



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 03:02 AM BST

PDB ID : 3MV0
Title : E. COLI (lacZ) BETA-GALACTOSIDASE (R599A) IN COMPLEX WITH D
-GALCTOPYRANOSYL-1-ONE
Authors : Dugdale, M.L.; Vance, M.; Driedger, M.L.; Nibber, A.; Tran, A.; Huber, R.E.
Deposited on : 2010-05-03
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

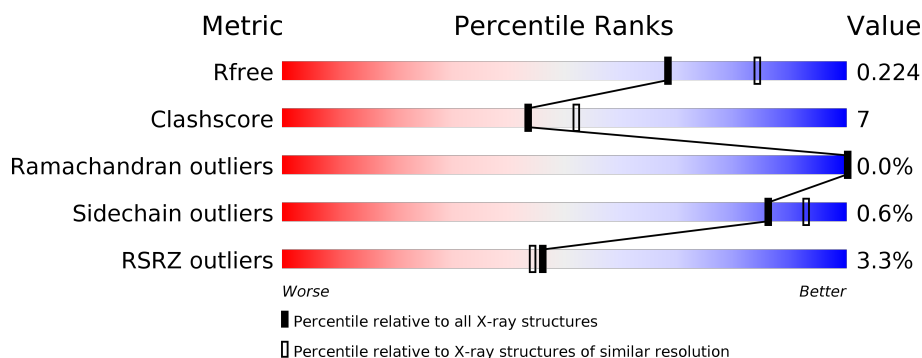
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1	1052	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div></div> </div> <div></div> </div>
1	2	1052	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div></div> </div> <div></div> </div>
1	3	1052	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div></div> </div> <div></div> </div>
1	4	1052	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>17%</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
5	DMS	1	5029	-	-	X	-
5	DMS	4	5007	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36190 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	1	1011	Total	C	N	O	S	0	0	0
			8119	5135	1437	1509	38			
1	2	1011	Total	C	N	O	S	0	0	0
			8119	5135	1437	1509	38			
1	3	1011	Total	C	N	O	S	0	0	0
			8119	5135	1437	1509	38			
1	4	1011	Total	C	N	O	S	0	0	0
			8119	5135	1437	1509	38			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-28	MET	-	expression tag	UNP B8LFD6
1	-27	GLY	-	expression tag	UNP B8LFD6
1	-26	GLY	-	expression tag	UNP B8LFD6
1	-25	SER	-	expression tag	UNP B8LFD6
1	-24	HIS	-	expression tag	UNP B8LFD6
1	-23	HIS	-	expression tag	UNP B8LFD6
1	-22	HIS	-	expression tag	UNP B8LFD6
1	-21	HIS	-	expression tag	UNP B8LFD6
1	-20	HIS	-	expression tag	UNP B8LFD6
1	-19	HIS	-	expression tag	UNP B8LFD6
1	-18	GLY	-	expression tag	UNP B8LFD6
1	-17	MET	-	expression tag	UNP B8LFD6
1	-16	ALA	-	expression tag	UNP B8LFD6
1	-15	SER	-	expression tag	UNP B8LFD6
1	-14	MET	-	expression tag	UNP B8LFD6
1	-13	THR	-	expression tag	UNP B8LFD6
1	-12	GLY	-	expression tag	UNP B8LFD6
1	-11	GLY	-	expression tag	UNP B8LFD6
1	-10	GLN	-	expression tag	UNP B8LFD6
1	-9	GLN	-	expression tag	UNP B8LFD6
1	-8	MET	-	expression tag	UNP B8LFD6

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Chain	Residue	Modelled	Actual	Comment	Reference
1	-7	GLY	-	expression tag	UNP B8LFD6
1	-6	ARG	-	expression tag	UNP B8LFD6
1	-5	ASP	-	expression tag	UNP B8LFD6
1	-4	LEU	-	expression tag	UNP B8LFD6
1	-3	TYR	-	expression tag	UNP B8LFD6
1	-2	ASP	-	expression tag	UNP B8LFD6
1	-1	ASP	-	expression tag	UNP B8LFD6
1	0	ASP	-	expression tag	UNP B8LFD6
1	1	ASP	-	expression tag	UNP B8LFD6
1	2	LYS	-	expression tag	UNP B8LFD6
1	3	ASP	-	expression tag	UNP B8LFD6
1	4	PRO	-	expression tag	UNP B8LFD6
1	5	MET	-	expression tag	UNP B8LFD6
1	6	ILE	-	expression tag	UNP B8LFD6
1	7	ASP	-	expression tag	UNP B8LFD6
1	8	PRO	-	expression tag	UNP B8LFD6
1	599	ALA	ARG	engineered mutation	UNP B8LFD6
2	-28	MET	-	expression tag	UNP B8LFD6
2	-27	GLY	-	expression tag	UNP B8LFD6
2	-26	GLY	-	expression tag	UNP B8LFD6
2	-25	SER	-	expression tag	UNP B8LFD6
2	-24	HIS	-	expression tag	UNP B8LFD6
2	-23	HIS	-	expression tag	UNP B8LFD6
2	-22	HIS	-	expression tag	UNP B8LFD6
2	-21	HIS	-	expression tag	UNP B8LFD6
2	-20	HIS	-	expression tag	UNP B8LFD6
2	-19	HIS	-	expression tag	UNP B8LFD6
2	-18	GLY	-	expression tag	UNP B8LFD6
2	-17	MET	-	expression tag	UNP B8LFD6
2	-16	ALA	-	expression tag	UNP B8LFD6
2	-15	SER	-	expression tag	UNP B8LFD6
2	-14	MET	-	expression tag	UNP B8LFD6
2	-13	THR	-	expression tag	UNP B8LFD6
2	-12	GLY	-	expression tag	UNP B8LFD6
2	-11	GLY	-	expression tag	UNP B8LFD6
2	-10	GLN	-	expression tag	UNP B8LFD6
2	-9	GLN	-	expression tag	UNP B8LFD6
2	-8	MET	-	expression tag	UNP B8LFD6
2	-7	GLY	-	expression tag	UNP B8LFD6
2	-6	ARG	-	expression tag	UNP B8LFD6
2	-5	ASP	-	expression tag	UNP B8LFD6
2	-4	LEU	-	expression tag	UNP B8LFD6

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Chain	Residue	Modelled	Actual	Comment	Reference
2	-3	TYR	-	expression tag	UNP B8LFD6
2	-2	ASP	-	expression tag	UNP B8LFD6
2	-1	ASP	-	expression tag	UNP B8LFD6
2	0	ASP	-	expression tag	UNP B8LFD6
2	1	ASP	-	expression tag	UNP B8LFD6
2	2	LYS	-	expression tag	UNP B8LFD6
2	3	ASP	-	expression tag	UNP B8LFD6
2	4	PRO	-	expression tag	UNP B8LFD6
2	5	MET	-	expression tag	UNP B8LFD6
2	6	ILE	-	expression tag	UNP B8LFD6
2	7	ASP	-	expression tag	UNP B8LFD6
2	8	PRO	-	expression tag	UNP B8LFD6
2	599	ALA	ARG	engineered mutation	UNP B8LFD6
3	-28	MET	-	expression tag	UNP B8LFD6
3	-27	GLY	-	expression tag	UNP B8LFD6
3	-26	GLY	-	expression tag	UNP B8LFD6
3	-25	SER	-	expression tag	UNP B8LFD6
3	-24	HIS	-	expression tag	UNP B8LFD6
3	-23	HIS	-	expression tag	UNP B8LFD6
3	-22	HIS	-	expression tag	UNP B8LFD6
3	-21	HIS	-	expression tag	UNP B8LFD6
3	-20	HIS	-	expression tag	UNP B8LFD6
3	-19	HIS	-	expression tag	UNP B8LFD6
3	-18	GLY	-	expression tag	UNP B8LFD6
3	-17	MET	-	expression tag	UNP B8LFD6
3	-16	ALA	-	expression tag	UNP B8LFD6
3	-15	SER	-	expression tag	UNP B8LFD6
3	-14	MET	-	expression tag	UNP B8LFD6
3	-13	THR	-	expression tag	UNP B8LFD6
3	-12	GLY	-	expression tag	UNP B8LFD6
3	-11	GLY	-	expression tag	UNP B8LFD6
3	-10	GLN	-	expression tag	UNP B8LFD6
3	-9	GLN	-	expression tag	UNP B8LFD6
3	-8	MET	-	expression tag	UNP B8LFD6
3	-7	GLY	-	expression tag	UNP B8LFD6
3	-6	ARG	-	expression tag	UNP B8LFD6
3	-5	ASP	-	expression tag	UNP B8LFD6
3	-4	LEU	-	expression tag	UNP B8LFD6
3	-3	TYR	-	expression tag	UNP B8LFD6
3	-2	ASP	-	expression tag	UNP B8LFD6
3	-1	ASP	-	expression tag	UNP B8LFD6
3	0	ASP	-	expression tag	UNP B8LFD6

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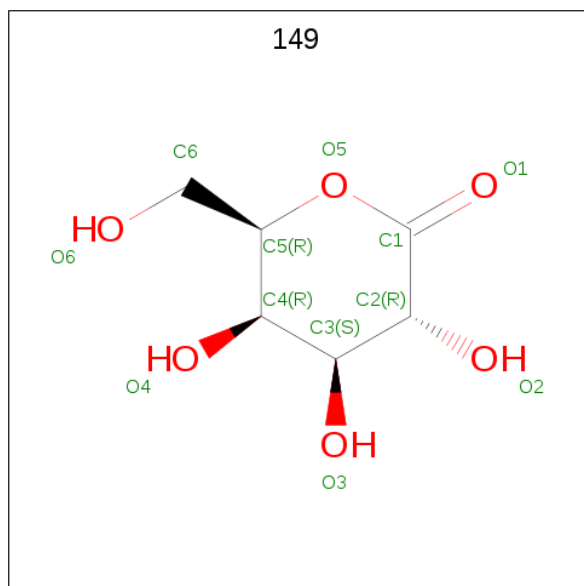
Chain	Residue	Modelled	Actual	Comment	Reference
3	1	ASP	-	expression tag	UNP B8LFD6
3	2	LYS	-	expression tag	UNP B8LFD6
3	3	ASP	-	expression tag	UNP B8LFD6
3	4	PRO	-	expression tag	UNP B8LFD6
3	5	MET	-	expression tag	UNP B8LFD6
3	6	ILE	-	expression tag	UNP B8LFD6
3	7	ASP	-	expression tag	UNP B8LFD6
3	8	PRO	-	expression tag	UNP B8LFD6
3	599	ALA	ARG	engineered mutation	UNP B8LFD6
4	-28	MET	-	expression tag	UNP B8LFD6
4	-27	GLY	-	expression tag	UNP B8LFD6
4	-26	GLY	-	expression tag	UNP B8LFD6
4	-25	SER	-	expression tag	UNP B8LFD6
4	-24	HIS	-	expression tag	UNP B8LFD6
4	-23	HIS	-	expression tag	UNP B8LFD6
4	-22	HIS	-	expression tag	UNP B8LFD6
4	-21	HIS	-	expression tag	UNP B8LFD6
4	-20	HIS	-	expression tag	UNP B8LFD6
4	-19	HIS	-	expression tag	UNP B8LFD6
4	-18	GLY	-	expression tag	UNP B8LFD6
4	-17	MET	-	expression tag	UNP B8LFD6
4	-16	ALA	-	expression tag	UNP B8LFD6
4	-15	SER	-	expression tag	UNP B8LFD6
4	-14	MET	-	expression tag	UNP B8LFD6
4	-13	THR	-	expression tag	UNP B8LFD6
4	-12	GLY	-	expression tag	UNP B8LFD6
4	-11	GLY	-	expression tag	UNP B8LFD6
4	-10	GLN	-	expression tag	UNP B8LFD6
4	-9	GLN	-	expression tag	UNP B8LFD6
4	-8	MET	-	expression tag	UNP B8LFD6
4	-7	GLY	-	expression tag	UNP B8LFD6
4	-6	ARG	-	expression tag	UNP B8LFD6
4	-5	ASP	-	expression tag	UNP B8LFD6
4	-4	LEU	-	expression tag	UNP B8LFD6
4	-3	TYR	-	expression tag	UNP B8LFD6
4	-2	ASP	-	expression tag	UNP B8LFD6
4	-1	ASP	-	expression tag	UNP B8LFD6
4	0	ASP	-	expression tag	UNP B8LFD6
4	1	ASP	-	expression tag	UNP B8LFD6
4	2	LYS	-	expression tag	UNP B8LFD6
4	3	ASP	-	expression tag	UNP B8LFD6
4	4	PRO	-	expression tag	UNP B8LFD6

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Chain	Residue	Modelled	Actual	Comment	Reference
4	5	MET	-	expression tag	UNP B8LFD6
4	6	ILE	-	expression tag	UNP B8LFD6
4	7	ASP	-	expression tag	UNP B8LFD6
4	8	PRO	-	expression tag	UNP B8LFD6
4	599	ALA	ARG	engineered mutation	UNP B8LFD6

- Molecule 2 is D-galactonolactone (three-letter code: 149) (formula: C₆H₁₀O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1	1	Total C O 12 6 6	0	0
2	2	1	Total C O 12 6 6	0	0
2	3	1	Total C O 12 6 6	0	0
2	4	1	Total C O 12 6 6	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	2	3	Total Mg 3 3	0	0
3	1	2	Total Mg 2 2	0	0

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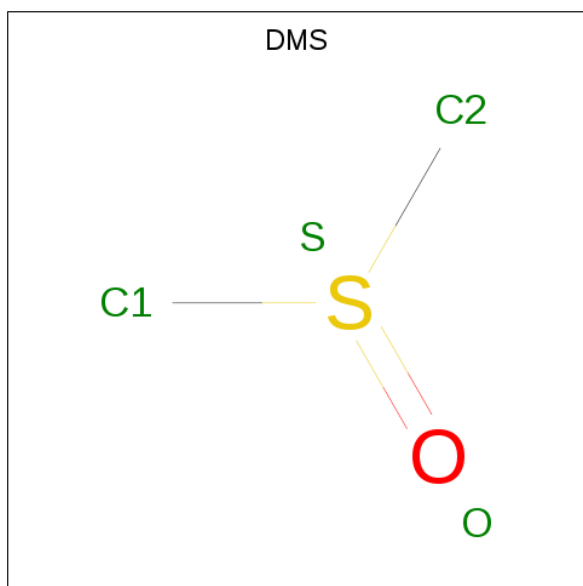
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	4	3	Total	Mg	0	0
			3	3		
3	3	3	Total	Mg	0	0
			3	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	2	4	Total	Na	0	0
			4	4		
4	1	4	Total	Na	0	0
			4	4		
4	4	4	Total	Na	0	0
			4	4		
4	3	4	Total	Na	0	0
			4	4		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	773	Total 773	O 773	0	0
6	2	858	Total 858	O 858	0	0
6	3	760	Total 760	O 760	0	0
6	4	760	Total 760	O 760	0	0

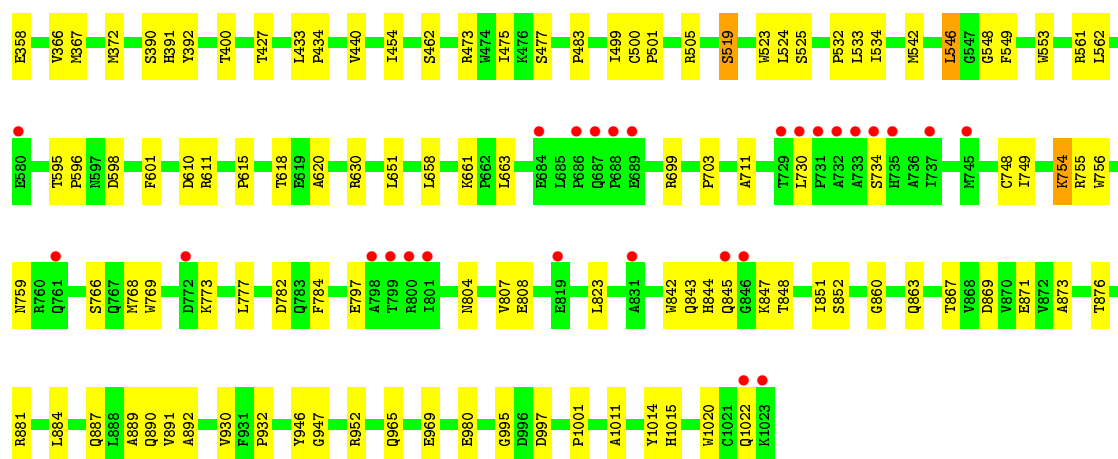
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain 1:

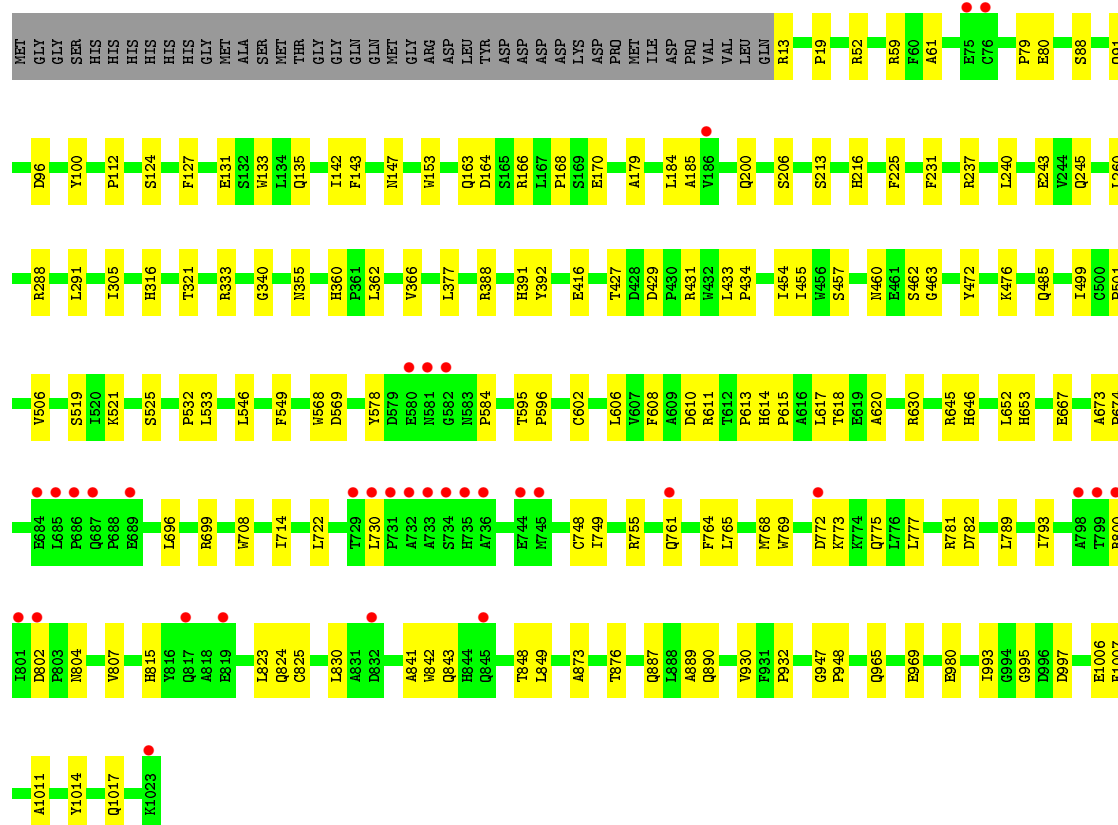
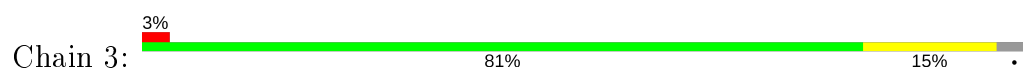
3% 80% 16%

Residue	State
K1023	Red
H844	Green
Q845	Red
G846	Red
K347	Yellow
T858	Yellow
D859	Green
G860	Green
S861	Yellow
G862	Yellow
Q863	Yellow
A873	Yellow
T876	Yellow
G883	Yellow
L884	Yellow
Q887	Yellow
L888	Green
A899	Green
Q890	Green
T891	Green
A892	Yellow
N896	Yellow
A912	Yellow
N945	Yellow
Y946	Yellow
G947	Yellow
F955	Yellow
I959	Red
Q965	Yellow
Y968	Yellow
E969	Yellow
H977	Red
E980	Yellow
D987	Yellow
S998	Yellow
A1011	Yellow
Y1014	Yellow
Q1017	Yellow
W1020	Yellow
C1021	Yellow
G1023	Yellow
E689	Red
V698	Yellow
P703	Yellow
W708	Yellow
L729	Red
L730	Red
W731	Red
A732	Red
A733	Red
S734	Red
H735	Red
A736	Red
W745	Red
D746	Yellow
I749	Yellow
E750	Yellow
L751	Yellow
G752	Green
N753	Yellow
K754	Yellow
R755	Yellow
W756	Yellow
N759	Yellow
W768	Yellow
W769	Yellow
I770	Yellow
G771	Red
D772	Red
K773	Red
K774	Red
L777	Yellow
D782	Yellow
P788	Yellow
G794	Yellow
E797	Yellow
A798	Red
W799	Red
R800	Red
I801	Red
R809	Yellow
Q817	Red
L823	Yellow
Q832	Yellow
Q833	Yellow
Q834	Yellow
L546	Red
H553	Yellow
R561	Yellow
L562	Yellow
H568	Yellow
D569	Yellow
Q573	Yellow
K577	Yellow
Y578	Yellow
D579	Yellow
E580	Red
H581	Red
G582	Yellow
N583	Yellow
P584	Yellow
A587	Yellow
D591	Yellow
T595	Yellow
P596	Yellow
C602	Yellow
A609	Yellow
D610	Yellow
R611	Yellow
T612	Yellow
P613	Yellow
H614	Yellow
A616	Yellow
L617	Yellow
T618	Yellow
E619	Yellow
Q625	Yellow
R630	Red
G634	Red
T635	Yellow
I636	Yellow
L651	Yellow
E661	Yellow
E684	Red
L685	Red
P686	Red
G687	Red
E688	Red
S88	Yellow
R292	Yellow
W301	Yellow
R333	Red
E334	Yellow
V335	Green
R336	Yellow
G340	Yellow
N345	Yellow
R352	Yellow
R356	Yellow
P361	Yellow
V366	Yellow
M367	Yellow
D368	Green
E369	Yellow
V373	Yellow
L377	Yellow
S390	Yellow
H391	Yellow
Y392	Yellow
Q163	Yellow
D164	Yellow
MET	Yellow
S165	Green
R166	Yellow
P430	Green
R431	Yellow
A432	Yellow
L433	Yellow
P434	Yellow
S452	Yellow
Y472	Yellow
K476	Yellow
L499	Yellow
G500	Green
P501	Yellow
M502	Yellow
S519	Yellow
L524	Yellow
S525	Yellow
P532	Yellow
L533	Yellow
E537	Yellow
E58	Yellow
Q91	Yellow
D96	Yellow
Y100	Yellow
Y105	Yellow
P112	Yellow
C122	Yellow
Y123	Green
S124	Yellow
F127	Yellow
N128	Yellow
V129	Yellow
D130	Red
E131	Yellow
Q135	Yellow
I142	Yellow
N147	Yellow
S148	Yellow
W153	Yellow
Q163	Yellow
D164	Yellow
MET	Yellow
S165	Green
R166	Yellow
E170	Yellow
G180	Yellow
L184	Yellow
A185	Yellow
G194	Yellow
E198	Yellow
D199	Yellow
Q200	Yellow
S206	Yellow
L240	Yellow
E241	Yellow
Q245	Yellow
G283	Yellow
G284	Yellow
E288	Yellow
E71	Red
S72	Yellow
W73	Yellow
E80	Red
V86	Yellow
D97	Yellow

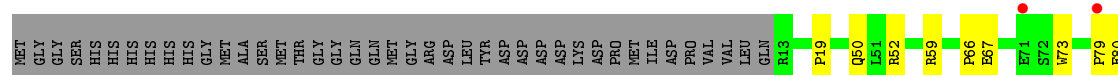
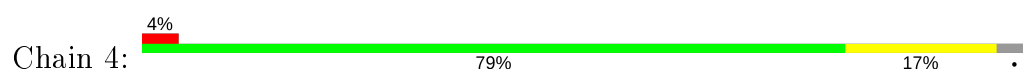
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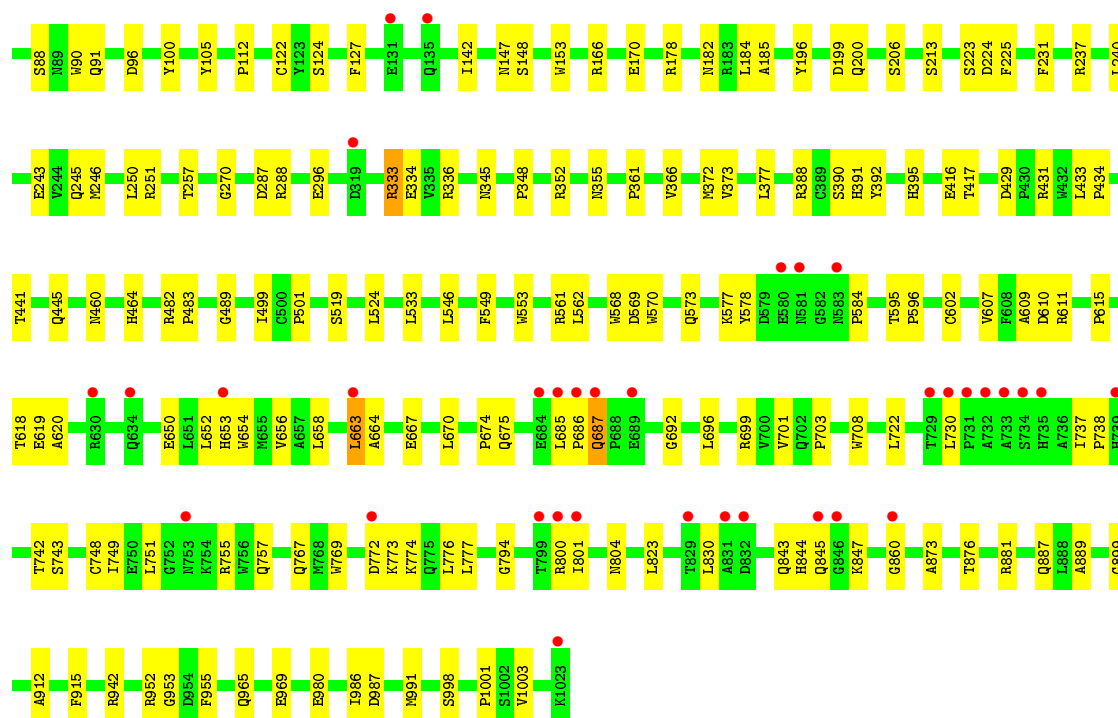


• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.84Å 166.31Å 201.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.23 – 2.20 21.23 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.1 (21.23-2.20) 92.1 (21.23-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.195 , 0.237 0.180 , 0.224	Depositor DCC
R_{free} test set	3358 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36190	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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 37.12 % 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 4.5024e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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, 149

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	1	0.33	0/8361	0.61	0/11408
1	2	0.33	0/8361	0.62	0/11408
1	3	0.33	0/8361	0.61	0/11408
1	4	0.33	0/8361	0.62	0/11408
All	All	0.33	0/33444	0.62	0/45632

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	1	8119	0	7708	109	0
1	2	8119	0	7708	107	0
1	3	8119	0	7708	110	0
1	4	8119	0	7708	118	0
2	1	12	0	9	0	0
2	2	12	0	9	0	0
2	3	12	0	9	0	0
2	4	12	0	9	0	0
3	1	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	3	0	0	0	0
3	3	3	0	0	0	0
3	4	3	0	0	0	0
4	1	4	0	0	0	0
4	2	4	0	0	0	0
4	3	4	0	0	0	0
4	4	4	0	0	0	0
5	1	112	0	168	6	0
5	2	124	0	186	1	0
5	3	136	0	204	1	0
5	4	116	0	174	0	0
6	1	773	0	0	4	0
6	2	858	0	0	5	0
6	3	760	0	0	3	0
6	4	760	0	0	2	0
All	All	36190	0	31600	435	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 7.

The worst 5 of 435 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)
1:3:142:ILE:HG12	1:3:170:GLU:HG2	1.50	0.94
1:1:142:ILE:HG12	1:1:170:GLU:HG2	1.57	0.84
1:4:687:GLN:NE2	1:4:687:GLN:H	1.76	0.83
1:1:823:LEU:O	1:2:730:LEU:HD21	1.80	0.81
1:1:283:GLY:HA3	5:1:5029:DMS:H12	1.63	0.79

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	1009/1052 (96%)	968 (96%)	40 (4%)	1 (0%)	51	60
1	2	1009/1052 (96%)	958 (95%)	51 (5%)	0	100	100
1	3	1009/1052 (96%)	966 (96%)	43 (4%)	0	100	100
1	4	1009/1052 (96%)	958 (95%)	51 (5%)	0	100	100
All	All	4036/4208 (96%)	3850 (95%)	185 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	798	ALA

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	1	863/897 (96%)	858 (99%)	5 (1%)	86	93
1	2	863/897 (96%)	859 (100%)	4 (0%)	88	94
1	3	863/897 (96%)	857 (99%)	6 (1%)	84	91
1	4	863/897 (96%)	857 (99%)	6 (1%)	84	91
All	All	3452/3588 (96%)	3431 (99%)	21 (1%)	86	93

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	333	ARG
1	3	546	LEU
1	4	546	LEU
1	2	754	LYS
1	4	663	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	2	1017	GLN
1	3	554	GLN
1	4	804	ASN
1	3	394	ASN
1	3	624	GLN

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 153 ligands modelled in this entry, 27 are monoatomic - leaving 126 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	4	5016	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	4	5001	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	4	5020	-	3,3,3	0.25	0	3,3,3	0.60	0
5	DMS	3	5025	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	1	5025	-	3,3,3	0.16	0	3,3,3	0.52	0
5	DMS	4	5008	-	3,3,3	0.26	0	3,3,3	0.61	0
5	DMS	2	5014	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	3	5013	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	2	5015	-	3,3,3	0.21	0	3,3,3	0.62	0
5	DMS	4	5027	-	3,3,3	0.22	0	3,3,3	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	4	5023	-	3,3,3	0.22	0	3,3,3	0.59	0
5	DMS	1	5029	-	3,3,3	0.23	0	3,3,3	0.57	0
5	DMS	3	5019	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	3	5005	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	1	5009	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	1	5024	-	3,3,3	0.24	0	3,3,3	0.61	0
2	149	4	2001	4	12,12,12	0.91	1 (8%)	15,17,17	0.77	0
5	DMS	4	5003	-	3,3,3	0.21	0	3,3,3	0.62	0
5	DMS	2	5033	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	2	5005	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	1	5028	-	3,3,3	0.27	0	3,3,3	0.61	0
5	DMS	2	5009	-	3,3,3	0.23	0	3,3,3	0.62	0
2	149	2	2001	4	12,12,12	1.20	2 (16%)	15,17,17	0.76	0
5	DMS	3	5021	4	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	3	5006	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	3	5008	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	3	5014	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	2	5001	-	3,3,3	0.27	0	3,3,3	0.64	0
5	DMS	1	5015	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	3	5030	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	3	5016	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	4	5013	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	4	5014	-	3,3,3	0.21	0	3,3,3	0.58	0
5	DMS	1	5007	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	4	5021	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	2	5023	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	3	5011	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	3	5015	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	4	5007	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	2	5028	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	1	5001	-	3,3,3	0.21	0	3,3,3	0.65	0
5	DMS	3	5034	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	3	1024	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	3	5010	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	2	5029	-	3,3,3	0.28	0	3,3,3	0.59	0
5	DMS	2	5017	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	3	5004	-	3,3,3	0.21	0	3,3,3	0.63	0
5	DMS	1	5012	-	3,3,3	0.21	0	3,3,3	0.59	0
5	DMS	1	5008	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	4	5017	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	3	5028	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	3	5018	-	3,3,3	0.23	0	3,3,3	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	4	5029	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	3	5007	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	1	5010	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	2	5021	4	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	1	5017	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	1	5019	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	4	5002	-	3,3,3	0.16	0	3,3,3	0.55	0
5	DMS	4	5028	-	3,3,3	0.32	0	3,3,3	0.57	0
5	DMS	3	5029	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	2	5010	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	4	5010	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	2	5031	-	3,3,3	0.28	0	3,3,3	0.63	0
5	DMS	2	5026	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	3	5017	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	4	5018	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	2	5020	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	2	5016	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	4	5024	-	3,3,3	0.22	0	3,3,3	0.63	0
5	DMS	4	5004	-	3,3,3	0.22	0	3,3,3	0.64	0
5	DMS	1	5003	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	1	5023	-	3,3,3	0.21	0	3,3,3	0.58	0
5	DMS	2	5025	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	4	5006	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	2	5022	-	3,3,3	0.21	0	3,3,3	0.60	0
5	DMS	3	5027	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	3	5024	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	2	5002	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	1	5022	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	1	5026	-	3,3,3	0.18	0	3,3,3	0.54	0
5	DMS	2	1024	-	3,3,3	0.27	0	3,3,3	0.64	0
5	DMS	2	5006	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	2	5019	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	1	5016	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	3	5001	-	3,3,3	0.21	0	3,3,3	0.62	0
5	DMS	3	5002	-	3,3,3	0.20	0	3,3,3	0.60	0
5	DMS	1	5004	-	3,3,3	0.22	0	3,3,3	0.63	0
5	DMS	2	5030	-	3,3,3	0.13	0	3,3,3	0.56	0
5	DMS	4	5030	-	3,3,3	0.28	0	3,3,3	0.54	0
5	DMS	2	5004	-	3,3,3	0.20	0	3,3,3	0.61	0
5	DMS	3	5023	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	2	5012	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	3	5020	-	3,3,3	0.21	0	3,3,3	0.60	0
5	DMS	4	5005	-	3,3,3	0.24	0	3,3,3	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	3	5033	-	3,3,3	0.31	0	3,3,3	0.61	0
5	DMS	1	5021	-	3,3,3	0.28	0	3,3,3	0.60	0
5	DMS	3	5003	-	3,3,3	0.26	0	3,3,3	0.60	0
5	DMS	4	5022	-	3,3,3	0.20	0	3,3,3	0.60	0
5	DMS	4	5025	-	3,3,3	0.26	0	3,3,3	0.59	0
5	DMS	1	5005	-	3,3,3	0.26	0	3,3,3	0.59	0
5	DMS	3	5012	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	1	5011	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	2	5027	-	3,3,3	0.25	0	3,3,3	0.61	0
2	149	3	2001	4	12,12,12	1.10	2 (16%)	15,17,17	0.78	0
2	149	1	2001	4	12,12,12	1.07	1 (8%)	15,17,17	0.80	0
5	DMS	2	5008	-	3,3,3	0.22	0	3,3,3	0.64	0
5	DMS	4	5019	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	1	5013	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	1	5020	-	3,3,3	0.20	0	3,3,3	0.61	0
5	DMS	4	5011	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	3	5032	-	3,3,3	0.13	0	3,3,3	0.64	0
5	DMS	4	5012	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	1	5018	4	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	3	5031	-	3,3,3	0.26	0	3,3,3	0.65	0
5	DMS	2	5024	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	1	5014	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	4	5026	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	2	5003	-	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	1	5002	-	3,3,3	0.19	0	3,3,3	0.62	0
5	DMS	2	5032	-	3,3,3	0.26	0	3,3,3	0.58	0
5	DMS	3	5022	-	3,3,3	0.20	0	3,3,3	0.61	0
5	DMS	3	5009	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	4	5009	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	2	5011	-	3,3,3	0.25	0	3,3,3	0.58	0
5	DMS	1	5006	-	3,3,3	0.22	0	3,3,3	0.61	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	149	2	2001	4	-	1/2/22/22	0/1/1/1
2	149	3	2001	4	-	1/2/22/22	0/1/1/1
2	149	1	2001	4	-	1/2/22/22	0/1/1/1
2	149	4	2001	4	-	1/2/22/22	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2001	149	O5-C1	2.78	1.38	1.34
2	1	2001	149	O5-C1	2.53	1.38	1.34
2	3	2001	149	O5-C1	2.41	1.38	1.34
2	2	2001	149	O5-C5	2.36	1.49	1.46
2	4	2001	149	O5-C1	2.20	1.38	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	3	2001	149	O5-C5-C6-O6
2	2	2001	149	O5-C5-C6-O6
2	1	2001	149	O5-C5-C6-O6
2	4	2001	149	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	5029	DMS	4	0
5	2	5033	DMS	1	0
5	3	5030	DMS	1	0
5	1	5012	DMS	2	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, 95th 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 ²)	Q<0.9
1	1	1011/1052 (96%)	-0.21	35 (3%) 44 42	13, 25, 46, 74	0
1	2	1011/1052 (96%)	-0.29	29 (2%) 51 49	13, 24, 45, 75	0
1	3	1011/1052 (96%)	-0.27	33 (3%) 46 44	14, 24, 45, 75	0
1	4	1011/1052 (96%)	-0.23	37 (3%) 41 39	13, 25, 46, 74	0
All	All	4044/4208 (96%)	-0.25	134 (3%) 46 44	13, 25, 46, 75	0

The worst 5 of 134 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	3	732	ALA	9.4
1	2	733	ALA	8.0
1	1	772	ASP	7.8
1	1	735	HIS	7.4
1	4	735	HIS	7.3

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, 95th 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(\AA^2)	Q<0.9
5	DMS	4	5007	4/4	0.32	0.52	113,113,113,114	0
3	MG	3	3003	1/1	0.49	0.14	78,78,78,78	0
5	DMS	2	5017	4/4	0.61	0.28	92,92,93,94	0
5	DMS	1	5007	4/4	0.66	0.25	90,90,90,91	0
5	DMS	3	5012	4/4	0.66	0.33	108,108,109,109	0
5	DMS	1	5013	4/4	0.72	0.35	96,96,97,97	0
5	DMS	4	5026	4/4	0.73	0.30	102,102,102,102	0
3	MG	4	3003	1/1	0.74	0.22	68,68,68,68	0
5	DMS	3	5016	4/4	0.80	0.22	71,72,72,73	0
5	DMS	3	5006	4/4	0.81	0.21	85,85,85,86	0
5	DMS	2	5025	4/4	0.81	0.29	93,93,93,94	0
5	DMS	3	5029	4/4	0.83	0.24	81,82,82,82	0
5	DMS	3	5024	4/4	0.84	0.32	76,77,77,77	0
5	DMS	3	5018	4/4	0.84	0.23	73,74,75,75	0
5	DMS	4	5016	4/4	0.84	0.23	59,59,61,62	0
5	DMS	3	5015	4/4	0.84	0.37	67,67,67,68	0
5	DMS	1	5021	4/4	0.85	0.31	70,71,72,72	0
5	DMS	3	5014	4/4	0.86	0.26	68,69,70,70	0
5	DMS	2	5020	4/4	0.86	0.18	69,70,70,70	0
3	MG	2	3003	1/1	0.87	0.13	45,45,45,45	0
5	DMS	3	5028	4/4	0.87	0.17	83,83,84,84	0
4	NA	1	3104	1/1	0.87	0.08	55,55,55,55	0
5	DMS	3	5034	4/4	0.87	0.20	66,66,66,67	0
5	DMS	2	5031	4/4	0.88	0.24	61,62,62,63	0
5	DMS	3	5027	4/4	0.89	0.29	79,80,80,80	0
5	DMS	4	5024	4/4	0.89	0.20	80,81,81,81	0
5	DMS	1	5015	4/4	0.89	0.17	65,65,66,66	0
5	DMS	3	5009	4/4	0.89	0.25	88,88,89,89	0
5	DMS	3	5030	4/4	0.90	0.24	79,79,80,80	0
5	DMS	2	5006	4/4	0.90	0.21	92,92,92,93	0
5	DMS	4	5013	4/4	0.90	0.40	86,86,86,86	0
5	DMS	1	5006	4/4	0.90	0.20	74,75,75,75	0
4	NA	2	3103	1/1	0.91	0.13	29,29,29,29	0
5	DMS	4	5017	4/4	0.91	0.20	72,73,73,74	0
5	DMS	3	5007	4/4	0.91	0.13	61,62,62,63	0
5	DMS	2	5026	4/4	0.91	0.13	63,63,63,65	0
5	DMS	3	5017	4/4	0.91	0.18	83,83,84,84	0
5	DMS	4	5006	4/4	0.91	0.14	46,47,48,49	0
5	DMS	1	5024	4/4	0.92	0.17	86,86,86,86	0
5	DMS	2	5033	4/4	0.92	0.26	72,72,73,73	0
5	DMS	4	5027	4/4	0.92	0.31	81,82,82,82	0
5	DMS	4	5023	4/4	0.92	0.22	90,90,90,91	0
5	DMS	1	5009	4/4	0.92	0.15	55,55,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	DMS	2	5024	4/4	0.92	0.17	78,78,78,79	0
5	DMS	1	5010	4/4	0.92	0.17	71,72,72,72	0
5	DMS	2	5021	4/4	0.92	0.36	89,89,89,90	0
5	DMS	2	5028	4/4	0.92	0.16	59,61,61,61	0
5	DMS	3	1024	4/4	0.92	0.19	74,74,75,75	0
5	DMS	4	5010	4/4	0.92	0.24	78,78,78,79	0
5	DMS	2	5015	4/4	0.93	0.14	56,56,56,57	0
5	DMS	3	5020	4/4	0.93	0.16	64,64,64,65	0
5	DMS	3	5033	4/4	0.93	0.21	59,60,61,61	0
5	DMS	4	5014	4/4	0.93	0.24	66,67,67,67	0
5	DMS	1	5019	4/4	0.93	0.26	82,83,83,83	0
5	DMS	1	5028	4/4	0.93	0.32	65,66,66,66	0
5	DMS	4	5019	4/4	0.93	0.18	64,64,64,64	0
5	DMS	4	5004	4/4	0.93	0.13	53,53,55,55	0
5	DMS	3	5031	4/4	0.93	0.20	58,59,60,60	0
5	DMS	1	5022	4/4	0.93	0.41	82,82,82,83	0
5	DMS	3	5021	4/4	0.93	0.23	64,64,65,66	0
5	DMS	1	5004	4/4	0.93	0.12	49,50,51,51	0
5	DMS	3	5013	4/4	0.94	0.17	55,56,56,56	0
5	DMS	1	5017	4/4	0.94	0.25	61,61,61,62	0
5	DMS	4	5018	4/4	0.94	0.11	72,72,73,73	0
5	DMS	4	5022	4/4	0.94	0.11	61,62,62,62	0
5	DMS	1	5025	4/4	0.94	0.15	45,46,47,49	0
4	NA	2	3104	1/1	0.94	0.08	34,34,34,34	0
4	NA	4	3104	1/1	0.94	0.11	41,41,41,41	0
5	DMS	2	5010	4/4	0.94	0.14	87,87,87,87	0
5	DMS	1	5018	4/4	0.94	0.18	68,68,69,69	0
5	DMS	3	5004	4/4	0.94	0.13	49,50,52,52	0
5	DMS	1	5014	4/4	0.94	0.13	65,65,66,66	0
5	DMS	1	5012	4/4	0.94	0.18	61,61,62,62	0
5	DMS	2	5004	4/4	0.94	0.13	49,50,51,52	0
5	DMS	4	5020	4/4	0.94	0.15	72,72,72,72	0
5	DMS	4	5009	4/4	0.94	0.13	60,60,60,61	0
2	149	1	2001	12/12	0.95	0.11	17,19,21,25	0
4	NA	4	3103	1/1	0.95	0.15	34,34,34,34	0
5	DMS	2	1024	4/4	0.95	0.15	59,60,61,61	0
5	DMS	2	5008	4/4	0.95	0.14	53,54,55,55	0
5	DMS	1	5016	4/4	0.95	0.12	65,65,65,65	0
5	DMS	2	5023	4/4	0.95	0.21	57,58,58,59	0
5	DMS	3	5019	4/4	0.95	0.18	63,63,64,64	0
5	DMS	3	5025	4/4	0.95	0.13	76,76,76,76	0
5	DMS	1	5002	4/4	0.95	0.12	45,46,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	DMS	2	5032	4/4	0.95	0.17	54,54,54,54	0
5	DMS	1	5011	4/4	0.95	0.12	47,48,49,50	0
5	DMS	4	5030	4/4	0.95	0.23	58,59,59,60	0
5	DMS	3	5002	4/4	0.96	0.12	26,29,30,33	0
2	149	3	2001	12/12	0.96	0.09	16,19,22,25	0
5	DMS	3	5008	4/4	0.96	0.14	62,62,63,63	0
5	DMS	2	5022	4/4	0.96	0.15	61,61,61,62	0
5	DMS	1	5008	4/4	0.96	0.12	46,47,47,48	0
5	DMS	4	5021	4/4	0.96	0.22	68,68,68,68	0
5	DMS	1	5020	4/4	0.96	0.12	54,55,55,56	0
4	NA	4	3102	1/1	0.96	0.07	20,20,20,20	0
5	DMS	4	5028	4/4	0.96	0.15	41,42,42,43	0
5	DMS	2	5016	4/4	0.96	0.30	54,54,54,55	0
2	149	2	2001	12/12	0.96	0.10	13,15,18,24	0
4	NA	3	3103	1/1	0.96	0.21	42,42,42,42	0
5	DMS	2	5029	4/4	0.96	0.11	56,56,57,57	0
5	DMS	2	5019	4/4	0.96	0.20	69,70,70,70	0
5	DMS	2	5005	4/4	0.96	0.16	38,38,39,40	0
3	MG	3	3001	1/1	0.96	0.04	19,19,19,19	0
5	DMS	3	5022	4/4	0.96	0.14	66,66,66,66	0
4	NA	1	3102	1/1	0.96	0.10	29,29,29,29	0
5	DMS	4	5008	4/4	0.96	0.23	49,50,50,51	0
5	DMS	2	5027	4/4	0.96	0.13	71,71,71,72	0
5	DMS	2	5001	4/4	0.97	0.14	29,29,30,33	0
5	DMS	4	5002	4/4	0.97	0.10	39,39,39,39	0
3	MG	4	3002	1/1	0.97	0.05	25,25,25,25	0
4	NA	1	3103	1/1	0.97	0.13	47,47,47,47	0
3	MG	2	3001	1/1	0.97	0.03	22,22,22,22	0
5	DMS	2	5030	4/4	0.97	0.12	38,39,39,39	0
5	DMS	3	5011	4/4	0.97	0.10	47,49,49,50	0
5	DMS	3	5032	4/4	0.97	0.15	42,43,44,46	0
5	DMS	4	5012	4/4	0.97	0.14	54,54,54,54	0
5	DMS	2	5014	4/4	0.97	0.17	48,49,49,49	0
4	NA	3	3104	1/1	0.97	0.06	42,42,42,42	0
3	MG	1	3002	1/1	0.97	0.05	24,24,24,24	0
5	DMS	2	5012	4/4	0.97	0.10	42,44,44,46	0
5	DMS	3	5001	4/4	0.97	0.13	31,31,31,35	0
5	DMS	1	5023	4/4	0.97	0.10	63,63,64,64	0
3	MG	2	3002	1/1	0.97	0.04	30,30,30,30	0
5	DMS	4	5029	4/4	0.97	0.15	60,61,61,61	0
4	NA	2	3101	1/1	0.97	0.07	18,18,18,18	0
5	DMS	4	5025	4/4	0.97	0.10	57,57,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	DMS	1	5029	4/4	0.97	0.22	51,52,53,54	0
2	149	4	2001	12/12	0.97	0.09	13,17,19,24	0
5	DMS	2	5009	4/4	0.97	0.14	56,56,56,56	0
5	DMS	3	5005	4/4	0.98	0.12	43,43,44,45	0
5	DMS	1	5005	4/4	0.98	0.11	39,39,40,40	0
3	MG	4	3001	1/1	0.98	0.06	23,23,23,23	0
5	DMS	1	5003	4/4	0.98	0.12	38,39,39,39	0
5	DMS	2	5002	4/4	0.98	0.08	32,33,34,37	0
4	NA	1	3101	1/1	0.98	0.05	21,21,21,21	0
5	DMS	2	5003	4/4	0.98	0.14	38,38,39,40	0
4	NA	3	3101	1/1	0.98	0.09	20,20,20,20	0
5	DMS	3	5010	4/4	0.98	0.14	40,41,42,42	0
5	DMS	1	5026	4/4	0.98	0.16	60,61,61,61	0
5	DMS	4	5011	4/4	0.98	0.11	41,41,42,43	0
3	MG	1	3001	1/1	0.98	0.09	20,20,20,20	0
4	NA	2	3102	1/1	0.98	0.04	18,18,18,18	0
5	DMS	2	5011	4/4	0.98	0.10	38,39,39,40	0
5	DMS	4	5003	4/4	0.98	0.13	42,42,43,44	0
4	NA	4	3101	1/1	0.99	0.06	16,16,16,16	0
4	NA	3	3102	1/1	0.99	0.10	24,24,24,24	0
5	DMS	3	5023	4/4	0.99	0.06	46,46,47,47	0
5	DMS	3	5003	4/4	0.99	0.18	35,36,36,37	0
5	DMS	4	5001	4/4	0.99	0.11	28,30,30,33	0
5	DMS	1	5001	4/4	0.99	0.18	26,27,28,29	0
5	DMS	4	5005	4/4	0.99	0.15	36,36,37,38	0
3	MG	3	3002	1/1	0.99	0.06	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.