



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2017 – 04:07 PM EDT

PDB ID : 2OZ3
Title : Crystal structure of L-Rhamnonate dehydratase from Azotobacter vinelandii
Authors : Patskovsky, Y.; Toro, R.; Sauder, J.M.; Freeman, J.C.; Bain, K.; Gheyi, T.;
Wu, B.; Wasserman, S.R.; Smith, D.; Gerlt, J.; Burley, S.K.; Almo, S.C.; New
York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : unknown
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

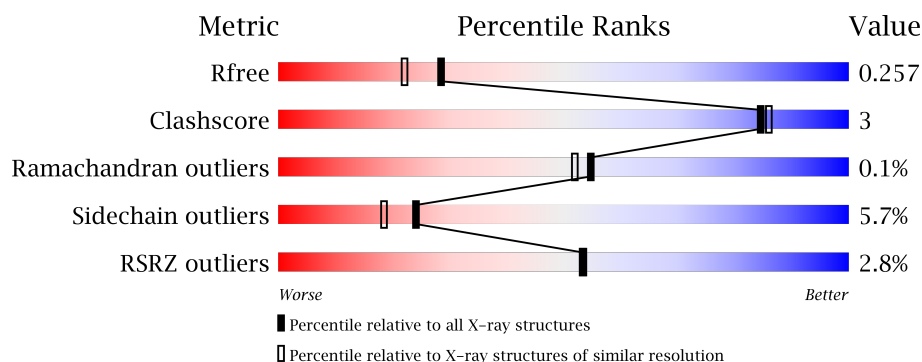
1 Overall quality at a glance

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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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 $\leq 5\%$. 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	404	
1	B	404	
1	C	404	
1	D	404	
1	E	404	

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Mol	Chain	Length	Quality of chain
1	F	404	 3% 87% 8% •
1	G	404	 3% 85% 11% ••
1	H	404	 3% 83% 11% • 5%

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
2	GOL	A	3016	-	-	-	X
2	GOL	A	3023	-	-	-	X
2	GOL	A	3024	-	-	-	X
2	GOL	A	3031	-	-	-	X
2	GOL	B	3002	-	-	-	X
2	GOL	B	3004	-	-	-	X
2	GOL	B	3021	-	-	-	X
2	GOL	C	3001	-	-	-	X
2	GOL	C	3020	-	-	-	X
2	GOL	C	3022	-	-	X	X
2	GOL	C	3027	-	-	-	X
2	GOL	D	3005	-	-	-	X
2	GOL	D	3007	-	-	-	X
2	GOL	D	3017	-	-	-	X
2	GOL	E	3010	-	-	-	X
2	GOL	F	3008	-	-	-	X
2	GOL	F	3011	-	-	-	X
2	GOL	G	3009	-	-	-	X
2	GOL	G	3013	-	-	-	X
2	GOL	H	3012	-	-	X	X
2	GOL	H	3018	-	-	-	X
2	GOL	H	3025	-	-	-	X
3	NA	D	2002	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26576 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	Se	0	4	0
			3143	1996	554	572	5	16			
1	B	396	Total	C	N	O	S	Se	0	4	0
			3143	1997	553	573	5	15			
1	C	388	Total	C	N	O	S	Se	0	3	0
			3083	1959	544	560	5	15			
1	D	395	Total	C	N	O	S	Se	0	4	0
			3132	1991	550	571	5	15			
1	E	396	Total	C	N	O	S	Se	0	2	0
			3137	1991	556	570	5	15			
1	F	387	Total	C	N	O	S	Se	0	4	0
			3080	1959	541	560	5	15			
1	G	395	Total	C	N	O	S	Se	5	4	0
			3131	1992	549	570	5	15			
1	H	383	Total	C	N	O	S	Se	0	6	0
			3063	1954	539	550	5	15			

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	CLONING ARTIFACT	UNP Q4J3N3
A	0	SER	-	CLONING ARTIFACT	UNP Q4J3N3
A	1	LEU	-	CLONING ARTIFACT	UNP Q4J3N3
A	38	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
A	108	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
A	171	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
A	178	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
A	201	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
A	212	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
A	217	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
A	262	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
A	263	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
A	278	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	282	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
A	341	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
A	342	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
A	352	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
A	368	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
A	395	GLU	-	CLONING ARTIFACT	UNP Q4J3N3
A	396	GLY	-	CLONING ARTIFACT	UNP Q4J3N3
A	397	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
A	398	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
A	399	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
A	400	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
A	401	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
A	402	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
B	-1	MSE	-	CLONING ARTIFACT	UNP Q4J3N3
B	0	SER	-	CLONING ARTIFACT	UNP Q4J3N3
B	1	LEU	-	CLONING ARTIFACT	UNP Q4J3N3
B	38	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
B	108	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
B	171	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
B	178	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
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B	341	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
B	342	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
B	352	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
B	368	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
B	395	GLU	-	CLONING ARTIFACT	UNP Q4J3N3
B	396	GLY	-	CLONING ARTIFACT	UNP Q4J3N3
B	397	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
B	398	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
B	399	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
B	400	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
B	401	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
B	402	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
C	-1	MSE	-	CLONING ARTIFACT	UNP Q4J3N3
C	0	SER	-	CLONING ARTIFACT	UNP Q4J3N3
C	1	LEU	-	CLONING ARTIFACT	UNP Q4J3N3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	38	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
C	108	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
C	171	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
C	178	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
C	201	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
C	212	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
C	217	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
C	262	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
C	263	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
C	278	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
C	282	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
C	341	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
C	342	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
C	352	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
C	368	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
C	395	GLU	-	CLONING ARTIFACT	UNP Q4J3N3
C	396	GLY	-	CLONING ARTIFACT	UNP Q4J3N3
C	397	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
C	398	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
C	399	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
C	400	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
C	401	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
C	402	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
D	-1	MSE	-	CLONING ARTIFACT	UNP Q4J3N3
D	0	SER	-	CLONING ARTIFACT	UNP Q4J3N3
D	1	LEU	-	CLONING ARTIFACT	UNP Q4J3N3
D	38	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
D	108	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
D	171	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
D	178	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
D	201	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
D	212	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
D	217	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
D	262	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
D	263	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
D	278	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
D	282	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
D	341	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
D	342	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
D	352	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
D	368	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
D	395	GLU	-	CLONING ARTIFACT	UNP Q4J3N3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	396	GLY	-	CLONING ARTIFACT	UNP Q4J3N3
D	397	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
D	398	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
D	399	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
D	400	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
D	401	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
D	402	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
E	-1	MSE	-	CLONING ARTIFACT	UNP Q4J3N3
E	0	SER	-	CLONING ARTIFACT	UNP Q4J3N3
E	1	LEU	-	CLONING ARTIFACT	UNP Q4J3N3
E	38	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
E	108	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
E	171	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
E	178	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
E	201	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
E	212	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
E	217	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
E	262	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
E	263	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
E	278	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
E	282	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
E	341	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
E	342	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
E	352	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
E	368	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
E	395	GLU	-	CLONING ARTIFACT	UNP Q4J3N3
E	396	GLY	-	CLONING ARTIFACT	UNP Q4J3N3
E	397	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
E	398	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
E	399	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
E	400	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
E	401	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
E	402	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
F	-1	MSE	-	CLONING ARTIFACT	UNP Q4J3N3
F	0	SER	-	CLONING ARTIFACT	UNP Q4J3N3
F	1	LEU	-	CLONING ARTIFACT	UNP Q4J3N3
F	38	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
F	108	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
F	171	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
F	178	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
F	201	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
F	212	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3

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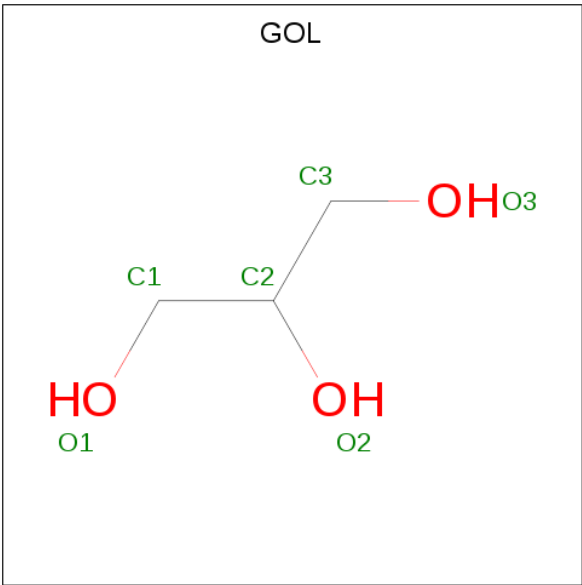
Chain	Residue	Modelled	Actual	Comment	Reference
F	217	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
F	262	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
F	263	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
F	278	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
F	282	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
F	341	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
F	342	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
F	352	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
F	368	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
F	395	GLU	-	CLONING ARTIFACT	UNP Q4J3N3
F	396	GLY	-	CLONING ARTIFACT	UNP Q4J3N3
F	397	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
F	398	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
F	399	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
F	400	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
F	401	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
F	402	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
G	-1	MSE	-	CLONING ARTIFACT	UNP Q4J3N3
G	0	SER	-	CLONING ARTIFACT	UNP Q4J3N3
G	1	LEU	-	CLONING ARTIFACT	UNP Q4J3N3
G	38	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
G	108	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
G	171	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
G	178	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
G	201	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
G	212	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
G	217	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
G	262	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
G	263	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
G	278	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
G	282	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
G	341	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
G	342	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
G	352	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
G	368	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
G	395	GLU	-	CLONING ARTIFACT	UNP Q4J3N3
G	396	GLY	-	CLONING ARTIFACT	UNP Q4J3N3
G	397	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
G	398	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
G	399	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
G	400	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
G	401	HIS	-	CLONING ARTIFACT	UNP Q4J3N3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	402	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
H	-1	MSE	-	CLONING ARTIFACT	UNP Q4J3N3
H	0	SER	-	CLONING ARTIFACT	UNP Q4J3N3
H	1	LEU	-	CLONING ARTIFACT	UNP Q4J3N3
H	38	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
H	108	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
H	171	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
H	178	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
H	201	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
H	212	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
H	217	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
H	262	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
H	263	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
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H	352	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
H	368	MSE	MET	MODIFIED RESIDUE	UNP Q4J3N3
H	395	GLU	-	CLONING ARTIFACT	UNP Q4J3N3
H	396	GLY	-	CLONING ARTIFACT	UNP Q4J3N3
H	397	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
H	398	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
H	399	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
H	400	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
H	401	HIS	-	CLONING ARTIFACT	UNP Q4J3N3
H	402	HIS	-	CLONING ARTIFACT	UNP Q4J3N3

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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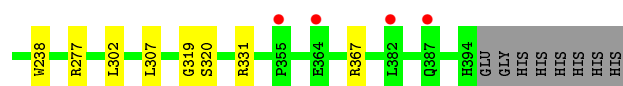
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

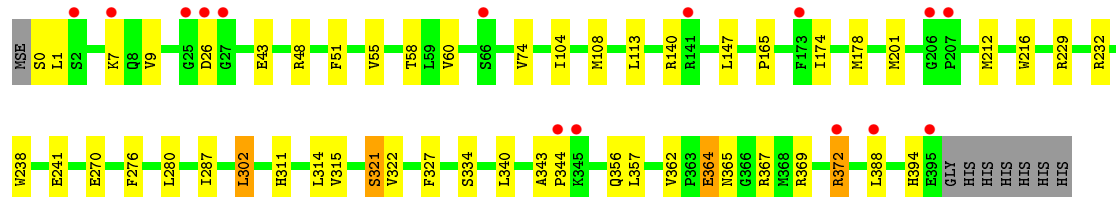
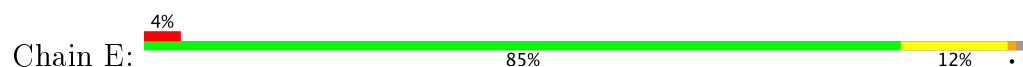
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

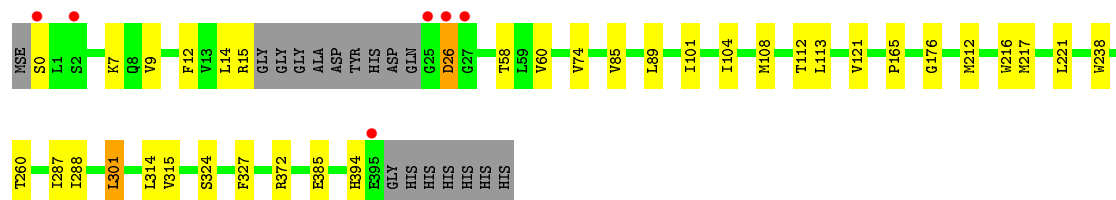
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	242	Total 242	O 242	0	0
4	B	228	Total 228	O 228	0	0
4	C	228	Total 228	O 228	0	0
4	D	149	Total 149	O 149	0	0
4	E	158	Total 158	O 158	0	0
4	F	166	Total 166	O 166	0	0
4	G	149	Total 149	O 149	0	0
4	H	156	Total 156	O 156	0	0



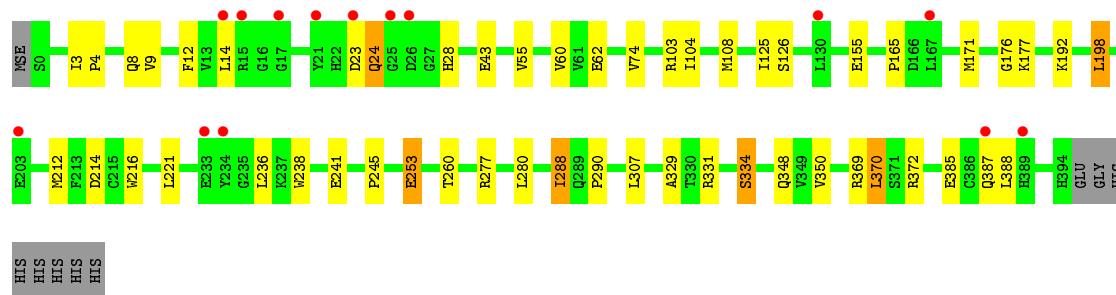
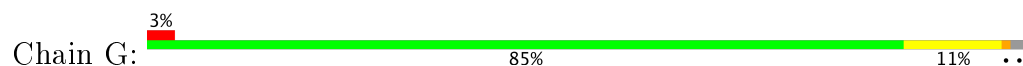
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



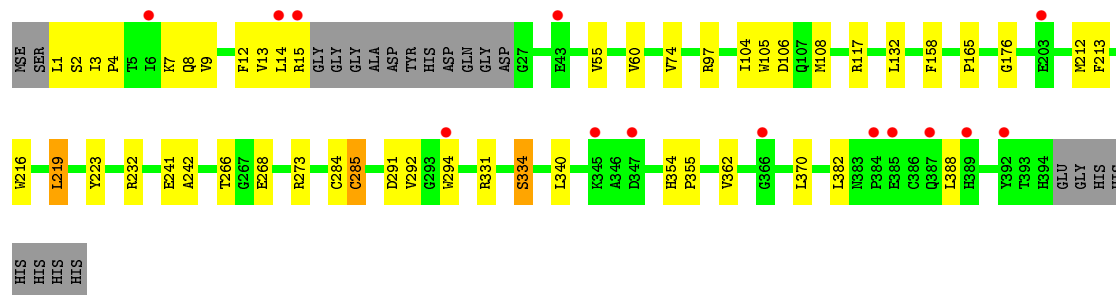
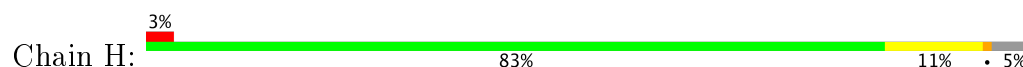
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.77Å 115.40Å 164.11Å 90.00° 96.06° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 31.46 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.9 (20.00-2.00) 96.9 (31.46-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.3.0028	Depositor
R, R_{free}	0.196 , 0.257 0.197 , 0.257	Depositor DCC
R_{free} test set	6225 reflections (3.11%)	DCC
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26576	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.43	0/3223	0.58	0/4346
1	B	0.42	0/3223	0.59	0/4346
1	C	0.42	0/3154	0.61	0/4251
1	D	0.40	0/3212	0.56	0/4333
1	E	0.40	0/3211	0.56	0/4329
1	F	0.39	0/3157	0.55	0/4255
1	G	0.39	0/3211	0.55	0/4331
1	H	0.40	0/3146	0.57	0/4240
All	All	0.40	0/25537	0.57	0/34431

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	0	2
1	B	0	1
1	C	0	3
1	D	1	1
1	E	0	1
1	F	0	2
1	G	0	1
1	H	0	3
All	All	1	14

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	26	ASP	CA

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	PHE	Peptide
1	A	284	CYS	Peptide
1	B	158	PHE	Peptide
1	C	12	PHE	Peptide
1	C	158	PHE	Peptide

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	3143	0	3074	15	0
1	B	3143	0	3074	18	0
1	C	3083	0	3019	14	0
1	D	3132	0	3063	15	0
1	E	3137	0	3065	18	0
1	F	3080	0	3022	12	0
1	G	3131	0	3066	22	0
1	H	3063	0	3028	19	0
2	A	54	0	72	1	0
2	B	24	0	32	2	0
2	C	36	0	48	7	0
2	D	24	0	32	1	0
2	E	6	0	8	0	0
2	F	12	0	16	0	0
2	G	12	0	16	0	0
2	H	18	0	24	4	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	242	0	0	2	0
4	B	228	0	0	1	0
4	C	228	0	0	1	0
4	D	149	0	0	1	0
4	E	158	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	166	0	0	0	0
4	G	149	0	0	0	0
4	H	156	0	0	0	0
All	All	26576	0	24659	132	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 3.

The worst 5 of 132 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:C:229[B]:ARG:HG2	1:C:229[B]:ARG:HH21	1.05	1.17
1:C:229[B]:ARG:NH2	1:C:229[B]:ARG:HG2	1.78	0.89
1:D:229:ARG:HG3	1:D:232:ARG:HH21	1.43	0.83
2:C:3022:GOL:H31	1:D:302:LEU:HD22	1.61	0.82
1:B:292:VAL:HG23	4:B:3233:HOH:O	1.86	0.74

There are no symmetry-related clashes.

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	398/404 (98%)	384 (96%)	14 (4%)	0	100	100
1	B	398/404 (98%)	391 (98%)	7 (2%)	0	100	100
1	C	387/404 (96%)	376 (97%)	10 (3%)	1 (0%)	44	40
1	D	397/404 (98%)	382 (96%)	13 (3%)	2 (0%)	32	26
1	E	396/404 (98%)	386 (98%)	9 (2%)	1 (0%)	44	40
1	F	387/404 (96%)	376 (97%)	11 (3%)	0	100	100
1	G	397/404 (98%)	385 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	385/404 (95%)	375 (97%)	10 (3%)	0	100	100
All	All	3145/3232 (97%)	3055 (97%)	86 (3%)	4 (0%)	55	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	13	VAL
1	D	26	ASP
1	E	321	SER
1	D	319	GLY

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	329/316 (104%)	317 (96%)	12 (4%)	40	38
1	B	329/316 (104%)	311 (94%)	18 (6%)	25	20
1	C	323/316 (102%)	308 (95%)	15 (5%)	31	27
1	D	328/316 (104%)	312 (95%)	16 (5%)	29	24
1	E	327/316 (104%)	305 (93%)	22 (7%)	19	13
1	F	324/316 (102%)	307 (95%)	17 (5%)	27	22
1	G	328/316 (104%)	303 (92%)	25 (8%)	15	10
1	H	323/316 (102%)	299 (93%)	24 (7%)	16	10
All	All	2611/2528 (103%)	2462 (94%)	149 (6%)	24	18

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	55	VAL
1	F	0	SER
1	H	216	TRP
1	E	178	MSE
1	E	241	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	257	ASN
1	D	311	HIS
1	G	24	GLN
1	C	257	ASN
1	C	311	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 33 ligands modelled in this entry, 2 are monoatomic - leaving 31 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	$\# Z > 2$
2	GOL	A	3003	-	5,5,5	0.30	0	5,5,5	0.20	0
2	GOL	A	3014	-	5,5,5	0.35	0	5,5,5	0.28	0
2	GOL	A	3016	-	5,5,5	0.35	0	5,5,5	0.38	0
2	GOL	A	3023	-	5,5,5	0.38	0	5,5,5	0.28	0
2	GOL	A	3024	-	5,5,5	0.36	0	5,5,5	0.12	0
2	GOL	A	3028	-	5,5,5	0.36	0	5,5,5	0.27	0
2	GOL	A	3030	-	5,5,5	0.35	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	3031	-	5,5,5	0.35	0	5,5,5	0.38	0
2	GOL	A	3032	-	5,5,5	0.35	0	5,5,5	0.32	0
2	GOL	B	3002	-	5,5,5	0.35	0	5,5,5	0.31	0
2	GOL	B	3004	-	5,5,5	0.32	0	5,5,5	0.40	0
2	GOL	B	3021	-	5,5,5	0.37	0	5,5,5	0.27	0
2	GOL	B	3029	-	5,5,5	0.35	0	5,5,5	0.15	0
2	GOL	C	3001	-	5,5,5	0.37	0	5,5,5	0.28	0
2	GOL	C	3019	-	5,5,5	0.35	0	5,5,5	0.33	0
2	GOL	C	3020	-	5,5,5	0.44	0	5,5,5	0.40	0
2	GOL	C	3022	-	5,5,5	0.34	0	5,5,5	0.69	0
2	GOL	C	3026	-	5,5,5	0.32	0	5,5,5	0.26	0
2	GOL	C	3027	-	5,5,5	0.36	0	5,5,5	0.33	0
2	GOL	D	3005	-	5,5,5	0.34	0	5,5,5	0.44	0
2	GOL	D	3006	-	5,5,5	0.30	0	5,5,5	0.29	0
2	GOL	D	3007	-	5,5,5	0.38	0	5,5,5	0.26	0
2	GOL	D	3017	-	5,5,5	0.35	0	5,5,5	0.21	0
2	GOL	E	3010	-	5,5,5	0.34	0	5,5,5	0.30	0
2	GOL	F	3008	-	5,5,5	0.34	0	5,5,5	0.29	0
2	GOL	F	3011	-	5,5,5	0.36	0	5,5,5	0.37	0
2	GOL	G	3009	-	5,5,5	0.34	0	5,5,5	0.22	0
2	GOL	G	3013	-	5,5,5	0.35	0	5,5,5	0.21	0
2	GOL	H	3012	-	5,5,5	0.57	0	5,5,5	0.32	0
2	GOL	H	3018	-	5,5,5	0.34	0	5,5,5	0.29	0
2	GOL	H	3025	-	5,5,5	0.32	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
2	GOL	A	3003	-	-	0/4/4/4	0/0/0/0
2	GOL	A	3014	-	-	0/4/4/4	0/0/0/0
2	GOL	A	3016	-	-	0/4/4/4	0/0/0/0
2	GOL	A	3023	-	-	0/4/4/4	0/0/0/0
2	GOL	A	3024	-	-	0/4/4/4	0/0/0/0
2	GOL	A	3028	-	-	0/4/4/4	0/0/0/0
2	GOL	A	3030	-	-	0/4/4/4	0/0/0/0
2	GOL	A	3031	-	-	0/4/4/4	0/0/0/0
2	GOL	A	3032	-	-	0/4/4/4	0/0/0/0
2	GOL	B	3002	-	-	0/4/4/4	0/0/0/0
2	GOL	B	3004	-	-	0/4/4/4	0/0/0/0
2	GOL	B	3021	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	3029	-	-	0/4/4/4	0/0/0/0
2	GOL	C	3001	-	-	0/4/4/4	0/0/0/0
2	GOL	C	3019	-	-	0/4/4/4	0/0/0/0
2	GOL	C	3020	-	-	0/4/4/4	0/0/0/0
2	GOL	C	3022	-	-	0/4/4/4	0/0/0/0
2	GOL	C	3026	-	-	0/4/4/4	0/0/0/0
2	GOL	C	3027	-	-	0/4/4/4	0/0/0/0
2	GOL	D	3005	-	-	0/4/4/4	0/0/0/0
2	GOL	D	3006	-	-	0/4/4/4	0/0/0/0
2	GOL	D	3007	-	-	0/4/4/4	0/0/0/0
2	GOL	D	3017	-	-	0/4/4/4	0/0/0/0
2	GOL	E	3010	-	-	0/4/4/4	0/0/0/0
2	GOL	F	3008	-	-	0/4/4/4	0/0/0/0
2	GOL	F	3011	-	-	0/4/4/4	0/0/0/0
2	GOL	G	3009	-	-	0/4/4/4	0/0/0/0
2	GOL	G	3013	-	-	0/4/4/4	0/0/0/0
2	GOL	H	3012	-	-	0/4/4/4	0/0/0/0
2	GOL	H	3018	-	-	0/4/4/4	0/0/0/0
2	GOL	H	3025	-	-	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.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3023	GOL	1	0
2	B	3004	GOL	1	0
2	B	3021	GOL	1	0
2	C	3020	GOL	2	0
2	C	3022	GOL	5	0
2	D	3007	GOL	1	0
2	H	3012	GOL	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	381/404 (94%)	-0.27	10 (2%) 56 56	13, 26, 58, 88	0
1	B	381/404 (94%)	-0.24	2 (0%) 90 90	15, 30, 52, 77	0
1	C	373/404 (92%)	-0.33	5 (1%) 77 77	15, 30, 51, 94	0
1	D	380/404 (94%)	0.14	17 (4%) 34 34	19, 39, 71, 104	0
1	E	381/404 (94%)	0.23	15 (3%) 40 40	25, 42, 66, 88	0
1	F	372/404 (92%)	-0.16	6 (1%) 72 71	18, 34, 59, 106	0
1	G	380/404 (94%)	0.15	14 (3%) 42 43	22, 41, 69, 94	0
1	H	368/404 (91%)	0.13	14 (3%) 41 41	20, 40, 62, 104	0
All	All	3016/3232 (93%)	-0.04	83 (2%) 53 53	13, 36, 63, 106	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	25	GLY	8.3
1	A	25	GLY	6.1
1	G	25	GLY	5.1
1	F	26	ASP	4.9
1	A	26	ASP	4.8

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 ⓘ

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, 95th 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
3	NA	D	2002	1/1	0.84	0.51	18.01	104,104,104,104	0
2	GOL	E	3010	6/6	0.87	0.26	10.87	61,66,73,74	0
2	GOL	F	3011	6/6	0.83	0.24	8.88	61,73,74,80	0
2	GOL	D	3005	6/6	0.87	0.21	8.74	56,56,57,60	0
2	GOL	D	3007	6/6	0.72	0.22	8.00	48,62,68,69	0
2	GOL	F	3008	6/6	0.88	0.21	6.99	41,54,58,74	0
2	GOL	C	3020	6/6	0.81	0.31	6.92	31,61,64,66	0
2	GOL	H	3018	6/6	0.84	0.25	6.85	53,55,63,68	0
2	GOL	H	3025	6/6	0.86	0.20	6.19	46,59,65,65	0
2	GOL	B	3021	6/6	0.89	0.21	6.15	38,54,58,60	0
2	GOL	B	3004	6/6	0.93	0.13	6.15	37,41,47,55	0
2	GOL	A	3024	6/6	0.86	0.17	4.85	54,57,64,64	0
2	GOL	C	3022	6/6	0.84	0.22	4.45	35,40,52,54	0
2	GOL	C	3001	6/6	0.92	0.15	4.37	42,55,60,65	0
2	GOL	C	3027	6/6	0.91	0.26	4.28	45,62,67,70	0
2	GOL	A	3023	6/6	0.83	0.19	4.24	38,62,66,69	0
2	GOL	B	3002	6/6	0.93	0.15	3.99	35,50,66,82	0
2	GOL	D	3017	6/6	0.91	0.27	3.54	46,51,58,63	0
2	GOL	A	3031	6/6	0.94	0.23	3.30	34,53,62,69	0
2	GOL	G	3013	6/6	0.83	0.23	3.02	38,40,45,50	0
2	GOL	G	3009	6/6	0.91	0.15	2.75	35,39,56,58	0
2	GOL	A	3016	6/6	0.90	0.17	2.68	57,63,68,74	0
2	GOL	H	3012	6/6	0.85	0.19	2.39	53,65,72,81	0
2	GOL	A	3014	6/6	0.86	0.17	1.92	54,60,62,70	0
2	GOL	A	3032	6/6	0.79	0.17	1.81	49,58,67,68	0
3	NA	B	2001	1/1	0.73	0.20	1.74	62,62,62,62	0
2	GOL	D	3006	6/6	0.90	0.15	0.70	46,57,62,64	0
2	GOL	C	3019	6/6	0.93	0.10	0.37	47,52,57,62	0
2	GOL	A	3003	6/6	0.95	0.09	-0.40	31,54,58,60	0
2	GOL	A	3030	6/6	0.92	0.34	-	57,60,71,72	0
2	GOL	C	3026	6/6	0.91	0.22	-	56,69,75,81	0
2	GOL	A	3028	6/6	0.92	0.26	-	48,60,69,75	0
2	GOL	B	3029	6/6	0.94	0.13	-	44,62,70,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.