



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:42 PM GMT

PDB ID : 2GD6  
Title : The 1,1-proton transfer reaction mechanism by alpha-methylacyl-CoA racemase 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 : 2.30 Å(reported)

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

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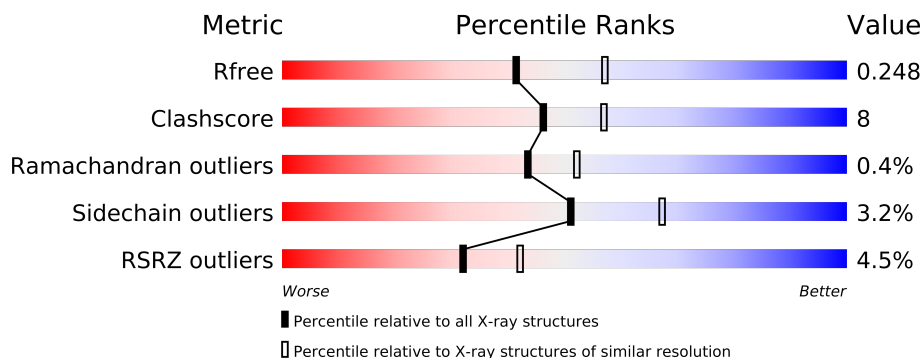
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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
2	ACO	B	752	-	X
3	GOL	C	1302	-	X

## 2 Entry composition i

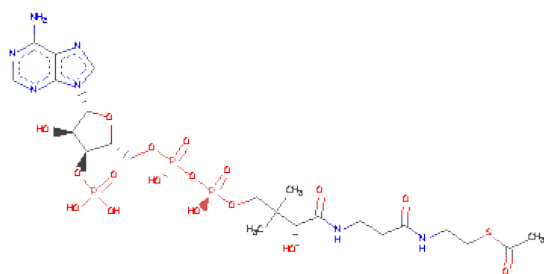
There are 4 unique types of molecules in this entry. The entry contains 11648 atoms, of which 0 are hydrogen and 0 are deuterium.

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	7	0
			2704	1694	488	506	16			
1	B	354	Total	C	N	O	S	0	4	0
			2696	1691	487	502	16			
1	C	354	Total	C	N	O	S	0	1	0
			2680	1683	481	501	15			
1	D	354	Total	C	N	O	S	0	1	0
			2680	1683	481	501	15			

- Molecule 2 is ACETYL COENZYME \*A (three-letter code: ACO) (formula: C<sub>23</sub>H<sub>38</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



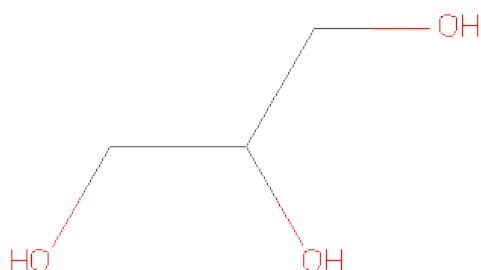
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			51	23	7	17	3 1		
2	B	1	Total	C	N	O	P S	0	0
			51	23	7	17	3 1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

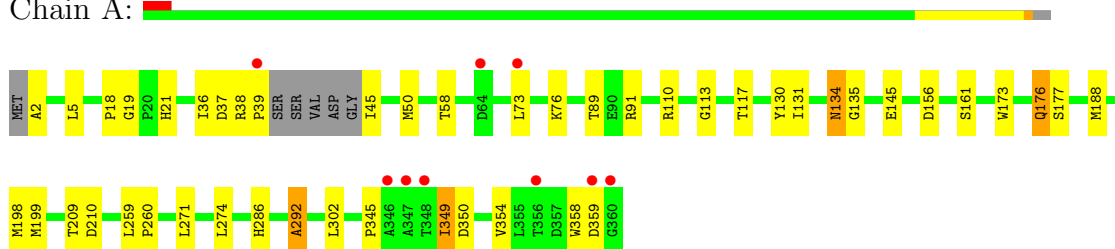
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	171	Total	O	0	0
			171	171		
4	B	185	Total	O	0	0
			185	185		
4	C	143	Total	O	0	0
			143	143		
4	D	173	Total	O	0	0
			173	173		

### 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.

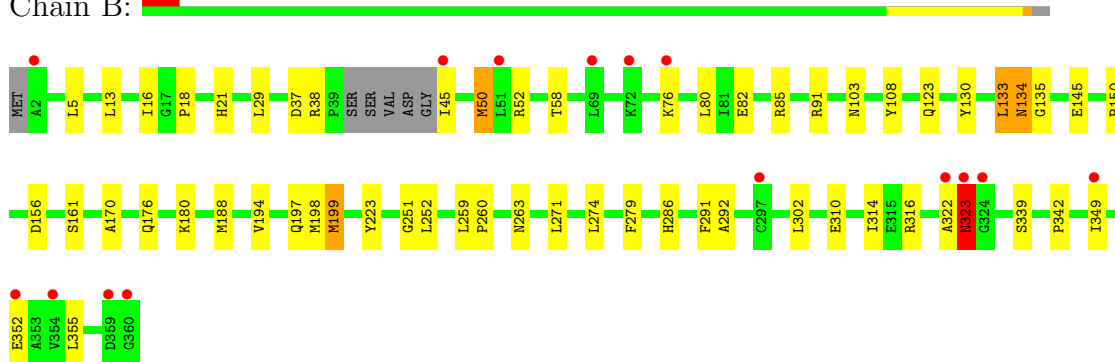
- Molecule 1: probable alpha-methylacyl-CoA racemase MCR

Chain A:



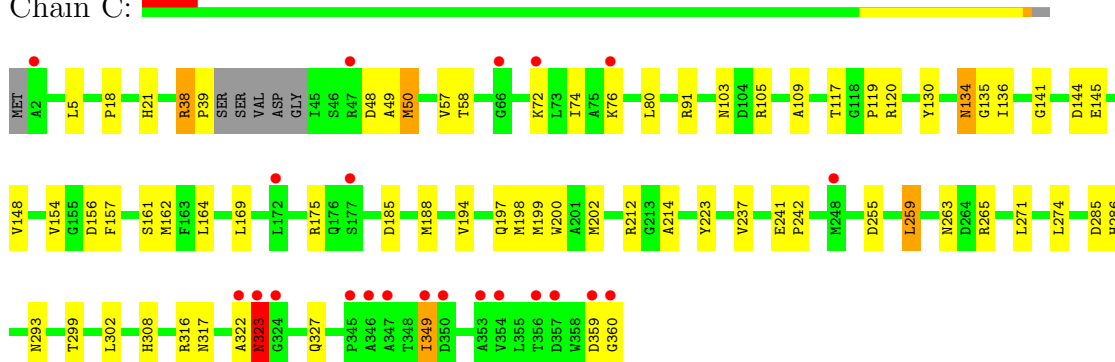
- Molecule 1: probable alpha-methylacyl-CoA racemase MCR

Chain B:



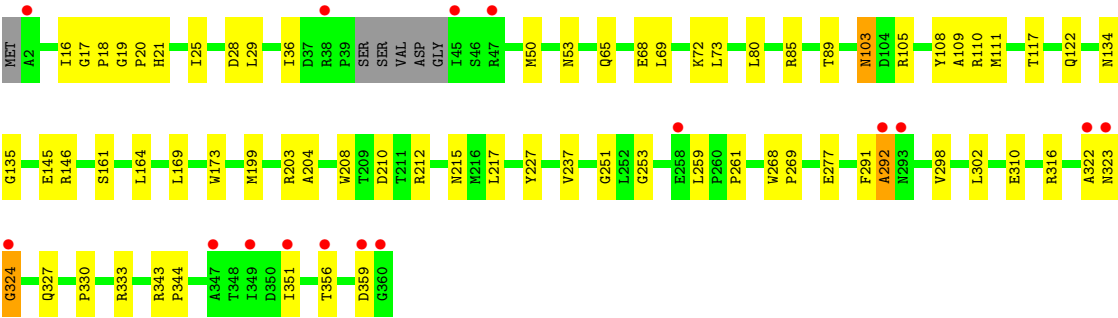
- Molecule 1: probable alpha-methylacyl-CoA racemase MCR

Chain C:



- Molecule 1: probable alpha-methylacyl-CoA racemase MCR

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.91Å 79.94Å 118.39Å 90.00° 91.03° 90.00°	Depositor
Resolution (Å)	19.71 – 2.30 19.71 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.71-2.30) 93.9 (19.71-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.98 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.219 , 0.270 0.231 , 0.248	Depositor DCC
$R_{free}$ test set	3713 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.6	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.8	EDS
Estimated twinning fraction	0.327 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 74229 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11648	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	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 56.28 % 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 2.7998e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>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, ACO

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	0.61	0/2801	0.69	0/3807
1	B	0.61	0/2778	0.70	1/3776 (0.0%)
1	C	0.57	0/2746	0.67	1/3735 (0.0%)
1	D	0.57	0/2746	0.66	0/3735
All	All	0.59	0/11071	0.68	2/15053 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	LEU	CA-CB-CG	5.92	128.91	115.30
1	C	259	LEU	CA-CB-CG	5.11	127.06	115.30

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	2704	0	2639	38	0
1	B	2696	0	2638	43	0
1	C	2680	0	2624	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2680	0	2624	56	0
2	A	51	0	34	2	0
2	B	51	0	34	3	0
2	C	51	0	34	9	0
2	D	51	0	34	2	0
3	A	6	0	8	2	0
3	C	6	0	8	0	0
4	A	171	0	0	10	0
4	B	185	0	0	8	0
4	C	143	0	0	15	0
4	D	173	0	0	15	0
All	All	11648	0	10677	178	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 (178) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:292:ALA:HA	4:D:850:HOH:O	1.68	0.94
1:C:91:ARG:HB2	4:C:1389:HOH:O	1.67	0.93
1:D:36:ILE:HD11	1:D:73:LEU:HD23	1.56	0.84
1:B:292:ALA:O	4:B:792:HOH:O	1.95	0.83
1:D:227:TYR:HE1	4:D:926:HOH:O	1.63	0.80
1:C:197:GLN:HE22	1:D:50:MET:HA	1.46	0.80
1:A:350:ASP:HB3	4:A:1440:HOH:O	1.82	0.79
2:C:753:ACO:H141	2:C:753:ACO:H32	1.64	0.79
1:A:173:TRP:O	1:A:176:GLN:HG3	1.83	0.79
1:B:286:HIS:HE1	4:B:775:HOH:O	1.65	0.79
1:A:286:HIS:HE1	4:A:1446:HOH:O	1.66	0.78
2:A:751:ACO:O	4:A:1472:HOH:O	2.00	0.78
1:C:91:ARG:NH1	2:C:753:ACO:O7A	2.18	0.77
1:B:322:ALA:O	1:B:323:ASN:C	2.23	0.76
1:D:68:GLU:O	1:D:72:LYS:HG3	1.88	0.74
1:D:261:PRO:HA	4:D:791:HOH:O	1.88	0.72
1:A:21:HIS:HD2	1:A:161:SER:OG	1.72	0.72
2:A:751:ACO:H141	2:A:751:ACO:O5P	1.89	0.72
4:A:1420:HOH:O	1:B:50:MET:HE3	1.89	0.72
1:B:91:ARG:NH1	2:B:752:ACO:O9A	2.24	0.70
1:D:109:ALA:HB1	1:D:164:LEU:HD11	1.73	0.70
1:C:285:ASP:OD2	4:C:1406:HOH:O	2.09	0.69
1:D:103:ASN:HD22	1:D:103:ASN:C	1.96	0.68
1:A:2:ALA:HB1	4:A:1406:HOH:O	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:754:ACO:H141	2:D:754:ACO:H31	1.75	0.68
1:C:48:ASP:OD1	1:C:50:MET:HB3	1.93	0.68
1:B:21:HIS:HA	1:B:50:MET:HE1	1.77	0.67
1:C:223:TYR:OH	1:C:263:ASN:ND2	2.27	0.67
1:C:148:VAL:HB	4:D:915:HOH:O	1.96	0.66
2:D:754:ACO:S1P	4:D:826:HOH:O	2.54	0.65
1:A:145:GLU:OE2	1:B:145:GLU:OE2	2.15	0.65
1:C:322:ALA:O	1:C:323:ASN:C	2.36	0.64
1:C:76:LYS:HE3	1:C:360:GLY:HA2	1.80	0.64
1:C:130:TYR:HE2	2:C:753:ACO:CH3	2.11	0.63
1:A:349:ILE:HD11	1:A:354:VAL:HG23	1.80	0.63
1:D:237:VAL:HB	4:D:926:HOH:O	1.99	0.62
1:B:322:ALA:O	1:B:323:ASN:O	2.17	0.62
1:C:316:ARG:HD2	1:D:117:THR:O	2.00	0.61
1:C:38:ARG:CZ	1:C:39:PRO:O	2.48	0.61
1:B:85:ARG:HD3	4:B:774:HOH:O	2.01	0.61
1:C:302:LEU:HD12	4:D:917:HOH:O	1.99	0.61
1:D:53:ASN:OD1	1:D:343:ARG:NH1	2.34	0.60
1:B:21:HIS:HD2	1:B:161:SER:OG	1.84	0.60
1:C:130:TYR:HE2	2:C:753:ACO:HH33	1.67	0.58
1:B:130:TYR:CE2	1:B:188:MET:HE3	2.39	0.58
1:D:19:GLY:HA3	4:D:799:HOH:O	2.04	0.58
1:C:185:ASP:HB3	1:D:333:ARG:HB2	1.85	0.57
1:B:259:LEU:HD13	1:B:274:LEU:HD13	1.88	0.56
2:C:753:ACO:HN4	2:C:753:ACO:HH33	1.71	0.55
1:A:36:ILE:HD11	1:A:73:LEU:HD23	1.88	0.55
1:C:5:LEU:HD23	1:D:173:TRP:CD1	2.42	0.55
1:A:19:GLY:HA3	4:A:1405:HOH:O	2.07	0.55
1:A:37:ASP:OD1	1:A:38:ARG:N	2.39	0.54
1:A:259:LEU:HD22	1:A:274:LEU:HD13	1.90	0.54
1:A:58:THR:HG23	4:A:1377:HOH:O	2.07	0.54
1:A:176:GLN:HE21	1:B:176:GLN:NE2	2.06	0.54
1:C:109:ALA:HB1	1:C:164:LEU:HD11	1.89	0.54
1:C:120:ARG:NH2	1:D:310:GLU:OE2	2.31	0.54
1:C:18:PRO:HB3	1:C:156:ASP:O	2.08	0.53
1:D:80:LEU:HD23	1:D:108:TYR:CE1	2.43	0.53
1:C:259:LEU:HD12	1:C:271:LEU:CD1	2.38	0.53
1:D:103:ASN:HD22	1:D:105:ARG:H	1.56	0.53
1:C:302:LEU:O	1:D:135:GLY:HA2	2.09	0.53
1:D:103:ASN:C	1:D:103:ASN:ND2	2.63	0.53
1:B:180:LYS:HG3	4:B:862:HOH:O	2.08	0.53
1:D:103:ASN:ND2	1:D:105:ARG:H	2.07	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:169:LEU:HB3	1:D:169:LEU:HB3	1.90	0.52
1:B:45:ILE:HG23	1:B:45:ILE:O	2.10	0.51
1:A:210:ASP:N	3:A:1301:GOL:O1	2.32	0.51
1:B:251:GLY:HA3	1:B:291:PHE:CE2	2.45	0.51
1:C:308:HIS:HA	4:C:1367:HOH:O	2.11	0.51
1:B:198:MET:HE2	1:B:199:MET:HE1	1.93	0.51
1:C:214:ALA:O	1:C:265:ARG:NH2	2.36	0.51
1:C:241:GLU:N	1:C:241:GLU:OE1	2.37	0.51
1:A:135:GLY:HA2	1:B:302:LEU:O	2.11	0.50
1:C:197:GLN:NE2	1:D:50:MET:HA	2.20	0.50
1:C:197:GLN:HE22	1:D:50:MET:CA	2.21	0.50
1:C:198:MET:HG2	1:C:202:MET:HE2	1.94	0.50
1:C:134:ASN:HD22	1:C:134:ASN:C	2.14	0.50
1:C:91:ARG:CB	4:C:1389:HOH:O	2.40	0.50
1:C:194:VAL:O	1:D:21:HIS:HE1	1.95	0.50
1:A:173:TRP:CD1	1:B:5:LEU:HD23	2.47	0.49
1:B:16:ILE:HG22	2:B:752:ACO:S1P	2.53	0.49
1:A:286:HIS:HD2	1:D:253:GLY:HA2	1.77	0.49
1:C:21:HIS:HD2	1:C:161:SER:OG	1.95	0.49
1:D:18:PRO:HB2	1:D:111:MET:HG2	1.94	0.49
1:D:322:ALA:HB1	4:D:901:HOH:O	2.11	0.49
1:C:286:HIS:HE1	4:C:1371:HOH:O	1.95	0.49
1:D:203:ARG:NH2	4:D:896:HOH:O	2.47	0.48
1:C:57:VAL:HG12	1:C:349:ILE:O	2.13	0.48
1:D:65:GLN:HG2	1:D:69:LEU:HD12	1.96	0.48
1:D:292:ALA:CA	4:D:850:HOH:O	2.41	0.48
1:C:188:MET:CE	2:C:753:ACO:HH32	2.44	0.48
1:D:85:ARG:NH1	1:D:122:GLN:OE1	2.47	0.48
1:B:286:HIS:CE1	4:B:775:HOH:O	2.51	0.47
4:C:1403:HOH:O	1:D:173:TRP:HZ3	1.97	0.47
1:B:260:PRO:HG2	1:B:271:LEU:HB2	1.95	0.47
1:C:74:ILE:HG12	1:C:80:LEU:HD13	1.95	0.47
1:C:119:PRO:HB2	4:D:888:HOH:O	2.15	0.47
1:C:72:LYS:HA	4:C:1402:HOH:O	2.14	0.47
1:B:352:GLU:HA	1:B:355:LEU:HD12	1.97	0.47
1:A:349:ILE:HD11	1:A:354:VAL:CG2	2.43	0.47
1:B:85:ARG:HB2	2:B:752:ACO:O2A	2.15	0.47
1:A:38:ARG:HG2	1:A:39:PRO:HD2	1.95	0.47
1:C:286:HIS:CE1	4:C:1371:HOH:O	2.68	0.47
1:A:117:THR:O	1:B:316:ARG:HD2	2.15	0.47
1:D:16:ILE:HG23	4:D:772:HOH:O	2.14	0.47
1:C:255:ASP:O	1:C:259:LEU:HD23	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:227:TYR:CE1	4:D:926:HOH:O	2.51	0.46
1:D:251:GLY:HA3	1:D:291:PHE:CE2	2.49	0.46
1:C:317:ASN:N	1:C:317:ASN:HD22	2.14	0.46
4:C:1399:HOH:O	1:D:204:ALA:HB2	2.15	0.46
1:A:76:LYS:HE2	1:A:358:TRP:O	2.14	0.46
1:B:52:ARG:HG3	1:B:342:PRO:HB3	1.97	0.46
1:D:69:LEU:HB3	1:D:351:ILE:HD13	1.96	0.46
1:A:130:TYR:CE2	1:A:188:MET:HE3	2.51	0.46
1:D:145:GLU:O	1:D:212:ARG:NH2	2.47	0.45
1:C:105:ARG:HB3	1:C:175:ARG:HH11	1.81	0.45
1:D:89:THR:OG1	1:D:110:ARG:NH2	2.50	0.45
1:C:117:THR:O	1:D:316:ARG:HD2	2.17	0.45
1:B:223:TYR:OH	1:B:263:ASN:ND2	2.43	0.45
1:C:299:THR:HG23	4:C:1352:HOH:O	2.17	0.45
1:A:349:ILE:HD12	1:A:350:ASP:O	2.16	0.45
1:A:131:ILE:HA	1:A:134:ASN:HD21	1.81	0.45
4:C:1417:HOH:O	1:D:217:LEU:HB3	2.17	0.45
1:C:145:GLU:O	1:C:212:ARG:NH2	2.44	0.45
1:B:252:LEU:HD21	1:B:279:PHE:CE1	2.52	0.45
1:A:198:MET:HB2	4:A:1420:HOH:O	2.16	0.45
1:B:150:PRO:HG2	4:B:753:HOH:O	2.17	0.45
1:D:323:ASN:O	1:D:324:GLY:O	2.35	0.44
1:B:286:HIS:HD2	4:B:885:HOH:O	1.99	0.44
1:B:18:PRO:HB3	1:B:156:ASP:O	2.17	0.44
1:C:259:LEU:HD13	1:C:274:LEU:HD13	2.00	0.44
1:A:50:MET:HA	1:B:197:GLN:HE22	1.83	0.44
1:D:208:TRP:CZ3	1:D:215:ASN:HB3	2.52	0.44
1:C:141:GLY:HA3	4:C:1374:HOH:O	2.17	0.44
1:A:302:LEU:O	1:B:135:GLY:HA2	2.17	0.44
1:D:18:PRO:HB2	1:D:111:MET:CG	2.47	0.44
1:D:203:ARG:HD2	1:D:210:ASP:OD1	2.18	0.44
1:B:13:LEU:HD12	1:B:82:GLU:HB3	2.00	0.44
1:C:157:PHE:O	1:C:162:MET:HG2	2.18	0.44
1:C:135:GLY:HA2	1:D:302:LEU:O	2.18	0.43
1:A:209:THR:HB	3:A:1301:GOL:H12	2.00	0.43
1:D:277:GLU:HG3	4:D:909:HOH:O	2.18	0.43
1:A:286:HIS:CE1	4:A:1446:HOH:O	2.54	0.43
1:A:21:HIS:CD2	1:A:161:SER:OG	2.62	0.43
1:A:21:HIS:HE1	1:B:194:VAL:O	2.01	0.43
1:C:49:ALA:HB1	1:C:327:GLN:OE1	2.18	0.43
1:D:237:VAL:HG22	1:D:298:VAL:HG22	2.00	0.43
1:B:263:ASN:ND2	4:B:899:HOH:O	2.50	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:17:GLY:O	1:D:20:PRO:HD2	2.18	0.43
1:A:292:ALA:O	1:B:123:GLN:NE2	2.50	0.43
1:A:113:GLY:HA3	1:A:130:TYR:CZ	2.53	0.43
1:C:130:TYR:HE2	2:C:753:ACO:HH31	1.82	0.42
1:B:80:LEU:HD23	1:B:108:TYR:CE1	2.54	0.42
1:A:89:THR:OG1	1:A:110:ARG:NH2	2.53	0.42
1:B:310:GLU:O	1:B:314:ILE:HG13	2.18	0.42
1:D:268:TRP:N	1:D:269:PRO:CD	2.83	0.42
1:C:242:PRO:HD2	4:C:1343:HOH:O	2.19	0.42
2:C:753:ACO:N4P	2:C:753:ACO:HH33	2.35	0.42
1:C:200:TRP:C	1:D:327:GLN:HE22	2.23	0.42
1:D:25:ILE:O	1:D:29:LEU:HG	2.20	0.41
1:A:345:PRO:HB3	4:A:1463:HOH:O	2.20	0.41
1:C:91:ARG:CG	4:C:1389:HOH:O	2.67	0.41
1:A:5:LEU:HD21	1:B:170:ALA:HA	2.02	0.41
1:D:145:GLU:HG3	1:D:146:ARG:O	2.20	0.41
1:B:134:ASN:HD22	1:B:134:ASN:C	2.23	0.41
1:C:156:ASP:OD1	2:C:753:ACO:HH32	2.20	0.41
1:C:223:TYR:O	1:C:237:VAL:HG12	2.21	0.41
1:A:18:PRO:HB3	1:A:156:ASP:O	2.21	0.41
1:A:260:PRO:HG2	1:A:271:LEU:HB2	2.03	0.41
1:B:156:ASP:HA	1:B:188:MET:SD	2.61	0.40
1:C:144:ASP:OD1	4:C:1419:HOH:O	2.22	0.40
1:D:343:ARG:HA	1:D:344:PRO:HD2	1.82	0.40
1:D:21:HIS:HD2	1:D:161:SER:OG	2.05	0.40
1:B:29:LEU:HA	1:B:339:SER:OG	2.20	0.40
1:D:28:ASP:HB3	1:D:330:PRO:HB3	2.03	0.40
1:C:136:ILE:HG21	1:C:154:VAL:HG11	2.03	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	357/360 (99%)	341 (96%)	15 (4%)	1 (0%)	50 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	354/360 (98%)	338 (96%)	15 (4%)	1 (0%)	50 60
1	C	351/360 (98%)	335 (95%)	15 (4%)	1 (0%)	50 60
1	D	351/360 (98%)	333 (95%)	16 (5%)	2 (1%)	33 39
All	All	1413/1440 (98%)	1347 (95%)	61 (4%)	5 (0%)	43 52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	292	ALA
1	A	292	ALA
1	B	323	ASN
1	D	324	GLY
1	C	323	ASN

### 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	277/275 (101%)	269 (97%)	8 (3%)	55 71
1	B	274/275 (100%)	263 (96%)	11 (4%)	42 56
1	C	271/275 (98%)	261 (96%)	10 (4%)	45 60
1	D	271/275 (98%)	265 (98%)	6 (2%)	64 81
All	All	1093/1100 (99%)	1058 (97%)	35 (3%)	51 67

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

Mol	Chain	Res	Type
1	A	45	ILE
1	A	91	ARG
1	A	134	ASN
1	A	176	GLN
1	A	177	SER
1	A	199	MET
1	A	349	ILE

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Mol	Chain	Res	Type
1	A	359	ASP
1	B	37	ASP
1	B	38	ARG
1	B	50	MET
1	B	58	THR
1	B	76	LYS
1	B	103	ASN
1	B	133	LEU
1	B	134	ASN
1	B	199	MET
1	B	323	ASN
1	B	349	ILE
1	C	38	ARG
1	C	50	MET
1	C	58	THR
1	C	103	ASN
1	C	134	ASN
1	C	199	MET
1	C	293	ASN
1	C	323	ASN
1	C	349	ILE
1	C	359	ASP
1	D	103	ASN
1	D	134	ASN
1	D	199	MET
1	D	259	LEU
1	D	356	THR
1	D	359	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) 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	327	GLN
1	B	21	HIS
1	B	103	ASN
1	B	134	ASN

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Mol	Chain	Res	Type
1	B	176	GLN
1	B	263	ASN
1	B	286	HIS
1	C	21	HIS
1	C	65	GLN
1	C	103	ASN
1	C	134	ASN
1	C	263	ASN
1	C	317	ASN
1	D	21	HIS
1	D	65	GLN
1	D	103	ASN
1	D	123	GLN
1	D	134	ASN
1	D	263	ASN
1	D	286	HIS
1	D	327	GLN
1	D	341	GLN

### 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 ⓘ

6 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	$\# Z  > 2$
3	GOL	A	1301	-	5,5,5	0.83	0	5,5,5	1.98	2 (40%)
2	ACO	A	751	-	53,53,53	0.91	2 (3%)	79,79,79	1.55	8 (10%)
2	ACO	B	752	-	53,53,53	0.94	2 (3%)	79,79,79	1.54	8 (10%)
3	GOL	C	1302	-	5,5,5	0.29	0	5,5,5	0.35	0
2	ACO	C	753	-	53,53,53	0.94	2 (3%)	79,79,79	1.51	10 (12%)
2	ACO	D	754	-	53,53,53	0.99	3 (5%)	79,79,79	1.71	10 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1301	-	-	0/4/4/4	0/0/0/0
2	ACO	A	751	-	-	1/51/67/67	0/1/3/3
2	ACO	B	752	-	-	0/51/67/67	0/1/3/3
3	GOL	C	1302	-	-	0/4/4/4	0/0/0/0
2	ACO	C	753	-	-	2/51/67/67	0/1/3/3
2	ACO	D	754	-	-	0/51/67/67	0/1/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	753	ACO	C5A-C4A	3.56	1.48	1.40
2	B	752	ACO	C5A-C4A	3.33	1.48	1.40
2	D	754	ACO	C5A-C4A	3.24	1.47	1.40
2	A	751	ACO	C5A-C4A	3.19	1.47	1.40
2	D	754	ACO	C4A-N9A	-2.51	1.34	1.37
2	D	754	ACO	O4B-C1B	2.29	1.44	1.41
2	B	752	ACO	C4A-N9A	-2.21	1.34	1.37
2	A	751	ACO	C4A-N9A	-2.21	1.34	1.37
2	C	753	ACO	C4A-N9A	-2.20	1.34	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	753	ACO	N3A-C2A-N1A	-6.67	123.13	128.71
2	A	751	ACO	N3A-C2A-N1A	-6.66	123.14	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	754	ACO	N3A-C2A-N1A	-6.64	123.16	128.71
2	B	752	ACO	N3A-C2A-N1A	-6.39	123.36	128.71
2	B	752	ACO	N3A-C4A-N9A	5.44	135.25	125.43
2	C	753	ACO	N3A-C4A-N9A	5.25	134.92	125.43
2	D	754	ACO	N3A-C4A-N9A	5.20	134.81	125.43
2	A	751	ACO	N3A-C4A-N9A	5.16	134.75	125.43
2	D	754	ACO	CBP-CAP-C9P	4.59	117.18	112.73
2	D	754	ACO	C4A-C5A-N7A	-4.53	105.64	109.52
2	D	754	ACO	O4B-C1B-N9A	4.37	112.51	108.44
2	A	751	ACO	C4A-C5A-N7A	-4.04	106.06	109.52
2	B	752	ACO	C4A-C5A-N7A	-3.62	106.42	109.52
2	D	754	ACO	C5A-C4A-N3A	-3.55	117.97	125.70
2	B	752	ACO	C5A-C4A-N3A	-3.43	118.23	125.70
2	C	753	ACO	C4A-C5A-N7A	-3.42	106.59	109.52
2	A	751	ACO	C5A-C4A-N3A	-3.34	118.44	125.70
2	D	754	ACO	C2P-S1P-C	3.29	114.76	101.38
3	A	1301	GOL	O3-C3-C2	-3.26	93.79	109.71
2	C	753	ACO	C5A-C4A-N3A	-3.08	118.98	125.70
3	A	1301	GOL	O1-C1-C2	-2.91	95.50	109.71
2	C	753	ACO	C2P-S1P-C	2.91	113.22	101.38
2	D	754	ACO	C2A-N3A-C4A	2.82	122.04	114.01
2	B	752	ACO	C2P-S1P-C	2.81	112.80	101.38
2	B	752	ACO	O4B-C1B-C2B	-2.68	102.67	106.77
2	B	752	ACO	O4B-C1B-N9A	2.64	110.89	108.44
2	D	754	ACO	CDP-CBP-CAP	2.63	113.37	108.82
2	A	751	ACO	C2A-N3A-C4A	2.62	121.46	114.01
2	B	752	ACO	C2A-N3A-C4A	2.62	121.45	114.01
2	A	751	ACO	C6P-C7P-N8P	2.61	117.50	111.87
2	C	753	ACO	C2A-N3A-C4A	2.46	121.01	114.01
2	C	753	ACO	O4B-C1B-C2B	-2.42	103.06	106.77
2	A	751	ACO	O8A-P3B-O3B	-2.29	100.48	107.09
2	A	751	ACO	P2A-O3A-P1A	-2.25	125.08	131.68
2	C	753	ACO	C8A-N9A-C4A	2.24	108.61	106.90
2	D	754	ACO	C7P-C6P-C5P	-2.15	108.60	112.25
2	C	753	ACO	O9A-P3B-O3B	-2.14	100.92	107.09
2	C	753	ACO	CEP-CBP-CCP	-2.10	105.73	108.76

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	753	ACO	CH3-C-S1P-C2P

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Mol	Chain	Res	Type	Atoms
2	C	753	ACO	O-C-S1P-C2P
2	A	751	ACO	CAP-C9P-N8P-C7P

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	354/360 (98%)	0.60	9 (2%) 54 65	29, 35, 41, 49	1 (0%)
1	B	354/360 (98%)	0.65	15 (4%) 35 45	30, 35, 41, 47	7 (1%)
1	C	354/360 (98%)	0.63	22 (6%) 20 28	29, 35, 41, 47	12 (3%)
1	D	354/360 (98%)	0.62	16 (4%) 32 42	30, 35, 41, 48	12 (3%)
All	All	1416/1440 (98%)	0.62	62 (4%) 32 43	29, 35, 41, 49	32 (2%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	360	GLY	7.6
1	C	360	GLY	6.5
1	A	360	GLY	5.7
1	C	359	ASP	4.7
1	D	360	GLY	4.6
1	B	359	ASP	4.6
1	A	346	ALA	4.2
1	B	324	GLY	4.1
1	A	347	ALA	3.8
1	C	322	ALA	3.8
1	D	322	ALA	3.8
1	C	323	ASN	3.8
1	C	347	ALA	3.7
1	C	346	ALA	3.5
1	B	45	ILE	3.4
1	C	2	ALA	3.3
1	A	359	ASP	3.3
1	C	349	ILE	3.3
1	D	359	ASP	3.2
1	C	353	ALA	3.2
1	B	323	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	349	ILE	3.0
1	A	73	LEU	2.8
1	D	323	ASN	2.7
1	C	47	ARG	2.7
1	D	47	ARG	2.6
1	D	347	ALA	2.6
1	D	324	GLY	2.6
1	A	356	THR	2.6
1	C	345	PRO	2.5
1	B	349	ILE	2.5
1	A	39	PRO	2.5
1	C	357	ASP	2.5
1	D	45	ILE	2.4
1	C	72	LYS	2.4
1	C	324	GLY	2.4
1	C	350	ASP	2.4
1	D	356	THR	2.4
1	B	69	LEU	2.4
1	B	76	LYS	2.3
1	B	322	ALA	2.3
1	C	177	SER	2.3
1	C	356	THR	2.2
1	C	354	VAL	2.2
1	A	64	ASP	2.2
1	D	38	ARG	2.2
1	D	351	ILE	2.2
1	D	2	ALA	2.2
1	C	172	LEU	2.2
1	A	348	THR	2.2
1	B	72	LYS	2.1
1	C	76	LYS	2.1
1	D	293	ASN	2.1
1	D	292	ALA	2.1
1	B	352	GLU	2.1
1	B	51	LEU	2.1
1	C	66	GLY	2.1
1	D	258	GLU	2.1
1	C	248	MET	2.0
1	B	297	CYS	2.0
1	B	2	ALA	2.0
1	B	354	VAL	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ACO	B	752	51/51	0.27	2.63	58,62,68,68	0
3	GOL	C	1302	6/6	0.23	2.56	58,62,63,64	0
2	ACO	C	753	51/51	0.25	1.95	51,57,73,74	0
2	ACO	A	751	51/51	0.25	1.84	56,60,76,77	0
3	GOL	A	1301	6/6	0.19	0.53	21,29,32,32	0
2	ACO	D	754	51/51	0.19	0.29	54,58,66,66	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.