



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:45 AM UTC

PDB ID : 1W0D / pdb_00001w0d
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 Structural Genomics Consortium (TBSGC)
Deposited on : 2004-06-03
Resolution : 1.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

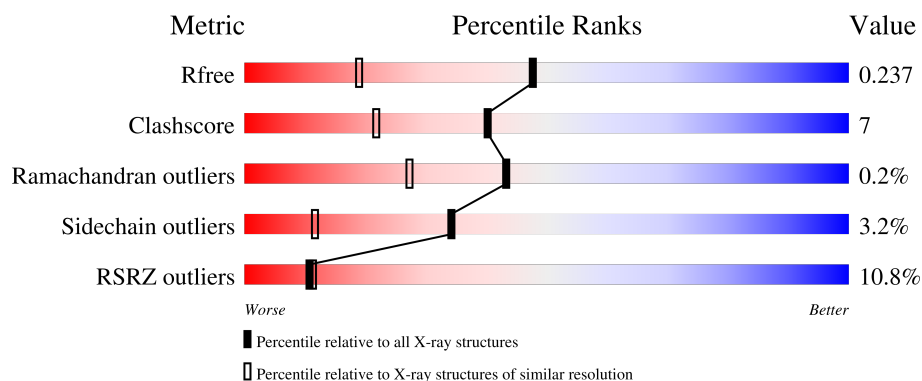
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	337	4% 83% 15% ..
1	B	337	21% 82% 16% .
1	C	337	9% 90% 9% .
1	D	337	8% 86% 12% ..

2 Entry composition [i](#)

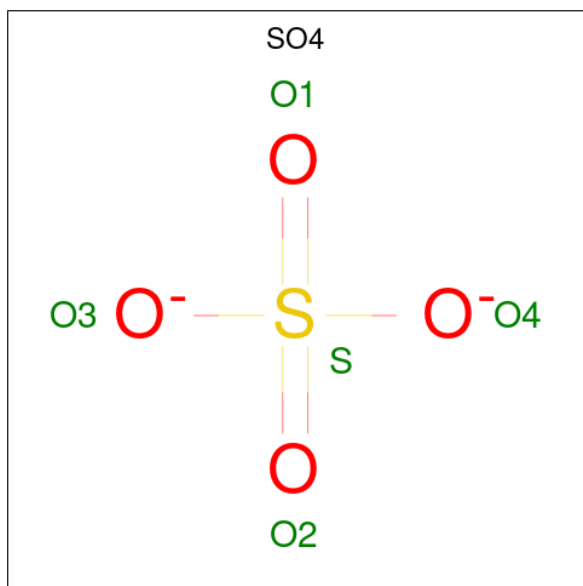
There are 3 unique types of molecules in this entry. The entry contains 10609 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 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 (CCD ID: SO4) (formula: O₄S).



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

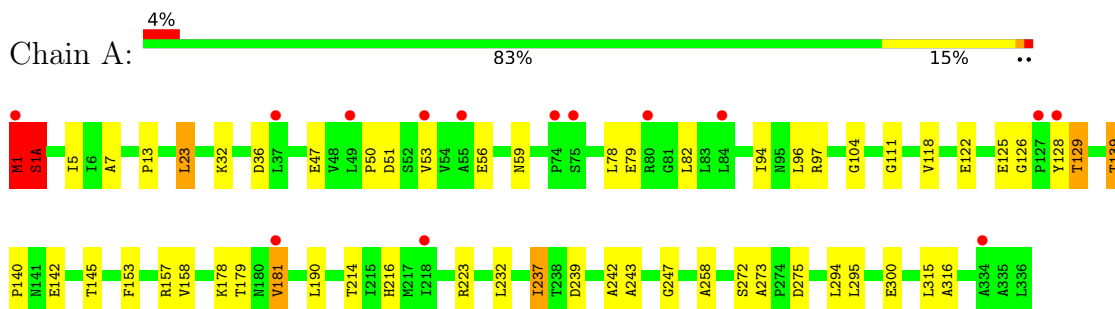
- Molecule 3 is water.

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

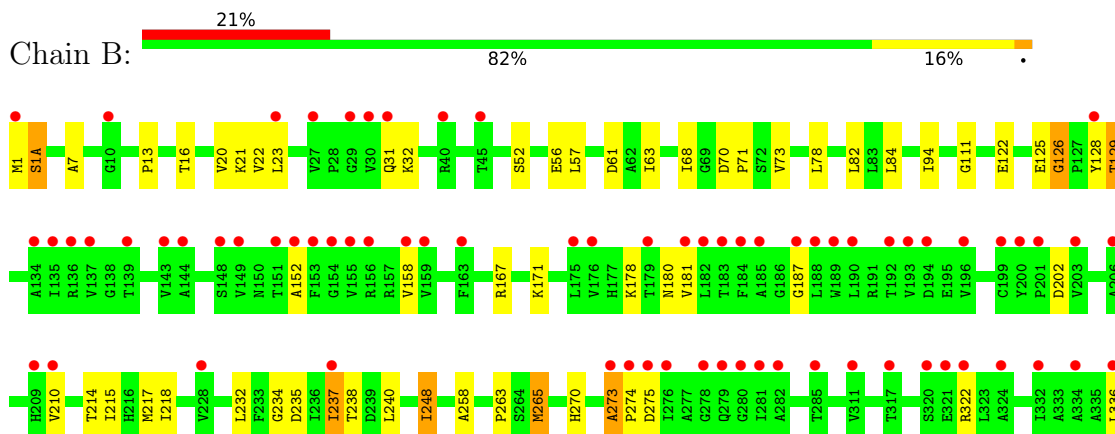
3 Residue-property plots [i](#)

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.

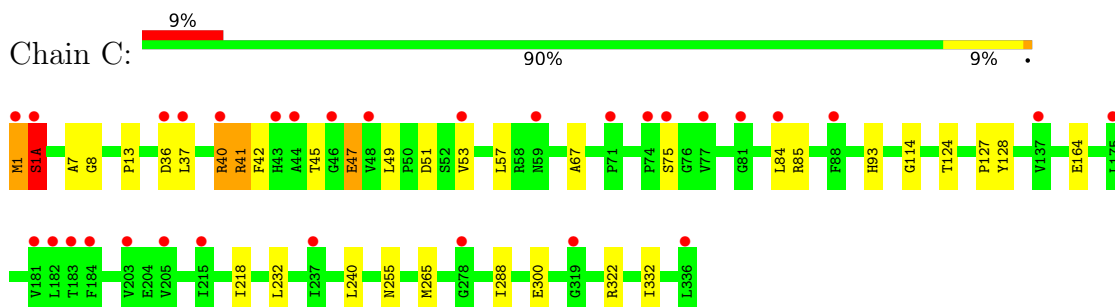
• Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE



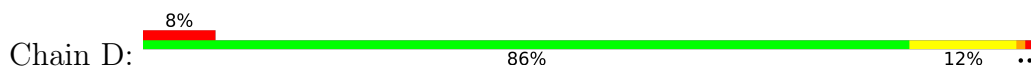
• Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE

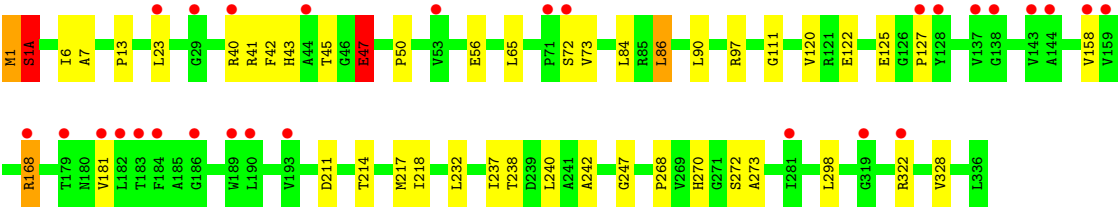


• Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE



• Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE





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 30.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	93.1 (30.00-1.65) 93.1 (30.00-1.65)	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 0.211 , 0.237	Depositor DCC
R_{free} test set	3127 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.99	2/2567 (0.1%)	1.12	5/3495 (0.1%)
1	B	0.89	1/2548 (0.0%)	1.06	5/3471 (0.1%)
1	C	1.05	2/2559 (0.1%)	1.15	1/3485 (0.0%)
1	D	1.01	0/2559	1.16	5/3485 (0.1%)
All	All	0.99	5/10233 (0.0%)	1.12	16/13936 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	265	MET	SD-CE	-9.35	1.56	1.79
1	A	139	THR	C-O	-7.24	1.18	1.24
1	B	265	MET	SD-CE	5.46	1.93	1.79
1	C	255	ASN	C-O	-5.10	1.18	1.24
1	A	1	MET	SD-CE	5.06	1.92	1.79

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	THR	N-CA-C	8.04	122.35	112.54
1	A	111	GLY	N-CA-C	7.75	127.34	114.48
1	D	47	GLU	N-CA-C	7.36	121.82	110.20
1	D	127	PRO	N-CA-C	6.96	122.59	114.03
1	C	127	PRO	N-CA-C	6.21	121.65	114.20
1	D	328	VAL	N-CA-C	-5.86	104.80	110.72
1	D	247	GLY	CA-C-O	-5.71	118.20	122.37
1	D	120	VAL	N-CA-C	-5.69	98.94	107.37
1	A	242	ALA	N-CA-C	-5.61	105.25	111.36
1	B	273	ALA	O-C-N	5.57	124.09	121.53
1	A	129	THR	N-CA-C	5.41	119.88	113.28
1	B	187	GLY	N-CA-C	-5.32	106.35	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	GLY	N-CA-C	5.22	116.91	111.95
1	B	126	GLY	CA-C-N	5.12	124.81	119.64
1	B	126	GLY	C-N-CA	5.12	124.81	119.64
1	A	237	ILE	CB-CG1-CD1	-5.09	103.12	113.80

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	2511	0	2518	50	0
1	B	2500	0	2504	48	0
1	C	2507	0	2513	25	0
1	D	2507	0	2513	33	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	133	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 7.

All (133) 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:168:ARG:HH11	1:D:168:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1:MET:O	1:A:1(A):SER:HB2	1.98	0.64
1:C:41:ARG:O	1:C:45:THR:OG1	2.14	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:232:LEU:C	1:A:232:LEU:HD23	2.24	0.62
1:B:217:MET:HE1	1:B:237:ILE:HD13	1.83	0.60
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: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:294:LEU:C	1:A:294:LEU:HD23	2.31	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:22:VAL:HG13	1:B:336:LEU:HD11	1.93	0.50
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:248:ILE:CD1	1:B:270:HIS:HA	2.41	0.50
1:C:232:LEU:C	1:C:232:LEU:HD23	2.36	0.50
1:B:111:GLY:HA2	1:D:111:GLY:HA2	1.93	0.50
1:D:84:LEU:HD22	3:D:2073:HOH:O	2.11	0.50
1:A:78:LEU:O	1:A:82:LEU:HB3	2.10	0.50
1:B:111:GLY:CA	1:D:111:GLY:HA2	2.41	0.50
1:D:47:GLU:HB2	1:D:50:PRO:HD3	1.95	0.49
1:D:232:LEU:C	1:D:232:LEU:HD23	2.38	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:B:232:LEU:HD23	1:B:232:LEU:C	2.38	0.48
1:C:7:ALA:HB1	1:C:13:PRO:HA	1.96	0.48
1:C:40:ARG:C	1:C:42:PHE:N	2.72	0.47
1:D:217:MET:HE1	1:D:237:ILE:HD13	1.97	0.47
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:D:1:MET:HE2	1:D:1(A):SER:H	1.79	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:A:142:GLU:HB3	1:B:152:ALA:HB2	1.99	0.45
1:A:237:ILE:C	1:A:237:ILE:HD12	2.41	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:B:122:GLU:CD	1:B:125:GLU:HG2	2.42	0.44
1:C:53:VAL:O	1:C:57:LEU:HG	2.17	0.44
1:D:41:ARG:NH1	1:D:47:GLU:OE2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:HIS:HE1	1:D:72:SER:O	1.99	0.44
1:B:84:LEU:HD12	1:B:84:LEU:HA	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:A:214:THR:HG21	1:B:240:LEU:HB2	1.99	0.43
1:D:1:MET:HG2	1:D:298:LEU:HD12	2.00	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:D:43:HIS:CE1	1:D:72:SER:O	2.71	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:D:122:GLU:CD	1:D:125:GLU:HG2	2.44	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:B:202:ASP:OD1	1:B:202:ASP:N	2.53	0.41
1:D:84:LEU:CD2	3:D:2073:HOH:O	2.68	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:5:ILE:HD12	1:A:32:LYS:HB3	2.02	0.41
1:A:272:SER:O	1:A:273:ALA:C	2.62	0.41
1:B:32:LYS:HE2	1:B:32:LYS:HB2	1.86	0.41
1:D:97[A]:ARG:CZ	1:D:97[A]:ARG:HB3	2.51	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:A:295:LEU:HD23	1:A:295:LEU:HA	1.88	0.41
1:C:8:GLY:HA3	1:C:67:ALA:O	2.21	0.41
1:C:41:ARG:HD3	1:C:47:GLU:HB3	2.03	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:A:181:VAL:HG11	1:B:128:TYR:CD1	2.54	0.41
1:B:68:ILE:HG21	1:B:82:LEU:HD23	2.03	0.41
1:C:40:ARG:CD	3:C:2020:HOH:O	2.68	0.41
1:A:122:GLU:CD	1:A:125:GLU:HG2	2.46	0.40
1:B:73:VAL:HG11	1:B:78:LEU:HG	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:SER:O	1:D:273:ALA:C	2.64	0.40
1:B:16:THR:O	1:B:20:VAL:HG23	2.21	0.40
1:D:268:PRO:HB2	1:D:270:HIS:CD2	2.57	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)
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%)	36	21
1	B	336/337 (100%)	326 (97%)	10 (3%)	0	100	100
1	C	337/337 (100%)	320 (95%)	16 (5%)	1 (0%)	36	21
1	D	337/337 (100%)	322 (96%)	14 (4%)	1 (0%)	36	21
All	All	1348/1348 (100%)	1293 (96%)	52 (4%)	3 (0%)	43	27

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%)	254 (98%)	6 (2%)	44	21
1	B	258/257 (100%)	249 (96%)	9 (4%)	32	10
1	C	259/257 (101%)	250 (96%)	9 (4%)	32	10
1	D	259/257 (101%)	250 (96%)	9 (4%)	32	10
All	All	1036/1028 (101%)	1003 (97%)	33 (3%)	34	12

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	1(A)	SER
1	A	23	LEU
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	322	ARG

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Mol	Chain	Res	Type
1	D	1	MET
1	D	1(A)	SER
1	D	23	LEU
1	D	40	ARG
1	D	47	GLU
1	D	56	GLU
1	D	86	LEU
1	D	168	ARG
1	D	322	ARG

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	60	HIS
1	A	208	GLN
1	B	59	ASN
1	B	279	GLN
1	C	279	GLN
1	D	208	GLN
1	D	231	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 [i](#)

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	0.30	0	6,6,6	0.32	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	337/337 (100%)	0.43	14 (4%) 40 44	7, 16, 28, 39	3 (0%)
1	B	337/337 (100%)	1.26	72 (21%) 2 3	7, 17, 26, 37	1 (0%)
1	C	337/337 (100%)	0.73	31 (9%) 14 16	8, 16, 32, 39	2 (0%)
1	D	337/337 (100%)	0.66	28 (8%) 17 19	8, 16, 28, 38	2 (0%)
All	All	1348/1348 (100%)	0.77	145 (10%) 11 11	7, 16, 29, 39	8 (0%)

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	44	ALA	6.6
1	B	1	MET	6.0
1	B	184	PHE	5.0
1	B	149	VAL	4.4
1	B	128	TYR	4.3
1	B	181	VAL	4.0
1	B	324	ALA	4.0
1	B	189	TRP	3.9
1	A	128	TYR	3.9
1	B	336	LEU	3.8
1	C	278	GLY	3.7
1	C	88	PHE	3.7
1	B	185	ALA	3.7
1	B	311	VAL	3.7
1	C	40	ARG	3.6
1	B	278	GLY	3.4
1	D	71	PRO	3.4
1	B	23	LEU	3.4
1	B	188	LEU	3.4
1	A	75	SER	3.4
1	B	151	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	3.4
1	B	190	LEU	3.3
1	B	143	VAL	3.3
1	B	135	ILE	3.3
1	B	152	ALA	3.3
1	B	187	GLY	3.2
1	C	77	VAL	3.2
1	B	196	VAL	3.2
1	D	29	GLY	3.1
1	B	45	THR	3.1
1	B	183	THR	3.1
1	B	320	SER	3.0
1	B	159	VAL	3.0
1	D	128	TYR	3.0
1	C	71	PRO	3.0
1	A	181	VAL	3.0
1	B	158	VAL	2.9
1	B	281	ILE	2.9
1	B	332	ILE	2.9
1	B	274	PRO	2.9
1	A	334	ALA	2.9
1	A	80	ARG	2.8
1	D	138	GLY	2.8
1	D	319	GLY	2.8
1	B	175	LEU	2.8
1	B	182	LEU	2.8
1	B	179	THR	2.8
1	A	84	LEU	2.8
1	A	37	LEU	2.8
1	D	182	LEU	2.8
1	B	153	PHE	2.7
1	B	210	VAL	2.7
1	C	48	VAL	2.7
1	B	276	ILE	2.7
1	C	36	ASP	2.7
1	B	334	ALA	2.7
1	C	74	PRO	2.6
1	B	192	THR	2.6
1	D	322	ARG	2.6
1	D	137	VAL	2.6
1	C	319	GLY	2.6
1	C	184	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	203	VAL	2.6
1	C	59	ASN	2.6
1	C	53	VAL	2.5
1	C	181	VAL	2.5
1	A	127	PRO	2.5
1	B	134	ALA	2.5
1	B	322	ARG	2.5
1	C	84	LEU	2.5
1	B	137	VAL	2.5
1	B	155	VAL	2.5
1	B	273	ALA	2.5
1	D	53	VAL	2.5
1	D	143	VAL	2.5
1	A	1	MET	2.5
1	D	72	SER	2.5
1	B	31	GLN	2.5
1	B	29	GLY	2.5
1	A	218	ILE	2.5
1	B	317	THR	2.5
1	A	49	LEU	2.4
1	B	163	PHE	2.4
1	A	74	PRO	2.4
1	B	136	ARG	2.4
1	D	183	THR	2.4
1	D	23	LEU	2.4
1	B	282	ALA	2.4
1	B	176	VAL	2.4
1	C	215	ILE	2.4
1	C	81	GLY	2.4
1	C	75	SER	2.4
1	B	27	VAL	2.4
1	B	30	VAL	2.4
1	C	203	VAL	2.4
1	C	46	GLY	2.3
1	B	194	ASP	2.3
1	B	228	VAL	2.3
1	C	137	VAL	2.3
1	B	206	ALA	2.3
1	C	336	LEU	2.3
1	D	190	LEU	2.3
1	B	156	ARG	2.3
1	D	159	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	275	ASP	2.2
1	D	186	GLY	2.2
1	B	237	ILE	2.2
1	D	281	ILE	2.2
1	B	199	CYS	2.2
1	C	37	LEU	2.2
1	B	154	GLY	2.2
1	B	280	GLY	2.2
1	A	53	VAL	2.2
1	C	205	VAL	2.2
1	B	148	SER	2.2
1	D	144	ALA	2.2
1	B	139	THR	2.2
1	B	193	VAL	2.1
1	B	201	PRO	2.1
1	B	321	GLU	2.1
1	B	10	GLY	2.1
1	C	175	LEU	2.1
1	B	279	GLN	2.1
1	C	1(A)	SER	2.1
1	D	189	TRP	2.1
1	B	40	ARG	2.1
1	D	179	THR	2.1
1	D	127	PRO	2.1
1	B	200	TYR	2.1
1	C	237	ILE	2.1
1	D	44	ALA	2.1
1	D	158	VAL	2.1
1	D	40	ARG	2.1
1	D	168	ARG	2.1
1	C	183	THR	2.1
1	D	184	PHE	2.1
1	A	55	ALA	2.0
1	C	182	LEU	2.0
1	B	209	HIS	2.0
1	B	285	THR	2.0
1	B	144	ALA	2.0
1	D	181	VAL	2.0
1	D	193	VAL	2.0
1	C	43	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	1337	5/5	0.83	0.19	27,29,32,35	5

6.5 Other polymers [i](#)

There are no such residues in this entry.