



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 03:54 am BST

PDB ID : 4QRO  
Title : CRYSTAL STRUCTURE of DIHYDROXYBENZOIC ACID DECARBOXYLASE BPRO\_2061 (TARGET EFI-500288) FROM POLAROMONAS SP. JS666 WITH BOUND MANGANESE AND AN INHIBITOR, 2-NITRORESORCINOL  
Authors : Patskovsky, Y.; Vladimirova, A.; Toro, R.; Bhosle, R.; Gerlt, J.A.; Raushel, M.; Almo, S.C.  
Deposited on : 2014-07-01  
Resolution : 1.65 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

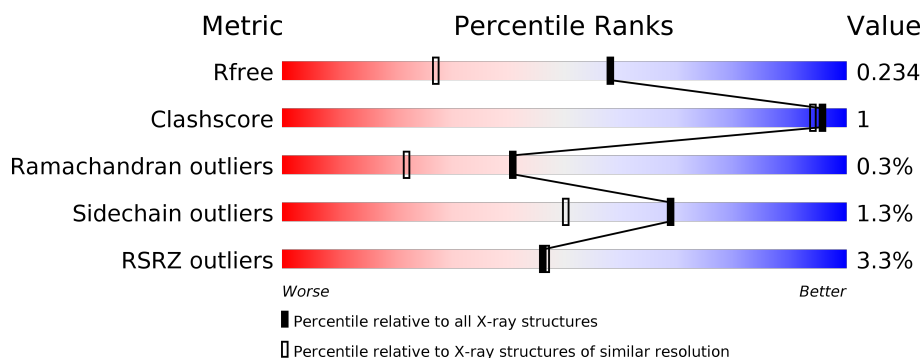
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	348	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
1	B	348	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>•</div> <div>7%</div> </div> </div>
1	C	348	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>•</div> <div>7%</div> </div> </div>
1	D	348	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>•</div> <div>7%</div> </div> </div>
1	E	348	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>•</div> <div>7%</div> </div> </div>
1	F	348	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	348	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>89%</div><div>5%6%</div></div></div>
1	H	348	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>89%</div><div>•7%</div></div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23784 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 Gamma-resorcylate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	6	0
			2729	1745	481	493	10			
1	B	324	Total	C	N	O	S	0	5	0
			2655	1699	465	481	10			
1	C	325	Total	C	N	O	S	0	3	0
			2648	1692	463	483	10			
1	D	323	Total	C	N	O	S	0	2	0
			2628	1681	459	479	9			
1	E	324	Total	C	N	O	S	0	5	0
			2645	1691	461	484	9			
1	F	324	Total	C	N	O	S	0	5	0
			2660	1700	468	482	10			
1	G	327	Total	C	N	O	S	0	7	0
			2702	1732	469	491	10			
1	H	324	Total	C	N	O	S	0	8	0
			2671	1707	469	485	10			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	ALA	-	EXPRESSION TAG	UNP Q12BV1
A	328	GLU	-	EXPRESSION TAG	UNP Q12BV1
A	329	ASN	-	EXPRESSION TAG	UNP Q12BV1
A	330	LEU	-	EXPRESSION TAG	UNP Q12BV1
A	331	TYR	-	EXPRESSION TAG	UNP Q12BV1
A	332	PHE	-	EXPRESSION TAG	UNP Q12BV1
A	333	GLN	-	EXPRESSION TAG	UNP Q12BV1
A	334	SER	-	EXPRESSION TAG	UNP Q12BV1
A	335	HIS	-	EXPRESSION TAG	UNP Q12BV1
A	336	HIS	-	EXPRESSION TAG	UNP Q12BV1
A	337	HIS	-	EXPRESSION TAG	UNP Q12BV1
A	338	HIS	-	EXPRESSION TAG	UNP Q12BV1
A	339	HIS	-	EXPRESSION TAG	UNP Q12BV1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	340	HIS	-	EXPRESSION TAG	UNP Q12BV1
A	341	TRP	-	EXPRESSION TAG	UNP Q12BV1
A	342	SER	-	EXPRESSION TAG	UNP Q12BV1
A	343	HIS	-	EXPRESSION TAG	UNP Q12BV1
A	344	PRO	-	EXPRESSION TAG	UNP Q12BV1
A	345	GLN	-	EXPRESSION TAG	UNP Q12BV1
A	346	PHE	-	EXPRESSION TAG	UNP Q12BV1
A	347	GLU	-	EXPRESSION TAG	UNP Q12BV1
A	348	LYS	-	EXPRESSION TAG	UNP Q12BV1
B	327	ALA	-	EXPRESSION TAG	UNP Q12BV1
B	328	GLU	-	EXPRESSION TAG	UNP Q12BV1
B	329	ASN	-	EXPRESSION TAG	UNP Q12BV1
B	330	LEU	-	EXPRESSION TAG	UNP Q12BV1
B	331	TYR	-	EXPRESSION TAG	UNP Q12BV1
B	332	PHE	-	EXPRESSION TAG	UNP Q12BV1
B	333	GLN	-	EXPRESSION TAG	UNP Q12BV1
B	334	SER	-	EXPRESSION TAG	UNP Q12BV1
B	335	HIS	-	EXPRESSION TAG	UNP Q12BV1
B	336	HIS	-	EXPRESSION TAG	UNP Q12BV1
B	337	HIS	-	EXPRESSION TAG	UNP Q12BV1
B	338	HIS	-	EXPRESSION TAG	UNP Q12BV1
B	339	HIS	-	EXPRESSION TAG	UNP Q12BV1
B	340	HIS	-	EXPRESSION TAG	UNP Q12BV1
B	341	TRP	-	EXPRESSION TAG	UNP Q12BV1
B	342	SER	-	EXPRESSION TAG	UNP Q12BV1
B	343	HIS	-	EXPRESSION TAG	UNP Q12BV1
B	344	PRO	-	EXPRESSION TAG	UNP Q12BV1
B	345	GLN	-	EXPRESSION TAG	UNP Q12BV1
B	346	PHE	-	EXPRESSION TAG	UNP Q12BV1
B	347	GLU	-	EXPRESSION TAG	UNP Q12BV1
B	348	LYS	-	EXPRESSION TAG	UNP Q12BV1
C	327	ALA	-	EXPRESSION TAG	UNP Q12BV1
C	328	GLU	-	EXPRESSION TAG	UNP Q12BV1
C	329	ASN	-	EXPRESSION TAG	UNP Q12BV1
C	330	LEU	-	EXPRESSION TAG	UNP Q12BV1
C	331	TYR	-	EXPRESSION TAG	UNP Q12BV1
C	332	PHE	-	EXPRESSION TAG	UNP Q12BV1
C	333	GLN	-	EXPRESSION TAG	UNP Q12BV1
C	334	SER	-	EXPRESSION TAG	UNP Q12BV1
C	335	HIS	-	EXPRESSION TAG	UNP Q12BV1
C	336	HIS	-	EXPRESSION TAG	UNP Q12BV1
C	337	HIS	-	EXPRESSION TAG	UNP Q12BV1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	338	HIS	-	EXPRESSION TAG	UNP Q12BV1
C	339	HIS	-	EXPRESSION TAG	UNP Q12BV1
C	340	HIS	-	EXPRESSION TAG	UNP Q12BV1
C	341	TRP	-	EXPRESSION TAG	UNP Q12BV1
C	342	SER	-	EXPRESSION TAG	UNP Q12BV1
C	343	HIS	-	EXPRESSION TAG	UNP Q12BV1
C	344	PRO	-	EXPRESSION TAG	UNP Q12BV1
C	345	GLN	-	EXPRESSION TAG	UNP Q12BV1
C	346	PHE	-	EXPRESSION TAG	UNP Q12BV1
C	347	GLU	-	EXPRESSION TAG	UNP Q12BV1
C	348	LYS	-	EXPRESSION TAG	UNP Q12BV1
D	327	ALA	-	EXPRESSION TAG	UNP Q12BV1
D	328	GLU	-	EXPRESSION TAG	UNP Q12BV1
D	329	ASN	-	EXPRESSION TAG	UNP Q12BV1
D	330	LEU	-	EXPRESSION TAG	UNP Q12BV1
D	331	TYR	-	EXPRESSION TAG	UNP Q12BV1
D	332	PHE	-	EXPRESSION TAG	UNP Q12BV1
D	333	GLN	-	EXPRESSION TAG	UNP Q12BV1
D	334	SER	-	EXPRESSION TAG	UNP Q12BV1
D	335	HIS	-	EXPRESSION TAG	UNP Q12BV1
D	336	HIS	-	EXPRESSION TAG	UNP Q12BV1
D	337	HIS	-	EXPRESSION TAG	UNP Q12BV1
D	338	HIS	-	EXPRESSION TAG	UNP Q12BV1
D	339	HIS	-	EXPRESSION TAG	UNP Q12BV1
D	340	HIS	-	EXPRESSION TAG	UNP Q12BV1
D	341	TRP	-	EXPRESSION TAG	UNP Q12BV1
D	342	SER	-	EXPRESSION TAG	UNP Q12BV1
D	343	HIS	-	EXPRESSION TAG	UNP Q12BV1
D	344	PRO	-	EXPRESSION TAG	UNP Q12BV1
D	345	GLN	-	EXPRESSION TAG	UNP Q12BV1
D	346	PHE	-	EXPRESSION TAG	UNP Q12BV1
D	347	GLU	-	EXPRESSION TAG	UNP Q12BV1
D	348	LYS	-	EXPRESSION TAG	UNP Q12BV1
E	327	ALA	-	EXPRESSION TAG	UNP Q12BV1
E	328	GLU	-	EXPRESSION TAG	UNP Q12BV1
E	329	ASN	-	EXPRESSION TAG	UNP Q12BV1
E	330	LEU	-	EXPRESSION TAG	UNP Q12BV1
E	331	TYR	-	EXPRESSION TAG	UNP Q12BV1
E	332	PHE	-	EXPRESSION TAG	UNP Q12BV1
E	333	GLN	-	EXPRESSION TAG	UNP Q12BV1
E	334	SER	-	EXPRESSION TAG	UNP Q12BV1
E	335	HIS	-	EXPRESSION TAG	UNP Q12BV1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	336	HIS	-	EXPRESSION TAG	UNP Q12BV1
E	337	HIS	-	EXPRESSION TAG	UNP Q12BV1
E	338	HIS	-	EXPRESSION TAG	UNP Q12BV1
E	339	HIS	-	EXPRESSION TAG	UNP Q12BV1
E	340	HIS	-	EXPRESSION TAG	UNP Q12BV1
E	341	TRP	-	EXPRESSION TAG	UNP Q12BV1
E	342	SER	-	EXPRESSION TAG	UNP Q12BV1
E	343	HIS	-	EXPRESSION TAG	UNP Q12BV1
E	344	PRO	-	EXPRESSION TAG	UNP Q12BV1
E	345	GLN	-	EXPRESSION TAG	UNP Q12BV1
E	346	PHE	-	EXPRESSION TAG	UNP Q12BV1
E	347	GLU	-	EXPRESSION TAG	UNP Q12BV1
E	348	LYS	-	EXPRESSION TAG	UNP Q12BV1
F	327	ALA	-	EXPRESSION TAG	UNP Q12BV1
F	328	GLU	-	EXPRESSION TAG	UNP Q12BV1
F	329	ASN	-	EXPRESSION TAG	UNP Q12BV1
F	330	LEU	-	EXPRESSION TAG	UNP Q12BV1
F	331	TYR	-	EXPRESSION TAG	UNP Q12BV1
F	332	PHE	-	EXPRESSION TAG	UNP Q12BV1
F	333	GLN	-	EXPRESSION TAG	UNP Q12BV1
F	334	SER	-	EXPRESSION TAG	UNP Q12BV1
F	335	HIS	-	EXPRESSION TAG	UNP Q12BV1
F	336	HIS	-	EXPRESSION TAG	UNP Q12BV1
F	337	HIS	-	EXPRESSION TAG	UNP Q12BV1
F	338	HIS	-	EXPRESSION TAG	UNP Q12BV1
F	339	HIS	-	EXPRESSION TAG	UNP Q12BV1
F	340	HIS	-	EXPRESSION TAG	UNP Q12BV1
F	341	TRP	-	EXPRESSION TAG	UNP Q12BV1
F	342	SER	-	EXPRESSION TAG	UNP Q12BV1
F	343	HIS	-	EXPRESSION TAG	UNP Q12BV1
F	344	PRO	-	EXPRESSION TAG	UNP Q12BV1
F	345	GLN	-	EXPRESSION TAG	UNP Q12BV1
F	346	PHE	-	EXPRESSION TAG	UNP Q12BV1
F	347	GLU	-	EXPRESSION TAG	UNP Q12BV1
F	348	LYS	-	EXPRESSION TAG	UNP Q12BV1
G	327	ALA	-	EXPRESSION TAG	UNP Q12BV1
G	328	GLU	-	EXPRESSION TAG	UNP Q12BV1
G	329	ASN	-	EXPRESSION TAG	UNP Q12BV1
G	330	LEU	-	EXPRESSION TAG	UNP Q12BV1
G	331	TYR	-	EXPRESSION TAG	UNP Q12BV1
G	332	PHE	-	EXPRESSION TAG	UNP Q12BV1
G	333	GLN	-	EXPRESSION TAG	UNP Q12BV1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	334	SER	-	EXPRESSION TAG	UNP Q12BV1
G	335	HIS	-	EXPRESSION TAG	UNP Q12BV1
G	336	HIS	-	EXPRESSION TAG	UNP Q12BV1
G	337	HIS	-	EXPRESSION TAG	UNP Q12BV1
G	338	HIS	-	EXPRESSION TAG	UNP Q12BV1
G	339	HIS	-	EXPRESSION TAG	UNP Q12BV1
G	340	HIS	-	EXPRESSION TAG	UNP Q12BV1
G	341	TRP	-	EXPRESSION TAG	UNP Q12BV1
G	342	SER	-	EXPRESSION TAG	UNP Q12BV1
G	343	HIS	-	EXPRESSION TAG	UNP Q12BV1
G	344	PRO	-	EXPRESSION TAG	UNP Q12BV1
G	345	GLN	-	EXPRESSION TAG	UNP Q12BV1
G	346	PHE	-	EXPRESSION TAG	UNP Q12BV1
G	347	GLU	-	EXPRESSION TAG	UNP Q12BV1
G	348	LYS	-	EXPRESSION TAG	UNP Q12BV1
H	327	ALA	-	EXPRESSION TAG	UNP Q12BV1
H	328	GLU	-	EXPRESSION TAG	UNP Q12BV1
H	329	ASN	-	EXPRESSION TAG	UNP Q12BV1
H	330	LEU	-	EXPRESSION TAG	UNP Q12BV1
H	331	TYR	-	EXPRESSION TAG	UNP Q12BV1
H	332	PHE	-	EXPRESSION TAG	UNP Q12BV1
H	333	GLN	-	EXPRESSION TAG	UNP Q12BV1
H	334	SER	-	EXPRESSION TAG	UNP Q12BV1
H	335	HIS	-	EXPRESSION TAG	UNP Q12BV1
H	336	HIS	-	EXPRESSION TAG	UNP Q12BV1
H	337	HIS	-	EXPRESSION TAG	UNP Q12BV1
H	338	HIS	-	EXPRESSION TAG	UNP Q12BV1
H	339	HIS	-	EXPRESSION TAG	UNP Q12BV1
H	340	HIS	-	EXPRESSION TAG	UNP Q12BV1
H	341	TRP	-	EXPRESSION TAG	UNP Q12BV1
H	342	SER	-	EXPRESSION TAG	UNP Q12BV1
H	343	HIS	-	EXPRESSION TAG	UNP Q12BV1
H	344	PRO	-	EXPRESSION TAG	UNP Q12BV1
H	345	GLN	-	EXPRESSION TAG	UNP Q12BV1
H	346	PHE	-	EXPRESSION TAG	UNP Q12BV1
H	347	GLU	-	EXPRESSION TAG	UNP Q12BV1
H	348	LYS	-	EXPRESSION TAG	UNP Q12BV1

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	1
			12	6	6		
2	B	1	Total	C	O	0	1
			12	6	6		
2	C	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	1
			12	6	6		
2	H	1	Total	C	O	0	1
			12	6	6		

- Molecule 3 is MANGANESE (II) ION (three-letter code: Mn) (formula: Mn).

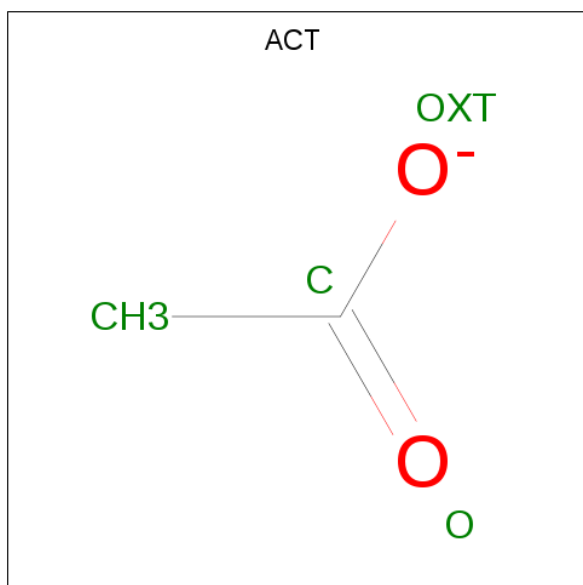
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		
3	H	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	F	1	Total	Mn	0	0
			1	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $\text{C}_2\text{H}_3\text{O}_2$ ).



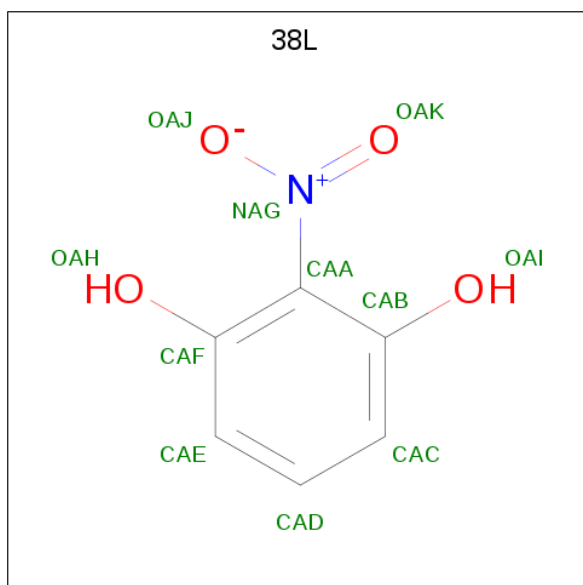
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		

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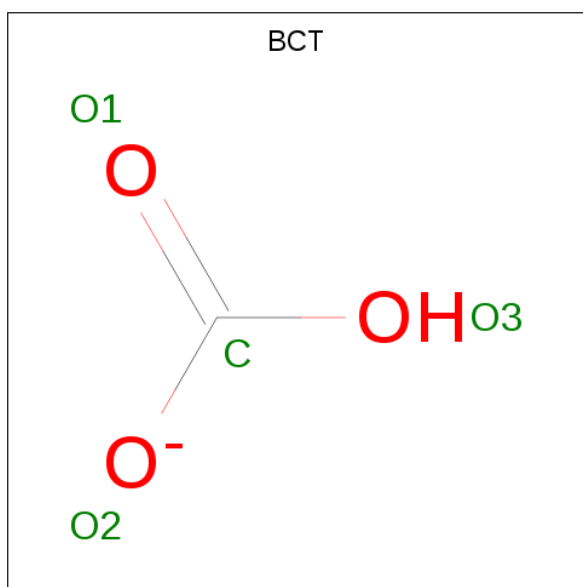
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2-nitrobenzene-1,3-diol (three-letter code: 38L) (formula:  $C_6H_5NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			11	6	1	4		
5	B	1	Total	C	N	O	0	0
			11	6	1	4		
5	C	1	Total	C	N	O	0	0
			11	6	1	4		
5	D	1	Total	C	N	O	0	0
			11	6	1	4		
5	E	1	Total	C	N	O	0	0
			11	6	1	4		
5	F	1	Total	C	N	O	0	0
			11	6	1	4		
5	G	1	Total	C	N	O	0	0
			11	6	1	4		
5	H	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 6 is BICARBONATE ION (three-letter code: BCT) (formula:  $CHO_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			4	1	3		

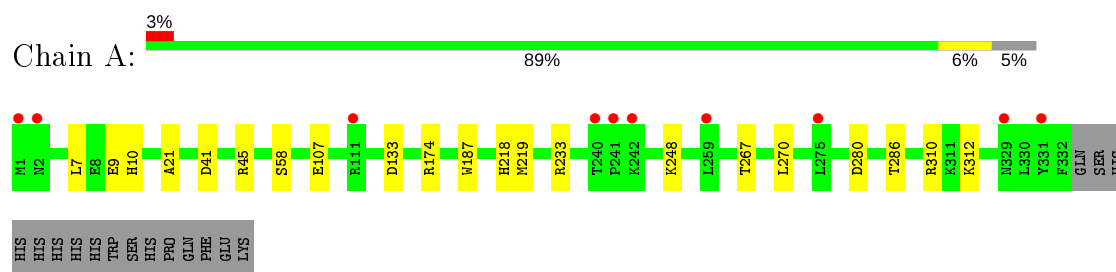
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	287	Total	O	0	1
			288	288		
7	B	245	Total	O	0	0
			245	245		
7	C	273	Total	O	0	0
			273	273		
7	D	240	Total	O	0	0
			240	240		
7	E	312	Total	O	0	0
			312	312		
7	F	290	Total	O	0	0
			290	290		
7	G	310	Total	O	0	0
			310	310		
7	H	284	Total	O	0	0
			284	284		

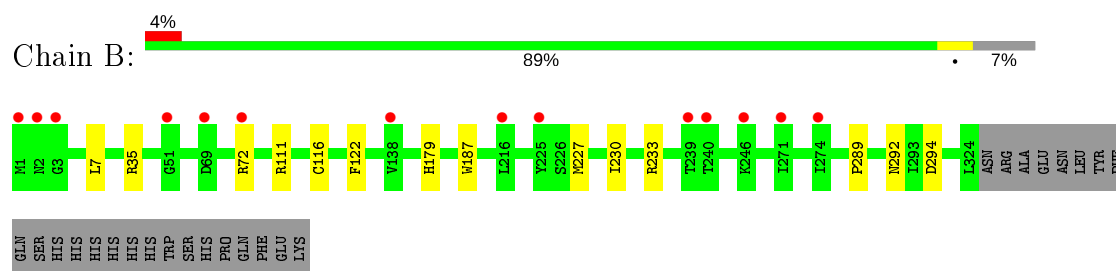
### 3 Residue-property plots [i](#)

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

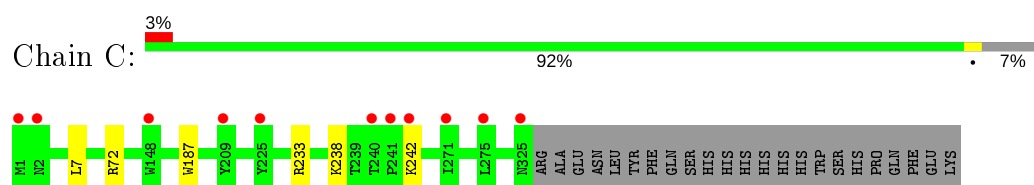
- Molecule 1: Gamma-resorcyate decarboxylase



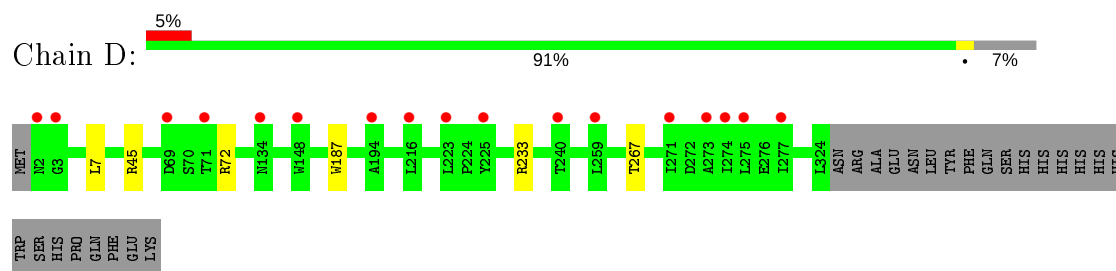
- Molecule 1: Gamma-resorcyate decarboxylase



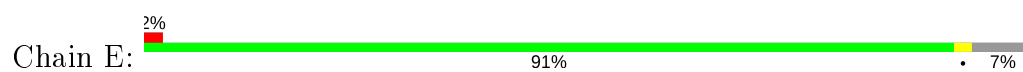
- Molecule 1: Gamma-resorcyate decarboxylase



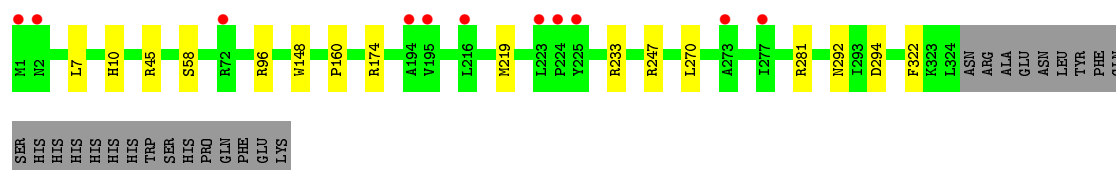
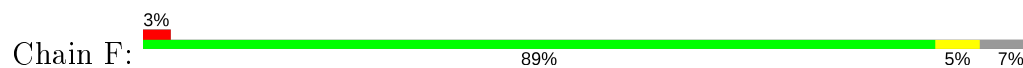
- Molecule 1: Gamma-resorcyate decarboxylase



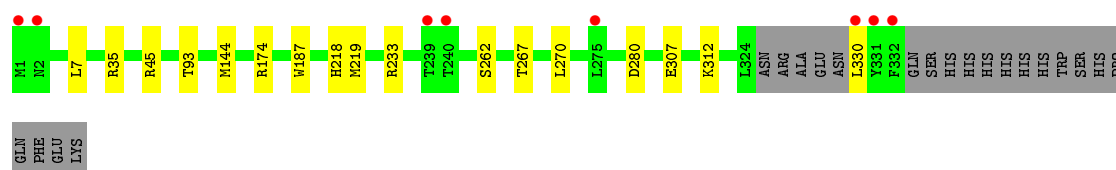
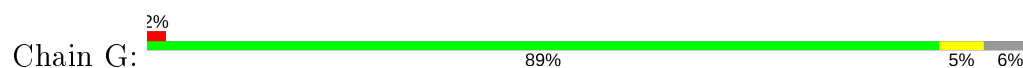
- Molecule 1: Gamma-resorcyate decarboxylase



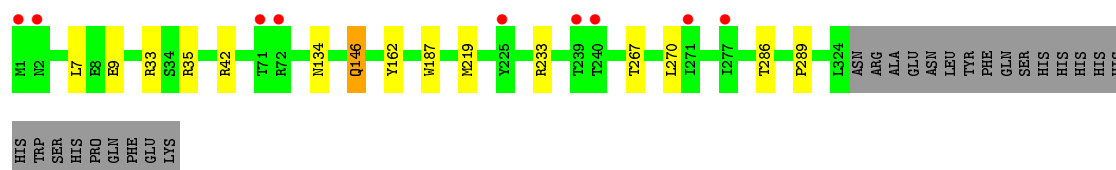
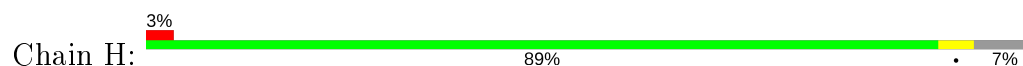
- Molecule 1: Gamma-resorcyate decarboxylase



- Molecule 1: Gamma-resorcyate decarboxylase



- Molecule 1: Gamma-resorcyate decarboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.96Å 151.06Å 143.83Å 90.00° 92.15° 90.00°	Depositor
Resolution (Å)	50.00 – 1.65 44.33 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-1.65) 99.5 (44.33-1.65)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, $R_{free}$	0.189 , 0.223 0.203 , 0.234	Depositor DCC
$R_{free}$ test set	12433 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.9	Xtriage
Anisotropy	0.807	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 55.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.105 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	23784	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3262e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, GOL, MN, 38L, ACT

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	0.56	0/2813	0.70	4/3819 (0.1%)
1	B	0.54	0/2740	0.65	0/3720
1	C	0.55	0/2721	0.69	0/3696
1	D	0.58	2/2704 (0.1%)	0.69	0/3674
1	E	0.74	0/2727	0.75	2/3705 (0.1%)
1	F	0.69	1/2742 (0.0%)	0.73	1/3723 (0.0%)
1	G	0.73	0/2788	0.80	5/3783 (0.1%)
1	H	0.70	0/2759	0.72	0/3746
All	All	0.64	3/21994 (0.0%)	0.72	12/29866 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	148	TRP	CB-CG	5.93	1.60	1.50
1	D	45[A]	ARG	N-CA	5.14	1.56	1.46
1	D	45[B]	ARG	N-CA	5.14	1.56	1.46

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	45	ARG	NE-CZ-NH2	8.92	124.76	120.30
1	A	174	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	G	45	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	133	ASP	CB-CG-OD1	5.53	123.28	118.30
1	F	247	ARG	NE-CZ-NH2	-5.34	117.63	120.30

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	2729	0	2654	9	0
1	B	2655	0	2592	5	0
1	C	2648	0	2567	1	0
1	D	2628	0	2548	1	0
1	E	2645	0	2565	4	0
1	F	2660	0	2591	7	0
1	G	2702	0	2630	8	0
1	H	2671	0	2603	8	0
2	A	18	0	24	4	0
2	B	12	0	16	0	0
2	C	6	0	8	0	0
2	F	12	0	16	1	0
2	H	12	0	16	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	4	0	3	1	0
4	B	4	0	3	0	0
4	C	8	0	6	0	0
4	D	4	0	3	0	0
4	E	8	0	6	0	0
4	F	4	0	3	0	0
4	G	4	0	3	0	0
4	H	8	0	6	0	0
5	A	11	0	3	0	0
5	B	11	0	4	0	0
5	C	11	0	3	0	0
5	D	11	0	3	0	0
5	E	11	0	3	0	0
5	F	11	0	3	0	0
5	G	11	0	3	0	0
5	H	11	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	4	0	0	0	0
7	A	288	0	0	5	0
7	B	245	0	0	1	0
7	C	273	0	0	1	0
7	D	240	0	0	0	0
7	E	312	0	0	1	0
7	F	290	0	0	2	0
7	G	310	0	0	2	0
7	H	284	0	0	2	0
All	All	23784	0	20888	46	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 1.

The worst 5 of 46 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)
4:A:404:ACT:H1	7:A:783:HOH:O	1.80	0.79
2:F:401[A]:GOL:H32	1:G:267:THR:OG1	1.84	0.78
1:H:267:THR:OG1	2:H:401[A]:GOL:H32	1.83	0.78
1:A:41:ASP:OD1	1:A:45[A]:ARG:NH1	2.20	0.74
1:H:146:GLN:HE21	1:H:146:GLN:H	1.36	0.73

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	336/348 (97%)	328 (98%)	7 (2%)	1 (0%)	41 22
1	B	327/348 (94%)	317 (97%)	9 (3%)	1 (0%)	41 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	326/348 (94%)	317 (97%)	8 (2%)	1 (0%)	41	22
1	D	323/348 (93%)	314 (97%)	8 (2%)	1 (0%)	41	22
1	E	327/348 (94%)	318 (97%)	8 (2%)	1 (0%)	41	22
1	F	327/348 (94%)	319 (98%)	8 (2%)	0	100	100
1	G	330/348 (95%)	321 (97%)	8 (2%)	1 (0%)	41	22
1	H	330/348 (95%)	322 (98%)	7 (2%)	1 (0%)	41	22
All	All	2626/2784 (94%)	2556 (97%)	63 (2%)	7 (0%)	41	22

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	187	TRP
1	A	187	TRP
1	B	187	TRP
1	C	187	TRP
1	E	187	TRP

### 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	281/294 (96%)	278 (99%)	3 (1%)	73	57
1	B	276/294 (94%)	272 (99%)	4 (1%)	67	46
1	C	273/294 (93%)	269 (98%)	4 (2%)	65	44
1	D	272/294 (92%)	269 (99%)	3 (1%)	73	57
1	E	274/294 (93%)	270 (98%)	4 (2%)	65	44
1	F	276/294 (94%)	272 (99%)	4 (1%)	67	46
1	G	281/294 (96%)	277 (99%)	4 (1%)	67	46
1	H	277/294 (94%)	273 (99%)	4 (1%)	67	46
All	All	2210/2352 (94%)	2180 (99%)	30 (1%)	69	46

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	233	ARG
1	E	233	ARG
1	H	146	GLN
1	E	72	ARG
1	E	307	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	254	ASN
1	E	2	ASN
1	G	254	ASN
1	D	179	HIS
1	H	132	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 38 ligands modelled in this entry, 8 are monoatomic - leaving 30 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	F	401[A]	-	5,5,5	0.47	0	5,5,5	0.86	0
4	ACT	E	402	-	1,3,3	2.46	1 (100%)	0,3,3	0.00	-
5	38L	A	405	3	10,11,11	0.88	1 (10%)	11,15,15	1.22	2 (18%)
2	GOL	H	401[A]	-	5,5,5	0.46	0	5,5,5	0.46	0
2	GOL	H	401[B]	-	5,5,5	0.38	0	5,5,5	0.89	0
2	GOL	C	401	-	5,5,5	0.31	0	5,5,5	0.21	0
2	GOL	A	401	-	5,5,5	0.27	0	5,5,5	0.41	0
4	ACT	H	403	-	1,3,3	2.33	1 (100%)	0,3,3	0.00	-
4	ACT	E	403	-	1,3,3	1.50	0	0,3,3	0.00	-
5	38L	B	404	3	10,11,11	1.16	1 (10%)	11,15,15	0.87	0
4	ACT	D	402	-	1,3,3	0.74	0	0,3,3	0.00	-
5	38L	H	405	3	10,11,11	1.02	1 (10%)	11,15,15	1.01	1 (9%)
5	38L	G	403	3	10,11,11	1.59	1 (10%)	11,15,15	1.03	2 (18%)
2	GOL	B	401[B]	-	5,5,5	0.43	0	5,5,5	0.34	0
2	GOL	B	401[A]	-	5,5,5	0.31	0	5,5,5	0.37	0
4	ACT	H	404	-	1,3,3	1.43	0	0,3,3	0.00	-
5	38L	C	405	3	10,11,11	0.61	0	11,15,15	1.21	2 (18%)
4	ACT	A	404	-	1,3,3	1.79	0	0,3,3	0.00	-
4	ACT	C	404	-	1,3,3	1.39	0	0,3,3	0.00	-
2	GOL	A	402[B]	-	5,5,5	0.28	0	5,5,5	0.65	0
5	38L	E	404	3	10,11,11	1.13	1 (10%)	11,15,15	1.21	2 (18%)
2	GOL	A	402[A]	-	5,5,5	0.47	0	5,5,5	0.30	0
4	ACT	G	402	-	1,3,3	3.59	1 (100%)	0,3,3	0.00	-
6	BCT	G	404	-	0,3,3	0.00	-	0,3,3	0.00	-
5	38L	F	404	3	10,11,11	1.22	2 (20%)	11,15,15	0.94	1 (9%)
4	ACT	F	403	-	1,3,3	1.93	0	0,3,3	0.00	-
4	ACT	C	403	-	1,3,3	1.60	0	0,3,3	0.00	-
4	ACT	B	403	-	1,3,3	1.94	0	0,3,3	0.00	-
2	GOL	F	401[B]	-	5,5,5	0.24	0	5,5,5	0.38	0
5	38L	D	403	3	10,11,11	0.94	1 (10%)	11,15,15	1.32	1 (9%)

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	C	401	-	-	4/4/4/4	-
2	GOL	B	401[B]	-	-	4/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	402[B]	-	-	3/4/4/4	-
2	GOL	F	401[A]	-	-	4/4/4/4	-
5	38L	B	404	3	-	0/2/4/4	0/1/1/1
5	38L	A	405	3	-	0/2/4/4	0/1/1/1
2	GOL	B	401[A]	-	-	4/4/4/4	-
5	38L	F	404	3	-	0/2/4/4	0/1/1/1
5	38L	C	405	3	-	0/2/4/4	0/1/1/1
2	GOL	H	401[A]	-	-	4/4/4/4	-
2	GOL	A	402[A]	-	-	4/4/4/4	-
2	GOL	H	401[B]	-	-	2/4/4/4	-
5	38L	H	405	3	-	0/2/4/4	0/1/1/1
5	38L	G	403	3	-	0/2/4/4	0/1/1/1
5	38L	E	404	3	-	0/2/4/4	0/1/1/1
2	GOL	F	401[B]	-	-	4/4/4/4	-
5	38L	D	403	3	-	0/2/4/4	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	403	38L	CAA-NAG	-4.00	1.38	1.45
4	G	402	ACT	CH3-C	3.59	1.53	1.48
5	B	404	38L	CAA-NAG	-2.84	1.40	1.45
5	E	404	38L	CAA-NAG	-2.72	1.40	1.45
5	D	403	38L	CAA-NAG	-2.56	1.41	1.45

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	403	38L	CAC-CAB-CAA	2.65	120.47	118.30
5	C	405	38L	CAE-CAF-CAA	2.64	120.46	118.30
5	A	405	38L	CAE-CAF-CAA	2.59	120.42	118.30
5	A	405	38L	CAC-CAB-CAA	2.44	120.30	118.30
5	E	404	38L	CAE-CAF-CAA	2.39	120.26	118.30

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	401[A]	GOL	O2-C2-C3-O3
2	H	401[B]	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	401[B]	GOL	O1-C1-C2-C3
2	B	401[B]	GOL	C1-C2-C3-O3
2	B	401[A]	GOL	O1-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401[A]	GOL	1	0
2	H	401[A]	GOL	1	0
2	H	401[B]	GOL	2	0
4	A	404	ACT	1	0
2	A	402[B]	GOL	1	0
2	A	402[A]	GOL	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	332/348 (95%)	0.20	10 (3%) 50 51	28, 36, 57, 77	0
1	B	324/348 (93%)	0.31	14 (4%) 35 34	29, 39, 59, 82	0
1	C	325/348 (93%)	0.24	11 (3%) 45 45	28, 36, 56, 105	0
1	D	323/348 (92%)	0.33	17 (5%) 26 25	29, 38, 59, 78	0
1	E	324/348 (93%)	0.06	6 (1%) 66 69	18, 25, 44, 88	0
1	F	324/348 (93%)	0.13	11 (3%) 45 45	20, 28, 44, 79	0
1	G	327/348 (93%)	0.13	8 (2%) 59 59	19, 26, 47, 95	0
1	H	324/348 (93%)	0.09	9 (2%) 53 53	19, 28, 46, 72	0
All	All	2603/2784 (93%)	0.19	86 (3%) 46 47	18, 33, 54, 105	0

The worst 5 of 86 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	330	LEU	6.3
1	G	331	TYR	6.2
1	D	2	ASN	5.8
1	G	332	PHE	5.3
1	C	325	ASN	5.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	C	401	6/6	0.70	0.35	62,71,80,106	0
4	ACT	C	404	4/4	0.76	0.16	39,45,51,52	0
2	GOL	B	401[B]	6/6	0.87	0.21	34,42,66,77	6
2	GOL	B	401[A]	6/6	0.87	0.21	34,41,56,80	6
2	GOL	F	401[A]	6/6	0.87	0.18	20,28,44,72	6
2	GOL	F	401[B]	6/6	0.87	0.18	25,29,64,64	6
6	BCT	G	404	4/4	0.88	0.20	34,38,59,100	0
4	ACT	E	403	4/4	0.88	0.21	31,37,45,96	0
2	GOL	A	402[A]	6/6	0.89	0.17	25,42,64,84	6
4	ACT	H	404	4/4	0.89	0.17	42,43,47,50	0
2	GOL	A	402[B]	6/6	0.89	0.17	29,42,52,63	6
4	ACT	B	403	4/4	0.90	0.13	39,42,43,46	0
4	ACT	G	402	4/4	0.90	0.11	27,29,31,32	0
2	GOL	A	401	6/6	0.91	0.18	39,63,75,79	0
2	GOL	H	401[A]	6/6	0.91	0.20	22,30,44,56	6
4	ACT	C	403	4/4	0.91	0.12	35,40,41,46	0
2	GOL	H	401[B]	6/6	0.91	0.20	21,29,45,71	6
5	38L	A	405	11/11	0.91	0.10	35,37,44,94	0
5	38L	D	403	11/11	0.91	0.09	32,37,55,65	0
5	38L	B	404	11/11	0.92	0.09	32,41,57,67	0
4	ACT	A	404	4/4	0.93	0.11	35,38,44,44	0
4	ACT	D	402	4/4	0.93	0.18	37,42,44,47	0
4	ACT	H	403	4/4	0.93	0.14	30,30,30,33	0
4	ACT	F	403	4/4	0.93	0.14	32,33,33,37	0
5	38L	F	404	11/11	0.94	0.08	26,29,35,57	0
4	ACT	E	402	4/4	0.94	0.10	27,30,31,39	0
5	38L	H	405	11/11	0.95	0.09	25,29,35,67	0
5	38L	C	405	11/11	0.95	0.08	35,41,50,71	0
5	38L	E	404	11/11	0.95	0.09	23,27,32,72	0
5	38L	G	403	11/11	0.95	0.11	21,28,29,79	0
3	MN	D	401	1/1	0.99	0.08	34,34,34,34	0
3	MN	B	402	1/1	0.99	0.06	33,33,33,33	0
3	MN	C	402	1/1	0.99	0.06	32,32,32,32	0
3	MN	A	403	1/1	0.99	0.06	31,31,31,31	0
3	MN	F	402	1/1	1.00	0.09	22,22,22,22	0
3	MN	G	401	1/1	1.00	0.07	21,21,21,21	0
3	MN	E	401	1/1	1.00	0.09	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MN	H	402	1/1	1.00	0.07	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.