WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 11:47 PM GMT

PDB ID : 2GD0

Title : The 1,1-proton transfer reaction mechanism by alpha-methylacyl-CoA race-mase is catalyzed by an aspartate/histidine pair and involves a smooth, methionine-rich surface for binding the fatty acyl moiety

Authors : Bhaumik, P.; Wierenga, R.K.

Deposited on : 2006-03-15

Resolution : 1.70 Å(reported)

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 1.70 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		0.233
Clashscore		8
Ramachandran outliers		0.5%
Sidechain outliers		3.2%
RSRZ outliers		2.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

❘ Percentile relative to X-ray structures of similar resolution
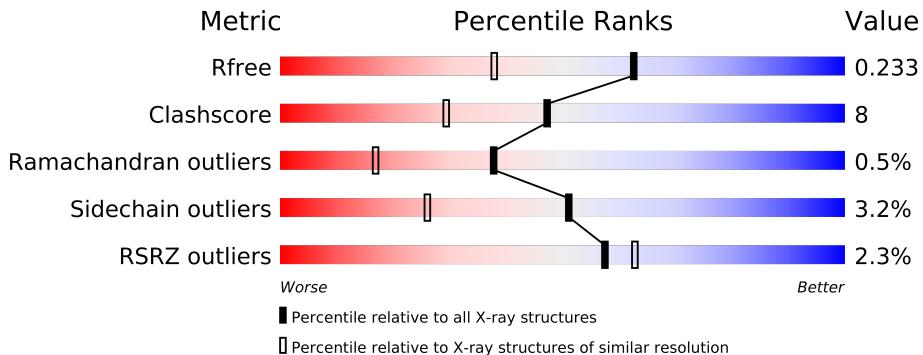
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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	360	
1	B	360	
1	C	360	
1	D	360	
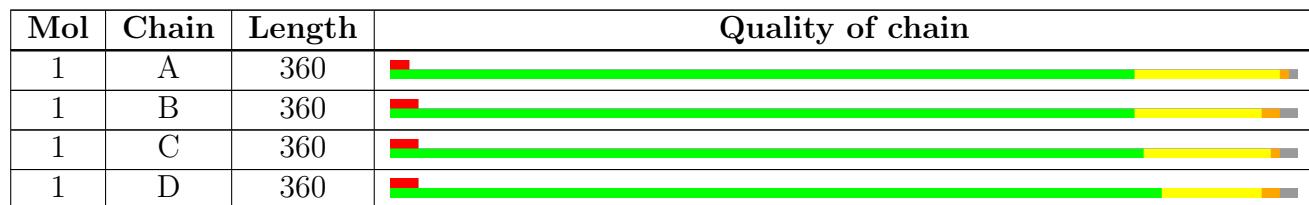
The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	A	2306	-	X
3	GOL	B	2304	-	X
3	GOL	C	2302	-	X

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 12376 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 probable alpha-methylacyl-CoA racemase MCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2679	1683	481	500	15			
1	B	354	Total	C	N	O	S	0	0	0
			2679	1683	481	500	15			
1	C	354	Total	C	N	O	S	0	0	0
			2679	1683	481	500	15			
1	D	354	Total	C	N	O	S	0	0	0
			2679	1683	481	500	15			

- Molecule 2 is (S)-2-METHYLMYRISTOYL-COENZYMEA (three-letter code: MRS) (formula: $C_{36}H_{64}N_7O_{17}P_3S$).
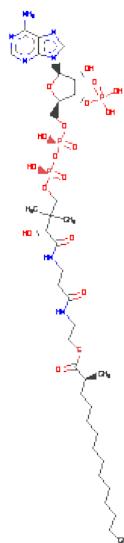
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		

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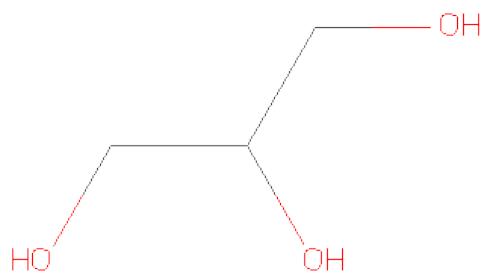
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	349	Total	O	0	0
			349	349		
4	B	341	Total	O	0	0
			341	341		
4	C	357	Total	O	0	0
			357	357		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	333	Total O 333 333		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: probable alpha-methylacyl-CoA racemase MCR

Chain A:
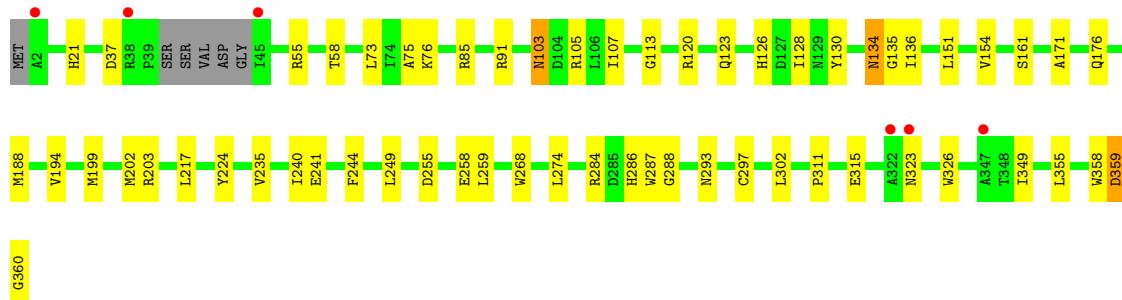
• Molecule 1: probable alpha-methylacyl-CoA racemase MCR

Chain B:
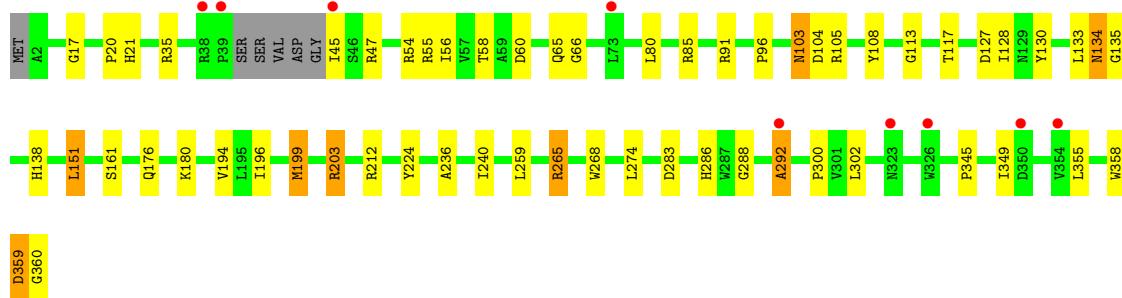
• Molecule 1: probable alpha-methylacyl-CoA racemase MCR

Chain C:
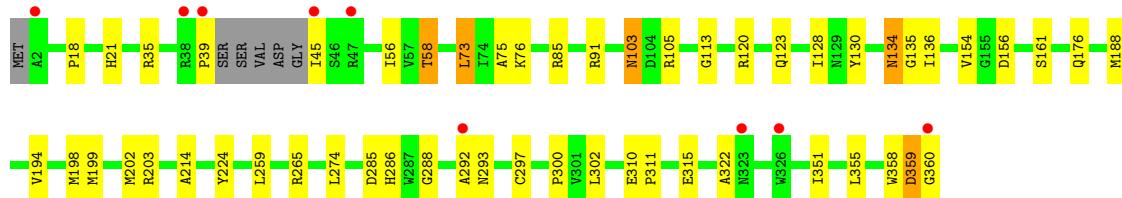
• Molecule 1: probable alpha-methylacyl-CoA racemase MCR

Chain D:
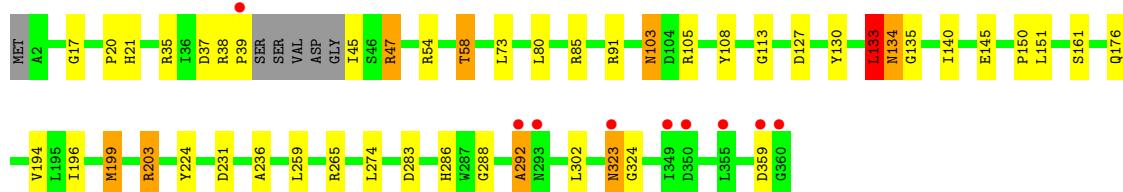
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	215.74Å 79.75Å 117.92Å 90.00° 123.14° 90.00°	Depositor
Resolution (Å)	19.80 – 1.70 19.79 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.80-1.70) 97.4 (19.79-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	4.07 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.236 , 0.276 0.215 , 0.233	Depositor DCC
R_{free} test set	8946 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	19.0	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 51.1	EDS
Estimated twinning fraction	0.477 for -h-2*l,-k,l	Xtriage
L-test for twinning	$< |L| > = 0.48, < L^2 > = 0.30$	Xtriage
Outliers	0 of 179089 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12376	wwPDB-VP
Average B, all atoms (Å^2)	28.0	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 76.91 % 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 9.4635e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities 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: GOL, MRS

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	0.89	4/2740 (0.1%)	0.84	1/3727 (0.0%)
1	B	0.87	4/2740 (0.1%)	0.84	3/3727 (0.1%)
1	C	0.88	3/2740 (0.1%)	0.83	0/3727
1	D	0.85	2/2740 (0.1%)	0.85	5/3727 (0.1%)
All	All	0.87	13/10960 (0.1%)	0.84	9/14908 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	TYR	CE1-CZ	7.33	1.48	1.38
1	C	297	CYS	CB-SG	-7.07	1.70	1.82
1	C	224	TYR	CE1-CZ	6.99	1.47	1.38
1	A	297	CYS	CB-SG	-6.90	1.70	1.82
1	A	224	TYR	CG-CD2	6.36	1.47	1.39
1	D	224	TYR	CG-CD2	5.93	1.46	1.39
1	C	224	TYR	CG-CD2	5.81	1.46	1.39
1	B	128	ILE	CB-CG2	5.42	1.69	1.52
1	B	224	TYR	CE1-CZ	5.23	1.45	1.38
1	D	224	TYR	CE1-CZ	5.22	1.45	1.38
1	B	224	TYR	CG-CD2	5.14	1.45	1.39
1	A	268	TRP	CG-CD1	5.11	1.44	1.36
1	B	268	TRP	CG-CD1	5.04	1.43	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	127	ASP	CB-CG-OD2	-8.47	110.68	118.30
1	B	127	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	D	265	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	203	ARG	NE-CZ-NH1	5.83	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	203	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	203	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	265	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	D	133	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	D	127	ASP	OD1-CG-OD2	5.07	132.93	123.30

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	2679	0	2623	54	0
1	B	2679	0	2623	47	0
1	C	2679	0	2623	51	0
1	D	2679	0	2623	40	0
2	A	64	0	60	5	0
2	B	64	0	60	2	0
2	C	64	0	60	2	0
2	D	64	0	60	1	0
3	A	6	0	8	2	0
3	B	6	0	8	1	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	A	349	0	0	14	0
4	B	341	0	0	20	0
4	C	357	0	0	10	0
4	D	333	0	0	16	0
All	All	12376	0	10764	174	0

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 8.

All (174) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:292:ALA:HB1	4:B:2640:HOH:O	1.14	1.27
1:D:35:ARG:HB2	4:D:2633:HOH:O	1.47	1.15
1:B:35:ARG:HB2	4:B:2641:HOH:O	1.43	1.14
1:D:283:ASP:HB2	4:D:2628:HOH:O	1.55	1.06
1:B:345:PRO:HG2	4:B:2636:HOH:O	1.68	0.94
1:D:288:GLY:O	4:D:2624:HOH:O	1.92	0.88
1:B:288:GLY:O	4:B:2412:HOH:O	1.92	0.86
1:B:283:ASP:HB2	4:B:2638:HOH:O	1.75	0.85
1:C:286:HIS:CD2	4:C:2652:HOH:O	2.29	0.84
1:D:288:GLY:HA2	4:D:2461:HOH:O	1.75	0.83
1:B:288:GLY:HA2	4:B:2427:HOH:O	1.81	0.79
1:C:176:GLN:HE21	1:D:176:GLN:HE21	1.32	0.76
1:A:315:GLU:HG3	4:A:2448:HOH:O	1.84	0.75
1:C:300:PRO:HB3	4:C:2501:HOH:O	1.87	0.75
1:B:259:LEU:HD22	1:B:274:LEU:HD13	1.69	0.74
1:A:176:GLN:HE21	1:B:176:GLN:HE21	1.34	0.73
1:C:120:ARG:HH11	1:C:123:GLN:HE22	1.34	0.72
1:A:259:LEU:HD22	1:A:274:LEU:HD13	1.72	0.72
1:C:355:LEU:HD22	1:C:360:GLY:HA3	1.71	0.70
1:D:259:LEU:HD22	1:D:274:LEU:HD13	1.74	0.69
1:B:85:ARG:HH12	1:B:91:ARG:HH22	1.39	0.69
1:A:91:ARG:NH1	2:A:1751:MRS:O7A	2.22	0.69
1:A:287:TRP:HB2	4:A:2650:HOH:O	1.93	0.69
1:A:85:ARG:NH1	4:A:2456:HOH:O	2.19	0.68
1:C:358:TRP:O	1:C:359:ASP:HB2	1.94	0.68
1:A:286:HIS:HE1	4:A:2398:HOH:O	1.77	0.67
1:A:284:ARG:HA	4:A:2650:HOH:O	1.95	0.67
1:C:286:HIS:HE1	4:C:2355:HOH:O	1.78	0.67
1:D:286:HIS:HE1	4:D:2427:HOH:O	1.79	0.65
1:D:47:ARG:HG2	4:D:2572:HOH:O	1.96	0.65
1:A:85:ARG:HD3	4:A:2351:HOH:O	1.97	0.64
1:C:259:LEU:HD22	1:C:274:LEU:HD13	1.80	0.64
1:A:235:VAL:CG1	4:A:2650:HOH:O	2.44	0.63
1:D:38:ARG:HD3	4:D:2549:HOH:O	1.97	0.63
1:A:120:ARG:HH11	1:A:123:GLN:HE22	1.46	0.62
1:C:85:ARG:HD3	4:C:2348:HOH:O	2.00	0.62
1:B:286:HIS:HE1	4:B:2414:HOH:O	1.82	0.62
1:A:311:PRO:O	1:A:315:GLU:HG2	2.00	0.61
1:A:358:TRP:O	1:A:359:ASP:HB2	2.02	0.58
1:B:292:ALA:HA	4:B:2412:HOH:O	2.04	0.57
1:D:91:ARG:NH1	2:D:1754:MRS:O7A	2.26	0.57
1:A:76:LYS:HE3	1:A:359:ASP:O	2.04	0.57
1:B:55:ARG:HD2	1:B:349:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:85:ARG:NH1	4:D:2618:HOH:O	2.37	0.56
1:A:286:HIS:HD2	4:C:2438:HOH:O	1.89	0.55
1:C:91:ARG:NH1	2:C:1753:MRS:O7A	2.38	0.55
1:D:134:ASN:C	1:D:134:ASN:HD22	2.09	0.55
1:A:55:ARG:HD2	1:A:349:ILE:HD11	1.88	0.55
1:C:21:HIS:HD2	1:C:161:SER:OG	1.90	0.54
2:A:1751:MRS:H72	4:B:2431:HOH:O	2.06	0.54
1:A:113:GLY:HA3	1:A:130:TYR:CZ	2.42	0.54
1:D:140:ILE:HD13	1:D:150:PRO:HG3	1.90	0.54
1:C:176:GLN:NE2	1:D:176:GLN:HE21	2.04	0.54
1:A:288:GLY:HA2	4:A:2606:HOH:O	2.07	0.54
1:C:285:ASP:OD1	4:C:2650:HOH:O	2.19	0.54
1:A:103:ASN:HD22	1:A:103:ASN:C	2.11	0.53
1:C:302:LEU:O	1:D:135:GLY:HA2	2.07	0.53
1:C:176:GLN:HG2	4:D:2634:HOH:O	2.08	0.53
1:B:358:TRP:O	1:B:359:ASP:HB2	2.08	0.53
1:D:103:ASN:ND2	1:D:105:ARG:H	2.07	0.53
1:A:302:LEU:O	1:B:135:GLY:HA2	2.09	0.53
1:D:292:ALA:HA	4:D:2624:HOH:O	2.09	0.53
1:C:322:ALA:HB1	4:C:2643:HOH:O	2.09	0.52
1:B:134:ASN:C	1:B:134:ASN:HD22	2.11	0.52
1:C:113:GLY:HA3	1:C:130:TYR:CZ	2.44	0.51
1:C:176:GLN:HE21	1:D:176:GLN:NE2	2.05	0.51
1:D:323:ASN:HB2	4:D:2497:HOH:O	2.10	0.51
1:C:103:ASN:HD22	1:C:103:ASN:C	2.12	0.51
1:A:21:HIS:HD2	1:A:161:SER:OG	1.92	0.51
1:A:235:VAL:HG13	4:A:2650:HOH:O	2.08	0.51
1:D:37:ASP:O	1:D:58:THR:HA	2.11	0.51
1:B:300:PRO:HB3	4:B:2427:HOH:O	2.10	0.50
1:A:103:ASN:ND2	1:A:105:ARG:H	2.09	0.50
1:B:103:ASN:ND2	1:B:105:ARG:H	2.10	0.50
1:C:120:ARG:NH1	1:C:123:GLN:HE22	2.04	0.50
1:C:76:LYS:HE3	1:C:359:ASP:O	2.12	0.50
1:C:45:ILE:O	1:C:45:ILE:HG23	2.11	0.50
1:B:288:GLY:CA	4:B:2427:HOH:O	2.52	0.49
1:C:214:ALA:O	1:C:265:ARG:NH2	2.45	0.49
1:C:203:ARG:NH2	4:C:2540:HOH:O	2.45	0.49
1:C:286:HIS:CE1	4:C:2355:HOH:O	2.61	0.48
4:A:2498:HOH:O	1:C:286:HIS:HD2	1.95	0.48
1:D:85:ARG:HD3	4:D:2360:HOH:O	2.13	0.48
1:A:176:GLN:NE2	1:B:176:GLN:HE21	2.08	0.48
1:A:103:ASN:HD22	1:A:105:ARG:H	1.59	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:103:ASN:ND2	1:C:105:ARG:H	2.11	0.48
1:A:113:GLY:HA3	1:A:130:TYR:CE1	2.49	0.48
1:C:135:GLY:HA2	1:D:302:LEU:O	2.12	0.47
1:B:17:GLY:O	1:B:20:PRO:HD2	2.14	0.47
1:C:39:PRO:O	4:C:2651:HOH:O	2.20	0.47
1:D:54:ARG:NE	4:D:2633:HOH:O	2.48	0.47
1:A:176:GLN:HE21	1:B:176:GLN:NE2	2.08	0.47
1:D:286:HIS:HD2	4:D:2396:HOH:O	1.97	0.47
1:C:35:ARG:HB3	1:C:56:ILE:HD13	1.97	0.47
1:A:130:TYR:CE2	1:A:188:MET:HE3	2.50	0.47
1:A:194:VAL:O	1:B:21:HIS:HE1	1.97	0.47
1:B:355:LEU:HD22	1:B:360:GLY:HA3	1.97	0.47
1:A:176:GLN:HG2	4:B:2597:HOH:O	2.15	0.47
1:D:21:HIS:HD2	1:D:161:SER:OG	1.97	0.47
1:A:135:GLY:HA2	1:B:302:LEU:O	2.14	0.47
1:A:85:ARG:NE	2:A:1751:MRS:O1A	2.48	0.46
1:C:176:GLN:HG2	1:D:176:GLN:NE2	2.30	0.46
1:D:85:ARG:HG3	4:D:2590:HOH:O	2.16	0.46
1:A:126:HIS:HA	2:A:1751:MRS:H22	1.98	0.46
1:D:196:ILE:HG12	1:D:199:MET:HB2	1.97	0.46
1:B:80:LEU:HD23	1:B:108:TYR:CE1	2.51	0.46
1:C:134:ASN:C	1:C:134:ASN:HD22	2.19	0.46
1:C:39:PRO:HA	1:C:58:THR:CG2	2.46	0.46
1:A:355:LEU:HD22	1:A:360:GLY:HA3	1.98	0.46
1:B:265:ARG:NH1	4:B:2379:HOH:O	2.43	0.45
1:D:324:GLY:C	4:D:2614:HOH:O	2.53	0.45
1:C:103:ASN:HD22	1:C:105:ARG:H	1.64	0.45
1:D:80:LEU:HD23	1:D:108:TYR:CE1	2.51	0.45
1:B:117:THR:HB	4:B:2559:HOH:O	2.15	0.45
1:B:196:ILE:HG12	1:B:199:MET:HB2	1.97	0.45
1:D:231:ASP:N	1:D:231:ASP:OD1	2.50	0.45
1:A:134:ASN:C	1:A:134:ASN:HD22	2.18	0.45
1:A:240:ILE:CG2	3:A:2306:GOL:H31	2.47	0.45
1:D:113:GLY:HA3	1:D:130:TYR:CZ	2.52	0.45
2:C:1753:MRS:H71	2:C:1753:MRS:H41	1.78	0.45
1:C:176:GLN:CG	1:D:176:GLN:HE21	2.31	0.44
1:C:39:PRO:HA	1:C:58:THR:HG21	1.99	0.44
1:C:194:VAL:O	1:D:21:HIS:HE1	2.00	0.44
1:A:120:ARG:NH1	1:A:123:GLN:HE22	2.14	0.44
1:C:21:HIS:HE1	1:D:194:VAL:O	2.01	0.44
1:C:113:GLY:HA3	1:C:130:TYR:CE1	2.52	0.44
1:A:21:HIS:HE1	1:B:194:VAL:O	2.01	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:85:ARG:CZ	4:B:2568:HOH:O	2.66	0.44
1:A:287:TRP:HD1	4:A:2650:HOH:O	2.00	0.44
1:A:176:GLN:HG2	1:B:176:GLN:NE2	2.33	0.44
1:B:113:GLY:HA3	1:B:130:TYR:CE1	2.53	0.44
1:B:265:ARG:NH2	4:B:2626:HOH:O	1.92	0.44
1:A:255:ASP:HB3	1:A:258:GLU:HG3	1.99	0.44
1:B:47:ARG:HB2	4:B:2599:HOH:O	2.18	0.43
1:B:96:PRO:HG2	4:B:2552:HOH:O	2.18	0.43
1:A:188:MET:HE1	2:A:1751:MRS:H21	2.00	0.43
4:A:2476:HOH:O	2:B:1752:MRS:H72	2.18	0.43
1:B:60:ASP:O	1:B:66:GLY:HA3	2.19	0.43
1:D:113:GLY:HA3	1:D:130:TYR:CE1	2.54	0.43
1:B:54:ARG:NE	4:B:2641:HOH:O	2.52	0.42
1:D:17:GLY:O	1:D:20:PRO:HD2	2.19	0.42
1:B:113:GLY:HA3	1:B:130:TYR:CZ	2.53	0.42
1:D:39:PRO:HG3	1:D:58:THR:HG23	2.01	0.42
1:C:130:TYR:CE2	1:C:188:MET:HE3	2.55	0.42
1:A:103:ASN:C	1:A:103:ASN:ND2	2.73	0.42
1:B:240:ILE:O	3:B:2304:GOL:H32	2.20	0.42
1:A:235:VAL:HG11	4:A:2650:HOH:O	2.13	0.42
1:B:286:HIS:HD2	4:B:2375:HOH:O	2.02	0.42
1:C:310:GLU:HG2	1:D:133:LEU:HD13	2.01	0.42
1:C:103:ASN:ND2	1:C:103:ASN:C	2.72	0.41
1:A:249:LEU:HD23	1:A:249:LEU:HA	1.88	0.41
1:A:241:GLU:HB2	1:A:244:PHE:CD2	2.56	0.41
1:C:311:PRO:O	1:C:315:GLU:HG3	2.19	0.41
1:A:75:ALA:HA	1:A:103:ASN:HB2	2.02	0.41
1:A:136:ILE:HG21	1:A:154:VAL:HG11	2.01	0.41
1:C:136:ILE:HG21	1:C:154:VAL:HG11	2.03	0.41
1:B:104:ASP:OD2	1:B:180:LYS:HE3	2.20	0.41
1:B:85:ARG:NH1	1:B:91:ARG:HH22	2.11	0.41
1:B:21:HIS:HD2	1:B:161:SER:OG	2.04	0.41
1:A:326:TRP:HD1	4:A:2630:HOH:O	2.03	0.41
1:A:202:MET:HG2	2:B:1752:MRS:H122	2.01	0.41
1:C:73:LEU:CD2	1:C:351:ILE:HD11	2.51	0.41
1:A:240:ILE:HG22	3:A:2306:GOL:H31	2.02	0.41
1:A:217:LEU:O	1:B:151:LEU:HA	2.21	0.41
1:C:18:PRO:HB3	1:C:156:ASP:O	2.21	0.41
1:C:75:ALA:HA	1:C:103:ASN:HB2	2.03	0.40
1:C:198:MET:HG2	1:C:202:MET:HE2	2.03	0.40
1:B:138:HIS:O	1:B:212:ARG:HD3	2.21	0.40
1:B:35:ARG:HB3	1:B:56:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:128:ILE:HG12	1:B:236:ALA:HB1	2.02	0.40
1:C:128:ILE:HG12	1:D:236:ALA:HB1	2.03	0.40
1:A:107:ILE:HD12	1:A:171:ALA:HB1	2.04	0.40
1:C:288:GLY:O	1:C:292:ALA:HB2	2.20	0.40
1:C:85:ARG:HH12	1:C:91:ARG:NH2	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	350/360 (97%)	335 (96%)	13 (4%)	2 (1%)	33	13
1	B	350/360 (97%)	334 (95%)	14 (4%)	2 (1%)	33	13
1	C	350/360 (97%)	335 (96%)	14 (4%)	1 (0%)	50	27
1	D	350/360 (97%)	336 (96%)	12 (3%)	2 (1%)	33	13
All	All	1400/1440 (97%)	1340 (96%)	53 (4%)	7 (0%)	38	17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	292	ALA
1	C	359	ASP
1	D	292	ALA
1	A	359	ASP
1	A	151	LEU
1	B	151	LEU
1	D	151	LEU

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	270/275 (98%)	262 (97%)	8 (3%)	53	29
1	B	270/275 (98%)	261 (97%)	9 (3%)	50	25
1	C	270/275 (98%)	264 (98%)	6 (2%)	64	43
1	D	270/275 (98%)	258 (96%)	12 (4%)	39	15
All	All	1080/1100 (98%)	1045 (97%)	35 (3%)	51	26

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	58	THR
1	A	73	LEU
1	A	103	ASN
1	A	134	ASN
1	A	199	MET
1	A	293	ASN
1	A	323	ASN
1	B	45	ILE
1	B	58	THR
1	B	65	GLN
1	B	103	ASN
1	B	133	LEU
1	B	134	ASN
1	B	199	MET
1	B	203	ARG
1	B	359	ASP
1	C	58	THR
1	C	73	LEU
1	C	103	ASN
1	C	134	ASN
1	C	199	MET
1	C	293	ASN
1	D	45	ILE
1	D	47	ARG
1	D	58	THR
1	D	73	LEU
1	D	103	ASN
1	D	133	LEU
1	D	134	ASN

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Mol	Chain	Res	Type
1	D	145	GLU
1	D	199	MET
1	D	203	ARG
1	D	323	ASN
1	D	359	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	103	ASN
1	A	123	GLN
1	A	134	ASN
1	A	176	GLN
1	A	286	HIS
1	A	293	ASN
1	A	323	ASN
1	B	21	HIS
1	B	103	ASN
1	B	134	ASN
1	B	176	GLN
1	B	263	ASN
1	B	286	HIS
1	C	21	HIS
1	C	103	ASN
1	C	123	GLN
1	C	134	ASN
1	C	286	HIS
1	D	21	HIS
1	D	103	ASN
1	D	134	ASN
1	D	176	GLN
1	D	263	ASN
1	D	286	HIS

5.3.3   RNA (i)

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 ⓘ

8 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	MRS	A	1751	-	66,66,66	1.09	3 (4%)	93,93,93	1.90	14 (15%)
3	GOL	A	2306	-	5,5,5	0.27	0	5,5,5	0.75	0
2	MRS	B	1752	-	66,66,66	1.12	3 (4%)	93,93,93	1.80	15 (16%)
3	GOL	B	2304	-	5,5,5	0.25	0	5,5,5	0.76	0
2	MRS	C	1753	-	66,66,66	1.05	2 (3%)	93,93,93	1.90	11 (11%)
3	GOL	C	2302	-	5,5,5	0.35	0	5,5,5	0.45	0
2	MRS	D	1754	-	66,66,66	1.10	4 (6%)	93,93,93	1.77	14 (15%)
3	GOL	D	2303	-	5,5,5	0.31	0	5,5,5	0.89	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	MRS	A	1751	-	-	0/67/83/83	0/1/3/3
3	GOL	A	2306	-	-	0/4/4/4	0/0/0/0
2	MRS	B	1752	-	-	0/67/83/83	0/1/3/3
3	GOL	B	2304	-	-	0/4/4/4	0/0/0/0
2	MRS	C	1753	-	-	1/67/83/83	0/1/3/3
3	GOL	C	2302	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MRS	D	1754	-	-	0/67/83/83	0/1/3/3
3	GOL	D	2303	-	-	0/4/4/4	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1752	MRS	C1-S1P	-6.33	1.68	1.76
2	D	1754	MRS	C1-S1P	-5.99	1.69	1.76
2	A	1751	MRS	C1-S1P	-5.60	1.69	1.76
2	C	1753	MRS	C1-S1P	-5.25	1.70	1.76
2	A	1751	MRS	C4A-N9A	-2.70	1.33	1.37
2	D	1754	MRS	C4A-N9A	-2.52	1.34	1.37
2	C	1753	MRS	C4A-N9A	-2.47	1.34	1.37
2	D	1754	MRS	O1-C1	2.38	1.23	1.20
2	B	1752	MRS	C4A-N9A	-2.38	1.34	1.37
2	B	1752	MRS	O1-C1	2.29	1.23	1.20
2	A	1751	MRS	P1A-O3A	2.16	1.63	1.59
2	D	1754	MRS	P1A-O3A	2.04	1.63	1.59

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1753	MRS	C2-C1-S1P	10.41	122.68	112.85
2	A	1751	MRS	C2-C1-S1P	10.21	122.50	112.85
2	B	1752	MRS	C2-C1-S1P	9.09	121.44	112.85
2	D	1754	MRS	C2-C1-S1P	8.75	121.12	112.85
2	A	1751	MRS	N3A-C2A-N1A	-7.65	122.32	128.71
2	D	1754	MRS	N3A-C2A-N1A	-7.45	122.48	128.71
2	C	1753	MRS	N3A-C2A-N1A	-7.33	122.58	128.71
2	B	1752	MRS	N3A-C2A-N1A	-7.15	122.73	128.71
2	C	1753	MRS	O1-C1-C2	-4.83	115.61	123.50
2	A	1751	MRS	C7P-N8P-C9P	4.33	131.47	122.57
2	A	1751	MRS	O1-C1-C2	-4.32	116.45	123.50
2	B	1752	MRS	N3A-C4A-N9A	4.28	133.16	125.43
2	B	1752	MRS	O1-C1-S1P	-4.16	120.06	123.67
2	C	1753	MRS	N3A-C4A-N9A	4.14	132.91	125.43
2	D	1754	MRS	N3A-C4A-N9A	4.14	132.90	125.43
2	A	1751	MRS	N3A-C4A-N9A	3.94	132.54	125.43
2	D	1754	MRS	C7P-N8P-C9P	3.83	130.44	122.57
2	C	1753	MRS	C7P-N8P-C9P	3.77	130.31	122.57
2	C	1753	MRS	C2P-S1P-C1	3.45	115.13	101.31
2	D	1754	MRS	O1-C1-S1P	-3.35	120.77	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1754	MRS	O1-C1-C2	-3.30	118.11	123.50
2	B	1752	MRS	C7P-N8P-C9P	3.28	129.31	122.57
2	B	1752	MRS	O1-C1-C2	-3.06	118.50	123.50
2	A	1751	MRS	O1-C1-S1P	-3.02	121.05	123.67
2	B	1752	MRS	CDP-CBP-CAP	2.98	113.99	108.82
2	B	1752	MRS	C5A-C4A-N3A	-2.93	119.33	125.70
2	A	1751	MRS	C2P-S1P-C1	2.89	112.86	101.31
2	C	1753	MRS	C5A-C4A-N3A	-2.80	119.60	125.70
2	D	1754	MRS	C5A-C4A-N3A	-2.80	119.60	125.70
2	A	1751	MRS	C5A-C4A-N3A	-2.77	119.67	125.70
2	B	1752	MRS	C3P-N4P-C5P	2.74	128.41	122.84
2	D	1754	MRS	C3P-N4P-C5P	2.70	128.33	122.84
2	A	1751	MRS	C2A-N3A-C4A	2.63	121.48	114.01
2	A	1751	MRS	C4A-C5A-N7A	-2.62	107.28	109.52
2	D	1754	MRS	C2A-N3A-C4A	2.61	121.44	114.01
2	A	1751	MRS	CDP-CBP-CCP	-2.58	105.03	108.76
2	B	1752	MRS	C2A-N3A-C4A	2.58	121.36	114.01
2	C	1753	MRS	C2A-N3A-C4A	2.55	121.26	114.01
2	A	1751	MRS	C2P-C3P-N4P	-2.55	106.74	112.50
2	C	1753	MRS	C4A-C5A-N7A	-2.50	107.38	109.52
2	B	1752	MRS	C4A-C5A-N7A	-2.43	107.44	109.52
2	D	1754	MRS	CDP-CBP-CAP	2.42	113.01	108.82
2	B	1752	MRS	C8A-N9A-C4A	2.28	108.64	106.90
2	A	1751	MRS	C3P-N4P-C5P	2.27	127.47	122.84
2	C	1753	MRS	C8A-N9A-C4A	2.27	108.63	106.90
2	C	1753	MRS	O1-C1-S1P	-2.27	121.70	123.67
2	D	1754	MRS	CBP-CAP-C9P	2.22	114.88	112.73
2	D	1754	MRS	C8A-N9A-C4A	2.20	108.58	106.90
2	A	1751	MRS	C8A-N9A-C4A	2.15	108.54	106.90
2	D	1754	MRS	C4A-C5A-N7A	-2.11	107.72	109.52
2	B	1752	MRS	C2P-C3P-N4P	-2.10	107.76	112.50
2	D	1754	MRS	O9A-P3B-O3B	-2.10	101.06	107.09
2	B	1752	MRS	O4B-C1B-N9A	2.08	110.38	108.44
2	B	1752	MRS	O5A-P2A-O3A	2.04	114.81	105.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1753	MRS	C3-C2-C1-S1P

There are no ring outliers.

5.7 Other polymers (i)

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	354/360 (98%)	0.14	6 (1%)	67	72	9, 24, 46, 57	0
1	B	354/360 (98%)	0.18	9 (2%)	54	60	9, 25, 49, 59	0
1	C	354/360 (98%)	0.08	9 (2%)	54	60	9, 25, 46, 56	0
1	D	354/360 (98%)	0.14	9 (2%)	54	60	9, 25, 49, 59	0
All	All	1416/1440 (98%)	0.14	33 (2%)	57	63	9, 25, 48, 59	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	ILE	5.6
1	B	323	ASN	4.9
1	B	39	PRO	4.4
1	C	360	GLY	4.0
1	C	45	ILE	3.9
1	D	292	ALA	3.6
1	C	323	ASN	3.6
1	A	347	ALA	3.5
1	C	39	PRO	3.4
1	B	350	ASP	3.3
1	B	292	ALA	3.3
1	D	360	GLY	3.3
1	C	326	TRP	3.2
1	D	350	ASP	3.0
1	D	293	ASN	2.9
1	A	322	ALA	2.8
1	D	355	LEU	2.8
1	C	38	ARG	2.6
1	D	39	PRO	2.6
1	A	323	ASN	2.6
1	D	323	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	349	ILE	2.5
1	B	354	VAL	2.5
1	C	292	ALA	2.4
1	C	2	ALA	2.4
1	B	45	ILE	2.3
1	B	38	ARG	2.3
1	C	47	ARG	2.2
1	D	359	ASP	2.2
1	A	38	ARG	2.1
1	B	326	TRP	2.1
1	A	2	ALA	2.0
1	B	73	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
3	GOL	C	2302	6/6	0.19	7.27	39,42,42,43	0
3	GOL	A	2306	6/6	0.16	6.71	38,42,42,45	0
3	GOL	B	2304	6/6	0.13	3.80	39,40,42,43	0
2	MRS	D	1754	64/64	0.18	1.92	38,52,59,61	0
2	MRS	C	1753	64/64	0.18	1.74	39,50,65,65	0
2	MRS	B	1752	64/64	0.16	1.46	36,50,63,63	0
3	GOL	D	2303	6/6	0.10	1.39	30,34,35,35	0
2	MRS	A	1751	64/64	0.15	1.15	36,50,58,59	0

6.5 Other polymers (i)

There are no such residues in this entry.