



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:23 PM GMT

PDB ID : 1JYN  
Title : E. COLI (lacZ) BETA-GALACTOSIDASE (E537Q) IN COMPLEX WITH LACTOSE  
Authors : Juers, D.H.; Matthews, B.W.  
Deposited on : 2001-09-13  
Resolution : 1.80 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

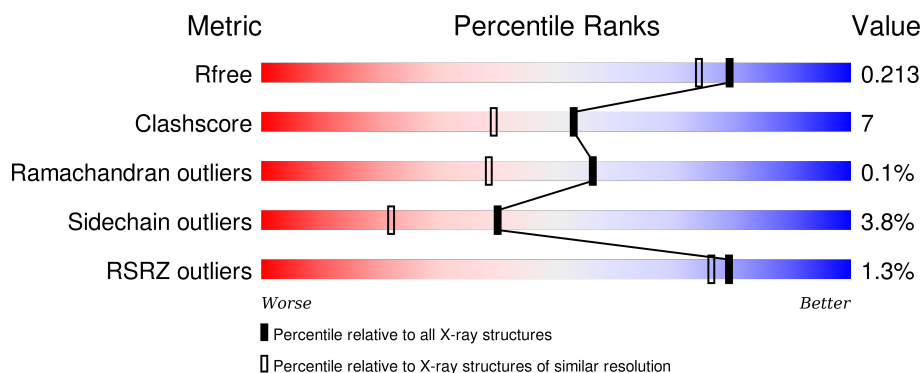
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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. 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	1023	<div> <div>2%</div> <div>74%</div> <div>21%</div> <div>• •</div> </div>
1	B	1023	<div> <div>2%</div> <div>75%</div> <div>21%</div> <div>• •</div> </div>
1	C	1023	<div> <div>2%</div> <div>74%</div> <div>21%</div> <div>• •</div> </div>
1	D	1023	<div> <div>2%</div> <div>74%</div> <div>21%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LAT	A	2001	-	-	-	X
2	LAT	B	2001	-	-	-	X
2	LAT	D	2001	-	-	-	X
5	DMS	A	8406	-	-	-	X
5	DMS	A	8407	-	-	-	X
5	DMS	A	8419	-	-	-	X
5	DMS	A	8420	-	-	-	X
5	DMS	A	8423	-	-	-	X
5	DMS	A	8504	-	-	-	X
5	DMS	A	8507	-	-	-	X
5	DMS	B	8405	-	-	-	X
5	DMS	B	8407	-	-	-	X
5	DMS	B	8408	-	-	-	X
5	DMS	B	8417	-	-	-	X
5	DMS	B	8420	-	-	-	X
5	DMS	B	8423	-	-	-	X
5	DMS	B	8425	-	-	-	X
5	DMS	B	8502	-	-	-	X
5	DMS	B	8508	-	-	-	X
5	DMS	C	8405	-	-	-	X
5	DMS	C	8407	-	-	-	X
5	DMS	C	8417	-	-	-	X
5	DMS	C	8419	-	-	-	X
5	DMS	C	8420	-	-	-	X
5	DMS	C	8423	-	-	-	X
5	DMS	C	8425	-	-	-	X
5	DMS	C	8501	-	-	-	X
5	DMS	D	8404	-	-	-	X
5	DMS	D	8406	-	-	-	X
5	DMS	D	8407	-	-	-	X
5	DMS	D	8419	-	-	-	X
5	DMS	D	8423	-	-	-	X
5	DMS	D	8703	-	-	-	X
5	DMS	D	8704	-	-	-	X
5	DMS	D	8705	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37546 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	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	B	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	C	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	D	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			

There are 36 discrepancies between the modelled and reference sequences:

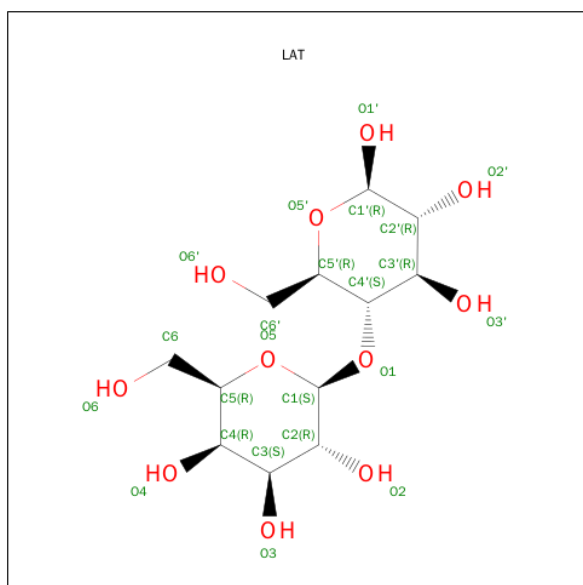
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	THR	CLONING ARTIFACT	? P00722
A	2	SER	MET	CLONING ARTIFACT	? P00722
A	3	HIS	ILE	CLONING ARTIFACT	? P00722
A	4	MET	THR	CLONING ARTIFACT	? P00722
A	5	LEU	ASP	CLONING ARTIFACT	? P00722
A	6	GLU	SER	CLONING ARTIFACT	? P00722
A	7	ASP	LEU	CLONING ARTIFACT	? P00722
A	8	PRO	ALA	CLONING ARTIFACT	? P00722
A	537	GLN	GLU	ENGINEERED	? P00722
B	1	GLY	THR	CLONING ARTIFACT	? P00722
B	2	SER	MET	CLONING ARTIFACT	? P00722
B	3	HIS	ILE	CLONING ARTIFACT	? P00722
B	4	MET	THR	CLONING ARTIFACT	? P00722
B	5	LEU	ASP	CLONING ARTIFACT	? P00722
B	6	GLU	SER	CLONING ARTIFACT	? P00722
B	7	ASP	LEU	CLONING ARTIFACT	? P00722
B	8	PRO	ALA	CLONING ARTIFACT	? P00722
B	537	GLN	GLU	ENGINEERED	? P00722
C	1	GLY	THR	CLONING ARTIFACT	? P00722
C	2	SER	MET	CLONING ARTIFACT	? P00722
C	3	HIS	ILE	CLONING ARTIFACT	? P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	THR	CLONING ARTIFACT	? P00722
C	5	LEU	ASP	CLONING ARTIFACT	? P00722
C	6	GLU	SER	CLONING ARTIFACT	? P00722
C	7	ASP	LEU	CLONING ARTIFACT	? P00722
C	8	PRO	ALA	CLONING ARTIFACT	? P00722
C	537	GLN	GLU	ENGINEERED	? P00722
D	1	GLY	THR	CLONING ARTIFACT	? P00722
D	2	SER	MET	CLONING ARTIFACT	? P00722
D	3	HIS	ILE	CLONING ARTIFACT	? P00722
D	4	MET	THR	CLONING ARTIFACT	? P00722
D	5	LEU	ASP	CLONING ARTIFACT	? P00722
D	6	GLU	SER	CLONING ARTIFACT	? P00722
D	7	ASP	LEU	CLONING ARTIFACT	? P00722
D	8	PRO	ALA	CLONING ARTIFACT	? P00722
D	537	GLN	GLU	ENGINEERED	? P00722

- Molecule 2 is SUGAR (LACTOSE) (three-letter code: LAT) (formula: C<sub>12</sub>H<sub>22</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		

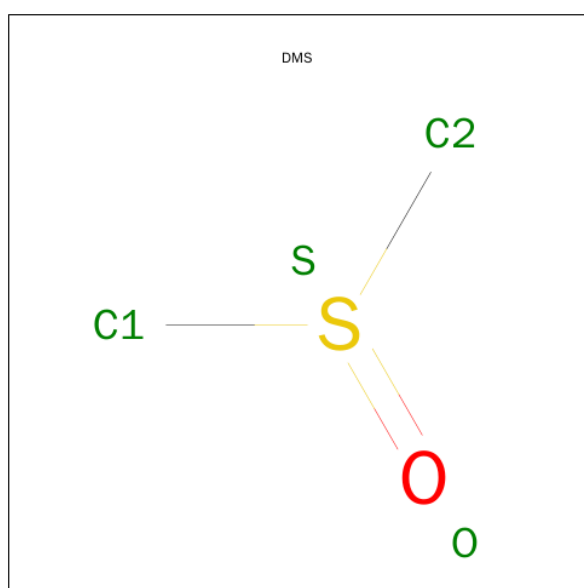
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	4	Total	Mg	0	0
			4	4		
3	D	4	Total	Mg	0	0
			4	4		
3	C	4	Total	Mg	0	0
			4	4		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

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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	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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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
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	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	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
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	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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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

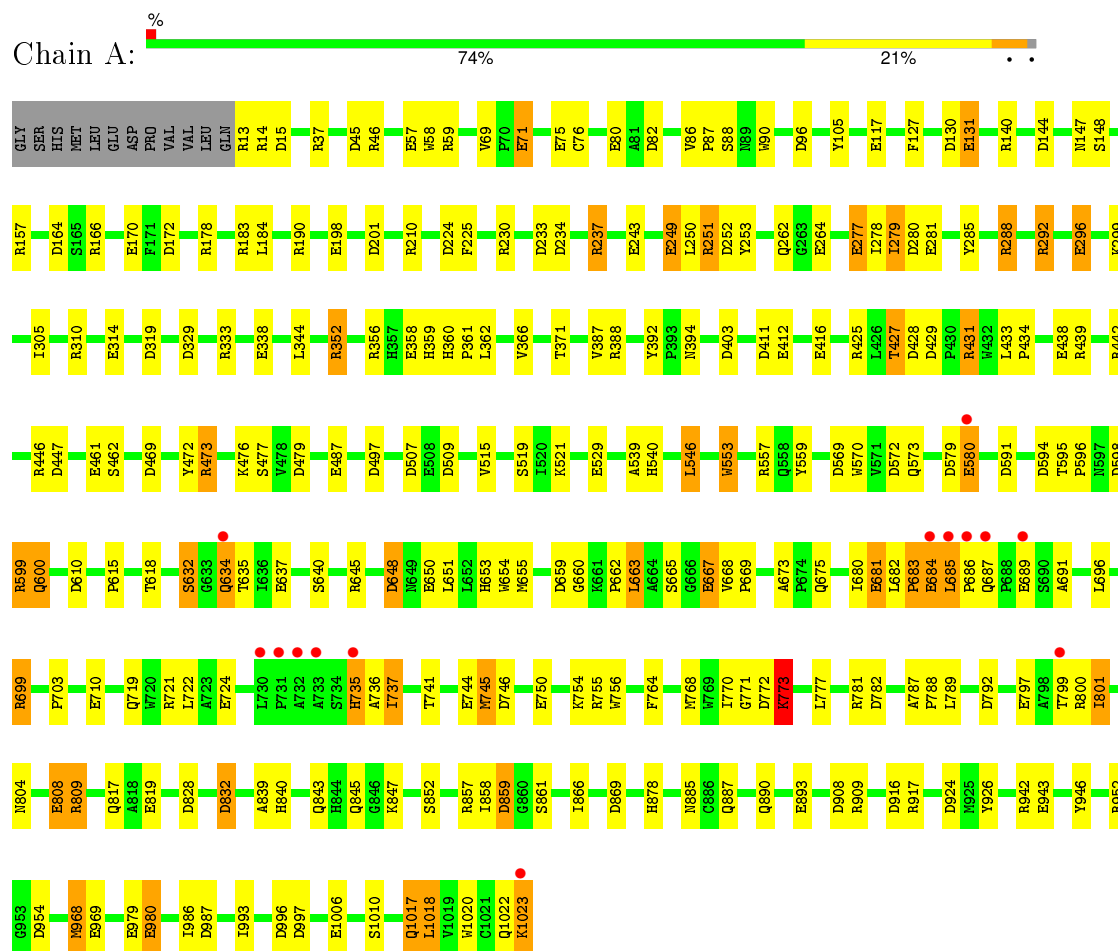
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1136	Total 1136	O 1136	0	0
6	B	1151	Total 1151	O 1151	0	0
6	C	1133	Total 1133	O 1133	0	0
6	D	1109	Total 1109	O 1109	0	0

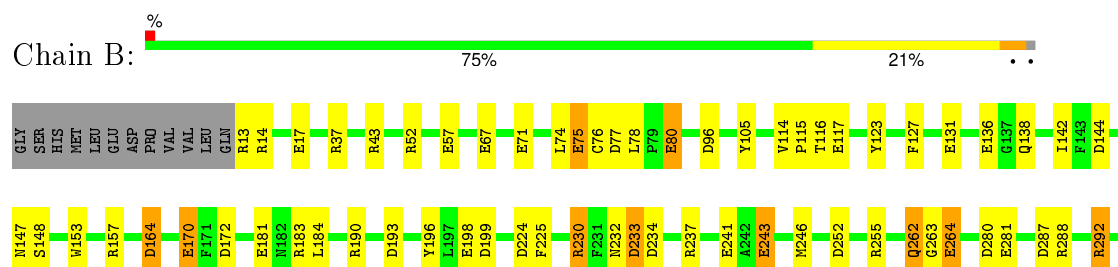
### 3 Residue-property plots

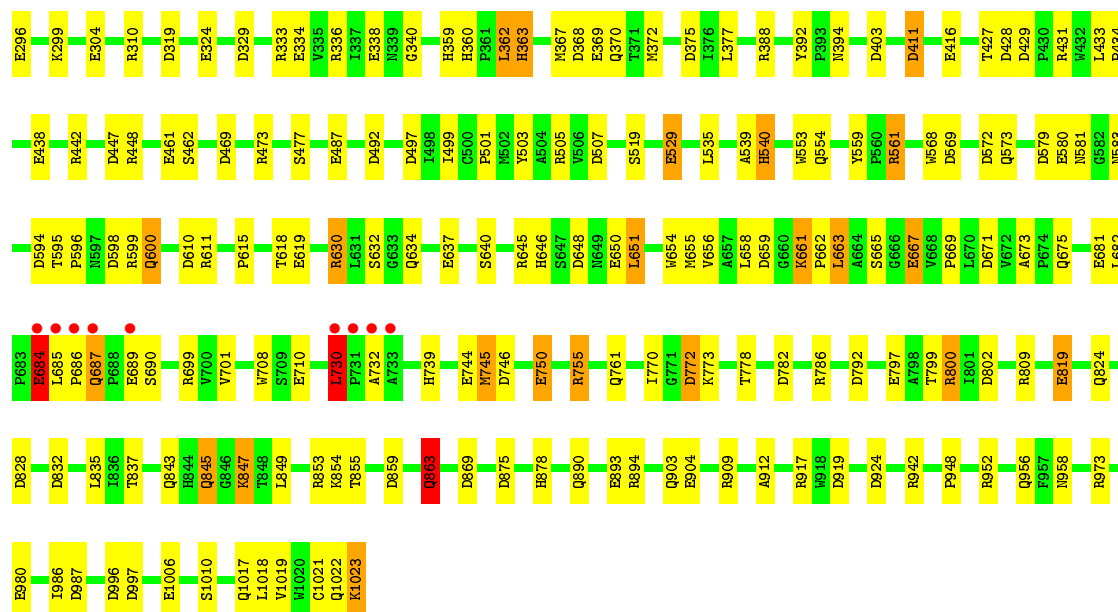
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

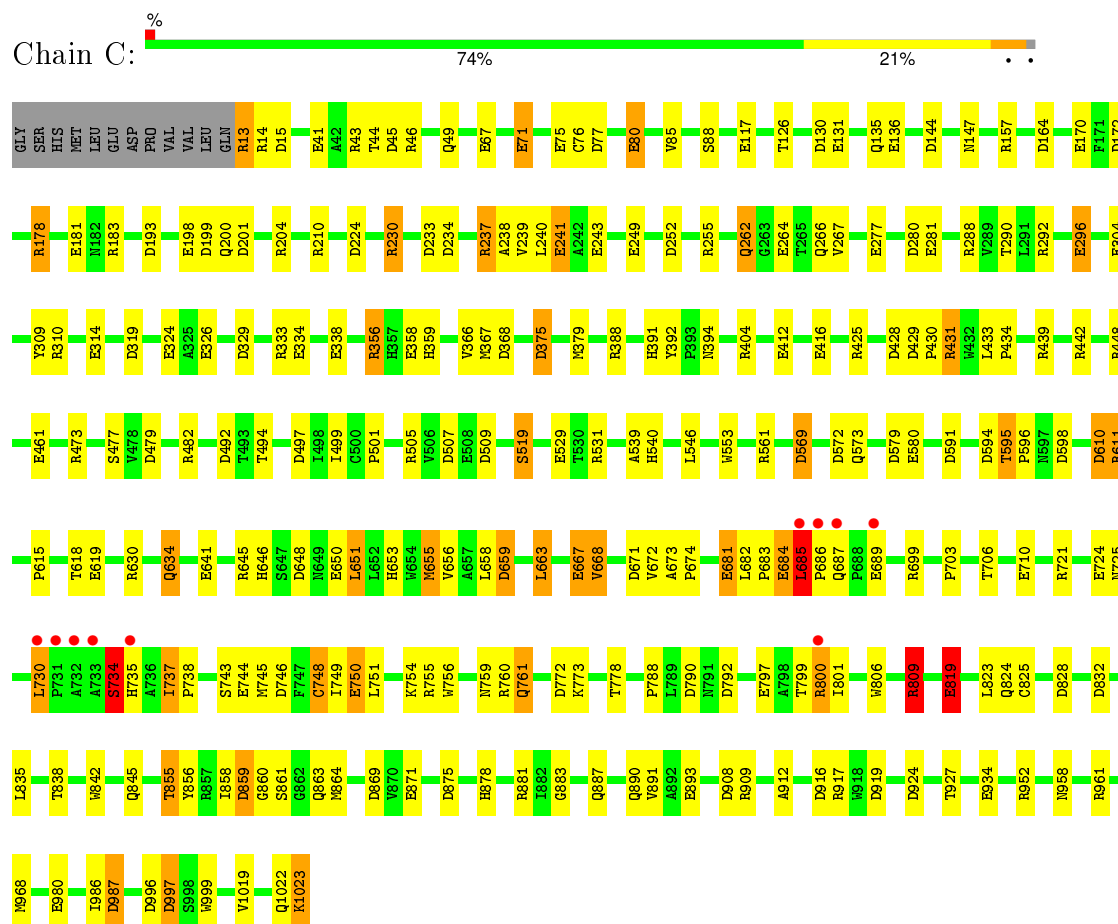


#### • Molecule 1: Beta-Galactosidase





• 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, $\alpha$ , $\beta$ , $\gamma$	149.55Å 168.63Å 200.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 1.80 16.99 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.0 (17.00-1.80) 93.5 (16.99-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 1.80Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.155 , 0.219 0.153 , 0.213	Depositor DCC
$R_{free}$ test set	6261 reflections (1.46%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.7	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 90.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 433670 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	37546	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	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 35.20 % 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 6.0529e-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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LAT, 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	1.13	43/8383 (0.5%)	1.66	175/11437 (1.5%)
1	B	1.15	42/8383 (0.5%)	1.64	159/11437 (1.4%)
1	C	1.13	46/8383 (0.5%)	1.66	171/11437 (1.5%)
1	D	1.13	41/8383 (0.5%)	1.64	173/11437 (1.5%)
All	All	1.14	172/33532 (0.5%)	1.65	678/45748 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	1	0

The worst 5 of 172 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	71	GLU	CD-OE2	10.67	1.37	1.25
1	B	71	GLU	CD-OE2	9.89	1.36	1.25
1	B	487	GLU	CD-OE2	9.46	1.36	1.25
1	D	243	GLU	CD-OE2	9.36	1.35	1.25
1	A	296	GLU	CD-OE2	9.25	1.35	1.25

The worst 5 of 678 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	442	ARG	NE-CZ-NH2	-20.09	110.26	120.30
1	D	183	ARG	NE-CZ-NH1	-15.78	112.41	120.30
1	A	755	ARG	NE-CZ-NH1	13.86	127.23	120.30
1	B	809	ARG	NE-CZ-NH2	-13.62	113.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	178	ARG	NE-CZ-NH1	13.44	127.02	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	687	GLN	CA

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	8128	0	7712	106	0
1	B	8128	0	7712	102	0
1	C	8128	0	7712	97	0
1	D	8128	0	7712	110	0
2	A	23	0	21	0	0
2	B	23	0	21	0	0
2	C	23	0	21	0	0
2	D	23	0	21	0	0
3	A	4	0	0	1	0
3	B	2	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	3	0	0	0	0
5	A	92	0	138	6	0
5	B	96	0	144	5	0
5	C	100	0	150	5	0
5	D	96	0	144	5	0
6	A	1136	0	0	15	1
6	B	1151	0	0	19	0
6	C	1133	0	0	11	0
6	D	1109	0	0	9	1
All	All	37546	0	31508	425	1

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 7.

The worst 5 of 425 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)
5:B:8508:DMS:C1	5:B:8508:DMS:S	2.01	1.46
1:A:634:GLN:H	1:A:634:GLN:NE2	1.41	1.18
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.43	1.16
1:B:655:MET:HE2	1:B:665:SER:HB3	1.16	1.12
1:C:237:ARG:HB3	1:C:237:ARG:HH11	1.24	1.02

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:9583:HOH:O	6:D:9783:HOH:O[4_545]	2.05	0.15

## 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	1011/1023 (99%)	972 (96%)	38 (4%)	1 (0%)	56	38
1	B	1011/1023 (99%)	974 (96%)	35 (4%)	2 (0%)	52	35
1	C	1011/1023 (99%)	979 (97%)	31 (3%)	1 (0%)	56	38
1	D	1011/1023 (99%)	973 (96%)	37 (4%)	1 (0%)	56	38
All	All	4044/4092 (99%)	3898 (96%)	141 (4%)	5 (0%)	56	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	732	ALA

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Mol	Chain	Res	Type
1	D	164	ASP
1	B	164	ASP
1	C	734	SER
1	A	683	PRO

### 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	865/875 (99%)	834 (96%)	31 (4%)	42	24
1	B	865/875 (99%)	835 (96%)	30 (4%)	43	25
1	C	865/875 (99%)	832 (96%)	33 (4%)	40	22
1	D	865/875 (99%)	829 (96%)	36 (4%)	36	18
All	All	3460/3500 (99%)	3330 (96%)	130 (4%)	40	22

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	863	GLN
1	C	546	LEU
1	D	773	LYS
1	B	1023	LYS
1	C	237	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	804	ASN
1	C	646	HIS
1	D	824	GLN
1	C	266	GLN
1	C	653	HIS

### 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 129 ligands modelled in this entry, 29 are monoatomic - leaving 100 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	LAT	A	2001	4	24,24,24	0.61	0	35,35,35	1.40	7 (20%)
5	DMS	A	8401	-	3,3,3	0.65	0	3,3,3	0.26	0
5	DMS	A	8402	-	3,3,3	0.87	0	3,3,3	0.51	0
5	DMS	A	8403	-	3,3,3	1.12	0	3,3,3	0.36	0
5	DMS	A	8404	-	3,3,3	0.75	0	3,3,3	0.10	0
5	DMS	A	8405	-	3,3,3	0.26	0	3,3,3	0.61	0
5	DMS	A	8406	-	3,3,3	0.19	0	3,3,3	0.44	0
5	DMS	A	8407	-	3,3,3	1.08	0	3,3,3	0.87	0
5	DMS	A	8408	-	3,3,3	0.92	0	3,3,3	0.58	0
5	DMS	A	8409	-	3,3,3	1.03	0	3,3,3	0.14	0
5	DMS	A	8410	-	3,3,3	0.26	0	3,3,3	0.29	0
5	DMS	A	8411	-	3,3,3	0.30	0	3,3,3	0.40	0
5	DMS	A	8412	-	3,3,3	0.20	0	3,3,3	0.20	0
5	DMS	A	8413	-	3,3,3	1.63	0	3,3,3	0.43	0
5	DMS	A	8414	-	3,3,3	0.80	0	3,3,3	0.16	0
5	DMS	A	8419	-	3,3,3	0.46	0	3,3,3	0.37	0
5	DMS	A	8420	-	3,3,3	0.35	0	3,3,3	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	DMS	A	8421	-	3,3,3	0.50	0	3,3,3	0.56	0
5	DMS	A	8423	-	3,3,3	0.91	0	3,3,3	0.32	0
5	DMS	A	8425	4	3,3,3	1.40	0	3,3,3	0.28	0
5	DMS	A	8501	-	3,3,3	0.90	0	3,3,3	0.13	0
5	DMS	A	8503	-	3,3,3	0.45	0	3,3,3	0.15	0
5	DMS	A	8504	-	3,3,3	0.23	0	3,3,3	0.16	0
5	DMS	A	8507	-	3,3,3	1.42	0	3,3,3	0.36	0
2	LAT	B	2001	4	24,24,24	0.71	1 (4%)	35,35,35	1.59	6 (17%)
5	DMS	B	8401	-	3,3,3	0.80	0	3,3,3	0.39	0
5	DMS	B	8402	-	3,3,3	1.20	0	3,3,3	0.28	0
5	DMS	B	8403	-	3,3,3	1.13	0	3,3,3	0.42	0
5	DMS	B	8404	-	3,3,3	0.84	0	3,3,3	0.30	0
5	DMS	B	8405	-	3,3,3	0.90	0	3,3,3	0.23	0
5	DMS	B	8407	-	3,3,3	1.30	0	3,3,3	0.25	0
5	DMS	B	8408	-	3,3,3	0.75	0	3,3,3	0.83	0
5	DMS	B	8409	-	3,3,3	1.16	0	3,3,3	0.30	0
5	DMS	B	8410	-	3,3,3	1.01	0	3,3,3	0.77	0
5	DMS	B	8411	-	3,3,3	0.83	0	3,3,3	0.22	0
5	DMS	B	8412	-	3,3,3	0.31	0	3,3,3	0.15	0
5	DMS	B	8413	-	3,3,3	1.62	1 (33%)	3,3,3	0.39	0
5	DMS	B	8414	-	3,3,3	0.25	0	3,3,3	0.19	0
5	DMS	B	8415	-	3,3,3	0.84	0	3,3,3	0.53	0
5	DMS	B	8416	-	3,3,3	0.76	0	3,3,3	0.17	0
5	DMS	B	8417	-	3,3,3	0.48	0	3,3,3	0.09	0
5	DMS	B	8420	-	3,3,3	0.57	0	3,3,3	0.23	0
5	DMS	B	8421	-	3,3,3	0.53	0	3,3,3	0.38	0
5	DMS	B	8423	-	3,3,3	0.26	0	3,3,3	0.44	0
5	DMS	B	8425	4	3,3,3	1.38	1 (33%)	3,3,3	0.64	0
5	DMS	B	8502	-	3,3,3	0.90	0	3,3,3	1.15	0
5	DMS	B	8504	-	3,3,3	0.12	0	3,3,3	0.25	0
5	DMS	B	8508	-	3,3,3	2.08	1 (33%)	3,3,3	0.59	0
5	DMS	B	8601	-	3,3,3	0.89	0	3,3,3	0.44	0
2	LAT	C	2001	4	24,24,24	0.85	0	35,35,35	1.34	6 (17%)
5	DMS	C	8401	-	3,3,3	0.61	0	3,3,3	0.27	0
5	DMS	C	8402	-	3,3,3	1.39	1 (33%)	3,3,3	0.32	0
5	DMS	C	8403	-	3,3,3	0.52	0	3,3,3	0.39	0
5	DMS	C	8404	-	3,3,3	0.91	0	3,3,3	0.63	0
5	DMS	C	8405	-	3,3,3	1.16	0	3,3,3	0.35	0
5	DMS	C	8407	-	3,3,3	0.93	0	3,3,3	0.15	0
5	DMS	C	8408	-	3,3,3	1.02	0	3,3,3	0.36	0
5	DMS	C	8409	-	3,3,3	0.95	0	3,3,3	0.22	0
5	DMS	C	8410	-	3,3,3	0.91	0	3,3,3	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	DMS	C	8411	-	3,3,3	0.56	0	3,3,3	0.11	0
5	DMS	C	8412	-	3,3,3	0.78	0	3,3,3	0.39	0
5	DMS	C	8413	-	3,3,3	1.28	0	3,3,3	0.24	0
5	DMS	C	8414	-	3,3,3	1.02	0	3,3,3	0.60	0
5	DMS	C	8415	-	3,3,3	1.23	0	3,3,3	0.39	0
5	DMS	C	8416	-	3,3,3	0.92	0	3,3,3	0.19	0
5	DMS	C	8417	-	3,3,3	0.64	0	3,3,3	0.35	0
5	DMS	C	8419	-	3,3,3	0.44	0	3,3,3	0.19	0
5	DMS	C	8420	-	3,3,3	0.48	0	3,3,3	0.26	0
5	DMS	C	8421	-	3,3,3	0.76	0	3,3,3	0.47	0
5	DMS	C	8423	-	3,3,3	0.62	0	3,3,3	0.43	0
5	DMS	C	8425	4	3,3,3	0.95	0	3,3,3	0.29	0
5	DMS	C	8501	-	3,3,3	0.53	0	3,3,3	0.60	0
5	DMS	C	8504	-	3,3,3	0.65	0	3,3,3	0.17	0
5	DMS	C	8601	-	3,3,3	0.87	0	3,3,3	0.34	0
5	DMS	C	8602	-	3,3,3	0.58	0	3,3,3	0.20	0
2	LAT	D	2001	4	24,24,24	0.77	0	35,35,35	1.21	3 (8%)
5	DMS	D	8401	-	3,3,3	1.09	0	3,3,3	0.35	0
5	DMS	D	8402	-	3,3,3	0.76	0	3,3,3	0.24	0
5	DMS	D	8403	-	3,3,3	0.54	0	3,3,3	0.22	0
5	DMS	D	8404	-	3,3,3	1.19	0	3,3,3	0.13	0
5	DMS	D	8405	-	3,3,3	0.38	0	3,3,3	0.37	0
5	DMS	D	8406	-	3,3,3	0.86	0	3,3,3	0.56	0
5	DMS	D	8407	-	3,3,3	1.83	2 (66%)	3,3,3	0.60	0
5	DMS	D	8408	-	3,3,3	0.90	0	3,3,3	0.06	0
5	DMS	D	8409	-	3,3,3	1.19	0	3,3,3	0.94	0
5	DMS	D	8410	-	3,3,3	0.62	0	3,3,3	0.25	0
5	DMS	D	8411	-	3,3,3	0.48	0	3,3,3	0.52	0
5	DMS	D	8412	-	3,3,3	0.25	0	3,3,3	0.24	0
5	DMS	D	8413	-	3,3,3	0.97	0	3,3,3	0.25	0
5	DMS	D	8414	-	3,3,3	0.14	0	3,3,3	0.25	0
5	DMS	D	8416	-	3,3,3	0.39	0	3,3,3	0.20	0
5	DMS	D	8419	-	3,3,3	0.33	0	3,3,3	0.22	0
5	DMS	D	8421	-	3,3,3	0.14	0	3,3,3	0.17	0
5	DMS	D	8423	-	3,3,3	0.74	0	3,3,3	0.17	0
5	DMS	D	8501	-	3,3,3	0.55	0	3,3,3	0.09	0
5	DMS	D	8508	-	3,3,3	0.81	0	3,3,3	0.22	0
5	DMS	D	8701	-	3,3,3	1.62	0	3,3,3	0.41	0
5	DMS	D	8703	-	3,3,3	0.70	0	3,3,3	0.55	0
5	DMS	D	8704	-	3,3,3	0.35	0	3,3,3	0.36	0
5	DMS	D	8705	-	3,3,3	1.14	0	3,3,3	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LAT	A	2001	4	-	0/8/48/48	0/2/2/2
5	DMS	A	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8413	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8419	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8420	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8425	4	-	0/0/0/0	0/0/0/0
5	DMS	A	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8503	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8507	-	-	0/0/0/0	0/0/0/0
2	LAT	B	2001	4	-	0/8/48/48	0/2/2/2
5	DMS	B	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8413	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8415	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	B	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8420	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8425	4	-	0/0/0/0	0/0/0/0
5	DMS	B	8502	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8508	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8601	-	-	0/0/0/0	0/0/0/0
2	LAT	C	2001	4	-	0/8/48/48	0/2/2/2
5	DMS	C	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8413	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8415	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8419	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8420	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8425	4	-	0/0/0/0	0/0/0/0
5	DMS	C	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8601	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8602	-	-	0/0/0/0	0/0/0/0
2	LAT	D	2001	4	-	0/8/48/48	0/2/2/2
5	DMS	D	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8405	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	D	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8413	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8419	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8508	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8701	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8703	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8704	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8705	-	-	0/0/0/0	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	LAT	C1'-C2'	-2.23	1.48	1.52
5	C	8402	DMS	C2-S	2.09	1.91	1.75
5	B	8425	DMS	O-S	2.13	1.64	1.50
5	B	8413	DMS	O-S	2.13	1.64	1.50
5	D	8407	DMS	C2-S	2.13	1.92	1.75

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	LAT	O1'-C1'-C2'	-4.09	98.24	109.21
2	B	2001	LAT	O5'-C1'-C2'	-4.02	103.38	109.80
2	C	2001	LAT	O1'-C1'-O5'	-3.67	100.20	110.25
2	C	2001	LAT	O1-C1-O5	-3.28	102.38	110.68
2	A	2001	LAT	O3'-C3'-C2'	-3.18	103.17	110.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8408	DMS	1	0
5	A	8412	DMS	3	0
5	A	8420	DMS	1	0
5	A	8425	DMS	1	0
5	B	8410	DMS	2	0
5	B	8417	DMS	2	0
5	B	8508	DMS	1	0
5	C	8408	DMS	2	0
5	C	8420	DMS	2	0
5	C	8602	DMS	1	0
5	D	8412	DMS	2	0
5	D	8421	DMS	1	0
5	D	8508	DMS	1	0
5	D	8703	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	1011/1023 (98%)	-0.78	14 (1%) 78 74	6, 13, 41, 100	0
1	B	1011/1023 (98%)	-0.78	9 (0%) 85 83	6, 12, 40, 94	0
1	C	1011/1023 (98%)	-0.78	10 (0%) 84 82	6, 13, 42, 100	0
1	D	1011/1023 (98%)	-0.74	19 (1%) 70 66	6, 13, 43, 95	0
All	All	4044/4092 (98%)	-0.77	52 (1%) 79 76	6, 13, 42, 100	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	HIS	8.0
1	D	735	HIS	7.4
1	D	732	ALA	6.3
1	A	686	PRO	6.2
1	A	689	GLU	6.1

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMS	B	8420	4/4	0.93	0.15	15.69	41,43,64,72	0
5	DMS	A	8507	4/4	0.84	0.16	14.19	23,26,35,72	0
5	DMS	D	8704	4/4	0.93	0.16	13.90	32,63,100,100	0
5	DMS	C	8420	4/4	0.94	0.14	11.85	26,32,43,64	0
5	DMS	B	8508	4/4	0.94	0.15	11.61	15,34,46,47	0
5	DMS	B	8423	4/4	0.95	0.13	9.97	24,28,46,100	0
5	DMS	C	8419	4/4	0.95	0.12	9.39	33,39,43,54	0
5	DMS	B	8407	4/4	0.95	0.16	8.84	30,31,36,37	0
5	DMS	C	8425	4/4	0.96	0.17	6.95	32,40,40,41	0
5	DMS	C	8501	4/4	0.95	0.11	6.57	18,35,37,38	0
5	DMS	A	8406	4/4	0.94	0.12	6.40	23,42,59,61	0
5	DMS	A	8420	4/4	0.96	0.12	6.28	30,33,39,44	0
2	LAT	A	2001	23/23	0.96	0.08	6.05	8,13,26,42	0
5	DMS	D	8703	4/4	0.87	0.16	5.92	29,55,61,61	0
5	DMS	D	8423	4/4	0.93	0.17	5.69	27,46,56,65	0
5	DMS	D	8404	4/4	0.96	0.10	5.56	17,17,42,58	0
5	DMS	D	8406	4/4	0.97	0.09	5.24	18,19,22,29	0
5	DMS	D	8407	4/4	0.95	0.12	4.80	27,31,37,44	0
5	DMS	A	8504	4/4	0.98	0.10	4.55	19,33,55,100	0
2	LAT	D	2001	23/23	0.97	0.07	4.39	7,12,27,100	0
5	DMS	B	8425	4/4	0.93	0.15	4.21	21,26,37,42	0
5	DMS	A	8419	4/4	0.97	0.10	3.91	34,37,38,42	0
5	DMS	C	8423	4/4	0.92	0.12	3.74	31,31,46,51	0
5	DMS	C	8417	4/4	0.92	0.14	3.56	25,27,63,74	0
5	DMS	B	8408	4/4	0.98	0.10	3.49	17,26,29,46	0
5	DMS	A	8407	4/4	0.97	0.09	3.30	16,24,25,33	0
5	DMS	A	8423	4/4	0.93	0.12	3.08	27,33,43,56	0
5	DMS	C	8405	4/4	0.98	0.09	3.07	16,22,25,27	0
5	DMS	C	8407	4/4	0.98	0.12	3.00	26,26,31,32	0
5	DMS	B	8502	4/4	0.98	0.10	2.84	19,24,33,33	0
5	DMS	B	8417	4/4	0.92	0.12	2.75	22,32,68,74	0
2	LAT	B	2001	23/23	0.97	0.07	2.61	2,9,26,32	0
5	DMS	B	8405	4/4	0.99	0.11	2.37	22,26,31,34	0
5	DMS	D	8419	4/4	0.98	0.09	2.22	22,33,39,41	0
5	DMS	D	8705	4/4	0.87	0.13	2.17	30,37,42,43	0
5	DMS	A	8404	4/4	0.98	0.07	1.96	18,21,27,27	0
2	LAT	C	2001	23/23	0.97	0.07	1.88	4,7,29,45	23
5	DMS	D	8408	4/4	0.99	0.09	1.84	16,27,27,31	0
5	DMS	C	8411	4/4	0.99	0.09	1.78	16,21,23,28	0
5	DMS	C	8602	4/4	0.97	0.10	1.77	46,51,58,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMS	A	8408	4/4	0.98	0.08	1.69	23,25,29,41	0
4	NA	C	3104	1/1	0.97	0.11	1.65	26,26,26,26	0
5	DMS	A	8412	4/4	0.95	0.13	1.58	34,44,51,54	0
5	DMS	B	8404	4/4	0.98	0.07	1.49	17,25,28,31	0
5	DMS	D	8501	4/4	0.95	0.08	1.11	21,29,32,50	0
5	DMS	A	8425	4/4	0.94	0.12	1.09	26,35,37,40	0
5	DMS	D	8701	4/4	0.99	0.07	1.07	9,12,16,32	0
5	DMS	D	8508	4/4	0.94	0.10	1.00	29,34,36,53	0
5	DMS	C	8403	4/4	0.99	0.07	0.89	16,17,18,18	0
5	DMS	A	8501	4/4	0.97	0.08	0.79	11,24,32,36	0
4	NA	A	3104	1/1	0.97	0.09	0.72	26,26,26,26	0
5	DMS	C	8412	4/4	0.98	0.08	0.65	23,29,32,56	0
5	DMS	C	8404	4/4	0.99	0.06	0.64	15,18,18,25	0
5	DMS	C	8408	4/4	0.97	0.07	0.42	15,20,28,29	0
5	DMS	B	8504	4/4	0.97	0.07	0.31	17,25,33,36	0
5	DMS	A	8403	4/4	0.99	0.06	0.14	15,15,16,20	0
4	NA	B	3104	1/1	0.95	0.08	0.09	27,27,27,27	0
5	DMS	B	8411	4/4	0.99	0.06	0.04	18,22,22,80	0
5	DMS	B	8412	4/4	0.98	0.07	0.01	22,30,32,32	0
5	DMS	D	8405	4/4	0.99	0.06	-0.06	21,23,31,36	0
5	DMS	B	8401	4/4	0.99	0.05	-0.09	11,12,14,16	0
5	DMS	C	8402	4/4	0.99	0.06	-0.14	11,16,21,24	0
5	DMS	A	8405	4/4	0.99	0.06	-0.23	16,22,25,57	0
5	DMS	D	8412	4/4	0.99	0.07	-0.24	21,25,30,46	0
5	DMS	A	8402	4/4	0.99	0.06	-0.30	12,19,20,21	0
4	NA	B	3102	1/1	1.00	0.05	-0.35	10,10,10,10	0
5	DMS	A	8401	4/4	1.00	0.05	-0.41	11,11,12,12	0
4	NA	A	3101	1/1	1.00	0.04	-0.49	10,10,10,10	0
5	DMS	D	8401	4/4	0.99	0.05	-0.55	11,11,14,15	0
5	DMS	D	8411	4/4	0.99	0.06	-0.57	15,17,22,48	0
5	DMS	B	8402	4/4	0.99	0.05	-0.60	9,16,17,20	0
3	MG	D	3001	1/1	0.99	0.04	-0.73	9,9,9,9	0
4	NA	D	3103	1/1	0.98	0.06	-0.77	26,26,26,26	0
5	DMS	B	8403	4/4	0.99	0.05	-0.78	14,15,20,20	0
4	NA	A	3103	1/1	0.98	0.05	-1.05	21,21,21,21	0
4	NA	C	3103	1/1	0.99	0.05	-1.24	19,19,19,19	0
4	NA	B	3101	1/1	1.00	0.04	-1.31	11,11,11,11	0
3	MG	B	3002	1/1	0.99	0.04	-1.32	13,13,13,13	0
5	DMS	A	8411	4/4	0.99	0.06	-1.32	17,17,22,36	0
5	DMS	D	8403	4/4	0.99	0.04	-1.36	13,20,20,22	0
3	MG	A	3002	1/1	1.00	0.04	-1.53	12,12,12,12	0
4	NA	C	3102	1/1	1.00	0.04	-1.55	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NA	B	3103	1/1	0.99	0.04	-1.62	19,19,19,19	0
5	DMS	D	8402	4/4	0.99	0.05	-1.79	13,15,18,19	0
4	NA	D	3102	1/1	1.00	0.03	-1.90	10,10,10,10	0
5	DMS	C	8401	4/4	0.99	0.04	-1.96	8,10,16,21	0
3	MG	D	3002	1/1	0.99	0.04	-2.27	12,12,12,12	0
4	NA	A	3102	1/1	1.00	0.03	-2.52	12,12,12,12	0
4	NA	C	3101	1/1	1.00	0.04	-3.00	9,9,9,9	0
4	NA	D	3101	1/1	1.00	0.03	-3.80	10,10,10,10	0
3	MG	B	3001	1/1	1.00	0.03	-4.44	8,8,8,8	0
3	MG	A	3001	1/1	1.00	0.03	-4.53	10,10,10,10	0
3	MG	C	3001	1/1	1.00	0.02	-4.82	10,10,10,10	0
3	MG	C	3002	1/1	1.00	0.03	-5.00	9,9,9,9	0
5	DMS	B	8409	4/4	0.97	0.11	-	28,28,31,32	0
3	MG	D	3003	1/1	0.90	0.24	-	55,55,55,55	0
5	DMS	B	8415	4/4	0.92	0.14	-	21,31,32,59	0
5	DMS	A	8503	4/4	0.97	0.16	-	34,37,46,50	0
5	DMS	B	8421	4/4	0.97	0.13	-	22,46,51,73	0
5	DMS	A	8410	4/4	0.98	0.06	-	18,28,29,35	0
5	DMS	B	8413	4/4	0.94	0.15	-	27,36,38,39	0
5	DMS	C	8413	4/4	0.97	0.12	-	25,31,31,32	0
5	DMS	D	8413	4/4	0.98	0.12	-	27,27,27,31	0
5	DMS	C	8416	4/4	0.96	0.18	-	31,34,36,40	0
5	DMS	B	8416	4/4	0.97	0.13	-	28,35,43,58	0
5	DMS	A	8414	4/4	0.97	0.12	-	26,26,43,100	0
5	DMS	D	8409	4/4	0.97	0.09	-	25,28,30,33	0
5	DMS	C	8504	4/4	0.94	0.10	-	29,32,45,52	0
5	DMS	D	8410	4/4	0.99	0.05	-	15,25,28,34	0
5	DMS	A	8413	4/4	0.96	0.14	-	24,26,32,41	0
3	MG	D	3005	1/1	0.98	0.08	-	21,21,21,21	0
3	MG	C	3004	1/1	0.96	0.15	-	37,37,37,37	0
5	DMS	A	8421	4/4	0.95	0.20	-	36,42,50,59	0
5	DMS	B	8601	4/4	0.97	0.13	-	35,35,39,48	0
5	DMS	C	8601	4/4	0.97	0.14	-	43,43,55,81	0
5	DMS	D	8416	4/4	0.96	0.18	-	22,36,46,100	0
5	DMS	C	8415	4/4	0.94	0.14	-	15,33,50,60	0
5	DMS	A	8409	4/4	0.97	0.11	-	26,26,26,40	0
5	DMS	C	8421	4/4	0.97	0.12	-	31,35,46,100	0
5	DMS	C	8409	4/4	0.97	0.10	-	27,32,37,38	0
5	DMS	B	8410	4/4	0.97	0.09	-	15,37,37,38	0
3	MG	C	3006	1/1	0.97	0.15	-	27,27,27,27	0
5	DMS	B	8414	4/4	0.98	0.10	-	21,42,100,100	0
3	MG	A	3005	1/1	0.95	0.08	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	A	3105	1/1	0.89	0.10	-	77,77,77,77	0
5	DMS	C	8414	4/4	0.98	0.09	-	16,36,37,51	0
5	DMS	D	8421	4/4	0.98	0.12	-	33,46,52,100	0
5	DMS	C	8410	4/4	0.98	0.07	-	25,28,31,35	0
5	DMS	D	8414	4/4	0.98	0.11	-	21,36,100,100	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.