



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:29 am BST

PDB ID : 3SEP  
Title : E. coli (lacZ) beta-galactosidase (S796A)  
Authors : Jancewicz, L.J.; Wheatley, R.W.; Sutendra, G.; Lee, M.; Fraser, M.; Huber, R.E.  
Deposited on : 2011-06-10  
Resolution : 2.05 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

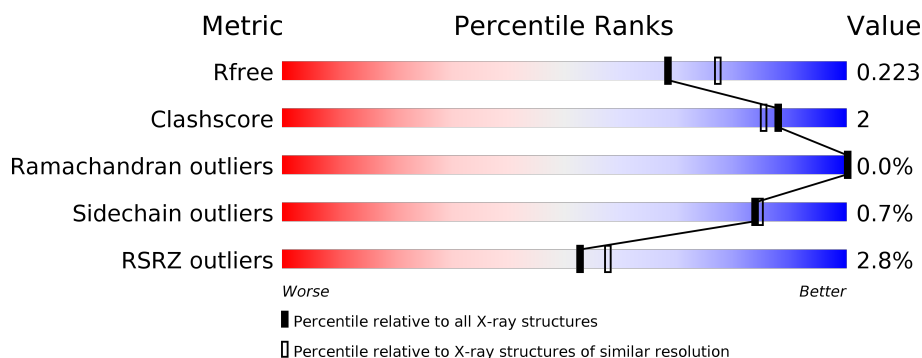
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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>89%</div> <div>7%</div> <div></div> </div> <div></div> </div>
1	B	1052	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div></div> </div> <div></div> </div>
1	C	1052	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div></div> <div></div> </div> <div></div> </div>
1	D	1052	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div></div> </div> <div></div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DMS	B	8012	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 37044 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
			8156	5159	1445	1514	38			
1	B	1015	Total	C	N	O	S	0	0	0
			8156	5159	1445	1514	38			
1	C	1015	Total	C	N	O	S	0	0	0
			8156	5159	1445	1514	38			
1	D	1015	Total	C	N	O	S	0	0	0
			8156	5159	1445	1514	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	796	ALA	SER	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	796	ALA	SER	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	796	ALA	SER	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	796	ALA	SER	ENGINEERED MUTATION	UNP P00722

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

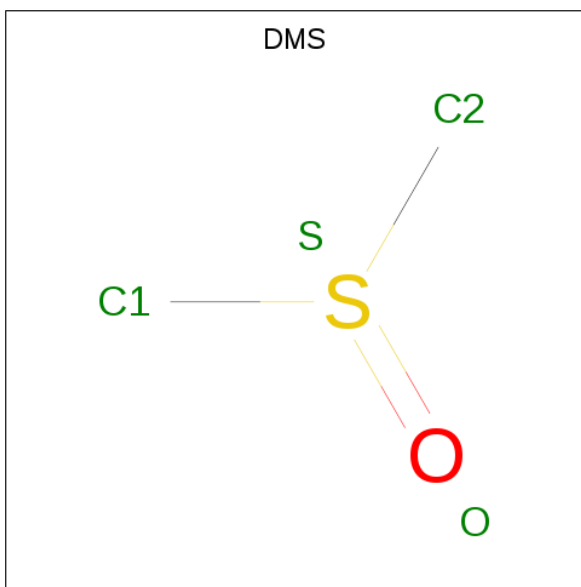
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mg 3 3	0	0
2	A	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0

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

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

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).





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

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

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

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

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

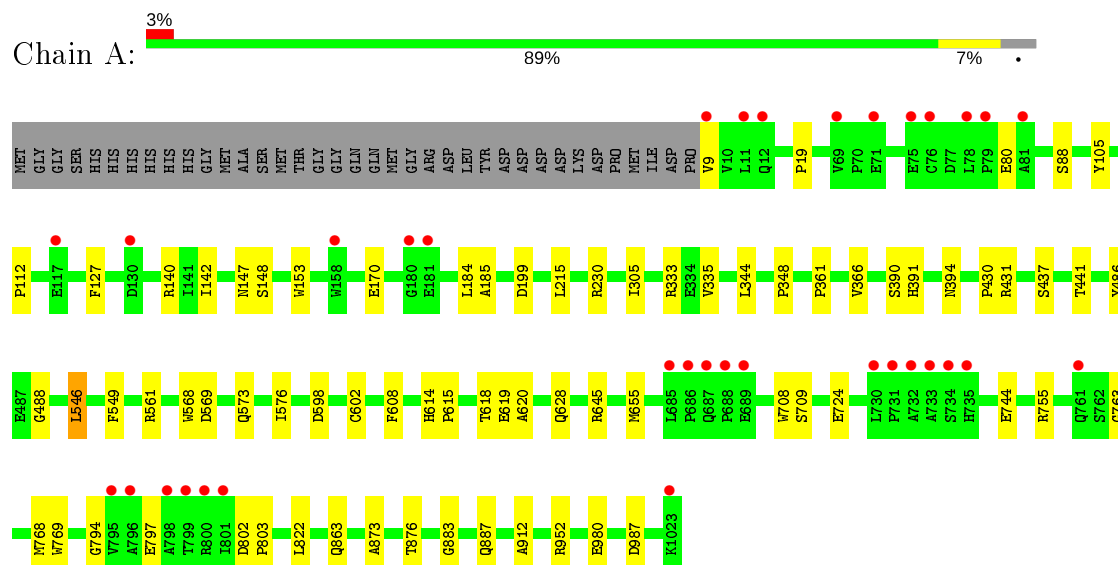
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	910	Total	O	0	0
			910	910		
5	B	1130	Total	O	0	0
			1130	1130		
5	C	1120	Total	O	0	0
			1120	1120		
5	D	925	Total	O	0	0
			925	925		

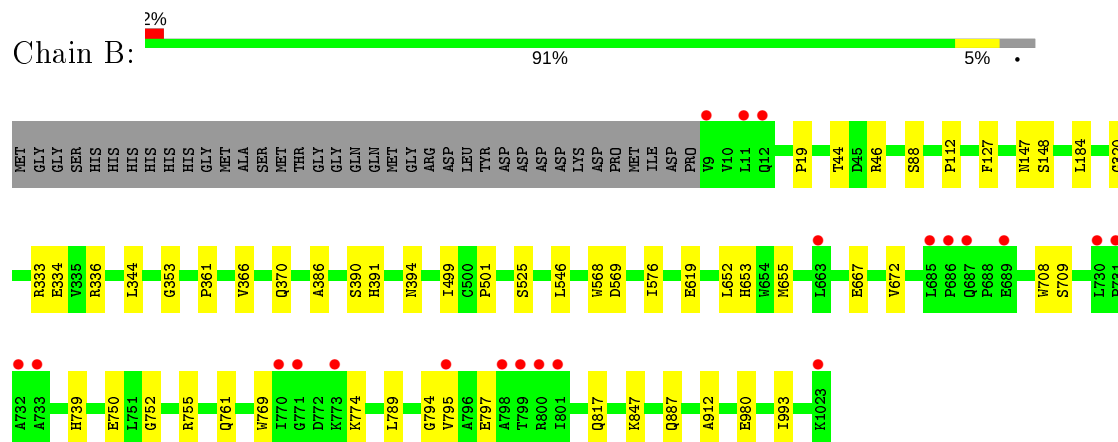
### 3 Residue-property plots [i](#)

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.

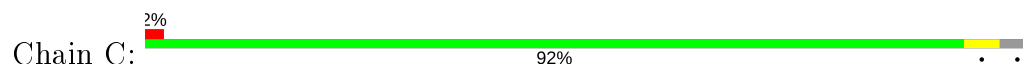
#### • Molecule 1: Beta-galactosidase

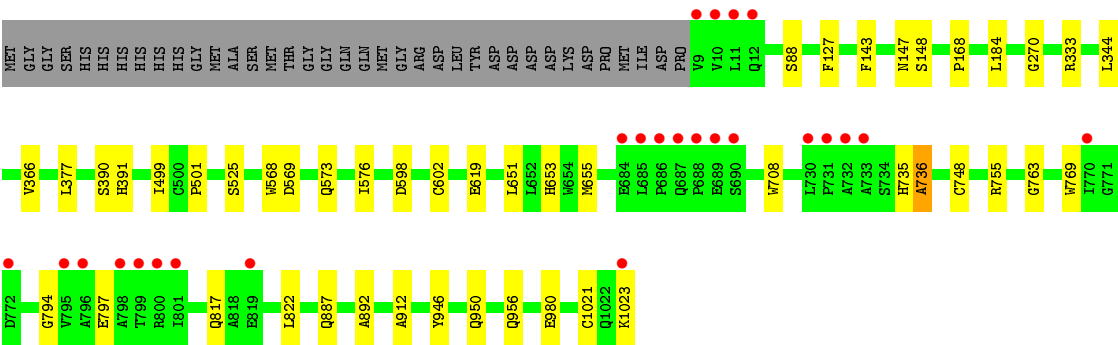


#### • Molecule 1: Beta-galactosidase

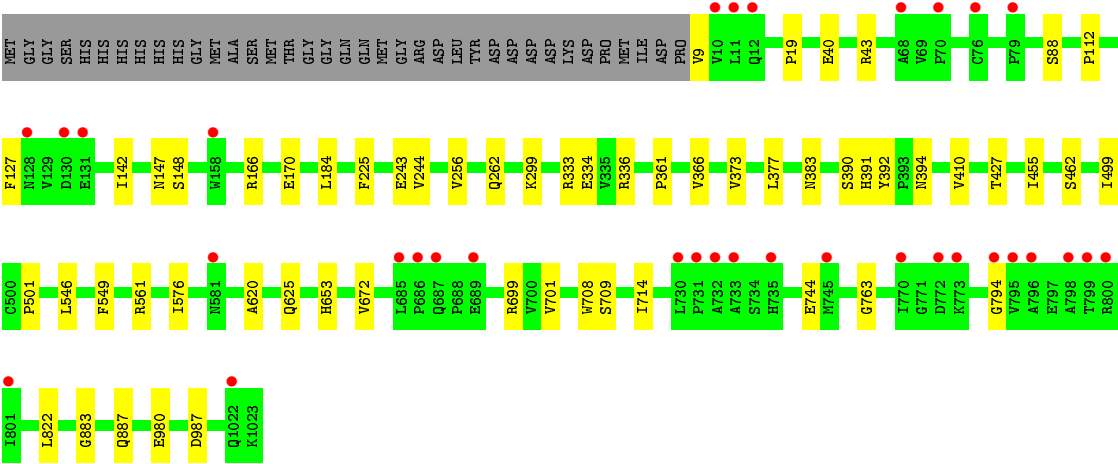
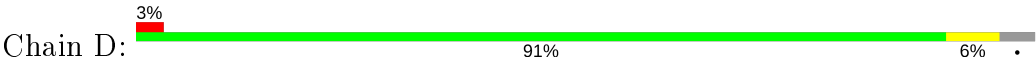


#### • Molecule 1: Beta-galactosidase





• Molecule 1: Beta-galactosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.34Å 163.16Å 203.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.00 – 2.05 84.58 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (80.00-2.05) 90.1 (84.58-2.05)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.05Å)	Xtrriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, $R_{free}$	0.172 , 0.221 0.175 , 0.223	Depositor DCC
$R_{free}$ test set	4086 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtrriage
Anisotropy	0.283	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	37044	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9261e-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

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	0/8398	0.53	0/11457
1	B	0.40	0/8398	0.54	0/11457
1	C	0.41	0/8398	0.54	0/11457
1	D	0.38	0/8398	0.53	0/11457
All	All	0.39	0/33592	0.53	0/45828

There are no bond length outliers.

There are no bond angle outliers.

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	8156	0	7753	41	0
1	B	8156	0	7753	28	0
1	C	8156	0	7753	27	0
1	D	8156	0	7753	36	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
4	A	84	0	126	1	0
4	B	92	0	138	1	0
4	C	80	0	120	3	0
4	D	56	0	84	2	0
5	A	910	0	0	5	0
5	B	1130	0	0	5	0
5	C	1120	0	0	5	0
5	D	925	0	0	2	0
All	All	37044	0	31480	129	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.

All (129) 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:A:142:ILE:HG12	1:A:170:GLU:HG2	1.60	0.84
1:C:887:GLN:NE2	1:C:980:GLU:O	2.13	0.81
4:C:8003:DMS:H23	5:C:4238:HOH:O	1.83	0.78
1:C:127:PHE:CE1	1:C:184:LEU:HG	2.25	0.71
1:C:735:HIS:O	1:C:736:ALA:HB3	1.97	0.64
1:B:127:PHE:CE1	1:B:184:LEU:HG	2.33	0.64
1:C:735:HIS:O	1:C:736:ALA:CB	2.48	0.61
1:D:887:GLN:NE2	1:D:980:GLU:O	2.32	0.61
1:C:655:MET:HB2	5:C:4796:HOH:O	2.00	0.61
1:C:127:PHE:HE1	1:C:184:LEU:HG	1.65	0.60
1:D:262:GLN:HE22	1:D:299:LYS:CE	2.14	0.60
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.84	0.59
1:B:127:PHE:HE1	1:B:184:LEU:HG	1.67	0.57
1:D:653:HIS:HD2	1:D:701:VAL:HG21	1.69	0.57
1:A:655:MET:HB2	5:A:4752:HOH:O	2.04	0.56
1:A:153:TRP:HB2	1:A:185:ALA:HB3	1.88	0.55
1:D:262:GLN:HE22	1:D:299:LYS:HE2	1.71	0.55
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.89	0.54
1:B:887:GLN:NE2	1:B:980:GLU:O	2.36	0.54
1:D:262:GLN:NE2	1:D:299:LYS:CE	2.70	0.54
1:C:619:GLU:HA	1:C:912:ALA:HB2	1.90	0.53
1:B:739:HIS:HB2	5:B:4995:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:950:GLN:HB2	1:C:1023:LYS:HB3	1.90	0.53
1:A:863:GLN:OE1	1:A:952:ARG:NH2	2.42	0.52
1:B:655:MET:HB2	5:B:4878:HOH:O	2.08	0.52
1:A:431:ARG:NH2	5:A:4394:HOH:O	2.41	0.52
1:D:127:PHE:CE1	1:D:184:LEU:HG	2.45	0.52
1:C:270:GLY:HA3	4:C:8005:DMS:O	2.09	0.51
1:D:383:ASN:HA	4:D:8003:DMS:H11	1.91	0.51
1:C:748:CYS:HB3	5:C:5091:HOH:O	2.11	0.51
1:A:608:PHE:CE2	1:A:614:HIS:HD2	2.29	0.51
1:C:598:ASP:OD1	1:C:797:GLU:HA	2.11	0.51
1:A:598:ASP:OD1	1:A:797:GLU:HA	2.10	0.50
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.94	0.50
1:D:361:PRO:HB2	1:D:576:ILE:HG12	1.93	0.50
1:C:1021:CYS:HB2	5:C:4910:HOH:O	2.11	0.50
1:C:88:SER:HA	1:C:366:VAL:HG21	1.94	0.50
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.94	0.49
1:A:573:GLN:HB2	1:A:602:CYS:O	2.12	0.49
1:A:724:GLU:O	1:B:847:LYS:NZ	2.45	0.49
1:D:653:HIS:CD2	1:D:701:VAL:HG21	2.46	0.49
1:A:88:SER:HA	1:A:366:VAL:HG21	1.94	0.49
1:A:755:ARG:HB3	1:A:769:TRP:HB2	1.94	0.48
1:C:576:ILE:HD12	4:C:8010:DMS:O	2.13	0.48
1:D:127:PHE:HE1	1:D:184:LEU:HG	1.78	0.48
1:A:147:ASN:HA	1:A:148:SER:HA	1.64	0.48
1:A:127:PHE:HE1	1:A:184:LEU:HG	1.78	0.48
1:B:794:GLY:HA3	5:B:4316:HOH:O	2.13	0.48
1:A:19:PRO:HD3	1:A:112:PRO:HB3	1.95	0.48
1:A:887:GLN:NE2	1:A:980:GLU:O	2.46	0.48
1:C:755:ARG:HB3	1:C:769:TRP:HB2	1.96	0.48
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.49	0.47
1:A:561:ARG:HD3	1:B:525:SER:O	2.14	0.47
1:A:794:GLY:HA2	5:A:4309:HOH:O	2.15	0.47
1:B:88:SER:HA	1:B:366:VAL:HG21	1.95	0.47
1:D:147:ASN:HA	1:D:148:SER:HA	1.65	0.47
1:C:794:GLY:HA3	5:C:4339:HOH:O	2.15	0.47
1:B:653:HIS:CE1	1:B:667:GLU:HG2	2.50	0.47
1:C:763:GLY:HA3	1:C:822:LEU:HD13	1.97	0.46
1:D:244:VAL:HG21	1:D:256:VAL:HG11	1.96	0.46
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.50	0.46
1:A:873:ALA:O	1:A:876:THR:HG22	2.16	0.46
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:PRO:HG3	4:D:8014:DMS:H23	1.97	0.46
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.97	0.46
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.51	0.46
1:D:883:GLY:HA3	1:D:987:ASP:HA	1.98	0.46
1:B:619:GLU:HA	1:B:912:ALA:HB2	1.97	0.45
1:D:40:GLU:OE2	1:D:43:ARG:NH2	2.47	0.45
1:B:370:GLN:HB2	5:B:4876:HOH:O	2.14	0.45
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.51	0.45
1:B:44:THR:OG1	1:B:46:ARG:HG3	2.16	0.45
1:B:750:GLU:HG2	1:B:755:ARG:HG3	1.99	0.45
1:C:147:ASN:HA	1:C:148:SER:HA	1.70	0.45
1:A:127:PHE:CE1	1:A:184:LEU:HG	2.51	0.45
1:A:546:LEU:HA	5:A:4126:HOH:O	2.17	0.45
1:A:619:GLU:HA	1:A:912:ALA:HB2	1.99	0.45
1:A:883:GLY:HA3	1:A:987:ASP:HA	1.99	0.45
1:D:427:THR:HG21	1:D:462:SER:HB3	1.98	0.45
1:A:361:PRO:HB2	1:A:576:ILE:HG12	1.98	0.45
1:D:262:GLN:NE2	1:D:299:LYS:HE3	2.31	0.45
1:D:410:VAL:HG22	1:D:455:ILE:HB	1.99	0.45
1:D:625:GLN:NE2	5:D:4225:HOH:O	2.49	0.45
1:D:794:GLY:HA3	5:D:4324:HOH:O	2.16	0.45
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.51	0.44
1:B:334:GLU:OE1	1:B:336:ARG:NH1	2.43	0.44
1:B:320:GLY:HA2	4:B:8006:DMS:O	2.17	0.44
1:B:353:GLY:HA2	1:B:386:ALA:O	2.17	0.44
1:D:225:PHE:HA	1:D:243:GLU:O	2.18	0.44
1:D:653:HIS:HD2	1:D:701:VAL:CG2	2.30	0.44
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.99	0.44
1:A:105:TYR:CE1	1:A:199:ASP:HB2	2.53	0.44
1:A:140:ARG:HG2	1:A:215:LEU:HB3	1.98	0.43
1:A:486:TYR:CE2	1:A:488:GLY:HA3	2.52	0.43
1:A:763:GLY:HA3	1:A:822:LEU:HD13	1.99	0.43
1:C:892:ALA:HB3	1:C:946:TYR:CE1	2.53	0.43
1:A:437:SER:O	1:A:441:THR:HG23	2.19	0.43
1:B:361:PRO:HB2	1:B:576:ILE:HG12	2.01	0.43
1:B:755:ARG:NH1	5:B:5110:HOH:O	2.52	0.43
1:B:789:LEU:HD11	1:B:993:ILE:HG22	2.01	0.43
1:D:166:ARG:HG3	1:D:392:TYR:HB2	2.00	0.43
1:A:230:ARG:HG2	5:A:4748:HOH:O	2.18	0.43
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.00	0.42
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:VAL:HG22	1:A:344:LEU:HD12	2.02	0.42
1:A:390:SER:HA	1:A:391:HIS:HA	1.76	0.42
1:A:615:PRO:O	1:A:618:THR:HG22	2.20	0.42
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.54	0.42
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.49	0.42
1:B:390:SER:HA	1:B:391:HIS:HA	1.86	0.42
1:A:9:VAL:HG12	1:D:9:VAL:HG12	2.02	0.41
1:D:763:GLY:HA3	1:D:822:LEU:HD13	2.01	0.41
1:C:573:GLN:HB2	1:C:602:CYS:O	2.20	0.41
1:D:19:PRO:HD3	1:D:112:PRO:CB	2.50	0.41
1:A:802:ASP:HA	1:A:803:PRO:HD2	1.97	0.41
1:C:390:SER:HA	1:C:391:HIS:HA	1.92	0.41
1:B:147:ASN:HA	1:B:148:SER:HA	1.70	0.41
1:D:699:ARG:HH11	1:D:714:ILE:HG21	1.86	0.41
1:C:525:SER:O	1:D:561:ARG:HD3	2.20	0.41
1:D:373:VAL:O	1:D:377:LEU:HG	2.20	0.41
1:D:390:SER:HA	1:D:391:HIS:HA	1.87	0.41
1:B:708:TRP:CE3	1:B:709:SER:HB3	2.55	0.41
1:D:88:SER:HA	1:D:366:VAL:HG21	2.02	0.41
1:B:795:VAL:HG13	1:B:797:GLU:O	2.21	0.41
1:B:755:ARG:HB3	1:B:769:TRP:HB2	2.02	0.41
1:A:628:GLN:NE2	4:A:8002:DMS:O	2.49	0.40
1:C:143:PHE:O	1:C:168:PRO:HA	2.22	0.40
1:A:768:MET:HE2	1:A:768:MET:HB2	1.90	0.40
1:B:19:PRO:HD3	1:B:112:PRO:CB	2.52	0.40

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%)	981 (97%)	32 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1013/1052 (96%)	980 (97%)	32 (3%)	1 (0%)	51	45
1	C	1013/1052 (96%)	985 (97%)	27 (3%)	1 (0%)	51	45
1	D	1013/1052 (96%)	976 (96%)	37 (4%)	0	100	100
All	All	4052/4208 (96%)	3922 (97%)	128 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	736	ALA
1	B	752	GLY

### 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	867/897 (97%)	861 (99%)	6 (1%)	84	84
1	B	867/897 (97%)	858 (99%)	9 (1%)	76	75
1	C	867/897 (97%)	863 (100%)	4 (0%)	88	89
1	D	867/897 (97%)	862 (99%)	5 (1%)	86	87
All	All	3468/3588 (97%)	3444 (99%)	24 (1%)	84	84

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	333	ARG
1	A	348	PRO
1	A	394	ASN
1	A	546	LEU
1	A	744	GLU
1	B	333	ARG
1	B	344	LEU
1	B	394	ASN

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Mol	Chain	Res	Type
1	B	546	LEU
1	B	652	LEU
1	B	672	VAL
1	B	761	GLN
1	B	774	LYS
1	B	817	GLN
1	C	333	ARG
1	C	344	LEU
1	C	817	GLN
1	C	956	GLN
1	D	333	ARG
1	D	394	ASN
1	D	546	LEU
1	D	672	VAL
1	D	744	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	693	GLN
1	A	757	GLN
1	B	1017	GLN
1	C	583	ASN
1	D	262	GLN
1	D	890	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 101 ligands modelled in this entry, 23 are monoatomic - leaving 78 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
4	DMS	C	8020	-	3,3,3	2.64	1 (33%)	3,3,3	0.51	0
4	DMS	C	8012	-	3,3,3	2.59	1 (33%)	3,3,3	0.60	0
4	DMS	D	8004	-	3,3,3	2.58	1 (33%)	3,3,3	0.52	0
4	DMS	C	8011	-	3,3,3	2.61	1 (33%)	3,3,3	0.23	0
4	DMS	B	8023	-	3,3,3	2.63	1 (33%)	3,3,3	0.53	0
4	DMS	D	8010	-	3,3,3	2.64	1 (33%)	3,3,3	0.54	0
4	DMS	C	8001	-	3,3,3	2.63	1 (33%)	3,3,3	0.89	0
4	DMS	B	8013	-	3,3,3	2.64	1 (33%)	3,3,3	0.60	0
4	DMS	D	8007	-	3,3,3	2.66	1 (33%)	3,3,3	0.66	0
4	DMS	C	8003	-	3,3,3	2.58	1 (33%)	3,3,3	0.25	0
4	DMS	B	8020	-	3,3,3	2.83	1 (33%)	3,3,3	0.76	0
4	DMS	A	8004	-	3,3,3	2.61	1 (33%)	3,3,3	0.49	0
4	DMS	A	8010	-	3,3,3	2.61	1 (33%)	3,3,3	0.52	0
4	DMS	B	8009	-	3,3,3	2.66	1 (33%)	3,3,3	0.57	0
4	DMS	C	8018	-	3,3,3	2.65	1 (33%)	3,3,3	0.58	0
4	DMS	D	8002	-	3,3,3	2.55	1 (33%)	3,3,3	0.55	0
4	DMS	B	8016	-	3,3,3	2.64	1 (33%)	3,3,3	0.55	0
4	DMS	D	8008	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
4	DMS	D	8012	-	3,3,3	2.64	1 (33%)	3,3,3	0.67	0
4	DMS	B	8018	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
4	DMS	B	8012	-	3,3,3	2.70	1 (33%)	3,3,3	0.64	0
4	DMS	A	8001	-	3,3,3	2.58	1 (33%)	3,3,3	0.63	0
4	DMS	D	8005	-	3,3,3	2.56	1 (33%)	3,3,3	0.30	0
4	DMS	C	8008	-	3,3,3	2.67	1 (33%)	3,3,3	0.65	0
4	DMS	A	8015	-	3,3,3	2.68	1 (33%)	3,3,3	0.54	0
4	DMS	C	8019	-	3,3,3	2.64	1 (33%)	3,3,3	0.52	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DMS	A	8002	-	3,3,3	2.61	1 (33%)	3,3,3	0.49	0
4	DMS	A	8012	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
4	DMS	B	8017	-	3,3,3	2.60	1 (33%)	3,3,3	0.49	0
4	DMS	C	8014	-	3,3,3	2.62	1 (33%)	3,3,3	0.58	0
4	DMS	B	8014	-	3,3,3	2.63	1 (33%)	3,3,3	0.50	0
4	DMS	A	8019	-	3,3,3	2.66	1 (33%)	3,3,3	0.50	0
4	DMS	B	8010	-	3,3,3	2.55	1 (33%)	3,3,3	0.33	0
4	DMS	C	8017	-	3,3,3	2.61	1 (33%)	3,3,3	0.38	0
4	DMS	D	8009	-	3,3,3	2.61	1 (33%)	3,3,3	0.51	0
4	DMS	A	8006	-	3,3,3	2.66	1 (33%)	3,3,3	0.56	0
4	DMS	A	8016	-	3,3,3	2.66	1 (33%)	3,3,3	0.52	0
4	DMS	C	8016	-	3,3,3	2.64	1 (33%)	3,3,3	0.59	0
4	DMS	A	8018	-	3,3,3	2.62	1 (33%)	3,3,3	0.44	0
4	DMS	D	8013	-	3,3,3	2.62	1 (33%)	3,3,3	0.46	0
4	DMS	C	8015	-	3,3,3	2.65	1 (33%)	3,3,3	0.58	0
4	DMS	B	8008	-	3,3,3	2.74	1 (33%)	3,3,3	0.60	0
4	DMS	B	8019	-	3,3,3	2.69	1 (33%)	3,3,3	0.59	0
4	DMS	C	8002	-	3,3,3	2.56	1 (33%)	3,3,3	0.54	0
4	DMS	D	8003	-	3,3,3	2.61	1 (33%)	3,3,3	0.56	0
4	DMS	C	8009	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
4	DMS	D	8014	-	3,3,3	2.64	1 (33%)	3,3,3	0.46	0
4	DMS	C	8010	-	3,3,3	2.61	1 (33%)	3,3,3	0.47	0
4	DMS	A	8007	-	3,3,3	2.66	1 (33%)	3,3,3	0.59	0
4	DMS	A	8021	-	3,3,3	2.64	1 (33%)	3,3,3	0.52	0
4	DMS	A	8017	-	3,3,3	2.69	1 (33%)	3,3,3	0.61	0
4	DMS	A	8003	-	3,3,3	2.63	1 (33%)	3,3,3	0.59	0
4	DMS	C	8013	-	3,3,3	2.67	1 (33%)	3,3,3	0.72	0
4	DMS	B	8002	-	3,3,3	2.62	1 (33%)	3,3,3	0.51	0
4	DMS	A	8013	-	3,3,3	2.65	1 (33%)	3,3,3	0.62	0
4	DMS	D	8011	-	3,3,3	2.63	1 (33%)	3,3,3	0.51	0
4	DMS	B	8005	-	3,3,3	2.64	1 (33%)	3,3,3	0.28	0
4	DMS	D	8001	-	3,3,3	2.65	1 (33%)	3,3,3	0.84	0
4	DMS	B	8001	-	3,3,3	2.52	1 (33%)	3,3,3	0.44	0
4	DMS	B	8006	-	3,3,3	2.64	1 (33%)	3,3,3	0.65	0
4	DMS	B	8022	-	3,3,3	2.68	1 (33%)	3,3,3	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DMS	A	8022	-	3,3,3	2.64	1 (33%)	3,3,3	0.59	0
4	DMS	C	8006	-	3,3,3	2.63	1 (33%)	3,3,3	0.47	0
4	DMS	A	8009	-	3,3,3	2.69	1 (33%)	3,3,3	0.64	0
4	DMS	B	8004	-	3,3,3	2.63	1 (33%)	3,3,3	0.58	0
4	DMS	C	8007	-	3,3,3	2.67	1 (33%)	3,3,3	0.67	0
4	DMS	B	8021	-	3,3,3	2.68	1 (33%)	3,3,3	0.58	0
4	DMS	B	8015	-	3,3,3	2.58	1 (33%)	3,3,3	0.54	0
4	DMS	B	8003	-	3,3,3	2.62	1 (33%)	3,3,3	0.48	0
4	DMS	C	8004	-	3,3,3	2.64	1 (33%)	3,3,3	0.64	0
4	DMS	B	8007	-	3,3,3	2.62	1 (33%)	3,3,3	0.57	0
4	DMS	B	8011	-	3,3,3	2.65	1 (33%)	3,3,3	0.57	0
4	DMS	A	8011	-	3,3,3	2.63	1 (33%)	3,3,3	0.57	0
4	DMS	A	8005	-	3,3,3	2.56	1 (33%)	3,3,3	0.52	0
4	DMS	D	8006	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
4	DMS	A	8008	-	3,3,3	2.70	1 (33%)	3,3,3	0.51	0
4	DMS	C	8005	-	3,3,3	2.59	1 (33%)	3,3,3	0.41	0
4	DMS	A	8020	-	3,3,3	2.66	1 (33%)	3,3,3	0.51	0

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8020	DMS	O-S	4.76	1.82	1.50
4	B	8008	DMS	O-S	4.60	1.81	1.50
4	B	8012	DMS	O-S	4.52	1.80	1.50
4	A	8008	DMS	O-S	4.51	1.80	1.50
4	D	8008	DMS	O-S	4.51	1.80	1.50
4	A	8009	DMS	O-S	4.50	1.80	1.50
4	B	8021	DMS	O-S	4.50	1.80	1.50
4	B	8019	DMS	O-S	4.50	1.80	1.50
4	D	8006	DMS	O-S	4.49	1.80	1.50
4	B	8022	DMS	O-S	4.49	1.80	1.50
4	A	8017	DMS	O-S	4.49	1.80	1.50
4	A	8012	DMS	O-S	4.49	1.80	1.50
4	A	8015	DMS	O-S	4.49	1.80	1.50
4	C	8007	DMS	O-S	4.48	1.80	1.50
4	C	8008	DMS	O-S	4.48	1.80	1.50
4	A	8016	DMS	O-S	4.47	1.80	1.50
4	C	8013	DMS	O-S	4.46	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	8019	DMS	O-S	4.46	1.80	1.50
4	D	8014	DMS	O-S	4.46	1.80	1.50
4	B	8009	DMS	O-S	4.46	1.80	1.50
4	A	8020	DMS	O-S	4.46	1.80	1.50
4	A	8006	DMS	O-S	4.45	1.80	1.50
4	C	8009	DMS	O-S	4.45	1.80	1.50
4	D	8007	DMS	O-S	4.45	1.80	1.50
4	B	8018	DMS	O-S	4.45	1.80	1.50
4	A	8007	DMS	O-S	4.45	1.80	1.50
4	C	8019	DMS	O-S	4.45	1.80	1.50
4	C	8015	DMS	O-S	4.44	1.80	1.50
4	B	8011	DMS	O-S	4.44	1.80	1.50
4	D	8010	DMS	O-S	4.44	1.80	1.50
4	C	8020	DMS	O-S	4.44	1.80	1.50
4	A	8022	DMS	O-S	4.44	1.80	1.50
4	C	8016	DMS	O-S	4.43	1.80	1.50
4	B	8023	DMS	O-S	4.43	1.80	1.50
4	B	8005	DMS	O-S	4.43	1.80	1.50
4	C	8018	DMS	O-S	4.43	1.80	1.50
4	B	8006	DMS	O-S	4.43	1.80	1.50
4	B	8013	DMS	O-S	4.43	1.80	1.50
4	D	8001	DMS	O-S	4.43	1.80	1.50
4	C	8001	DMS	O-S	4.42	1.80	1.50
4	A	8013	DMS	O-S	4.42	1.80	1.50
4	A	8011	DMS	O-S	4.42	1.80	1.50
4	D	8012	DMS	O-S	4.42	1.80	1.50
4	A	8021	DMS	O-S	4.42	1.80	1.50
4	C	8006	DMS	O-S	4.42	1.80	1.50
4	C	8004	DMS	O-S	4.42	1.80	1.50
4	D	8013	DMS	O-S	4.42	1.80	1.50
4	B	8016	DMS	O-S	4.42	1.80	1.50
4	A	8003	DMS	O-S	4.41	1.80	1.50
4	B	8014	DMS	O-S	4.41	1.80	1.50
4	A	8004	DMS	O-S	4.40	1.80	1.50
4	C	8014	DMS	O-S	4.40	1.80	1.50
4	B	8003	DMS	O-S	4.40	1.80	1.50
4	D	8011	DMS	O-S	4.40	1.80	1.50
4	B	8002	DMS	O-S	4.40	1.79	1.50
4	C	8017	DMS	O-S	4.40	1.79	1.50
4	B	8004	DMS	O-S	4.40	1.79	1.50
4	A	8002	DMS	O-S	4.39	1.79	1.50
4	D	8003	DMS	O-S	4.39	1.79	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	8011	DMS	O-S	4.39	1.79	1.50
4	A	8018	DMS	O-S	4.38	1.79	1.50
4	B	8007	DMS	O-S	4.38	1.79	1.50
4	C	8010	DMS	O-S	4.37	1.79	1.50
4	A	8010	DMS	O-S	4.37	1.79	1.50
4	C	8003	DMS	O-S	4.37	1.79	1.50
4	D	8009	DMS	O-S	4.36	1.79	1.50
4	B	8017	DMS	O-S	4.36	1.79	1.50
4	B	8015	DMS	O-S	4.35	1.79	1.50
4	C	8012	DMS	O-S	4.33	1.79	1.50
4	D	8004	DMS	O-S	4.32	1.79	1.50
4	C	8005	DMS	O-S	4.32	1.79	1.50
4	A	8001	DMS	O-S	4.32	1.79	1.50
4	C	8002	DMS	O-S	4.32	1.79	1.50
4	D	8005	DMS	O-S	4.30	1.79	1.50
4	B	8010	DMS	O-S	4.29	1.79	1.50
4	D	8002	DMS	O-S	4.29	1.79	1.50
4	A	8005	DMS	O-S	4.28	1.79	1.50
4	B	8001	DMS	O-S	4.22	1.78	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	8003	DMS	1	0
4	A	8002	DMS	1	0
4	D	8003	DMS	1	0
4	D	8014	DMS	1	0
4	C	8010	DMS	1	0
4	B	8006	DMS	1	0
4	C	8005	DMS	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	1015/1052 (96%)	-0.08	34 (3%)	46	50	15, 27, 53, 86	0
1	B	1015/1052 (96%)	-0.24	21 (2%)	63	67	12, 21, 46, 88	0
1	C	1015/1052 (96%)	-0.23	25 (2%)	57	61	12, 22, 47, 89	0
1	D	1015/1052 (96%)	-0.03	33 (3%)	46	50	15, 29, 53, 91	0
All	All	4060/4208 (96%)	-0.14	113 (2%)	53	58	12, 25, 51, 91	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	731	PRO	5.9
1	C	686	PRO	5.5
1	D	11	LEU	5.3
1	B	799	THR	5.2
1	A	799	THR	5.2
1	D	687	GLN	5.2
1	A	689	GLU	5.0
1	A	9	VAL	4.9
1	C	1023	LYS	4.9
1	B	689	GLU	4.8
1	C	731	PRO	4.7
1	A	687	GLN	4.6
1	C	689	GLU	4.5
1	B	686	PRO	4.5
1	A	686	PRO	4.5
1	A	801	ILE	4.4
1	B	795	VAL	4.4
1	B	732	ALA	4.3
1	D	686	PRO	4.2
1	D	799	THR	4.1
1	D	731	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	689	GLU	4.0
1	D	10	VAL	4.0
1	C	795	VAL	4.0
1	B	9	VAL	3.9
1	B	770	ILE	3.9
1	D	76	CYS	3.9
1	C	770	ILE	3.9
1	C	11	LEU	3.9
1	D	730	LEU	3.9
1	D	735	HIS	3.8
1	C	801	ILE	3.7
1	A	733	ALA	3.7
1	B	11	LEU	3.7
1	A	685	LEU	3.6
1	B	730	LEU	3.6
1	C	798	ALA	3.6
1	C	730	LEU	3.6
1	A	730	LEU	3.6
1	A	795	VAL	3.6
1	D	732	ALA	3.5
1	A	11	LEU	3.5
1	D	795	VAL	3.5
1	A	796	ALA	3.5
1	A	735	HIS	3.4
1	A	12	GLN	3.4
1	D	801	ILE	3.4
1	B	687	GLN	3.4
1	B	12	GLN	3.4
1	A	732	ALA	3.3
1	C	687	GLN	3.3
1	D	130	ASP	3.3
1	B	733	ALA	3.1
1	B	1023	LYS	3.1
1	D	79	PRO	3.1
1	C	9	VAL	3.1
1	D	772	ASP	3.1
1	C	10	VAL	3.1
1	C	800	ARG	3.1
1	B	801	ILE	2.9
1	A	731	PRO	2.9
1	A	158	TRP	2.9
1	D	794	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	684	GLU	2.9
1	A	79	PRO	2.8
1	A	800	ARG	2.8
1	A	1023	LYS	2.7
1	D	12	GLN	2.7
1	B	800	ARG	2.7
1	D	770	ILE	2.7
1	C	690	SER	2.7
1	A	688	PRO	2.6
1	C	12	GLN	2.6
1	D	685	LEU	2.6
1	C	688	PRO	2.6
1	D	68	ALA	2.6
1	D	773	LYS	2.5
1	D	1022	GLN	2.5
1	A	81	ALA	2.5
1	B	798	ALA	2.5
1	D	800	ARG	2.4
1	D	70	PRO	2.4
1	B	685	LEU	2.4
1	A	76	CYS	2.4
1	A	69	VAL	2.4
1	C	733	ALA	2.4
1	A	71	GLU	2.4
1	A	734	SER	2.4
1	C	685	LEU	2.4
1	D	581	ASN	2.4
1	A	75	GLU	2.4
1	D	796	ALA	2.4
1	A	181	GLU	2.3
1	D	131	GLU	2.3
1	A	117	GLU	2.3
1	D	798	ALA	2.3
1	C	796	ALA	2.2
1	A	761	GLN	2.2
1	A	798	ALA	2.2
1	C	799	THR	2.2
1	A	78	LEU	2.2
1	C	772	ASP	2.2
1	B	771	GLY	2.2
1	A	130	ASP	2.2
1	C	732	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	663	LEU	2.1
1	B	773	LYS	2.1
1	C	819	GLU	2.1
1	D	733	ALA	2.1
1	A	180	GLY	2.1
1	D	745	MET	2.0
1	D	128	ASN	2.0
1	D	158	TRP	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
4	DMS	B	8012	4/4	0.14	0.58	108,109,109,111	0
4	DMS	B	8020	4/4	0.61	0.30	44,52,56,61	0
4	DMS	D	8006	4/4	0.67	0.32	75,77,79,82	0
4	DMS	A	8009	4/4	0.70	0.29	89,90,90,92	0
4	DMS	A	8012	4/4	0.72	0.34	88,88,89,91	0
4	DMS	B	8009	4/4	0.74	0.31	78,78,80,80	0
4	DMS	A	8020	4/4	0.76	0.28	77,78,78,82	0
4	DMS	B	8016	4/4	0.77	0.24	55,58,61,66	0
4	DMS	C	8019	4/4	0.79	0.23	60,60,65,70	0
4	DMS	D	8013	4/4	0.79	0.21	57,60,63,63	0
4	DMS	C	8004	4/4	0.79	0.27	44,46,52,53	0
4	DMS	A	8006	4/4	0.81	0.23	62,62,64,70	0
4	DMS	D	8008	4/4	0.81	0.24	66,66,67,70	0
4	DMS	A	8013	4/4	0.82	0.34	66,69,69,70	0
4	DMS	A	8017	4/4	0.83	0.26	71,72,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	D	3002	1/1	0.84	0.12	31,31,31,31	0
2	MG	A	3002	1/1	0.85	0.10	33,33,33,33	0
4	DMS	C	8016	4/4	0.85	0.21	61,61,64,65	0
4	DMS	C	8013	4/4	0.86	0.26	43,47,49,56	0
4	DMS	C	8012	4/4	0.87	0.23	53,53,54,56	0
4	DMS	C	8017	4/4	0.87	0.23	77,77,78,78	0
4	DMS	C	8009	4/4	0.87	0.25	70,72,73,74	0
4	DMS	D	8002	4/4	0.87	0.32	54,59,62,62	0
4	DMS	A	8016	4/4	0.87	0.19	68,69,71,72	0
4	DMS	A	8015	4/4	0.89	0.22	72,74,75,75	0
4	DMS	C	8008	4/4	0.89	0.23	57,58,60,61	0
4	DMS	D	8011	4/4	0.89	0.34	72,72,74,75	0
4	DMS	B	8021	4/4	0.89	0.17	60,61,62,67	0
4	DMS	A	8021	4/4	0.89	0.19	71,73,73,74	0
4	DMS	D	8001	4/4	0.90	0.22	42,45,48,52	0
4	DMS	A	8018	4/4	0.90	0.25	64,65,65,65	0
4	DMS	D	8009	4/4	0.90	0.21	49,51,52,55	0
4	DMS	A	8008	4/4	0.91	0.19	49,53,55,57	0
4	DMS	D	8014	4/4	0.91	0.34	69,71,74,75	0
4	DMS	D	8004	4/4	0.91	0.20	53,54,54,58	0
4	DMS	A	8004	4/4	0.91	0.14	53,54,55,59	0
4	DMS	C	8011	4/4	0.91	0.25	51,54,57,58	0
4	DMS	B	8015	4/4	0.91	0.27	41,42,45,55	0
4	DMS	C	8020	4/4	0.92	0.16	50,52,52,55	0
4	DMS	D	8012	4/4	0.92	0.17	48,49,51,58	0
4	DMS	C	8007	4/4	0.92	0.24	53,54,59,62	0
4	DMS	C	8006	4/4	0.92	0.19	56,58,61,61	0
4	DMS	B	8018	4/4	0.92	0.24	56,58,59,62	0
4	DMS	A	8019	4/4	0.92	0.19	64,64,66,67	0
4	DMS	C	8015	4/4	0.92	0.16	58,59,61,62	0
4	DMS	D	8007	4/4	0.93	0.20	52,53,53,55	0
4	DMS	C	8001	4/4	0.93	0.21	28,33,39,40	0
4	DMS	C	8005	4/4	0.93	0.21	37,40,44,47	0
4	DMS	B	8022	4/4	0.93	0.14	49,52,53,53	0
4	DMS	B	8013	4/4	0.93	0.21	47,51,54,56	0
4	DMS	A	8007	4/4	0.93	0.23	45,47,50,51	0
3	NA	B	3103	1/1	0.93	0.11	48,48,48,48	0
4	DMS	B	8006	4/4	0.93	0.20	39,46,46,49	0
4	DMS	B	8023	4/4	0.93	0.18	58,59,61,61	0
4	DMS	B	8019	4/4	0.94	0.15	30,31,41,43	0
4	DMS	C	8018	4/4	0.94	0.13	35,37,41,43	0
4	DMS	B	8008	4/4	0.94	0.15	38,43,45,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NA	D	3102	1/1	0.94	0.11	24,24,24,24	0
4	DMS	C	8010	4/4	0.94	0.21	33,34,40,47	0
4	DMS	D	8010	4/4	0.94	0.17	51,54,56,57	0
4	DMS	C	8014	4/4	0.94	0.21	53,55,56,56	0
3	NA	C	3102	1/1	0.94	0.12	22,22,22,22	0
4	DMS	D	8005	4/4	0.94	0.21	43,45,49,49	0
4	DMS	B	8014	4/4	0.95	0.16	50,53,54,57	0
4	DMS	C	8002	4/4	0.95	0.15	30,31,36,41	0
4	DMS	A	8010	4/4	0.95	0.17	47,48,48,51	0
4	DMS	B	8004	4/4	0.95	0.12	22,26,33,34	0
2	MG	B	3002	1/1	0.95	0.16	21,21,21,21	0
2	MG	B	3007	1/1	0.95	0.15	46,46,46,46	0
2	MG	B	3001	1/1	0.96	0.07	17,17,17,17	0
3	NA	A	3103	1/1	0.96	0.16	41,41,41,41	0
3	NA	C	3103	1/1	0.96	0.14	43,43,43,43	0
4	DMS	B	8017	4/4	0.96	0.16	38,40,41,43	0
3	NA	A	3101	1/1	0.96	0.09	29,29,29,29	0
4	DMS	D	8003	4/4	0.96	0.19	38,41,42,43	0
3	NA	D	3103	1/1	0.96	0.12	49,49,49,49	0
4	DMS	B	8002	4/4	0.96	0.14	23,29,30,34	0
4	DMS	A	8011	4/4	0.96	0.18	50,51,53,56	0
4	DMS	A	8002	4/4	0.96	0.17	32,35,37,40	0
2	MG	C	3001	1/1	0.96	0.09	17,17,17,17	0
3	NA	C	3104	1/1	0.96	0.13	35,35,35,35	0
3	NA	D	3101	1/1	0.97	0.09	29,29,29,29	0
2	MG	C	3002	1/1	0.97	0.12	21,21,21,21	0
4	DMS	A	8003	4/4	0.97	0.11	36,36,39,42	0
4	DMS	B	8007	4/4	0.97	0.14	36,38,39,44	0
4	DMS	A	8005	4/4	0.97	0.14	34,39,40,41	0
4	DMS	B	8011	4/4	0.97	0.13	44,45,46,49	0
4	DMS	A	8022	4/4	0.97	0.19	57,57,58,58	0
3	NA	B	3104	1/1	0.97	0.10	35,35,35,35	0
4	DMS	B	8010	4/4	0.98	0.17	32,35,38,40	0
3	NA	B	3102	1/1	0.98	0.09	21,21,21,21	0
4	DMS	C	8003	4/4	0.98	0.16	34,38,39,41	0
3	NA	C	3101	1/1	0.98	0.09	23,23,23,23	0
4	DMS	B	8003	4/4	0.98	0.13	32,36,36,37	0
3	NA	B	3101	1/1	0.98	0.08	20,20,20,20	0
2	MG	A	3001	1/1	0.98	0.08	24,24,24,24	0
4	DMS	B	8005	4/4	0.98	0.16	34,37,37,38	0
4	DMS	B	8001	4/4	0.98	0.12	22,26,27,29	0
2	MG	D	3001	1/1	0.99	0.06	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DMS	A	8001	4/4	0.99	0.11	23,30,31,32	0
3	NA	A	3102	1/1	0.99	0.09	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.