



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:35 PM UTC

PDB ID : 8DHE / pdb\_00008dhe  
Title : Tannerella forsythia beta-glucuronidase (mL1)  
Authors : Lietzan, A.D.; Redinbo, M.R.  
Deposited on : 2022-06-27  
Resolution : 2.20 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

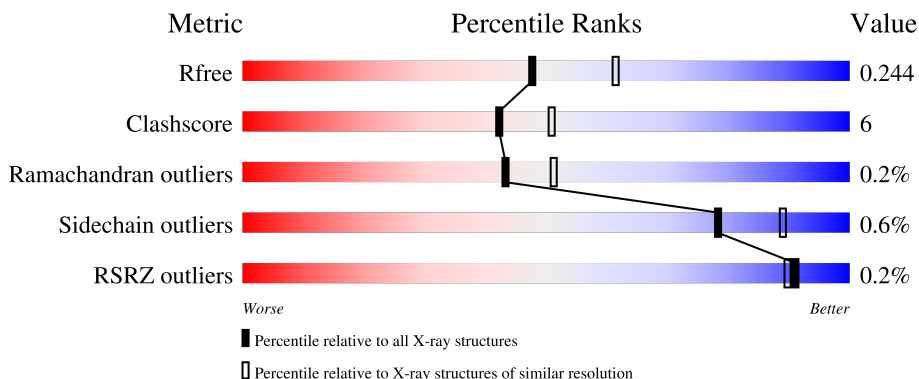
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 of 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	687	81% 14% .
1	B	687	81% 15% .
1	C	687	79% 16% .
1	D	687	80% 16% .

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22005 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 Glycosyl hydrolase family 2, sugar bindingdomain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	660	5331	3373	954	986	18	0	3	0
1	B	660	5309	3361	947	983	18	0	0	0
1	C	657	5285	3349	937	981	18	0	0	0
1	D	660	5289	3350	939	982	18	0	1	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A0E4FP39
A	2	HIS	-	expression tag	UNP A0A0E4FP39
A	3	HIS	-	expression tag	UNP A0A0E4FP39
A	4	HIS	-	expression tag	UNP A0A0E4FP39
A	5	HIS	-	expression tag	UNP A0A0E4FP39
A	6	HIS	-	expression tag	UNP A0A0E4FP39
A	7	HIS	-	expression tag	UNP A0A0E4FP39
A	8	SER	-	expression tag	UNP A0A0E4FP39
A	9	SER	-	expression tag	UNP A0A0E4FP39
A	10	GLY	-	expression tag	UNP A0A0E4FP39
A	11	VAL	-	expression tag	UNP A0A0E4FP39
A	12	ASP	-	expression tag	UNP A0A0E4FP39
A	13	LEU	-	expression tag	UNP A0A0E4FP39
A	14	GLY	-	expression tag	UNP A0A0E4FP39
A	15	THR	-	expression tag	UNP A0A0E4FP39
A	16	GLU	-	expression tag	UNP A0A0E4FP39
A	17	ASN	-	expression tag	UNP A0A0E4FP39
A	18	LEU	-	expression tag	UNP A0A0E4FP39
A	19	TYR	-	expression tag	UNP A0A0E4FP39
A	20	PHE	-	expression tag	UNP A0A0E4FP39
A	21	GLN	-	expression tag	UNP A0A0E4FP39

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	-	expression tag	UNP A0A0E4FP39
A	23	ASN	-	expression tag	UNP A0A0E4FP39
B	1	MET	-	initiating methionine	UNP A0A0E4FP39
B	2	HIS	-	expression tag	UNP A0A0E4FP39
B	3	HIS	-	expression tag	UNP A0A0E4FP39
B	4	HIS	-	expression tag	UNP A0A0E4FP39
B	5	HIS	-	expression tag	UNP A0A0E4FP39
B	6	HIS	-	expression tag	UNP A0A0E4FP39
B	7	HIS	-	expression tag	UNP A0A0E4FP39
B	8	SER	-	expression tag	UNP A0A0E4FP39
B	9	SER	-	expression tag	UNP A0A0E4FP39
B	10	GLY	-	expression tag	UNP A0A0E4FP39
B	11	VAL	-	expression tag	UNP A0A0E4FP39
B	12	ASP	-	expression tag	UNP A0A0E4FP39
B	13	LEU	-	expression tag	UNP A0A0E4FP39
B	14	GLY	-	expression tag	UNP A0A0E4FP39
B	15	THR	-	expression tag	UNP A0A0E4FP39
B	16	GLU	-	expression tag	UNP A0A0E4FP39
B	17	ASN	-	expression tag	UNP A0A0E4FP39
B	18	LEU	-	expression tag	UNP A0A0E4FP39
B	19	TYR	-	expression tag	UNP A0A0E4FP39
B	20	PHE	-	expression tag	UNP A0A0E4FP39
B	21	GLN	-	expression tag	UNP A0A0E4FP39
B	22	SER	-	expression tag	UNP A0A0E4FP39
B	23	ASN	-	expression tag	UNP A0A0E4FP39
C	1	MET	-	initiating methionine	UNP A0A0E4FP39
C	2	HIS	-	expression tag	UNP A0A0E4FP39
C	3	HIS	-	expression tag	UNP A0A0E4FP39
C	4	HIS	-	expression tag	UNP A0A0E4FP39
C	5	HIS	-	expression tag	UNP A0A0E4FP39
C	6	HIS	-	expression tag	UNP A0A0E4FP39
C	7	HIS	-	expression tag	UNP A0A0E4FP39
C	8	SER	-	expression tag	UNP A0A0E4FP39
C	9	SER	-	expression tag	UNP A0A0E4FP39
C	10	GLY	-	expression tag	UNP A0A0E4FP39
C	11	VAL	-	expression tag	UNP A0A0E4FP39
C	12	ASP	-	expression tag	UNP A0A0E4FP39
C	13	LEU	-	expression tag	UNP A0A0E4FP39
C	14	GLY	-	expression tag	UNP A0A0E4FP39
C	15	THR	-	expression tag	UNP A0A0E4FP39
C	16	GLU	-	expression tag	UNP A0A0E4FP39
C	17	ASN	-	expression tag	UNP A0A0E4FP39

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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	LEU	-	expression tag	UNP A0A0E4FP39
C	19	TYR	-	expression tag	UNP A0A0E4FP39
C	20	PHE	-	expression tag	UNP A0A0E4FP39
C	21	GLN	-	expression tag	UNP A0A0E4FP39
C	22	SER	-	expression tag	UNP A0A0E4FP39
C	23	ASN	-	expression tag	UNP A0A0E4FP39
D	1	MET	-	initiating methionine	UNP A0A0E4FP39
D	2	HIS	-	expression tag	UNP A0A0E4FP39
D	3	HIS	-	expression tag	UNP A0A0E4FP39
D	4	HIS	-	expression tag	UNP A0A0E4FP39
D	5	HIS	-	expression tag	UNP A0A0E4FP39
D	6	HIS	-	expression tag	UNP A0A0E4FP39
D	7	HIS	-	expression tag	UNP A0A0E4FP39
D	8	SER	-	expression tag	UNP A0A0E4FP39
D	9	SER	-	expression tag	UNP A0A0E4FP39
D	10	GLY	-	expression tag	UNP A0A0E4FP39
D	11	VAL	-	expression tag	UNP A0A0E4FP39
D	12	ASP	-	expression tag	UNP A0A0E4FP39
D	13	LEU	-	expression tag	UNP A0A0E4FP39
D	14	GLY	-	expression tag	UNP A0A0E4FP39
D	15	THR	-	expression tag	UNP A0A0E4FP39
D	16	GLU	-	expression tag	UNP A0A0E4FP39
D	17	ASN	-	expression tag	UNP A0A0E4FP39
D	18	LEU	-	expression tag	UNP A0A0E4FP39
D	19	TYR	-	expression tag	UNP A0A0E4FP39
D	20	PHE	-	expression tag	UNP A0A0E4FP39
D	21	GLN	-	expression tag	UNP A0A0E4FP39
D	22	SER	-	expression tag	UNP A0A0E4FP39
D	23	ASN	-	expression tag	UNP A0A0E4FP39

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	189	Total O 189 189	0	0

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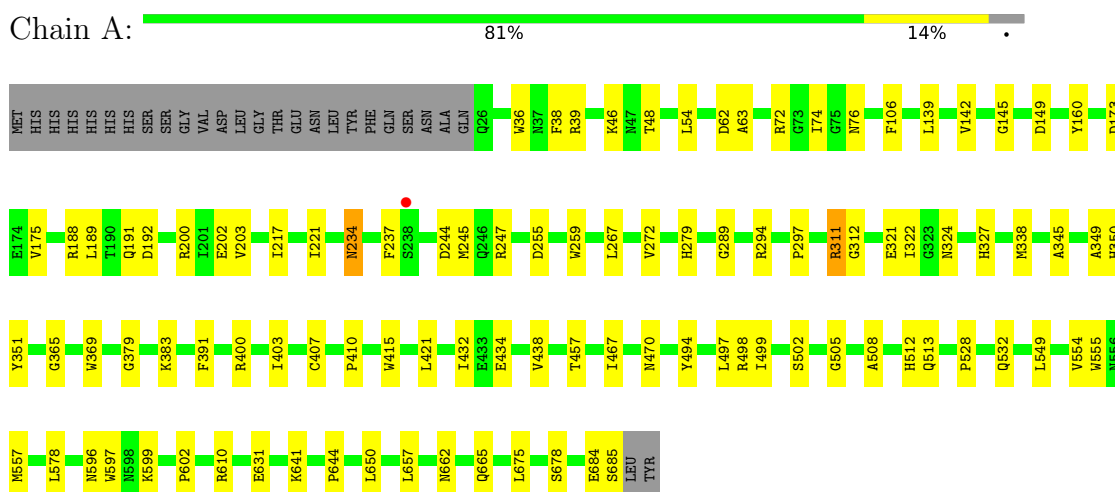
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	B	187	Total 187	O 187	0	0
5	C	174	Total 174	O 174	0	0
5	D	189	Total 189	O 189	0	0

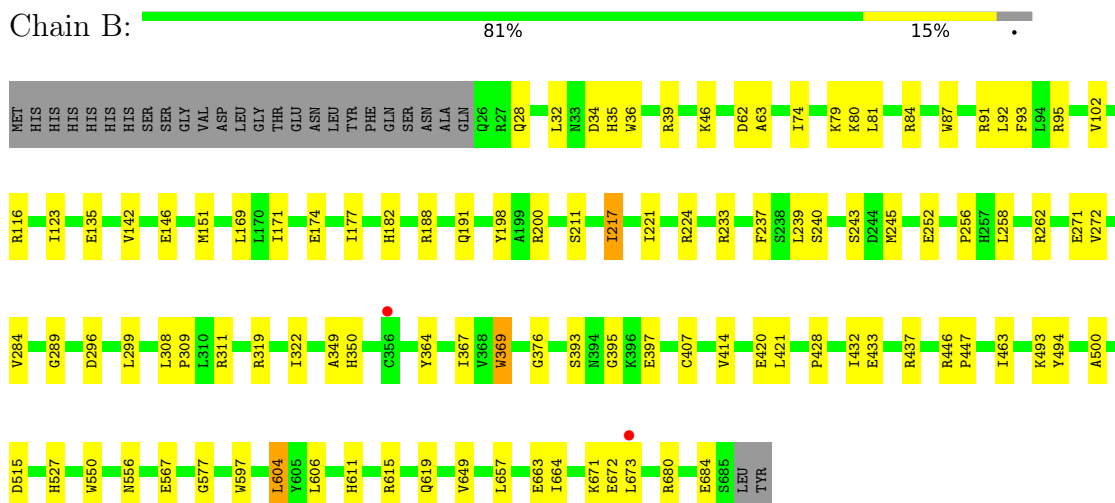
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

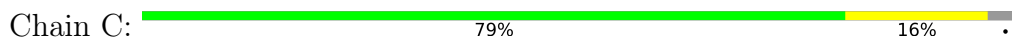
- Molecule 1: Glycosyl hydrolase family 2, sugar bindingdomain protein

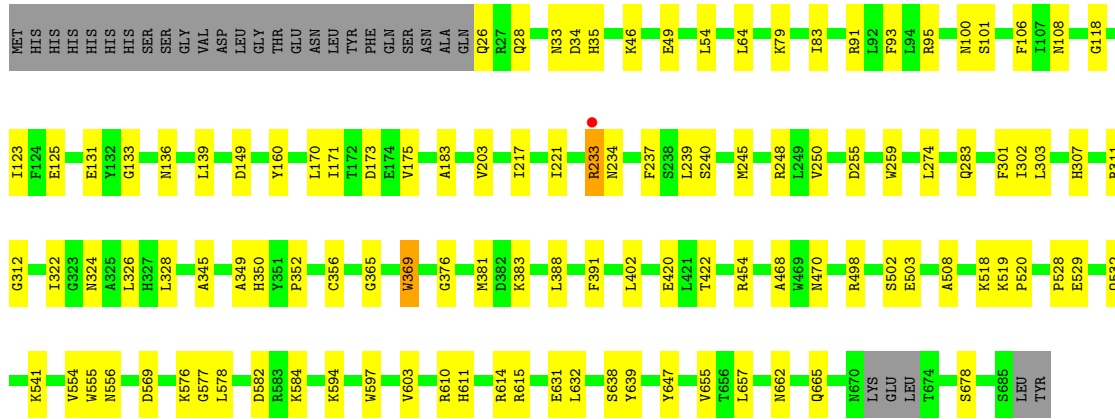


- Molecule 1: Glycosyl hydrolase family 2, sugar bindingdomain protein



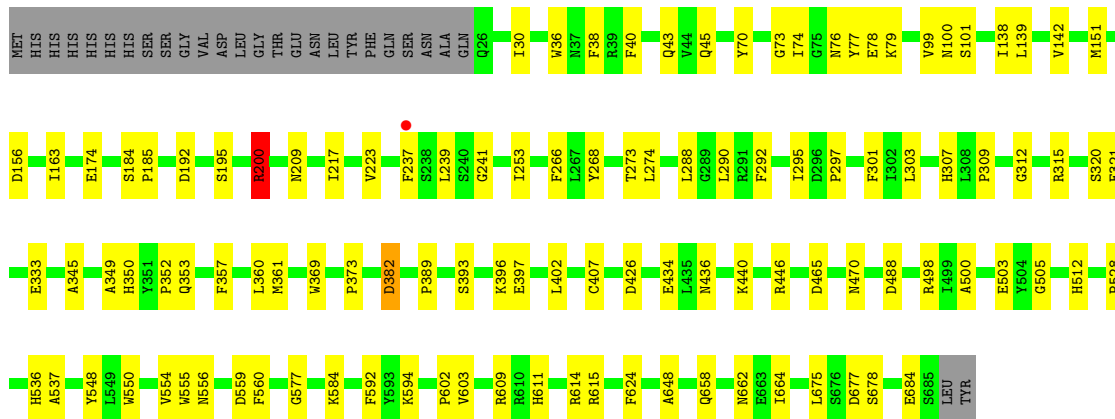
- Molecule 1: Glycosyl hydrolase family 2, sugar bindingdomain protein





● Molecule 1: Glycosyl hydrolase family 2, sugar binding domain protein

Chain D: 80% 16%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.44Å 139.65Å 109.82Å 90.00° 94.50° 90.00°	Depositor
Resolution (Å)	51.71 – 2.20 51.71 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.7 (51.71-2.20) 96.7 (51.71-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.205 , 0.244 0.206 , 0.244	Depositor DCC
$R_{free}$ test set	2008 reflections (1.31%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtrriage
Anisotropy	0.618	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 29.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22005	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: GOL, EDO, CL

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	0.44	1/5479 (0.0%)	0.62	0/7441
1	B	0.40	0/5451	0.60	1/7404 (0.0%)
1	C	0.41	1/5426 (0.0%)	0.60	0/7369
1	D	0.38	0/5431	0.58	1/7382 (0.0%)
All	All	0.41	2/21787 (0.0%)	0.60	2/29596 (0.0%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	ASP	C-O	-11.77	1.18	1.23
1	C	255	ASP	C-O	-5.24	1.21	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	200	ARG	CB-CG-CD	-5.31	99.09	111.30
1	B	604	LEU	CD1-CG-CD2	5.16	122.14	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	233	ARG	Sidechain
1	D	200	ARG	Sidechain

## 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	5331	0	5045	58	0
1	B	5309	0	5007	63	0
1	C	5285	0	4986	77	0
1	D	5289	0	4978	69	0
2	A	12	0	18	1	0
2	B	4	0	6	1	0
2	D	8	0	12	2	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	1	0
4	D	1	0	0	0	0
5	A	189	0	0	4	0
5	B	187	0	0	4	0
5	C	174	0	0	7	0
5	D	189	0	0	8	0
All	All	22005	0	20084	261	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 6.

The worst 5 of 261 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:576:LYS:NZ	5:C:801:HOH:O	2.02	0.91
1:D:192:ASP:OD2	1:D:200:ARG:NH2	2.05	0.89
1:A:245:MET:HE3	1:A:247:ARG:HD3	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:GLU:H	1:C:136:ASN:HD21	1.23	0.85
1:C:233:ARG:NH2	1:C:250:VAL:O	2.18	0.77

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	661/687 (96%)	630 (95%)	30 (4%)	1 (0%)	43	51
1	B	658/687 (96%)	626 (95%)	31 (5%)	1 (0%)	43	51
1	C	653/687 (95%)	627 (96%)	25 (4%)	1 (0%)	43	51
1	D	659/687 (96%)	632 (96%)	25 (4%)	2 (0%)	36	42
All	All	2631/2748 (96%)	2515 (96%)	111 (4%)	5 (0%)	43	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	HIS
1	C	35	HIS
1	D	382	ASP
1	D	426	ASP
1	B	35	HIS

### 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	553/594 (93%)	548 (99%)	5 (1%)	70	84
1	B	547/594 (92%)	542 (99%)	5 (1%)	70	84
1	C	546/594 (92%)	544 (100%)	2 (0%)	84	92
1	D	546/594 (92%)	544 (100%)	2 (0%)	84	92
All	All	2192/2376 (92%)	2178 (99%)	14 (1%)	78	89

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	369	TRP
1	B	604	LEU
1	D	369	TRP
1	C	369	TRP
1	D	273	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	307	HIS
1	D	324	ASN
1	D	491	HIS
1	B	234	ASN
1	B	109	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	EDO	A	801	-	3,3,3	0.45	0	2,2,2	0.67	0
2	EDO	D	702	-	3,3,3	0.56	0	2,2,2	0.16	0
2	EDO	A	803	-	3,3,3	0.57	0	2,2,2	0.18	0
3	GOL	A	802	-	5,5,5	1.03	0	5,5,5	1.14	0
3	GOL	D	701	-	5,5,5	0.81	0	5,5,5	1.50	1 (20%)
2	EDO	B	702	-	3,3,3	0.49	0	2,2,2	0.38	0
3	GOL	B	701	-	5,5,5	0.83	0	5,5,5	1.24	0
3	GOL	C	701	-	5,5,5	1.03	1 (20%)	5,5,5	1.24	1 (20%)
2	EDO	A	804	-	3,3,3	0.54	0	2,2,2	0.21	0
2	EDO	D	703	-	3,3,3	0.32	0	2,2,2	0.76	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	EDO	A	801	-	-	0/1/1/1	-
2	EDO	D	702	-	-	0/1/1/1	-
2	EDO	A	803	-	-	0/1/1/1	-
3	GOL	A	802	-	-	4/4/4/4	-
3	GOL	D	701	-	-	0/4/4/4	-
2	EDO	B	702	-	-	0/1/1/1	-
3	GOL	B	701	-	-	2/4/4/4	-
3	GOL	C	701	-	-	0/4/4/4	-
2	EDO	A	804	-	-	0/1/1/1	-
2	EDO	D	703	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	701	GOL	C1-C2	2.13	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	D	701	GOL	C3-C2-C1	-2.76	101.67	111.80
3	C	701	GOL	C3-C2-C1	-2.03	104.35	111.80

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	701	GOL	O1-C1-C2-C3
3	A	802	GOL	O2-C2-C3-O3
3	A	802	GOL	O1-C1-C2-C3
3	A	802	GOL	C1-C2-C3-O3
3	B	701	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	EDO	1	0
2	D	702	EDO	2	0
3	D	701	GOL	1	0
2	B	702	EDO	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 [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, 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	660/687 (96%)	-0.24	1 (0%) 91 90	16, 33, 53, 82	3 (0%)
1	B	660/687 (96%)	-0.23	2 (0%) 90 88	24, 36, 52, 77	0
1	C	657/687 (95%)	-0.20	1 (0%) 91 90	24, 35, 50, 68	0
1	D	660/687 (96%)	-0.13	1 (0%) 91 90	16, 37, 55, 82	1 (0%)
All	All	2637/2748 (95%)	-0.20	5 (0%) 91 90	16, 35, 53, 82	4 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	356	CYS	2.5
1	A	238	SER	2.3
1	B	673	LEU	2.3
1	D	237	PHE	2.1
1	C	233	ARG	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	EDO	A	801	4/4	0.88	0.10	27,29,32,40	0
3	GOL	C	701	6/6	0.90	0.10	35,38,41,46	0
3	GOL	A	802	6/6	0.91	0.10	38,41,42,43	0
2	EDO	A	804	4/4	0.91	0.10	35,36,39,43	0
2	EDO	D	702	4/4	0.92	0.12	39,42,44,48	0
3	GOL	D	701	6/6	0.92	0.09	32,38,40,42	0
2	EDO	B	702	4/4	0.93	0.08	45,46,46,50	0
2	EDO	A	803	4/4	0.93	0.10	39,39,40,50	0
2	EDO	D	703	4/4	0.93	0.08	39,39,41,43	0
3	GOL	B	701	6/6	0.95	0.07	33,36,40,42	0
4	CL	C	702	1/1	0.97	0.05	41,41,41,41	0
4	CL	D	704	1/1	0.97	0.06	40,40,40,40	0
4	CL	A	805	1/1	0.99	0.03	41,41,41,41	0
4	CL	B	703	1/1	0.99	0.03	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.