



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 27, 2017 – 05:25 PM EDT

PDB ID : 1JZ4
Title : E. COLI (lacZ) BETA-GALACTOSIDASE-TRAPPED 2-DEOXY-GALACTOSYL-ENZYME INTERMEDIATE (Low Bis-Tris)
Authors : Juers, D.H.; Matthews, B.W.
Deposited on : unknown
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

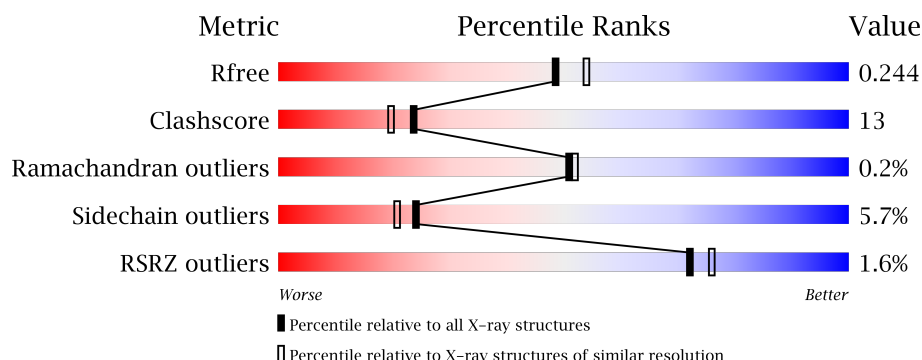
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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. 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>64%</div> <div>29%</div> <div>5%</div> <div>..</div> </div>
1	B	1023	<div> <div>%</div> <div>62%</div> <div>30%</div> <div>5%</div> <div>..</div> </div>
1	C	1023	<div> <div>2%</div> <div>63%</div> <div>28%</div> <div>7%</div> <div>..</div> </div>
1	D	1023	<div> <div>2%</div> <div>63%</div> <div>30%</div> <div>5%</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
2	2DG	B	2001	-	-	-	X
4	NA	D	3103	-	-	-	X
5	DMS	A	8406	-	-	-	X
5	DMS	A	8407	-	-	-	X
5	DMS	A	8417	-	-	-	X
5	DMS	A	8420	-	-	-	X
5	DMS	A	8502	-	-	-	X
5	DMS	A	8504	-	-	-	X
5	DMS	B	8404	-	-	-	X
5	DMS	B	8405	-	-	-	X
5	DMS	B	8406	-	-	-	X
5	DMS	B	8407	-	-	-	X
5	DMS	B	8408	-	-	-	X
5	DMS	B	8420	-	-	-	X
5	DMS	B	8423	-	-	-	X
5	DMS	B	8508	-	X	-	X
5	DMS	C	8419	-	-	-	X
5	DMS	C	8420	-	-	-	X
5	DMS	C	8501	-	-	-	X
5	DMS	C	8506	-	-	X	-
5	DMS	C	8602	-	-	-	X
5	DMS	D	8408	-	-	-	X
5	DMS	D	8412	-	-	X	-
5	DMS	D	8703	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36890 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	0	0
			8125	5138	1440	1509	38			
1	B	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			
1	C	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			

There are 32 discrepancies between the modelled and reference sequences:

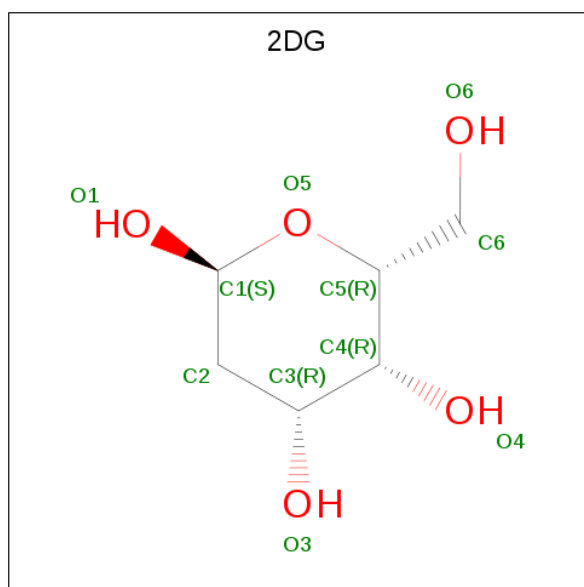
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	THR	CLONING ARTIFACT	? P00722
A	2	SER	MET	CLONING ARTIFACT	? P00722
A	3	HIS	ILE	CLONING ARTIFACT	? P00722
A	4	MET	THR	CLONING ARTIFACT	? P00722
A	5	LEU	ASP	CLONING ARTIFACT	? P00722
A	6	GLU	SER	CLONING ARTIFACT	? P00722
A	7	ASP	LEU	CLONING ARTIFACT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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	GLU	SER	CLONING ARTIFACT	? P00722
C	7	ASP	LEU	CLONING ARTIFACT	? P00722
C	8	PRO	ALA	CLONING ARTIFACT	? 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

- Molecule 2 is 2-DEOXY-BETA-D-GALACTOSE (three-letter code: 2DG) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		
2	D	1	Total	C	O	0	0
			10	6	4		

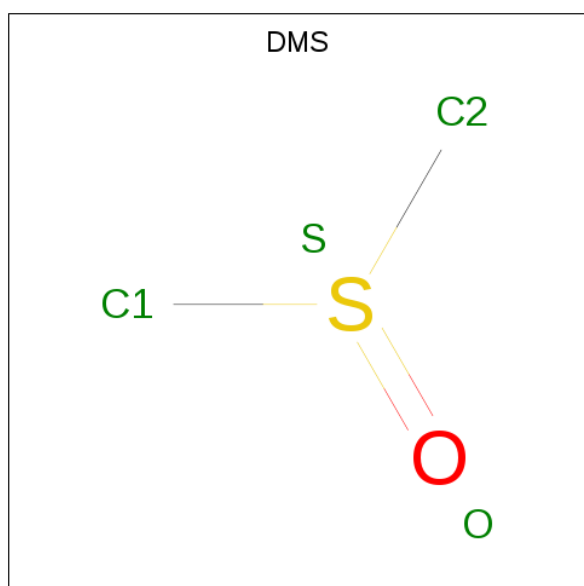
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

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



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

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	992	Total	O	0	0
			992	992		
6	B	995	Total	O	0	0
			995	995		

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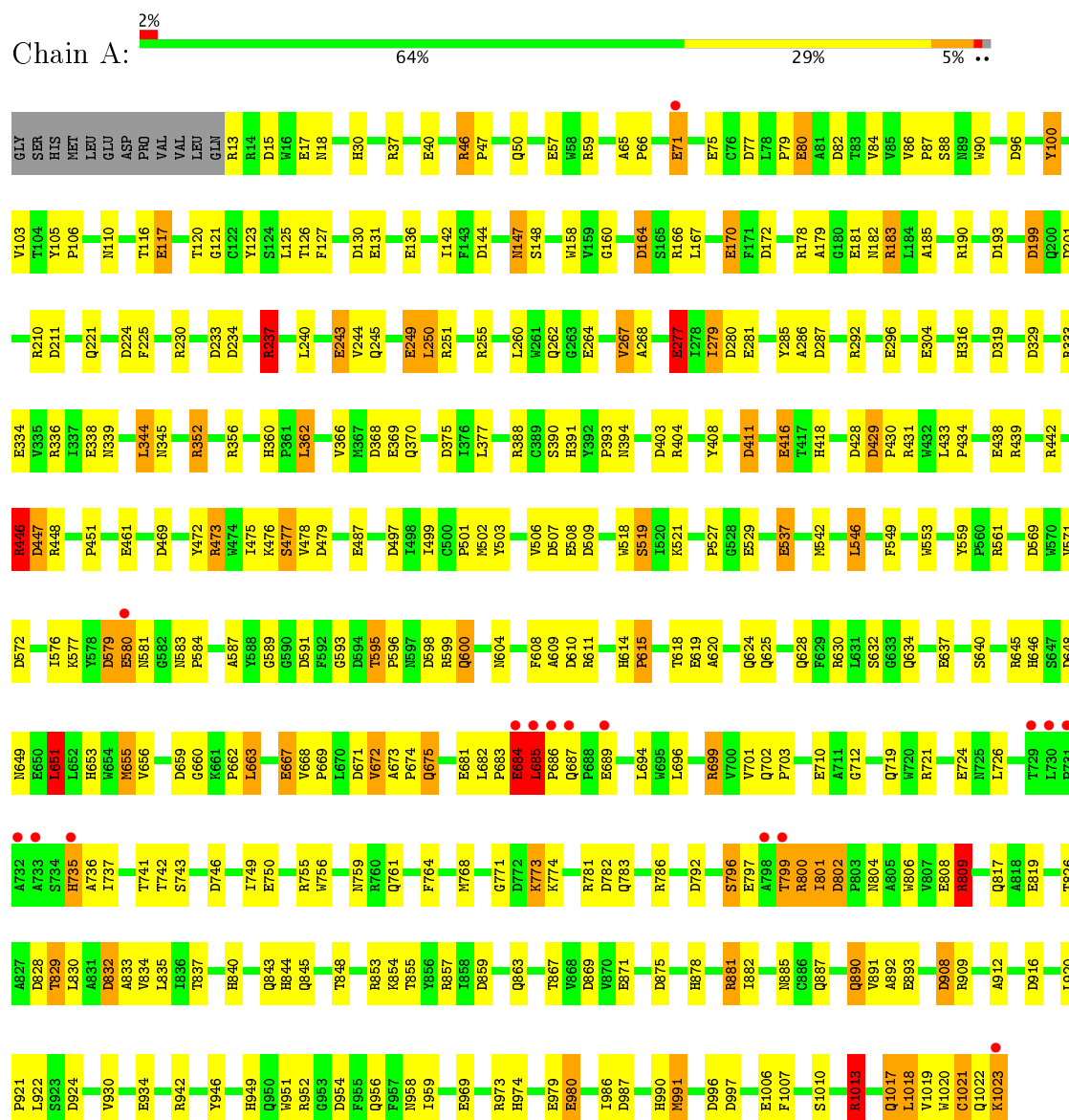
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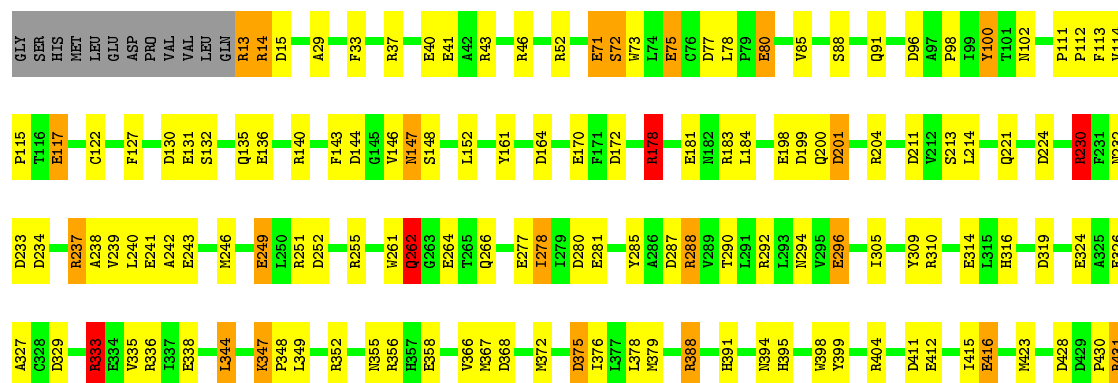
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	946	Total 946	O 946	0	0
6	D	980	Total 980	O 980	0	0

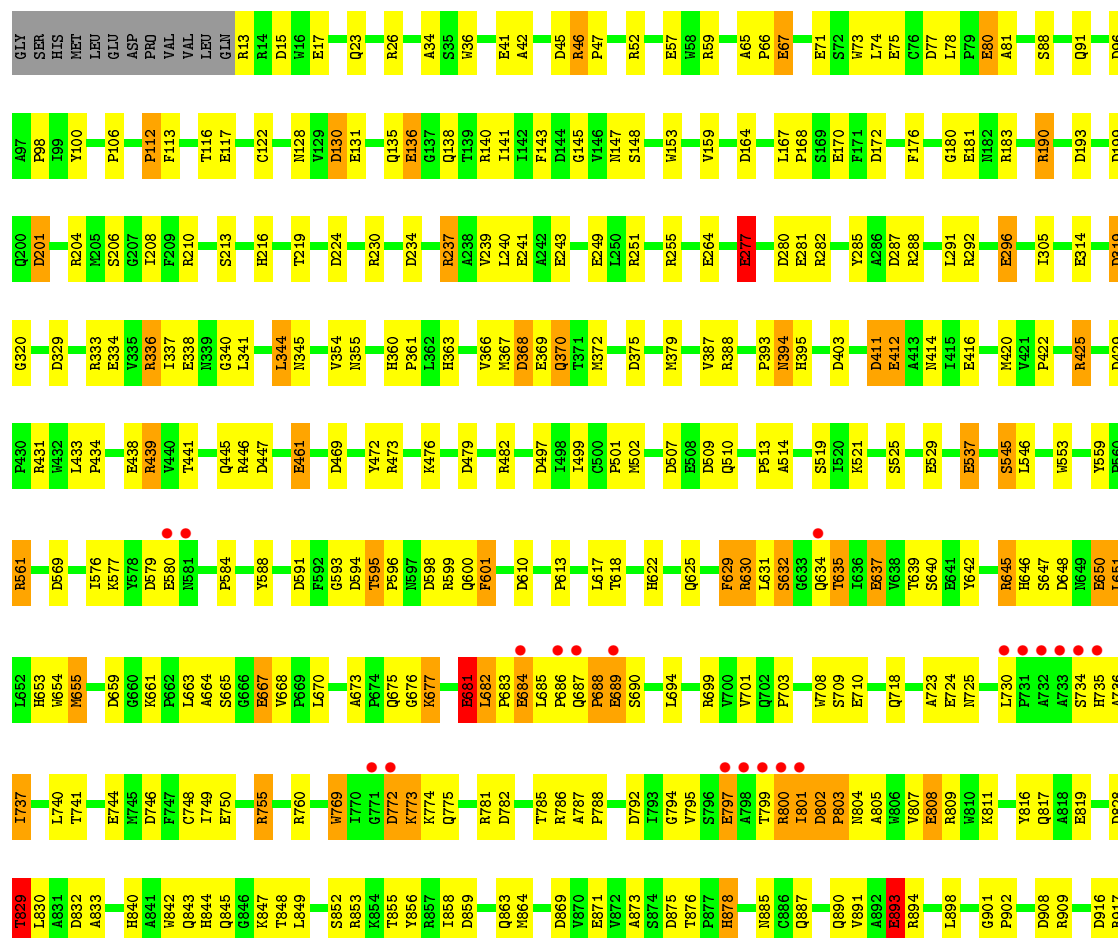
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Beta-Galactosidase







R918	D919	L920	P921	E934	R942	E943	L944	N945	H949	Q950	W951	R952	G953	D954	F955	Q956	I959	S960	R961	Y962	M968	E969	H972	R973	H974	E979	E980	G981	L984	R985	I986	D987	D996	D997	S1004	S1010	R1013	L1018	V1019	W1020	C1021	Q1022	K1023
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.50 Å 169.00 Å 200.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 19.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.0 (40.00-2.10) 86.4 (19.99-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.09 Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.164 , 0.267 0.152 , 0.244	Depositor DCC
R_{free} test set	3669 reflections (1.46%)	DCC
Wilson B-factor (Å ²)	11.5	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 95.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36890	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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 36.06 % 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 5.3009e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, DMS, 2DG

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	1.09	43/8367 (0.5%)	1.73	174/11415 (1.5%)
1	B	1.11	48/8367 (0.6%)	1.69	165/11415 (1.4%)
1	C	1.11	42/8367 (0.5%)	1.75	177/11415 (1.6%)
1	D	1.11	48/8367 (0.6%)	1.69	151/11415 (1.3%)
All	All	1.10	181/33468 (0.5%)	1.71	667/45660 (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	B	0	1
1	D	1	0
All	All	1	1

The worst 5 of 181 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	277	GLU	CD-OE2	10.41	1.37	1.25
1	C	281	GLU	CD-OE2	10.15	1.36	1.25
1	D	71	GLU	CD-OE2	10.14	1.36	1.25
1	C	684	GLU	CD-OE2	9.88	1.36	1.25
1	C	296	GLU	CD-OE2	9.86	1.36	1.25

The worst 5 of 667 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	809	ARG	NE-CZ-NH1	19.72	130.16	120.30
1	C	442	ARG	NE-CZ-NH2	-17.27	111.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	786	ARG	NE-CZ-NH1	15.02	127.81	120.30
1	C	721	ARG	NE-CZ-NH1	15.00	127.80	120.30
1	A	46	ARG	NE-CZ-NH1	15.00	127.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	689	GLU	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	329	ASP	Sidechain

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	8125	0	7716	188	1
1	B	8125	0	7716	201	0
1	C	8125	0	7716	219	0
1	D	8125	0	7716	208	0
2	A	10	0	9	0	0
2	B	10	0	9	1	0
2	C	10	0	9	0	0
2	D	10	0	9	2	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	3	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	100	0	150	9	0
5	B	108	0	162	10	0
5	C	112	0	168	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	92	0	138	13	0
6	A	992	0	0	21	0
6	B	995	0	0	14	0
6	C	946	0	0	14	1
6	D	980	0	0	18	0
All	All	36890	0	31518	810	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 13.

The worst 5 of 810 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:C:634:GLN:NE2	1:C:634:GLN:H	1.47	1.13
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.33	1.10
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.54	1.05
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.37	1.02
1:B:797:GLU:HG2	1:B:799:THR:HG23	1.35	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)
1:A:773:LYS:NZ	6:C:9410:HOH:O[3_544]	2.18	0.02

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	1009/1023 (99%)	964 (96%)	44 (4%)	1 (0%)	55 57
1	B	1009/1023 (99%)	956 (95%)	48 (5%)	5 (0%)	32 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1009/1023 (99%)	963 (95%)	46 (5%)	0	100	100
1	D	1009/1023 (99%)	962 (95%)	43 (4%)	4 (0%)	38	35
All	All	4036/4092 (99%)	3845 (95%)	181 (4%)	10 (0%)	51	52

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	690	SER
1	B	731	PRO
1	D	688	PRO
1	D	801	ILE
1	B	688	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	864/875 (99%)	816 (94%)	48 (6%)	25	21
1	B	864/875 (99%)	815 (94%)	49 (6%)	24	21
1	C	864/875 (99%)	817 (95%)	47 (5%)	26	23
1	D	864/875 (99%)	812 (94%)	52 (6%)	22	19
All	All	3456/3500 (99%)	3260 (94%)	196 (6%)	24	21

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	824	GLN
1	C	333	ARG
1	D	772	ASP
1	B	847	LYS
1	C	75	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	646	HIS
1	C	102	ASN
1	D	878	HIS
1	B	757	GLN
1	B	824	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 132 ligands modelled in this entry, 25 are monoatomic - leaving 107 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	2DG	A	2001	1,4	10,10,11	1.02	1 (10%)	10,13,15	1.82	2 (20%)
5	DMS	A	8401	-	3,3,3	1.93	1 (33%)	3,3,3	0.12	0
5	DMS	A	8402	-	3,3,3	1.55	1 (33%)	3,3,3	0.14	0
5	DMS	A	8403	-	3,3,3	0.96	0	3,3,3	0.73	0
5	DMS	A	8404	-	3,3,3	1.80	1 (33%)	3,3,3	0.30	0
5	DMS	A	8405	-	3,3,3	1.49	1 (33%)	3,3,3	0.23	0
5	DMS	A	8406	-	3,3,3	1.85	1 (33%)	3,3,3	0.45	0
5	DMS	A	8407	-	3,3,3	1.73	2 (66%)	3,3,3	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	8408	-	3,3,3	1.04	0	3,3,3	0.23	0
5	DMS	A	8409	-	3,3,3	2.32	2 (66%)	3,3,3	0.35	0
5	DMS	A	8410	-	3,3,3	0.71	0	3,3,3	0.09	0
5	DMS	A	8411	-	3,3,3	1.54	1 (33%)	3,3,3	0.15	0
5	DMS	A	8412	-	3,3,3	0.75	0	3,3,3	0.20	0
5	DMS	A	8413	-	3,3,3	2.01	2 (66%)	3,3,3	0.16	0
5	DMS	A	8414	-	3,3,3	0.75	0	3,3,3	0.44	0
5	DMS	A	8415	-	3,3,3	1.91	1 (33%)	3,3,3	0.15	0
5	DMS	A	8417	-	3,3,3	1.11	0	3,3,3	0.50	0
5	DMS	A	8419	-	3,3,3	0.65	0	3,3,3	0.39	0
5	DMS	A	8420	-	3,3,3	1.55	1 (33%)	3,3,3	1.01	0
5	DMS	A	8421	-	3,3,3	0.88	0	3,3,3	0.97	0
5	DMS	A	8425	4	3,3,3	1.40	1 (33%)	3,3,3	0.55	0
5	DMS	A	8501	-	3,3,3	1.43	1 (33%)	3,3,3	0.31	0
5	DMS	A	8502	-	3,3,3	1.15	0	3,3,3	1.35	1 (33%)
5	DMS	A	8503	-	3,3,3	0.65	0	3,3,3	0.17	0
5	DMS	A	8504	-	3,3,3	0.34	0	3,3,3	0.42	0
5	DMS	A	8602	-	3,3,3	0.86	0	3,3,3	0.82	0
2	2DG	B	2001	1,4	10,10,11	1.41	1 (10%)	10,13,15	1.37	1 (10%)
5	DMS	B	8401	-	3,3,3	0.65	0	3,3,3	0.42	0
5	DMS	B	8402	-	3,3,3	1.87	2 (66%)	3,3,3	0.18	0
5	DMS	B	8403	-	3,3,3	1.44	0	3,3,3	1.24	1 (33%)
5	DMS	B	8404	-	3,3,3	0.80	0	3,3,3	0.35	0
5	DMS	B	8405	-	3,3,3	0.88	0	3,3,3	0.38	0
5	DMS	B	8406	-	3,3,3	1.24	1 (33%)	3,3,3	0.25	0
5	DMS	B	8407	-	3,3,3	1.50	0	3,3,3	0.25	0
5	DMS	B	8408	-	3,3,3	1.40	0	3,3,3	0.40	0
5	DMS	B	8409	-	3,3,3	0.71	0	3,3,3	1.27	1 (33%)
5	DMS	B	8410	-	3,3,3	1.29	0	3,3,3	0.48	0
5	DMS	B	8411	-	3,3,3	0.36	0	3,3,3	0.75	0
5	DMS	B	8412	-	3,3,3	1.89	1 (33%)	3,3,3	0.17	0
5	DMS	B	8413	-	3,3,3	2.20	2 (66%)	3,3,3	0.82	0
5	DMS	B	8414	-	3,3,3	0.55	0	3,3,3	0.75	0
5	DMS	B	8415	-	3,3,3	1.09	0	3,3,3	1.32	1 (33%)
5	DMS	B	8416	-	3,3,3	1.29	0	3,3,3	0.06	0
5	DMS	B	8417	-	3,3,3	1.17	0	3,3,3	0.47	0
5	DMS	B	8420	-	3,3,3	1.28	1 (33%)	3,3,3	0.39	0
5	DMS	B	8421	-	3,3,3	0.83	0	3,3,3	0.14	0
5	DMS	B	8423	-	3,3,3	0.57	0	3,3,3	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	8425	4	3,3,3	1.91	1 (33%)	3,3,3	0.37	0
5	DMS	B	8427	-	3,3,3	0.87	0	3,3,3	0.61	0
5	DMS	B	8502	-	3,3,3	0.73	0	3,3,3	1.25	1 (33%)
5	DMS	B	8504	-	3,3,3	0.11	0	3,3,3	0.08	0
5	DMS	B	8506	-	3,3,3	1.38	0	3,3,3	0.78	0
5	DMS	B	8508	-	3,3,3	2.47	3 (100%)	3,3,3	0.38	0
5	DMS	B	8601	-	3,3,3	0.42	0	3,3,3	0.28	0
2	2DG	C	2001	1,4	10,10,11	1.27	1 (10%)	10,13,15	1.99	1 (10%)
5	DMS	C	8401	-	3,3,3	0.87	0	3,3,3	0.75	0
5	DMS	C	8402	-	3,3,3	2.05	1 (33%)	3,3,3	0.72	0
5	DMS	C	8403	-	3,3,3	0.83	0	3,3,3	0.42	0
5	DMS	C	8404	-	3,3,3	1.29	0	3,3,3	0.67	0
5	DMS	C	8405	-	3,3,3	1.82	1 (33%)	3,3,3	0.25	0
5	DMS	C	8407	-	3,3,3	1.15	0	3,3,3	0.10	0
5	DMS	C	8408	-	3,3,3	0.67	0	3,3,3	0.25	0
5	DMS	C	8409	-	3,3,3	1.57	1 (33%)	3,3,3	0.37	0
5	DMS	C	8410	-	3,3,3	1.09	0	3,3,3	0.36	0
5	DMS	C	8411	-	3,3,3	1.66	1 (33%)	3,3,3	0.33	0
5	DMS	C	8412	-	3,3,3	0.86	0	3,3,3	0.55	0
5	DMS	C	8413	-	3,3,3	2.93	2 (66%)	3,3,3	0.43	0
5	DMS	C	8414	-	3,3,3	1.56	1 (33%)	3,3,3	0.35	0
5	DMS	C	8415	-	3,3,3	1.55	1 (33%)	3,3,3	0.96	0
5	DMS	C	8416	-	3,3,3	1.10	0	3,3,3	0.71	0
5	DMS	C	8417	-	3,3,3	0.85	0	3,3,3	0.51	0
5	DMS	C	8419	-	3,3,3	1.38	0	3,3,3	0.18	0
5	DMS	C	8420	-	3,3,3	1.28	0	3,3,3	0.65	0
5	DMS	C	8421	-	3,3,3	0.60	0	3,3,3	0.23	0
5	DMS	C	8423	-	3,3,3	1.29	0	3,3,3	0.31	0
5	DMS	C	8425	4	3,3,3	1.47	1 (33%)	3,3,3	1.63	1 (33%)
5	DMS	C	8427	-	3,3,3	0.89	0	3,3,3	0.09	0
5	DMS	C	8501	-	3,3,3	1.50	0	3,3,3	1.18	1 (33%)
5	DMS	C	8503	-	3,3,3	0.79	0	3,3,3	0.41	0
5	DMS	C	8504	-	3,3,3	1.09	0	3,3,3	0.22	0
5	DMS	C	8506	-	3,3,3	1.56	1 (33%)	3,3,3	1.24	1 (33%)
5	DMS	C	8601	-	3,3,3	1.08	0	3,3,3	0.61	0
5	DMS	C	8602	-	3,3,3	1.04	0	3,3,3	0.15	0
2	2DG	D	2001	1,4	10,10,11	1.38	2 (20%)	10,13,15	2.50	3 (30%)
5	DMS	D	8401	-	3,3,3	1.77	1 (33%)	3,3,3	0.32	0
5	DMS	D	8402	-	3,3,3	1.14	0	3,3,3	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	D	8403	-	3,3,3	0.51	0	3,3,3	0.31	0
5	DMS	D	8404	-	3,3,3	1.56	1 (33%)	3,3,3	0.51	0
5	DMS	D	8405	-	3,3,3	0.82	0	3,3,3	0.24	0
5	DMS	D	8406	-	3,3,3	1.01	0	3,3,3	0.37	0
5	DMS	D	8408	-	3,3,3	1.12	0	3,3,3	0.31	0
5	DMS	D	8409	-	3,3,3	2.21	1 (33%)	3,3,3	0.58	0
5	DMS	D	8410	-	3,3,3	1.28	0	3,3,3	0.48	0
5	DMS	D	8411	-	3,3,3	0.92	0	3,3,3	0.49	0
5	DMS	D	8412	-	3,3,3	1.48	1 (33%)	3,3,3	0.59	0
5	DMS	D	8413	-	3,3,3	0.89	0	3,3,3	0.65	0
5	DMS	D	8414	-	3,3,3	1.20	0	3,3,3	0.08	0
5	DMS	D	8416	-	3,3,3	0.75	0	3,3,3	0.23	0
5	DMS	D	8417	-	3,3,3	1.25	0	3,3,3	0.72	0
5	DMS	D	8419	-	3,3,3	0.87	0	3,3,3	0.36	0
5	DMS	D	8421	-	3,3,3	1.02	0	3,3,3	0.08	0
5	DMS	D	8501	-	3,3,3	0.83	0	3,3,3	0.89	0
5	DMS	D	8503	-	3,3,3	1.33	1 (33%)	3,3,3	0.77	0
5	DMS	D	8508	-	3,3,3	0.56	0	3,3,3	0.59	0
5	DMS	D	8701	-	3,3,3	2.87	2 (66%)	3,3,3	0.74	0
5	DMS	D	8703	-	3,3,3	0.83	0	3,3,3	0.32	0
5	DMS	D	8705	-	3,3,3	1.22	0	3,3,3	0.21	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	2DG	A	2001	1,4	-	0/2/16/18	0/1/1/1
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	8415	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8417	-	-	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	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	8502	-	-	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	8602	-	-	0/0/0/0	0/0/0/0
2	2DG	B	2001	1,4	-	0/2/16/18	0/1/1/1
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	8406	-	-	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
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	8427	-	-	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	8506	-	-	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	2DG	C	2001	1,4	-	0/2/16/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	8427	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8503	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8506	-	-	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	2DG	D	2001	1,4	-	0/2/16/18	0/1/1/1
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
5	DMS	D	8406	-	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	D	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8417	-	-	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	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8503	-	-	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	8705	-	-	0/0/0/0	0/0/0/0

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	8406	DMS	C2-S	-3.20	1.51	1.75
5	C	8414	DMS	C1-S	-2.54	1.56	1.75
5	A	8407	DMS	O-S	2.00	1.63	1.50
5	C	8411	DMS	C1-S	2.02	1.91	1.75
5	D	8412	DMS	O-S	2.03	1.64	1.50

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	2DG	C3-C4-C5	-5.69	104.22	109.91
2	A	2001	2DG	C3-C4-C5	-4.66	105.25	109.91
2	D	2001	2DG	C3-C4-C5	-4.14	105.77	109.91
2	A	2001	2DG	O4-C4-C3	-2.41	105.64	110.02
2	B	2001	2DG	O3-C3-C2	-2.06	104.93	110.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

31 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8406	DMS	1	0
5	A	8410	DMS	1	0
5	A	8414	DMS	1	0
5	A	8420	DMS	2	0
5	A	8502	DMS	3	0
5	A	8602	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	2DG	1	0
5	B	8402	DMS	1	0
5	B	8406	DMS	1	0
5	B	8412	DMS	1	0
5	B	8415	DMS	2	0
5	B	8417	DMS	1	0
5	B	8504	DMS	1	0
5	B	8506	DMS	2	0
5	B	8601	DMS	1	0
5	C	8412	DMS	2	0
5	C	8420	DMS	2	0
5	C	8427	DMS	1	0
5	C	8503	DMS	3	0
5	C	8504	DMS	1	0
5	C	8506	DMS	4	0
5	C	8601	DMS	1	0
5	C	8602	DMS	1	0
2	D	2001	2DG	2	0
5	D	8412	DMS	4	0
5	D	8413	DMS	1	0
5	D	8416	DMS	3	0
5	D	8419	DMS	1	0
5	D	8503	DMS	2	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, 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	A	1011/1023 (98%)	-0.76	16 (1%) 72 76	5, 15, 44, 98	0
1	B	1011/1023 (98%)	-0.73	11 (1%) 80 84	5, 15, 45, 100	0
1	C	1011/1023 (98%)	-0.70	17 (1%) 70 75	6, 15, 46, 100	0
1	D	1011/1023 (98%)	-0.70	20 (1%) 65 70	4, 16, 46, 99	0
All	All	4044/4092 (98%)	-0.72	64 (1%) 72 76	4, 15, 45, 100	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	731	PRO	8.1
1	A	735	HIS	8.1
1	A	686	PRO	7.9
1	B	731	PRO	7.2
1	D	732	ALA	6.7

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	D	8703	4/4	0.89	0.20	12.90	24,53,80,80	0
5	DMS	A	8417	4/4	0.93	0.17	9.23	25,26,61,100	0
5	DMS	A	8406	4/4	0.96	0.13	9.02	7,53,55,100	0
5	DMS	C	8420	4/4	0.98	0.12	9.01	34,36,53,100	0
5	DMS	A	8407	4/4	0.95	0.13	7.94	28,40,42,43	0
5	DMS	B	8407	4/4	0.95	0.17	7.22	34,34,63,66	0
5	DMS	B	8420	4/4	0.96	0.13	6.63	36,45,63,100	0
5	DMS	B	8508	4/4	0.90	0.11	5.84	27,31,46,64	0
5	DMS	A	8504	4/4	0.98	0.10	5.55	23,35,38,100	0
5	DMS	B	8406	4/4	0.92	0.19	5.50	34,40,61,78	0
5	DMS	B	8423	4/4	0.96	0.10	5.16	28,44,71,87	0
5	DMS	C	8501	4/4	0.98	0.12	4.88	23,23,34,38	0
5	DMS	B	8408	4/4	0.94	0.17	4.33	15,25,43,60	0
5	DMS	C	8602	4/4	0.95	0.11	4.25	27,32,53,77	0
5	DMS	C	8419	4/4	0.94	0.14	4.05	33,44,54,61	0
2	2DG	B	2001	10/11	0.97	0.11	2.99	13,15,19,24	0
5	DMS	B	8405	4/4	0.99	0.11	2.60	23,28,62,71	0
5	DMS	A	8420	4/4	0.98	0.09	2.49	33,35,39,46	0
5	DMS	A	8502	4/4	0.93	0.12	2.48	14,21,75,84	0
5	DMS	B	8404	4/4	0.99	0.07	2.29	16,20,30,40	0
5	DMS	D	8408	4/4	0.99	0.10	2.10	14,27,28,36	0
4	NA	D	3103	1/1	0.91	0.11	2.10	38,38,38,38	0
5	DMS	D	8417	4/4	0.94	0.14	1.87	18,26,39,73	0
5	DMS	A	8419	4/4	0.98	0.12	1.77	24,26,55,100	0
5	DMS	B	8425	4/4	0.95	0.13	1.71	22,30,32,54	0
5	DMS	C	8407	4/4	0.98	0.11	1.71	35,39,51,52	0
5	DMS	A	8401	4/4	0.99	0.09	1.68	6,13,16,19	0
5	DMS	B	8506	4/4	0.98	0.10	1.63	31,39,63,100	0
5	DMS	C	8423	4/4	0.95	0.10	1.58	26,27,32,61	0
5	DMS	C	8405	4/4	0.99	0.09	1.53	16,23,25,38	0
5	DMS	B	8403	4/4	0.99	0.12	1.47	12,12,18,21	0
5	DMS	D	8403	4/4	0.99	0.09	1.46	21,26,27,45	0
5	DMS	C	8403	4/4	0.99	0.10	1.44	10,12,16,19	0
5	DMS	D	8701	4/4	0.98	0.09	1.38	15,17,22,37	0
5	DMS	C	8425	4/4	0.96	0.11	1.29	33,37,39,48	0
5	DMS	A	8412	4/4	0.98	0.10	1.25	24,33,37,37	0
5	DMS	A	8403	4/4	0.99	0.09	1.12	15,20,21,23	0
5	DMS	B	8502	4/4	0.96	0.09	1.09	13,30,45,50	0
5	DMS	B	8412	4/4	0.96	0.11	1.05	21,33,34,38	0
4	NA	A	3103	1/1	0.98	0.10	0.98	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	2DG	C	2001	10/11	0.97	0.08	0.97	7,15,26,27	0
5	DMS	C	8417	4/4	0.95	0.10	0.95	24,51,57,58	0
5	DMS	A	8425	4/4	0.95	0.16	0.82	34,40,45,45	0
5	DMS	C	8401	4/4	0.99	0.08	0.80	10,11,21,30	0
5	DMS	B	8504	4/4	0.98	0.10	0.74	31,37,51,52	0
5	DMS	D	8404	4/4	0.99	0.07	0.70	14,19,26,80	0
2	2DG	A	2001	10/11	0.97	0.07	0.65	10,15,18,25	0
5	DMS	D	8705	4/4	0.96	0.12	0.62	24,32,51,51	0
5	DMS	A	8408	4/4	0.99	0.08	0.55	14,23,31,82	0
5	DMS	D	8405	4/4	0.99	0.08	0.55	18,23,42,100	0
5	DMS	B	8401	4/4	0.99	0.07	0.54	13,13,21,22	0
5	DMS	D	8406	4/4	0.96	0.08	0.52	18,19,20,34	0
5	DMS	C	8408	4/4	0.97	0.09	0.51	13,35,46,83	0
2	2DG	D	2001	10/11	0.96	0.08	0.47	9,15,24,24	0
5	DMS	B	8417	4/4	0.96	0.10	0.46	26,31,34,63	0
5	DMS	D	8410	4/4	0.98	0.10	0.44	22,35,39,100	0
5	DMS	D	8501	4/4	0.97	0.09	0.37	16,34,36,46	0
5	DMS	A	8411	4/4	0.98	0.08	0.33	24,26,28,100	0
5	DMS	C	8404	4/4	0.99	0.06	0.21	11,13,21,21	0
5	DMS	D	8508	4/4	0.98	0.08	0.20	19,46,50,80	0
3	MG	B	3001	1/1	0.98	0.06	0.15	11,11,11,11	0
5	DMS	D	8412	4/4	0.98	0.10	0.10	15,25,32,33	0
5	DMS	C	8411	4/4	0.99	0.08	0.03	18,20,34,50	0
4	NA	C	3104	1/1	0.97	0.09	-0.06	26,26,26,26	0
5	DMS	B	8402	4/4	0.98	0.07	-0.13	8,21,25,29	0
5	DMS	D	8401	4/4	0.99	0.06	-0.21	10,11,20,27	0
5	DMS	A	8501	4/4	0.97	0.08	-0.21	12,13,29,33	0
5	DMS	A	8410	4/4	0.99	0.09	-0.26	28,39,55,58	0
5	DMS	D	8402	4/4	0.98	0.07	-0.27	9,23,27,32	0
4	NA	B	3104	1/1	0.96	0.09	-0.32	37,37,37,37	0
5	DMS	A	8402	4/4	0.98	0.07	-0.32	11,26,30,47	0
5	DMS	C	8412	4/4	0.99	0.07	-0.41	18,31,67,100	0
5	DMS	C	8402	4/4	0.99	0.07	-0.43	6,31,38,40	0
5	DMS	D	8419	4/4	0.98	0.07	-0.53	18,32,40,44	0
3	MG	D	3002	1/1	0.98	0.07	-0.55	19,19,19,19	0
4	NA	B	3101	1/1	0.98	0.06	-0.55	13,13,13,13	0
4	NA	A	3101	1/1	0.98	0.05	-0.65	13,13,13,13	0
5	DMS	A	8404	4/4	0.99	0.06	-0.80	9,22,22,30	0
4	NA	D	3101	1/1	0.99	0.04	-0.82	16,16,16,16	0
4	NA	B	3102	1/1	0.99	0.06	-0.84	13,13,13,13	0
4	NA	C	3103	1/1	0.97	0.06	-0.86	22,22,22,22	0
3	MG	C	3002	1/1	0.99	0.05	-0.88	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NA	A	3104	1/1	0.99	0.06	-0.96	21,21,21,21	0
5	DMS	A	8405	4/4	0.99	0.05	-1.13	11,22,25,27	0
4	NA	C	3101	1/1	0.98	0.05	-1.22	11,11,11,11	0
5	DMS	D	8411	4/4	0.99	0.05	-1.27	11,27,27,100	0
4	NA	D	3102	1/1	0.99	0.06	-1.30	18,18,18,18	0
5	DMS	B	8411	4/4	0.99	0.05	-1.38	15,17,32,100	0
4	NA	A	3102	1/1	0.99	0.04	-1.53	15,15,15,15	0
3	MG	A	3002	1/1	0.98	0.05	-1.68	14,14,14,14	0
4	NA	B	3103	1/1	0.99	0.03	-1.83	19,19,19,19	0
4	NA	C	3102	1/1	0.99	0.04	-2.03	16,16,16,16	0
3	MG	B	3002	1/1	0.99	0.04	-3.01	14,14,14,14	0
3	MG	C	3001	1/1	0.99	0.03	-4.34	12,12,12,12	0
3	MG	A	3001	1/1	0.99	0.02	-7.96	13,13,13,13	0
3	MG	D	3001	1/1	0.99	0.02	-8.37	15,15,15,15	0
5	DMS	C	8416	4/4	0.96	0.26	-	31,33,49,64	0
3	MG	A	3005	1/1	0.89	0.05	-	36,36,36,36	0
5	DMS	B	8409	4/4	0.97	0.09	-	18,32,33,38	0
5	DMS	D	8413	4/4	0.98	0.13	-	21,24,34,35	0
5	DMS	B	8410	4/4	0.98	0.09	-	18,27,41,54	0
5	DMS	D	8414	4/4	0.97	0.14	-	17,32,44,92	0
5	DMS	C	8414	4/4	0.98	0.08	-	17,18,23,39	0
5	DMS	C	8409	4/4	0.97	0.09	-	23,35,41,41	0
5	DMS	C	8504	4/4	0.98	0.08	-	32,34,42,64	0
5	DMS	A	8414	4/4	0.98	0.10	-	16,37,47,100	0
5	DMS	D	8503	4/4	0.97	0.17	-	33,53,64,100	0
5	DMS	C	8410	4/4	0.99	0.07	-	21,35,37,43	0
5	DMS	C	8413	4/4	0.95	0.15	-	31,32,34,38	0
5	DMS	C	8601	4/4	0.96	0.14	-	31,53,55,100	0
5	DMS	A	8602	4/4	0.98	0.18	-	42,45,100,100	0
5	DMS	A	8415	4/4	0.94	0.10	-	24,27,28,70	0
5	DMS	C	8503	4/4	0.96	0.19	-	20,31,54,100	0
5	DMS	C	8506	4/4	0.96	0.10	-	15,24,47,89	0
5	DMS	C	8415	4/4	0.95	0.11	-	20,26,33,52	0
5	DMS	B	8421	4/4	0.97	0.10	-	14,46,60,85	0
5	DMS	D	8421	4/4	0.97	0.12	-	36,45,48,52	0
5	DMS	B	8415	4/4	0.94	0.12	-	22,26,33,67	0
5	DMS	B	8601	4/4	0.97	0.12	-	36,60,100,100	0
5	DMS	A	8413	4/4	0.97	0.12	-	34,34,53,100	0
5	DMS	C	8427	4/4	0.98	0.15	-	37,43,81,82	0
5	DMS	B	8414	4/4	0.97	0.14	-	24,43,49,100	0
5	DMS	D	8416	4/4	0.97	0.21	-	16,34,42,89	0
5	DMS	D	8409	4/4	0.96	0.08	-	25,30,39,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	B	8416	4/4	0.97	0.12	-	35,42,52,88	0
3	MG	D	3005	1/1	0.97	0.05	-	43,43,43,43	0
5	DMS	B	8427	4/4	0.93	0.10	-	28,31,42,65	0
5	DMS	A	8503	4/4	0.97	0.20	-	42,47,48,100	0
5	DMS	A	8421	4/4	0.95	0.19	-	42,43,67,100	0
5	DMS	B	8413	4/4	0.93	0.15	-	22,32,35,42	0
5	DMS	C	8421	4/4	0.98	0.11	-	26,26,41,64	0
5	DMS	A	8409	4/4	0.96	0.11	-	24,27,39,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.