Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 02:20 am BST

PDB ID	:	1X74
Title	:	Alpha-methylacyl-CoA racemase from Mycobacterium tuberculosis- mutational and structural characterization of the fold and active site
Authors	:	Kalle, S.; Bhaumik, P.; Schmitz, W.; Kotti, T.J.; Conzelmann, E.; Wierenga, R.K.; Hiltunen, J.K.
Deposited on	:	2004-08-13
Resolution	:	1.79 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	Percentile Ranks	Value
Rfree		0.222
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		2.4%
RSRZ outliers		9.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
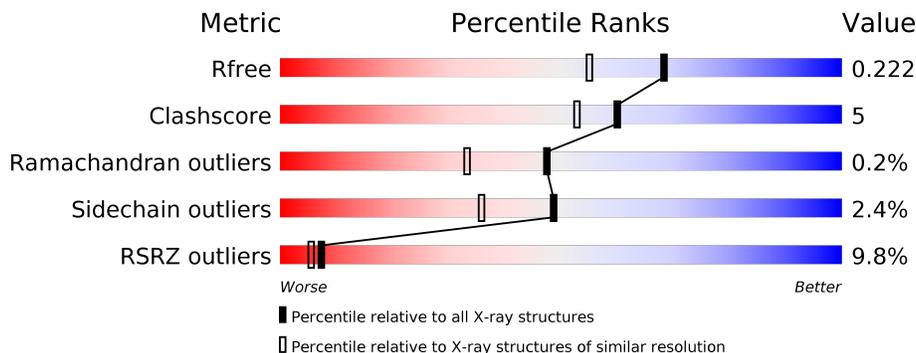
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol	Chain	Length	Quality of chain
1	A	360	9% / 91% / 7% ··
1	B	360	9% / 85% / 11% ··
1	C	360	9% / 86% / 10% ··
1	D	360	10% / 88% / 9% ··

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12445 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-methylacyl-CoA racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total 2708	C 1696	N 489	O 507	S 16	0	8	0
1	B	354	Total 2725	C 1705	N 493	O 511	S 16	0	13	0
1	C	354	Total 2730	C 1707	N 495	O 512	S 16	0	13	0
1	D	354	Total 2729	C 1706	N 496	O 511	S 16	0	13	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
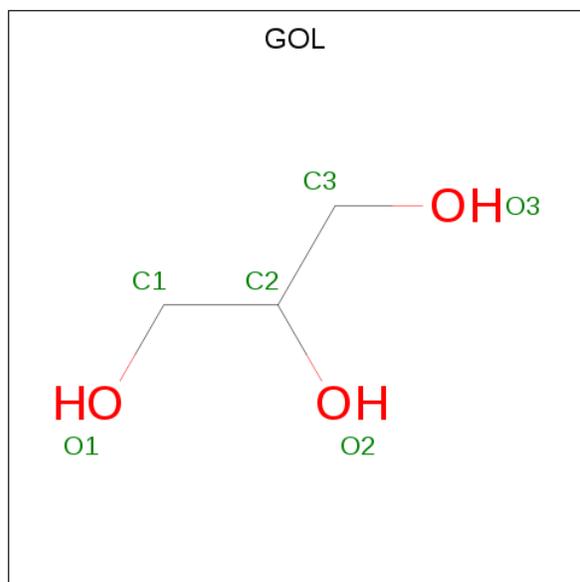
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
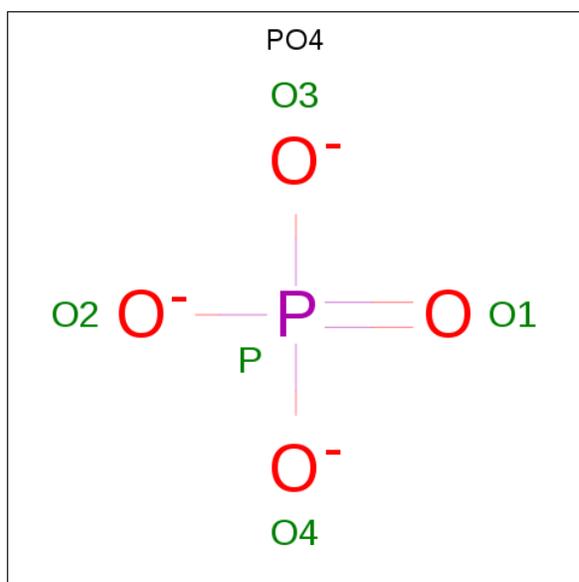
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total 5	O 4	P 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	371	Total 371	O 371	0	0
4	B	368	Total 368	O 368	0	0
4	C	351	Total 351	O 351	0	0
4	D	368	Total 368	O 368	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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-methylacyl-CoA racemase
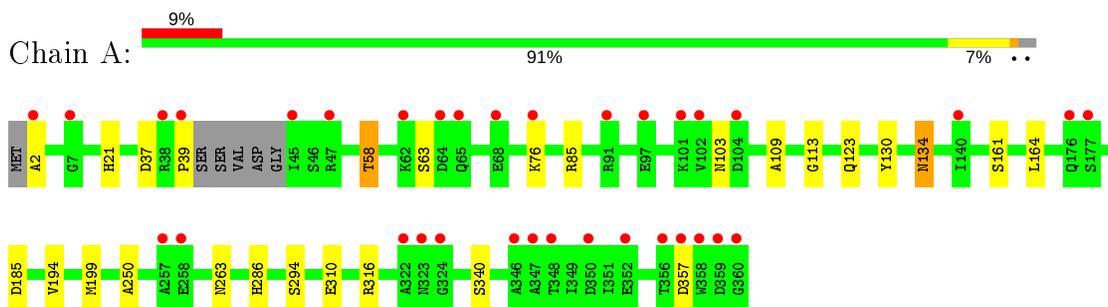
- Molecule 1: 2-methylacyl-CoA racemase
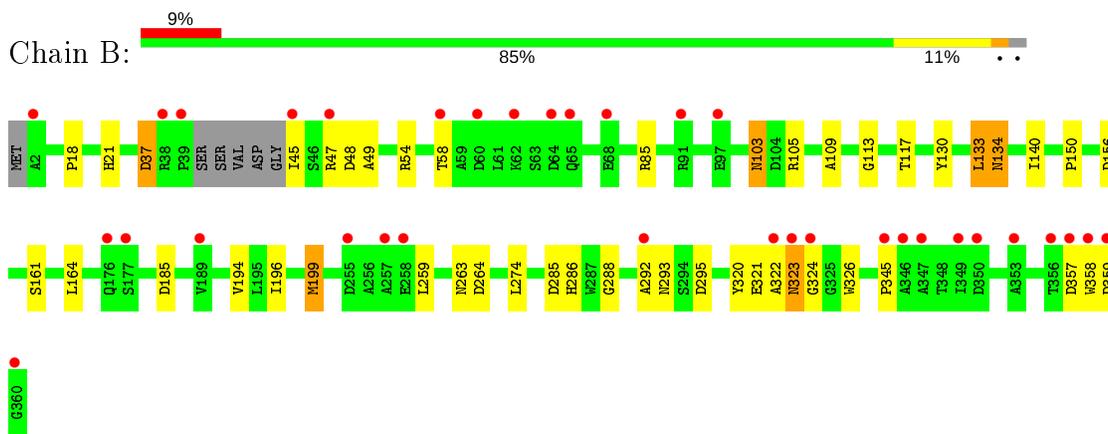
- Molecule 1: 2-methylacyl-CoA racemase
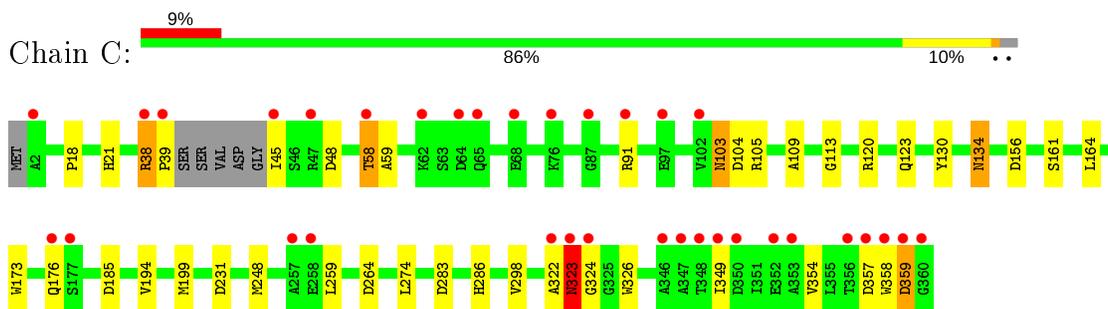
- Molecule 1: 2-methylacyl-CoA racemase
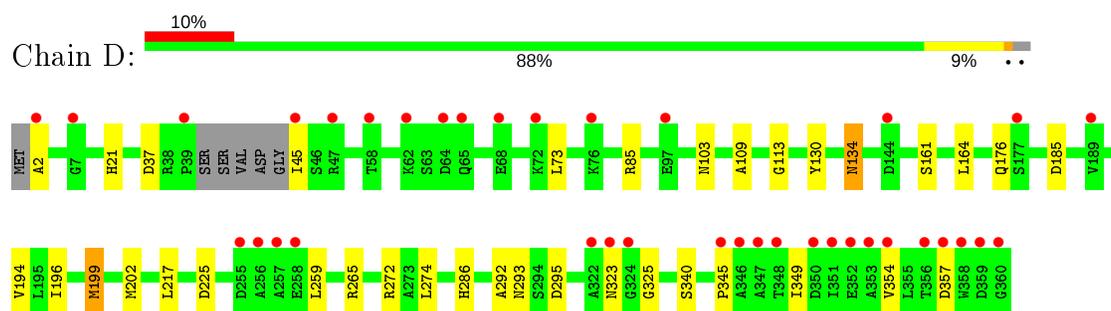
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	180.07Å 79.78Å 117.62Å 90.00° 92.04° 90.00°	Depositor
Resolution (Å)	19.96 – 1.79 19.96 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.96-1.79) 99.5 (19.96-1.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$<I/\sigma(I)>$ [1]	2.33 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.160 , 0.193 0.200 , 0.222	Depositor DCC
R_{free} test set	7826 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	18.6	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 58.7	EDS
L-test for twinning [2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.139 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12445	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0137e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4

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	0.62	0/2810	0.79	2/3819 (0.1%)
1	B	0.62	0/2836	0.81	4/3854 (0.1%)
1	C	0.61	0/2840	0.78	8/3859 (0.2%)
1	D	0.62	0/2836	0.80	3/3854 (0.1%)
All	All	0.62	0/11322	0.79	17/15386 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	185	ASP	CB-CG-OD2	6.69	124.32	118.30
1	B	185	ASP	CB-CG-OD2	6.34	124.01	118.30
1	B	295	ASP	CB-CG-OD2	6.28	123.96	118.30
1	A	357	ASP	CB-CG-OD2	6.28	123.95	118.30
1	D	295	ASP	CB-CG-OD2	6.17	123.86	118.30
1	B	357	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	185	ASP	CB-CG-OD2	5.95	123.65	118.30
1	D	357	ASP	CB-CG-OD2	5.76	123.48	118.30
1	C	264	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	357	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	231	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	185	ASP	CB-CG-OD2	5.35	123.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	283[A]	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	283[B]	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	264	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	104	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	359	ASP	CB-CG-OD2	5.15	122.94	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	54	ARG	Peptide

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	2708	0	2643	17	0
1	B	2725	0	2653	32	0
1	C	2730	0	2660	30	0
1	D	2729	0	2659	32	0
2	A	12	0	16	0	0
2	B	30	0	40	0	0
2	C	24	0	32	4	0
2	D	24	0	32	1	0
3	D	5	0	0	0	0
4	A	371	0	0	4	2
4	B	368	0	0	11	2
4	C	351	0	0	7	0
4	D	368	0	0	11	0
All	All	12445	0	10735	101	2

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 (101) 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:263[B]:ASN:ND2	4:A:2498:HOH:O	1.94	0.97
1:C:48:ASP:HA	4:C:2470:HOH:O	1.66	0.95
1:A:85:ARG:NH1	4:A:2677:HOH:O	2.07	0.85
1:B:48:ASP:HA	4:B:2676:HOH:O	1.85	0.77
1:D:292[A]:ALA:O	4:D:2613:HOH:O	2.03	0.77
1:B:37:ASP:OD1	4:B:2675:HOH:O	2.02	0.75
1:B:322[B]:ALA:O	1:B:323[B]:ASN:C	2.25	0.74
1:B:263:ASN:ND2	4:B:2673:HOH:O	1.99	0.73
1:B:85:ARG:NH1	4:B:2672:HOH:O	2.23	0.72
1:B:292[B]:ALA:O	4:B:2657:HOH:O	2.07	0.71
2:C:2315:GOL:H11	1:D:202:MET:CG	2.20	0.71
1:B:263:ASN:OD1	4:B:2493:HOH:O	2.08	0.69
1:B:286:HIS:HD2	4:B:2428:HOH:O	1.77	0.66
1:D:85:ARG:HD3	4:D:2417:HOH:O	1.95	0.65
1:C:176[B]:GLN:CD	1:D:176[B]:GLN:NE2	2.50	0.65
1:A:37:ASP:HB2	4:A:2683:HOH:O	1.98	0.63
1:D:21:HIS:HD2	1:D:161:SER:OG	1.83	0.61
1:C:259:LEU:HD22	1:C:274:LEU:HD13	1.82	0.61
1:C:176[A]:GLN:NE2	1:D:176[A]:GLN:CD	2.54	0.60
1:A:2:ALA:N	1:A:340:SER:HG	2.00	0.60
1:C:322[B]:ALA:O	1:C:323[B]:ASN:C	2.40	0.59
1:B:21:HIS:HD2	1:B:161:SER:OG	1.86	0.59
1:C:21:HIS:HD2	1:C:161:SER:OG	1.85	0.59
1:D:286:HIS:HE1	4:D:2362:HOH:O	1.86	0.56
1:A:39:PRO:HA	1:A:58:THR:HG23	1.88	0.55
2:C:2315:GOL:H11	1:D:202:MET:HG2	1.88	0.55
1:C:59:ALA:N	4:C:2652:HOH:O	2.39	0.55
1:B:286:HIS:HE1	4:B:2366:HOH:O	1.89	0.54
1:A:21:HIS:HD2	1:A:161:SER:OG	1.90	0.54
1:A:294:SER:HB3	4:D:2524:HOH:O	2.06	0.53
1:C:21:HIS:HE1	1:D:194:VAL:O	1.93	0.52
1:A:39:PRO:HA	1:A:58:THR:CG2	2.40	0.51
1:B:285:ASP:OD1	4:B:2671:HOH:O	2.19	0.51
2:C:2315:GOL:H11	1:D:202:MET:HG3	1.91	0.51
1:C:113:GLY:HA3	1:C:130:TYR:CZ	2.47	0.50
1:A:286:HIS:HE1	4:D:2345:HOH:O	1.95	0.49
1:D:113:GLY:HA3	1:D:130:TYR:CZ	2.48	0.49
1:A:194:VAL:O	1:B:21:HIS:HE1	1.95	0.49
1:C:286:HIS:HE1	4:C:2399:HOH:O	1.95	0.49
1:C:58:THR:HG23	4:C:2652:HOH:O	2.13	0.49
1:B:259:LEU:HD22	1:B:274:LEU:HD13	1.95	0.48
1:A:113:GLY:HA3	1:A:130:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLY:HA3	1:B:130:TYR:CZ	2.50	0.47
1:D:323[B]:ASN:HB2	4:D:2456:HOH:O	2.14	0.47
1:A:310:GLU:HG2	1:B:133:LEU:HD13	1.97	0.47
1:B:109:ALA:HB1	1:B:164:LEU:HD11	1.98	0.46
1:C:326:TRP:HD1	4:C:2514:HOH:O	1.98	0.46
1:D:196:ILE:HG12	1:D:199:MET:HB2	1.97	0.46
2:D:2306:GOL:H31	4:D:2677:HOH:O	2.16	0.46
1:A:21:HIS:HE1	1:B:194:VAL:O	1.99	0.46
1:C:18:PRO:HB3	1:C:156:ASP:O	2.16	0.45
1:C:120:ARG:HG2	1:C:123[A]:GLN:NE2	2.32	0.45
1:C:248[B]:MET:HG3	1:C:298:VAL:CG2	2.46	0.45
1:D:259:LEU:HD22	1:D:274:LEU:HD13	1.98	0.45
1:C:109:ALA:HB1	1:C:164:LEU:HD11	1.99	0.45
2:C:2307:GOL:H11	1:D:217:LEU:HD11	1.98	0.45
1:C:358:TRP:O	1:C:359:ASP:HB2	2.16	0.45
1:A:316:ARG:HD2	1:B:117:THR:O	2.17	0.45
1:C:38:ARG:HB3	1:C:39:PRO:HD2	1.98	0.45
1:B:322[A]:ALA:O	1:B:324[A]:GLY:N	2.49	0.45
1:D:349:ILE:HD11	1:D:354:VAL:CG2	2.47	0.45
1:B:320:TYR:CE1	1:B:322[B]:ALA:HB2	2.52	0.44
1:C:194:VAL:O	1:D:21:HIS:HE1	2.01	0.44
1:C:176[B]:GLN:NE2	1:D:176[B]:GLN:NE2	2.64	0.44
1:C:349:ILE:HD11	1:C:354:VAL:CG2	2.48	0.44
4:A:2664:HOH:O	1:B:49:ALA:HB1	2.16	0.44
1:C:324[A]:GLY:HA3	4:C:2420:HOH:O	2.18	0.44
1:C:134:ASN:HD22	1:C:134:ASN:C	2.20	0.43
1:A:134:ASN:C	1:A:134:ASN:HD22	2.20	0.43
1:B:358:TRP:O	1:B:359:ASP:HB2	2.18	0.43
1:C:176[B]:GLN:NE2	1:D:176[B]:GLN:HE21	2.17	0.42
1:B:140:ILE:HD13	1:B:150:PRO:HG3	2.01	0.42
1:D:109:ALA:HB1	1:D:164:LEU:HD11	2.01	0.42
1:C:120:ARG:HG2	1:C:123[A]:GLN:HE22	1.85	0.42
1:B:196:ILE:HG12	1:B:199:MET:HB2	2.01	0.42
1:D:176[A]:GLN:NE2	4:D:2451:HOH:O	2.53	0.42
1:A:250:ALA:O	1:D:286:HIS:CD2	2.72	0.42
1:B:18:PRO:HB3	1:B:156:ASP:O	2.19	0.42
1:D:2:ALA:N	1:D:340:SER:HG	2.17	0.42
1:B:134:ASN:HD22	1:B:134:ASN:C	2.22	0.42
1:D:292[B]:ALA:O	1:D:293[B]:ASN:HB2	2.20	0.42
1:A:109:ALA:HB1	1:A:164:LEU:HD11	2.02	0.41
1:B:45:ILE:HG23	1:B:45:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323[B]:ASN:C	1:D:325[B]:GLY:N	2.72	0.41
1:C:45:ILE:HG22	4:C:2426:HOH:O	2.20	0.41
1:C:45:ILE:O	1:C:45:ILE:HG23	2.20	0.41
1:D:2:ALA:HB1	4:D:2610:HOH:O	2.21	0.41
1:B:288:GLY:HA2	4:B:2666:HOH:O	2.21	0.41
1:D:85:ARG:NH1	4:D:2531:HOH:O	2.54	0.41
1:B:103:ASN:HD22	1:B:105:ARG:H	1.69	0.41
1:C:103:ASN:ND2	1:C:105:ARG:H	2.18	0.41
1:B:345:PRO:HD3	4:B:2678:HOH:O	2.20	0.41
1:C:176[B]:GLN:OE1	1:D:176[B]:GLN:NE2	2.52	0.41
1:D:45:ILE:HD11	1:D:345:PRO:O	2.21	0.41
1:D:134:ASN:C	1:D:134:ASN:HD22	2.23	0.41
1:B:321:GLU:HG3	1:B:326:TRP:CH2	2.56	0.40
1:D:225:ASP:OD2	1:D:272:ARG:NH1	2.55	0.40

All (2) 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)
4:A:2498:HOH:O	4:B:2493:HOH:O[4_655]	2.12	0.08
4:A:2448:HOH:O	4:B:2674:HOH:O[2_655]	2.16	0.04

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	358/360 (99%)	348 (97%)	10 (3%)	0	100	100
1	B	363/360 (101%)	348 (96%)	11 (3%)	4 (1%)	14	4
1	C	363/360 (101%)	351 (97%)	10 (3%)	2 (1%)	25	12
1	D	363/360 (101%)	349 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1447/1440 (100%)	1396 (96%)	45 (3%)	6 (0%)	47 21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	293[A]	ASN
1	B	293[B]	ASN
1	C	323[A]	ASN
1	C	323[B]	ASN
1	B	323[A]	ASN
1	B	323[B]	ASN

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	278/275 (101%)	270 (97%)	8 (3%)	42	29
1	B	279/275 (102%)	272 (98%)	7 (2%)	47	34
1	C	280/275 (102%)	272 (97%)	8 (3%)	42	29
1	D	279/275 (102%)	274 (98%)	5 (2%)	59	48
All	All	1116/1100 (102%)	1088 (98%)	28 (2%)	49	34

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	63	SER
1	A	76	LYS
1	A	103	ASN
1	A	123[A]	GLN
1	A	123[B]	GLN
1	A	134	ASN
1	A	199	MET
1	B	37	ASP

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Mol	Chain	Res	Type
1	B	47	ARG
1	B	58	THR
1	B	103	ASN
1	B	133	LEU
1	B	134	ASN
1	B	199	MET
1	C	38	ARG
1	C	58	THR
1	C	91	ARG
1	C	103	ASN
1	C	134	ASN
1	C	199	MET
1	C	323[A]	ASN
1	C	323[B]	ASN
1	D	37	ASP
1	D	73	LEU
1	D	103	ASN
1	D	134	ASN
1	D	199	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	103	ASN
1	A	134	ASN
1	A	286	HIS
1	B	21	HIS
1	B	103	ASN
1	B	134	ASN
1	B	263	ASN
1	B	286	HIS
1	C	21	HIS
1	C	103	ASN
1	C	134	ASN
1	C	286	HIS
1	D	21	HIS
1	D	103	ASN
1	D	134	ASN
1	D	286	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	GOL	B	2303	-	5,5,5	0.32	0	5,5,5	0.74	0
2	GOL	B	2308	-	5,5,5	0.46	0	5,5,5	0.66	0
2	GOL	C	2301	-	5,5,5	0.35	0	5,5,5	0.54	0
2	GOL	C	2315	-	5,5,5	0.29	0	5,5,5	0.44	0
2	GOL	D	2306	-	5,5,5	0.39	0	5,5,5	0.32	0
2	GOL	A	2311	-	5,5,5	0.39	0	5,5,5	0.33	0
2	GOL	B	2302	-	5,5,5	0.49	0	5,5,5	0.65	0
2	GOL	D	2305	-	5,5,5	0.50	0	5,5,5	1.07	0
2	GOL	B	2312	-	5,5,5	0.28	0	5,5,5	0.70	0
2	GOL	C	2314	-	5,5,5	0.34	0	5,5,5	0.60	0
3	PO4	D	1600	-	4,4,4	1.27	0	6,6,6	0.58	0
2	GOL	C	2307	-	5,5,5	0.35	0	5,5,5	0.23	0
2	GOL	D	2309	-	5,5,5	0.46	0	5,5,5	0.64	0
2	GOL	B	2304	-	5,5,5	0.29	0	5,5,5	0.45	0
2	GOL	D	2310	-	5,5,5	0.36	0	5,5,5	0.46	0
2	GOL	A	2313	-	5,5,5	0.30	0	5,5,5	0.91	0

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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	GOL	B	2303	-	-	4/4/4/4	-
2	GOL	B	2308	-	-	0/4/4/4	-
2	GOL	C	2301	-	-	2/4/4/4	-
2	GOL	C	2315	-	-	3/4/4/4	-
2	GOL	D	2306	-	-	0/4/4/4	-
2	GOL	A	2311	-	-	0/4/4/4	-
2	GOL	B	2302	-	-	1/4/4/4	-
2	GOL	B	2304	-	-	0/4/4/4	-
2	GOL	D	2305	-	-	0/4/4/4	-
2	GOL	B	2312	-	-	2/4/4/4	-
2	GOL	C	2314	-	-	2/4/4/4	-
2	GOL	C	2307	-	-	2/4/4/4	-
2	GOL	A	2313	-	-	2/4/4/4	-
2	GOL	D	2309	-	-	4/4/4/4	-
2	GOL	D	2310	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2303	GOL	C1-C2-C3-O3
2	C	2315	GOL	C1-C2-C3-O3
2	C	2315	GOL	O2-C2-C3-O3
2	B	2312	GOL	O1-C1-C2-C3
2	C	2314	GOL	C1-C2-C3-O3
2	C	2307	GOL	C1-C2-C3-O3
2	A	2313	GOL	O1-C1-C2-C3
2	B	2303	GOL	O2-C2-C3-O3
2	C	2301	GOL	C1-C2-C3-O3
2	D	2309	GOL	O1-C1-C2-C3
2	D	2309	GOL	C1-C2-C3-O3
2	D	2309	GOL	O1-C1-C2-O2
2	D	2309	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	C	2307	GOL	O2-C2-C3-O3
2	A	2313	GOL	O1-C1-C2-O2
2	C	2314	GOL	O2-C2-C3-O3
2	B	2312	GOL	O1-C1-C2-O2
2	B	2303	GOL	O1-C1-C2-O2
2	C	2301	GOL	O2-C2-C3-O3
2	C	2315	GOL	O1-C1-C2-C3
2	B	2302	GOL	O1-C1-C2-C3
2	B	2303	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2315	GOL	3	0
2	D	2306	GOL	1	0
2	C	2307	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	354/360 (98%)	0.47	34 (9%)	8	6	3, 9, 22, 32	0
1	B	354/360 (98%)	0.51	34 (9%)	8	6	5, 9, 21, 26	0
1	C	354/360 (98%)	0.57	34 (9%)	8	6	2, 9, 22, 27	0
1	D	354/360 (98%)	0.53	37 (10%)	6	4	3, 9, 21, 26	0
All	All	1416/1440 (98%)	0.52	139 (9%)	7	5	2, 9, 22, 32	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	45	ILE	7.5
1	B	45	ILE	6.7
1	A	45	ILE	6.6
1	C	2	ALA	6.5
1	C	45	ILE	6.4
1	C	359	ASP	6.0
1	B	323[A]	ASN	6.0
1	B	2	ALA	5.9
1	D	360	GLY	5.8
1	C	39	PRO	5.5
1	A	360	GLY	5.3
1	C	360	GLY	5.3
1	C	356	THR	5.2
1	B	346	ALA	5.1
1	B	347	ALA	5.1
1	D	350	ASP	5.0
1	C	346	ALA	4.9
1	A	347	ALA	4.9
1	A	323	ASN	4.8
1	B	359	ASP	4.8
1	A	359	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	2	ALA	4.8
1	C	323[A]	ASN	4.8
1	D	323[A]	ASN	4.8
1	D	359	ASP	4.7
1	B	292[A]	ALA	4.7
1	A	356	THR	4.6
1	D	356	THR	4.6
1	A	2	ALA	4.5
1	A	324	GLY	4.5
1	C	91	ARG	4.3
1	B	356	THR	4.2
1	A	346	ALA	4.2
1	A	350	ASP	4.1
1	C	347	ALA	4.1
1	B	360	GLY	4.0
1	B	350	ASP	4.0
1	D	324[A]	GLY	3.9
1	D	39	PRO	3.9
1	C	47	ARG	3.8
1	B	39	PRO	3.7
1	D	65	GLN	3.6
1	C	350	ASP	3.6
1	B	47	ARG	3.6
1	A	91	ARG	3.6
1	D	353	ALA	3.6
1	A	39	PRO	3.6
1	D	346	ALA	3.6
1	A	47	ARG	3.6
1	C	64	ASP	3.5
1	D	47	ARG	3.5
1	C	65	GLN	3.4
1	C	38	ARG	3.4
1	A	64	ASP	3.3
1	B	91	ARG	3.3
1	D	347	ALA	3.3
1	B	357	ASP	3.3
1	A	65	GLN	3.3
1	D	348	THR	3.3
1	B	353	ALA	3.2
1	D	257	ALA	3.2
1	B	322[A]	ALA	3.2
1	C	357	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	353	ALA	3.1
1	B	258	GLU	3.1
1	B	65	GLN	3.1
1	B	345	PRO	3.1
1	D	258	GLU	3.1
1	B	38	ARG	3.0
1	D	64	ASP	3.0
1	C	177	SER	3.0
1	B	64	ASP	3.0
1	A	322	ALA	3.0
1	C	258	GLU	2.9
1	B	349	ILE	2.9
1	A	357	ASP	2.8
1	D	62	LYS	2.8
1	C	76	LYS	2.8
1	A	38	ARG	2.8
1	C	324[A]	GLY	2.8
1	D	357	ASP	2.8
1	A	62	LYS	2.8
1	A	68	GLU	2.7
1	C	257	ALA	2.7
1	B	189	VAL	2.6
1	C	322[A]	ALA	2.6
1	B	176[A]	GLN	2.6
1	B	324[A]	GLY	2.6
1	D	351	ILE	2.6
1	D	352	GLU	2.6
1	B	257	ALA	2.6
1	A	76	LYS	2.6
1	D	345	PRO	2.6
1	A	7	GLY	2.6
1	D	358	TRP	2.5
1	A	258	GLU	2.5
1	D	58	THR	2.5
1	C	349	ILE	2.5
1	C	62	LYS	2.5
1	A	257	ALA	2.5
1	D	177	SER	2.4
1	D	97	GLU	2.4
1	B	255	ASP	2.4
1	C	97	GLU	2.4
1	D	72	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	358	TRP	2.3
1	A	177	SER	2.3
1	C	352	GLU	2.3
1	B	62	LYS	2.3
1	D	76	LYS	2.2
1	C	176[A]	GLN	2.2
1	B	177	SER	2.2
1	B	58	THR	2.2
1	C	58	THR	2.2
1	D	68	GLU	2.2
1	B	97	GLU	2.2
1	A	348	THR	2.2
1	C	102	VAL	2.2
1	A	140	ILE	2.2
1	B	60	ASP	2.2
1	C	68	GLU	2.1
1	C	348	THR	2.1
1	D	256	ALA	2.1
1	A	102	VAL	2.1
1	D	255	ASP	2.1
1	B	68	GLU	2.1
1	A	176	GLN	2.1
1	D	7	GLY	2.1
1	A	358	TRP	2.1
1	D	189	VAL	2.1
1	D	322[A]	ALA	2.1
1	A	101	LYS	2.0
1	A	97	GLU	2.0
1	A	352	GLU	2.0
1	A	104	ASP	2.0
1	D	144	ASP	2.0
1	D	354	VAL	2.0
1	C	358	TRP	2.0
1	C	87	GLY	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.

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6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	C	2315	6/6	0.60	0.34	63,66,67,67	0
2	GOL	C	2314	6/6	0.70	0.21	43,43,45,46	0
2	GOL	A	2313	6/6	0.82	0.19	32,37,39,42	0
2	GOL	D	2309	6/6	0.87	0.15	23,32,35,36	0
2	GOL	D	2305	6/6	0.87	0.18	21,22,24,24	0
2	GOL	B	2308	6/6	0.88	0.18	26,29,30,31	0
2	GOL	B	2302	6/6	0.88	0.16	23,25,27,28	0
2	GOL	D	2306	6/6	0.89	0.16	24,25,28,30	0
2	GOL	B	2312	6/6	0.89	0.14	29,36,37,42	0
2	GOL	C	2301	6/6	0.90	0.19	29,30,31,31	0
2	GOL	C	2307	6/6	0.91	0.15	33,39,41,44	0
2	GOL	B	2303	6/6	0.91	0.17	23,39,42,44	0
2	GOL	A	2311	6/6	0.92	0.16	26,30,31,32	0
2	GOL	B	2304	6/6	0.94	0.16	28,30,32,34	0
2	GOL	D	2310	6/6	0.95	0.14	27,29,30,33	0
3	PO4	D	1600	5/5	0.97	0.17	42,43,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.