



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:59 AM UTC

PDB ID : 3MUZ / pdb_00003muz
Title : E.Coli (lacZ) beta-galactosidase (R599A) in complex with IPTG
Authors : Dugdale, M.L.; Vance, M.L.; Driedger, M.R.; Nibber, A.; Tran, A.; Huber, R.E.
Deposited on : 2010-05-03
Resolution : 1.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

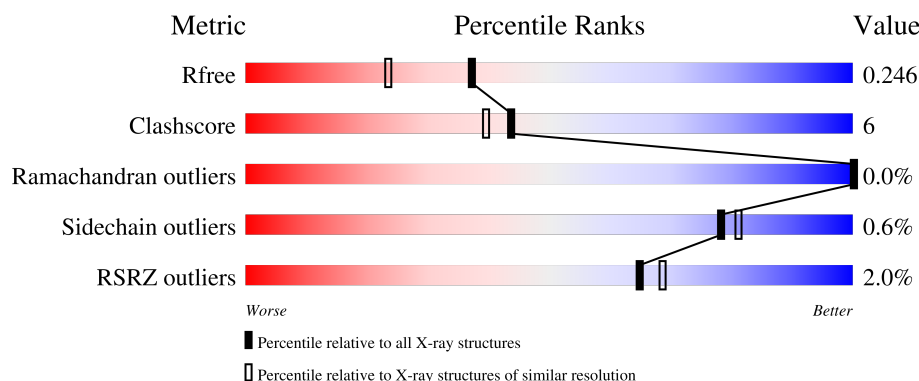
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 of 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	2% 78% 18% .
1	2	1052	2% 82% 13% ..
1	3	1052	2% 81% 14% ..
1	4	1052	2% 79% 16% .

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
5	DMS	2	6026	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37334 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	conflict	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	conflict	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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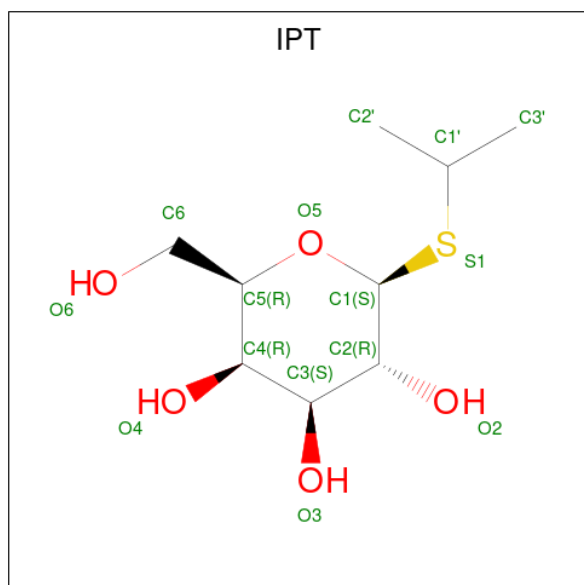
Chain	Residue	Modelled	Actual	Comment	Reference
3	1	ASP	-	expression tag	UNP B8LFD6
3	2	LYS	-	expression tag	UNP B8LFD6
3	3	ASP	-	expression tag	UNP B8LFD6
3	4	PRO	-	expression tag	UNP B8LFD6
3	5	MET	-	expression tag	UNP B8LFD6
3	6	ILE	-	expression tag	UNP B8LFD6
3	7	ASP	-	expression tag	UNP B8LFD6
3	8	PRO	-	expression tag	UNP B8LFD6
3	599	ALA	ARG	conflict	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	conflict	UNP B8LFD6

- Molecule 2 is 1-methylethyl 1-thio-beta-D-galactopyranoside (CCD ID: IPT) (formula: $C_9H_{18}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	1	1	Total	C	O	S	0	0
			15	9	5	1		
2	1	1	Total	C	O	S	0	0
			15	9	5	1		
2	2	1	Total	C	O	S	0	0
			15	9	5	1		
2	2	1	Total	C	O	S	0	0
			15	9	5	1		
2	3	1	Total	C	O	S	0	0
			15	9	5	1		
2	3	1	Total	C	O	S	0	0
			15	9	5	1		
2	4	1	Total	C	O	S	0	0
			15	9	5	1		
2	4	1	Total	C	O	S	0	0
			15	9	5	1		

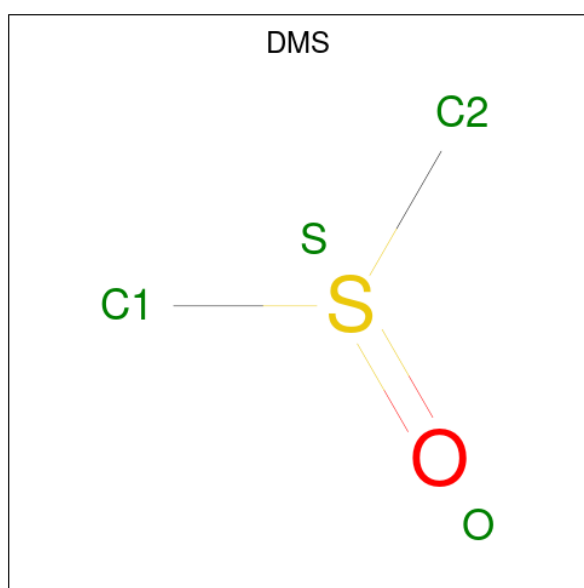
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

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

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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	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
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	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
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

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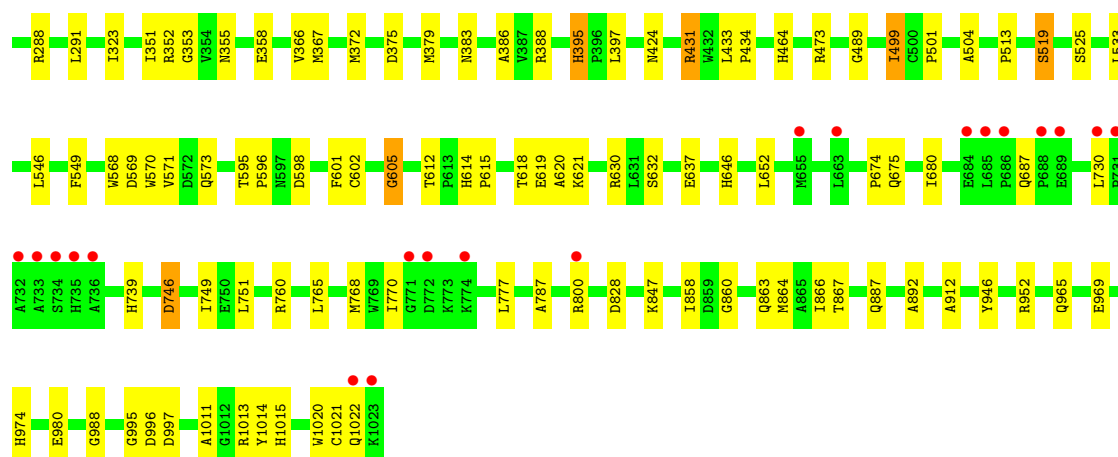
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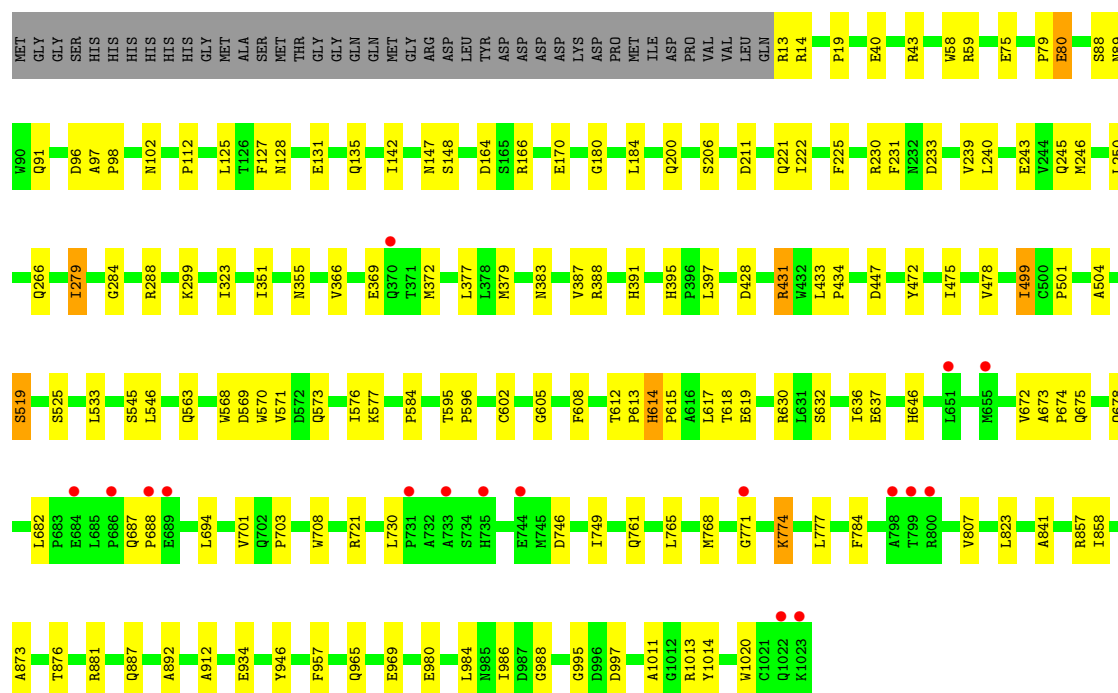
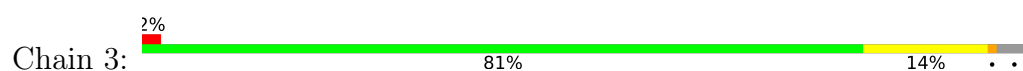
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	4	1	Total	C	O	S	0	0
			4	2	1	1		
5	4	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is water.

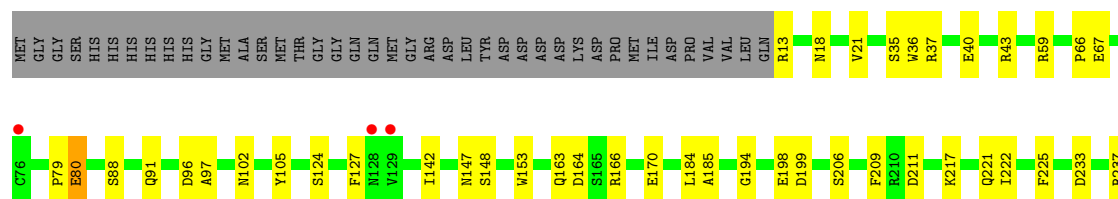
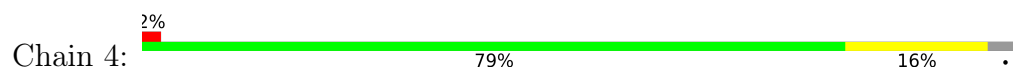
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	1022	Total	O	0	0
			1022	1022		
6	2	1089	Total	O	0	0
			1089	1089		
6	3	1051	Total	O	0	0
			1051	1051		
6	4	946	Total	O	0	0
			946	946		

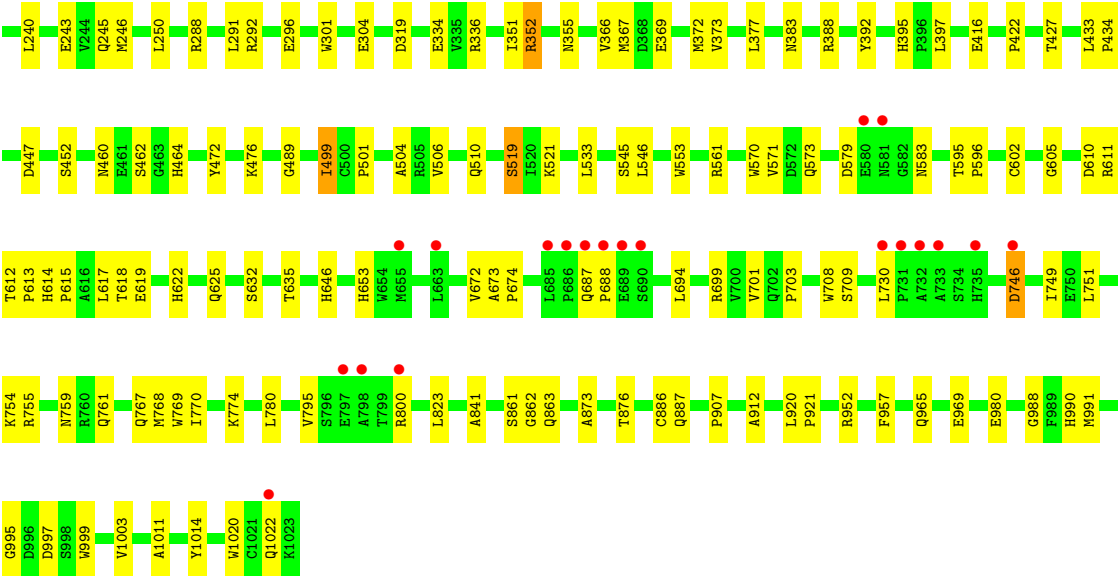


• Molecule 1: Beta-galactosidase



• 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	151.83Å 163.28Å 204.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.42 – 1.90 12.42 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.0 (12.42-1.90) 93.6 (12.42-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.90Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.219 , 0.248 0.217 , 0.246	Depositor DCC
R_{free} test set	5355 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 65.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	37334	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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 41.77 % 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 2.2481e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: IPT, DMS, NA, MG

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	0.86	25/11408 (0.2%)
1	2	0.35	0/8361	0.88	26/11408 (0.2%)
1	3	0.35	0/8361	0.89	29/11408 (0.3%)
1	4	0.32	0/8361	0.86	26/11408 (0.2%)
All	All	0.34	0/33444	0.87	106/45632 (0.2%)

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	1	0	1

There are no bond length outliers.

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	614	HIS	N-CA-C	-8.23	99.33	110.36
1	2	570	TRP	N-CA-C	8.17	120.10	111.03
1	3	97	ALA	N-CA-C	8.16	120.35	110.07
1	4	570	TRP	N-CA-C	8.12	120.05	111.03
1	1	570	TRP	N-CA-C	7.85	119.74	111.03

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	100	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	113	0
1	2	8119	0	7707	101	0
1	3	8119	0	7707	91	0
1	4	8119	0	7708	103	0
2	1	30	0	35	0	0
2	2	30	0	35	2	0
2	3	30	0	35	2	0
2	4	30	0	35	1	0
3	1	4	0	0	0	0
3	2	4	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	132	0	198	7	0
5	2	172	0	258	15	0
5	3	172	0	258	12	0
5	4	124	0	186	5	0
6	1	1022	0	0	13	0
6	2	1089	0	0	5	0
6	3	1051	0	0	6	0
6	4	946	0	0	3	0
All	All	37334	0	31870	397	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 6.

The worst 5 of 397 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)
1:2:431:ARG:HB2	1:2:431:ARG:HH21	1.33	0.93
1:4:142:ILE:HG12	1:4:170:GLU:HG2	1.52	0.91
1:1:142:ILE:HG12	1:1:170:GLU:HG2	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:142:ILE:HG12	1:3:170:GLU:HG2	1.59	0.84
1:2:770:ILE:HG21	1:2:1022:GLN:HE22	1.42	0.84

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%)	41 (4%)	0	100	100
1	2	1009/1052 (96%)	967 (96%)	42 (4%)	0	100	100
1	3	1009/1052 (96%)	972 (96%)	36 (4%)	1 (0%)	48	40
1	4	1009/1052 (96%)	969 (96%)	40 (4%)	0	100	100
All	All	4036/4208 (96%)	3876 (96%)	159 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3	164	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	863/897 (96%)	858 (99%)	5 (1%)	78	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	863/897 (96%)	859 (100%)	4 (0%)	81	84
1	3	863/897 (96%)	855 (99%)	8 (1%)	70	73
1	4	863/897 (96%)	858 (99%)	5 (1%)	78	81
All	All	3452/3588 (96%)	3430 (99%)	22 (1%)	78	81

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

Mol	Chain	Res	Type
1	3	687	GLN
1	4	80	GLU
1	3	774	LYS
1	4	519	SER
1	2	431	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	3	266	GLN
1	3	863	GLN
1	4	950	GLN
1	3	374	GLN
1	3	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 188 ligands modelled in this entry, 30 are monoatomic - leaving 158 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	2	6042	-	3,3,3	0.24	0	3,3,3	0.62	0
2	IPT	4	2002	-	15,15,15	0.90	1 (6%)	18,21,21	0.70	0
5	DMS	1	6017	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	2	6035	-	3,3,3	0.24	0	3,3,3	0.63	0
2	IPT	3	2001	4	15,15,15	0.89	1 (6%)	18,21,21	0.73	0
5	DMS	3	6027	-	3,3,3	0.19	0	3,3,3	0.64	0
5	DMS	3	6041	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	1	6006	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	4	6007	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	2	6043	-	3,3,3	0.26	0	3,3,3	0.61	0
5	DMS	3	6019	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	1	6002	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	4	6028	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	1	6023	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	1	6001	-	3,3,3	0.20	0	3,3,3	0.58	0
5	DMS	3	6004	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	4	6021	-	3,3,3	0.24	0	3,3,3	0.64	0
2	IPT	4	2001	4	15,15,15	0.87	1 (6%)	18,21,21	0.71	0
5	DMS	4	6014	-	3,3,3	0.23	0	3,3,3	0.62	0
2	IPT	1	2001	4	15,15,15	0.83	1 (6%)	18,21,21	0.70	0
5	DMS	1	6014	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	4	6012	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	2	6016	4	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	4	6029	-	3,3,3	0.23	0	3,3,3	0.63	0
2	IPT	1	2002	-	15,15,15	0.98	1 (6%)	18,21,21	0.71	0
5	DMS	1	6016	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	3	6006	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	3	6015	-	3,3,3	0.22	0	3,3,3	0.59	0
5	DMS	3	6020	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	3	6038	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	4	6030	-	3,3,3	0.24	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	3	6000	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	2	6005	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	3	6040	-	3,3,3	0.21	0	3,3,3	0.65	0
5	DMS	2	6007	-	3,3,3	0.27	0	3,3,3	0.64	0
5	DMS	2	6019	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	2	6023	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	2	6017	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	3	6005	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	3	6014	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	4	6013	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	1	6025	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	1	6018	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	3	6017	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	3	6035	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	3	6036	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	2	6027	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	4	6002	-	3,3,3	0.29	0	3,3,3	0.61	0
5	DMS	4	6026	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	2	6031	-	3,3,3	0.22	0	3,3,3	0.64	0
5	DMS	1	6024	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	1	6030	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	2	6004	-	3,3,3	0.24	0	3,3,3	0.57	0
5	DMS	3	6031	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	2	6011	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	3	6021	-	3,3,3	0.26	0	3,3,3	0.65	0
5	DMS	4	6023	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	1	6031	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	2	6022	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	1	6022	-	3,3,3	0.26	0	3,3,3	0.66	0
5	DMS	2	6014	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	2	6025	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	4	6005	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	1	6004	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	1	6005	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	4	6016	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	2	6036	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	3	6012	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	2	6020	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	3	6018	-	3,3,3	0.20	0	3,3,3	0.61	0
5	DMS	3	6002	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	1	6019	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	3	6037	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	2	6038	-	3,3,3	0.23	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	1	6008	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	2	6001	-	3,3,3	0.19	0	3,3,3	0.58	0
5	DMS	2	6010	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	1	6010	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	4	6015	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	4	6003	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	2	6026	-	3,3,3	0.35	0	3,3,3	0.66	0
5	DMS	2	6040	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	2	6034	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	1	6032	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	4	6011	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	4	6018	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	1	6007	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	3	6022	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	4	6019	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	2	6033	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	4	6008	-	3,3,3	0.28	0	3,3,3	0.62	0
5	DMS	2	6037	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	2	6029	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	3	6028	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	4	6024	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	3	6010	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	3	6001	-	3,3,3	0.19	0	3,3,3	0.59	0
5	DMS	2	6024	-	3,3,3	0.26	0	3,3,3	0.61	0
5	DMS	1	6012	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	3	6003	-	3,3,3	0.22	0	3,3,3	0.66	0
5	DMS	1	6011	-	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	1	6000	-	3,3,3	0.27	0	3,3,3	0.61	0
5	DMS	4	6017	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	4	6004	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	2	6002	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	3	6025	-	3,3,3	0.27	0	3,3,3	0.61	0
5	DMS	4	6009	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	3	1024	-	3,3,3	0.12	0	3,3,3	0.64	0
2	IPT	3	2002	-	15,15,15	0.91	1 (6%)	18,21,21	0.72	0
5	DMS	2	6006	-	3,3,3	0.21	0	3,3,3	0.63	0
5	DMS	3	6026	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	4	6010	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	1	6029	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	4	6006	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	1	6026	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	2	6032	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	3	6030	-	3,3,3	0.27	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	4	6025	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	1	6003	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	2	6028	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	2	6021	-	3,3,3	0.21	0	3,3,3	0.59	0
5	DMS	1	6027	-	3,3,3	0.28	0	3,3,3	0.63	0
5	DMS	4	6000	-	3,3,3	0.22	0	3,3,3	0.60	0
2	IPT	2	2001	4	15,15,15	0.90	1 (6%)	18,21,21	0.76	0
5	DMS	2	6009	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	3	6034	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	2	6039	-	3,3,3	0.21	0	3,3,3	0.67	0
5	DMS	2	6012	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	3	6024	-	3,3,3	0.24	0	3,3,3	0.62	0
2	IPT	2	2002	-	15,15,15	0.88	1 (6%)	18,21,21	0.72	0
5	DMS	4	6020	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	1	6020	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	3	6029	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	2	6013	-	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	4	6001	-	3,3,3	0.17	0	3,3,3	0.59	0
5	DMS	1	6009	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	1	6013	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	2	6015	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	1	6015	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	2	6003	-	3,3,3	0.26	0	3,3,3	0.67	0
5	DMS	2	6000	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	3	6007	-	3,3,3	0.29	0	3,3,3	0.62	0
5	DMS	2	6008	-	3,3,3	0.22	0	3,3,3	0.57	0
5	DMS	3	6039	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	1	6021	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	3	6016	4	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	3	6013	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	3	6009	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	3	6032	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	2	6030	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	3	6008	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	3	6011	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	4	6022	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	4	6027	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	1	6028	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	3	6033	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	2	6018	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	3	6023	-	3,3,3	0.25	0	3,3,3	0.62	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	IPT	2	2002	-	-	0/6/26/26	0/1/1/1
2	IPT	4	2002	-	-	0/6/26/26	0/1/1/1
2	IPT	1	2002	-	-	0/6/26/26	0/1/1/1
2	IPT	3	2001	4	-	3/6/26/26	0/1/1/1
2	IPT	3	2002	-	-	0/6/26/26	0/1/1/1
2	IPT	4	2001	4	-	3/6/26/26	0/1/1/1
2	IPT	2	2001	4	-	1/6/26/26	0/1/1/1
2	IPT	1	2001	4	-	1/6/26/26	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	2002	IPT	O5-C1	2.65	1.46	1.42
2	2	2001	IPT	O5-C1	2.62	1.46	1.42
2	3	2002	IPT	O5-C1	2.51	1.46	1.42
2	4	2001	IPT	O5-C1	2.36	1.46	1.42
2	4	2002	IPT	O5-C1	2.32	1.46	1.42

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	3	2001	IPT	C2'-C1'-S1-C1
2	3	2001	IPT	C3'-C1'-S1-C1
2	4	2001	IPT	C2'-C1'-S1-C1
2	2	2001	IPT	O5-C5-C6-O6
2	4	2001	IPT	O5-C5-C6-O6

There are no ring outliers.

35 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	3	6027	DMS	1	0
5	2	6043	DMS	1	0
5	1	6002	DMS	2	0
5	4	6021	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	4	2001	IPT	1	0
5	1	6014	DMS	1	0
5	3	6020	DMS	1	0
5	3	6040	DMS	1	0
5	2	6027	DMS	1	0
5	4	6002	DMS	1	0
5	2	6022	DMS	1	0
5	3	6018	DMS	1	0
5	1	6019	DMS	1	0
5	2	6010	DMS	1	0
5	2	6026	DMS	4	0
5	2	6040	DMS	2	0
5	1	6032	DMS	1	0
5	4	6009	DMS	1	0
5	3	1024	DMS	1	0
2	3	2002	IPT	2	0
5	3	6026	DMS	1	0
5	2	6032	DMS	2	0
5	3	6030	DMS	1	0
2	2	2001	IPT	1	0
5	2	6039	DMS	1	0
2	2	2002	IPT	1	0
5	3	6029	DMS	3	0
5	4	6001	DMS	1	0
5	1	6009	DMS	1	0
5	2	6015	DMS	1	0
5	1	6021	DMS	1	0
5	3	6016	DMS	1	0
5	3	6013	DMS	1	0
5	4	6027	DMS	1	0
5	2	6018	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, 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%)	-0.07	21 (2%) 63 67	10, 20, 40, 66	0
1	2	1011/1052 (96%)	-0.29	20 (1%) 65 69	8, 16, 36, 68	0
1	3	1011/1052 (96%)	-0.32	17 (1%) 69 72	9, 16, 33, 67	0
1	4	1011/1052 (96%)	-0.07	23 (2%) 61 65	10, 21, 39, 70	0
All	All	4044/4208 (96%)	-0.19	81 (2%) 65 69	8, 19, 37, 70	0

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	735	HIS	4.9
1	2	732	ALA	4.8
1	2	731	PRO	4.6
1	3	689	GLU	3.8
1	3	1023	LYS	3.8

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	DMS	2	6040	4/4	0.37	0.32	92,92,93,93	0
5	DMS	2	6042	4/4	0.40	0.22	95,96,96,96	0
5	DMS	3	6040	4/4	0.40	0.29	51,53,55,56	0
5	DMS	1	6019	4/4	0.41	0.38	99,99,100,100	0
5	DMS	3	6035	4/4	0.43	0.28	88,88,88,89	0
5	DMS	1	6025	4/4	0.47	0.24	82,83,83,83	0
5	DMS	2	6016	4/4	0.50	0.28	91,92,92,92	0
5	DMS	2	6012	4/4	0.56	0.30	77,78,79,79	0
5	DMS	3	6026	4/4	0.56	0.26	97,97,98,98	0
5	DMS	2	6029	4/4	0.58	0.25	80,81,81,82	0
5	DMS	4	6017	4/4	0.58	0.26	75,76,76,76	0
5	DMS	1	6032	4/4	0.60	0.29	75,76,76,76	0
5	DMS	3	6036	4/4	0.60	0.25	97,97,98,98	0
5	DMS	2	6031	4/4	0.61	0.22	75,76,76,77	0
5	DMS	4	6027	4/4	0.62	0.22	60,60,60,61	0
5	DMS	1	6029	4/4	0.64	0.19	67,68,69,69	0
5	DMS	3	6032	4/4	0.65	0.25	85,86,86,86	0
5	DMS	3	6041	4/4	0.65	0.24	77,78,78,79	0
5	DMS	4	6021	4/4	0.66	0.27	82,82,82,82	0
5	DMS	3	6037	4/4	0.66	0.23	74,75,75,75	0
5	DMS	2	6035	4/4	0.67	0.25	75,75,76,76	0
5	DMS	2	6038	4/4	0.68	0.20	55,55,55,57	0
5	DMS	4	6016	4/4	0.69	0.27	93,94,94,94	0
5	DMS	4	6029	4/4	0.70	0.17	73,73,74,75	0
3	MG	4	3003	1/1	0.71	0.14	65,65,65,65	0
5	DMS	1	6024	4/4	0.72	0.24	80,81,81,81	0
5	DMS	2	6033	4/4	0.72	0.20	92,92,92,92	0
5	DMS	4	6013	4/4	0.73	0.15	66,66,66,67	0
5	DMS	2	6015	4/4	0.73	0.20	85,85,85,85	0
5	DMS	2	6026	4/4	0.73	0.23	40,42,45,45	0
5	DMS	1	6028	4/4	0.74	0.18	70,71,71,71	0
2	IPT	1	2002	15/15	0.74	0.14	27,31,34,35	15
5	DMS	4	6018	4/4	0.74	0.21	80,81,81,81	0
5	DMS	2	6028	4/4	0.75	0.20	44,45,46,49	0
5	DMS	4	6007	4/4	0.75	0.18	74,74,74,74	0
5	DMS	1	6014	4/4	0.75	0.25	94,94,94,94	0
5	DMS	3	6038	4/4	0.76	0.18	68,68,69,70	0
5	DMS	1	6023	4/4	0.76	0.18	59,60,61,61	0
5	DMS	3	6014	4/4	0.76	0.18	60,60,60,61	0
5	DMS	4	6026	4/4	0.76	0.19	67,68,68,68	0
5	DMS	3	6025	4/4	0.76	0.19	60,60,61,61	0
5	DMS	1	6011	4/4	0.76	0.18	84,84,84,84	0
5	DMS	2	6025	4/4	0.77	0.20	66,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	1	6031	4/4	0.77	0.20	73,74,74,74	0
5	DMS	3	6018	4/4	0.77	0.22	59,59,60,61	0
5	DMS	2	6043	4/4	0.77	0.17	56,56,57,57	0
5	DMS	4	6012	4/4	0.78	0.18	79,79,79,80	0
5	DMS	2	6034	4/4	0.78	0.16	67,68,69,69	0
5	DMS	4	6028	4/4	0.78	0.18	89,89,90,90	0
5	DMS	1	6030	4/4	0.78	0.17	66,66,66,67	0
5	DMS	1	6026	4/4	0.79	0.16	76,76,76,77	0
5	DMS	3	6022	4/4	0.80	0.16	74,75,75,75	0
5	DMS	2	6022	4/4	0.80	0.19	81,81,82,82	0
5	DMS	3	6039	4/4	0.80	0.18	59,59,60,61	0
5	DMS	3	6005	4/4	0.80	0.16	53,53,53,54	0
3	MG	1	3003	1/1	0.80	0.13	59,59,59,59	0
5	DMS	4	6011	4/4	0.80	0.16	56,57,57,58	0
5	DMS	3	6015	4/4	0.80	0.19	70,71,71,71	0
5	DMS	2	6039	4/4	0.80	0.20	47,48,48,48	0
5	DMS	3	6031	4/4	0.81	0.17	84,84,84,85	0
5	DMS	3	6020	4/4	0.81	0.19	64,65,65,65	0
5	DMS	4	6030	4/4	0.81	0.19	81,82,82,82	0
5	DMS	1	6027	4/4	0.82	0.18	49,49,49,51	0
5	DMS	1	6018	4/4	0.82	0.16	64,64,65,65	0
5	DMS	2	6036	4/4	0.82	0.18	52,52,53,54	0
5	DMS	2	6037	4/4	0.82	0.15	74,74,75,75	0
2	IPT	4	2002	15/15	0.82	0.11	27,30,32,32	0
5	DMS	1	6010	4/4	0.82	0.15	58,58,58,59	0
5	DMS	3	6030	4/4	0.82	0.18	51,51,52,52	0
5	DMS	4	6024	4/4	0.83	0.18	67,68,68,68	0
5	DMS	3	6029	4/4	0.83	0.22	55,55,56,57	0
5	DMS	1	6017	4/4	0.83	0.17	38,41,42,46	0
5	DMS	3	6017	4/4	0.84	0.18	57,57,57,58	0
5	DMS	3	6016	4/4	0.84	0.18	65,65,65,65	0
5	DMS	2	6018	4/4	0.85	0.20	65,65,66,66	0
5	DMS	2	6023	4/4	0.85	0.15	72,72,72,73	0
5	DMS	4	6022	4/4	0.85	0.16	54,55,55,56	0
5	DMS	3	6034	4/4	0.85	0.12	57,57,58,59	0
5	DMS	4	6025	4/4	0.85	0.17	68,69,69,69	0
5	DMS	1	6022	4/4	0.86	0.17	54,54,54,54	0
5	DMS	2	6030	4/4	0.86	0.13	64,64,65,65	0
5	DMS	1	6015	4/4	0.86	0.17	70,70,70,70	0
5	DMS	2	6007	4/4	0.86	0.15	43,44,45,46	0
5	DMS	4	6015	4/4	0.86	0.17	63,63,63,64	0
5	DMS	1	6007	4/4	0.86	0.17	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	3	6019	4/4	0.86	0.15	77,77,77,77	0
5	DMS	3	6007	4/4	0.86	0.13	49,50,50,51	0
5	DMS	4	6019	4/4	0.86	0.15	63,64,64,64	0
5	DMS	3	6027	4/4	0.87	0.14	41,41,42,44	0
5	DMS	2	6019	4/4	0.87	0.14	63,63,64,64	0
5	DMS	2	6005	4/4	0.87	0.18	50,51,51,51	0
5	DMS	2	6006	4/4	0.87	0.14	43,44,44,45	0
2	IPT	2	2002	15/15	0.87	0.10	32,37,39,39	0
5	DMS	3	6033	4/4	0.87	0.17	66,67,67,67	0
2	IPT	4	2001	15/15	0.87	0.11	20,25,32,34	0
5	DMS	4	6014	4/4	0.87	0.17	91,91,91,91	0
5	DMS	1	6003	4/4	0.87	0.13	55,56,57,57	0
5	DMS	1	6020	4/4	0.87	0.14	63,63,63,63	0
2	IPT	1	2001	15/15	0.87	0.11	17,21,28,30	0
5	DMS	2	6032	4/4	0.88	0.15	42,46,47,48	0
4	NA	4	3103	1/1	0.88	0.07	37,37,37,37	0
3	MG	3	3003	1/1	0.88	0.19	74,74,74,74	0
5	DMS	2	6010	4/4	0.88	0.15	40,40,42,43	0
5	DMS	2	6020	4/4	0.88	0.15	60,60,60,61	0
5	DMS	1	6006	4/4	0.88	0.15	61,61,61,62	0
3	MG	2	3003	1/1	0.88	0.13	52,52,52,52	0
5	DMS	4	6002	4/4	0.88	0.18	43,45,45,46	0
5	DMS	3	6011	4/4	0.88	0.13	39,41,41,43	0
2	IPT	3	2002	15/15	0.89	0.10	32,36,38,39	0
5	DMS	3	6023	4/4	0.89	0.15	51,52,52,53	0
5	DMS	3	6024	4/4	0.89	0.14	60,60,60,60	0
5	DMS	3	1024	4/4	0.89	0.12	58,58,58,60	0
5	DMS	3	6001	4/4	0.89	0.15	29,31,33,33	0
5	DMS	1	6009	4/4	0.89	0.14	57,57,57,58	0
5	DMS	1	6002	4/4	0.90	0.15	39,40,40,41	0
5	DMS	1	6012	4/4	0.90	0.13	69,69,70,70	0
5	DMS	3	6012	4/4	0.90	0.14	57,57,57,57	0
5	DMS	1	6013	4/4	0.90	0.13	55,55,56,56	0
4	NA	3	3104	1/1	0.90	0.12	28,28,28,28	0
5	DMS	1	6021	4/4	0.90	0.15	59,59,59,60	0
4	NA	3	3103	1/1	0.90	0.07	34,34,34,34	0
5	DMS	4	6009	4/4	0.91	0.13	45,46,46,47	0
5	DMS	2	6001	4/4	0.91	0.17	27,29,29,30	0
5	DMS	1	6001	4/4	0.91	0.16	28,31,31,31	0
5	DMS	2	6011	4/4	0.91	0.12	59,59,60,60	0
5	DMS	4	6020	4/4	0.91	0.13	36,38,39,41	0
5	DMS	1	6016	4/4	0.91	0.12	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	3	6010	4/4	0.91	0.13	33,35,36,37	0
5	DMS	3	6013	4/4	0.92	0.11	54,54,55,55	0
5	DMS	2	6013	4/4	0.92	0.12	43,43,44,44	0
5	DMS	2	6017	4/4	0.92	0.13	61,61,62,62	0
5	DMS	3	6021	4/4	0.92	0.11	44,45,45,46	0
5	DMS	3	6003	4/4	0.92	0.11	37,37,38,39	0
4	NA	4	3104	1/1	0.92	0.07	35,35,35,35	0
5	DMS	4	6005	4/4	0.92	0.12	50,50,51,52	0
3	MG	1	3002	1/1	0.93	0.05	24,24,24,24	0
5	DMS	4	6001	4/4	0.93	0.15	35,36,36,37	0
5	DMS	2	6014	4/4	0.93	0.10	55,56,56,56	0
4	NA	2	3103	1/1	0.93	0.08	36,36,36,36	0
5	DMS	4	6006	4/4	0.93	0.11	45,46,46,46	0
2	IPT	2	2001	15/15	0.93	0.08	10,16,21,21	0
5	DMS	3	6006	4/4	0.93	0.10	46,47,47,47	0
5	DMS	4	6010	4/4	0.93	0.11	55,55,55,55	0
5	DMS	2	6027	4/4	0.93	0.11	44,44,44,45	0
4	NA	4	3102	1/1	0.94	0.07	16,16,16,16	0
5	DMS	4	6023	4/4	0.94	0.10	41,41,42,42	0
2	IPT	3	2001	15/15	0.94	0.08	12,18,23,26	0
4	NA	2	3104	1/1	0.94	0.08	31,31,31,31	0
5	DMS	2	6003	4/4	0.94	0.11	26,26,27,30	0
5	DMS	3	6009	4/4	0.94	0.11	38,38,39,39	0
5	DMS	3	6028	4/4	0.94	0.10	42,42,42,43	0
5	DMS	2	6024	4/4	0.94	0.09	31,32,33,35	0
5	DMS	4	6003	4/4	0.94	0.13	34,35,36,37	0
5	DMS	2	6009	4/4	0.95	0.12	34,35,36,37	0
5	DMS	1	6005	4/4	0.95	0.09	52,53,53,53	0
3	MG	2	3001	1/1	0.95	0.03	13,13,13,13	0
3	MG	1	3001	1/1	0.95	0.03	16,16,16,16	0
3	MG	2	3004	1/1	0.95	0.04	34,34,34,34	0
5	DMS	2	6002	4/4	0.96	0.09	31,32,32,34	0
4	NA	1	3103	1/1	0.96	0.05	29,29,29,29	0
4	NA	1	3104	1/1	0.96	0.05	32,32,32,32	0
5	DMS	4	6000	4/4	0.96	0.10	23,25,25,27	0
3	MG	4	3001	1/1	0.96	0.04	17,17,17,17	0
5	DMS	2	6000	4/4	0.96	0.10	16,21,23,23	0
5	DMS	2	6021	4/4	0.96	0.08	39,40,40,40	0
3	MG	1	3004	1/1	0.96	0.04	43,43,43,43	0
4	NA	4	3101	1/1	0.97	0.04	19,19,19,19	0
5	DMS	3	6002	4/4	0.97	0.07	30,31,32,32	0
5	DMS	2	6004	4/4	0.97	0.09	27,28,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	3	6004	4/4	0.97	0.10	25,25,26,26	0
3	MG	4	3002	1/1	0.97	0.07	23,23,23,23	0
5	DMS	4	6008	4/4	0.97	0.09	36,37,38,39	0
5	DMS	1	6008	4/4	0.97	0.07	36,36,37,37	0
4	NA	1	3101	1/1	0.98	0.05	18,18,18,18	0
4	NA	1	3102	1/1	0.98	0.02	12,12,12,12	0
5	DMS	3	6000	4/4	0.98	0.07	14,19,19,21	0
5	DMS	2	6008	4/4	0.98	0.07	24,25,27,27	0
5	DMS	1	6000	4/4	0.98	0.06	18,23,23,25	0
5	DMS	4	6004	4/4	0.98	0.06	28,29,30,30	0
3	MG	2	3002	1/1	0.98	0.07	15,15,15,15	0
4	NA	3	3101	1/1	0.98	0.02	13,13,13,13	0
4	NA	2	3101	1/1	0.99	0.05	15,15,15,15	0
4	NA	3	3102	1/1	0.99	0.02	14,14,14,14	0
5	DMS	1	6004	4/4	0.99	0.05	26,27,28,29	0
4	NA	2	3102	1/1	0.99	0.03	13,13,13,13	0
3	MG	3	3001	1/1	0.99	0.02	13,13,13,13	0
5	DMS	3	6008	4/4	0.99	0.05	20,22,22,22	0
3	MG	3	3002	1/1	0.99	0.04	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.