Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:29 PM GMT

PDB ID	:	3RCY
Title	:	CRYSTAL STRUCTURE OF Mandelate racemase/muconate lactonizing enzyme-like protein from Roseovarius sp. TM1035
Authors	:	Malashkevich, V.N.; Toro, R.; Seidel, R.; Garrett, S.; Foti, R.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2011-03-31
Resolution	:	1.99 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

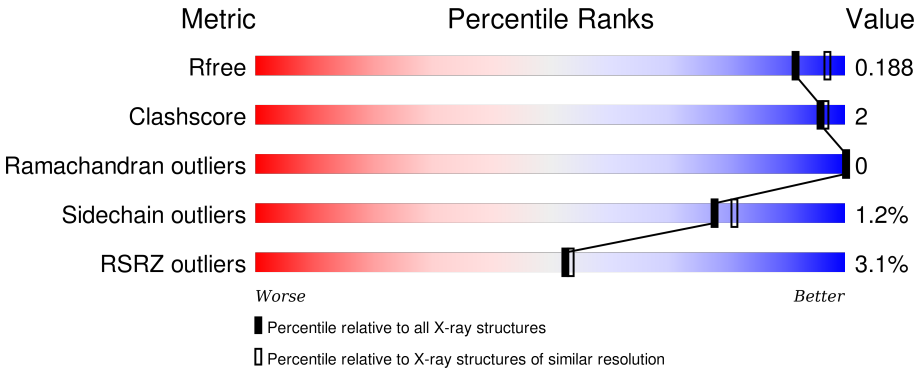
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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 >=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 <=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	433	3% 88% · 9%
1	B	433	3% 87% · 9%
1	C	433	2% 88% · 9%
1	D	433	2% 89% · 9%
1	E	433	3% 87% 5% 9%

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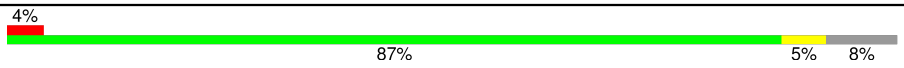
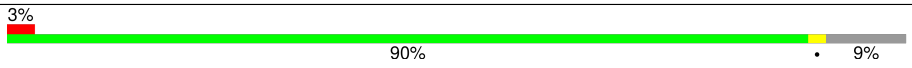
Mol	Chain	Length	Quality of chain
1	F	433	
1	G	433	
1	H	433	

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	D	433	-	-	-	X
3	GOL	E	501	-	-	-	X
3	GOL	F	501	-	-	-	X
3	GOL	G	501	-	-	X	X
4	RIB	A	433	X	-	-	X
4	RIB	A	505	X	-	-	X
4	RIB	B	505	X	-	-	X
4	RIB	D	505	X	-	-	X
4	RIB	E	505	X	-	-	X
4	RIB	G	505	X	-	-	X
4	RIB	H	433	X	-	-	X
4	RIB	H	505	X	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26806 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-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	4	0
			3042	1945	526	552	19			
1	B	395	Total	C	N	O	S	0	3	0
			3024	1934	522	549	19			
1	C	396	Total	C	N	O	S	0	6	0
			3044	1947	520	558	19			
1	D	396	Total	C	N	O	S	0	5	0
			3046	1948	523	556	19			
1	E	395	Total	C	N	O	S	0	3	0
			3027	1936	522	550	19			
1	F	397	Total	C	N	O	S	0	3	0
			3041	1944	524	554	19			
1	G	396	Total	C	N	O	S	0	7	0
			3062	1958	529	556	19			
1	H	395	Total	C	N	O	S	0	2	0
			3021	1932	522	548	19			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP A6DZ31
A	1	VAL	-	EXPRESSION TAG	UNP A6DZ31
A	411	ALA	-	EXPRESSION TAG	UNP A6DZ31
A	412	GLU	-	EXPRESSION TAG	UNP A6DZ31
A	413	ASN	-	EXPRESSION TAG	UNP A6DZ31
A	414	LEU	-	EXPRESSION TAG	UNP A6DZ31
A	415	TYR	-	EXPRESSION TAG	UNP A6DZ31
A	416	PHE	-	EXPRESSION TAG	UNP A6DZ31
A	417	GLN	-	EXPRESSION TAG	UNP A6DZ31
A	418	SER	-	EXPRESSION TAG	UNP A6DZ31
A	419	HIS	-	EXPRESSION TAG	UNP A6DZ31
A	420	HIS	-	EXPRESSION TAG	UNP A6DZ31
A	421	HIS	-	EXPRESSION TAG	UNP A6DZ31

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Chain	Residue	Modelled	Actual	Comment	Reference
A	422	HIS	-	EXPRESSION TAG	UNP A6DZ31
A	423	HIS	-	EXPRESSION TAG	UNP A6DZ31
A	424	HIS	-	EXPRESSION TAG	UNP A6DZ31
A	425	TRP	-	EXPRESSION TAG	UNP A6DZ31
A	426	SER	-	EXPRESSION TAG	UNP A6DZ31
A	427	HIS	-	EXPRESSION TAG	UNP A6DZ31
A	428	PRO	-	EXPRESSION TAG	UNP A6DZ31
A	429	GLN	-	EXPRESSION TAG	UNP A6DZ31
A	430	PHE	-	EXPRESSION TAG	UNP A6DZ31
A	431	GLU	-	EXPRESSION TAG	UNP A6DZ31
A	432	LYS	-	EXPRESSION TAG	UNP A6DZ31
B	0	MET	-	EXPRESSION TAG	UNP A6DZ31
B	1	VAL	-	EXPRESSION TAG	UNP A6DZ31
B	411	ALA	-	EXPRESSION TAG	UNP A6DZ31
B	412	GLU	-	EXPRESSION TAG	UNP A6DZ31
B	413	ASN	-	EXPRESSION TAG	UNP A6DZ31
B	414	LEU	-	EXPRESSION TAG	UNP A6DZ31
B	415	TYR	-	EXPRESSION TAG	UNP A6DZ31
B	416	PHE	-	EXPRESSION TAG	UNP A6DZ31
B	417	GLN	-	EXPRESSION TAG	UNP A6DZ31
B	418	SER	-	EXPRESSION TAG	UNP A6DZ31
B	419	HIS	-	EXPRESSION TAG	UNP A6DZ31
B	420	HIS	-	EXPRESSION TAG	UNP A6DZ31
B	421	HIS	-	EXPRESSION TAG	UNP A6DZ31
B	422	HIS	-	EXPRESSION TAG	UNP A6DZ31
B	423	HIS	-	EXPRESSION TAG	UNP A6DZ31
B	424	HIS	-	EXPRESSION TAG	UNP A6DZ31
B	425	TRP	-	EXPRESSION TAG	UNP A6DZ31
B	426	SER	-	EXPRESSION TAG	UNP A6DZ31
B	427	HIS	-	EXPRESSION TAG	UNP A6DZ31
B	428	PRO	-	EXPRESSION TAG	UNP A6DZ31
B	429	GLN	-	EXPRESSION TAG	UNP A6DZ31
B	430	PHE	-	EXPRESSION TAG	UNP A6DZ31
B	431	GLU	-	EXPRESSION TAG	UNP A6DZ31
B	432	LYS	-	EXPRESSION TAG	UNP A6DZ31
C	0	MET	-	EXPRESSION TAG	UNP A6DZ31
C	1	VAL	-	EXPRESSION TAG	UNP A6DZ31
C	411	ALA	-	EXPRESSION TAG	UNP A6DZ31
C	412	GLU	-	EXPRESSION TAG	UNP A6DZ31
C	413	ASN	-	EXPRESSION TAG	UNP A6DZ31
C	414	LEU	-	EXPRESSION TAG	UNP A6DZ31
C	415	TYR	-	EXPRESSION TAG	UNP A6DZ31

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Chain	Residue	Modelled	Actual	Comment	Reference
C	416	PHE	-	EXPRESSION TAG	UNP A6DZ31
C	417	GLN	-	EXPRESSION TAG	UNP A6DZ31
C	418	SER	-	EXPRESSION TAG	UNP A6DZ31
C	419	HIS	-	EXPRESSION TAG	UNP A6DZ31
C	420	HIS	-	EXPRESSION TAG	UNP A6DZ31
C	421	HIS	-	EXPRESSION TAG	UNP A6DZ31
C	422	HIS	-	EXPRESSION TAG	UNP A6DZ31
C	423	HIS	-	EXPRESSION TAG	UNP A6DZ31
C	424	HIS	-	EXPRESSION TAG	UNP A6DZ31
C	425	TRP	-	EXPRESSION TAG	UNP A6DZ31
C	426	SER	-	EXPRESSION TAG	UNP A6DZ31
C	427	HIS	-	EXPRESSION TAG	UNP A6DZ31
C	428	PRO	-	EXPRESSION TAG	UNP A6DZ31
C	429	GLN	-	EXPRESSION TAG	UNP A6DZ31
C	430	PHE	-	EXPRESSION TAG	UNP A6DZ31
C	431	GLU	-	EXPRESSION TAG	UNP A6DZ31
C	432	LYS	-	EXPRESSION TAG	UNP A6DZ31
D	0	MET	-	EXPRESSION TAG	UNP A6DZ31
D	1	VAL	-	EXPRESSION TAG	UNP A6DZ31
D	411	ALA	-	EXPRESSION TAG	UNP A6DZ31
D	412	GLU	-	EXPRESSION TAG	UNP A6DZ31
D	413	ASN	-	EXPRESSION TAG	UNP A6DZ31
D	414	LEU	-	EXPRESSION TAG	UNP A6DZ31
D	415	TYR	-	EXPRESSION TAG	UNP A6DZ31
D	416	PHE	-	EXPRESSION TAG	UNP A6DZ31
D	417	GLN	-	EXPRESSION TAG	UNP A6DZ31
D	418	SER	-	EXPRESSION TAG	UNP A6DZ31
D	419	HIS	-	EXPRESSION TAG	UNP A6DZ31
D	420	HIS	-	EXPRESSION TAG	UNP A6DZ31
D	421	HIS	-	EXPRESSION TAG	UNP A6DZ31
D	422	HIS	-	EXPRESSION TAG	UNP A6DZ31
D	423	HIS	-	EXPRESSION TAG	UNP A6DZ31
D	424	HIS	-	EXPRESSION TAG	UNP A6DZ31
D	425	TRP	-	EXPRESSION TAG	UNP A6DZ31
D	426	SER	-	EXPRESSION TAG	UNP A6DZ31
D	427	HIS	-	EXPRESSION TAG	UNP A6DZ31
D	428	PRO	-	EXPRESSION TAG	UNP A6DZ31
D	429	GLN	-	EXPRESSION TAG	UNP A6DZ31
D	430	PHE	-	EXPRESSION TAG	UNP A6DZ31
D	431	GLU	-	EXPRESSION TAG	UNP A6DZ31
D	432	LYS	-	EXPRESSION TAG	UNP A6DZ31
E	0	MET	-	EXPRESSION TAG	UNP A6DZ31

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1	VAL	-	EXPRESSION TAG	UNP A6DZ31
E	411	ALA	-	EXPRESSION TAG	UNP A6DZ31
E	412	GLU	-	EXPRESSION TAG	UNP A6DZ31
E	413	ASN	-	EXPRESSION TAG	UNP A6DZ31
E	414	LEU	-	EXPRESSION TAG	UNP A6DZ31
E	415	TYR	-	EXPRESSION TAG	UNP A6DZ31
E	416	PHE	-	EXPRESSION TAG	UNP A6DZ31
E	417	GLN	-	EXPRESSION TAG	UNP A6DZ31
E	418	SER	-	EXPRESSION TAG	UNP A6DZ31
E	419	HIS	-	EXPRESSION TAG	UNP A6DZ31
E	420	HIS	-	EXPRESSION TAG	UNP A6DZ31
E	421	HIS	-	EXPRESSION TAG	UNP A6DZ31
E	422	HIS	-	EXPRESSION TAG	UNP A6DZ31
E	423	HIS	-	EXPRESSION TAG	UNP A6DZ31
E	424	HIS	-	EXPRESSION TAG	UNP A6DZ31
E	425	TRP	-	EXPRESSION TAG	UNP A6DZ31
E	426	SER	-	EXPRESSION TAG	UNP A6DZ31
E	427	HIS	-	EXPRESSION TAG	UNP A6DZ31
E	428	PRO	-	EXPRESSION TAG	UNP A6DZ31
E	429	GLN	-	EXPRESSION TAG	UNP A6DZ31
E	430	PHE	-	EXPRESSION TAG	UNP A6DZ31
E	431	GLU	-	EXPRESSION TAG	UNP A6DZ31
E	432	LYS	-	EXPRESSION TAG	UNP A6DZ31
F	0	MET	-	EXPRESSION TAG	UNP A6DZ31
F	1	VAL	-	EXPRESSION TAG	UNP A6DZ31
F	411	ALA	-	EXPRESSION TAG	UNP A6DZ31
F	412	GLU	-	EXPRESSION TAG	UNP A6DZ31
F	413	ASN	-	EXPRESSION TAG	UNP A6DZ31
F	414	LEU	-	EXPRESSION TAG	UNP A6DZ31
F	415	TYR	-	EXPRESSION TAG	UNP A6DZ31
F	416	PHE	-	EXPRESSION TAG	UNP A6DZ31
F	417	GLN	-	EXPRESSION TAG	UNP A6DZ31
F	418	SER	-	EXPRESSION TAG	UNP A6DZ31
F	419	HIS	-	EXPRESSION TAG	UNP A6DZ31
F	420	HIS	-	EXPRESSION TAG	UNP A6DZ31
F	421	HIS	-	EXPRESSION TAG	UNP A6DZ31
F	422	HIS	-	EXPRESSION TAG	UNP A6DZ31
F	423	HIS	-	EXPRESSION TAG	UNP A6DZ31
F	424	HIS	-	EXPRESSION TAG	UNP A6DZ31
F	425	TRP	-	EXPRESSION TAG	UNP A6DZ31
F	426	SER	-	EXPRESSION TAG	UNP A6DZ31
F	427	HIS	-	EXPRESSION TAG	UNP A6DZ31

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Chain	Residue	Modelled	Actual	Comment	Reference
F	428	PRO	-	EXPRESSION TAG	UNP A6DZ31
F	429	GLN	-	EXPRESSION TAG	UNP A6DZ31
F	430	PHE	-	EXPRESSION TAG	UNP A6DZ31
F	431	GLU	-	EXPRESSION TAG	UNP A6DZ31
F	432	LYS	-	EXPRESSION TAG	UNP A6DZ31
G	0	MET	-	EXPRESSION TAG	UNP A6DZ31
G	1	VAL	-	EXPRESSION TAG	UNP A6DZ31
G	411	ALA	-	EXPRESSION TAG	UNP A6DZ31
G	412	GLU	-	EXPRESSION TAG	UNP A6DZ31
G	413	ASN	-	EXPRESSION TAG	UNP A6DZ31
G	414	LEU	-	EXPRESSION TAG	UNP A6DZ31
G	415	TYR	-	EXPRESSION TAG	UNP A6DZ31
G	416	PHE	-	EXPRESSION TAG	UNP A6DZ31
G	417	GLN	-	EXPRESSION TAG	UNP A6DZ31
G	418	SER	-	EXPRESSION TAG	UNP A6DZ31
G	419	HIS	-	EXPRESSION TAG	UNP A6DZ31
G	420	HIS	-	EXPRESSION TAG	UNP A6DZ31
G	421	HIS	-	EXPRESSION TAG	UNP A6DZ31
G	422	HIS	-	EXPRESSION TAG	UNP A6DZ31
G	423	HIS	-	EXPRESSION TAG	UNP A6DZ31
G	424	HIS	-	EXPRESSION TAG	UNP A6DZ31
G	425	TRP	-	EXPRESSION TAG	UNP A6DZ31
G	426	SER	-	EXPRESSION TAG	UNP A6DZ31
G	427	HIS	-	EXPRESSION TAG	UNP A6DZ31
G	428	PRO	-	EXPRESSION TAG	UNP A6DZ31
G	429	GLN	-	EXPRESSION TAG	UNP A6DZ31
G	430	PHE	-	EXPRESSION TAG	UNP A6DZ31
G	431	GLU	-	EXPRESSION TAG	UNP A6DZ31
G	432	LYS	-	EXPRESSION TAG	UNP A6DZ31
H	0	MET	-	EXPRESSION TAG	UNP A6DZ31
H	1	VAL	-	EXPRESSION TAG	UNP A6DZ31
H	411	ALA	-	EXPRESSION TAG	UNP A6DZ31
H	412	GLU	-	EXPRESSION TAG	UNP A6DZ31
H	413	ASN	-	EXPRESSION TAG	UNP A6DZ31
H	414	LEU	-	EXPRESSION TAG	UNP A6DZ31
H	415	TYR	-	EXPRESSION TAG	UNP A6DZ31
H	416	PHE	-	EXPRESSION TAG	UNP A6DZ31
H	417	GLN	-	EXPRESSION TAG	UNP A6DZ31
H	418	SER	-	EXPRESSION TAG	UNP A6DZ31
H	419	HIS	-	EXPRESSION TAG	UNP A6DZ31
H	420	HIS	-	EXPRESSION TAG	UNP A6DZ31
H	421	HIS	-	EXPRESSION TAG	UNP A6DZ31

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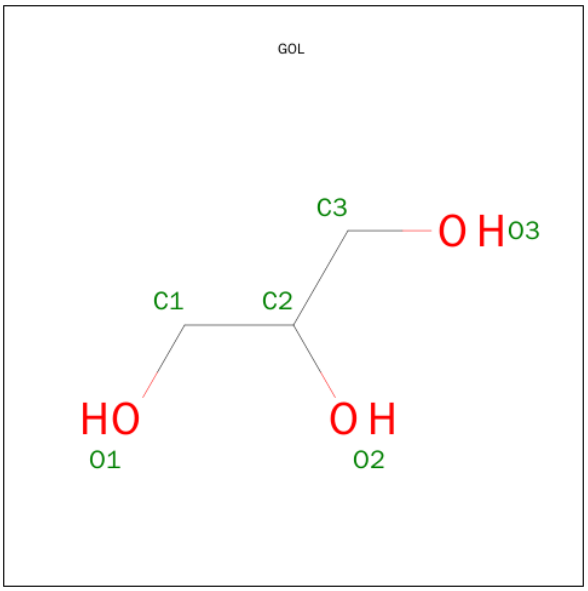
Chain	Residue	Modelled	Actual	Comment	Reference
H	422	HIS	-	EXPRESSION TAG	UNP A6DZ31
H	423	HIS	-	EXPRESSION TAG	UNP A6DZ31
H	424	HIS	-	EXPRESSION TAG	UNP A6DZ31
H	425	TRP	-	EXPRESSION TAG	UNP A6DZ31
H	426	SER	-	EXPRESSION TAG	UNP A6DZ31
H	427	HIS	-	EXPRESSION TAG	UNP A6DZ31
H	428	PRO	-	EXPRESSION TAG	UNP A6DZ31
H	429	GLN	-	EXPRESSION TAG	UNP A6DZ31
H	430	PHE	-	EXPRESSION TAG	UNP A6DZ31
H	431	GLU	-	EXPRESSION TAG	UNP A6DZ31
H	432	LYS	-	EXPRESSION TAG	UNP A6DZ31

- 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
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	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 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0

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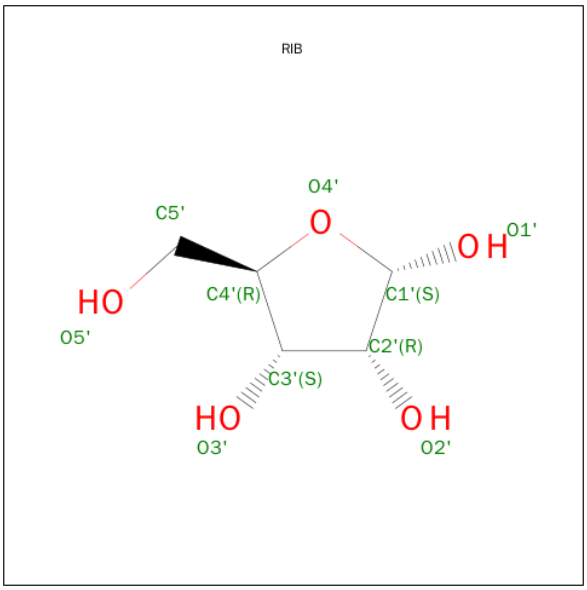
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0

- Molecule 4 is SUGAR (RIBOSE) (three-letter code: RIB) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 5 5	0	0
4	A	1	Total C O 10 5 5	0	0
4	B	1	Total C O 10 5 5	0	0
4	D	1	Total C O 10 5 5	0	0
4	E	1	Total C O 10 5 5	0	0
4	G	1	Total C O 10 5 5	0	0
4	H	1	Total C O 10 5 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is water.

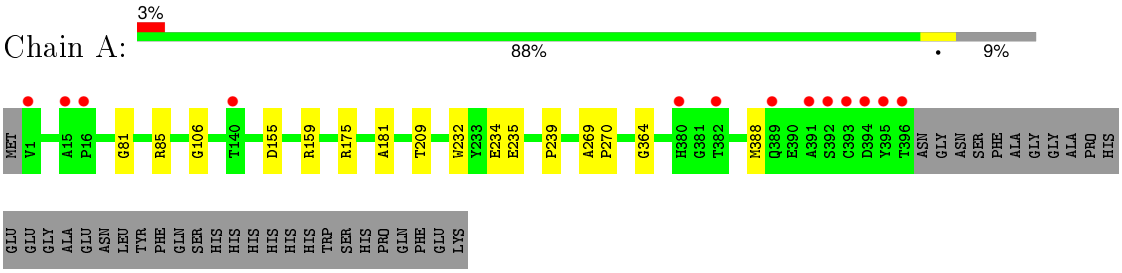
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	305	Total	O	0	0
			305	305		
5	B	284	Total	O	0	0
			284	284		
5	C	307	Total	O	0	0
			307	307		
5	D	333	Total	O	0	0
			333	333		
5	E	290	Total	O	0	0
			290	290		
5	F	269	Total	O	0	0
			269	269		
5	G	281	Total	O	0	0
			281	281		
5	H	234	Total	O	0	0
			234	234		

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.

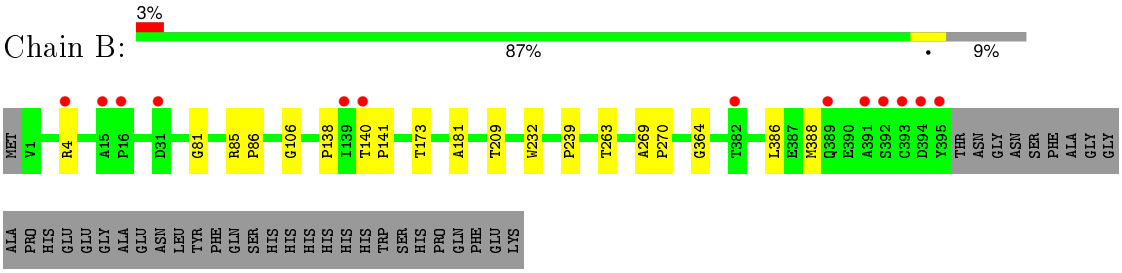
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme-like protein

Chain A:



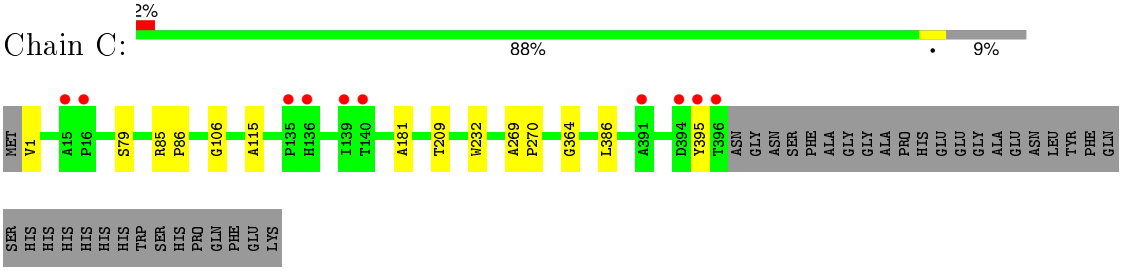
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme-like protein

Chain B:



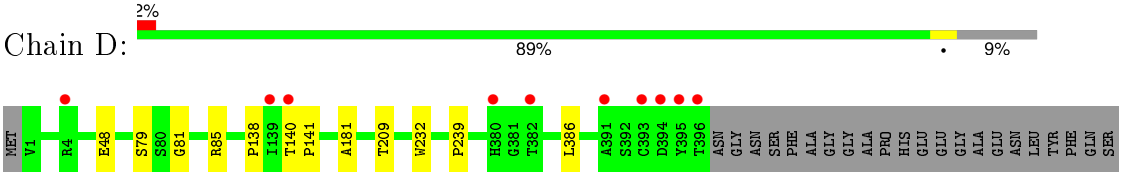
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme-like protein

Chain C:



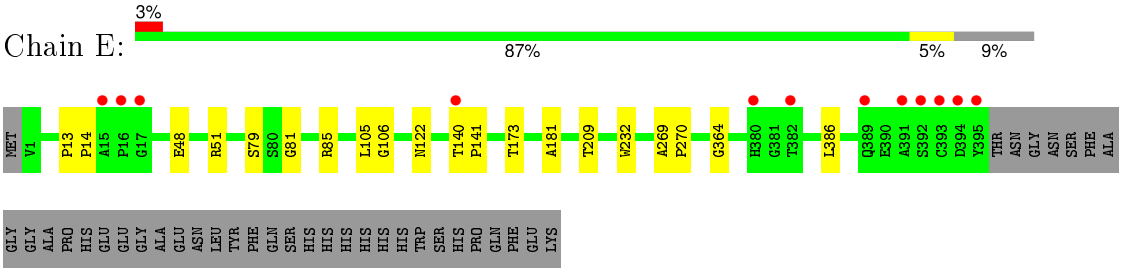
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme-like protein

Chain D:



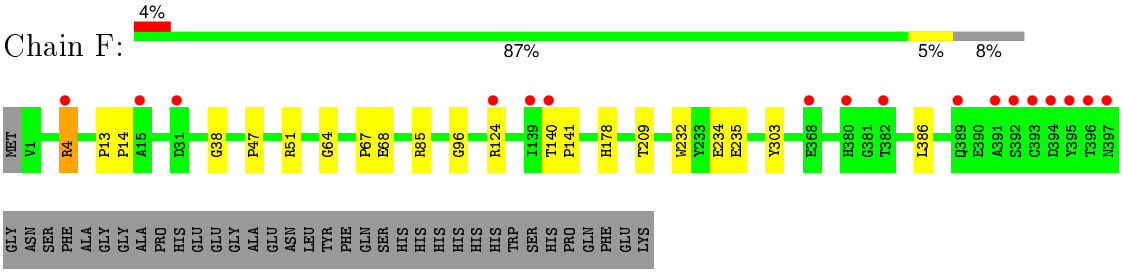
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme-like protein

Chain E:



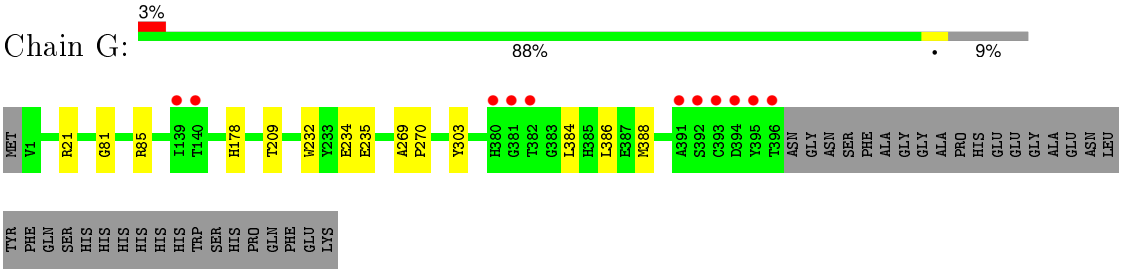
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme-like protein

Chain F:



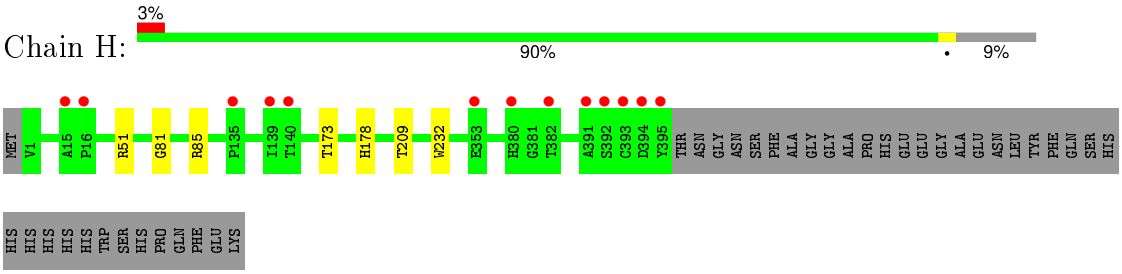
• Molecule 1: Mandelate racemase/muconate lactonizing enzyme-like protein

Chain G:



• Molecule 1: Mandelate racemase/muconate lactonizing enzyme-like protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	144.98Å 162.14Å 141.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.99 20.00 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.99) 99.7 (20.00-1.99)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.147 , 0.181 0.154 , 0.188	Depositor DCC
R_{free} test set	11321 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 46.7	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 225935 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26806	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, RIB

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	0.46	0/3139	0.55	0/4280
1	B	0.44	0/3118	0.54	0/4252
1	C	0.44	1/3147 (0.0%)	0.54	0/4292
1	D	0.44	0/3146	0.53	0/4290
1	E	0.42	0/3121	0.54	0/4256
1	F	0.41	0/3134	0.53	0/4272
1	G	0.41	0/3168	0.52	0/4318
1	H	0.40	0/3112	0.51	0/4244
All	All	0.43	1/25085 (0.0%)	0.53	0/34204

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	VAL	C-N	-5.03	1.22	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3042	0	3005	11	0
1	B	3024	0	2984	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3044	0	3001	9	0
1	D	3046	0	3004	8	0
1	E	3027	0	2985	15	0
1	F	3041	0	2996	15	0
1	G	3062	0	3030	11	0
1	H	3021	0	2979	4	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	2	0
3	B	18	0	24	2	0
3	C	12	0	16	5	0
3	D	18	0	24	2	0
3	E	12	0	16	2	0
3	F	6	0	8	0	0
3	G	24	0	32	8	0
3	H	6	0	8	0	0
4	A	20	0	20	2	0
4	B	10	0	10	1	0
4	D	10	0	10	1	0
4	E	10	0	10	0	0
4	G	10	0	10	0	0
4	H	20	0	20	0	0
5	A	305	0	0	1	0
5	B	284	0	0	0	0
5	C	307	0	0	0	0
5	D	333	0	0	0	0
5	E	290	0	0	0	0
5	F	269	0	0	3	0
5	G	281	0	0	2	0
5	H	234	0	0	4	0
All	All	26806	0	24208	75	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 2.

All (75) 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:G:303:TYR:HE1	3:G:501:GOL:H2	1.33	0.90
1:A:239:PRO:O	4:A:433:RIB:H2'	1.81	0.81
1:C:181:ALA:HB1	3:C:502:GOL:H31	1.69	0.74
4:A:433:RIB:O3'	1:C:86:PRO:HD2	1.88	0.73
1:G:303:TYR:CE1	3:G:501:GOL:H2	2.23	0.72
1:B:181:ALA:HB1	3:B:502:GOL:H12	1.72	0.72
1:E:181:ALA:HB1	3:E:502:GOL:H12	1.73	0.70
1:A:159[A]:ARG:NH1	5:A:2793:HOH:O	2.24	0.69
1:F:67:PRO:C	1:F:68:GLU:CA	2.62	0.67
1:A:175[B]:ARG:NH2	1:E:122:ASN:OD1	2.30	0.65
1:G:303:TYR:OH	3:G:501:GOL:H11	1.98	0.62
1:A:181:ALA:HB1	3:A:502:GOL:H12	1.81	0.62
1:D:181:ALA:HB1	3:D:502:GOL:H12	1.81	0.62
1:D:48[A]:GLU:OE2	1:D:48[A]:GLU:HA	2.02	0.59
1:F:303:TYR:OH	3:G:501:GOL:H12	2.02	0.58
1:E:48[A]:GLU:OE1	1:E:51[A]:ARG:HD2	2.04	0.56
1:H:178:HIS:HD2	5:H:448:HOH:O	1.85	0.56
1:G:178:HIS:HD2	5:G:2625:HOH:O	1.89	0.54
1:F:47:PRO:O	1:F:51:ARG:HG3	2.08	0.54
1:F:140:THR:HB	1:F:141:PRO:HD3	1.90	0.53
1:A:269:ALA:HB3	1:A:270:PRO:HD3	1.90	0.52
1:F:386:LEU:O	1:H:81:GLY:HA2	2.10	0.51
1:G:178:HIS:HE1	5:G:1891:HOH:O	1.94	0.51
1:B:106:GLY:HA3	1:B:364:GLY:HA2	1.92	0.50
1:B:269:ALA:HB3	1:B:270:PRO:HD3	1.94	0.50
1:F:178:HIS:HD2	5:F:744:HOH:O	1.95	0.50
1:B:140:THR:HB	1:B:141:PRO:HD3	1.94	0.49
1:E:48[A]:GLU:OE1	1:E:51[A]:ARG:NE	2.46	0.49
1:C:395:TYR:O	3:C:502:GOL:O2	2.21	0.48
1:A:155:ASP:OD2	1:A:159[A]:ARG:NH2	2.45	0.48
3:D:433:GOL:H31	5:H:457:HOH:O	2.13	0.48
1:C:181:ALA:HB1	3:C:502:GOL:C3	2.41	0.48
1:B:239:PRO:O	4:D:505:RIB:H2'	2.14	0.47
1:F:303:TYR:HE1	3:G:501:GOL:H31	1.80	0.47
1:H:178:HIS:HE1	5:H:466:HOH:O	1.97	0.47
1:B:81:GLY:HA2	1:D:386:LEU:O	2.15	0.47
1:A:388:MET:SD	1:C:79:SER:HB3	2.55	0.46
1:F:303:TYR:CE1	3:G:501:GOL:H31	2.50	0.46
1:E:269:ALA:HB3	1:E:270:PRO:HD3	1.98	0.46
3:B:503:GOL:H12	5:F:3010:HOH:O	2.15	0.45
1:A:81:GLY:HA2	1:C:386:LEU:O	2.16	0.45
1:E:48[A]:GLU:OE1	1:E:51[A]:ARG:CD	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48[A]:GLU:CD	1:E:51[A]:ARG:HE	2.19	0.45
1:F:178:HIS:HE1	5:F:1179:HOH:O	2.00	0.45
1:B:138:PRO:HB2	1:B:141:PRO:HD2	1.99	0.45
1:E:81:GLY:HA2	1:G:386:LEU:O	2.17	0.45
1:E:140:THR:HB	1:E:141:PRO:HD3	1.99	0.45
1:E:106:GLY:HA3	1:E:364:GLY:HA2	1.99	0.45
1:E:181:ALA:HB1	3:E:502:GOL:C1	2.45	0.44
1:E:386:LEU:O	1:G:81:GLY:HA2	2.17	0.44
1:F:38:GLY:HA3	1:F:96:GLY:O	2.17	0.44
1:G:269:ALA:HB3	1:G:270:PRO:HD3	1.99	0.44
1:C:106:GLY:HA3	1:C:364:GLY:HA2	1.98	0.44
3:C:501:GOL:H2	1:E:105:LEU:HD13	1.99	0.43
1:D:140:THR:HB	1:D:141:PRO:HD3	2.00	0.43
1:C:269:ALA:HB3	1:C:270:PRO:HD3	2.00	0.43
1:A:181:ALA:HB1	3:A:502:GOL:C1	2.47	0.43
4:B:505:RIB:H2'	1:D:239:PRO:O	2.19	0.43
1:A:106:GLY:HA3	1:A:364:GLY:HA2	2.00	0.43
1:F:303:TYR:CZ	3:G:501:GOL:H12	2.54	0.43
1:A:234:GLU:O	1:A:235:GLU:C	2.57	0.43
1:B:386:LEU:O	1:D:81:GLY:HA2	2.19	0.42
1:E:79:SER:HB3	1:G:388:MET:SD	2.59	0.42
1:B:388:MET:SD	1:D:79:SER:HB3	2.59	0.42
1:F:4:ARG:NH2	1:F:64:GLY:HA2	2.34	0.42
1:F:303:TYR:CE1	3:G:501:GOL:H12	2.54	0.42
1:H:51:ARG:NH2	5:H:1313:HOH:O	2.53	0.42
1:G:21:ARG:HD2	1:G:384:LEU:O	2.20	0.42
1:C:115:ALA:O	3:C:501:GOL:O2	2.34	0.42
1:D:138:PRO:HB2	1:D:141:PRO:HD2	2.03	0.41
1:G:234:GLU:O	1:G:235:GLU:C	2.59	0.41
1:F:234:GLU:O	1:F:235:GLU:C	2.59	0.41
1:B:86:PRO:HB3	1:B:263:THR:HG23	2.03	0.41
1:E:13:PRO:HA	1:E:14:PRO:HD3	1.99	0.40
1:F:13:PRO:HA	1:F:14:PRO:HD3	1.97	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	398/433 (92%)	384 (96%)	14 (4%)	0	100	100
1	B	396/433 (92%)	383 (97%)	13 (3%)	0	100	100
1	C	400/433 (92%)	386 (96%)	14 (4%)	0	100	100
1	D	399/433 (92%)	382 (96%)	17 (4%)	0	100	100
1	E	396/433 (92%)	382 (96%)	14 (4%)	0	100	100
1	F	396/433 (92%)	382 (96%)	14 (4%)	0	100	100
1	G	401/433 (93%)	389 (97%)	12 (3%)	0	100	100
1	H	395/433 (91%)	383 (97%)	12 (3%)	0	100	100
All	All	3181/3464 (92%)	3071 (96%)	110 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	306/332 (92%)	303 (99%)	3 (1%)	82	85
1	B	304/332 (92%)	299 (98%)	5 (2%)	70	73
1	C	308/332 (93%)	305 (99%)	3 (1%)	82	85
1	D	307/332 (92%)	304 (99%)	3 (1%)	82	85
1	E	304/332 (92%)	300 (99%)	4 (1%)	76	79
1	F	305/332 (92%)	300 (98%)	5 (2%)	70	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	309/332 (93%)	306 (99%)	3 (1%)	82 85
1	H	303/332 (91%)	299 (99%)	4 (1%)	76 79
All	All	2446/2656 (92%)	2416 (99%)	30 (1%)	78 81

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	ARG
1	A	209	THR
1	A	232	TRP
1	B	4	ARG
1	B	85	ARG
1	B	173	THR
1	B	209	THR
1	B	232	TRP
1	C	85	ARG
1	C	209	THR
1	C	232	TRP
1	D	85	ARG
1	D	209	THR
1	D	232	TRP
1	E	85	ARG
1	E	173	THR
1	E	209	THR
1	E	232	TRP
1	F	4	ARG
1	F	85	ARG
1	F	124	ARG
1	F	209	THR
1	F	232	TRP
1	G	85	ARG
1	G	209	THR
1	G	232	TRP
1	H	85	ARG
1	H	173	THR
1	H	209	THR
1	H	232	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	385	HIS
1	B	385	HIS
1	C	385	HIS
1	D	385	HIS
1	E	385	HIS
1	F	178	HIS
1	F	377	ASN
1	F	385	HIS
1	G	178	HIS
1	G	385	HIS
1	H	178	HIS
1	H	385	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 34 ligands modelled in this entry, 8 are monoatomic - leaving 26 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	$\#\|Z\| > 2$
4	RIB	A	433	-	10,10,10	0.67	0	12,14,14	1.03	1 (8%)
3	GOL	A	502	-	5,5,5	0.48	0	5,5,5	0.47	0
3	GOL	A	503	-	5,5,5	0.38	0	5,5,5	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	RIB	A	505	-	10,10,10	0.60	0	12,14,14	1.27	2 (16%)
3	GOL	B	433	-	5,5,5	0.30	0	5,5,5	0.58	0
3	GOL	B	502	-	5,5,5	0.46	0	5,5,5	0.49	0
3	GOL	B	503	-	5,5,5	0.42	0	5,5,5	0.24	0
4	RIB	B	505	-	10,10,10	0.59	0	12,14,14	1.03	1 (8%)
3	GOL	C	501	-	5,5,5	0.33	0	5,5,5	0.48	0
3	GOL	C	502	-	5,5,5	0.53	0	5,5,5	0.46	0
3	GOL	D	433	-	5,5,5	0.33	0	5,5,5	0.21	0
3	GOL	D	501	-	5,5,5	0.29	0	5,5,5	0.18	0
3	GOL	D	502	-	5,5,5	0.46	0	5,5,5	0.31	0
4	RIB	D	505	-	10,10,10	0.63	0	12,14,14	1.06	1 (8%)
3	GOL	E	501	-	5,5,5	0.27	0	5,5,5	0.15	0
3	GOL	E	502	-	5,5,5	0.45	0	5,5,5	0.45	0
4	RIB	E	505	-	10,10,10	0.59	0	12,14,14	1.22	1 (8%)
3	GOL	F	501	-	5,5,5	0.27	0	5,5,5	0.52	0
3	GOL	G	501	-	5,5,5	0.30	0	5,5,5	0.33	0
3	GOL	G	502	-	5,5,5	0.40	0	5,5,5	0.31	0
3	GOL	G	503	-	5,5,5	0.43	0	5,5,5	0.33	0
3	GOL	G	504	-	5,5,5	0.26	0	5,5,5	0.26	0
4	RIB	G	505	-	10,10,10	0.56	0	12,14,14	1.24	2 (16%)
4	RIB	H	433	-	10,10,10	0.56	0	12,14,14	1.27	2 (16%)
3	GOL	H	501	-	5,5,5	0.29	0	5,5,5	0.23	0
4	RIB	H	505	-	10,10,10	0.56	0	12,14,14	1.17	1 (8%)

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
4	RIB	A	433	-	1/1/4/4	0/2/18/18	0/1/1/1
3	GOL	A	502	-	-	0/4/4/4	0/0/0/0
3	GOL	A	503	-	-	0/4/4/4	0/0/0/0
4	RIB	A	505	-	1/1/4/4	0/2/18/18	0/1/1/1
3	GOL	B	433	-	-	0/4/4/4	0/0/0/0
3	GOL	B	502	-	-	0/4/4/4	0/0/0/0
3	GOL	B	503	-	-	0/4/4/4	0/0/0/0
4	RIB	B	505	-	1/1/4/4	0/2/18/18	0/1/1/1
3	GOL	C	501	-	-	0/4/4/4	0/0/0/0
3	GOL	C	502	-	-	0/4/4/4	0/0/0/0
3	GOL	D	433	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	501	-	-	0/4/4/4	0/0/0/0
3	GOL	D	502	-	-	0/4/4/4	0/0/0/0
4	RIB	D	505	-	1/1/4/4	0/2/18/18	0/1/1/1
3	GOL	E	501	-	-	0/4/4/4	0/0/0/0
3	GOL	E	502	-	-	0/4/4/4	0/0/0/0
4	RIB	E	505	-	1/1/4/4	0/2/18/18	0/1/1/1
3	GOL	F	501	-	-	0/4/4/4	0/0/0/0
3	GOL	G	501	-	-	0/4/4/4	0/0/0/0
3	GOL	G	502	-	-	0/4/4/4	0/0/0/0
3	GOL	G	503	-	-	0/4/4/4	0/0/0/0
3	GOL	G	504	-	-	0/4/4/4	0/0/0/0
4	RIB	G	505	-	1/1/4/4	0/2/18/18	0/1/1/1
4	RIB	H	433	-	1/1/4/4	0/2/18/18	0/1/1/1
3	GOL	H	501	-	-	0/4/4/4	0/0/0/0
4	RIB	H	505	-	1/1/4/4	0/2/18/18	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	505	RIB	C5'-C4'-C3'	-2.24	109.78	115.08
4	A	505	RIB	C5'-C4'-C3'	-2.19	109.91	115.08
4	H	433	RIB	C5'-C4'-C3'	-2.15	110.00	115.08
4	A	433	RIB	C1'-C2'-C3'	2.23	105.41	102.45
4	B	505	RIB	C1'-C2'-C3'	2.37	105.58	102.45
4	G	505	RIB	C1'-C2'-C3'	2.44	105.68	102.45
4	H	505	RIB	C1'-C2'-C3'	2.45	105.69	102.45
4	D	505	RIB	C1'-C2'-C3'	2.58	105.86	102.45
4	H	433	RIB	C1'-C2'-C3'	2.70	106.03	102.45
4	A	505	RIB	C1'-C2'-C3'	2.73	106.06	102.45
4	E	505	RIB	C1'-C2'-C3'	2.81	106.17	102.45

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	505	RIB	C1'
4	G	505	RIB	C1'
4	D	505	RIB	C1'
4	H	433	RIB	C1'
4	A	433	RIB	C1'
4	B	505	RIB	C1'
4	H	505	RIB	C1'

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Mol	Chain	Res	Type	Atom
4	E	505	RIB	C1'

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	433	RIB	2	0
3	A	502	GOL	2	0
3	B	502	GOL	1	0
3	B	503	GOL	1	0
4	B	505	RIB	1	0
3	C	501	GOL	2	0
3	C	502	GOL	3	0
3	D	433	GOL	1	0
3	D	502	GOL	1	0
4	D	505	RIB	1	0
3	E	502	GOL	2	0
3	G	501	GOL	8	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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^2)	Q<0.9
1	A	396/433 (91%)	-0.27	13 (3%)	50	51	10, 15, 27, 57	0
1	B	395/433 (91%)	-0.24	13 (3%)	50	51	11, 17, 31, 49	0
1	C	396/433 (91%)	-0.29	10 (2%)	61	61	11, 16, 29, 55	0
1	D	396/433 (91%)	-0.35	10 (2%)	61	61	10, 16, 27, 56	0
1	E	395/433 (91%)	-0.23	12 (3%)	54	55	12, 18, 30, 52	0
1	F	397/433 (91%)	-0.09	17 (4%)	39	40	13, 20, 35, 61	0
1	G	396/433 (91%)	-0.18	11 (2%)	56	57	13, 20, 32, 54	0
1	H	395/433 (91%)	-0.09	13 (3%)	50	51	12, 21, 37, 53	0
All	All	3166/3464 (91%)	-0.22	99 (3%)	52	53	10, 18, 32, 61	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	396	THR	7.9
1	F	396	THR	6.3
1	F	397	ASN	6.1
1	E	394	ASP	5.9
1	D	396	THR	5.8
1	F	391	ALA	5.7
1	C	396	THR	5.6
1	A	395	TYR	5.3
1	G	396	THR	5.2
1	E	391	ALA	5.0
1	A	393	CYS	5.0
1	A	394	ASP	5.0
1	E	392	SER	5.0
1	C	140	THR	4.8
1	G	140	THR	4.7
1	H	382	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	392	SER	4.6
1	A	392	SER	4.5
1	B	395	TYR	4.5
1	F	140	THR	4.4
1	E	395	TYR	4.3
1	H	393	CYS	4.3
1	A	15	ALA	4.3
1	A	380	HIS	4.2
1	H	15	ALA	4.0
1	F	380	HIS	3.9
1	H	395	TYR	3.9
1	F	394	ASP	3.9
1	F	382	THR	3.9
1	H	140	THR	3.9
1	C	135	PRO	3.7
1	H	139	ILE	3.7
1	E	393	CYS	3.7
1	G	380	HIS	3.7
1	A	391	ALA	3.6
1	B	140	THR	3.6
1	C	394	ASP	3.4
1	G	391	ALA	3.4
1	E	382	THR	3.3
1	D	393	CYS	3.3
1	H	380	HIS	3.2
1	D	394	ASP	3.2
1	C	395	TYR	3.2
1	H	135	PRO	3.2
1	C	391	ALA	3.2
1	H	391	ALA	3.1
1	G	381	GLY	3.1
1	F	393	CYS	3.1
1	B	394	ASP	3.1
1	H	394	ASP	3.1
1	G	393	CYS	3.1
1	H	392	SER	3.1
1	E	380	HIS	3.1
1	F	31	ASP	3.1
1	F	15	ALA	3.0
1	H	16	PRO	3.0
1	B	382	THR	2.9
1	B	15	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	139	ILE	2.9
1	D	140	THR	2.9
1	E	15	ALA	2.9
1	B	16	PRO	2.8
1	G	382	THR	2.8
1	A	382	THR	2.8
1	B	391	ALA	2.8
1	A	16	PRO	2.7
1	E	389	GLN	2.6
1	F	395	TYR	2.6
1	F	389	GLN	2.6
1	D	380	HIS	2.6
1	G	395	TYR	2.6
1	B	393	CYS	2.5
1	C	15	ALA	2.5
1	D	139	ILE	2.5
1	C	16	PRO	2.5
1	E	140	THR	2.5
1	E	16	PRO	2.5
1	D	391	ALA	2.5
1	B	392	SER	2.4
1	C	139	ILE	2.4
1	D	395	TYR	2.4
1	G	392	SER	2.4
1	F	4	ARG	2.4
1	B	389	GLN	2.3
1	A	140	THR	2.3
1	D	4[A]	ARG	2.3
1	C	136	HIS	2.3
1	F	139	ILE	2.3
1	A	1	VAL	2.2
1	F	368	GLU	2.2
1	A	389	GLN	2.2
1	B	4	ARG	2.2
1	B	139	ILE	2.2
1	F	124	ARG	2.2
1	D	382	THR	2.1
1	B	31	ASP	2.1
1	E	17	GLY	2.0
1	G	394	ASP	2.0
1	H	353	GLU	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^{th} 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^2)	Q<0.9
4	RIB	H	505	10/10	0.69	0.32	25.06	53,54,54,54	0
4	RIB	B	505	10/10	0.73	0.31	24.53	53,53,54,54	0
4	RIB	D	505	10/10	0.78	0.33	24.26	55,55,55,55	0
4	RIB	E	505	10/10	0.72	0.29	23.24	51,51,52,52	0
4	RIB	A	505	10/10	0.72	0.30	21.10	50,50,51,51	0
4	RIB	A	433	10/10	0.80	0.27	20.77	51,51,51,51	0
4	RIB	G	505	10/10	0.82	0.28	18.19	53,53,54,54	0
4	RIB	H	433	10/10	0.73	0.31	15.00	56,57,57,57	0
3	GOL	G	501	6/6	0.75	0.26	10.09	37,38,45,45	0
3	GOL	F	501	6/6	0.91	0.15	2.38	27,29,31,31	0
3	GOL	E	501	6/6	0.93	0.12	2.15	26,27,29,29	0
3	GOL	D	433	6/6	0.83	0.16	2.01	45,45,48,48	0
3	GOL	D	501	6/6	0.94	0.12	1.88	24,26,27,27	0
3	GOL	B	433	6/6	0.93	0.12	1.58	23,25,30,30	0
3	GOL	E	502	6/6	0.90	0.20	1.33	24,26,44,44	0
3	GOL	C	501	6/6	0.94	0.12	1.16	29,30,35,36	0
3	GOL	G	504	6/6	0.93	0.13	1.11	27,30,31,31	0
3	GOL	B	502	6/6	0.92	0.19	1.05	19,21,39,40	0
3	GOL	G	502	6/6	0.91	0.21	1.01	22,24,42,42	0
3	GOL	A	503	6/6	0.96	0.10	0.84	26,26,28,28	0
3	GOL	H	501	6/6	0.95	0.11	0.72	26,26,29,29	0
3	GOL	C	502	6/6	0.94	0.18	0.53	24,25,39,39	0
3	GOL	D	502	6/6	0.90	0.19	0.47	26,27,41,42	0
3	GOL	B	503	6/6	0.94	0.17	0.31	20,21,42,43	0
3	GOL	A	502	6/6	0.90	0.20	0.23	19,21,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MG	H	500	1/1	0.96	0.09	0.16	25,25,25,25	0
3	GOL	G	503	6/6	0.96	0.14	0.07	20,21,36,36	0
2	MG	A	500	1/1	0.98	0.07	-0.54	19,19,19,19	0
2	MG	E	500	1/1	0.96	0.08	-0.55	23,23,23,23	0
2	MG	B	500	1/1	0.97	0.07	-0.57	19,19,19,19	0
2	MG	F	500	1/1	0.99	0.07	-0.80	21,21,21,21	0
2	MG	C	500	1/1	0.98	0.07	-1.16	18,18,18,18	0
2	MG	G	500	1/1	0.99	0.05	-2.21	21,21,21,21	0
2	MG	D	500	1/1	0.99	0.03	-4.50	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.