



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 09:54 am BST

PDB ID : 5DT7  
Title : Crystal structure of the GH1 beta-glucosidase from *Exiguobacterium antarcticum* B7 in space group C2221  
Authors : Zanphorlin, L.M.; Giuseppe, P.O.; Tonoli, C.C.C.; Murakami, M.T.  
Deposited on : 2015-09-17  
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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

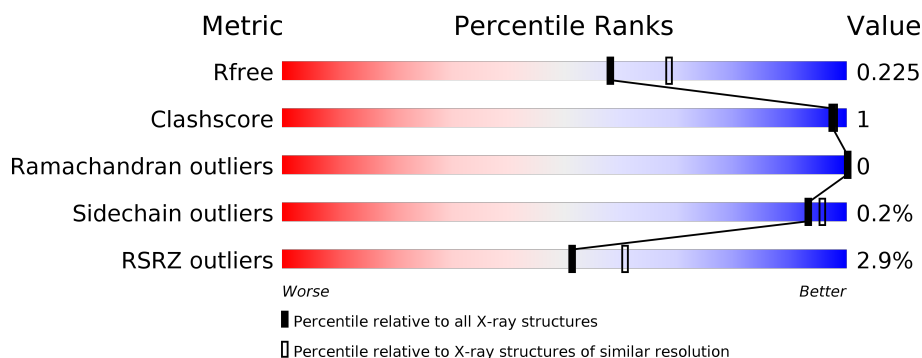
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	471	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>91%</span> <span>6%</span> </div> </div>
1	B	471	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>4%</span> <span>92%</span> <span>6%</span> </div> </div>
1	C	471	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>4%</span> <span>92%</span> <span>6%</span> </div> </div>
1	D	471	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>3%</span> <span>92%</span> <span>6%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15096 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 Beta-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3613	2319	603	676	15			
1	B	442	Total	C	N	O	S	0	0	0
			3601	2311	601	673	16			
1	C	445	Total	C	N	O	S	0	0	0
			3621	2325	604	676	16			
1	D	445	Total	C	N	O	S	0	0	0
			3621	2325	604	676	16			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP K0A8J9
A	-21	GLY	-	expression tag	UNP K0A8J9
A	-20	SER	-	expression tag	UNP K0A8J9
A	-19	SER	-	expression tag	UNP K0A8J9
A	-18	HIS	-	expression tag	UNP K0A8J9
A	-17	HIS	-	expression tag	UNP K0A8J9
A	-16	HIS	-	expression tag	UNP K0A8J9
A	-15	HIS	-	expression tag	UNP K0A8J9
A	-14	HIS	-	expression tag	UNP K0A8J9
A	-13	HIS	-	expression tag	UNP K0A8J9
A	-12	SER	-	expression tag	UNP K0A8J9
A	-11	SER	-	expression tag	UNP K0A8J9
A	-10	GLY	-	expression tag	UNP K0A8J9
A	-9	LEU	-	expression tag	UNP K0A8J9
A	-8	VAL	-	expression tag	UNP K0A8J9
A	-7	PRO	-	expression tag	UNP K0A8J9
A	-6	ARG	-	expression tag	UNP K0A8J9
A	-5	GLY	-	expression tag	UNP K0A8J9
A	-4	SER	-	expression tag	UNP K0A8J9
A	-3	HIS	-	expression tag	UNP K0A8J9
A	-2	MET	-	expression tag	UNP K0A8J9

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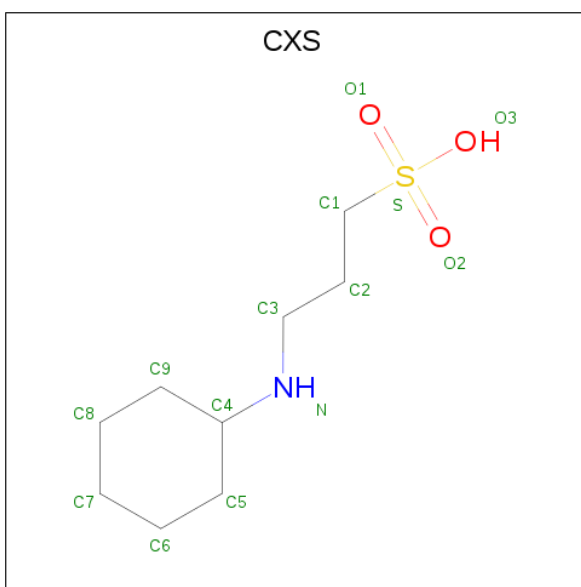
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP K0A8J9
A	0	SER	-	expression tag	UNP K0A8J9
B	-22	MET	-	initiating methionine	UNP K0A8J9
B	-21	GLY	-	expression tag	UNP K0A8J9
B	-20	SER	-	expression tag	UNP K0A8J9
B	-19	SER	-	expression tag	UNP K0A8J9
B	-18	HIS	-	expression tag	UNP K0A8J9
B	-17	HIS	-	expression tag	UNP K0A8J9
B	-16	HIS	-	expression tag	UNP K0A8J9
B	-15	HIS	-	expression tag	UNP K0A8J9
B	-14	HIS	-	expression tag	UNP K0A8J9
B	-13	HIS	-	expression tag	UNP K0A8J9
B	-12	SER	-	expression tag	UNP K0A8J9
B	-11	SER	-	expression tag	UNP K0A8J9
B	-10	GLY	-	expression tag	UNP K0A8J9
B	-9	LEU	-	expression tag	UNP K0A8J9
B	-8	VAL	-	expression tag	UNP K0A8J9
B	-7	PRO	-	expression tag	UNP K0A8J9
B	-6	ARG	-	expression tag	UNP K0A8J9
B	-5	GLY	-	expression tag	UNP K0A8J9
B	-4	SER	-	expression tag	UNP K0A8J9
B	-3	HIS	-	expression tag	UNP K0A8J9
B	-2	MET	-	expression tag	UNP K0A8J9
B	-1	ALA	-	expression tag	UNP K0A8J9
B	0	SER	-	expression tag	UNP K0A8J9
C	-22	MET	-	initiating methionine	UNP K0A8J9
C	-21	GLY	-	expression tag	UNP K0A8J9
C	-20	SER	-	expression tag	UNP K0A8J9
C	-19	SER	-	expression tag	UNP K0A8J9
C	-18	HIS	-	expression tag	UNP K0A8J9
C	-17	HIS	-	expression tag	UNP K0A8J9
C	-16	HIS	-	expression tag	UNP K0A8J9
C	-15	HIS	-	expression tag	UNP K0A8J9
C	-14	HIS	-	expression tag	UNP K0A8J9
C	-13	HIS	-	expression tag	UNP K0A8J9
C	-12	SER	-	expression tag	UNP K0A8J9
C	-11	SER	-	expression tag	UNP K0A8J9
C	-10	GLY	-	expression tag	UNP K0A8J9
C	-9	LEU	-	expression tag	UNP K0A8J9
C	-8	VAL	-	expression tag	UNP K0A8J9
C	-7	PRO	-	expression tag	UNP K0A8J9
C	-6	ARG	-	expression tag	UNP K0A8J9

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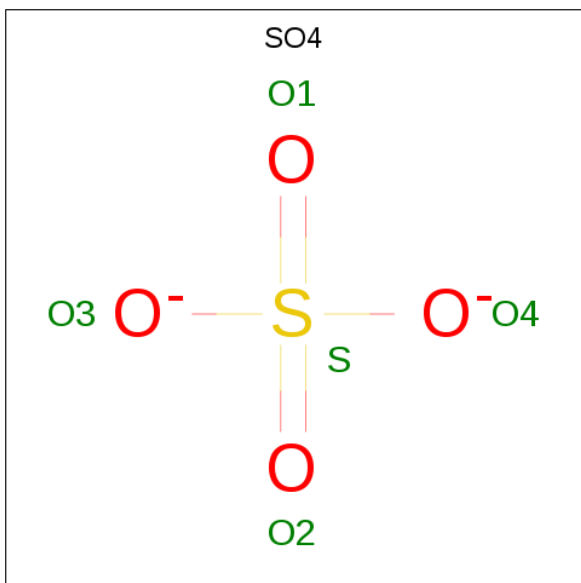
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	expression tag	UNP K0A8J9
C	-4	SER	-	expression tag	UNP K0A8J9
C	-3	HIS	-	expression tag	UNP K0A8J9
C	-2	MET	-	expression tag	UNP K0A8J9
C	-1	ALA	-	expression tag	UNP K0A8J9
C	0	SER	-	expression tag	UNP K0A8J9
D	-22	MET	-	initiating methionine	UNP K0A8J9
D	-21	GLY	-	expression tag	UNP K0A8J9
D	-20	SER	-	expression tag	UNP K0A8J9
D	-19	SER	-	expression tag	UNP K0A8J9
D	-18	HIS	-	expression tag	UNP K0A8J9
D	-17	HIS	-	expression tag	UNP K0A8J9
D	-16	HIS	-	expression tag	UNP K0A8J9
D	-15	HIS	-	expression tag	UNP K0A8J9
D	-14	HIS	-	expression tag	UNP K0A8J9
D	-13	HIS	-	expression tag	UNP K0A8J9
D	-12	SER	-	expression tag	UNP K0A8J9
D	-11	SER	-	expression tag	UNP K0A8J9
D	-10	GLY	-	expression tag	UNP K0A8J9
D	-9	LEU	-	expression tag	UNP K0A8J9
D	-8	VAL	-	expression tag	UNP K0A8J9
D	-7	PRO	-	expression tag	UNP K0A8J9
D	-6	ARG	-	expression tag	UNP K0A8J9
D	-5	GLY	-	expression tag	UNP K0A8J9
D	-4	SER	-	expression tag	UNP K0A8J9
D	-3	HIS	-	expression tag	UNP K0A8J9
D	-2	MET	-	expression tag	UNP K0A8J9
D	-1	ALA	-	expression tag	UNP K0A8J9
D	0	SER	-	expression tag	UNP K0A8J9

- Molecule 2 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (three-letter code: CXS) (formula: C<sub>9</sub>H<sub>19</sub>NO<sub>3</sub>S).



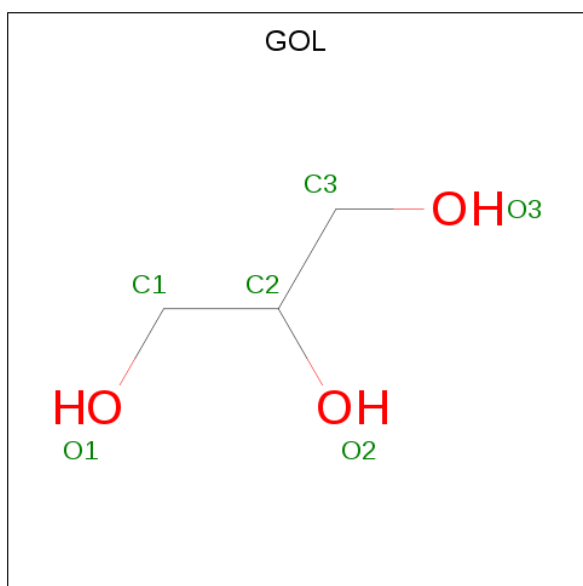
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	C	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	D	1	Total	C	N	O	S	0	0
			14	9	1	3	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	158	Total 158	O 158	0	0
5	B	115	Total 115	O 115	0	0
5	C	130	Total 130	O 130	0	0
5	D	116	Total 116	O 116	0	0

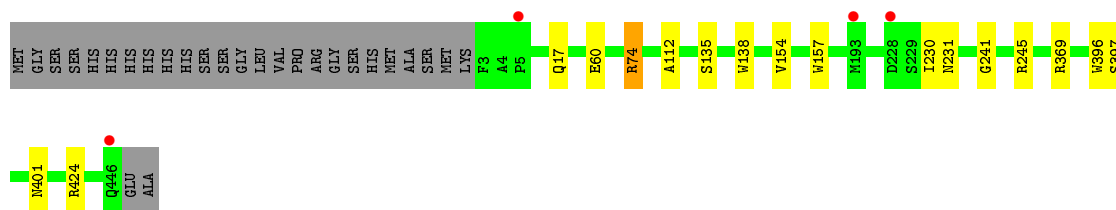


### 3 Residue-property plots [i](#)

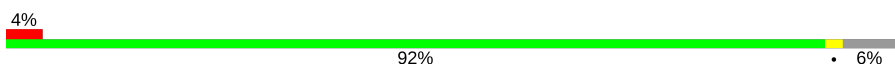
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

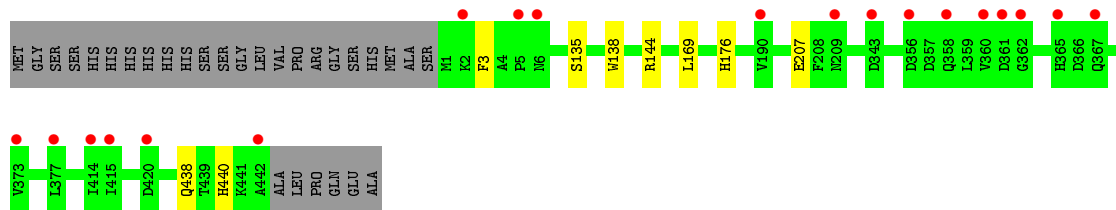
- Molecule 1: Beta-glucosidase

Chain A: 



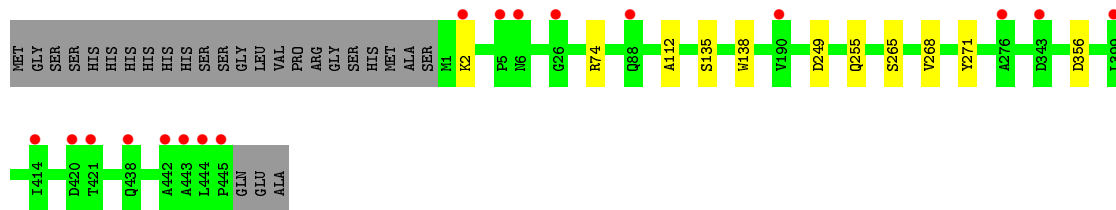
- Molecule 1: Beta-glucosidase

Chain B: 




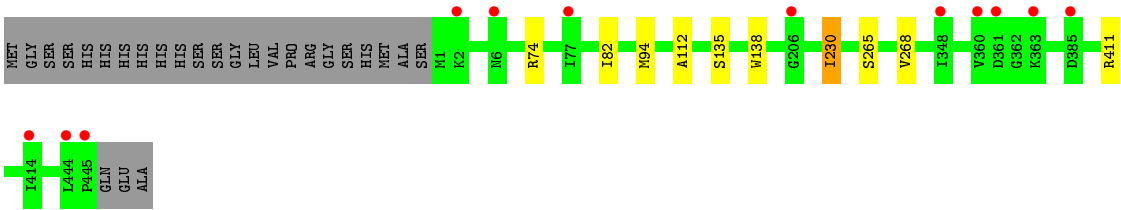
- Molecule 1: Beta-glucosidase

Chain C: 



- Molecule 1: Beta-glucosidase

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.97Å 376.12Å 109.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.15 19.98 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-2.15) 99.7 (19.98-2.15)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.188 , 0.217 0.197 , 0.225	Depositor DCC
$R_{free}$ test set	6550 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.2	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15096	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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, CXS, SO4

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	0.57	0/3730	0.74	2/5073 (0.0%)
1	B	0.56	0/3717	0.71	0/5052
1	C	0.57	0/3738	0.71	1/5082 (0.0%)
1	D	0.58	0/3738	0.71	1/5082 (0.0%)
All	All	0.57	0/14923	0.72	4/20289 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	D	411	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	369	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	356	ASP	CB-CG-OD1	5.11	122.90	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	3613	0	3344	8	0
1	B	3601	0	3338	4	0
1	C	3621	0	3361	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3621	0	3361	6	0
2	A	14	0	18	0	0
2	B	14	0	18	0	0
2	C	14	0	18	0	0
2	D	14	0	19	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
4	A	12	0	16	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	158	0	0	0	0
5	B	115	0	0	0	0
5	C	130	0	0	0	0
5	D	116	0	0	0	0
All	All	15096	0	13517	22	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.

All (22) 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:271:TYR:O	1:D:230:ILE:CD1	2.53	0.57
1:B:3:PHE:HB2	1:B:440:HIS:CD2	2.45	0.52
1:C:135:SER:HA	1:C:138:TRP:CE3	2.47	0.49
1:D:135:SER:HA	1:D:138:TRP:CE3	2.51	0.46
1:B:169:LEU:HD23	1:B:176:HIS:CE1	2.51	0.46
1:B:135:SER:HA	1:B:138:TRP:CE3	2.51	0.45
1:D:74:ARG:HA	1:D:112:ALA:O	2.16	0.45
1:A:135:SER:HA	1:A:138:TRP:CE3	2.53	0.44
1:A:74:ARG:HA	1:A:112:ALA:O	2.18	0.43
1:A:154:VAL:HG21	1:A:157:TRP:CE2	2.53	0.43
1:B:144:ARG:NH1	1:B:207:GLU:OE2	2.44	0.42
1:C:74:ARG:HA	1:C:112:ALA:O	2.20	0.42
1:C:265:SER:HA	1:C:268:VAL:O	2.20	0.41
1:A:230:ILE:HG13	1:A:231:ASN:N	2.34	0.41
1:A:241:GLY:HA2	1:A:245:ARG:HB2	2.02	0.41
1:A:396:TRP:HA	1:A:397:SER:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:OE2	1:A:424:ARG:HG2	2.21	0.41
1:C:249:ASP:HB3	1:C:255:GLN:O	2.21	0.41
1:D:82:ILE:HD12	1:D:94:MET:HG2	2.03	0.41
1:C:271:TYR:O	1:D:230:ILE:HD11	2.20	0.40
1:D:265:SER:HA	1:D:268:VAL:O	2.20	0.40
1:A:17:GLN:O	1:A:401:ASN:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/471 (94%)	431 (98%)	11 (2%)	0	100	100
1	B	440/471 (93%)	428 (97%)	12 (3%)	0	100	100
1	C	443/471 (94%)	427 (96%)	16 (4%)	0	100	100
1	D	443/471 (94%)	431 (97%)	12 (3%)	0	100	100
All	All	1768/1884 (94%)	1717 (97%)	51 (3%)	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	376/398 (94%)	376 (100%)	0	100	100
1	B	375/398 (94%)	374 (100%)	1 (0%)	92	95
1	C	377/398 (95%)	376 (100%)	1 (0%)	92	95
1	D	377/398 (95%)	376 (100%)	1 (0%)	92	95
All	All	1505/1592 (94%)	1502 (100%)	3 (0%)	93	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	438	GLN
1	C	2	LYS
1	D	230	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

16 ligands are modelled in this entry.

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
3	SO4	A	502	-	4,4,4	0.37	0	6,6,6	0.17	0
2	CXS	A	501	-	14,14,14	2.64	2 (14%)	18,18,18	1.49	3 (16%)
2	CXS	B	501	-	14,14,14	2.60	2 (14%)	18,18,18	1.40	3 (16%)
2	CXS	C	501	-	14,14,14	2.56	2 (14%)	18,18,18	1.47	4 (22%)
4	GOL	A	505	-	5,5,5	0.40	0	5,5,5	0.49	0
4	GOL	B	503	-	5,5,5	0.26	0	5,5,5	0.29	0
4	GOL	C	504	-	5,5,5	0.22	0	5,5,5	0.39	0
3	SO4	D	502	-	4,4,4	0.41	0	6,6,6	0.26	0
4	GOL	D	504	-	5,5,5	0.29	0	5,5,5	0.41	0
2	CXS	D	501	-	14,14,14	2.40	2 (14%)	18,18,18	1.80	5 (27%)
3	SO4	B	502	-	4,4,4	0.37	0	6,6,6	0.17	0
4	GOL	A	504	-	5,5,5	0.26	0	5,5,5	0.40	0
3	SO4	D	503	-	4,4,4	0.31	0	6,6,6	0.10	0
3	SO4	A	503	-	4,4,4	0.39	0	6,6,6	0.32	0
3	SO4	C	503	-	4,4,4	0.34	0	6,6,6	0.14	0
3	SO4	C	502	-	4,4,4	0.43	0	6,6,6	0.18	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
4	GOL	C	504	-	-	0/4/4/4	-
2	CXS	A	501	-	-	1/8/16/16	0/1/1/1
4	GOL	A	504	-	-	0/4/4/4	-
2	CXS	C	501	-	-	1/8/16/16	0/1/1/1
4	GOL	B	503	-	-	2/4/4/4	-
4	GOL	D	504	-	-	0/4/4/4	-
2	CXS	D	501	-	-	1/8/16/16	0/1/1/1
4	GOL	A	505	-	-	3/4/4/4	-
2	CXS	B	501	-	-	1/8/16/16	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	CXS	C1-S	-7.59	1.66	1.77
2	B	501	CXS	C1-S	-7.29	1.67	1.77
2	A	501	CXS	C1-S	-7.24	1.67	1.77
2	C	501	CXS	C1-S	-6.79	1.67	1.77
2	C	501	CXS	O1-S	6.44	1.64	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	CXS	O1-S	6.43	1.64	1.45
2	B	501	CXS	O2-S	6.13	1.63	1.45
2	D	501	CXS	O3-S	4.52	1.63	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	CXS	C3-N-C4	4.68	123.34	114.14
2	A	501	CXS	C3-N-C4	4.17	122.32	114.14
2	D	501	CXS	C2-C1-S	-3.39	108.04	113.25
2	B	501	CXS	O3-S-C1	3.32	111.13	105.77
2	C	501	CXS	O2-S-C1	3.15	110.70	106.92
2	A	501	CXS	O2-S-C1	3.09	110.64	106.92
2	B	501	CXS	C3-N-C4	2.98	120.00	114.14
2	C	501	CXS	C3-N-C4	2.96	119.95	114.14
2	B	501	CXS	O2-S-C1	2.81	110.30	106.92
2	D	501	CXS	O1-S-C1	2.59	110.03	106.92
2	D	501	CXS	O3-S-C1	2.52	109.84	105.77
2	A	501	CXS	O1-S-C1	2.33	109.72	106.92
2	D	501	CXS	O2-S-C1	2.29	109.67	106.92
2	C	501	CXS	O1-S-C1	2.20	109.56	106.92
2	C	501	CXS	O3-S-C1	2.09	109.15	105.77

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	GOL	O1-C1-C2-C3
2	A	501	CXS	C5-C4-N-C3
4	A	505	GOL	C1-C2-C3-O3
2	D	501	CXS	C5-C4-N-C3
4	B	503	GOL	O1-C1-C2-O2
4	A	505	GOL	O2-C2-C3-O3
2	C	501	CXS	C2-C3-N-C4
4	A	505	GOL	O1-C1-C2-O2
2	B	501	CXS	C2-C3-N-C4

There are no ring outliers.

No monomer is involved in short contacts.

## 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	444/471 (94%)	-0.17	4 (0%) 84 88	30, 39, 50, 79	0
1	B	442/471 (93%)	0.09	19 (4%) 35 45	30, 45, 63, 86	0
1	C	445/471 (94%)	0.04	17 (3%) 40 49	34, 44, 58, 94	1 (0%)
1	D	445/471 (94%)	0.09	12 (2%) 54 63	32, 43, 58, 78	0
All	All	1776/1884 (94%)	0.01	52 (2%) 51 61	30, 42, 59, 94	1 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	445	PRO	6.0
1	C	444	LEU	5.5
1	C	442	ALA	5.3
1	B	6	ASN	5.1
1	B	2	LYS	4.4
1	C	2	LYS	4.3
1	C	443	ALA	4.3
1	A	446	GLN	4.1
1	A	5	PRO	3.8
1	B	358	GLN	3.8
1	B	5	PRO	3.7
1	D	206	GLY	3.4
1	B	367	GLN	3.4
1	D	360	VAL	3.3
1	B	442	ALA	3.3
1	C	26	GLY	3.3
1	D	2	LYS	3.3
1	B	361	ASP	3.3
1	C	88	GLN	3.1
1	C	276	ALA	3.1
1	B	414	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	385	ASP	2.8
1	D	77	ILE	2.8
1	B	420	ASP	2.8
1	D	6	ASN	2.7
1	B	362	GLY	2.6
1	C	438	GLN	2.6
1	C	414	ILE	2.6
1	D	348	ILE	2.5
1	C	5	PRO	2.5
1	D	445	PRO	2.4
1	D	361	ASP	2.4
1	C	399	LEU	2.4
1	C	343	ASP	2.4
1	B	415	ILE	2.3
1	D	414	ILE	2.3
1	C	420	ASP	2.3
1	B	343	ASP	2.2
1	B	373	VAL	2.2
1	C	190	VAL	2.2
1	B	209	ASN	2.2
1	B	365	HIS	2.2
1	B	190	VAL	2.1
1	C	6	ASN	2.1
1	A	228	ASP	2.1
1	C	421	THR	2.1
1	D	363	LYS	2.1
1	B	360	VAL	2.1
1	A	193	MET	2.1
1	B	377	LEU	2.1
1	B	356	ASP	2.0
1	D	444	LEU	2.0

## 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
3	SO4	A	503	5/5	0.85	0.23	70,76,80,84	0
3	SO4	C	502	5/5	0.88	0.22	66,72,74,75	0
4	GOL	C	504	6/6	0.90	0.12	46,47,47,48	0
4	GOL	D	504	6/6	0.91	0.16	40,42,44,44	0
3	SO4	D	503	5/5	0.92	0.31	88,93,95,95	0
4	GOL	B	503	6/6	0.92	0.11	39,40,40,41	0
4	GOL	A	505	6/6	0.92	0.13	52,55,58,59	0
3	SO4	A	502	5/5	0.94	0.15	58,60,66,67	0
4	GOL	A	504	6/6	0.94	0.09	39,43,44,44	0
2	CXS	C	501	14/14	0.94	0.10	47,50,53,53	0
3	SO4	C	503	5/5	0.94	0.26	84,85,90,91	0
3	SO4	D	502	5/5	0.94	0.16	58,62,66,68	0
2	CXS	D	501	14/14	0.95	0.10	47,52,60,61	0
2	CXS	A	501	14/14	0.96	0.11	45,49,53,55	0
2	CXS	B	501	14/14	0.97	0.09	46,47,48,52	0
3	SO4	B	502	5/5	0.98	0.12	54,56,58,59	0

## 6.5 Other polymers

There are no such residues in this entry.