



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 06:04 pm GMT

PDB ID : 2GCI  
Title : The 1,1-proton transfer reaction mechanism by alpha-methylacyl-CoA race-  
mase is catalyzed by an asparte/histidine pair and involves a smooth,  
methionine-rich surface for binding the fatty acyl moiety  
Authors : Bhaumik, P.; Wierenga, R.K.  
Deposited on : 2006-03-14  
Resolution : 1.60 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](mailto: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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

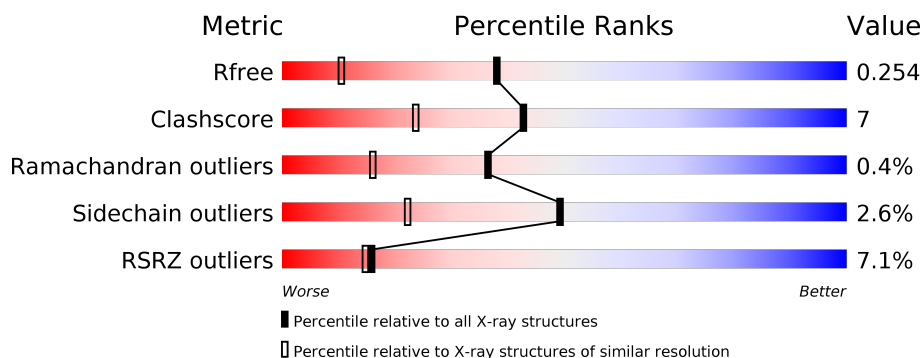
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
$R_{free}$	111664	2957 (1.60-1.60)
Clashscore	122126	3202 (1.60-1.60)
Ramachandran outliers	120053	3117 (1.60-1.60)
Sidechain outliers	120020	3116 (1.60-1.60)
RSRZ outliers	108989	2883 (1.60-1.60)

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. 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	360	<div> <div>9%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	B	360	<div> <div>11%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	C	360	<div> <div>5%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	D	360	<div> <div>3%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	C	1302	-	-	X	-

## 2 Entry composition [i](#)

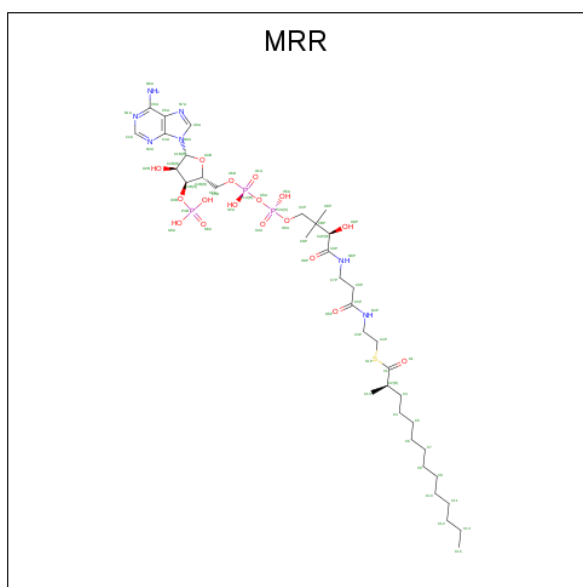
There are 4 unique types of molecules in this entry. The entry contains 12207 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 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 (R)-2-METHYLMYRISTOYL-COENZYME A (three-letter code: MRR) (formula: C<sub>36</sub>H<sub>64</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
			55	27	7	17	3 1		
2	B	1	Total	C	N	O	P S	0	1
			74	46	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
			54	26	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	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	246	Total	O	0	0
			246	246		

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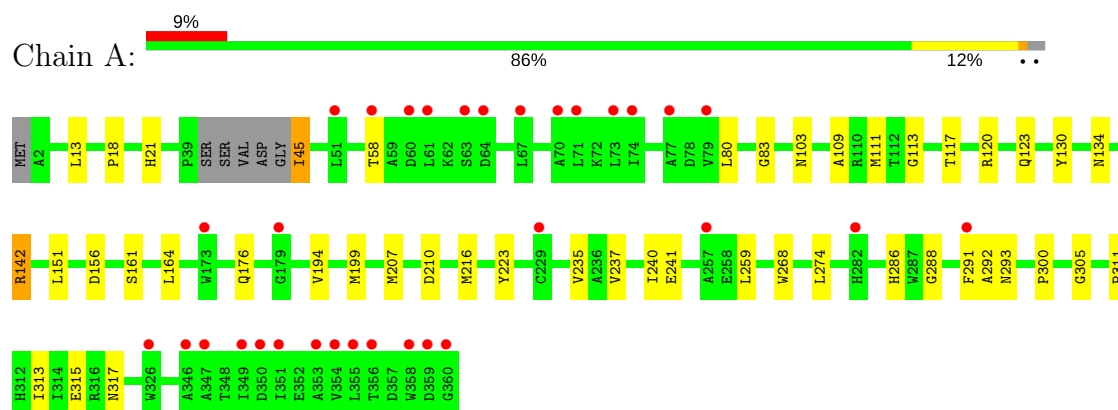
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	243	Total 243	O 243	0	0
4	C	349	Total 349	O 349	0	0
4	D	370	Total 370	O 370	0	0

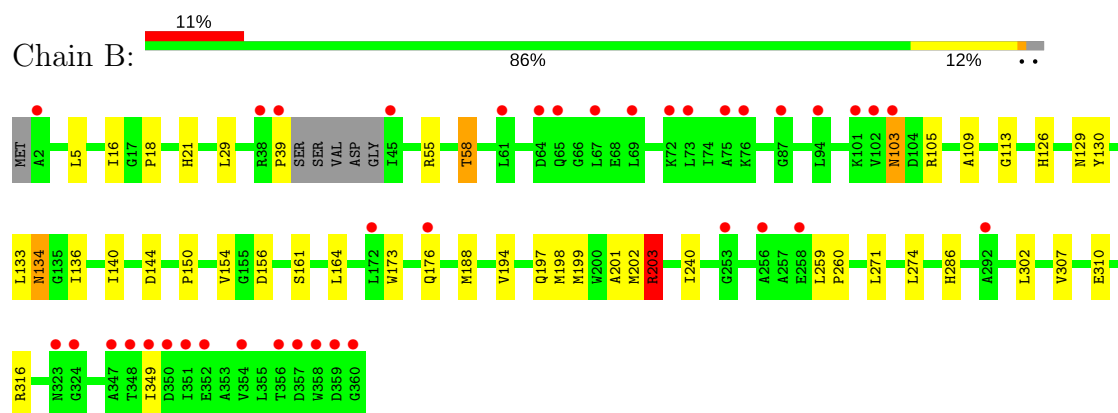
### 3 Residue-property plots [i](#)

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.

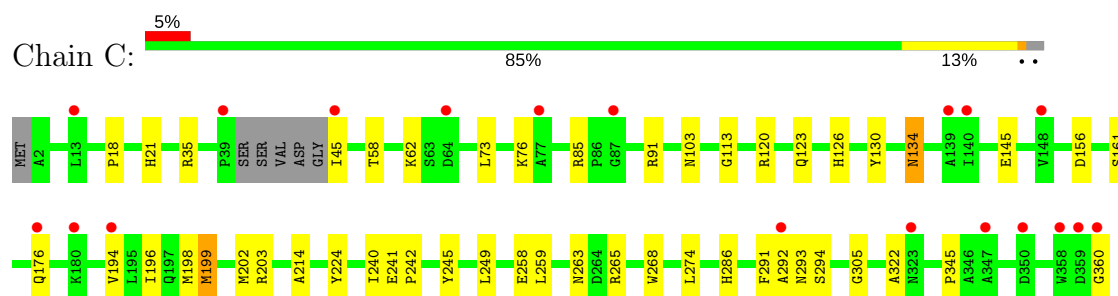
- Molecule 1: probable alpha-methylacyl-CoA racemase MCR



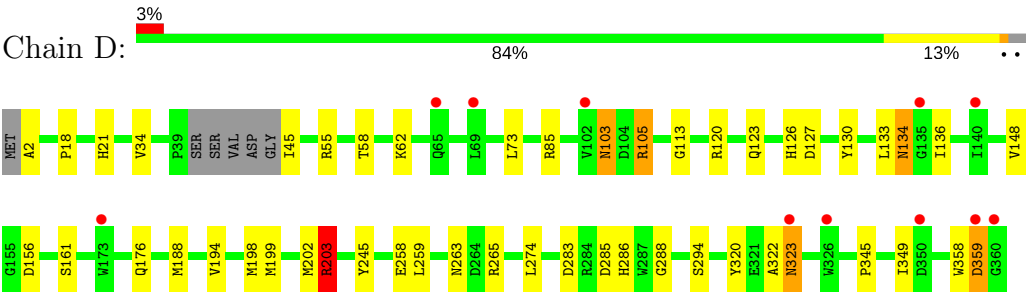
- Molecule 1: probable alpha-methylacyl-CoA racemase MCR



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.70Å 79.81Å 118.06Å 90.00° 89.93° 90.00°	Depositor
Resolution (Å)	19.83 – 1.60 19.83 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.83-1.60) 96.7 (19.83-1.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.210 , 0.244 0.244 , 0.254	Depositor DCC
$R_{free}$ test set	10825 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.7	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.458 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12207	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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 64.75 % 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 7.8953e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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

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	0.63	0/2740	0.73	1/3727 (0.0%)
1	B	0.64	0/2740	0.72	1/3727 (0.0%)
1	C	0.87	2/2740 (0.1%)	0.85	2/3727 (0.1%)
1	D	0.85	2/2740 (0.1%)	0.89	5/3727 (0.1%)
All	All	0.75	4/10960 (0.0%)	0.80	9/14908 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	105	ARG	CZ-NH1	5.82	1.40	1.33
1	C	268	TRP	CG-CD1	5.69	1.44	1.36
1	D	245	TYR	CE2-CZ	5.01	1.45	1.38
1	C	224	TYR	CG-CD2	5.00	1.45	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	203	ARG	NE-CZ-NH1	15.77	128.18	120.30
1	C	35	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	D	203	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	142	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	B	203	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	D	265	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	D	105	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	C	35	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	D	120	ARG	NE-CZ-NH2	-5.86	117.37	120.30

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	2679	0	2623	38	0
1	B	2679	0	2623	36	0
1	C	2679	0	2623	46	1
1	D	2679	0	2623	49	0
2	A	55	0	39	0	0
2	B	74	0	46	8	0
2	C	54	0	39	3	0
2	D	64	0	60	14	0
3	A	6	0	8	2	0
3	B	12	0	16	1	1
3	C	12	0	16	7	0
3	D	6	0	8	1	1
4	A	246	0	0	20	1
4	B	243	0	0	6	0
4	C	349	0	0	12	1
4	D	370	0	0	16	1
All	All	12207	0	10724	162	3

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 (162) 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:237:VAL:HG12	4:A:1988:HOH:O	1.31	1.29
1:A:300:PRO:HA	4:A:1986:HOH:O	1.13	1.25
1:C:242:PRO:HD3	2:D:1754:MRR:H151	1.32	1.10
1:D:283:ASP:HB2	4:D:2112:HOH:O	1.54	1.07
1:C:202:MET:HE2	4:C:2002:HOH:O	1.57	1.04
1:D:285:ASP:OD1	4:D:2051:HOH:O	1.76	1.00
1:D:156:ASP:OD2	2:D:1754:MRR:H2	1.63	0.98
3:C:1302:GOL:O2	2:D:1754:MRR:H153	1.70	0.91
1:C:242:PRO:CD	2:D:1754:MRR:H151	2.02	0.90
1:D:198:MET:HG2	1:D:202:MET:HE2	1.54	0.89
4:A:1946:HOH:O	2:B:1752[B]:MRR:H142	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLN:NE2	4:B:1988:HOH:O	2.09	0.83
3:C:1301:GOL:H11	1:D:202:MET:HG2	1.62	0.80
1:C:199:MET:SD	4:C:2002:HOH:O	2.39	0.80
2:C:1753:MRR:C5A	2:C:1753:MRR:N3A	2.45	0.78
1:C:176:GLN:HE21	1:D:176:GLN:HE21	1.34	0.76
1:A:288:GLY:HA2	4:A:1984:HOH:O	1.84	0.76
1:B:129:ASN:OD1	4:B:1983:HOH:O	2.03	0.75
1:C:241:GLU:HG3	2:D:1754:MRR:H142	1.68	0.75
3:C:1301:GOL:H11	1:D:202:MET:CG	2.18	0.74
1:C:305:GLY:HA2	1:D:203:ARG:HH22	1.54	0.73
1:A:305:GLY:HA2	1:B:203:ARG:HH22	1.54	0.73
1:A:240:ILE:O	3:A:1306:GOL:H31	1.90	0.72
1:A:291:PHE:O	1:A:293:ASN:N	2.22	0.72
1:C:291:PHE:O	1:C:293:ASN:N	2.22	0.72
1:A:142:ARG:NH2	4:A:1985:HOH:O	2.12	0.71
1:C:203:ARG:NH2	4:C:1860:HOH:O	2.20	0.70
2:B:1752[A]:MRR:H141	2:B:1752[A]:MRR:H72	1.74	0.69
1:A:311:PRO:O	1:A:315:GLU:HG2	1.92	0.69
1:D:259:LEU:HD22	1:D:274:LEU:HD13	1.74	0.68
1:C:259:LEU:HD22	1:C:274:LEU:HD13	1.74	0.68
1:C:21:HIS:HD2	1:C:161:SER:OG	1.77	0.68
1:B:16:ILE:HG21	2:B:1752[A]:MRR:H82	1.75	0.67
1:B:140:ILE:HD13	1:B:150:PRO:HG3	1.77	0.67
1:C:76:LYS:HE3	1:C:360:GLY:HA2	1.78	0.66
1:C:45:ILE:HG23	4:C:1973:HOH:O	1.95	0.66
1:A:120:ARG:HH11	1:A:123:GLN:HE22	1.42	0.65
1:A:223:TYR:O	4:A:1988:HOH:O	2.14	0.65
4:A:1993:HOH:O	1:B:302:LEU:HD12	1.95	0.65
1:D:85:ARG:HD2	4:D:1909:HOH:O	1.96	0.65
1:D:126:HIS:HB3	2:D:1754:MRR:H133	1.79	0.65
1:D:358:TRP:O	1:D:359:ASP:HB2	1.95	0.65
1:D:127:ASP:H	2:D:1754:MRR:H132	1.62	0.64
1:B:113:GLY:HA2	1:B:188:MET:HB2	1.79	0.64
1:B:198:MET:HG2	1:B:202:MET:HE2	1.80	0.64
1:C:120:ARG:HH11	1:C:123:GLN:HE22	1.46	0.64
1:C:258:GLU:HG3	4:C:1960:HOH:O	1.97	0.63
1:A:21:HIS:HD2	1:A:161:SER:OG	1.81	0.62
1:D:188:MET:SD	4:D:2019:HOH:O	2.56	0.60
1:D:288:GLY:HA2	4:D:2027:HOH:O	2.02	0.59
1:C:126:HIS:HB3	2:C:1753:MRR:H133	1.84	0.59
1:C:45:ILE:HD11	4:C:1859:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:HG12	4:A:1986:HOH:O	2.03	0.59
1:A:240:ILE:O	3:A:1306:GOL:C3	2.51	0.58
1:B:173:TRP:HA	1:B:176:GLN:HE21	1.68	0.58
1:D:258:GLU:HG3	4:D:2029:HOH:O	2.03	0.58
1:D:62:LYS:HE2	4:D:2017:HOH:O	2.03	0.58
1:D:21:HIS:HD2	1:D:161:SER:OG	1.88	0.57
1:A:120:ARG:NH1	1:A:123:GLN:HE22	2.02	0.57
1:A:216:MET:HE1	2:B:1752[B]:MRR:H152	1.86	0.57
1:B:136:ILE:HG21	1:B:154:VAL:HG11	1.87	0.56
1:B:201:ALA:HB2	4:B:1988:HOH:O	2.06	0.56
1:C:214:ALA:O	1:C:265:ARG:NH2	2.39	0.55
1:B:21:HIS:HD2	1:B:161:SER:OG	1.89	0.55
1:D:286:HIS:HE1	4:D:1815:HOH:O	1.89	0.55
1:D:320:TYR:CE1	1:D:322:ALA:HB2	2.42	0.55
1:D:286:HIS:HD2	4:D:1950:HOH:O	1.90	0.54
1:A:286:HIS:HE1	4:A:1888:HOH:O	1.91	0.54
1:A:113:GLY:HA3	1:A:130:TYR:CZ	2.43	0.54
1:A:286:HIS:HD2	4:C:1816:HOH:O	1.90	0.53
1:C:198:MET:HG2	4:C:2002:HOH:O	2.08	0.53
1:B:286:HIS:HE1	4:B:1771:HOH:O	1.92	0.53
1:B:260:PRO:HG2	1:B:271:LEU:HB2	1.90	0.53
1:A:259:LEU:HD22	1:A:274:LEU:HD13	1.90	0.53
1:C:241:GLU:HA	2:D:1754:MRR:H142	1.90	0.52
1:A:109:ALA:HB1	1:A:164:LEU:HD11	1.91	0.52
1:D:345:PRO:HD3	4:D:2119:HOH:O	2.08	0.52
1:A:313:ILE:HG22	4:A:1830:HOH:O	2.08	0.52
1:B:109:ALA:HB1	1:B:164:LEU:HD11	1.92	0.52
1:C:198:MET:HE3	4:C:2002:HOH:O	2.07	0.52
1:D:127:ASP:HA	4:D:2019:HOH:O	2.09	0.52
1:A:216:MET:CE	2:B:1752[B]:MRR:H152	2.41	0.51
1:A:21:HIS:HE1	1:B:194:VAL:O	1.94	0.51
1:D:156:ASP:OD2	2:D:1754:MRR:C2	2.50	0.51
1:A:176:GLN:NE2	4:A:1930:HOH:O	2.43	0.50
1:D:263:ASN:OD1	3:D:1303:GOL:H32	2.11	0.50
3:C:1302:GOL:O2	2:D:1754:MRR:C15	2.50	0.50
1:C:305:GLY:HA2	1:D:203:ARG:NH2	2.25	0.50
1:A:241:GLU:OE2	2:B:1752[A]:MRR:H92	2.11	0.50
1:C:45:ILE:HD11	1:C:345:PRO:O	2.12	0.50
1:D:55:ARG:HD2	1:D:349:ILE:HD11	1.93	0.49
1:C:242:PRO:CD	2:D:1754:MRR:C15	2.84	0.49
1:D:2:ALA:HA	4:D:2052:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:GLU:HA	2:D:1754:MRR:C14	2.42	0.49
1:C:286:HIS:HE1	4:C:1982:HOH:O	1.94	0.49
1:A:235:VAL:HA	4:A:1986:HOH:O	2.12	0.49
1:C:62:LYS:NZ	4:C:2071:HOH:O	2.46	0.49
1:D:18:PRO:HB3	1:D:156:ASP:O	2.12	0.49
1:B:5:LEU:HD12	1:B:29:LEU:HB2	1.95	0.49
1:C:263:ASN:HD21	3:C:1302:GOL:C3	2.26	0.49
1:B:126:HIS:HB2	4:B:1983:HOH:O	2.13	0.48
1:A:194:VAL:O	1:B:21:HIS:HE1	1.95	0.48
1:C:240:ILE:O	3:C:1302:GOL:H31	2.13	0.48
1:C:176:GLN:HG2	1:D:176:GLN:NE2	2.28	0.48
4:A:1774:HOH:O	1:C:286:HIS:HD2	1.95	0.48
1:A:120:ARG:HH11	1:A:123:GLN:NE2	2.10	0.48
1:B:134:ASN:C	1:B:134:ASN:HD22	2.17	0.47
1:A:13:LEU:HG	1:A:80:LEU:HD11	1.97	0.47
1:C:156:ASP:OD2	2:C:1753:MRR:H2	2.14	0.47
1:D:127:ASP:H	2:D:1754:MRR:C13	2.27	0.47
1:D:113:GLY:HA3	1:D:130:TYR:CZ	2.50	0.46
1:C:113:GLY:HA3	1:C:130:TYR:CZ	2.50	0.46
1:B:259:LEU:HD22	1:B:274:LEU:HD13	1.97	0.46
1:C:194:VAL:O	1:D:21:HIS:HE1	1.99	0.46
1:B:240:ILE:O	3:B:1304:GOL:H2	2.16	0.46
1:D:134:ASN:HD22	1:D:134:ASN:C	2.19	0.45
1:A:207:MET:HE1	2:B:1752[B]:MRR:H112	1.99	0.45
1:B:18:PRO:HB3	1:B:156:ASP:O	2.17	0.45
1:C:21:HIS:HE1	1:D:194:VAL:O	1.99	0.45
1:D:85:ARG:HG2	4:D:2011:HOH:O	2.17	0.45
1:D:103:ASN:ND2	1:D:105:ARG:H	2.14	0.45
1:B:103:ASN:ND2	1:B:105:ARG:H	2.16	0.44
1:B:113:GLY:HA3	1:B:130:TYR:CZ	2.52	0.44
1:B:286:HIS:HD2	4:B:1869:HOH:O	2.00	0.44
1:D:130:TYR:HD2	4:D:2019:HOH:O	2.00	0.44
1:A:18:PRO:HB3	1:A:156:ASP:O	2.17	0.44
1:D:136:ILE:HG21	1:D:154:VAL:HG11	2.00	0.44
1:D:320:TYR:OH	4:D:2116:HOH:O	2.09	0.44
1:A:268:TRP:HD1	4:A:1769:HOH:O	2.01	0.44
1:B:103:ASN:HD22	1:B:105:ARG:H	1.66	0.44
1:D:148:VAL:HG22	1:D:149:PRO:HD2	2.00	0.43
1:C:91:ARG:NH2	4:C:2089:HOH:O	2.14	0.43
1:D:34:VAL:HG11	1:D:73:LEU:HD21	2.00	0.43
1:C:241:GLU:HG3	2:D:1754:MRR:H102	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1993:HOH:O	1:B:302:LEU:CD1	2.61	0.43
1:C:134:ASN:HD22	1:C:134:ASN:C	2.21	0.43
1:C:18:PRO:HB3	1:C:156:ASP:O	2.19	0.42
1:C:245:TYR:CE2	1:C:249:LEU:HD11	2.53	0.42
1:A:45:ILE:N	4:A:1994:HOH:O	2.52	0.42
4:A:1993:HOH:O	1:B:307:VAL:HA	2.20	0.42
3:C:1301:GOL:H11	1:D:202:MET:HG3	2.00	0.42
1:A:210:ASP:OD2	4:A:1982:HOH:O	2.22	0.42
1:A:305:GLY:HA2	1:B:203:ARG:NH2	2.30	0.42
1:D:103:ASN:HD22	1:D:105:ARG:H	1.67	0.42
1:C:196:ILE:HG12	1:C:199:MET:HB2	2.01	0.41
1:A:317:ASN:HA	4:A:1858:HOH:O	2.19	0.41
1:C:291:PHE:C	1:C:293:ASN:N	2.73	0.41
1:D:322:ALA:O	1:D:323:ASN:C	2.57	0.41
1:C:294:SER:O	1:D:123:GLN:HG3	2.21	0.41
4:A:1993:HOH:O	1:B:310:GLU:HB2	2.21	0.41
1:B:39:PRO:HA	1:B:58:THR:HG21	2.03	0.41
1:D:148:VAL:CG2	1:D:149:PRO:HD2	2.51	0.41
1:C:76:LYS:HE3	1:C:360:GLY:CA	2.47	0.41
1:C:120:ARG:NH1	1:C:123:GLN:HE22	2.16	0.41
1:D:203:ARG:NH2	4:D:1969:HOH:O	2.53	0.41
1:A:117:THR:O	1:B:316:ARG:HD2	2.21	0.41
1:B:55:ARG:HD2	1:B:349:ILE:HD11	2.02	0.41
1:C:305:GLY:CA	1:D:203:ARG:HH22	2.29	0.40
1:A:83:GLY:HA2	1:A:111:MET:O	2.20	0.40

All (3) 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:D:1303:GOL:C3	4:C:1853:HOH:O[4_543]	1.94	0.26
1:C:265:ARG:NH2	4:D:1881:HOH:O[4_553]	2.11	0.09
3:B:1304:GOL:C3	4:A:1810:HOH:O[4_554]	2.15	0.05

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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%)	338 (97%)	10 (3%)	2 (1%)	27	9
1	B	350/360 (97%)	337 (96%)	13 (4%)	0	100	100
1	C	350/360 (97%)	336 (96%)	12 (3%)	2 (1%)	27	9
1	D	350/360 (97%)	337 (96%)	12 (3%)	1 (0%)	43	22
All	All	1400/1440 (97%)	1348 (96%)	47 (3%)	5 (0%)	36	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ALA
1	C	292	ALA
1	D	323	ASN
1	C	322	ALA
1	A	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%)	265 (98%)	5 (2%)	60	36
1	B	270/275 (98%)	263 (97%)	7 (3%)	49	22
1	C	270/275 (98%)	263 (97%)	7 (3%)	49	22
1	D	270/275 (98%)	261 (97%)	9 (3%)	41	15
All	All	1080/1100 (98%)	1052 (97%)	28 (3%)	49	22

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

Mol	Chain	Res	Type
1	A	45	ILE

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Mol	Chain	Res	Type
1	A	58	THR
1	A	103	ASN
1	A	134	ASN
1	A	199	MET
1	B	58	THR
1	B	103	ASN
1	B	133	LEU
1	B	134	ASN
1	B	144	ASP
1	B	199	MET
1	B	203	ARG
1	C	58	THR
1	C	73	LEU
1	C	85	ARG
1	C	103	ASN
1	C	134	ASN
1	C	145	GLU
1	C	199	MET
1	D	45	ILE
1	D	58	THR
1	D	103	ASN
1	D	133	LEU
1	D	134	ASN
1	D	199	MET
1	D	203	ARG
1	D	294	SER
1	D	359	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) 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	263	ASN
1	A	286	HIS
1	B	21	HIS
1	B	103	ASN
1	B	134	ASN
1	B	176	GLN
1	B	286	HIS

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Mol	Chain	Res	Type
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	286	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

11 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	1306	-	5,5,5	0.36	0	5,5,5	0.55	0
2	MRR	A	1751	-	48,57,66	0.78	0	59,84,93	1.59	6 (10%)
3	GOL	B	1304	-	5,5,5	0.39	0	5,5,5	0.27	0
3	GOL	B	1305	-	5,5,5	0.29	0	5,5,5	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MRR	B	1752[A]	-	57,66,66	0.77	0	68,93,93	1.49	8 (11%)
2	MRR	B	1752[B]	-	57,66,66	0.76	0	68,93,93	1.50	8 (11%)
3	GOL	C	1301	-	5,5,5	0.33	0	5,5,5	0.47	0
3	GOL	C	1302	-	5,5,5	0.39	0	5,5,5	0.41	0
2	MRR	C	1753	-	45,54,66	1.58	5 (11%)	58,76,93	1.78	8 (13%)
3	GOL	D	1303	-	5,5,5	0.50	0	5,5,5	0.43	0
2	MRR	D	1754	-	57,66,66	0.84	3 (5%)	68,93,93	1.49	5 (7%)

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	1306	-	-	0/4/4/4	0/0/0/0
2	MRR	A	1751	-	-	0/53/74/83	0/3/3/3
3	GOL	B	1304	-	-	0/4/4/4	0/0/0/0
3	GOL	B	1305	-	-	0/4/4/4	0/0/0/0
2	MRR	B	1752[A]	-	-	0/62/83/83	0/3/3/3
2	MRR	B	1752[B]	-	-	0/62/83/83	0/3/3/3
3	GOL	C	1301	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1302	-	-	0/4/4/4	0/0/0/0
2	MRR	C	1753	-	-	0/56/72/83	0/1/1/3
3	GOL	D	1303	-	-	0/4/4/4	0/0/0/0
2	MRR	D	1754	-	-	0/62/83/83	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1753	MRR	C5A-N7A	-6.35	1.36	1.47
2	C	1753	MRR	C2A-N1A	-4.13	1.34	1.45
2	C	1753	MRR	C8A-N9A	-3.98	1.34	1.45
2	C	1753	MRR	C8A-N7A	-3.53	1.35	1.45
2	D	1754	MRR	C1-S1P	-2.22	1.67	1.74
2	D	1754	MRR	O4B-C1B	2.03	1.44	1.41
2	D	1754	MRR	O1-C1	2.11	1.24	1.20
2	C	1753	MRR	C1B-N9A	2.50	1.48	1.41

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1751	MRR	N3A-C2A-N1A	-7.94	122.07	128.86
2	B	1752[B]	MRR	N3A-C2A-N1A	-7.57	122.38	128.86
2	B	1752[A]	MRR	N3A-C2A-N1A	-7.57	122.38	128.86
2	D	1754	MRR	N3A-C2A-N1A	-7.47	122.47	128.86
2	C	1753	MRR	O1-C1-S1P	-4.58	117.44	123.76
2	D	1754	MRR	O1-C1-S1P	-4.47	117.59	123.76
2	B	1752[B]	MRR	O1-C1-S1P	-4.08	118.13	123.76
2	B	1752[A]	MRR	O1-C1-S1P	-4.08	118.13	123.76
2	A	1751	MRR	O1-C1-S1P	-4.03	118.19	123.76
2	C	1753	MRR	N7A-C8A-N9A	-2.76	110.22	113.49
2	B	1752[B]	MRR	C6P-C7P-N8P	-2.33	107.12	111.85
2	B	1752[A]	MRR	C6P-C7P-N8P	-2.33	107.12	111.85
2	D	1754	MRR	O5P-C5P-C6P	-2.28	117.77	122.00
2	B	1752[B]	MRR	C4A-C5A-N7A	-2.24	107.24	109.41
2	B	1752[A]	MRR	C4A-C5A-N7A	-2.24	107.24	109.41
2	B	1752[B]	MRR	C2P-C3P-N4P	-2.21	107.65	112.46
2	B	1752[A]	MRR	C2P-C3P-N4P	-2.21	107.65	112.46
2	A	1751	MRR	C4A-C5A-N7A	-2.10	107.38	109.41
2	A	1751	MRR	C2P-S1P-C1	2.12	108.60	101.80
2	C	1753	MRR	CDP-CBP-CAP	2.15	112.56	108.82
2	C	1753	MRR	C3P-N4P-C5P	2.28	127.17	122.85
2	D	1754	MRR	C3P-N4P-C5P	2.44	127.48	122.85
2	B	1752[B]	MRR	C2P-S1P-C1	2.46	109.70	101.80
2	B	1752[A]	MRR	C2P-S1P-C1	2.46	109.70	101.80
2	A	1751	MRR	C3P-N4P-C5P	3.12	128.75	122.85
2	B	1752[B]	MRR	C3P-N4P-C5P	3.24	128.99	122.85
2	B	1752[A]	MRR	C3P-N4P-C5P	3.24	128.99	122.85
2	D	1754	MRR	C7P-N8P-C9P	3.50	129.01	122.59
2	B	1752[B]	MRR	C7P-N8P-C9P	3.61	129.22	122.59
2	B	1752[A]	MRR	C7P-N8P-C9P	3.61	129.22	122.59
2	A	1751	MRR	C7P-N8P-C9P	3.95	129.84	122.59
2	C	1753	MRR	C7P-N8P-C9P	3.98	129.89	122.59
2	C	1753	MRR	C2A-N1A-C6A	4.33	122.27	114.08
2	C	1753	MRR	C5A-C6A-N1A	5.48	119.87	110.27
2	C	1753	MRR	N3A-C2A-N1A	7.10	121.62	113.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1306	GOL	2	0
3	B	1304	GOL	1	1
2	B	1752[A]	MRR	4	0
2	B	1752[B]	MRR	4	0
3	C	1301	GOL	3	0
3	C	1302	GOL	4	0
2	C	1753	MRR	3	0
3	D	1303	GOL	1	1
2	D	1754	MRR	14	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 ⓘ

### 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%)	0.80	32 (9%) 9 8	20, 29, 42, 46	0
1	B	354/360 (98%)	0.86	38 (10%) 6 5	19, 28, 40, 48	0
1	C	354/360 (98%)	0.74	19 (5%) 26 24	16, 22, 34, 44	0
1	D	354/360 (98%)	0.63	12 (3%) 45 42	16, 22, 33, 42	0
All	All	1416/1440 (98%)	0.76	101 (7%) 16 15	16, 26, 37, 48	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	GLY	6.2
1	A	351	ILE	5.7
1	B	360	GLY	5.5
1	B	73	LEU	5.4
1	A	356	THR	5.1
1	B	347	ALA	4.9
1	B	350	ASP	4.9
1	D	360	GLY	4.9
1	B	102	VAL	4.7
1	C	292	ALA	4.3
1	B	323	ASN	4.1
1	D	359	ASP	4.0
1	B	349	ILE	4.0
1	B	359	ASP	3.6
1	A	64	ASP	3.5
1	D	323	ASN	3.5
1	C	350	ASP	3.5
1	C	39	PRO	3.4
1	A	179	GLY	3.4
1	A	346	ALA	3.3
1	C	360	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	359	ASP	3.1
1	B	45	ILE	3.1
1	B	2	ALA	3.1
1	B	292	ALA	3.1
1	A	229	CYS	3.0
1	B	69	LEU	3.0
1	C	323	ASN	2.9
1	C	358	TRP	2.9
1	A	355	LEU	2.9
1	A	350	ASP	2.8
1	B	358	TRP	2.8
1	B	356	THR	2.8
1	B	354	VAL	2.8
1	C	359	ASP	2.8
1	A	257	ALA	2.8
1	A	60	ASP	2.7
1	A	291	PHE	2.7
1	C	176	GLN	2.7
1	B	38	ARG	2.6
1	B	72	LYS	2.6
1	A	71	LEU	2.6
1	D	151	LEU	2.6
1	D	326	TRP	2.6
1	D	102	VAL	2.6
1	A	74	ILE	2.5
1	C	45	ILE	2.5
1	A	173	TRP	2.5
1	A	51	LEU	2.5
1	B	76	LYS	2.5
1	B	324	GLY	2.5
1	B	61	LEU	2.5
1	B	253	GLY	2.5
1	B	64	ASP	2.4
1	A	326	TRP	2.4
1	A	77	ALA	2.4
1	B	256	ALA	2.4
1	B	67	LEU	2.4
1	C	64	ASP	2.4
1	B	352	GLU	2.4
1	A	353	ALA	2.3
1	B	348	THR	2.3
1	B	172	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	69	LEU	2.3
1	B	65	GLN	2.3
1	A	63	SER	2.3
1	A	347	ALA	2.3
1	B	357	ASP	2.3
1	C	180	LYS	2.3
1	D	173	TRP	2.2
1	A	58	THR	2.2
1	C	148	VAL	2.2
1	A	354	VAL	2.2
1	A	73	LEU	2.2
1	D	140	ILE	2.2
1	B	87	GLY	2.2
1	B	258	GLU	2.2
1	D	350	ASP	2.2
1	C	139	ALA	2.2
1	A	67	LEU	2.1
1	B	94	LEU	2.1
1	C	140	ILE	2.1
1	D	65	GLN	2.1
1	B	39	PRO	2.1
1	A	79	VAL	2.1
1	C	347	ALA	2.1
1	B	176	GLN	2.1
1	C	194	VAL	2.1
1	C	13	LEU	2.1
1	A	282	HIS	2.1
1	A	358	TRP	2.1
1	C	77	ALA	2.1
1	C	87	GLY	2.1
1	A	349	ILE	2.1
1	B	351	ILE	2.1
1	D	135	GLY	2.0
1	B	103	ASN	2.0
1	A	70	ALA	2.0
1	B	75	ALA	2.0
1	B	101	LYS	2.0
1	A	61	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 [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, 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	1304	6/6	0.58	0.24	56,57,58,58	0
2	MRR	A	1751	55/64	0.66	0.24	54,62,65,66	0
3	GOL	C	1301	6/6	0.67	0.29	85,85,86,86	0
2	MRR	B	1752[A]	64/64	0.69	0.25	34,57,69,69	10
2	MRR	B	1752[B]	64/64	0.69	0.25	18,57,69,69	10
3	GOL	A	1306	6/6	0.71	0.19	39,40,41,42	0
3	GOL	B	1305	6/6	0.75	0.16	54,59,61,64	0
3	GOL	C	1302	6/6	0.79	0.15	30,33,36,37	0
2	MRR	C	1753	54/64	0.80	0.16	34,45,51,52	0
2	MRR	D	1754	64/64	0.81	0.15	31,41,49,52	0
3	GOL	D	1303	6/6	0.83	0.18	38,40,43,44	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.