEU:HD23	1:C:85:ARG:HG2	1.80	0.64
1:A:216:HIS:HB3	1:A:223:ARG:HD3	1.80	0.63
1:A:153:PHE:O	1:A:157[A]:ARG:HG3	2.02	0.60
1:C:40:ARG:CZ	3:C:2023:HOH:O	2.50	0.59
1:A:47:GLU:HB3	1:A:50:PRO:HG3	1.84	0.59
1:A:232:LEU:HD23	1:A:232:LEU:C	2.24	0.57
1:A:97[B]:ARG:NH2	1:A:239:ASP:OD1	2.35	0.57
1:A:181:VAL:HG22	1:B:128:TYR:HA	1.86	0.56
1:D:42:PHE:CD2	1:D:73:VAL:HG22	2.40	0.56
1:A:1:MET:N	1:A:300:GLU:OE2	2.39	0.56
1:C:40:ARG:HD2	3:C:2020:HOH:O	2.07	0.55
1:B:63:ILE:HB	1:B:265:MET:HG3	1.89	0.55
1:C:36:ASP:OD1	1:C:40:ARG:HD3	2.06	0.55
1:B:63:ILE:CG2	1:B:265:MET:HG3	2.38	0.54
1:A:181:VAL:HG21	1:B:128:TYR:HB3	1.89	0.54
1:D:42:PHE:HD2	1:D:73:VAL:HG22	1.73	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:93:HIS:HA	1:C:124:THR:HG23	1.91	0.53
1:C:1:MET:N	1:C:300:GLU:OE2	2.43	0.52
1:A:181:VAL:HG11	1:B:128:TYR:CG	2.45	0.52
1:A:128:TYR:HA	1:B:181:VAL:CG2	2.40	0.51
1:A:50:PRO:HB2	1:A:53:VAL:HG23	1.93	0.51
1:A:94:ILE:HD12	1:A:258:ALA:HB2	1.93	0.51
1:A:36:ASP:O	1:A:36:ASP:OD2	2.28	0.51
1:D:168:ARG:HH11	1:D:168:ARG:CG	2.14	0.51
1:D:97[B]:ARG:NH2	1:D:238:THR:O	2.44	0.51
1:D:7:ALA:HB1	1:D:13:PRO:HA	1.93	0.51
1:C:36:ASP:O	1:C:41:ARG:CB	2.59	0.50
1:C:41:ARG:HG3	1:C:47:GLU:O	2.11	0.50
1:B:22:VAL:HG13	1:B:336:LEU:HD11	1.93	0.50
1:B:248:ILE:CD1	1:B:270:HIS:HA	2.41	0.50
1:B:111:GLY:HA2	1:D:111:GLY:HA2	1.93	0.50
1:A:294:LEU:C	1:A:294:LEU:HD23	2.31	0.50
1:D:84:LEU:HD22	3:D:2073:HOH:O	2.11	0.50
1:B:111:GLY:CA	1:D:111:GLY:HA2	2.41	0.50
1:A:78:LEU:O	1:A:82:LEU:HB3	2.10	0.50
1:D:47:GLU:HB2	1:D:50:PRO:HD3	1.95	0.49
1:A:122:GLU:HG2	1:A:158:VAL:HG21	1.95	0.49
1:D:97[B]:ARG:NH2	1:D:242:ALA:HB2	2.27	0.48
1:B:234:GLY:O	1:B:238:THR:HG23	2.13	0.48
1:A:258:ALA:HB3	3:A:2036:HOH:O	2.11	0.48
1:C:128:TYR:CG	1:D:181:VAL:HG11	2.48	0.48
1:C:7:ALA:HB1	1:C:13:PRO:HA	1.96	0.48
1:A:179:THR:HG21	1:A:190:LEU:HG	1.96	0.47
1:B:7:ALA:HB1	1:B:13:PRO:HA	1.97	0.47
1:B:178:LYS:HG3	1:B:181:VAL:HG12	1.97	0.47
1:D:86:LEU:HD22	1:D:90:LEU:CD1	2.45	0.46
1:A:56:GLU:O	1:A:59:ASN:HB2	2.15	0.46
1:A:7:ALA:HB1	1:A:13:PRO:HA	1.96	0.46
1:A:94:ILE:CD1	1:A:258:ALA:HB2	2.45	0.46
1:A:1:MET:HB3	1:A:1(A):SER:H	1.52	0.46
1:A:96:LEU:HD11	1:A:118:VAL:HG11	1.97	0.46
1:A:145:THR:HG23	3:A:2068:HOH:O	2.16	0.46
1:C:232:LEU:C	1:C:232:LEU:HD23	2.36	0.45
1:A:142:GLU:HB3	1:B:152:ALA:HB2	1.99	0.45
1:D:97[B]:ARG:HH21	1:D:242:ALA:HB2	1.82	0.45
1:B:57:LEU:O	1:B:263:PRO:HG3	2.17	0.44
1:D:41:ARG:NH1	1:D:47:GLU:OE2	2.49	0.44
1:C:53:VAL:O	1:C:57:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:232:LEU:HD23	1:D:232:LEU:C	2.38	0.44
1:D:43:HIS:HE1	1:D:72:SER:O	1.99	0.44
1:B:84:LEU:HA	1:B:84:LEU:HD12	1.82	0.44
1:D:6:ILE:O	1:D:65:LEU:HA	2.17	0.44
1:A:178:LYS:NZ	1:B:235:ASP:OD2	2.49	0.44
1:C:37:LEU:HD21	1:C:53:VAL:HG11	2.00	0.44
1:D:1:MET:HG2	1:D:298:LEU:HD12	2.00	0.43
1:A:214:THR:HG21	1:B:240:LEU:HB2	1.99	0.43
1:A:316:ALA:O	1:C:114:GLY:HA3	2.17	0.43
1:B:94:ILE:CD1	1:B:258:ALA:HB2	2.49	0.43
1:B:232:LEU:C	1:B:232:LEU:HD23	2.38	0.43
1:D:43:HIS:CE1	1:D:72:SER:O	2.71	0.43
1:C:40:ARG:C	1:C:42:PHE:N	2.72	0.43
1:B:63:ILE:CB	1:B:265:MET:HG3	2.49	0.42
1:A:128:TYR:HA	1:B:181:VAL:HG22	2.00	0.42
1:B:273:ALA:N	1:B:274:PRO:HD3	2.34	0.42
1:A:23:LEU:CD1	1:A:295:LEU:HD21	2.50	0.42
1:A:139:THR:HB	1:A:140:PRO:HD2	2.02	0.42
1:C:288:ILE:HG21	1:C:332:ILE:HG21	2.01	0.42
1:C:218:ILE:HD11	1:C:240:LEU:HD11	2.01	0.41
1:D:211:ASP:O	1:D:214:THR:HB	2.20	0.41
1:D:84:LEU:CD2	3:D:2073:HOH:O	2.68	0.41
1:B:202:ASP:N	1:B:202:ASP:OD1	2.53	0.41
1:A:104:GLY:HA3	1:A:315:LEU:O	2.20	0.41
1:B:70:ASP:HA	1:B:71:PRO:HD2	1.87	0.41
1:B:126:GLY:O	1:B:129:THR:HG23	2.20	0.41
1:A:237:ILE:C	1:A:237:ILE:HD12	2.41	0.41
1:A:5:ILE:HD12	1:A:32:LYS:HB3	2.02	0.41
1:D:97[A]:ARG:HB3	1:D:97[A]:ARG:CZ	2.51	0.41
1:B:32:LYS:HB2	1:B:32:LYS:HE2	1.86	0.41
1:A:47:GLU:HB3	1:A:50:PRO:CG	2.48	0.41
1:A:239:ASP:HB3	1:B:215:ILE:HD11	2.03	0.41
1:B:1(A):SER:HA	1:B:61:ASP:OD1	2.21	0.41
1:C:41:ARG:HD3	1:C:47:GLU:HB3	2.03	0.41
1:A:295:LEU:HA	1:A:295:LEU:HD23	1.88	0.41
1:C:8:GLY:HA3	1:C:67:ALA:O	2.21	0.41
1:A:181:VAL:HG11	1:B:128:TYR:CD1	2.54	0.41
1:A:181:VAL:CG1	1:B:128:TYR:CG	3.04	0.41
1:A:181:VAL:HG22	1:B:128:TYR:CA	2.51	0.41
1:C:40:ARG:CD	3:C:2020:HOH:O	2.68	0.41
1:B:68:ILE:HG21	1:B:82:LEU:HD23	2.03	0.41
1:B:73:VAL:HG11	1:B:78:LEU:HG	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:268:PRO:HB2	1:D:270:HIS:CD2	2.57	0.40
1:B:16:THR:O	1:B:20:VAL:HG23	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	Distance(Å)	Clash(Å)
3:B:2009:HOH:O	3:C:2079:HOH:O[2_564]	2.14	0.06

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	338/337 (100%)	325 (96%)	12 (4%)	1 (0%)	50	24
1	B	336/337 (100%)	326 (97%)	10 (3%)	0	100	100
1	C	337/337 (100%)	320 (95%)	16 (5%)	1 (0%)	50	24
1	D	337/337 (100%)	322 (96%)	14 (4%)	1 (0%)	50	24
All	All	1348/1348 (100%)	1293 (96%)	52 (4%)	3 (0%)	56	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1(A)	SER
1	C	1(A)	SER
1	D	1(A)	SER

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	260/257 (101%)	255 (98%)	5 (2%)	69	43
1	B	258/257 (100%)	249 (96%)	9 (4%)	48	16
1	C	259/257 (101%)	248 (96%)	11 (4%)	40	12
1	D	259/257 (101%)	253 (98%)	6 (2%)	63	33
All	All	1036/1028 (101%)	1005 (97%)	31 (3%)	53	21

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	1(A)	SER
1	A	51	ASP
1	A	181	VAL
1	A	275	ASP
1	B	1	MET
1	B	1(A)	SER
1	B	21	LYS
1	B	23	LEU
1	B	31	GLN
1	B	237	ILE
1	B	248	ILE
1	B	275	ASP
1	B	322	ARG
1	C	1	MET
1	C	1(A)	SER
1	C	40	ARG
1	C	41	ARG
1	C	47	GLU
1	C	51	ASP
1	C	75	SER
1	C	84	LEU
1	C	85	ARG
1	C	164	GLU
1	C	322	ARG
1	D	1	MET
1	D	47	GLU
1	D	56	GLU
1	D	86	LEU
1	D	168	ARG
1	D	322	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	208	GLN
1	B	279	GLN
1	C	141	ASN
1	C	279	GLN
1	D	141	ASN
1	D	231	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	D	1337	-	4,4,4	0.31	0	6,6,6	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	D	1337	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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	337/337 (100%)	0.68	31 (9%) 9 7	10, 16, 28, 39	0
1	B	337/337 (100%)	1.17	71 (21%) 1 1	9, 17, 26, 37	0
1	C	337/337 (100%)	0.81	44 (13%) 4 3	9, 16, 32, 39	0
1	D	337/337 (100%)	0.73	40 (11%) 5 4	10, 16, 28, 38	0
All	All	1348/1348 (100%)	0.85	186 (13%) 4 3	9, 16, 29, 39	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	10.7
1	B	323	LEU	7.3
1	D	322	ARG	6.7
1	B	320	SER	6.5
1	B	281	ILE	6.4
1	B	322	ARG	6.4
1	B	324	ALA	6.3
1	C	44	ALA	6.2
1	B	336	LEU	6.1
1	B	334	ALA	5.7
1	B	45	THR	5.7
1	A	75	SER	5.1
1	B	274	PRO	5.1
1	D	319	GLY	5.0
1	B	29	GLY	4.5
1	B	311	VAL	4.5
1	B	332	ILE	4.4
1	C	71	PRO	4.4
1	C	322	ARG	4.3
1	D	29	GLY	4.3
1	B	23	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	275	ASP	4.1
1	B	276	ILE	4.1
1	B	321	GLU	4.1
1	D	320	SER	4.1
1	B	71	PRO	4.1
1	D	71	PRO	4.0
1	B	278	GLY	4.0
1	B	273	ALA	4.0
1	D	321	GLU	3.9
1	B	44	ALA	3.9
1	C	77	VAL	3.8
1	A	51	ASP	3.8
1	B	27	VAL	3.8
1	B	77	VAL	3.8
1	C	75	SER	3.7
1	B	279	GLN	3.7
1	C	233	PHE	3.7
1	C	59	ASN	3.6
1	B	31	GLN	3.6
1	B	30	VAL	3.6
1	B	319	GLY	3.6
1	A	74	PRO	3.5
1	D	44	ALA	3.5
1	A	49	LEU	3.5
1	D	75	SER	3.5
1	A	1	MET	3.5
1	C	1	MET	3.5
1	C	45	THR	3.5
1	B	59	ASN	3.5
1	B	309	ARG	3.5
1	C	46	GLY	3.4
1	C	1(A)	SER	3.4
1	B	42	PHE	3.4
1	A	322	ARG	3.3
1	A	278	GLY	3.3
1	A	275	ASP	3.3
1	B	128	TYR	3.3
1	B	317	THR	3.3
1	C	40	ARG	3.3
1	B	333	ALA	3.3
1	B	75	SER	3.3
1	C	96	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	327	ASP	3.3
1	D	233	PHE	3.2
1	D	96	LEU	3.2
1	C	51	ASP	3.2
1	B	25	ALA	3.1
1	C	74	PRO	3.1
1	C	321	GLU	3.1
1	A	281	ILE	3.1
1	C	94	ILE	3.1
1	A	336	LEU	3.1
1	D	46	GLY	3.0
1	D	120	VAL	3.0
1	C	319	GLY	3.0
1	B	330	GLU	3.0
1	C	158	VAL	3.0
1	C	119	VAL	3.0
1	B	40	ARG	2.9
1	C	320	SER	2.9
1	B	105	VAL	2.9
1	C	50	PRO	2.9
1	C	48	VAL	2.9
1	B	104	GLY	2.9
1	D	97[A]	ARG	2.8
1	C	42	PHE	2.8
1	C	53	VAL	2.8
1	D	158	VAL	2.8
1	D	252	ALA	2.8
1	C	281	ILE	2.8
1	B	305	ALA	2.8
1	B	302	ASP	2.8
1	D	182	LEU	2.8
1	A	50	PRO	2.8
1	D	254	GLY	2.7
1	D	127	PRO	2.7
1	C	72	SER	2.7
1	B	280	GLY	2.7
1	B	10	GLY	2.6
1	D	123	GLY	2.6
1	B	299	GLY	2.6
1	A	53	VAL	2.6
1	B	112	ASN	2.6
1	C	47	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	301	HIS	2.6
1	B	335	ALA	2.6
1	D	72	SER	2.6
1	A	59	ASN	2.6
1	A	119	VAL	2.6
1	A	232	LEU	2.6
1	B	41	ARG	2.6
1	B	282	ALA	2.6
1	D	159	VAL	2.5
1	C	336	LEU	2.5
1	D	128	TYR	2.5
1	B	313	ALA	2.5
1	D	229	THR	2.5
1	B	318	ARG	2.5
1	D	149	VAL	2.5
1	A	128	TYR	2.5
1	B	55	ALA	2.5
1	B	113	PRO	2.5
1	D	53	VAL	2.4
1	B	21	LYS	2.4
1	A	237	ILE	2.4
1	D	94	ILE	2.4
1	C	254	GLY	2.4
1	C	278	GLY	2.4
1	C	147	VAL	2.4
1	C	182	LEU	2.4
1	B	102	TYR	2.4
1	B	34	SER	2.4
1	B	2	LYS	2.4
1	A	25	ALA	2.4
1	C	88	PHE	2.4
1	B	73	VAL	2.4
1	B	306	ARG	2.4
1	D	42	PHE	2.4
1	C	232	LEU	2.3
1	C	293	LEU	2.3
1	A	55	ALA	2.3
1	C	97[A]	ARG	2.3
1	A	302	ASP	2.3
1	B	331	ARG	2.3
1	D	151	THR	2.3
1	A	126	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	238	THR	2.3
1	D	232	LEU	2.3
1	C	256	ILE	2.3
1	B	1(A)	SER	2.3
1	C	149	VAL	2.3
1	A	97[A]	ARG	2.3
1	B	26	VAL	2.3
1	D	119	VAL	2.3
1	B	325	THR	2.3
1	D	28	PRO	2.2
1	C	41	ARG	2.2
1	C	52	SER	2.2
1	A	28	PRO	2.2
1	C	31	GLN	2.2
1	B	76	GLY	2.2
1	A	305	ALA	2.2
1	B	329	GLY	2.2
1	D	126	GLY	2.2
1	D	65	LEU	2.2
1	B	72	SER	2.2
1	B	35	TYR	2.2
1	C	229	THR	2.2
1	B	315	LEU	2.1
1	A	276	ILE	2.1
1	B	36	ASP	2.1
1	A	47	GLU	2.1
1	D	189	TRP	2.1
1	D	236	ILE	2.1
1	D	281	ILE	2.1
1	D	234	GLY	2.1
1	A	73	VAL	2.1
1	D	148	SER	2.1
1	D	49	LEU	2.1
1	D	98	PRO	2.0
1	A	44	ALA	2.0
1	C	253	SER	2.0
1	A	80	ARG	2.0
1	B	314	HIS	2.0
1	A	84	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	D	1337	5/5	0.20	-	27,29,32,35	5

6.5 Other polymers

There are no such residues in this entry.