



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 04:51 PM BST

PDB ID : 1O66  
Title : Crystal structure of 3-methyl-2-oxobutanoate hydroxymethyltransferase  
Authors : Structural GenomiX  
Deposited on : 2003-10-23  
Resolution : 1.75 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
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) : 2.13

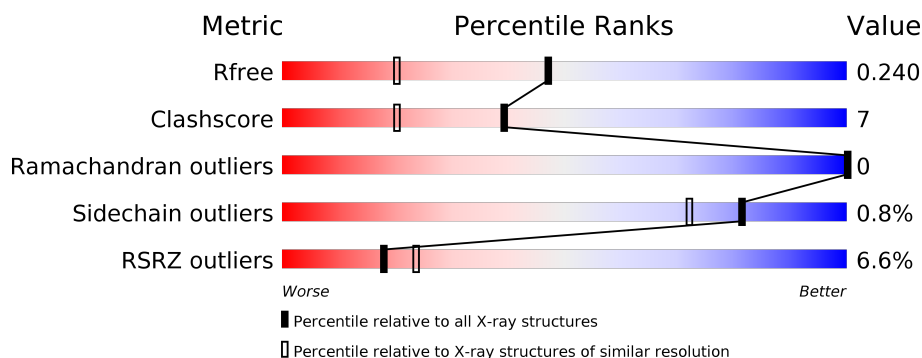
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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

Mol	Chain	Length	Quality of chain
1	A	275	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>9%</div> </div> </div>
1	B	275	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>10%</div> </div> </div>
1	C	275	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>11%</div> </div> </div>
1	D	275	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>9%</div> </div> </div>
1	E	275	<div> <div>11%</div> <div> <div></div> <div>67%</div> <div>19%</div> <div>14%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9550 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-methyl-2-oxobutanoate hydroxymethyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	Se	0	3	0
			1818	1147	306	342	6	17			
1	B	248	Total	C	N	O	S	Se	0	4	0
			1793	1130	299	341	7	16			
1	C	246	Total	C	N	O	S	Se	0	5	0
			1810	1145	300	342	6	17			
1	D	249	Total	C	N	O	S	Se	0	4	0
			1816	1146	306	342	6	16			
1	E	237	Total	C	N	O	S	Se	0	2	0
			1713	1081	288	322	6	16			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	cloning artifact	UNP Q9JZW6
A	0	SER	-	cloning artifact	UNP Q9JZW6
A	1	LEU	-	cloning artifact	UNP Q9JZW6
A	10	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	19	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	31	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	38	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	47	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	63	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	78	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	103	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	109	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	118	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	127	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	178	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	213	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	216	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	232	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
A	264	GLU	-	cloning artifact	UNP Q9JZW6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	-	cloning artifact	UNP Q9JZW6
A	266	GLY	-	cloning artifact	UNP Q9JZW6
A	267	SER	-	cloning artifact	UNP Q9JZW6
A	268	HIS	-	cloning artifact	UNP Q9JZW6
A	269	HIS	-	cloning artifact	UNP Q9JZW6
A	270	HIS	-	cloning artifact	UNP Q9JZW6
A	271	HIS	-	cloning artifact	UNP Q9JZW6
A	272	HIS	-	cloning artifact	UNP Q9JZW6
A	273	HIS	-	cloning artifact	UNP Q9JZW6
B	-1	MSE	-	cloning artifact	UNP Q9JZW6
B	0	SER	-	cloning artifact	UNP Q9JZW6
B	1	LEU	-	cloning artifact	UNP Q9JZW6
B	10	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	19	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	31	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	38	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	47	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	63	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	78	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	103	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
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B	127	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	178	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	213	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	216	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	232	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
B	264	GLU	-	cloning artifact	UNP Q9JZW6
B	265	GLY	-	cloning artifact	UNP Q9JZW6
B	266	GLY	-	cloning artifact	UNP Q9JZW6
B	267	SER	-	cloning artifact	UNP Q9JZW6
B	268	HIS	-	cloning artifact	UNP Q9JZW6
B	269	HIS	-	cloning artifact	UNP Q9JZW6
B	270	HIS	-	cloning artifact	UNP Q9JZW6
B	271	HIS	-	cloning artifact	UNP Q9JZW6
B	272	HIS	-	cloning artifact	UNP Q9JZW6
B	273	HIS	-	cloning artifact	UNP Q9JZW6
C	-1	MSE	-	cloning artifact	UNP Q9JZW6
C	0	SER	-	cloning artifact	UNP Q9JZW6
C	1	LEU	-	cloning artifact	UNP Q9JZW6
C	10	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	19	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	31	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	38	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	47	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	63	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	78	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	103	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	109	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	118	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	127	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	178	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	213	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	216	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	232	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
C	264	GLU	-	cloning artifact	UNP Q9JZW6
C	265	GLY	-	cloning artifact	UNP Q9JZW6
C	266	GLY	-	cloning artifact	UNP Q9JZW6
C	267	SER	-	cloning artifact	UNP Q9JZW6
C	268	HIS	-	cloning artifact	UNP Q9JZW6
C	269	HIS	-	cloning artifact	UNP Q9JZW6
C	270	HIS	-	cloning artifact	UNP Q9JZW6
C	271	HIS	-	cloning artifact	UNP Q9JZW6
C	272	HIS	-	cloning artifact	UNP Q9JZW6
C	273	HIS	-	cloning artifact	UNP Q9JZW6
D	-1	MSE	-	cloning artifact	UNP Q9JZW6
D	0	SER	-	cloning artifact	UNP Q9JZW6
D	1	LEU	-	cloning artifact	UNP Q9JZW6
D	10	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	19	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	31	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	38	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	47	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	63	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	78	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	103	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	109	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	118	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	127	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	178	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	213	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	216	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	232	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
D	264	GLU	-	cloning artifact	UNP Q9JZW6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	265	GLY	-	cloning artifact	UNP Q9JZW6
D	266	GLY	-	cloning artifact	UNP Q9JZW6
D	267	SER	-	cloning artifact	UNP Q9JZW6
D	268	HIS	-	cloning artifact	UNP Q9JZW6
D	269	HIS	-	cloning artifact	UNP Q9JZW6
D	270	HIS	-	cloning artifact	UNP Q9JZW6
D	271	HIS	-	cloning artifact	UNP Q9JZW6
D	272	HIS	-	cloning artifact	UNP Q9JZW6
D	273	HIS	-	cloning artifact	UNP Q9JZW6
E	-1	MSE	-	cloning artifact	UNP Q9JZW6
E	0	SER	-	cloning artifact	UNP Q9JZW6
E	1	LEU	-	cloning artifact	UNP Q9JZW6
E	10	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
E	19	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
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E	38	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
E	47	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
E	63	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
E	78	MSE	MET	MODIFIED RESIDUE	UNP Q9JZW6
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E	266	GLY	-	cloning artifact	UNP Q9JZW6
E	267	SER	-	cloning artifact	UNP Q9JZW6
E	268	HIS	-	cloning artifact	UNP Q9JZW6
E	269	HIS	-	cloning artifact	UNP Q9JZW6
E	270	HIS	-	cloning artifact	UNP Q9JZW6
E	271	HIS	-	cloning artifact	UNP Q9JZW6
E	272	HIS	-	cloning artifact	UNP Q9JZW6
E	273	HIS	-	cloning artifact	UNP Q9JZW6

- Molecule 2 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
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		

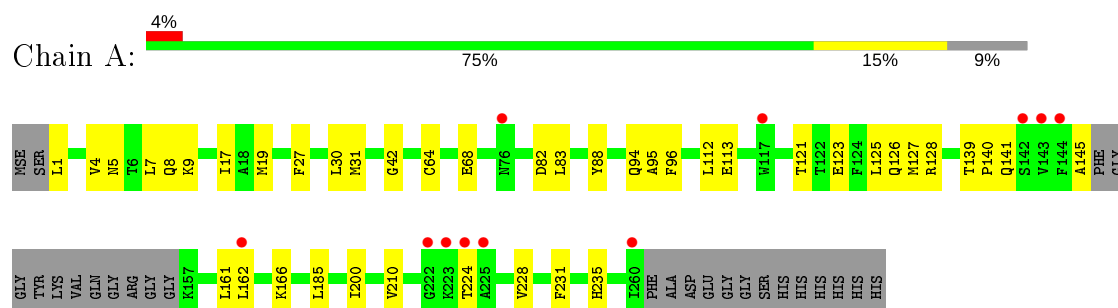
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	148	Total	O	0	0
			148	148		
3	B	98	Total	O	0	0
			98	98		
3	C	148	Total	O	0	0
			148	148		
3	D	103	Total	O	0	0
			103	103		
3	E	73	Total	O	0	0
			73	73		

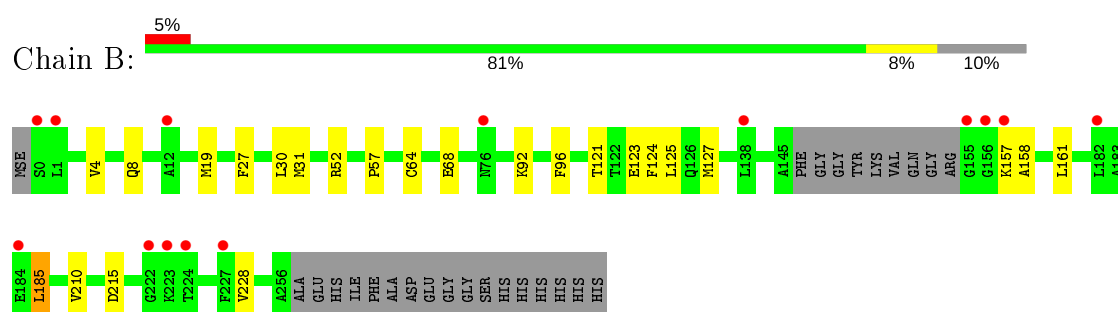
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

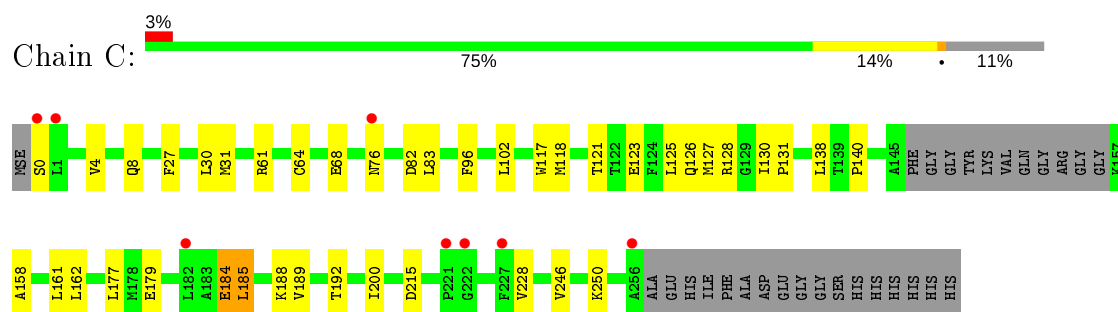
- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase



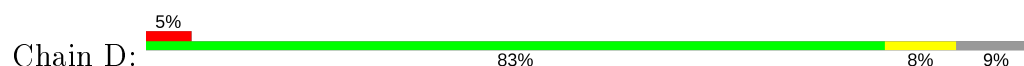
- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase



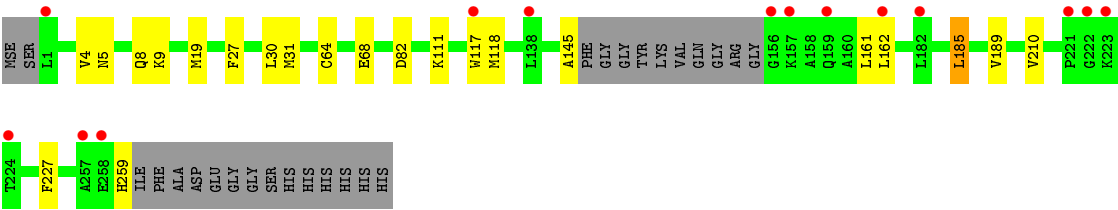
- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase



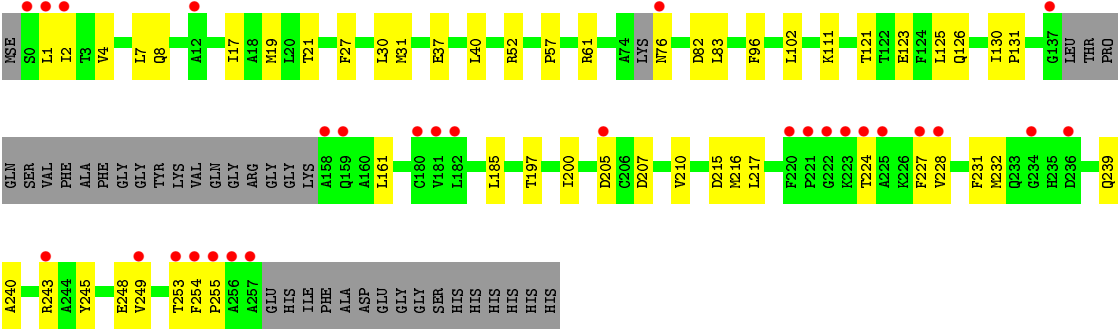
- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase







● Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	165.19 Å   111.49 Å   99.08 Å 90.00°   122.65°   90.00°	Depositor
Resolution (Å)	43.44 – 1.75 43.50 – 1.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.44-1.75) 99.8 (43.50-1.75)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 1.75 Å)	Xtriage
Refinement program	REFMAC 4.0	Depositor
R, $R_{free}$	0.231   ,   0.250 0.220   ,   0.240	Depositor DCC
$R_{free}$ test set	15130 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.0	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9550	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.29	0/1850	0.56	0/2476
1	B	0.29	0/1823	0.56	0/2440
1	C	0.30	0/1851	0.58	0/2476
1	D	0.30	0/1850	0.57	0/2475
1	E	0.27	0/1731	0.52	0/2313
All	All	0.29	0/9105	0.56	0/12180

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1818	0	1821	32	0
1	B	1793	0	1773	15	0
1	C	1810	0	1807	34	0
1	D	1816	0	1806	18	0
1	E	1713	0	1708	39	1
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	6	0	8	0	0
2	E	6	0	8	0	0
3	A	148	0	0	4	0
3	B	98	0	0	1	0
3	C	148	0	0	2	0
3	D	103	0	0	0	0
3	E	73	0	0	1	0
All	All	9550	0	8955	133	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127[B]:MSE:HE3	1:A:128:ARG:HH12	1.10	1.11
1:C:127[A]:MSE:HE3	1:C:128:ARG:HH12	1.32	0.90
1:A:127[B]:MSE:HE3	1:A:128:ARG:NH1	1.93	0.83
1:C:161:LEU:HD23	1:C:185:LEU:HD22	1.64	0.80
1:D:5:ASN:HD21	1:D:9:LYS:HE2	1.50	0.76
1:A:123:GLU:HG2	1:A:127[A]:MSE:HE2	1.67	0.75
1:A:121:THR:O	1:A:125[B]:LEU:HD23	1.87	0.74
1:D:82:ASP:OD1	1:D:111:LYS:HE3	1.88	0.73
1:C:96:PHE:HA	1:C:125[A]:LEU:HD11	1.70	0.72
1:D:5:ASN:ND2	1:D:9:LYS:HE2	2.05	0.72
1:D:117[B]:TRP:CZ3	1:D:118:MSE:HE3	2.25	0.71
1:E:52:ARG:HD3	1:E:57:PRO:HG2	1.70	0.71
1:D:117[B]:TRP:CE3	1:D:118:MSE:HE3	2.26	0.71
1:E:96:PHE:HA	1:E:125[A]:LEU:HD11	1.73	0.70
1:E:2:ILE:HD11	1:E:7:LEU:HD21	1.74	0.69
1:B:96:PHE:HA	1:B:125[B]:LEU:HD11	1.75	0.69
1:C:117[B]:TRP:CZ3	1:C:118:MSE:HE3	2.28	0.69
1:E:2:ILE:HG22	1:E:76:ASN:O	1.93	0.68
1:C:127[A]:MSE:HE3	1:C:128:ARG:NH1	2.07	0.68
1:A:96:PHE:HA	1:A:125[B]:LEU:HD11	1.76	0.66
1:A:94:GLN:HB3	3:A:411:HOH:O	1.96	0.64
1:C:117[B]:TRP:CE3	1:C:118:MSE:HE3	2.33	0.63
1:D:162:LEU:HD23	1:D:189:VAL:HG22	1.79	0.63
1:E:245:TYR:O	1:E:249:VAL:HG23	1.99	0.63
1:A:161:LEU:HD23	1:A:185:LEU:HD22	1.80	0.62
1:A:95:ALA:N	3:A:411:HOH:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:LEU:HD23	1:E:185:LEU:HD22	1.82	0.61
1:B:92:LYS:HE3	3:B:363:HOH:O	2.01	0.61
1:B:27:PHE:HB3	1:B:31:MSE:HE2	1.84	0.60
1:A:140:PRO:HB2	3:A:394:HOH:O	2.03	0.59
1:A:123:GLU:O	1:A:127[A]:MSE:HG3	2.03	0.58
1:B:161:LEU:HD23	1:B:185:LEU:HD13	1.84	0.58
1:C:184:GLU:HG3	1:C:185:LEU:N	2.20	0.57
1:E:82:ASP:OD1	1:E:111:LYS:HE2	2.05	0.56
1:E:52:ARG:HD3	1:E:57:PRO:CG	2.34	0.56
1:C:83:LEU:HD23	1:C:102:LEU:HD12	1.88	0.55
1:A:1:LEU:HD22	1:A:1:LEU:N	2.22	0.55
1:A:5:ASN:HD21	1:A:9:LYS:HE3	1.72	0.55
1:D:27:PHE:HB3	1:D:31:MSE:HE2	1.87	0.55
1:D:161:LEU:HD23	1:D:185:LEU:HD22	1.88	0.55
1:E:4:VAL:O	1:E:8:GLN:HG3	2.07	0.55
1:B:4:VAL:O	1:B:8:GLN:HG3	2.07	0.55
1:E:231:PHE:CE2	1:E:245:TYR:HA	2.42	0.55
1:E:248:GLU:HB3	1:E:253:THR:HB	1.90	0.54
1:E:161:LEU:HD23	1:E:185:LEU:CD2	2.38	0.54
1:C:246:VAL:O	1:C:250:LYS:HG2	2.08	0.54
1:E:30:LEU:C	1:E:30:LEU:HD23	2.29	0.53
1:E:19:MSE:O	1:E:210:VAL:HA	2.09	0.53
1:E:121:THR:O	1:E:125[A]:LEU:HD23	2.09	0.52
1:D:118:MSE:HE2	1:D:118:MSE:HA	1.92	0.52
1:C:188:LYS:O	1:C:192:THR:HG23	2.10	0.52
1:E:83:LEU:HD23	1:E:102:LEU:HD12	1.91	0.52
1:A:162:LEU:O	1:A:166:LYS:HG3	2.11	0.51
1:A:88:TYR:HA	3:A:411:HOH:O	2.11	0.51
1:A:42:GLY:HA2	1:A:82:ASP:OD2	2.10	0.51
1:A:161:LEU:HD23	1:A:185:LEU:CD2	2.40	0.51
1:A:27:PHE:HB3	1:A:31:MSE:HE2	1.93	0.50
1:B:92:LYS:HD2	1:B:124:PHE:CD1	2.47	0.50
1:C:158:ALA:HA	1:C:185:LEU:HD11	1.94	0.50
1:C:125[A]:LEU:HD12	1:C:130:ILE:HD12	1.95	0.49
1:E:83:LEU:HD23	1:E:102:LEU:CD1	2.42	0.49
1:E:200:ILE:O	1:E:200:ILE:HG23	2.13	0.49
1:E:185:LEU:O	1:E:185:LEU:HD23	2.13	0.49
1:C:4:VAL:O	1:C:8:GLN:HG3	2.14	0.48
1:C:64:CYS:O	1:C:68:GLU:HG3	2.14	0.48
1:B:64:CYS:O	1:B:68:GLU:HG3	2.13	0.48
1:D:64:CYS:O	1:D:68:GLU:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LYS:HG3	1:B:158:ALA:N	2.29	0.48
1:B:30:LEU:C	1:B:30:LEU:HD23	2.34	0.48
1:C:179:GLU:HG3	1:C:200:ILE:HG23	1.95	0.48
1:A:30:LEU:C	1:A:30:LEU:HD23	2.34	0.47
1:E:2:ILE:HD11	1:E:7:LEU:CD2	2.44	0.47
1:D:4:VAL:O	1:D:8:GLN:HG3	2.15	0.47
1:E:254:PHE:CD1	1:E:255:PRO:HA	2.50	0.47
1:E:7:LEU:HD22	1:E:17:ILE:HD13	1.98	0.46
1:C:161:LEU:HD23	1:C:185:LEU:CD2	2.39	0.46
1:B:19:MSE:HG2	1:B:210:VAL:HG23	1.98	0.46
1:E:27:PHE:HB3	1:E:31:MSE:HE2	1.96	0.46
1:A:1:LEU:H1	1:A:1:LEU:HD22	1.81	0.46
1:C:128:ARG:HG2	1:D:117[B]:TRP:CZ3	2.51	0.45
1:C:162:LEU:HD23	1:C:189:VAL:HG22	1.98	0.45
1:C:30:LEU:HD23	1:C:30:LEU:C	2.37	0.45
1:A:113:GLU:OE2	1:A:139:THR:HB	2.16	0.45
1:B:121:THR:O	1:B:125[B]:LEU:HD23	2.16	0.45
1:A:200:ILE:HG23	1:A:200:ILE:O	2.17	0.45
1:E:19:MSE:HG2	1:E:210:VAL:HG23	1.99	0.45
1:A:123:GLU:O	1:A:126:GLN:HG3	2.16	0.44
1:E:205:ASP:HB2	3:E:339:HOH:O	2.16	0.44
1:A:128:ARG:HG2	1:C:117[B]:TRP:CZ3	2.52	0.44
1:E:240:ALA:HA	1:E:243:ARG:HE	1.82	0.44
1:B:158:ALA:HA	1:B:185:LEU:HD11	2.00	0.44
1:E:227:PHE:CD1	1:E:228:VAL:HG23	2.53	0.44
1:E:1:LEU:HD23	1:E:76:ASN:HA	1.99	0.44
1:C:0:SER:C	1:C:76:ASN:HD22	2.21	0.44
1:E:2:ILE:CD1	1:E:37:GLU:HB3	2.48	0.44
1:C:215:ASP:HB3	1:C:228:VAL:HG11	2.00	0.44
1:E:217:LEU:O	1:E:232:MSE:HG3	2.18	0.44
1:A:83:LEU:HD12	1:A:112:LEU:HB3	1.99	0.43
1:A:4:VAL:O	1:A:8:GLN:HG3	2.19	0.43
1:C:27:PHE:HB3	1:C:31:MSE:HE2	2.01	0.43
1:D:19:MSE:HG2	1:D:210:VAL:HG23	2.01	0.43
1:E:123:GLU:O	1:E:126:GLN:HG3	2.18	0.43
1:C:200:ILE:HG23	1:C:200:ILE:O	2.18	0.43
1:E:224:THR:HG22	1:E:228:VAL:HB	2.01	0.43
1:C:61:ARG:NH1	3:C:318:HOH:O	2.51	0.43
1:C:138:LEU:HD13	1:C:138:LEU:C	2.40	0.43
1:A:231:PHE:O	1:A:235:HIS:HD2	2.01	0.42
1:A:113:GLU:OE2	1:A:141:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ARG:HG2	1:D:117[B]:TRP:CH2	2.55	0.42
1:C:125[A]:LEU:CD1	1:C:130:ILE:HD12	2.49	0.42
1:E:2:ILE:HD12	1:E:37:GLU:HB3	2.01	0.42
1:A:7:LEU:HD22	1:A:17:ILE:HD13	2.01	0.42
1:A:19:MSE:O	1:A:210:VAL:HA	2.20	0.41
1:E:216:MSE:SE	1:E:217:LEU:HG	2.70	0.41
1:C:121:THR:O	1:C:125[A]:LEU:HD23	2.20	0.41
1:C:131:PRO:HG3	1:D:145:ALA:HA	2.03	0.41
1:C:177:LEU:HD23	1:C:177:LEU:C	2.41	0.41
1:E:21:THR:HA	1:E:40:LEU:O	2.21	0.41
1:C:140:PRO:HB2	3:C:354:HOH:O	2.21	0.41
1:D:30:LEU:C	1:D:30:LEU:HD23	2.41	0.41
1:E:125[A]:LEU:CD1	1:E:130:ILE:HD12	2.50	0.41
1:A:145:ALA:HA	1:E:131:PRO:HG3	2.02	0.41
1:A:64:CYS:O	1:A:68:GLU:HG3	2.21	0.41
1:E:197:THR:O	1:E:207:ASP:HB2	2.21	0.41
1:B:215:ASP:HB3	1:B:228:VAL:HG11	2.01	0.41
1:B:52:ARG:HD3	1:B:57:PRO:HB2	2.02	0.41
1:C:83:LEU:HD23	1:C:102:LEU:CD1	2.50	0.41
1:E:215:ASP:HB3	1:E:228:VAL:HG11	2.03	0.41
1:B:123:GLU:O	1:B:127[B]:MSE:HG3	2.21	0.40
1:D:227:PHE:HA	1:D:259:HIS:HB3	2.02	0.40
1:C:123:GLU:O	1:C:127[B]:MSE:HG3	2.21	0.40
1:A:224:THR:HG22	1:A:228:VAL:HB	2.03	0.40
1:D:19:MSE:O	1:D:210:VAL:HA	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:ARG:NH1	1:E:61:ARG:NH1[2_656]	2.12	0.08

## 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	249/275 (90%)	245 (98%)	4 (2%)	0	100	100
1	B	248/275 (90%)	245 (99%)	3 (1%)	0	100	100
1	C	248/275 (90%)	244 (98%)	4 (2%)	0	100	100
1	D	249/275 (90%)	246 (99%)	3 (1%)	0	100	100
1	E	233/275 (85%)	227 (97%)	6 (3%)	0	100	100
All	All	1227/1375 (89%)	1207 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	185/189 (98%)	185 (100%)	0	100	100
1	B	180/189 (95%)	179 (99%)	1 (1%)	86	79
1	C	185/189 (98%)	181 (98%)	4 (2%)	52	29
1	D	184/189 (97%)	183 (100%)	1 (0%)	88	83
1	E	170/189 (90%)	169 (99%)	1 (1%)	86	79
All	All	904/945 (96%)	897 (99%)	7 (1%)	81	72

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	185	LEU
1	C	82	ASP
1	C	126	GLN
1	C	184	GLU
1	C	185	LEU
1	D	185	LEU
1	E	239	GLN



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	235	HIS
1	B	233	GLN
1	B	235	HIS
1	C	5	ASN
1	C	233	GLN
1	D	5	ASN
1	E	8	GLN
1	E	76	ASN
1	E	159	GLN
1	E	163	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 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	274	2	5,5,5	0.25	0	5,5,5	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	A	274	2	5,5,5	0.25	0	5,5,5	0.15	0
2	GOL	D	274	2	5,5,5	0.24	0	5,5,5	0.16	0
2	GOL	C	274	2	5,5,5	0.24	0	5,5,5	0.16	0
2	GOL	E	274	-	5,5,5	0.30	0	5,5,5	0.20	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	GOL	B	274	2	-	0/4/4/4	-
2	GOL	A	274	2	-	0/4/4/4	-
2	GOL	D	274	2	-	0/4/4/4	-
2	GOL	C	274	2	-	0/4/4/4	-
2	GOL	E	274	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	234/275 (85%)	0.38	11 (4%) 31 37	7, 16, 31, 39	0
1	B	233/275 (84%)	0.48	14 (6%) 21 27	8, 17, 30, 42	0
1	C	231/275 (84%)	0.21	8 (3%) 44 50	6, 14, 27, 36	0
1	D	234/275 (85%)	0.31	14 (5%) 21 27	7, 15, 29, 40	0
1	E	222/275 (80%)	0.98	29 (13%) 3 5	9, 26, 41, 47	0
All	All	1154/1375 (83%)	0.47	76 (6%) 18 24	6, 17, 35, 47	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	224	THR	9.0
1	E	223	LYS	6.8
1	D	156	GLY	6.6
1	B	155	GLY	6.2
1	E	221	PRO	6.0
1	A	260	ILE	5.9
1	E	257	ALA	5.9
1	E	256	ALA	5.6
1	A	223	LYS	5.5
1	B	0	SER	5.2
1	E	222	GLY	5.2
1	D	224	THR	5.1
1	E	253	THR	5.1
1	B	156	GLY	5.0
1	B	182	LEU	4.9
1	E	1	LEU	4.5
1	E	0	SER	4.4
1	E	180	CYS	4.4
1	C	0	SER	4.3
1	E	227	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	205	ASP	4.0
1	B	1	LEU	3.9
1	A	224	THR	3.9
1	E	236	ASP	3.9
1	B	138	LEU	3.8
1	B	222	GLY	3.8
1	D	1	LEU	3.6
1	D	257	ALA	3.4
1	D	221	PRO	3.3
1	B	12	ALA	3.3
1	B	227	PHE	3.2
1	C	256	ALA	3.2
1	E	158	ALA	3.1
1	C	1	LEU	3.1
1	B	223	LYS	3.0
1	A	222	GLY	3.0
1	D	117[A]	TRP	3.0
1	E	137	GLY	2.9
1	E	225	ALA	2.9
1	C	76	ASN	2.9
1	B	76	ASN	2.8
1	C	227	PHE	2.7
1	E	76	ASN	2.7
1	C	222	GLY	2.6
1	D	222	GLY	2.6
1	E	254	PHE	2.6
1	E	249	VAL	2.5
1	A	144	PHE	2.5
1	A	162	LEU	2.5
1	D	223	LYS	2.4
1	A	76	ASN	2.4
1	D	182	LEU	2.4
1	E	181	VAL	2.4
1	C	221	PRO	2.4
1	B	184	GLU	2.4
1	E	182	LEU	2.3
1	E	159	GLN	2.3
1	B	224	THR	2.3
1	D	258	GLU	2.2
1	E	234	GLY	2.2
1	B	157	LYS	2.2
1	E	2	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	117	TRP	2.2
1	A	142	SER	2.1
1	E	243	ARG	2.1
1	A	143	VAL	2.1
1	E	228	VAL	2.1
1	D	162	LEU	2.1
1	E	220	PHE	2.1
1	E	255	PRO	2.1
1	D	157	LYS	2.0
1	D	138	LEU	2.0
1	A	225	ALA	2.0
1	E	12	ALA	2.0
1	D	159	GLN	2.0
1	C	182	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å <sup>2</sup> )	Q<0.9
2	GOL	B	274	6/6	0.73	0.20	21,21,21,21	6
2	GOL	A	274	6/6	0.73	0.20	21,21,21,21	6
2	GOL	D	274	6/6	0.78	0.20	17,17,17,17	6
2	GOL	C	274	6/6	0.78	0.20	17,17,17,17	6
2	GOL	E	274	6/6	0.94	0.13	22,23,23,24	6

## 6.5 Other polymers [i](#)

There are no such residues in this entry.