



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 12:25 pm BST

PDB ID : 3UHJ
Title : Crystal structure of a probable glycerol dehydrogenase from Sinorhizobium meliloti 1021
Authors : Agarwal, R.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRG)
Deposited on : 2011-11-03
Resolution : 2.34 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (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

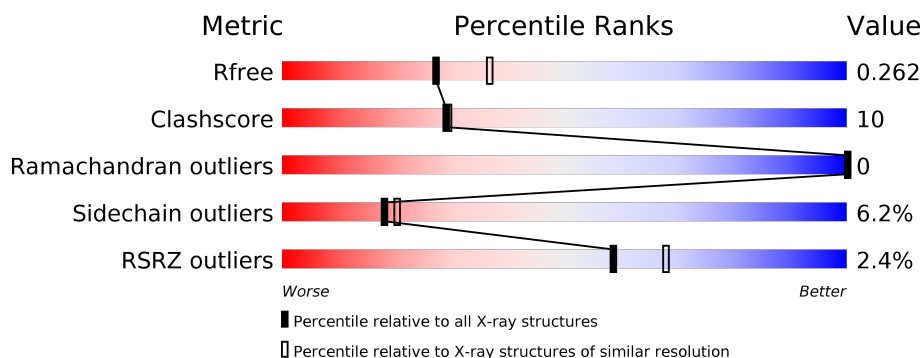
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 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	387	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	387	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>•</div> <div>8%</div> </div> </div>
1	C	387	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>•</div> <div>8%</div> </div> </div>
1	D	387	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>•</div> <div>8%</div> </div> </div>
1	E	387	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>•</div> <div>8%</div> </div> </div>
1	F	387	<div> <div>8%</div> <div> <div></div> <div>74%</div> <div>15%</div> <div>•</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	387	
1	H	387	

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	487	-	-	X	-
2	GOL	E	487	-	-	X	-
2	GOL	G	487	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21320 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 Probable glycerol dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	Se	0	0	0
			2633	1660	468	492	9	4			
1	B	356	Total	C	N	O	S	Se	0	0	0
			2571	1621	455	483	9	3			
1	C	355	Total	C	N	O	S	Se	0	0	0
			2585	1632	453	488	9	3			
1	D	357	Total	C	N	O	S	Se	0	0	0
			2617	1647	467	491	9	3			
1	E	355	Total	C	N	O	S	Se	0	0	0
			2601	1638	462	489	9	3			
1	F	351	Total	C	N	O	S	Se	0	0	0
			2532	1591	452	477	9	3			
1	G	356	Total	C	N	O	S	Se	0	0	0
			2597	1639	459	487	9	3			
1	H	355	Total	C	N	O	S	Se	0	0	0
			2601	1641	459	489	9	3			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	EXPRESSION TAG	UNP Q92MR2
A	2	HIS	-	EXPRESSION TAG	UNP Q92MR2
A	3	HIS	-	EXPRESSION TAG	UNP Q92MR2
A	4	HIS	-	EXPRESSION TAG	UNP Q92MR2
A	5	HIS	-	EXPRESSION TAG	UNP Q92MR2
A	6	HIS	-	EXPRESSION TAG	UNP Q92MR2
A	7	HIS	-	EXPRESSION TAG	UNP Q92MR2
A	8	SER	-	EXPRESSION TAG	UNP Q92MR2
A	9	SER	-	EXPRESSION TAG	UNP Q92MR2
A	10	GLY	-	EXPRESSION TAG	UNP Q92MR2
A	11	VAL	-	EXPRESSION TAG	UNP Q92MR2
A	12	ASP	-	EXPRESSION TAG	UNP Q92MR2
A	13	LEU	-	EXPRESSION TAG	UNP Q92MR2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	14	GLY	-	EXPRESSION TAG	UNP Q92MR2
A	15	THR	-	EXPRESSION TAG	UNP Q92MR2
A	16	GLU	-	EXPRESSION TAG	UNP Q92MR2
A	17	ASN	-	EXPRESSION TAG	UNP Q92MR2
A	18	LEU	-	EXPRESSION TAG	UNP Q92MR2
A	19	TYR	-	EXPRESSION TAG	UNP Q92MR2
A	20	PHE	-	EXPRESSION TAG	UNP Q92MR2
A	21	GLN	-	EXPRESSION TAG	UNP Q92MR2
A	22	SER	-	EXPRESSION TAG	UNP Q92MR2
A	23	MSE	-	EXPRESSION TAG	UNP Q92MR2
B	1	MSE	-	EXPRESSION TAG	UNP Q92MR2
B	2	HIS	-	EXPRESSION TAG	UNP Q92MR2
B	3	HIS	-	EXPRESSION TAG	UNP Q92MR2
B	4	HIS	-	EXPRESSION TAG	UNP Q92MR2
B	5	HIS	-	EXPRESSION TAG	UNP Q92MR2
B	6	HIS	-	EXPRESSION TAG	UNP Q92MR2
B	7	HIS	-	EXPRESSION TAG	UNP Q92MR2
B	8	SER	-	EXPRESSION TAG	UNP Q92MR2
B	9	SER	-	EXPRESSION TAG	UNP Q92MR2
B	10	GLY	-	EXPRESSION TAG	UNP Q92MR2
B	11	VAL	-	EXPRESSION TAG	UNP Q92MR2
B	12	ASP	-	EXPRESSION TAG	UNP Q92MR2
B	13	LEU	-	EXPRESSION TAG	UNP Q92MR2
B	14	GLY	-	EXPRESSION TAG	UNP Q92MR2
B	15	THR	-	EXPRESSION TAG	UNP Q92MR2
B	16	GLU	-	EXPRESSION TAG	UNP Q92MR2
B	17	ASN	-	EXPRESSION TAG	UNP Q92MR2
B	18	LEU	-	EXPRESSION TAG	UNP Q92MR2
B	19	TYR	-	EXPRESSION TAG	UNP Q92MR2
B	20	PHE	-	EXPRESSION TAG	UNP Q92MR2
B	21	GLN	-	EXPRESSION TAG	UNP Q92MR2
B	22	SER	-	EXPRESSION TAG	UNP Q92MR2
B	23	MSE	-	EXPRESSION TAG	UNP Q92MR2
C	1	MSE	-	EXPRESSION TAG	UNP Q92MR2
C	2	HIS	-	EXPRESSION TAG	UNP Q92MR2
C	3	HIS	-	EXPRESSION TAG	UNP Q92MR2
C	4	HIS	-	EXPRESSION TAG	UNP Q92MR2
C	5	HIS	-	EXPRESSION TAG	UNP Q92MR2
C	6	HIS	-	EXPRESSION TAG	UNP Q92MR2
C	7	HIS	-	EXPRESSION TAG	UNP Q92MR2
C	8	SER	-	EXPRESSION TAG	UNP Q92MR2
C	9	SER	-	EXPRESSION TAG	UNP Q92MR2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	10	GLY	-	EXPRESSION TAG	UNP Q92MR2
C	11	VAL	-	EXPRESSION TAG	UNP Q92MR2
C	12	ASP	-	EXPRESSION TAG	UNP Q92MR2
C	13	LEU	-	EXPRESSION TAG	UNP Q92MR2
C	14	GLY	-	EXPRESSION TAG	UNP Q92MR2
C	15	THR	-	EXPRESSION TAG	UNP Q92MR2
C	16	GLU	-	EXPRESSION TAG	UNP Q92MR2
C	17	ASN	-	EXPRESSION TAG	UNP Q92MR2
C	18	LEU	-	EXPRESSION TAG	UNP Q92MR2
C	19	TYR	-	EXPRESSION TAG	UNP Q92MR2
C	20	PHE	-	EXPRESSION TAG	UNP Q92MR2
C	21	GLN	-	EXPRESSION TAG	UNP Q92MR2
C	22	SER	-	EXPRESSION TAG	UNP Q92MR2
C	23	MSE	-	EXPRESSION TAG	UNP Q92MR2
D	1	MSE	-	EXPRESSION TAG	UNP Q92MR2
D	2	HIS	-	EXPRESSION TAG	UNP Q92MR2
D	3	HIS	-	EXPRESSION TAG	UNP Q92MR2
D	4	HIS	-	EXPRESSION TAG	UNP Q92MR2
D	5	HIS	-	EXPRESSION TAG	UNP Q92MR2
D	6	HIS	-	EXPRESSION TAG	UNP Q92MR2
D	7	HIS	-	EXPRESSION TAG	UNP Q92MR2
D	8	SER	-	EXPRESSION TAG	UNP Q92MR2
D	9	SER	-	EXPRESSION TAG	UNP Q92MR2
D	10	GLY	-	EXPRESSION TAG	UNP Q92MR2
D	11	VAL	-	EXPRESSION TAG	UNP Q92MR2
D	12	ASP	-	EXPRESSION TAG	UNP Q92MR2
D	13	LEU	-	EXPRESSION TAG	UNP Q92MR2
D	14	GLY	-	EXPRESSION TAG	UNP Q92MR2
D	15	THR	-	EXPRESSION TAG	UNP Q92MR2
D	16	GLU	-	EXPRESSION TAG	UNP Q92MR2
D	17	ASN	-	EXPRESSION TAG	UNP Q92MR2
D	18	LEU	-	EXPRESSION TAG	UNP Q92MR2
D	19	TYR	-	EXPRESSION TAG	UNP Q92MR2
D	20	PHE	-	EXPRESSION TAG	UNP Q92MR2
D	21	GLN	-	EXPRESSION TAG	UNP Q92MR2
D	22	SER	-	EXPRESSION TAG	UNP Q92MR2
D	23	MSE	-	EXPRESSION TAG	UNP Q92MR2
E	1	MSE	-	EXPRESSION TAG	UNP Q92MR2
E	2	HIS	-	EXPRESSION TAG	UNP Q92MR2
E	3	HIS	-	EXPRESSION TAG	UNP Q92MR2
E	4	HIS	-	EXPRESSION TAG	UNP Q92MR2
E	5	HIS	-	EXPRESSION TAG	UNP Q92MR2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	6	HIS	-	EXPRESSION TAG	UNP Q92MR2
E	7	HIS	-	EXPRESSION TAG	UNP Q92MR2
E	8	SER	-	EXPRESSION TAG	UNP Q92MR2
E	9	SER	-	EXPRESSION TAG	UNP Q92MR2
E	10	GLY	-	EXPRESSION TAG	UNP Q92MR2
E	11	VAL	-	EXPRESSION TAG	UNP Q92MR2
E	12	ASP	-	EXPRESSION TAG	UNP Q92MR2
E	13	LEU	-	EXPRESSION TAG	UNP Q92MR2
E	14	GLY	-	EXPRESSION TAG	UNP Q92MR2
E	15	THR	-	EXPRESSION TAG	UNP Q92MR2
E	16	GLU	-	EXPRESSION TAG	UNP Q92MR2
E	17	ASN	-	EXPRESSION TAG	UNP Q92MR2
E	18	LEU	-	EXPRESSION TAG	UNP Q92MR2
E	19	TYR	-	EXPRESSION TAG	UNP Q92MR2
E	20	PHE	-	EXPRESSION TAG	UNP Q92MR2
E	21	GLN	-	EXPRESSION TAG	UNP Q92MR2
E	22	SER	-	EXPRESSION TAG	UNP Q92MR2
E	23	MSE	-	EXPRESSION TAG	UNP Q92MR2
F	1	MSE	-	EXPRESSION TAG	UNP Q92MR2
F	2	HIS	-	EXPRESSION TAG	UNP Q92MR2
F	3	HIS	-	EXPRESSION TAG	UNP Q92MR2
F	4	HIS	-	EXPRESSION TAG	UNP Q92MR2
F	5	HIS	-	EXPRESSION TAG	UNP Q92MR2
F	6	HIS	-	EXPRESSION TAG	UNP Q92MR2
F	7	HIS	-	EXPRESSION TAG	UNP Q92MR2
F	8	SER	-	EXPRESSION TAG	UNP Q92MR2
F	9	SER	-	EXPRESSION TAG	UNP Q92MR2
F	10	GLY	-	EXPRESSION TAG	UNP Q92MR2
F	11	VAL	-	EXPRESSION TAG	UNP Q92MR2
F	12	ASP	-	EXPRESSION TAG	UNP Q92MR2
F	13	LEU	-	EXPRESSION TAG	UNP Q92MR2
F	14	GLY	-	EXPRESSION TAG	UNP Q92MR2
F	15	THR	-	EXPRESSION TAG	UNP Q92MR2
F	16	GLU	-	EXPRESSION TAG	UNP Q92MR2
F	17	ASN	-	EXPRESSION TAG	UNP Q92MR2
F	18	LEU	-	EXPRESSION TAG	UNP Q92MR2
F	19	TYR	-	EXPRESSION TAG	UNP Q92MR2
F	20	PHE	-	EXPRESSION TAG	UNP Q92MR2
F	21	GLN	-	EXPRESSION TAG	UNP Q92MR2
F	22	SER	-	EXPRESSION TAG	UNP Q92MR2
F	23	MSE	-	EXPRESSION TAG	UNP Q92MR2
G	1	MSE	-	EXPRESSION TAG	UNP Q92MR2

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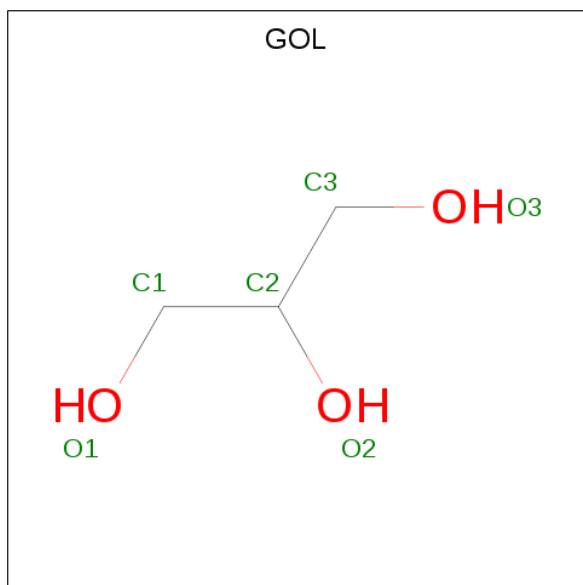
Chain	Residue	Modelled	Actual	Comment	Reference
G	2	HIS	-	EXPRESSION TAG	UNP Q92MR2
G	3	HIS	-	EXPRESSION TAG	UNP Q92MR2
G	4	HIS	-	EXPRESSION TAG	UNP Q92MR2
G	5	HIS	-	EXPRESSION TAG	UNP Q92MR2
G	6	HIS	-	EXPRESSION TAG	UNP Q92MR2
G	7	HIS	-	EXPRESSION TAG	UNP Q92MR2
G	8	SER	-	EXPRESSION TAG	UNP Q92MR2
G	9	SER	-	EXPRESSION TAG	UNP Q92MR2
G	10	GLY	-	EXPRESSION TAG	UNP Q92MR2
G	11	VAL	-	EXPRESSION TAG	UNP Q92MR2
G	12	ASP	-	EXPRESSION TAG	UNP Q92MR2
G	13	LEU	-	EXPRESSION TAG	UNP Q92MR2
G	14	GLY	-	EXPRESSION TAG	UNP Q92MR2
G	15	THR	-	EXPRESSION TAG	UNP Q92MR2
G	16	GLU	-	EXPRESSION TAG	UNP Q92MR2
G	17	ASN	-	EXPRESSION TAG	UNP Q92MR2
G	18	LEU	-	EXPRESSION TAG	UNP Q92MR2
G	19	TYR	-	EXPRESSION TAG	UNP Q92MR2
G	20	PHE	-	EXPRESSION TAG	UNP Q92MR2
G	21	GLN	-	EXPRESSION TAG	UNP Q92MR2
G	22	SER	-	EXPRESSION TAG	UNP Q92MR2
G	23	MSE	-	EXPRESSION TAG	UNP Q92MR2
H	1	MSE	-	EXPRESSION TAG	UNP Q92MR2
H	2	HIS	-	EXPRESSION TAG	UNP Q92MR2
H	3	HIS	-	EXPRESSION TAG	UNP Q92MR2
H	4	HIS	-	EXPRESSION TAG	UNP Q92MR2
H	5	HIS	-	EXPRESSION TAG	UNP Q92MR2
H	6	HIS	-	EXPRESSION TAG	UNP Q92MR2
H	7	HIS	-	EXPRESSION TAG	UNP Q92MR2
H	8	SER	-	EXPRESSION TAG	UNP Q92MR2
H	9	SER	-	EXPRESSION TAG	UNP Q92MR2
H	10	GLY	-	EXPRESSION TAG	UNP Q92MR2
H	11	VAL	-	EXPRESSION TAG	UNP Q92MR2
H	12	ASP	-	EXPRESSION TAG	UNP Q92MR2
H	13	LEU	-	EXPRESSION TAG	UNP Q92MR2
H	14	GLY	-	EXPRESSION TAG	UNP Q92MR2
H	15	THR	-	EXPRESSION TAG	UNP Q92MR2
H	16	GLU	-	EXPRESSION TAG	UNP Q92MR2
H	17	ASN	-	EXPRESSION TAG	UNP Q92MR2
H	18	LEU	-	EXPRESSION TAG	UNP Q92MR2
H	19	TYR	-	EXPRESSION TAG	UNP Q92MR2
H	20	PHE	-	EXPRESSION TAG	UNP Q92MR2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	21	GLN	-	EXPRESSION TAG	UNP Q92MR2
H	22	SER	-	EXPRESSION TAG	UNP Q92MR2
H	23	MSE	-	EXPRESSION TAG	UNP Q92MR2

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	Zn 1	0	0
3	H	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	A	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0

- Molecule 4 is SELENIUM ATOM (three-letter code: SE) (formula: Se).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total 1	Se 1	0	0
4	E	1	Total 1	Se 1	0	0

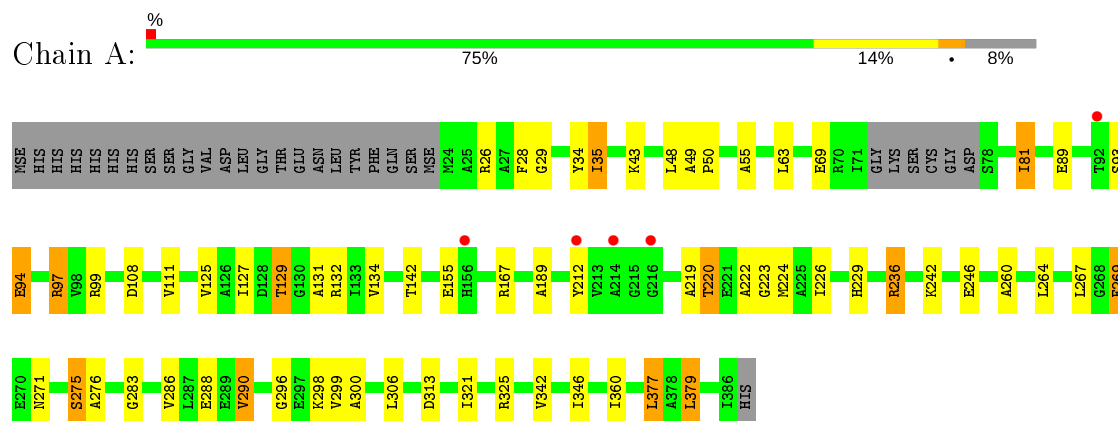
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total 79	O 79	0	0
5	B	80	Total 80	O 80	0	0
5	C	65	Total 65	O 65	0	0
5	D	54	Total 54	O 54	0	0
5	E	79	Total 79	O 79	0	0
5	F	55	Total 55	O 55	0	0
5	G	78	Total 78	O 78	0	0
5	H	47	Total 47	O 47	0	0

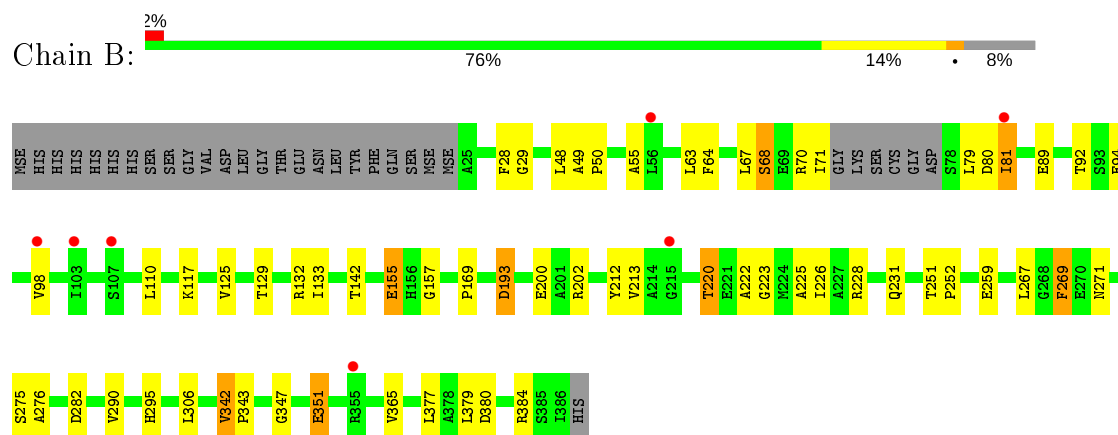
3 Residue-property plots [i](#)

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.

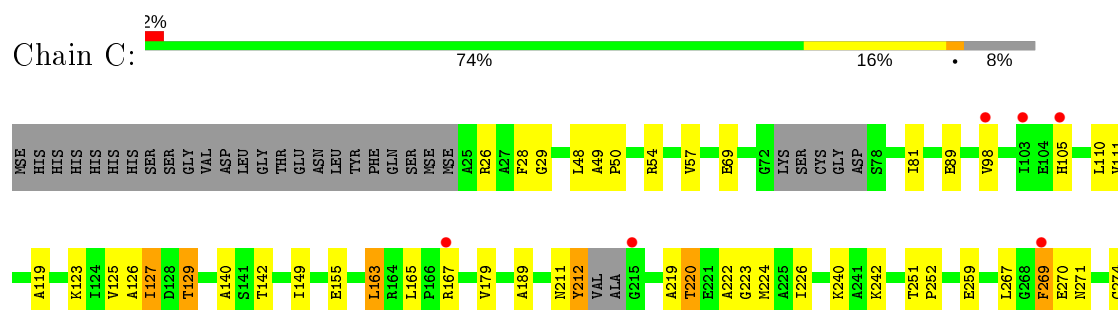
• Molecule 1: Probable glycerol dehydrogenase



• Molecule 1: Probable glycerol dehydrogenase

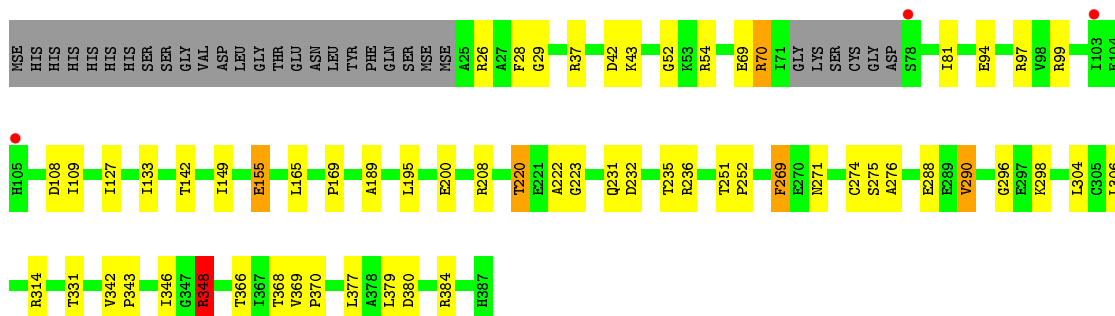
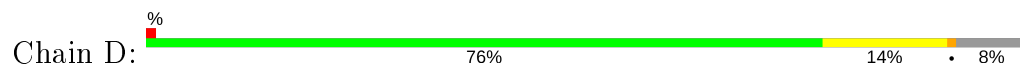


• Molecule 1: Probable glycerol dehydrogenase

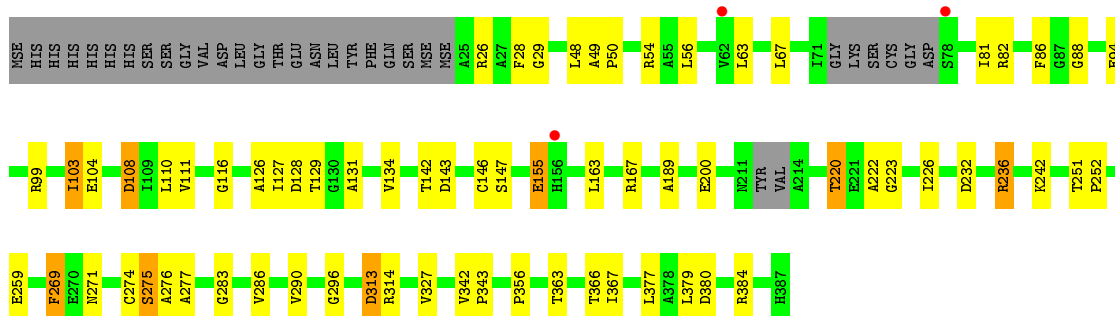
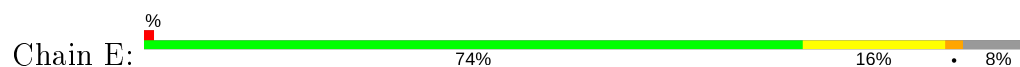




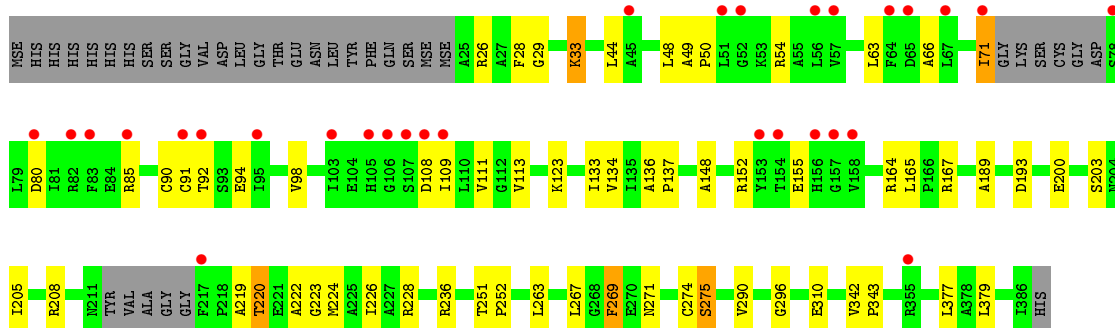
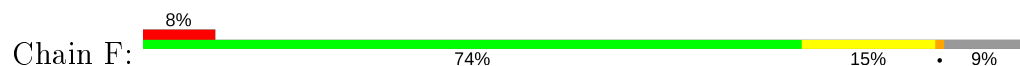
- Molecule 1: Probable glycerol dehydrogenase



- Molecule 1: Probable glycerol dehydrogenase

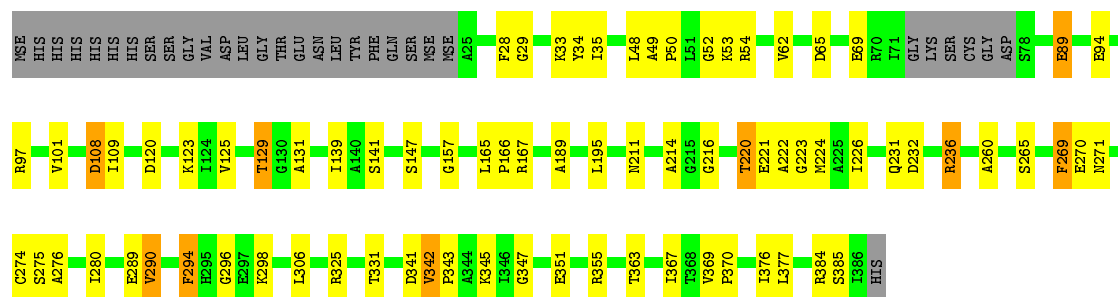


- Molecule 1: Probable glycerol dehydrogenase

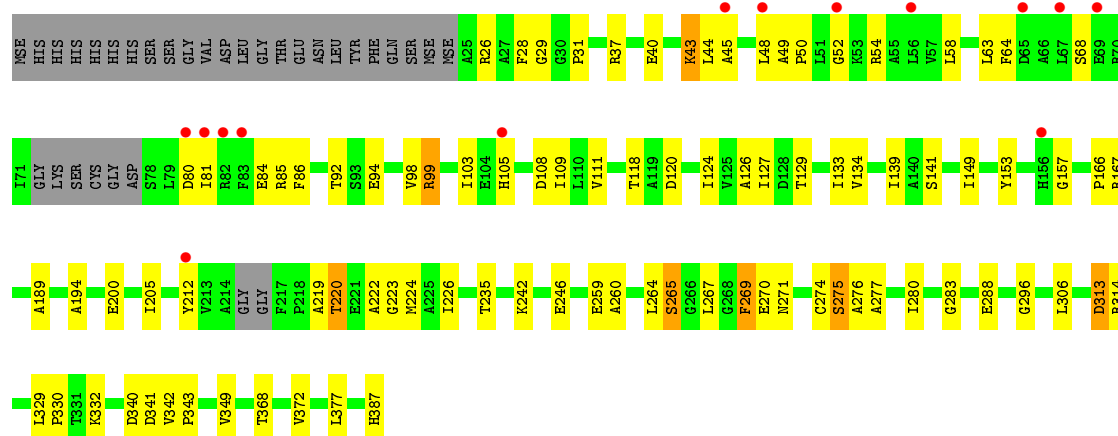


- Molecule 1: Probable glycerol dehydrogenase





- Molecule 1: Probable glycerol dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.48 Å 99.00 Å 104.73 Å 76.94° 83.38° 71.47°	Depositor
Resolution (Å)	45.98 – 2.34 45.97 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.2 (45.98-2.34) 98.2 (45.97-2.34)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.34 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.197 , 0.264 0.201 , 0.262	Depositor DCC
R_{free} test set	6116 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21320	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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, ZN, SE

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	1.04	1/2670 (0.0%)	0.91	2/3622 (0.1%)
1	B	0.96	2/2607 (0.1%)	0.88	3/3544 (0.1%)
1	C	0.95	2/2621 (0.1%)	0.85	1/3559 (0.0%)
1	D	0.92	3/2654 (0.1%)	0.91	3/3601 (0.1%)
1	E	0.95	3/2637 (0.1%)	0.86	2/3578 (0.1%)
1	F	0.86	0/2567	0.83	4/3488 (0.1%)
1	G	0.99	1/2633 (0.0%)	0.89	1/3576 (0.0%)
1	H	0.87	0/2638	0.85	3/3582 (0.1%)
All	All	0.94	12/21027 (0.1%)	0.87	19/28550 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	146	CYS	CB-SG	-5.77	1.72	1.81
1	G	34	TYR	CD2-CE2	-5.76	1.30	1.39
1	D	69	GLU	CG-CD	5.70	1.60	1.51
1	D	155	GLU	CG-CD	5.49	1.60	1.51
1	B	155	GLU	CG-CD	5.41	1.60	1.51

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	379	LEU	CA-CB-CG	-5.99	101.53	115.30
1	C	26	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	F	228	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	B	202	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	G	384	ARG	NE-CZ-NH2	-5.54	117.53	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	2633	0	2654	54	0
1	B	2571	0	2546	51	0
1	C	2585	0	2571	50	0
1	D	2617	0	2620	47	0
1	E	2601	0	2602	49	0
1	F	2532	0	2482	40	0
1	G	2597	0	2601	57	0
1	H	2601	0	2595	64	0
2	A	6	0	8	4	0
2	B	6	0	8	3	0
2	C	6	0	8	2	0
2	D	6	0	8	1	0
2	E	6	0	8	4	0
2	G	6	0	8	2	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	E	1	0	0	0	0
4	H	1	0	0	0	0
5	A	79	0	0	1	0
5	B	80	0	0	1	0
5	C	65	0	0	1	0
5	D	54	0	0	4	0
5	E	79	0	0	2	0
5	F	55	0	0	3	0
5	G	78	0	0	2	0
5	H	47	0	0	3	0
All	All	21320	0	20719	398	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 10.

The worst 5 of 398 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:149:ILE:HD13	1:C:269:PHE:HE2	1.06	1.19
1:A:290:VAL:HG12	1:A:298:LYS:HE2	1.32	1.09
1:B:220:THR:HG22	1:B:223:GLY:H	1.17	1.05
1:G:29:GLY:H	1:G:271:ASN:HD21	1.05	1.02
1:C:149:ILE:HD13	1:C:269:PHE:CE2	1.95	1.01

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	353/387 (91%)	338 (96%)	15 (4%)	0	100	100
1	B	352/387 (91%)	341 (97%)	11 (3%)	0	100	100
1	C	349/387 (90%)	336 (96%)	13 (4%)	0	100	100
1	D	353/387 (91%)	342 (97%)	11 (3%)	0	100	100
1	E	349/387 (90%)	340 (97%)	9 (3%)	0	100	100
1	F	345/387 (89%)	329 (95%)	16 (5%)	0	100	100
1	G	352/387 (91%)	339 (96%)	13 (4%)	0	100	100
1	H	349/387 (90%)	332 (95%)	17 (5%)	0	100	100
All	All	2802/3096 (90%)	2697 (96%)	105 (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	265/292 (91%)	245 (92%)	20 (8%)	13	14
1	B	251/292 (86%)	235 (94%)	16 (6%)	17	19
1	C	256/292 (88%)	242 (94%)	14 (6%)	21	25
1	D	262/292 (90%)	252 (96%)	10 (4%)	33	41
1	E	260/292 (89%)	246 (95%)	14 (5%)	22	26
1	F	245/292 (84%)	228 (93%)	17 (7%)	15	16
1	G	258/292 (88%)	238 (92%)	20 (8%)	12	12
1	H	260/292 (89%)	244 (94%)	16 (6%)	18	20
All	All	2057/2336 (88%)	1930 (94%)	127 (6%)	18	20

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	348	ARG
1	E	356	PRO
1	H	99	ARG
1	D	377	LEU
1	E	108	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	231	GLN
1	E	271	ASN
1	G	231	GLN
1	D	271	ASN
1	G	271	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 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	C	487	-	5,5,5	0.47	0	5,5,5	0.75	0
2	GOL	A	487	-	5,5,5	0.49	0	5,5,5	0.35	0
2	GOL	G	487	-	5,5,5	0.48	0	5,5,5	1.15	1 (20%)
2	GOL	E	487	-	5,5,5	0.50	0	5,5,5	0.71	0
2	GOL	B	487	-	5,5,5	0.77	0	5,5,5	0.78	0
2	GOL	D	487	-	5,5,5	0.47	0	5,5,5	1.53	1 (20%)

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	487	-	-	4/4/4/4	-
2	GOL	A	487	-	-	4/4/4/4	-
2	GOL	G	487	-	-	0/4/4/4	-
2	GOL	E	487	-	-	4/4/4/4	-
2	GOL	B	487	-	-	0/4/4/4	-
2	GOL	D	487	-	-	4/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	487	GOL	C3-C2-C1	-2.64	101.45	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	487	GOL	O1-C1-C2	-2.04	100.40	110.20

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	487	GOL	O1-C1-C2-C3
2	C	487	GOL	C1-C2-C3-O3
2	C	487	GOL	O2-C2-C3-O3
2	A	487	GOL	C1-C2-C3-O3
2	A	487	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	487	GOL	2	0
2	A	487	GOL	4	0
2	G	487	GOL	2	0
2	E	487	GOL	4	0
2	B	487	GOL	3	0
2	D	487	GOL	1	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, 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	353/387 (91%)	-0.01	5 (1%) 75 82	19, 32, 50, 56	0
1	B	353/387 (91%)	0.05	7 (1%) 65 74	20, 34, 57, 72	0
1	C	352/387 (90%)	0.02	7 (1%) 65 74	20, 35, 51, 62	0
1	D	354/387 (91%)	-0.08	3 (0%) 86 90	20, 35, 53, 64	0
1	E	352/387 (90%)	-0.09	3 (0%) 84 89	20, 35, 51, 61	0
1	F	348/387 (89%)	0.34	30 (8%) 10 16	25, 40, 66, 74	0
1	G	353/387 (91%)	-0.19	0 100 100	22, 34, 50, 56	0
1	H	352/387 (90%)	0.21	14 (3%) 38 49	23, 40, 60, 70	0
All	All	2817/3096 (90%)	0.03	69 (2%) 59 68	19, 35, 57, 74	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	156	HIS	5.0
1	F	56	LEU	4.9
1	H	81	ILE	4.7
1	B	56	LEU	4.6
1	F	103	ILE	4.5

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, 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	B-factors(Å ²)	Q<0.9
2	GOL	G	487	6/6	0.78	0.48	24,26,27,28	6
3	ZN	F	388	1/1	0.85	0.09	37,37,37,37	1
2	GOL	C	487	6/6	0.86	0.45	34,35,36,40	6
2	GOL	D	487	6/6	0.86	0.62	34,37,38,39	6
2	GOL	E	487	6/6	0.89	0.38	29,35,38,40	6
2	GOL	B	487	6/6	0.90	0.42	27,33,35,37	6
2	GOL	A	487	6/6	0.92	0.28	34,36,40,40	6
3	ZN	H	389	1/1	0.93	0.10	44,44,44,44	1
3	ZN	G	388	1/1	0.93	0.15	36,36,36,36	1
3	ZN	C	388	1/1	0.94	0.14	41,41,41,41	1
3	ZN	B	388	1/1	0.96	0.08	47,47,47,47	1
4	SE	H	388	1/1	0.96	0.04	75,75,75,75	0
3	ZN	A	388	1/1	0.97	0.04	38,38,38,38	1
4	SE	E	388	1/1	0.98	0.09	69,69,69,69	0
3	ZN	E	389	1/1	0.98	0.12	39,39,39,39	1
3	ZN	D	388	1/1	0.98	0.07	42,42,42,42	1

6.5 Other polymers ⓘ

There are no such residues in this entry.