



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 05:00 PM BST

PDB ID : 3TJI  
Title : CRYSTAL STRUCTURE OF AN ENOLASE FROM ENTEROBACTER sp. 638 (EFI TARGET EFI-501662) with BOUND MG  
Authors : Vetting, M.W.; Toro, R.; Bhosle, R.; Wasserman, S.R.; Morisco, L.L.; Hilerich, B.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Zencheck, W.D.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)  
Deposited on : 2011-08-24  
Resolution : 1.80 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	:	2.13.1
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

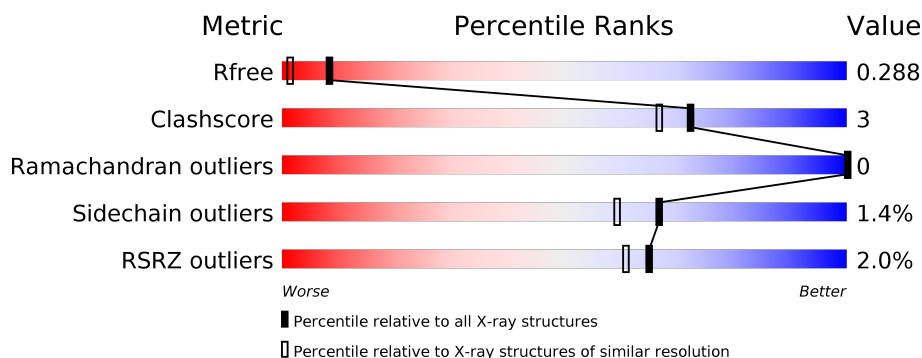
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	422	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>5%</div> </div> </div>
1	B	422	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>5%</div> </div> </div>
1	C	422	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>• 5%</div> </div> </div>
1	D	422	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14219 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 Mandelate racemase/muconate lactonizing enzyme, N-terminal domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	9	0
			3224	2069	570	569	16			
1	B	399	Total	C	N	O	S	0	7	0
			3208	2053	566	573	16			
1	C	399	Total	C	N	O	S	0	6	0
			3198	2048	564	570	16			
1	D	399	Total	C	N	O	S	0	8	0
			3214	2061	565	572	16			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP A4W7D6
A	-21	HIS	-	EXPRESSION TAG	UNP A4W7D6
A	-20	HIS	-	EXPRESSION TAG	UNP A4W7D6
A	-19	HIS	-	EXPRESSION TAG	UNP A4W7D6
A	-18	HIS	-	EXPRESSION TAG	UNP A4W7D6
A	-17	HIS	-	EXPRESSION TAG	UNP A4W7D6
A	-16	HIS	-	EXPRESSION TAG	UNP A4W7D6
A	-15	SER	-	EXPRESSION TAG	UNP A4W7D6
A	-14	SER	-	EXPRESSION TAG	UNP A4W7D6
A	-13	GLY	-	EXPRESSION TAG	UNP A4W7D6
A	-12	VAL	-	EXPRESSION TAG	UNP A4W7D6
A	-11	ASP	-	EXPRESSION TAG	UNP A4W7D6
A	-10	LEU	-	EXPRESSION TAG	UNP A4W7D6
A	-9	GLY	-	EXPRESSION TAG	UNP A4W7D6
A	-8	THR	-	EXPRESSION TAG	UNP A4W7D6
A	-7	GLU	-	EXPRESSION TAG	UNP A4W7D6
A	-6	ASN	-	EXPRESSION TAG	UNP A4W7D6
A	-5	LEU	-	EXPRESSION TAG	UNP A4W7D6
A	-4	TYR	-	EXPRESSION TAG	UNP A4W7D6
A	-3	PHE	-	EXPRESSION TAG	UNP A4W7D6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLN	-	EXPRESSION TAG	UNP A4W7D6
A	-1	SER	-	EXPRESSION TAG	UNP A4W7D6
A	0	MET	-	EXPRESSION TAG	UNP A4W7D6
B	-22	MET	-	EXPRESSION TAG	UNP A4W7D6
B	-21	HIS	-	EXPRESSION TAG	UNP A4W7D6
B	-20	HIS	-	EXPRESSION TAG	UNP A4W7D6
B	-19	HIS	-	EXPRESSION TAG	UNP A4W7D6
B	-18	HIS	-	EXPRESSION TAG	UNP A4W7D6
B	-17	HIS	-	EXPRESSION TAG	UNP A4W7D6
B	-16	HIS	-	EXPRESSION TAG	UNP A4W7D6
B	-15	SER	-	EXPRESSION TAG	UNP A4W7D6
B	-14	SER	-	EXPRESSION TAG	UNP A4W7D6
B	-13	GLY	-	EXPRESSION TAG	UNP A4W7D6
B	-12	VAL	-	EXPRESSION TAG	UNP A4W7D6
B	-11	ASP	-	EXPRESSION TAG	UNP A4W7D6
B	-10	LEU	-	EXPRESSION TAG	UNP A4W7D6
B	-9	GLY	-	EXPRESSION TAG	UNP A4W7D6
B	-8	THR	-	EXPRESSION TAG	UNP A4W7D6
B	-7	GLU	-	EXPRESSION TAG	UNP A4W7D6
B	-6	ASN	-	EXPRESSION TAG	UNP A4W7D6
B	-5	LEU	-	EXPRESSION TAG	UNP A4W7D6
B	-4	TYR	-	EXPRESSION TAG	UNP A4W7D6
B	-3	PHE	-	EXPRESSION TAG	UNP A4W7D6
B	-2	GLN	-	EXPRESSION TAG	UNP A4W7D6
B	-1	SER	-	EXPRESSION TAG	UNP A4W7D6
B	0	MET	-	EXPRESSION TAG	UNP A4W7D6
C	-22	MET	-	EXPRESSION TAG	UNP A4W7D6
C	-21	HIS	-	EXPRESSION TAG	UNP A4W7D6
C	-20	HIS	-	EXPRESSION TAG	UNP A4W7D6
C	-19	HIS	-	EXPRESSION TAG	UNP A4W7D6
C	-18	HIS	-	EXPRESSION TAG	UNP A4W7D6
C	-17	HIS	-	EXPRESSION TAG	UNP A4W7D6
C	-16	HIS	-	EXPRESSION TAG	UNP A4W7D6
C	-15	SER	-	EXPRESSION TAG	UNP A4W7D6
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C	-12	VAL	-	EXPRESSION TAG	UNP A4W7D6
C	-11	ASP	-	EXPRESSION TAG	UNP A4W7D6
C	-10	LEU	-	EXPRESSION TAG	UNP A4W7D6
C	-9	GLY	-	EXPRESSION TAG	UNP A4W7D6
C	-8	THR	-	EXPRESSION TAG	UNP A4W7D6
C	-7	GLU	-	EXPRESSION TAG	UNP A4W7D6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ASN	-	EXPRESSION TAG	UNP A4W7D6
C	-5	LEU	-	EXPRESSION TAG	UNP A4W7D6
C	-4	TYR	-	EXPRESSION TAG	UNP A4W7D6
C	-3	PHE	-	EXPRESSION TAG	UNP A4W7D6
C	-2	GLN	-	EXPRESSION TAG	UNP A4W7D6
C	-1	SER	-	EXPRESSION TAG	UNP A4W7D6
C	0	MET	-	EXPRESSION TAG	UNP A4W7D6
D	-22	MET	-	EXPRESSION TAG	UNP A4W7D6
D	-21	HIS	-	EXPRESSION TAG	UNP A4W7D6
D	-20	HIS	-	EXPRESSION TAG	UNP A4W7D6
D	-19	HIS	-	EXPRESSION TAG	UNP A4W7D6
D	-18	HIS	-	EXPRESSION TAG	UNP A4W7D6
D	-17	HIS	-	EXPRESSION TAG	UNP A4W7D6
D	-16	HIS	-	EXPRESSION TAG	UNP A4W7D6
D	-15	SER	-	EXPRESSION TAG	UNP A4W7D6
D	-14	SER	-	EXPRESSION TAG	UNP A4W7D6
D	-13	GLY	-	EXPRESSION TAG	UNP A4W7D6
D	-12	VAL	-	EXPRESSION TAG	UNP A4W7D6
D	-11	ASP	-	EXPRESSION TAG	UNP A4W7D6
D	-10	LEU	-	EXPRESSION TAG	UNP A4W7D6
D	-9	GLY	-	EXPRESSION TAG	UNP A4W7D6
D	-8	THR	-	EXPRESSION TAG	UNP A4W7D6
D	-7	GLU	-	EXPRESSION TAG	UNP A4W7D6
D	-6	ASN	-	EXPRESSION TAG	UNP A4W7D6
D	-5	LEU	-	EXPRESSION TAG	UNP A4W7D6
D	-4	TYR	-	EXPRESSION TAG	UNP A4W7D6
D	-3	PHE	-	EXPRESSION TAG	UNP A4W7D6
D	-2	GLN	-	EXPRESSION TAG	UNP A4W7D6
D	-1	SER	-	EXPRESSION TAG	UNP A4W7D6
D	0	MET	-	EXPRESSION TAG	UNP A4W7D6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- 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	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Cl	0	0
			3	3		
4	A	4	Total	Cl	0	0
			4	4		
4	D	1	Total	Cl	0	0
			1	1		
4	C	4	Total	Cl	0	0
			4	4		


- Molecule 5 is water.

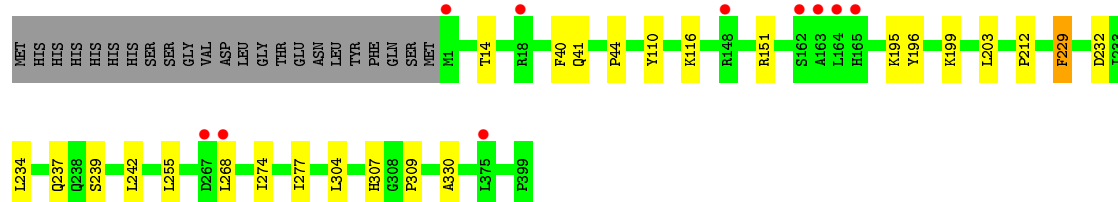
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	335	Total 335	O 335	0	0
5	B	344	Total 344	O 344	0	0
5	C	314	Total 314	O 314	0	0
5	D	336	Total 336	O 336	0	0

### 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.

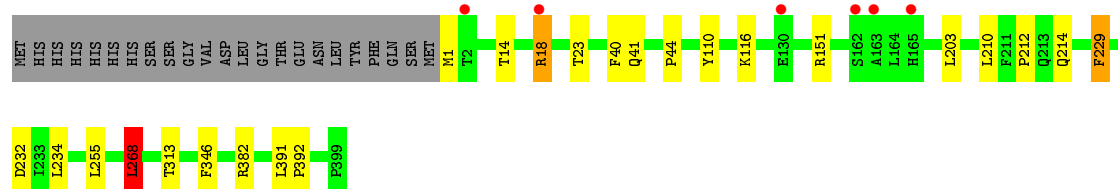
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, N-terminal domain protein

Chain A: 




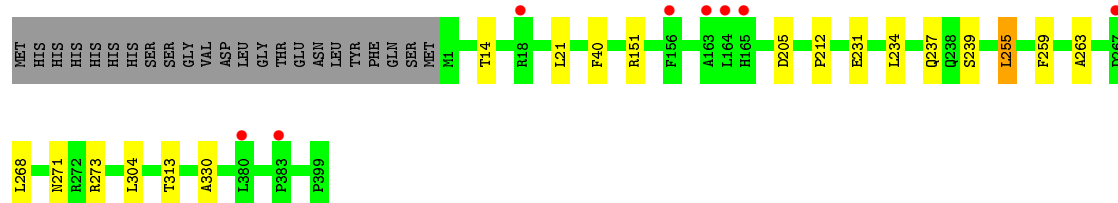
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, N-terminal domain protein

Chain B: 




- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, N-terminal domain protein

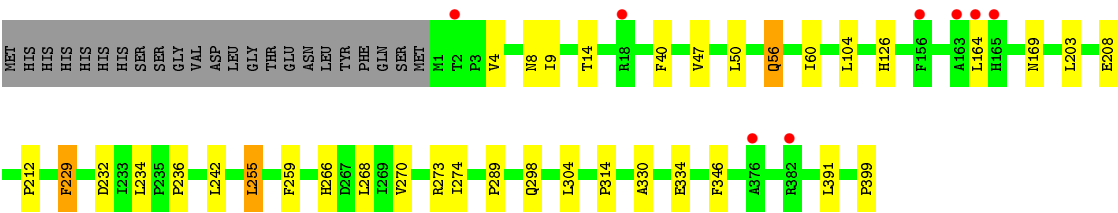
Chain C: 



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, N-terminal domain protein

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 <sub>2</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.15Å 182.15Å 104.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	128.80 – 1.80 128.80 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (128.80-1.80) 98.2 (128.80-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.252 , 0.282 0.256 , 0.288	Depositor DCC
$R_{free}$ test set	1966 reflections (1.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.5	Xtriage
Anisotropy	0.657	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 39.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14219	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	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 55.46 % 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 3.1538e-05. 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 [i](#)

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

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

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	0.53	0/3332	0.61	0/4547
1	B	0.55	0/3312	0.64	1/4520 (0.0%)
1	C	0.54	0/3299	0.61	0/4503
1	D	0.55	0/3322	0.62	0/4535
All	All	0.54	0/13265	0.62	1/18105 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	LEU	CA-CB-CG	6.04	129.20	115.30

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	3224	0	3171	24	0
1	B	3208	0	3137	13	0
1	C	3198	0	3131	18	0
1	D	3214	0	3149	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	12	0	16	3	0
4	A	4	0	0	2	0
4	B	3	0	0	0	0
4	C	4	0	0	0	0
4	D	1	0	0	0	0
5	A	335	0	0	1	0
5	B	344	0	0	3	0
5	C	314	0	0	4	1
5	D	336	0	0	7	0
All	All	14219	0	12628	88	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 3.

All (88) 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:242[B]:LEU:CD1	1:A:268[B]:LEU:HD21	1.82	1.09
1:A:242[B]:LEU:HD12	1:A:268[B]:LEU:HD21	1.36	1.06
1:D:259:PHE:HB3	5:D:1028:HOH:O	1.65	0.96
5:B:445:HOH:O	3:D:401:GOL:H2	1.66	0.95
1:A:242[B]:LEU:CD1	1:A:268[B]:LEU:CD2	2.47	0.92
1:C:273[B]:ARG:HH11	1:C:273[B]:ARG:CG	1.89	0.85
1:B:23[B]:THR:HG21	1:B:346:PHE:HE1	1.46	0.80
1:C:273[B]:ARG:HD3	5:C:1361:HOH:O	1.85	0.77
1:A:14:THR:HG22	5:A:1043:HOH:O	1.84	0.76
1:B:14:THR:HG22	5:B:1328:HOH:O	1.86	0.75
1:C:239:SER:HB2	1:C:268[B]:LEU:HD21	1.69	0.73
1:A:242[B]:LEU:HD12	1:A:268[B]:LEU:CD2	2.13	0.72
1:D:268[B]:LEU:HA	1:D:273[B]:ARG:HD3	1.72	0.71
1:B:23[B]:THR:HG21	1:B:346:PHE:CE1	2.26	0.70
1:D:9:ILE:H	1:D:56[A]:GLN:HE22	1.37	0.70
1:D:50:LEU:HD12	5:D:1055:HOH:O	1.92	0.69
1:C:273[B]:ARG:HG3	1:C:273[B]:ARG:HH11	1.58	0.68
1:B:23[B]:THR:HG22	1:B:313:THR:HG21	1.76	0.67
1:D:236:PRO:HB2	5:D:1018:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:445:HOH:O	3:D:401:GOL:C2	2.34	0.66
1:A:242[B]:LEU:HD13	1:A:268[B]:LEU:CD2	2.30	0.62
1:D:268[A]:LEU:HD11	1:D:274:ILE:HG23	1.81	0.61
1:A:239:SER:CB	1:A:268[B]:LEU:HD11	2.32	0.60
1:C:273[B]:ARG:HG2	1:C:273[B]:ARG:HH11	1.65	0.60
1:D:242:LEU:CD1	1:D:268[B]:LEU:HD21	2.34	0.57
1:D:9:ILE:H	1:D:56[A]:GLN:NE2	2.03	0.57
1:A:239:SER:HB2	1:A:268[B]:LEU:HD11	1.85	0.56
1:D:391:LEU:HD12	5:D:1047:HOH:O	2.07	0.55
1:A:234:LEU:HD12	1:A:242[A]:LEU:HD12	1.90	0.54
1:C:273[B]:ARG:CG	1:C:273[B]:ARG:NH1	2.59	0.54
1:D:14[A]:THR:HG22	5:D:1337:HOH:O	2.08	0.52
1:C:14[A]:THR:HG22	5:C:1145:HOH:O	2.09	0.52
1:C:263:ALA:HB3	5:C:1166:HOH:O	2.09	0.51
1:A:212:PRO:HA	1:A:234:LEU:HD21	1.93	0.51
1:D:268[B]:LEU:HA	1:D:273[B]:ARG:CD	2.41	0.50
1:D:47:VAL:HA	5:D:1055:HOH:O	2.12	0.50
1:D:56[A]:GLN:OE1	1:D:60:ILE:HD11	2.12	0.49
1:D:289:PRO:CB	3:D:401:GOL:H32	2.44	0.48
1:D:242:LEU:HD12	1:D:268[B]:LEU:HD21	1.95	0.48
1:B:255:LEU:HD23	1:B:268:LEU:HD11	1.96	0.47
1:B:232:ASP:HA	1:B:255:LEU:HD12	1.95	0.47
1:A:255[A]:LEU:HD23	1:A:268[A]:LEU:HD22	1.96	0.47
1:A:242[B]:LEU:HD13	1:A:268[B]:LEU:HD23	1.97	0.47
1:B:212:PRO:HA	1:B:234:LEU:HD21	1.96	0.47
1:B:110:TYR:CE1	1:B:116:LYS:HG3	2.50	0.46
1:A:268[A]:LEU:HD13	1:A:274:ILE:HG12	1.97	0.46
1:D:268[B]:LEU:HD23	1:D:273[B]:ARG:HG2	1.98	0.46
1:C:271:ASN:HB2	1:C:273[B]:ARG:HD2	1.97	0.46
1:D:208:GLU:OE2	1:D:399:PRO:O	2.34	0.46
1:C:205:ASP:HA	1:C:231:GLU:HB3	1.97	0.45
1:A:234:LEU:CD1	1:A:242[A]:LEU:HD12	2.46	0.45
1:D:304:LEU:HB2	1:D:330:ALA:HA	1.98	0.45
1:C:304:LEU:HB2	1:C:330:ALA:HA	1.97	0.45
1:A:232:ASP:HA	1:A:255[B]:LEU:HD12	1.98	0.45
1:C:255:LEU:HD23	1:C:259:PHE:CZ	2.53	0.44
1:C:212:PRO:HA	1:C:234:LEU:HD21	1.97	0.44
1:D:268[A]:LEU:HD11	1:D:274:ILE:CG2	2.48	0.44
4:A:404:CL:CL	1:C:237:GLN:HB2	2.55	0.43
1:D:232:ASP:HA	1:D:255:LEU:HD12	2.00	0.43
1:D:266:HIS:O	1:D:270:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:LEU:HD12	1:D:203:LEU:N	2.34	0.43
1:A:304:LEU:HB2	1:A:330:ALA:HA	1.99	0.43
1:A:110:TYR:CE1	1:A:116:LYS:HG3	2.54	0.43
1:B:203:LEU:HD23	1:B:229:PHE:CZ	2.53	0.43
1:C:268[B]:LEU:HA	1:C:268[B]:LEU:HD23	1.86	0.43
1:B:391:LEU:HB3	1:B:392:PRO:CD	2.48	0.42
1:B:41:GLN:O	1:B:44:PRO:HD3	2.19	0.42
1:D:268[A]:LEU:HD21	1:D:274:ILE:HD13	2.01	0.41
1:D:126:HIS:NE2	1:D:334:GLU:OE2	2.51	0.41
1:A:307:HIS:CE1	1:A:309:PRO:HG3	2.56	0.41
1:C:273[B]:ARG:HG2	1:C:273[B]:ARG:NH1	2.29	0.41
1:D:203:LEU:HD23	1:D:229:PHE:CZ	2.55	0.41
1:D:4:VAL:HG21	1:D:104[B]:LEU:HD11	2.02	0.41
1:D:314:PRO:HG2	1:D:346:PHE:HB2	2.02	0.41
1:A:195:LYS:HG2	1:A:196:TYR:CE2	2.56	0.41
1:A:239:SER:O	1:A:242[A]:LEU:HD13	2.21	0.41
1:C:273[B]:ARG:NH1	5:C:496:HOH:O	2.53	0.41
1:A:41:GLN:O	1:A:44:PRO:HD3	2.20	0.41
1:C:21:LEU:HB3	1:C:313:THR:HG22	2.02	0.41
1:D:212:PRO:HA	1:D:234:LEU:HD21	2.03	0.41
1:A:199:LYS:HB3	1:A:199:LYS:HE3	1.87	0.40
1:D:169:ASN:ND2	5:D:1207:HOH:O	2.54	0.40
1:D:8:ASN:OD1	1:D:56[A]:GLN:NE2	2.49	0.40
1:A:237:GLN:HB2	4:A:403:CL:CL	2.58	0.40
1:B:210:LEU:HB3	1:B:214:GLN:HB2	2.04	0.40
1:B:18:ARG:O	1:B:382:ARG:NH1	2.55	0.40
1:A:203:LEU:HD23	1:A:229:PHE:CZ	2.56	0.40
1:D:56[A]:GLN:HB2	1:D:56[A]:GLN:HE21	1.62	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)
5:C:963:HOH:O	5:C:963:HOH:O[7_556]	2.14	0.06

## 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	406/422 (96%)	396 (98%)	10 (2%)	0	100	100
1	B	404/422 (96%)	393 (97%)	11 (3%)	0	100	100
1	C	403/422 (96%)	394 (98%)	9 (2%)	0	100	100
1	D	405/422 (96%)	396 (98%)	9 (2%)	0	100	100
All	All	1618/1688 (96%)	1579 (98%)	39 (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	343/355 (97%)	339 (99%)	4 (1%)	71	65
1	B	341/355 (96%)	335 (98%)	6 (2%)	59	48
1	C	340/355 (96%)	337 (99%)	3 (1%)	78	75
1	D	342/355 (96%)	335 (98%)	7 (2%)	55	44
All	All	1366/1420 (96%)	1346 (98%)	20 (2%)	67	56

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	PHE
1	A	151	ARG

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Mol	Chain	Res	Type
1	A	229	PHE
1	A	277	ILE
1	B	1	MET
1	B	18	ARG
1	B	40	PHE
1	B	151	ARG
1	B	229	PHE
1	B	268	LEU
1	C	40	PHE
1	C	151	ARG
1	C	255	LEU
1	D	40	PHE
1	D	56[A]	GLN
1	D	56[B]	GLN
1	D	164	LEU
1	D	229	PHE
1	D	255	LEU
1	D	298	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	145	GLN
1	C	165	HIS
1	D	169	ASN
1	D	238	GLN

### 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 monosaccharides in this entry.



## 5.6 Ligand geometry

Of 21 ligands modelled in this entry, 16 are monoatomic - leaving 5 for Mogul analysis.

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	D	400	-	5,5,5	0.46	0	5,5,5	0.36	0
3	GOL	A	400	-	5,5,5	0.41	0	5,5,5	0.54	0
3	GOL	C	400	-	5,5,5	0.40	0	5,5,5	0.39	0
3	GOL	D	401	-	5,5,5	0.36	0	5,5,5	1.14	0
3	GOL	B	400	-	5,5,5	0.39	0	5,5,5	0.34	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
3	GOL	D	400	-	-	0/4/4/4	-
3	GOL	A	400	-	-	0/4/4/4	-
3	GOL	C	400	-	-	0/4/4/4	-
3	GOL	D	401	-	-	3/4/4/4	-
3	GOL	B	400	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	401	GOL	C1-C2-C3-O3
3	D	401	GOL	O2-C2-C3-O3
3	D	401	GOL	O1-C1-C2-C3
3	B	400	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	GOL	3	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	399/422 (94%)	0.13	10 (2%) 57 52	6, 11, 22, 33	0
1	B	399/422 (94%)	0.19	6 (1%) 73 70	6, 11, 21, 33	0
1	C	399/422 (94%)	0.07	8 (2%) 65 61	7, 11, 22, 42	0
1	D	399/422 (94%)	0.18	8 (2%) 65 61	6, 11, 22, 36	0
All	All	1596/1688 (94%)	0.14	32 (2%) 65 61	6, 11, 22, 42	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	165	HIS	4.4
1	D	156[A]	PHE	4.2
1	C	165	HIS	4.0
1	D	163	ALA	3.5
1	B	163	ALA	3.4
1	A	165[A]	HIS	3.4
1	B	165	HIS	3.4
1	D	18	ARG	3.3
1	A	267	ASP	3.2
1	C	164	LEU	3.1
1	D	2	THR	3.1
1	A	164	LEU	3.1
1	C	163	ALA	3.0
1	A	163	ALA	3.0
1	D	164	LEU	2.9
1	A	162	SER	2.8
1	A	18	ARG	2.6
1	A	268[A]	LEU	2.6
1	B	130	GLU	2.5
1	C	156	PHE	2.4
1	D	382	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	375	LEU	2.3
1	C	18	ARG	2.3
1	C	380	LEU	2.2
1	B	162	SER	2.2
1	D	376	ALA	2.2
1	B	18	ARG	2.1
1	C	383	PRO	2.1
1	C	267	ASP	2.1
1	A	148	ARG	2.1
1	A	1	MET	2.0
1	B	2	THR	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
3	GOL	D	401	6/6	0.79	0.27	13,22,25,25	0
3	GOL	B	400	6/6	0.89	0.12	10,12,14,16	0
3	GOL	D	400	6/6	0.89	0.13	12,13,14,19	0
3	GOL	C	400	6/6	0.91	0.13	14,15,17,19	0
3	GOL	A	400	6/6	0.91	0.11	13,14,15,15	0
4	CL	B	403	1/1	0.95	0.10	35,35,35,35	0
4	CL	A	402	1/1	0.96	0.07	22,22,22,22	0
4	CL	C	404	1/1	0.96	0.07	30,30,30,30	0
4	CL	A	403	1/1	0.97	0.07	19,19,19,19	0
4	CL	C	402	1/1	0.98	0.08	22,22,22,22	0
4	CL	A	404	1/1	0.98	0.06	21,21,21,21	0
4	CL	A	401	1/1	0.98	0.05	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	601	1/1	0.98	0.06	12,12,12,12	0
4	CL	B	402	1/1	0.98	0.06	17,17,17,17	0
4	CL	C	403	1/1	0.98	0.10	17,17,17,17	0
2	MG	C	601	1/1	0.99	0.06	11,11,11,11	0
4	CL	C	401	1/1	0.99	0.07	17,17,17,17	0
4	CL	D	402	1/1	0.99	0.04	23,23,23,23	0
2	MG	B	601	1/1	0.99	0.04	12,12,12,12	0
2	MG	D	601	1/1	0.99	0.07	10,10,10,10	0
4	CL	B	401	1/1	0.99	0.04	12,12,12,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.