



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:37 AM GMT

PDB ID : 2RDX  
Title : Crystal structure of mandelate racemase/muconate lactonizing enzyme from *Roseovarius nubinhibens* ISM  
Authors : Patskovsky, Y.; Bonanno, J.; Sauder, J.M.; Ozyurt, S.; Gilmore, M.; Lau, C.; Maletic, M.; Gheyi, T.; Wasserman, S.R.; Koss, J.; Gerlt, J.A.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2007-09-25  
Resolution : 2.00 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  
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

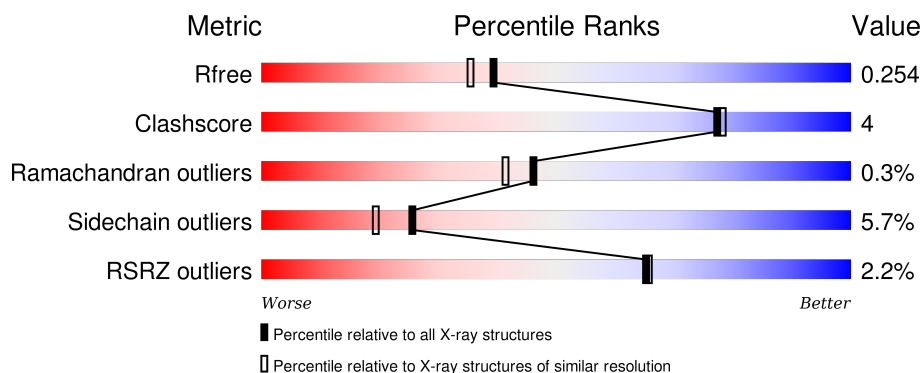
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	379	<div> <div>2%</div> <div>86%</div> <div>10%</div> <div>• •</div> </div>
1	B	379	<div> <div>%</div> <div>82%</div> <div>14%</div> <div>• •</div> </div>
1	C	379	<div> <div>2%</div> <div>84%</div> <div>11%</div> <div>• •</div> </div>
1	D	379	<div> <div>2%</div> <div>88%</div> <div>7%</div> <div>• •</div> </div>
1	E	379	<div> <div>3%</div> <div>85%</div> <div>10%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	379	
1	G	379	
1	H	379	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	380	-	-	-	X
3	GOL	C	379	-	-	-	X
3	GOL	G	379	-	-	-	X
3	GOL	H	379	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23975 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, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	10	0
			2890	1802	529	538	21			
1	B	369	Total	C	N	O	S	0	4	0
			2851	1776	519	536	20			
1	C	369	Total	C	N	O	S	0	6	0
			2872	1788	531	534	19			
1	D	369	Total	C	N	O	S	0	11	0
			2910	1812	542	537	19			
1	E	369	Total	C	N	O	S	0	6	0
			2865	1786	527	533	19			
1	F	369	Total	C	N	O	S	0	3	0
			2850	1774	522	535	19			
1	G	360	Total	C	N	O	S	0	3	0
			2793	1738	514	522	19			
1	H	369	Total	C	N	O	S	0	6	0
			2869	1788	528	534	19			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP A3SNF8
A	0	SER	-	EXPRESSION TAG	UNP A3SNF8
A	1	LEU	-	EXPRESSION TAG	UNP A3SNF8
A	370	GLU	-	EXPRESSION TAG	UNP A3SNF8
A	371	GLY	-	EXPRESSION TAG	UNP A3SNF8
A	372	HIS	-	EXPRESSION TAG	UNP A3SNF8
A	373	HIS	-	EXPRESSION TAG	UNP A3SNF8
A	374	HIS	-	EXPRESSION TAG	UNP A3SNF8
A	375	HIS	-	EXPRESSION TAG	UNP A3SNF8
A	376	HIS	-	EXPRESSION TAG	UNP A3SNF8
A	377	HIS	-	EXPRESSION TAG	UNP A3SNF8
B	-1	MET	-	EXPRESSION TAG	UNP A3SNF8
B	0	SER	-	EXPRESSION TAG	UNP A3SNF8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	LEU	-	EXPRESSION TAG	UNP A3SNF8
B	370	GLU	-	EXPRESSION TAG	UNP A3SNF8
B	371	GLY	-	EXPRESSION TAG	UNP A3SNF8
B	372	HIS	-	EXPRESSION TAG	UNP A3SNF8
B	373	HIS	-	EXPRESSION TAG	UNP A3SNF8
B	374	HIS	-	EXPRESSION TAG	UNP A3SNF8
B	375	HIS	-	EXPRESSION TAG	UNP A3SNF8
B	376	HIS	-	EXPRESSION TAG	UNP A3SNF8
B	377	HIS	-	EXPRESSION TAG	UNP A3SNF8
C	-1	MET	-	EXPRESSION TAG	UNP A3SNF8
C	0	SER	-	EXPRESSION TAG	UNP A3SNF8
C	1	LEU	-	EXPRESSION TAG	UNP A3SNF8
C	370	GLU	-	EXPRESSION TAG	UNP A3SNF8
C	371	GLY	-	EXPRESSION TAG	UNP A3SNF8
C	372	HIS	-	EXPRESSION TAG	UNP A3SNF8
C	373	HIS	-	EXPRESSION TAG	UNP A3SNF8
C	374	HIS	-	EXPRESSION TAG	UNP A3SNF8
C	375	HIS	-	EXPRESSION TAG	UNP A3SNF8
C	376	HIS	-	EXPRESSION TAG	UNP A3SNF8
C	377	HIS	-	EXPRESSION TAG	UNP A3SNF8
D	-1	MET	-	EXPRESSION TAG	UNP A3SNF8
D	0	SER	-	EXPRESSION TAG	UNP A3SNF8
D	1	LEU	-	EXPRESSION TAG	UNP A3SNF8
D	370	GLU	-	EXPRESSION TAG	UNP A3SNF8
D	371	GLY	-	EXPRESSION TAG	UNP A3SNF8
D	372	HIS	-	EXPRESSION TAG	UNP A3SNF8
D	373	HIS	-	EXPRESSION TAG	UNP A3SNF8
D	374	HIS	-	EXPRESSION TAG	UNP A3SNF8
D	375	HIS	-	EXPRESSION TAG	UNP A3SNF8
D	376	HIS	-	EXPRESSION TAG	UNP A3SNF8
D	377	HIS	-	EXPRESSION TAG	UNP A3SNF8
E	-1	MET	-	EXPRESSION TAG	UNP A3SNF8
E	0	SER	-	EXPRESSION TAG	UNP A3SNF8
E	1	LEU	-	EXPRESSION TAG	UNP A3SNF8
E	370	GLU	-	EXPRESSION TAG	UNP A3SNF8
E	371	GLY	-	EXPRESSION TAG	UNP A3SNF8
E	372	HIS	-	EXPRESSION TAG	UNP A3SNF8
E	373	HIS	-	EXPRESSION TAG	UNP A3SNF8
E	374	HIS	-	EXPRESSION TAG	UNP A3SNF8
E	375	HIS	-	EXPRESSION TAG	UNP A3SNF8
E	376	HIS	-	EXPRESSION TAG	UNP A3SNF8
E	377	HIS	-	EXPRESSION TAG	UNP A3SNF8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	MET	-	EXPRESSION TAG	UNP A3SNF8
F	0	SER	-	EXPRESSION TAG	UNP A3SNF8
F	1	LEU	-	EXPRESSION TAG	UNP A3SNF8
F	370	GLU	-	EXPRESSION TAG	UNP A3SNF8
F	371	GLY	-	EXPRESSION TAG	UNP A3SNF8
F	372	HIS	-	EXPRESSION TAG	UNP A3SNF8
F	373	HIS	-	EXPRESSION TAG	UNP A3SNF8
F	374	HIS	-	EXPRESSION TAG	UNP A3SNF8
F	375	HIS	-	EXPRESSION TAG	UNP A3SNF8
F	376	HIS	-	EXPRESSION TAG	UNP A3SNF8
F	377	HIS	-	EXPRESSION TAG	UNP A3SNF8
G	-1	MET	-	EXPRESSION TAG	UNP A3SNF8
G	0	SER	-	EXPRESSION TAG	UNP A3SNF8
G	1	LEU	-	EXPRESSION TAG	UNP A3SNF8
G	370	GLU	-	EXPRESSION TAG	UNP A3SNF8
G	371	GLY	-	EXPRESSION TAG	UNP A3SNF8
G	372	HIS	-	EXPRESSION TAG	UNP A3SNF8
G	373	HIS	-	EXPRESSION TAG	UNP A3SNF8
G	374	HIS	-	EXPRESSION TAG	UNP A3SNF8
G	375	HIS	-	EXPRESSION TAG	UNP A3SNF8
G	376	HIS	-	EXPRESSION TAG	UNP A3SNF8
G	377	HIS	-	EXPRESSION TAG	UNP A3SNF8
H	-1	MET	-	EXPRESSION TAG	UNP A3SNF8
H	0	SER	-	EXPRESSION TAG	UNP A3SNF8
H	1	LEU	-	EXPRESSION TAG	UNP A3SNF8
H	370	GLU	-	EXPRESSION TAG	UNP A3SNF8
H	371	GLY	-	EXPRESSION TAG	UNP A3SNF8
H	372	HIS	-	EXPRESSION TAG	UNP A3SNF8
H	373	HIS	-	EXPRESSION TAG	UNP A3SNF8
H	374	HIS	-	EXPRESSION TAG	UNP A3SNF8
H	375	HIS	-	EXPRESSION TAG	UNP A3SNF8
H	376	HIS	-	EXPRESSION TAG	UNP A3SNF8
H	377	HIS	-	EXPRESSION TAG	UNP A3SNF8

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

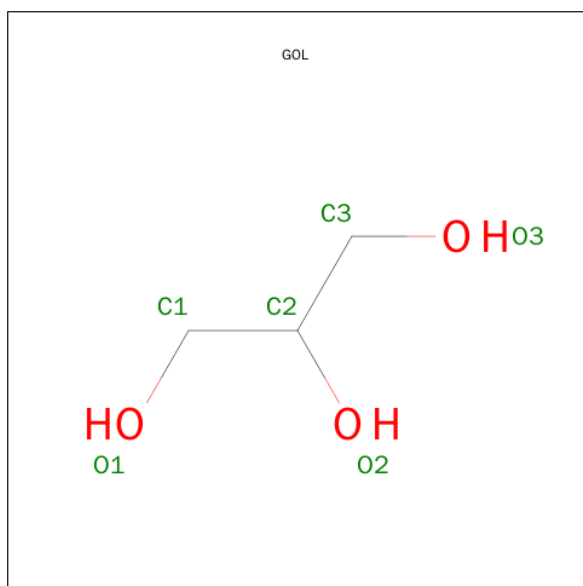
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	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	A	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	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 4 is water.

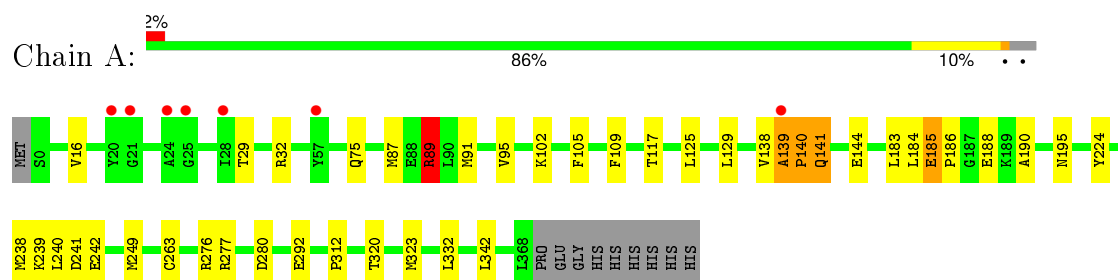
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	149	Total	O	0	0
			149	149		
4	B	126	Total	O	0	0
			126	126		
4	C	152	Total	O	0	0
			152	152		
4	D	135	Total	O	0	0
			135	135		
4	E	101	Total	O	0	0
			101	101		
4	F	94	Total	O	0	0
			94	94		
4	G	141	Total	O	0	0
			141	141		
4	H	127	Total	O	0	0
			127	127		



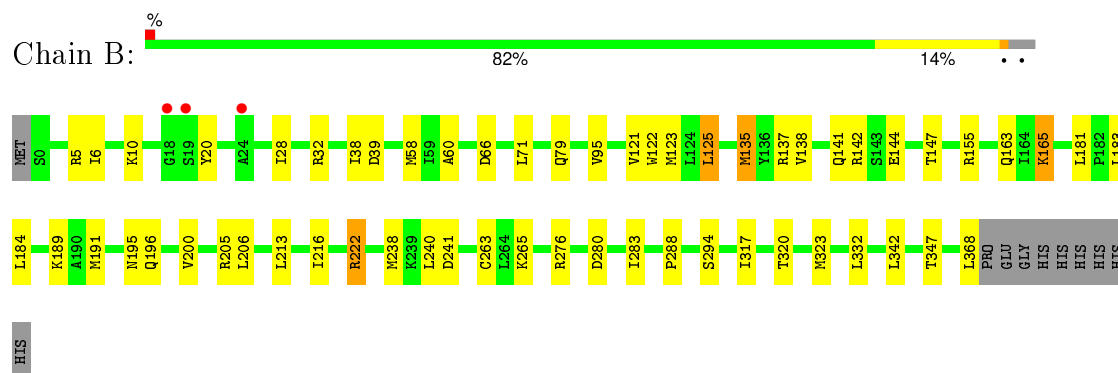
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

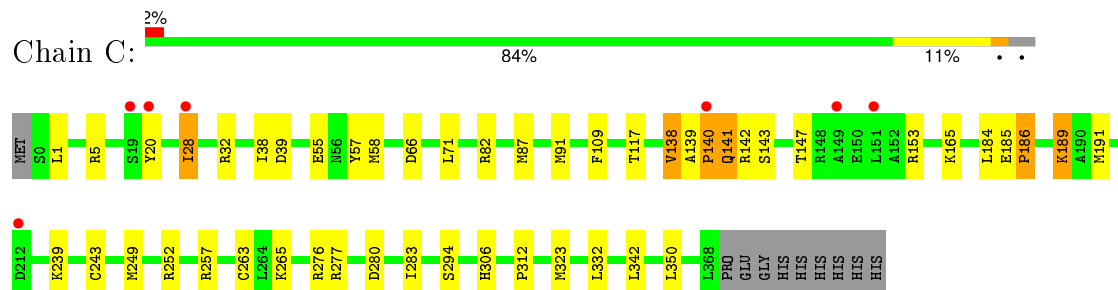
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative



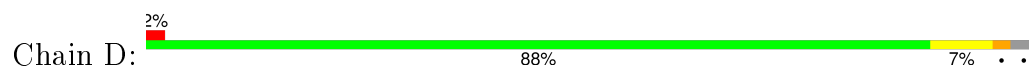
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative

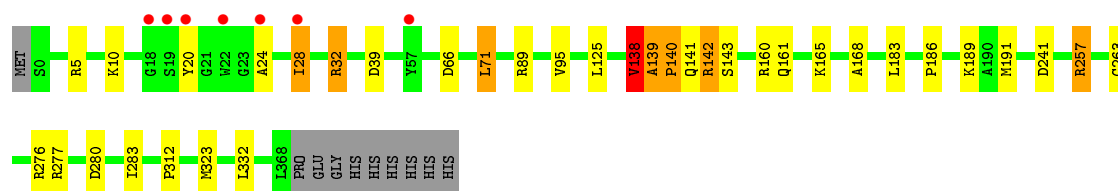


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative

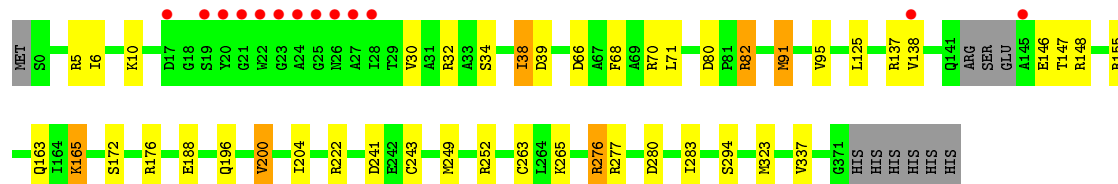
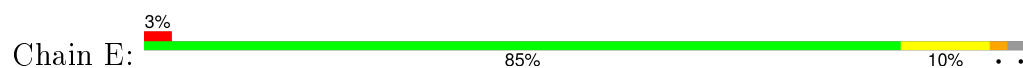


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative

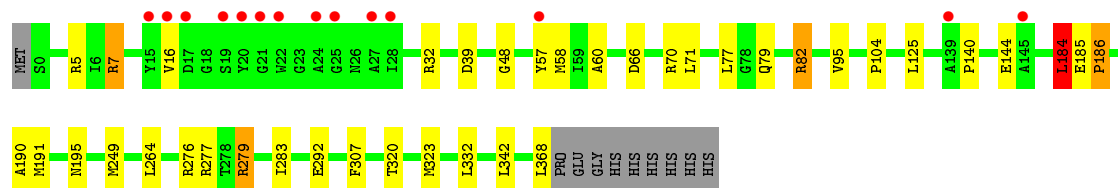
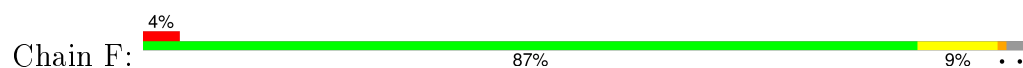




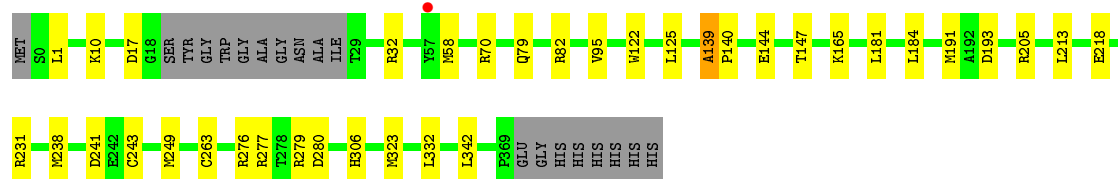
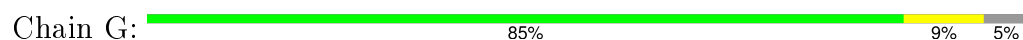
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative



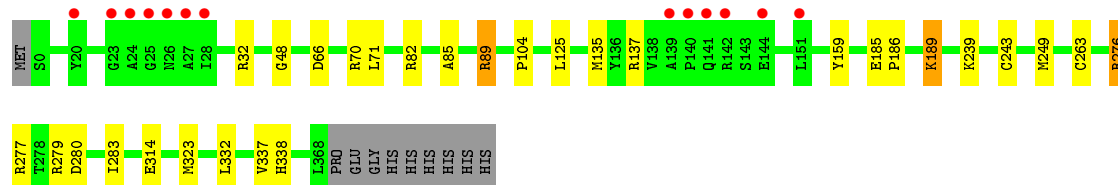
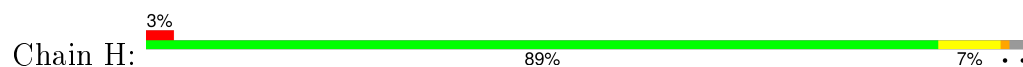
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme, putative



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.41Å 169.22Å 223.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 30.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (20.00-2.00) 97.9 (30.84-2.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, $R_{free}$	0.194 , 0.256 0.197 , 0.254	Depositor DCC
$R_{free}$ test set	6351 reflections (3.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 24.8	EDS
Estimated twinning fraction	0.051 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 210739 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	23975	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.96% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, MG

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	0.41	0/2976	0.66	2/4034 (0.0%)
1	B	0.39	0/2921	0.62	0/3962
1	C	0.42	0/2946	0.63	0/3994
1	D	0.45	0/2994	0.66	1/4056 (0.0%)
1	E	0.39	0/2942	0.61	0/3989
1	F	0.40	0/2915	0.62	1/3955 (0.0%)
1	G	0.41	0/2855	0.61	0/3871
1	H	0.42	0/2946	0.62	0/3994
All	All	0.41	0/23495	0.63	4/31855 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	C	0	1
1	D	0	2
All	All	1	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89[A]	ARG	N-CA-C	5.74	126.51	111.00
1	A	89[B]	ARG	N-CA-C	5.74	126.51	111.00
1	F	184	LEU	CA-CB-CG	5.51	127.97	115.30
1	D	138	VAL	CB-CA-C	-5.42	101.09	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	89[A]	ARG	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ALA	Peptide
1	A	185	GLU	Peptide
1	C	139	ALA	Peptide
1	D	138	VAL	Peptide
1	D	139	ALA	Peptide

## 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	2890	0	2852	33	0
1	B	2851	0	2797	21	0
1	C	2872	0	2828	29	0
1	D	2910	0	2877	22	0
1	E	2865	0	2819	21	0
1	F	2850	0	2788	20	0
1	G	2793	0	2744	21	0
1	H	2869	0	2828	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	12	0	16	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	F	6	0	8	0	0
3	G	6	0	8	0	0
3	H	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	149	0	0	3	0
4	B	126	0	0	1	0
4	C	152	0	0	3	0
4	D	135	0	0	0	0
4	E	101	0	0	0	0
4	F	94	0	0	1	0
4	G	141	0	0	3	0
4	H	127	0	0	1	0
All	All	23975	0	22589	167	0

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 4.

All (167) 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:185:GLU:HB2	1:A:186:PRO:HD3	1.26	1.09
1:A:185:GLU:HB2	1:A:186:PRO:CD	1.92	1.00
1:A:139:ALA:HB1	1:A:140:PRO:HD3	1.45	0.96
1:C:140:PRO:HG2	1:C:147:THR:HG22	1.52	0.90
1:G:139:ALA:HB1	1:G:140:PRO:HA	1.53	0.88
1:C:138:VAL:O	1:C:138:VAL:HG23	1.70	0.88
1:A:89[A]:ARG:HG3	1:A:89[A]:ARG:HH21	1.39	0.87
1:C:189:LYS:HD2	4:C:491:HOH:O	1.75	0.84
1:A:185:GLU:CB	1:A:186:PRO:HD3	1.93	0.81
1:E:82:ARG:HG3	1:E:82:ARG:HH11	1.46	0.80
1:A:185:GLU:O	1:A:188:GLU:HB2	1.88	0.74
1:D:257[A]:ARG:HG2	1:D:257[A]:ARG:HH21	1.55	0.71
1:H:338:HIS:HD2	4:H:480:HOH:O	1.76	0.69
1:G:139:ALA:CB	1:G:140:PRO:HA	2.25	0.67
1:C:140:PRO:CG	1:C:147:THR:HG22	2.24	0.67
1:H:279:ARG:NH1	1:H:280:ASP:OD1	2.28	0.67
1:E:68:PHE:HZ	1:E:91:MET:HG2	1.60	0.66
1:A:89[A]:ARG:CG	1:A:89[A]:ARG:HH21	2.09	0.66
1:G:139:ALA:HB1	1:G:140:PRO:CA	2.24	0.65
1:G:1:LEU:HD22	1:G:82:ARG:HD2	1.79	0.65
1:D:139:ALA:HB1	1:D:140:PRO:HB3	1.80	0.63
1:D:139:ALA:HB1	1:D:140:PRO:CG	2.29	0.63
1:F:7:ARG:HG2	4:F:388:HOH:O	2.00	0.62
1:A:184:LEU:HD11	1:A:190:ALA:HB2	1.81	0.62
1:F:185:GLU:HB2	1:F:186:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:85:ALA:O	1:H:89[B]:ARG:HG3	2.00	0.60
1:D:139:ALA:HB1	1:D:140:PRO:CB	2.31	0.59
1:A:141:GLN:CG	1:A:141:GLN:O	2.52	0.58
1:E:70[B]:ARG:HH12	1:F:70:ARG:HH22	1.52	0.58
1:A:138:VAL:HG12	4:A:434:HOH:O	2.04	0.56
1:E:68:PHE:HZ	1:E:91:MET:CG	2.18	0.56
1:F:7:ARG:NH1	1:F:39:ASP:OD2	2.39	0.55
1:D:20:TYR:HB3	1:D:28:ILE:HG23	1.88	0.54
1:C:87:MET:O	1:C:91:MET:HG3	2.07	0.54
1:E:68:PHE:CZ	1:E:91:MET:HG2	2.42	0.54
1:H:135:MET:HE2	1:H:159:TYR:HE2	1.71	0.54
1:E:155:ARG:HD3	1:E:188:GLU:OE2	2.07	0.54
1:C:1:LEU:HD22	1:C:82:ARG:HD2	1.88	0.54
1:A:185:GLU:CB	1:A:186:PRO:CD	2.63	0.54
1:E:277:ARG:HD2	1:G:280:ASP:HB3	1.91	0.53
1:A:292:GLU:HG2	1:A:320:THR:HG22	1.89	0.53
1:A:238[A]:MET:HE3	1:A:240:LEU:HD21	1.90	0.52
1:C:138:VAL:O	1:C:138:VAL:CG2	2.44	0.52
1:C:140:PRO:O	1:C:141:GLN:HG3	2.09	0.52
1:E:5:ARG:HB3	1:E:39:ASP:HB2	1.92	0.52
1:A:139:ALA:CB	1:A:140:PRO:HD3	2.22	0.52
1:F:184:LEU:HD21	1:F:190:ALA:HB2	1.92	0.52
1:A:95:VAL:CG2	1:A:102:LYS:HE3	2.40	0.52
1:A:280:ASP:HB3	1:C:277:ARG:HD2	1.92	0.51
1:B:280:ASP:HB3	1:F:277:ARG:HD2	1.92	0.51
1:A:241:ASP:HA	1:A:263:CYS:HB3	1.91	0.51
1:F:292:GLU:HG2	1:F:320:THR:HG22	1.92	0.51
1:E:80:ASP:OD1	1:E:82:ARG:NH1	2.43	0.51
1:A:95:VAL:HG22	1:A:102:LYS:CE	2.40	0.51
1:F:57:TYR:HE1	1:F:195:ASN:ND2	2.09	0.51
1:B:6:ILE:HG12	1:B:38:ILE:HD13	1.93	0.51
1:A:89[A]:ARG:NH2	4:A:439:HOH:O	2.44	0.50
1:B:122:TRP:CZ3	1:B:123:MET:HG2	2.47	0.50
1:H:185:GLU:HB3	1:H:186:PRO:HD2	1.93	0.49
1:E:146:GLU:HG3	1:E:176:ARG:HH21	1.76	0.49
1:F:57:TYR:CE1	1:F:195:ASN:ND2	2.80	0.49
1:E:138:VAL:HA	1:E:163:GLN:HB3	1.94	0.49
1:C:58:MET:HE1	1:C:265:LYS:HD2	1.94	0.49
1:C:5:ARG:HB3	1:C:39:ASP:HB2	1.95	0.49
1:E:280:ASP:HB3	1:G:277:ARG:HD2	1.94	0.49
1:B:205:ARG:CZ	1:C:189:LYS:HE3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:LEU:HD12	1:G:213:LEU:HD13	1.95	0.49
1:A:91:MET:HE1	1:A:105:PHE:HB3	1.96	0.48
1:C:57:TYR:CE2	1:C:58:MET:HE3	2.48	0.48
1:G:10:LYS:HD2	4:G:520:HOH:O	2.12	0.48
1:F:279:ARG:O	1:F:283:ILE:HG12	2.14	0.48
1:B:135:MET:HG2	1:B:320:THR:HA	1.94	0.48
1:A:117:THR:HB	1:C:117:THR:HB	1.95	0.48
1:F:279:ARG:HG2	1:F:307:PHE:CE1	2.49	0.48
1:G:122:TRP:H	1:G:306:HIS:HD2	1.59	0.48
1:B:10:LYS:HE2	4:B:394:HOH:O	2.14	0.47
1:C:185:GLU:HB2	1:C:186:PRO:HD2	1.96	0.47
1:A:91:MET:HE1	1:A:109:PHE:CE2	2.50	0.47
1:D:125:LEU:HD22	1:D:276[B]:ARG:HG3	1.96	0.47
1:G:205[A]:ARG:NH1	4:G:519:HOH:O	2.47	0.47
1:D:283:ILE:HG21	1:D:312:PRO:HG2	1.97	0.47
1:A:91:MET:HE1	1:A:109:PHE:HE2	1.80	0.46
1:G:243:CYS:O	1:G:249:MET:HG2	2.15	0.46
1:D:89[A]:ARG:HH22	1:H:314:GLU:HB2	1.81	0.46
1:B:265:LYS:HD3	1:B:294:SER:HA	1.98	0.46
1:E:125:LEU:HD22	1:E:276:ARG:HG3	1.98	0.46
1:D:277:ARG:HD2	1:H:280:ASP:HB3	1.98	0.46
1:B:141:GLN:HG3	1:B:165:LYS:HB3	1.97	0.46
1:F:58:MET:HG3	1:F:60:ALA:HB3	1.97	0.46
1:B:196:GLN:HB3	1:B:222:ARG:HA	1.98	0.46
1:F:77:LEU:HB3	1:F:368:LEU:HD13	1.97	0.46
1:B:181:LEU:HD12	1:B:213:LEU:HB3	1.98	0.46
1:B:191:MET:HB3	1:B:216:ILE:HB	1.97	0.46
1:G:140:PRO:HB2	1:G:147:THR:HG22	1.98	0.46
1:G:249:MET:HE3	1:G:249:MET:O	2.16	0.46
1:A:95:VAL:HG22	1:A:102:LYS:HE3	1.98	0.45
1:C:265:LYS:HD3	1:C:294:SER:HA	1.98	0.45
1:D:5:ARG:HB3	1:D:39:ASP:HB2	1.98	0.45
1:D:161:GLN:HG2	1:D:189:LYS:HB2	1.98	0.45
1:B:5:ARG:HB3	1:B:39:ASP:HB2	1.98	0.45
1:A:224:TYR:CG	1:A:249:MET:HE1	2.51	0.45
1:G:122:TRP:H	1:G:306:HIS:CD2	2.34	0.45
1:B:165:LYS:HE2	1:B:195:ASN:HD21	1.81	0.45
1:D:10:LYS:HE3	1:D:32:ARG:HD2	1.98	0.45
1:A:89[A]:ARG:CG	1:A:89[A]:ARG:NH2	2.77	0.45
1:F:48:GLY:HA3	1:F:104:PRO:O	2.17	0.45
1:C:1:LEU:CD2	1:C:82:ARG:HD2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276[A]:ARG:HH22	1:H:276:ARG:NH2	2.14	0.45
1:F:5:ARG:HE	1:F:7:ARG:HD3	1.81	0.44
1:C:55:GLU:HB3	1:D:71:LEU:HD11	1.99	0.44
1:F:264:LEU:HD13	1:F:279:ARG:HB3	1.99	0.44
1:D:142:ARG:HE	1:D:142:ARG:HB3	1.69	0.44
1:E:243:CYS:O	1:E:249:MET:HG2	2.18	0.44
1:D:241:ASP:HA	1:D:263:CYS:HB3	2.00	0.44
1:B:288:PRO:HB3	1:B:317:ILE:HD11	1.98	0.44
1:E:6:ILE:HG12	1:E:38:ILE:HD13	2.00	0.44
1:B:238:MET:HE3	1:B:240:LEU:HD21	1.99	0.44
1:C:306:HIS:HE1	1:C:350:LEU:O	2.01	0.44
1:E:10:LYS:NZ	1:E:34:SER:OG	2.50	0.44
1:D:280:ASP:HB3	1:H:277:ARG:HD2	1.99	0.44
1:E:138:VAL:HG23	1:E:165:LYS:HD3	1.99	0.43
1:C:283:ILE:HG21	1:C:312:PRO:HG2	2.01	0.43
1:E:200:VAL:O	1:E:204:ILE:HG12	2.19	0.43
1:C:20:TYR:HB3	1:C:28:ILE:HG23	2.00	0.43
1:A:224:TYR:CD2	1:A:249:MET:HE1	2.53	0.43
1:H:239:LYS:HE2	1:H:263:CYS:HB2	2.01	0.43
1:B:121:VAL:HG12	1:B:125:LEU:HD22	2.01	0.43
1:A:129:LEU:HB3	1:A:312:PRO:HA	2.01	0.43
1:D:24:ALA:HA	1:D:168:ALA:HA	2.00	0.43
1:D:139:ALA:HB1	1:D:140:PRO:HG3	1.98	0.42
1:H:89[A]:ARG:CG	1:H:89[A]:ARG:HH21	2.32	0.42
1:G:139:ALA:CB	1:G:140:PRO:CA	2.92	0.42
1:B:123:MET:HE1	1:F:82:ARG:HB2	2.01	0.42
1:F:5:ARG:HB3	1:F:39:ASP:HB2	2.01	0.42
1:F:249:MET:O	1:F:249:MET:HE3	2.19	0.42
1:E:241:ASP:HA	1:E:263:CYS:HB3	2.01	0.42
1:A:224:TYR:CG	1:A:249:MET:CE	3.03	0.42
1:G:193:ASP:HA	1:G:218:GLU:HB3	2.01	0.42
1:B:58:MET:HG3	1:B:60:ALA:HB3	2.02	0.42
1:H:137:ARG:HD3	1:H:137:ARG:HA	1.87	0.42
1:G:279:ARG:NH1	4:G:498:HOH:O	2.49	0.42
1:C:239:LYS:HE2	1:C:263:CYS:HB2	2.01	0.42
1:C:57:TYR:CD2	1:C:58:MET:HE3	2.55	0.42
1:C:239:LYS:NZ	4:C:528:HOH:O	2.52	0.42
1:G:241:ASP:HA	1:G:263:CYS:HB3	2.02	0.42
1:G:231:ARG:HD2	1:G:238:MET:HE2	2.02	0.41
4:C:476:HOH:O	1:H:189[A]:LYS:HE2	2.20	0.41
1:B:241:ASP:HA	1:B:263:CYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:ARG:HB2	1:C:143:SER:H	1.70	0.41
1:D:257[A]:ARG:HA	1:D:257[A]:ARG:HD3	1.81	0.41
1:E:196:GLN:HB3	1:E:222:ARG:HA	2.02	0.41
1:B:20:TYR:CD1	1:B:28:ILE:HD12	2.55	0.41
1:H:48:GLY:HA3	1:H:104:PRO:O	2.21	0.41
1:D:257[A]:ARG:HG2	1:D:257[A]:ARG:NH2	2.31	0.41
1:D:189:LYS:HZ3	1:G:205[B]:ARG:HH12	1.69	0.41
1:C:243:CYS:O	1:C:249:MET:HG2	2.21	0.41
1:A:195[B]:ASN:ND2	1:A:242:GLU:OE2	2.54	0.41
1:C:257[A]:ARG:HD2	1:C:257[A]:ARG:HA	1.85	0.41
1:G:70:ARG:HH22	1:H:70:ARG:HH22	1.67	0.41
1:A:239:LYS:NZ	4:A:508:HOH:O	2.54	0.41
1:E:265:LYS:HD3	1:E:294:SER:HA	2.03	0.41
1:A:277:ARG:HD2	1:C:280:ASP:HB3	2.03	0.41
1:H:243:CYS:O	1:H:249:MET:HG2	2.21	0.41
1:A:87:MET:O	1:A:91:MET:HG3	2.21	0.41
1:C:38:ILE:HD13	1:C:109:PHE:CE1	2.56	0.40
1:F:5:ARG:NE	1:F:7:ARG:HD3	2.36	0.40
1:B:163:GLN:OE1	1:B:165:LYS:HE3	2.22	0.40

There are no symmetry-related clashes.

## 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	377/379 (100%)	363 (96%)	13 (3%)	1 (0%)	46	41
1	B	371/379 (98%)	358 (96%)	13 (4%)	0	100	100
1	C	373/379 (98%)	357 (96%)	12 (3%)	4 (1%)	17	9
1	D	378/379 (100%)	362 (96%)	13 (3%)	3 (1%)	24	15
1	E	371/379 (98%)	356 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	370/379 (98%)	353 (95%)	15 (4%)	2 (0%)	34	26
1	G	359/379 (95%)	346 (96%)	12 (3%)	1 (0%)	46	41
1	H	373/379 (98%)	361 (97%)	12 (3%)	0	100	100
All	All	2972/3032 (98%)	2856 (96%)	105 (4%)	11 (0%)	46	33

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	140	PRO
1	C	141	GLN
1	D	140	PRO
1	G	139	ALA
1	A	140	PRO
1	C	186	PRO
1	D	186[A]	PRO
1	D	186[B]	PRO
1	C	138	VAL
1	F	140	PRO
1	F	186	PRO

### 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	298/297 (100%)	283 (95%)	15 (5%)	30	24
1	B	292/297 (98%)	265 (91%)	27 (9%)	11	6
1	C	294/297 (99%)	278 (95%)	16 (5%)	27	21
1	D	298/297 (100%)	281 (94%)	17 (6%)	25	19
1	E	293/297 (99%)	273 (93%)	20 (7%)	20	13
1	F	291/297 (98%)	274 (94%)	17 (6%)	25	19
1	G	287/297 (97%)	273 (95%)	14 (5%)	31	25
1	H	294/297 (99%)	280 (95%)	14 (5%)	31	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2347/2376 (99%)	2207 (94%)	140 (6%)	25	17

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	29	THR
1	A	32	ARG
1	A	75[A]	GLN
1	A	75[B]	GLN
1	A	89[A]	ARG
1	A	89[B]	ARG
1	A	125	LEU
1	A	141	GLN
1	A	144	GLU
1	A	183	LEU
1	A	276	ARG
1	A	323	MET
1	A	332	LEU
1	A	342	LEU
1	B	32	ARG
1	B	66	ASP
1	B	71	LEU
1	B	79	GLN
1	B	95	VAL
1	B	125	LEU
1	B	135	MET
1	B	137	ARG
1	B	138	VAL
1	B	142	ARG
1	B	144	GLU
1	B	147	THR
1	B	155	ARG
1	B	165	LYS
1	B	183	LEU
1	B	184	LEU
1	B	189	LYS
1	B	200	VAL
1	B	206	LEU
1	B	222	ARG
1	B	276	ARG
1	B	283	ILE

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Mol	Chain	Res	Type
1	B	323	MET
1	B	332	LEU
1	B	342	LEU
1	B	347	THR
1	B	368	LEU
1	C	28	ILE
1	C	32	ARG
1	C	66	ASP
1	C	71	LEU
1	C	153	ARG
1	C	165	LYS
1	C	184	LEU
1	C	189	LYS
1	C	191	MET
1	C	252[A]	ARG
1	C	252[B]	ARG
1	C	276[A]	ARG
1	C	276[B]	ARG
1	C	323	MET
1	C	332	LEU
1	C	342	LEU
1	D	28	ILE
1	D	32	ARG
1	D	66	ASP
1	D	71	LEU
1	D	95	VAL
1	D	138	VAL
1	D	141	GLN
1	D	142	ARG
1	D	143	SER
1	D	160	ARG
1	D	165	LYS
1	D	183	LEU
1	D	191	MET
1	D	257[A]	ARG
1	D	257[B]	ARG
1	D	323	MET
1	D	332	LEU
1	E	30	VAL
1	E	32	ARG
1	E	38	ILE
1	E	66	ASP

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Mol	Chain	Res	Type
1	E	71	LEU
1	E	82	ARG
1	E	91	MET
1	E	95	VAL
1	E	137	ARG
1	E	147	THR
1	E	148	ARG
1	E	165	LYS
1	E	172	SER
1	E	200	VAL
1	E	252[A]	ARG
1	E	252[B]	ARG
1	E	276	ARG
1	E	283	ILE
1	E	323	MET
1	E	337	VAL
1	F	7	ARG
1	F	16	VAL
1	F	32	ARG
1	F	66	ASP
1	F	71	LEU
1	F	79	GLN
1	F	82	ARG
1	F	95	VAL
1	F	125	LEU
1	F	144	GLU
1	F	184	LEU
1	F	191	MET
1	F	276	ARG
1	F	279	ARG
1	F	323	MET
1	F	332	LEU
1	F	342	LEU
1	G	17	ASP
1	G	32	ARG
1	G	58	MET
1	G	79	GLN
1	G	95	VAL
1	G	125	LEU
1	G	144	GLU
1	G	165	LYS
1	G	184	LEU

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Mol	Chain	Res	Type
1	G	191	MET
1	G	276	ARG
1	G	323	MET
1	G	332	LEU
1	G	342	LEU
1	H	32	ARG
1	H	66	ASP
1	H	71	LEU
1	H	82	ARG
1	H	89[A]	ARG
1	H	89[B]	ARG
1	H	125	LEU
1	H	189[A]	LYS
1	H	189[B]	LYS
1	H	276	ARG
1	H	283	ILE
1	H	323	MET
1	H	332	LEU
1	H	337	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	306	HIS
1	B	79	GLN
1	B	195	ASN
1	B	357	ASN
1	C	306	HIS
1	D	196	GLN
1	D	306	HIS
1	D	357	ASN
1	E	75	GLN
1	E	79	GLN
1	E	306	HIS
1	F	75	GLN
1	F	79	GLN
1	F	195	ASN
1	F	306	HIS
1	G	306	HIS
1	G	357	ASN
1	H	141	GLN

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Mol	Chain	Res	Type
1	H	338	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	A	379	-	5,5,5	0.34	0	5,5,5	0.43	0
3	GOL	A	380	-	5,5,5	0.40	0	5,5,5	0.33	0
3	GOL	C	379	-	5,5,5	0.31	0	5,5,5	0.20	0
3	GOL	D	379	-	5,5,5	0.35	0	5,5,5	0.80	0
3	GOL	F	379	-	5,5,5	0.36	0	5,5,5	0.54	0
3	GOL	G	379	-	5,5,5	0.44	0	5,5,5	0.62	0
3	GOL	H	379	-	5,5,5	0.39	0	5,5,5	0.44	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	A	379	-	-	0/4/4/4	0/0/0/0
3	GOL	A	380	-	-	0/4/4/4	0/0/0/0
3	GOL	C	379	-	-	0/4/4/4	0/0/0/0
3	GOL	D	379	-	-	0/4/4/4	0/0/0/0
3	GOL	F	379	-	-	0/4/4/4	0/0/0/0
3	GOL	G	379	-	-	0/4/4/4	0/0/0/0
3	GOL	H	379	-	-	0/4/4/4	0/0/0/0

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	369/379 (97%)	-0.47	7 (1%) 70 70	14, 24, 54, 85	0
1	B	369/379 (97%)	-0.46	3 (0%) 87 88	15, 25, 44, 73	0
1	C	369/379 (97%)	-0.41	7 (1%) 70 70	12, 24, 56, 91	0
1	D	369/379 (97%)	-0.36	7 (1%) 70 70	15, 25, 53, 98	0
1	E	369/379 (97%)	-0.25	13 (3%) 48 49	11, 24, 65, 109	0
1	F	369/379 (97%)	-0.06	14 (3%) 44 45	10, 25, 59, 86	0
1	G	360/379 (94%)	-0.49	1 (0%) 94 94	14, 25, 51, 69	0
1	H	369/379 (97%)	-0.34	13 (3%) 48 49	8, 24, 67, 111	0
All	All	2943/3032 (97%)	-0.35	65 (2%) 65 66	8, 25, 57, 111	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	25	GLY	8.6
1	E	28	ILE	6.9
1	E	24	ALA	6.8
1	F	27	ALA	6.2
1	E	20	TYR	6.1
1	H	27	ALA	6.1
1	E	19	SER	6.0
1	E	21	GLY	5.9
1	D	28	ILE	5.7
1	E	27	ALA	5.7
1	E	138	VAL	5.0
1	F	16	VAL	4.8
1	A	25	GLY	4.8
1	H	140	PRO	4.5
1	H	28	ILE	4.4
1	D	24	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	19	SER	3.9
1	E	145	ALA	3.8
1	C	140	PRO	3.8
1	D	18	GLY	3.7
1	A	28	ILE	3.7
1	F	28	ILE	3.6
1	D	22	TRP	3.5
1	D	20	TYR	3.5
1	B	19	SER	3.2
1	A	24	ALA	3.1
1	C	20	TYR	3.0
1	H	24	ALA	3.0
1	D	57	TYR	3.0
1	F	24	ALA	3.0
1	F	15	TYR	3.0
1	E	23	GLY	2.9
1	H	142	ARG	2.9
1	F	20	TYR	2.9
1	E	26	ASN	2.9
1	B	18	GLY	2.9
1	H	139	ALA	2.9
1	H	20	TYR	2.8
1	D	19	SER	2.7
1	G	57	TYR	2.7
1	C	149	ALA	2.5
1	F	145	ALA	2.5
1	C	19	SER	2.5
1	A	20	TYR	2.5
1	H	151	LEU	2.5
1	H	26	ASN	2.5
1	C	151	LEU	2.5
1	F	17	ASP	2.4
1	E	17	ASP	2.4
1	F	139	ALA	2.4
1	A	21	GLY	2.4
1	F	57	TYR	2.4
1	H	141	GLN	2.3
1	A	139	ALA	2.3
1	E	22	TRP	2.3
1	F	21	GLY	2.2
1	F	25	GLY	2.2
1	A	57	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	22	TRP	2.2
1	H	144	GLU	2.2
1	C	212	ASP	2.1
1	H	25	GLY	2.1
1	B	24	ALA	2.1
1	H	23	GLY	2.0
1	C	28	ILE	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 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	A	380	6/6	0.97	0.22	8.69	20,34,59,92	0
3	GOL	G	379	6/6	0.95	0.14	6.76	26,34,43,58	0
3	GOL	H	379	6/6	0.96	0.24	2.33	25,47,62,71	0
3	GOL	C	379	6/6	0.94	0.15	2.17	21,51,64,71	0
3	GOL	A	379	6/6	0.95	0.18	1.21	31,59,64,64	0
3	GOL	F	379	6/6	0.96	0.18	1.17	21,43,55,59	0
3	GOL	D	379	6/6	0.94	0.14	0.24	20,43,49,54	0
2	MG	G	378	1/1	0.99	0.06	-1.16	19,19,19,19	0
2	MG	D	378	1/1	0.97	0.04	-1.50	20,20,20,20	0
2	MG	A	378	1/1	0.98	0.03	-1.66	23,23,23,23	0
2	MG	F	378	1/1	0.98	0.03	-1.75	30,30,30,30	0
2	MG	H	378	1/1	0.98	0.04	-1.82	22,22,22,22	0
2	MG	E	378	1/1	0.98	0.04	-2.11	24,24,24,24	0
2	MG	C	378	1/1	0.98	0.03	-3.51	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	B	378	1/1	0.99	0.02	-3.87	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.