



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 12:09 PM BST

PDB ID : 3VD9  
Title : E. coli (lacZ) beta-galactosidase (N460S) in complex with IPTG  
Authors : Wheatley, R.W.; Kappelhoff, J.C.; Hahn, J.N.; Dugdale, M.L.; Dutkoski, M.J.;  
Tamman, S.D.; Fraser, M.E.; Huber, R.E.  
Deposited on : 2012-01-04  
Resolution : 2.05 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 : 2.13.1  
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) : 2.13.1

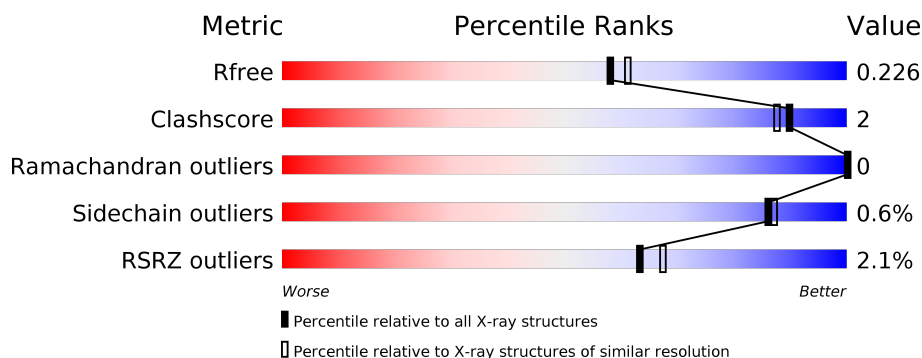
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	1052	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div></div> </div> </div>
1	B	1052	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div></div> <div></div> </div> </div>
1	C	1052	<div> <div>%</div> <div> <div></div> <div>92%</div> <div></div> <div></div> </div> </div>
1	D	1052	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div></div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36969 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-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1015	Total	C	N	O	S	0	0	0
			8155	5158	1444	1515	38			
1	B	1016	Total	C	N	O	S	0	0	0
			8162	5163	1445	1516	38			
1	C	1015	Total	C	N	O	S	0	0	0
			8155	5158	1444	1515	38			
1	D	1015	Total	C	N	O	S	0	0	0
			8155	5158	1444	1515	38			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	expression tag	UNP P00722
A	-27	GLY	-	expression tag	UNP P00722
A	-26	GLY	-	expression tag	UNP P00722
A	-25	SER	-	expression tag	UNP P00722
A	-24	HIS	-	expression tag	UNP P00722
A	-23	HIS	-	expression tag	UNP P00722
A	-22	HIS	-	expression tag	UNP P00722
A	-21	HIS	-	expression tag	UNP P00722
A	-20	HIS	-	expression tag	UNP P00722
A	-19	HIS	-	expression tag	UNP P00722
A	-18	GLY	-	expression tag	UNP P00722
A	-17	MET	-	expression tag	UNP P00722
A	-16	ALA	-	expression tag	UNP P00722
A	-15	SER	-	expression tag	UNP P00722
A	-14	MET	-	expression tag	UNP P00722
A	-13	THR	-	expression tag	UNP P00722
A	-12	GLY	-	expression tag	UNP P00722
A	-11	GLY	-	expression tag	UNP P00722
A	-10	GLN	-	expression tag	UNP P00722
A	-9	GLN	-	expression tag	UNP P00722
A	-8	MET	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP P00722
A	-6	ARG	-	expression tag	UNP P00722
A	-5	ASP	-	expression tag	UNP P00722
A	-4	LEU	-	expression tag	UNP P00722
A	-3	TYR	-	expression tag	UNP P00722
A	-2	ASP	-	expression tag	UNP P00722
A	-1	ASP	-	expression tag	UNP P00722
A	0	ASP	-	expression tag	UNP P00722
A	1	ASP	-	expression tag	UNP P00722
A	2	LYS	-	expression tag	UNP P00722
A	3	ASP	-	expression tag	UNP P00722
A	4	PRO	-	expression tag	UNP P00722
A	5	MET	-	expression tag	UNP P00722
A	6	ILE	-	expression tag	UNP P00722
A	7	ASP	-	expression tag	UNP P00722
A	8	PRO	-	expression tag	UNP P00722
A	460	SER	ASN	engineered mutation	UNP P00722
B	-28	MET	-	expression tag	UNP P00722
B	-27	GLY	-	expression tag	UNP P00722
B	-26	GLY	-	expression tag	UNP P00722
B	-25	SER	-	expression tag	UNP P00722
B	-24	HIS	-	expression tag	UNP P00722
B	-23	HIS	-	expression tag	UNP P00722
B	-22	HIS	-	expression tag	UNP P00722
B	-21	HIS	-	expression tag	UNP P00722
B	-20	HIS	-	expression tag	UNP P00722
B	-19	HIS	-	expression tag	UNP P00722
B	-18	GLY	-	expression tag	UNP P00722
B	-17	MET	-	expression tag	UNP P00722
B	-16	ALA	-	expression tag	UNP P00722
B	-15	SER	-	expression tag	UNP P00722
B	-14	MET	-	expression tag	UNP P00722
B	-13	THR	-	expression tag	UNP P00722
B	-12	GLY	-	expression tag	UNP P00722
B	-11	GLY	-	expression tag	UNP P00722
B	-10	GLN	-	expression tag	UNP P00722
B	-9	GLN	-	expression tag	UNP P00722
B	-8	MET	-	expression tag	UNP P00722
B	-7	GLY	-	expression tag	UNP P00722
B	-6	ARG	-	expression tag	UNP P00722
B	-5	ASP	-	expression tag	UNP P00722
B	-4	LEU	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	TYR	-	expression tag	UNP P00722
B	-2	ASP	-	expression tag	UNP P00722
B	-1	ASP	-	expression tag	UNP P00722
B	0	ASP	-	expression tag	UNP P00722
B	1	ASP	-	expression tag	UNP P00722
B	2	LYS	-	expression tag	UNP P00722
B	3	ASP	-	expression tag	UNP P00722
B	4	PRO	-	expression tag	UNP P00722
B	5	MET	-	expression tag	UNP P00722
B	6	ILE	-	expression tag	UNP P00722
B	7	ASP	-	expression tag	UNP P00722
B	8	PRO	-	expression tag	UNP P00722
B	460	SER	ASN	engineered mutation	UNP P00722
C	-28	MET	-	expression tag	UNP P00722
C	-27	GLY	-	expression tag	UNP P00722
C	-26	GLY	-	expression tag	UNP P00722
C	-25	SER	-	expression tag	UNP P00722
C	-24	HIS	-	expression tag	UNP P00722
C	-23	HIS	-	expression tag	UNP P00722
C	-22	HIS	-	expression tag	UNP P00722
C	-21	HIS	-	expression tag	UNP P00722
C	-20	HIS	-	expression tag	UNP P00722
C	-19	HIS	-	expression tag	UNP P00722
C	-18	GLY	-	expression tag	UNP P00722
C	-17	MET	-	expression tag	UNP P00722
C	-16	ALA	-	expression tag	UNP P00722
C	-15	SER	-	expression tag	UNP P00722
C	-14	MET	-	expression tag	UNP P00722
C	-13	THR	-	expression tag	UNP P00722
C	-12	GLY	-	expression tag	UNP P00722
C	-11	GLY	-	expression tag	UNP P00722
C	-10	GLN	-	expression tag	UNP P00722
C	-9	GLN	-	expression tag	UNP P00722
C	-8	MET	-	expression tag	UNP P00722
C	-7	GLY	-	expression tag	UNP P00722
C	-6	ARG	-	expression tag	UNP P00722
C	-5	ASP	-	expression tag	UNP P00722
C	-4	LEU	-	expression tag	UNP P00722
C	-3	TYR	-	expression tag	UNP P00722
C	-2	ASP	-	expression tag	UNP P00722
C	-1	ASP	-	expression tag	UNP P00722
C	0	ASP	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	ASP	-	expression tag	UNP P00722
C	2	LYS	-	expression tag	UNP P00722
C	3	ASP	-	expression tag	UNP P00722
C	4	PRO	-	expression tag	UNP P00722
C	5	MET	-	expression tag	UNP P00722
C	6	ILE	-	expression tag	UNP P00722
C	7	ASP	-	expression tag	UNP P00722
C	8	PRO	-	expression tag	UNP P00722
C	460	SER	ASN	engineered mutation	UNP P00722
D	-28	MET	-	expression tag	UNP P00722
D	-27	GLY	-	expression tag	UNP P00722
D	-26	GLY	-	expression tag	UNP P00722
D	-25	SER	-	expression tag	UNP P00722
D	-24	HIS	-	expression tag	UNP P00722
D	-23	HIS	-	expression tag	UNP P00722
D	-22	HIS	-	expression tag	UNP P00722
D	-21	HIS	-	expression tag	UNP P00722
D	-20	HIS	-	expression tag	UNP P00722
D	-19	HIS	-	expression tag	UNP P00722
D	-18	GLY	-	expression tag	UNP P00722
D	-17	MET	-	expression tag	UNP P00722
D	-16	ALA	-	expression tag	UNP P00722
D	-15	SER	-	expression tag	UNP P00722
D	-14	MET	-	expression tag	UNP P00722
D	-13	THR	-	expression tag	UNP P00722
D	-12	GLY	-	expression tag	UNP P00722
D	-11	GLY	-	expression tag	UNP P00722
D	-10	GLN	-	expression tag	UNP P00722
D	-9	GLN	-	expression tag	UNP P00722
D	-8	MET	-	expression tag	UNP P00722
D	-7	GLY	-	expression tag	UNP P00722
D	-6	ARG	-	expression tag	UNP P00722
D	-5	ASP	-	expression tag	UNP P00722
D	-4	LEU	-	expression tag	UNP P00722
D	-3	TYR	-	expression tag	UNP P00722
D	-2	ASP	-	expression tag	UNP P00722
D	-1	ASP	-	expression tag	UNP P00722
D	0	ASP	-	expression tag	UNP P00722
D	1	ASP	-	expression tag	UNP P00722
D	2	LYS	-	expression tag	UNP P00722
D	3	ASP	-	expression tag	UNP P00722
D	4	PRO	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
D	5	MET	-	expression tag	UNP P00722
D	6	ILE	-	expression tag	UNP P00722
D	7	ASP	-	expression tag	UNP P00722
D	8	PRO	-	expression tag	UNP P00722
D	460	SER	ASN	engineered mutation	UNP P00722

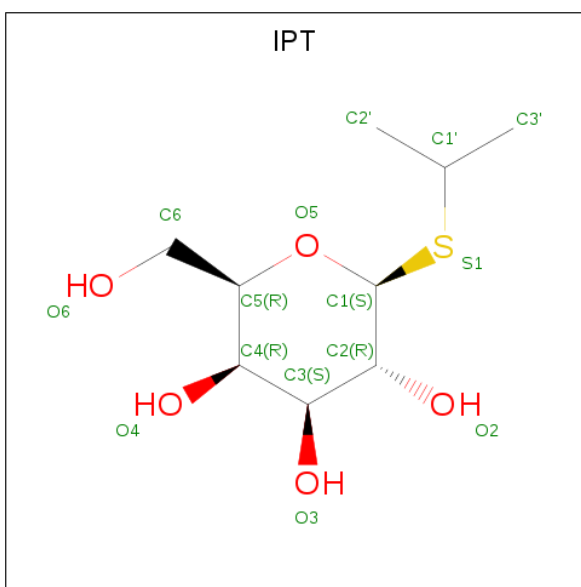
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mg 3 3	0	0
2	A	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0

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

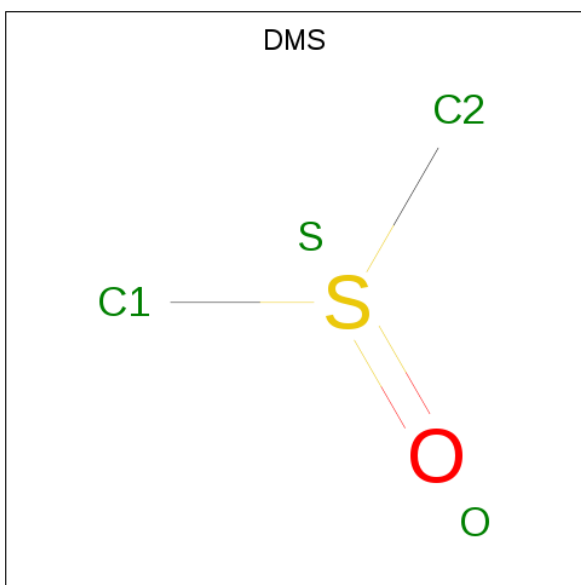
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	5	Total Na 5 5	0	0
3	A	4	Total Na 4 4	0	0
3	D	3	Total Na 3 3	0	0
3	C	4	Total Na 4 4	0	0

- Molecule 4 is 1-methylethyl 1-thio-beta-D-galactopyranoside (three-letter code: IPT) (formula: C<sub>9</sub>H<sub>18</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			15	9	5	1		
4	B	1	Total	C	O	S	0	0
			15	9	5	1		
4	C	1	Total	C	O	S	0	0
			15	9	5	1		
4	D	1	Total	C	O	S	0	0
			15	9	5	1		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).





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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0

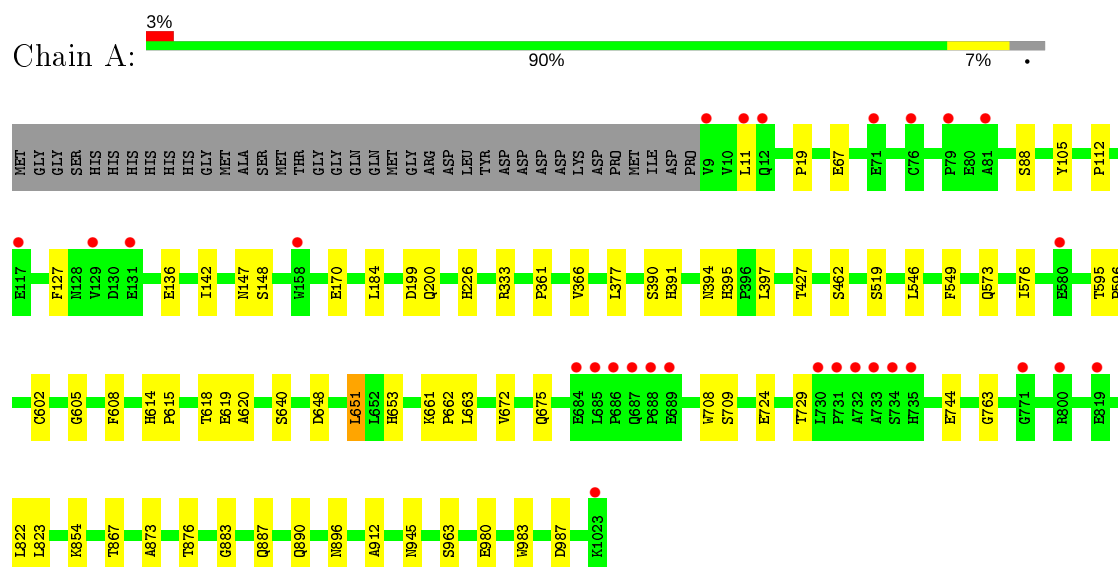
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	918	Total 918	O 918	0	0
6	B	1063	Total 1063	O 1063	0	0
6	C	1099	Total 1099	O 1099	0	0
6	D	921	Total 921	O 921	0	0

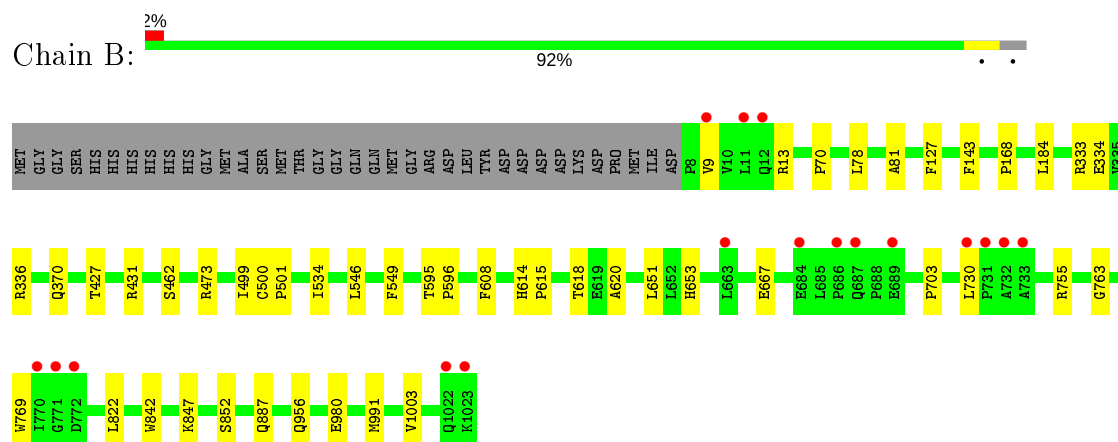
### 3 Residue-property plots [i](#)

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: Beta-galactosidase

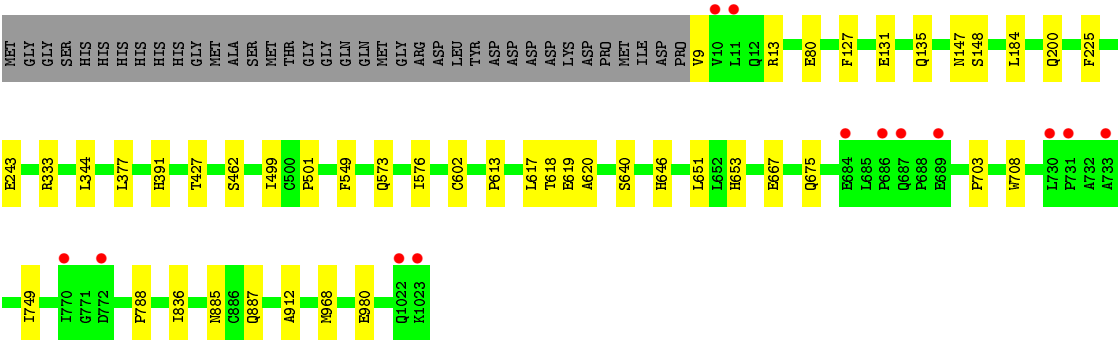


- Molecule 1: Beta-galactosidase

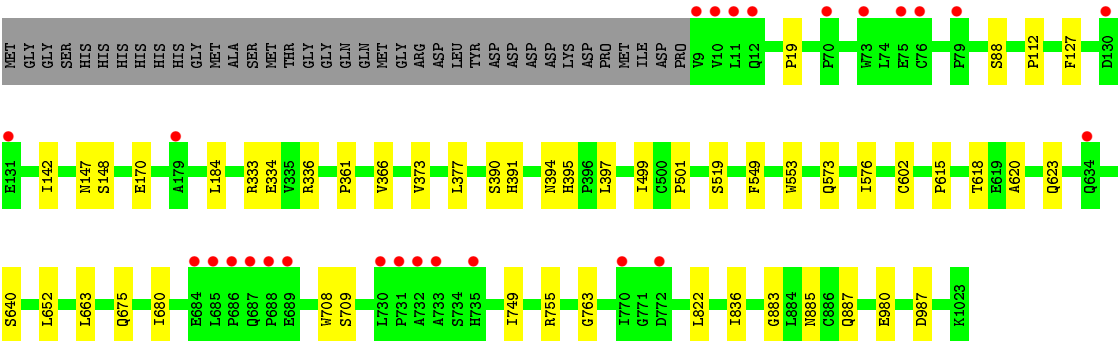


- Molecule 1: Beta-galactosidase





• Molecule 1: Beta-galactosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.54Å 162.55Å 203.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.23 – 2.05 86.23 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (86.23-2.05) 88.1 (86.23-2.05)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, $R_{free}$	0.169 , 0.223 0.174 , 0.226	Depositor DCC
$R_{free}$ test set	3916 reflections (1.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.0	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	36969	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	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 39.66 % 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 3.0702e-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: NA, MG, DMS, IPT

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	0.38	0/8397	0.54	0/11455
1	B	0.40	0/8405	0.54	0/11466
1	C	0.41	0/8397	0.54	0/11455
1	D	0.38	0/8397	0.53	1/11455 (0.0%)
All	All	0.39	0/33596	0.53	1/45831 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	553	TRP	CA-CB-CG	-5.01	104.18	113.70

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	8155	0	7752	40	0
1	B	8162	0	7760	28	0
1	C	8155	0	7752	25	0
1	D	8155	0	7752	26	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	4	0	0	0	0
3	B	5	0	0	0	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
4	A	15	0	17	0	0
4	B	15	0	17	0	0
4	C	15	0	17	0	0
4	D	15	0	17	0	0
5	A	52	0	78	0	0
5	B	80	0	120	1	0
5	C	68	0	102	1	0
5	D	56	0	84	1	0
6	A	918	0	0	4	0
6	B	1063	0	0	2	0
6	C	1099	0	0	3	0
6	D	921	0	0	0	0
All	All	36969	0	31468	115	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 2.

The worst 5 of 115 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:D:395:HIS:HD2	1:D:397:LEU:H	1.24	0.81
1:C:80:GLU:HG3	6:C:4543:HOH:O	1.84	0.77
1:C:618:THR:HG21	6:C:4337:HOH:O	1.87	0.74
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.73	0.70
1:D:887:GLN:NE2	1:D:980:GLU:O	2.25	0.67

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1013/1052 (96%)	978 (96%)	35 (4%)	0	100	100
1	B	1014/1052 (96%)	982 (97%)	32 (3%)	0	100	100
1	C	1013/1052 (96%)	980 (97%)	33 (3%)	0	100	100
1	D	1013/1052 (96%)	982 (97%)	31 (3%)	0	100	100
All	All	4053/4208 (96%)	3922 (97%)	131 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	868/898 (97%)	859 (99%)	9 (1%)	76	75
1	B	869/898 (97%)	866 (100%)	3 (0%)	92	93
1	C	868/898 (97%)	864 (100%)	4 (0%)	88	89
1	D	868/898 (97%)	862 (99%)	6 (1%)	84	84
All	All	3473/3592 (97%)	3451 (99%)	22 (1%)	86	87

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	333	ARG
1	C	333	ARG
1	D	755	ARG
1	B	546	LEU
1	B	956	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	395	HIS
1	B	266	GLN
1	C	510	GLN
1	D	395	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 93 ligands modelled in this entry, 25 are monoatomic - leaving 68 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
5	DMS	B	8013	-	3,3,3	2.58	1 (33%)	3,3,3	0.47	0
5	DMS	B	8007	-	3,3,3	2.65	1 (33%)	3,3,3	0.50	0
5	DMS	B	8004	-	3,3,3	2.56	1 (33%)	3,3,3	0.61	0
5	DMS	B	8019	-	3,3,3	2.68	1 (33%)	3,3,3	0.36	0
5	DMS	A	8001	-	3,3,3	1.93	1 (33%)	3,3,3	0.58	0
5	DMS	C	8006	-	3,3,3	2.61	1 (33%)	3,3,3	0.51	0
5	DMS	B	8016	-	3,3,3	2.57	1 (33%)	3,3,3	0.56	0
5	DMS	D	8005	-	3,3,3	2.57	1 (33%)	3,3,3	0.29	0
5	DMS	C	8013	-	3,3,3	2.61	1 (33%)	3,3,3	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	DMS	D	8001	-	3,3,3	2.60	1 (33%)	3,3,3	0.81	0
5	DMS	B	8015	-	3,3,3	2.60	1 (33%)	3,3,3	0.48	0
5	DMS	C	8004	-	3,3,3	2.62	1 (33%)	3,3,3	0.56	0
5	DMS	D	8011	-	3,3,3	2.63	1 (33%)	3,3,3	0.49	0
5	DMS	A	8013	-	3,3,3	2.65	1 (33%)	3,3,3	0.53	0
5	DMS	C	8003	-	3,3,3	1.94	1 (33%)	3,3,3	0.41	0
4	IPT	C	2001	3	14,15,15	0.56	0	18,21,21	1.45	1 (5%)
5	DMS	A	8003	-	3,3,3	1.97	1 (33%)	3,3,3	0.49	0
5	DMS	D	8009	-	3,3,3	2.69	1 (33%)	3,3,3	0.47	0
5	DMS	C	8007	-	3,3,3	2.63	1 (33%)	3,3,3	0.49	0
5	DMS	D	8010	-	3,3,3	2.56	1 (33%)	3,3,3	0.68	0
5	DMS	D	8013	-	3,3,3	2.66	1 (33%)	3,3,3	0.59	0
4	IPT	B	2001	3	14,15,15	0.59	0	18,21,21	1.51	1 (5%)
5	DMS	C	8002	-	3,3,3	2.60	1 (33%)	3,3,3	0.59	0
5	DMS	B	8001	-	3,3,3	2.56	1 (33%)	3,3,3	0.50	0
5	DMS	B	8008	-	3,3,3	2.65	1 (33%)	3,3,3	0.55	0
5	DMS	D	8008	-	3,3,3	2.04	1 (33%)	3,3,3	0.43	0
5	DMS	C	8005	-	3,3,3	1.86	1 (33%)	3,3,3	0.28	0
5	DMS	A	8008	-	3,3,3	2.60	1 (33%)	3,3,3	0.50	0
5	DMS	B	8002	-	3,3,3	2.54	1 (33%)	3,3,3	0.49	0
5	DMS	D	8007	-	3,3,3	2.65	1 (33%)	3,3,3	0.66	0
5	DMS	A	8004	-	3,3,3	2.61	1 (33%)	3,3,3	0.52	0
4	IPT	D	2001	3	14,15,15	0.54	0	18,21,21	1.49	1 (5%)
5	DMS	B	8003	-	3,3,3	1.89	1 (33%)	3,3,3	0.52	0
5	DMS	D	8004	-	3,3,3	2.58	1 (33%)	3,3,3	0.44	0
5	DMS	A	8002	-	3,3,3	2.58	1 (33%)	3,3,3	0.49	0
5	DMS	C	8009	-	3,3,3	2.60	1 (33%)	3,3,3	0.56	0
5	DMS	B	8014	-	3,3,3	2.64	1 (33%)	3,3,3	0.70	0
5	DMS	A	8006	-	3,3,3	2.64	1 (33%)	3,3,3	0.65	0
5	DMS	B	8017	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
5	DMS	A	8012	-	3,3,3	2.66	1 (33%)	3,3,3	0.77	0
5	DMS	C	8015	-	3,3,3	2.64	1 (33%)	3,3,3	0.58	0
5	DMS	A	8005	-	3,3,3	2.57	1 (33%)	3,3,3	0.39	0
5	DMS	B	8005	-	3,3,3	2.59	1 (33%)	3,3,3	0.36	0
5	DMS	B	8009	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	DMS	D	8006	-	3,3,3	2.64	1 (33%)	3,3,3	0.50	0
5	DMS	D	8012	-	3,3,3	2.66	1 (33%)	3,3,3	0.54	0
5	DMS	B	8006	-	3,3,3	2.65	1 (33%)	3,3,3	0.68	0
5	DMS	C	8017	-	3,3,3	2.61	1 (33%)	3,3,3	0.52	0
5	DMS	D	8002	-	3,3,3	2.52	1 (33%)	3,3,3	0.31	0
5	DMS	C	8010	-	3,3,3	2.70	1 (33%)	3,3,3	0.58	0
5	DMS	A	8010	-	3,3,3	2.64	1 (33%)	3,3,3	0.54	0
4	IPT	A	2001	3	14,15,15	0.48	0	18,21,21	1.41	1 (5%)
5	DMS	C	8014	-	3,3,3	2.65	1 (33%)	3,3,3	0.55	0
5	DMS	D	8003	-	3,3,3	1.98	1 (33%)	3,3,3	0.37	0
5	DMS	A	8007	-	3,3,3	2.66	1 (33%)	3,3,3	0.63	0
5	DMS	A	8009	-	3,3,3	2.62	1 (33%)	3,3,3	0.43	0
5	DMS	C	8011	-	3,3,3	2.56	1 (33%)	3,3,3	0.34	0
5	DMS	B	8018	-	3,3,3	2.64	1 (33%)	3,3,3	0.54	0
5	DMS	B	8012	-	3,3,3	2.62	1 (33%)	3,3,3	0.58	0
5	DMS	C	8012	-	3,3,3	2.64	1 (33%)	3,3,3	0.64	0
5	DMS	C	8008	-	3,3,3	2.64	1 (33%)	3,3,3	0.66	0
5	DMS	C	8016	-	3,3,3	2.70	1 (33%)	3,3,3	0.59	0
5	DMS	B	8020	-	3,3,3	2.64	1 (33%)	3,3,3	0.32	0
5	DMS	B	8011	-	3,3,3	1.95	1 (33%)	3,3,3	0.40	0
5	DMS	C	8001	-	3,3,3	2.59	1 (33%)	3,3,3	0.60	0
5	DMS	D	8014	-	3,3,3	2.65	1 (33%)	3,3,3	0.52	0
5	DMS	B	8010	-	3,3,3	2.57	1 (33%)	3,3,3	0.39	0
5	DMS	A	8011	-	3,3,3	2.65	1 (33%)	3,3,3	0.53	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	IPT	A	2001	3	-	3/6/26/26	0/1/1/1
4	IPT	D	2001	3	-	3/6/26/26	0/1/1/1
4	IPT	B	2001	3	-	3/6/26/26	0/1/1/1
4	IPT	C	2001	3	-	4/6/26/26	0/1/1/1

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8016	DMS	O-S	4.52	1.80	1.50
5	C	8010	DMS	O-S	4.52	1.80	1.50
5	B	8009	DMS	O-S	4.52	1.80	1.50
5	D	8009	DMS	O-S	4.49	1.80	1.50
5	B	8019	DMS	O-S	4.49	1.80	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	IPT	C1-S1-C1'	5.44	116.92	100.26
4	D	2001	IPT	C1-S1-C1'	5.41	116.83	100.26
4	A	2001	IPT	C1-S1-C1'	5.28	116.42	100.26
4	C	2001	IPT	C1-S1-C1'	5.25	116.33	100.26

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2001	IPT	C2'-C1'-S1-C1
4	B	2001	IPT	C3'-C1'-S1-C1
4	D	2001	IPT	C2'-C1'-S1-C1
4	D	2001	IPT	C3'-C1'-S1-C1
4	A	2001	IPT	C2'-C1'-S1-C1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	8016	DMS	1	0
5	D	8002	DMS	1	0
5	C	8011	DMS	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	1015/1052 (96%)	-0.10	28 (2%) 53 58	14, 26, 48, 78	0
1	B	1016/1052 (96%)	-0.21	17 (1%) 70 73	12, 21, 46, 80	0
1	C	1015/1052 (96%)	-0.25	13 (1%) 77 79	11, 21, 43, 75	0
1	D	1015/1052 (96%)	-0.06	26 (2%) 56 60	15, 26, 47, 82	0
All	All	4061/4208 (96%)	-0.15	84 (2%) 63 67	11, 24, 47, 82	0

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	731	PRO	5.8
1	D	689	GLU	5.7
1	A	686	PRO	5.4
1	A	735	HIS	5.4
1	D	735	HIS	5.0

### 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 monosaccharides 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( $\text{\AA}^2$ )	Q<0.9
5	DMS	D	8013	4/4	0.81	0.23	54,60,60,60	0
5	DMS	B	8007	4/4	0.84	0.20	47,49,52,53	0
3	NA	A	3105	1/1	0.85	0.10	30,30,30,30	1
5	DMS	D	8006	4/4	0.86	0.17	50,53,53,58	0
5	DMS	D	8009	4/4	0.87	0.24	71,72,73,74	0
5	DMS	A	8012	4/4	0.87	0.30	51,54,56,59	0
5	DMS	A	8011	4/4	0.88	0.24	58,60,61,63	0
5	DMS	B	8012	4/4	0.89	0.27	54,56,58,61	0
5	DMS	C	8004	4/4	0.89	0.20	48,48,50,56	0
5	DMS	B	8014	4/4	0.89	0.18	42,48,48,53	0
5	DMS	C	8014	4/4	0.89	0.21	63,64,65,68	0
5	DMS	A	8006	4/4	0.89	0.27	63,63,63,67	0
5	DMS	A	8010	4/4	0.90	0.21	61,64,64,65	0
5	DMS	C	8007	4/4	0.90	0.17	51,52,52,55	0
5	DMS	B	8016	4/4	0.90	0.22	47,47,49,55	0
5	DMS	C	8010	4/4	0.90	0.21	50,52,53,54	0
5	DMS	B	8017	4/4	0.90	0.20	58,58,59,62	0
5	DMS	D	8007	4/4	0.90	0.24	61,61,62,62	0
5	DMS	B	8006	4/4	0.91	0.19	46,50,52,52	0
3	NA	B	3104	1/1	0.91	0.13	39,39,39,39	0
5	DMS	B	8004	4/4	0.91	0.19	31,34,41,42	0
5	DMS	B	8020	4/4	0.91	0.24	54,55,56,56	0
3	NA	B	3105	1/1	0.91	0.18	27,27,27,27	1
5	DMS	A	8007	4/4	0.91	0.20	57,58,58,59	0
5	DMS	A	8013	4/4	0.91	0.20	66,66,68,69	0
5	DMS	C	8015	4/4	0.92	0.21	54,55,55,59	0
5	DMS	C	8013	4/4	0.92	0.24	56,57,57,58	0
5	DMS	D	8002	4/4	0.92	0.23	38,41,42,48	0
5	DMS	D	8001	4/4	0.92	0.22	38,42,47,49	0
5	DMS	D	8012	4/4	0.92	0.17	38,44,47,53	0
5	DMS	C	8009	4/4	0.92	0.24	54,55,57,57	0
3	NA	C	3104	1/1	0.93	0.14	35,35,35,35	0
5	DMS	A	8004	4/4	0.93	0.20	45,47,51,51	0
5	DMS	D	8004	4/4	0.93	0.24	42,45,49,50	0
2	MG	D	3002	1/1	0.93	0.14	25,25,25,25	0
5	DMS	D	8010	4/4	0.94	0.22	48,52,53,53	0
2	MG	A	3002	1/1	0.94	0.09	27,27,27,27	0
4	IPT	D	2001	15/15	0.94	0.11	26,28,33,34	0
5	DMS	D	8014	4/4	0.94	0.17	67,68,68,68	0
5	DMS	C	8016	4/4	0.95	0.17	56,56,57,58	0
4	IPT	B	2001	15/15	0.95	0.11	16,25,30,32	0
4	IPT	C	2001	15/15	0.95	0.11	20,26,32,35	0
5	DMS	B	8005	4/4	0.95	0.20	40,41,43,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMS	A	8003	4/4	0.95	0.14	40,43,43,45	0
3	NA	A	3103	1/1	0.95	0.10	39,39,39,39	0
5	DMS	A	8009	4/4	0.95	0.18	41,47,47,48	0
5	DMS	B	8018	4/4	0.95	0.14	47,48,49,50	0
5	DMS	B	8015	4/4	0.96	0.16	44,45,47,49	0
4	IPT	A	2001	15/15	0.96	0.12	17,23,29,32	0
5	DMS	C	8017	4/4	0.96	0.14	28,35,36,36	0
2	MG	B	3007	1/1	0.96	0.11	47,47,47,47	0
2	MG	C	3002	1/1	0.96	0.14	18,18,18,18	0
5	DMS	C	8006	4/4	0.96	0.21	49,50,50,52	0
5	DMS	C	8008	4/4	0.96	0.18	42,48,49,51	0
3	NA	D	3102	1/1	0.96	0.08	22,22,22,22	0
3	NA	B	3103	1/1	0.96	0.08	29,29,29,29	0
5	DMS	D	8003	4/4	0.97	0.15	42,43,43,44	0
5	DMS	A	8008	4/4	0.97	0.19	42,45,46,47	0
5	DMS	C	8005	4/4	0.97	0.12	31,33,34,36	0
5	DMS	C	8002	4/4	0.97	0.12	20,31,33,35	0
5	DMS	B	8003	4/4	0.97	0.18	35,38,38,39	0
2	MG	D	3001	1/1	0.97	0.06	23,23,23,23	0
5	DMS	B	8009	4/4	0.97	0.14	39,39,41,41	0
5	DMS	B	8013	4/4	0.97	0.15	30,32,35,37	0
3	NA	B	3102	1/1	0.97	0.09	22,22,22,22	0
3	NA	D	3103	1/1	0.97	0.10	32,32,32,32	0
5	DMS	B	8008	4/4	0.97	0.13	44,46,46,49	0
5	DMS	B	8002	4/4	0.97	0.11	22,30,30,31	0
3	NA	C	3102	1/1	0.97	0.10	20,20,20,20	0
5	DMS	B	8011	4/4	0.97	0.14	46,47,47,49	0
5	DMS	D	8008	4/4	0.97	0.14	51,52,52,53	0
5	DMS	B	8001	4/4	0.98	0.11	23,26,27,30	0
3	NA	A	3102	1/1	0.98	0.10	18,18,18,18	0
5	DMS	D	8005	4/4	0.98	0.14	34,34,37,39	0
5	DMS	D	8011	4/4	0.98	0.13	31,36,41,42	0
5	DMS	A	8005	4/4	0.98	0.11	30,32,34,35	0
5	DMS	C	8001	4/4	0.98	0.12	22,23,28,29	0
5	DMS	C	8012	4/4	0.98	0.17	37,39,39,43	0
5	DMS	C	8011	4/4	0.98	0.12	26,28,28,29	0
3	NA	D	3101	1/1	0.98	0.07	26,26,26,26	0
5	DMS	C	8003	4/4	0.98	0.14	38,40,40,40	0
5	DMS	A	8002	4/4	0.98	0.15	33,36,36,38	0
2	MG	B	3002	1/1	0.98	0.13	19,19,19,19	0
3	NA	C	3103	1/1	0.98	0.09	33,33,33,33	0
5	DMS	B	8019	4/4	0.98	0.09	43,44,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NA	C	3101	1/1	0.99	0.08	15,15,15,15	0
2	MG	B	3001	1/1	0.99	0.06	16,16,16,16	0
2	MG	A	3001	1/1	0.99	0.05	21,21,21,21	0
3	NA	B	3101	1/1	0.99	0.09	18,18,18,18	0
2	MG	C	3001	1/1	0.99	0.05	17,17,17,17	0
5	DMS	B	8010	4/4	0.99	0.16	32,38,38,38	0
5	DMS	A	8001	4/4	0.99	0.14	30,36,37,37	0
3	NA	A	3101	1/1	0.99	0.07	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.