



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 17, 2021 – 06:16 AM EDT

PDB ID : 1JZ8
Title : E. COLI (lacZ) BETA-GALACTOSIDASE (E537Q) IN COMPLEX WITH ALLOLACTOSE
Authors : Juers, D.H.; Matthews, B.W.
Deposited on : 2001-09-13
Resolution : 1.50 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 : 2.23.2
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) : 2.23.2

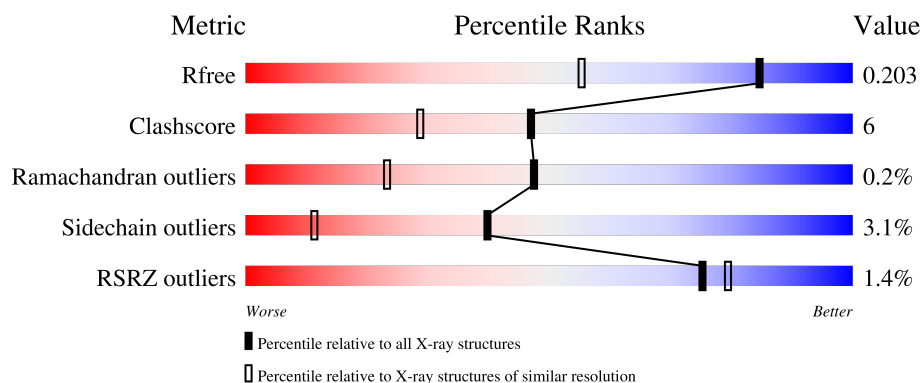
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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.




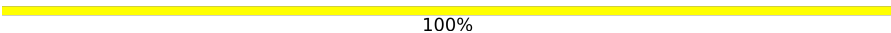

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	A	1023	<div> <div>0%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>..</div> </div> </div>
1	B	1023	<div> <div>0%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>..</div> </div> </div>
1	C	1023	<div> <div>0%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>..</div> </div> </div>
1	D	1023	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>..</div> </div> </div>
2	E	2	<div> <div></div> <div>100%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	2	 50% 50%
2	G	2	 100%
2	H	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BGC	F	1[A]	X	-	-	-
5	DMS	A	8413	-	X	-	-
5	DMS	A	8425	-	X	-	-
5	DMS	A	8502	-	X	-	-
5	DMS	B	8415	-	-	X	-
5	DMS	B	8418	-	-	X	-
5	DMS	B	8501	-	-	X	-
5	DMS	C	8418	-	-	X	-
5	DMS	D	8701	-	X	-	-
5	DMS	D	8705	-	-	X	-
6	BGC	B	2002[B]	X	-	-	-
7	TAR	B	2003[C]	X	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 37685 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-Galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	B	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	C	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	D	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			

There are 36 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-6)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	1	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mg	0	0
			4	4		
3	B	3	Total	Mg	0	0
			3	3		
3	C	5	Total	Mg	0	0
			5	5		

Continued on next page...

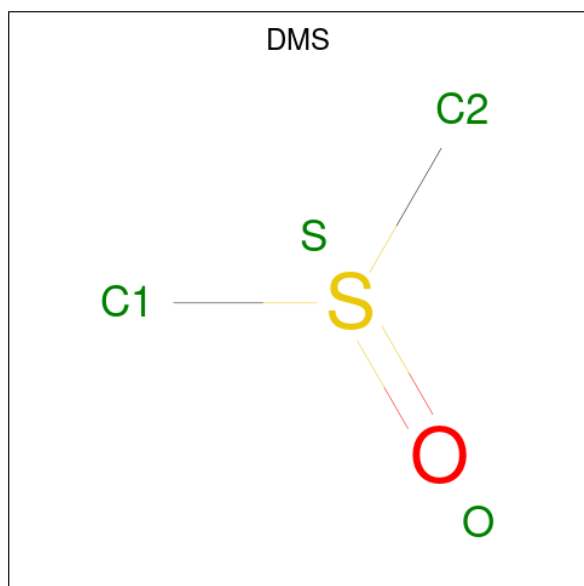
Continued from previous page...

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

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

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

Continued on next page...

[illegible]

Continued on next page...

Continued from previous page...

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	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

Continued on next page...

Continued from previous page...

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	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	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

Continued on next page...

[illegible]

Continued on next page...

Continued from previous page...

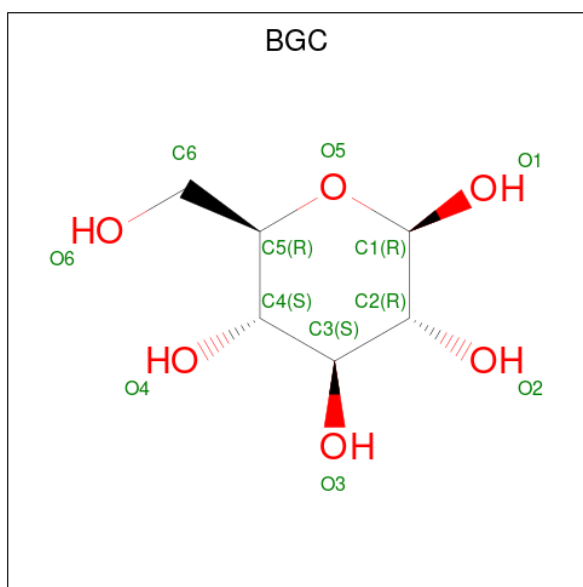
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2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

Continued on next page...

Continued from previous page...

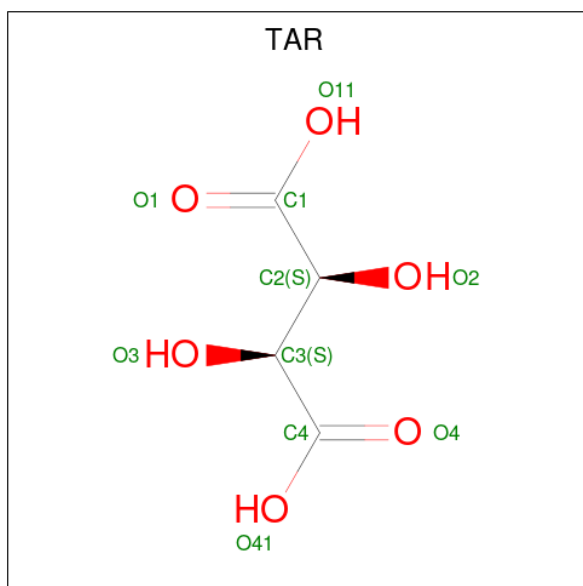
[illegible]

- Molecule 6 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	1
			9	4	5		

- Molecule 7 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	1
			9	4	5		

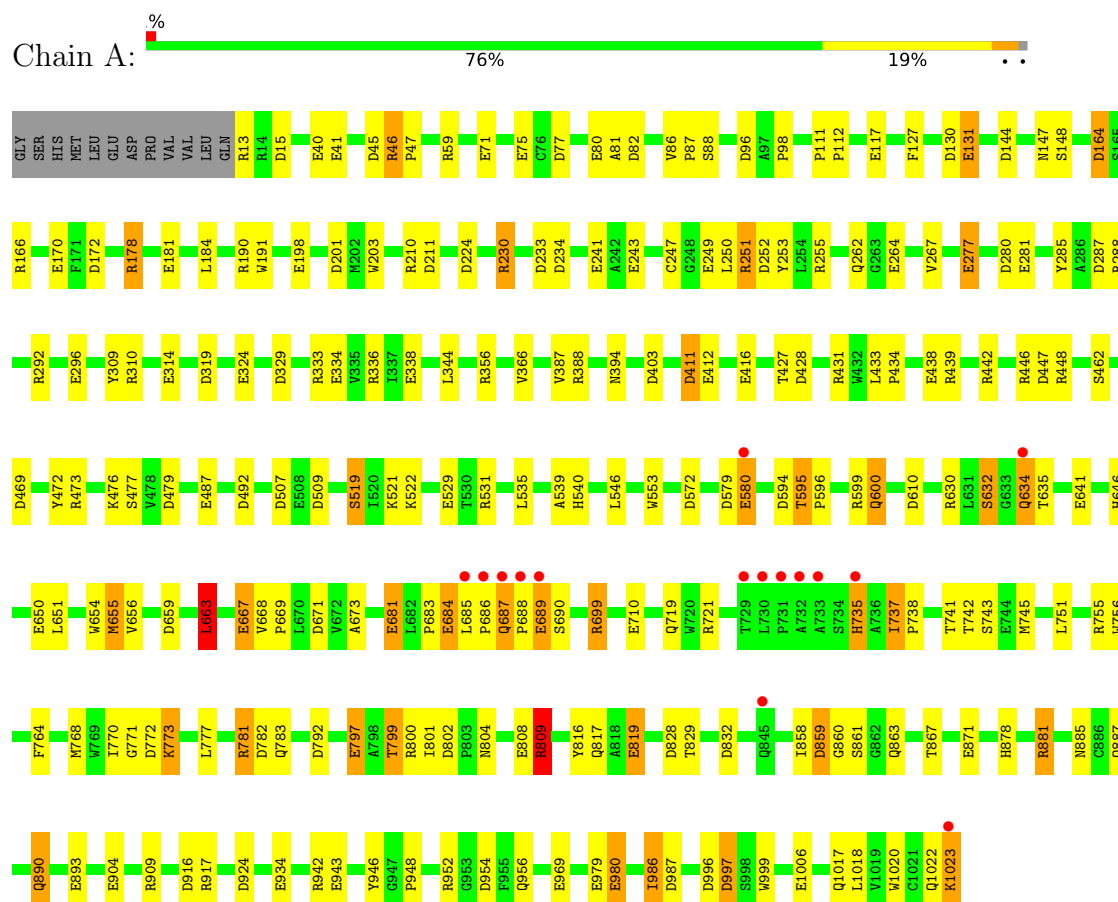
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1144	Total 1144	O 1144	0	0
8	B	1148	Total 1148	O 1148	0	0
8	C	1126	Total 1126	O 1126	0	0
8	D	1105	Total 1105	O 1105	0	0

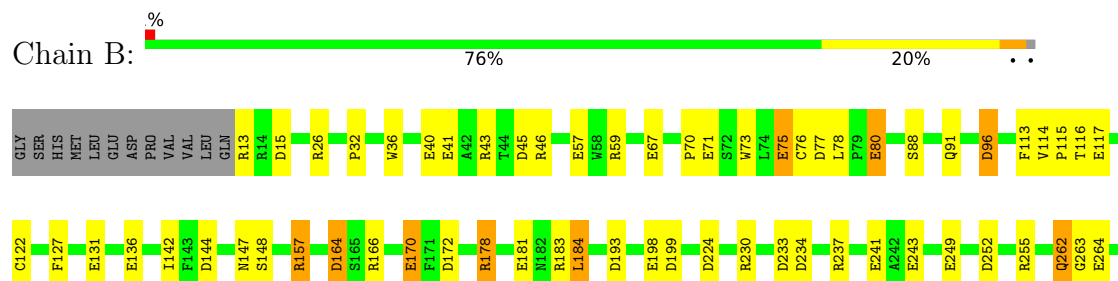
3 Residue-property plots

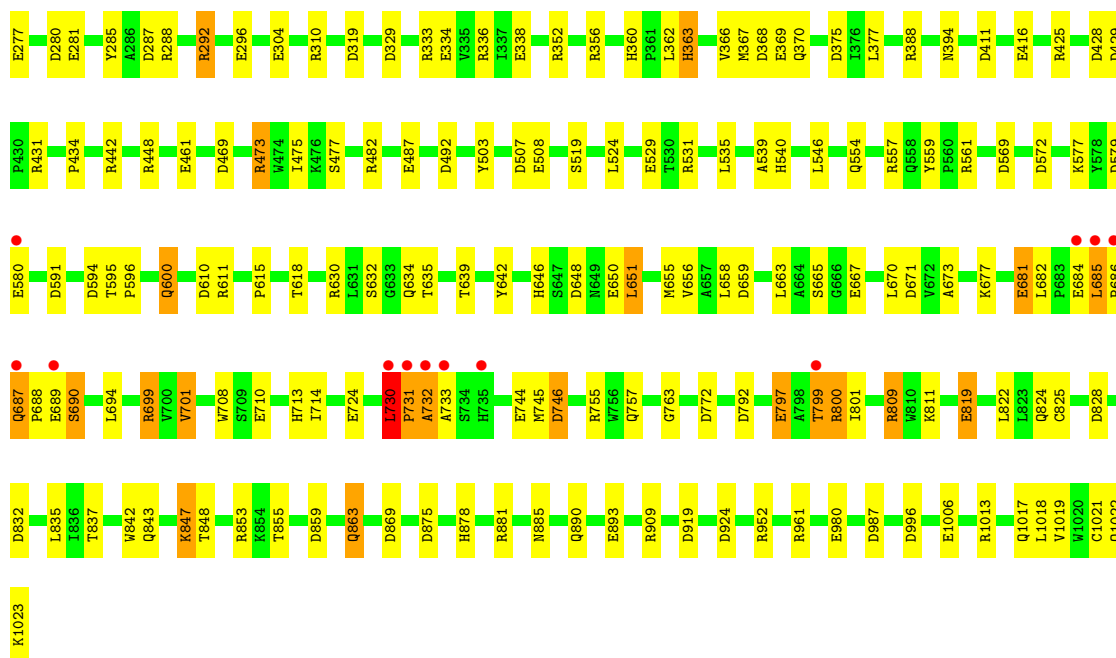
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Beta-Galactosidase

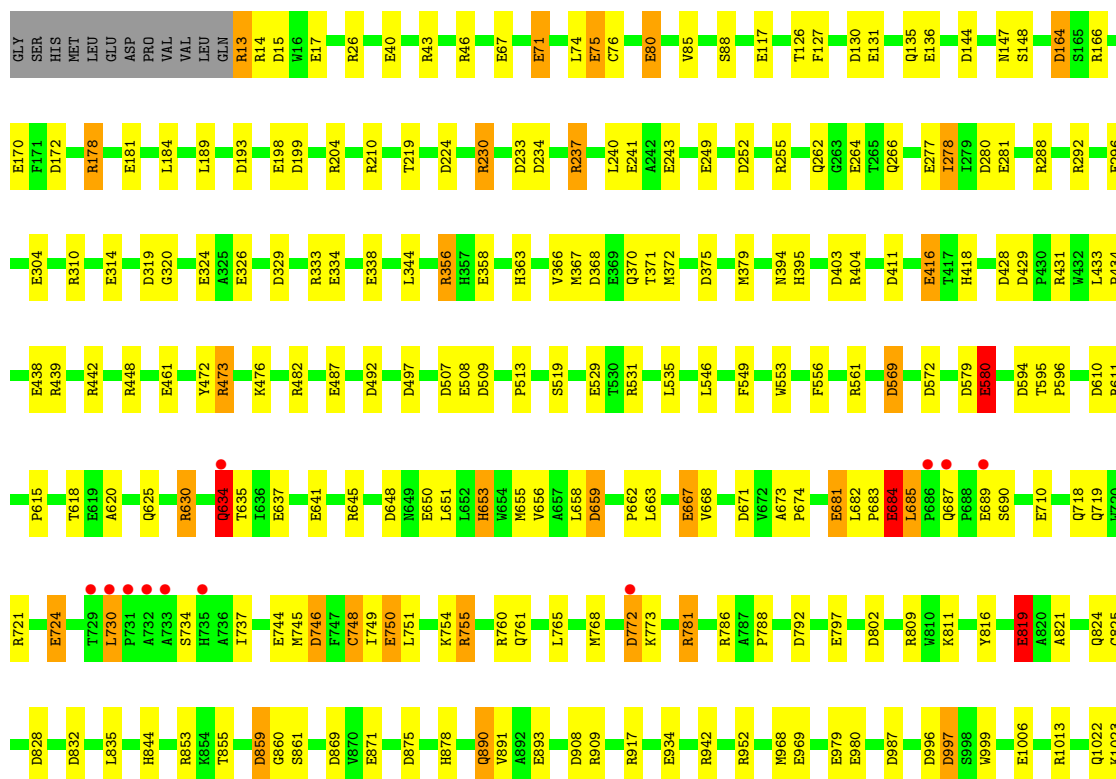
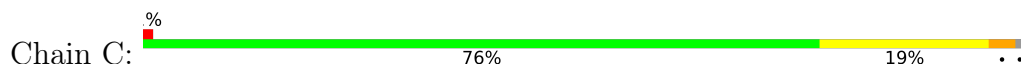


• Molecule 1: Beta-Galactosidase

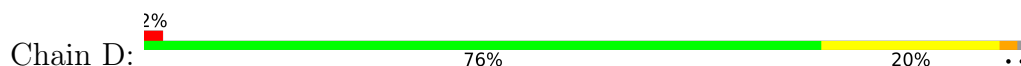


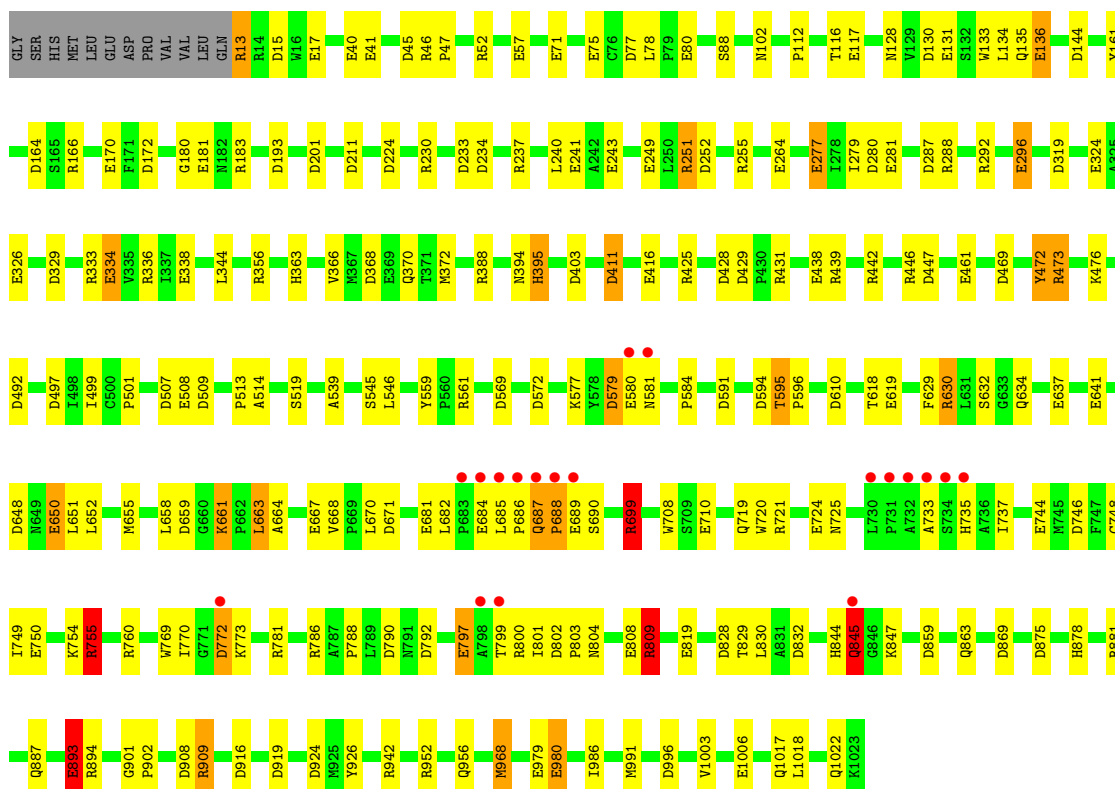


• Molecule 1: Beta-Galactosidase



• Molecule 1: Beta-Galactosidase





- Molecule 2: beta-D-galactopyranose-(1-6)-beta-D-glucopyranose

Chain E: 100%



- Molecule 2: beta-D-galactopyranose-(1-6)-beta-D-glucopyranose

Chain F: 50% 50%



- Molecule 2: beta-D-galactopyranose-(1-6)-beta-D-glucopyranose

Chain G:  100%



- Molecule 2: beta-D-galactopyranose-(1-6)-beta-D-glucopyranose

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.39Å 168.71Å 200.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 1.50 18.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.2 (18.00-1.50) 97.8 (18.00-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 1.51Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.165 , 0.208 0.162 , 0.203	Depositor DCC
R_{free} test set	11385 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 82.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	37685	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.54 % 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 5.7464e-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 ⓘ

5.1 Standard geometry ⓘ

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

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	1.19	52/8383 (0.6%)	1.53	143/11437 (1.3%)
1	B	1.21	46/8383 (0.5%)	1.51	154/11437 (1.3%)
1	C	1.21	52/8383 (0.6%)	1.54	152/11437 (1.3%)
1	D	1.21	51/8383 (0.6%)	1.50	146/11437 (1.3%)
All	All	1.20	201/33532 (0.6%)	1.52	595/45748 (1.3%)

The worst 5 of 201 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	893	GLU	CD-OE2	11.37	1.38	1.25
1	D	71	GLU	CD-OE2	10.62	1.37	1.25
1	A	296	GLU	CD-OE2	10.38	1.37	1.25
1	C	684	GLU	CD-OE2	9.95	1.36	1.25
1	C	80	GLU	CD-OE2	9.65	1.36	1.25

The worst 5 of 595 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	630	ARG	NE-CZ-NH1	26.47	133.53	120.30
1	C	442	ARG	NE-CZ-NH2	-17.31	111.64	120.30
1	A	431	ARG	NE-CZ-NH2	-17.25	111.67	120.30
1	D	473	ARG	NE-CZ-NH1	13.79	127.19	120.30
1	A	442	ARG	NE-CZ-NH2	-12.96	113.82	120.30

There are no chirality outliers.

There are no planarity outliers.

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	A	8128	0	7712	98	0
1	B	8128	0	7712	96	0
1	C	8128	0	7712	98	0
1	D	8128	0	7712	80	0
2	E	23	0	20	0	0
2	F	23	0	14	0	0
2	G	23	0	20	0	0
2	H	23	0	20	1	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	5	0	0	0	0
3	D	4	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	120	0	180	12	0
5	B	128	0	192	22	0
5	C	128	0	192	14	0
5	D	132	0	195	20	0
6	B	9	0	5	3	0
7	B	9	0	5	9	0
8	A	1144	0	0	11	0
8	B	1148	0	0	13	0
8	C	1126	0	0	14	0
8	D	1105	0	0	12	0
All	All	37685	0	31691	404	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 404 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:8403:DMS:C2	5:A:8403:DMS:S	2.02	1.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:8423:DMS:S	5:D:8423:DMS:C1	2.01	1.47
5:C:8415:DMS:S	5:C:8415:DMS:C2	2.01	1.46
5:B:8407:DMS:C2	5:B:8407:DMS:S	2.05	1.45
5:B:8601:DMS:C2	5:B:8601:DMS:S	2.04	1.44

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	A	1011/1023 (99%)	977 (97%)	33 (3%)	1 (0%)	51	25
1	B	1011/1023 (99%)	976 (96%)	31 (3%)	4 (0%)	34	13
1	C	1011/1023 (99%)	979 (97%)	31 (3%)	1 (0%)	51	25
1	D	1011/1023 (99%)	978 (97%)	29 (3%)	4 (0%)	34	13
All	All	4044/4092 (99%)	3910 (97%)	124 (3%)	10 (0%)	47	23

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	731	PRO
1	B	732	ALA
1	B	690	SER
1	D	688	PRO
1	D	539[A]	ALA

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	A	865/875 (99%)	836 (97%)	29 (3%)	37	9
1	B	865/875 (99%)	844 (98%)	21 (2%)	49	19
1	C	865/875 (99%)	835 (96%)	30 (4%)	36	9
1	D	865/875 (99%)	837 (97%)	28 (3%)	39	10
All	All	3460/3500 (99%)	3352 (97%)	108 (3%)	40	11

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	333	ARG
1	C	687	GLN
1	D	773	LYS
1	C	370	GLN
1	C	634	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	878	HIS
1	D	878	HIS
1	C	977	HIS
1	D	624	GLN
1	D	977	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 ⓘ

8 monosaccharides are modelled in this entry.

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	BGC	E	1	2	12,12,12	0.82	0	17,17,17	1.10	2 (11%)
2	GAL	E	2	4,2	11,11,12	1.66	3 (27%)	15,15,17	1.52	4 (26%)
2	GAL	F	2	4,2	11,11,12	1.52	2 (18%)	15,15,17	1.57	4 (26%)
2	BGC	G	1	2	12,12,12	1.19	1 (8%)	17,17,17	1.34	2 (11%)
2	GAL	G	2	4,2	11,11,12	1.61	2 (18%)	15,15,17	1.19	2 (13%)
2	BGC	H	1	2	12,12,12	1.15	1 (8%)	17,17,17	0.86	0
2	GAL	H	2	4,2	11,11,12	1.60	3 (27%)	15,15,17	1.20	1 (6%)

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	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	GAL	E	2	4,2	-	1/2/19/22	0/1/1/1
2	BGC	F	1[A]	-	1/1/5/5	-	-
2	GAL	F	2	4,2	-	1/2/19/22	0/1/1/1
2	BGC	G	1	2	-	2/2/22/22	0/1/1/1
2	GAL	G	2	4,2	-	1/2/19/22	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	GAL	H	2	4,2	-	1/2/19/22	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	GAL	O4-C4	3.47	1.51	1.43
2	H	2	GAL	O4-C4	3.37	1.50	1.43
2	E	2	GAL	O4-C4	3.27	1.50	1.43
2	G	2	GAL	O4-C4	3.04	1.50	1.43
2	G	1	BGC	O2-C2	2.77	1.49	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	GAL	O2-C2-C1	-3.38	102.24	109.15
2	E	2	GAL	O3-C3-C2	-3.19	103.88	109.99
2	H	2	GAL	O2-C2-C1	-3.08	102.85	109.15
2	F	2	GAL	O3-C3-C2	-3.00	104.24	109.99
2	G	2	GAL	O2-C2-C1	-2.93	103.16	109.15

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	1[A]	BGC	C2

5 of 6 torsion outliers are listed below:

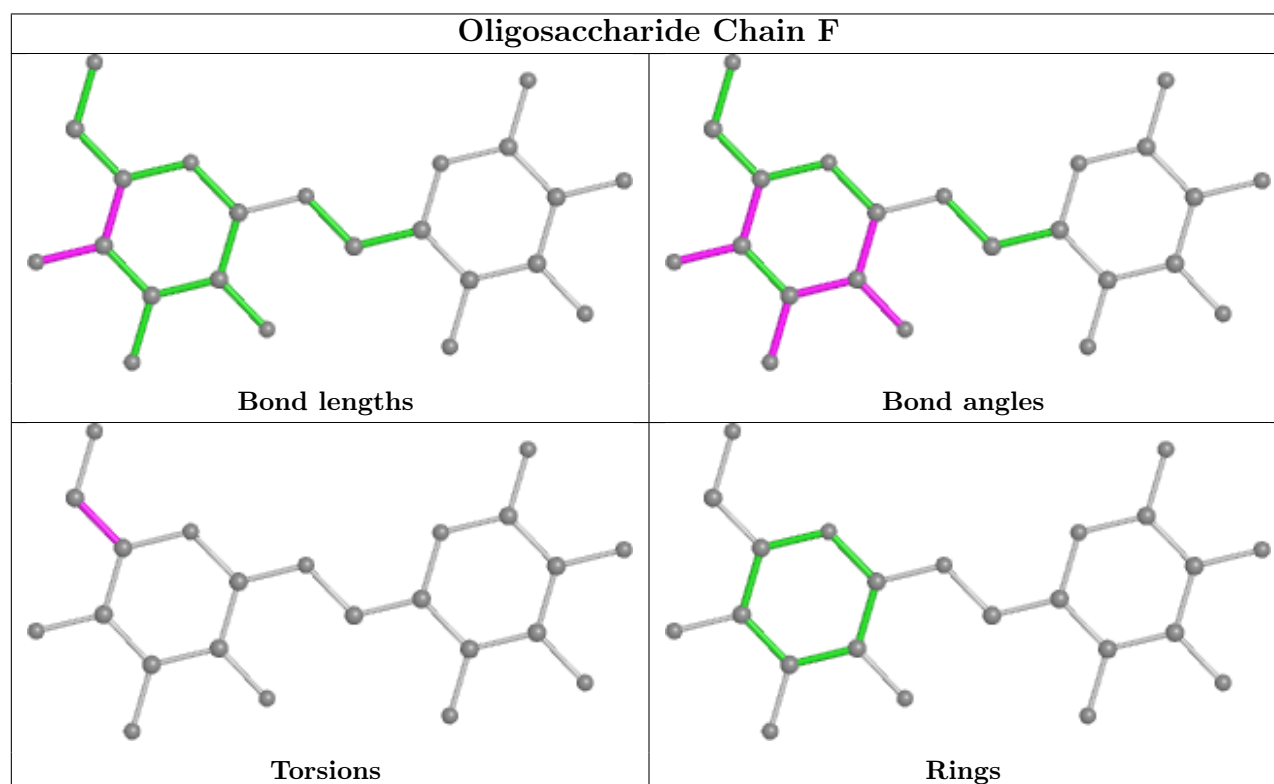
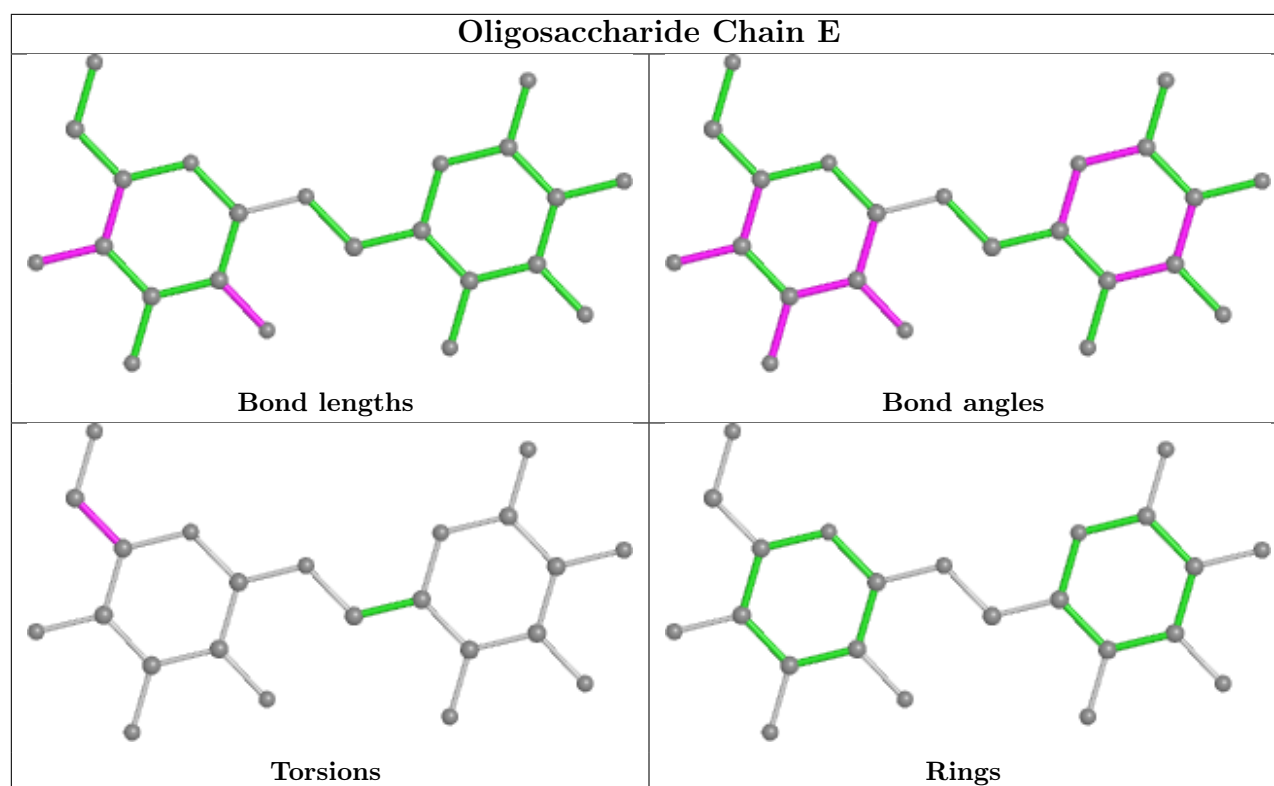
Mol	Chain	Res	Type	Atoms
2	E	2	GAL	O5-C5-C6-O6
2	G	2	GAL	O5-C5-C6-O6
2	H	2	GAL	O5-C5-C6-O6
2	G	1	BGC	C4-C5-C6-O6
2	F	2	GAL	O5-C5-C6-O6

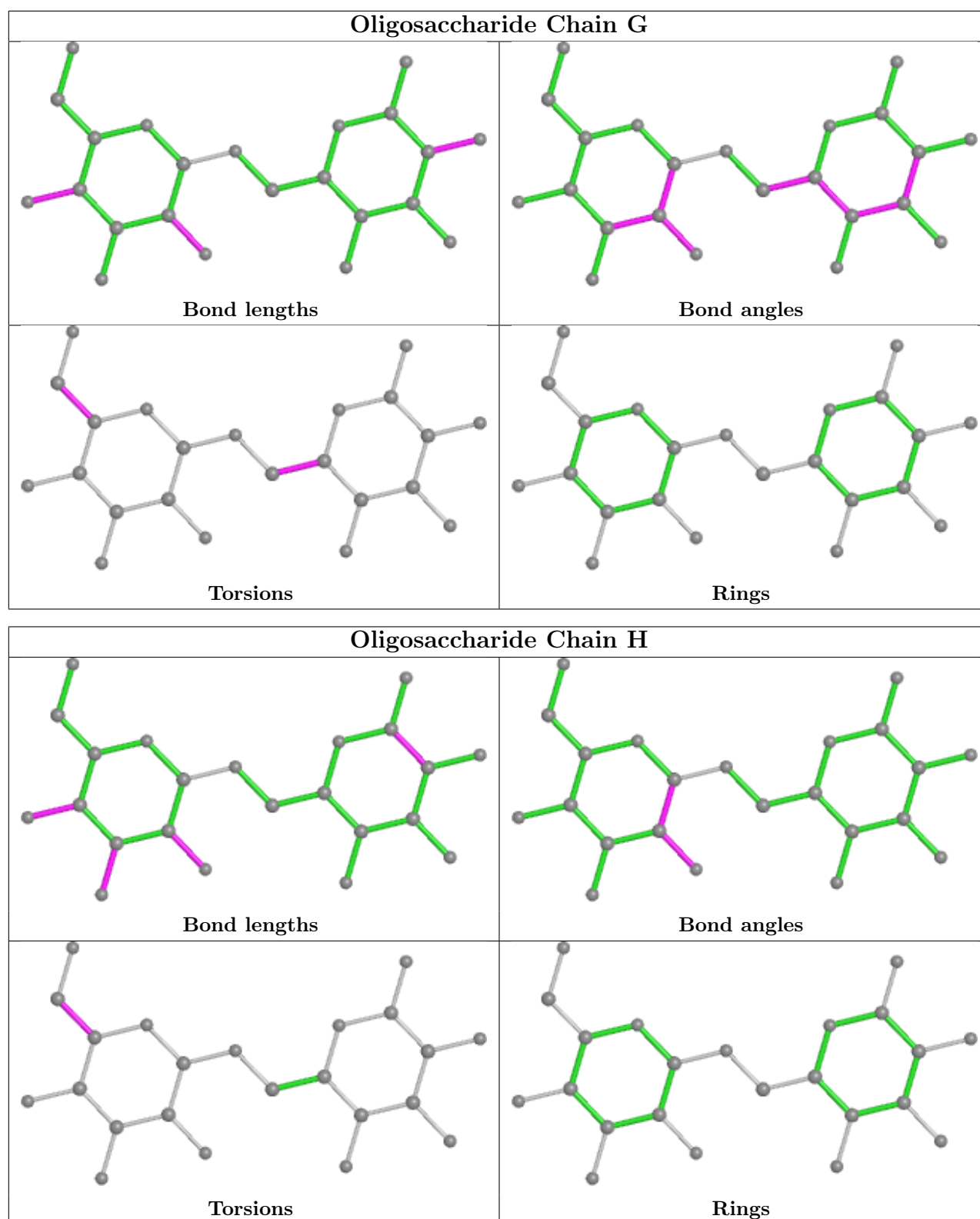
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	GAL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

Of 161 ligands modelled in this entry, 32 are monoatomic - leaving 129 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	A	8406	-	3,3,3	0.93	0	3,3,3	0.88	0
5	DMS	B	8502	-	3,3,3	1.20	0	3,3,3	2.05	1 (33%)
5	DMS	A	8423	-	3,3,3	2.05	2 (66%)	3,3,3	0.46	0
5	DMS	D	8412	-	3,3,3	0.82	0	3,3,3	0.60	0
5	DMS	D	8414	-	3,3,3	0.44	0	3,3,3	0.29	0
5	DMS	B	8428	-	3,3,3	1.59	1 (33%)	3,3,3	0.34	0
5	DMS	D	8508	-	3,3,3	1.77	1 (33%)	3,3,3	0.81	0
5	DMS	B	8402	-	3,3,3	1.95	2 (66%)	3,3,3	0.53	0
5	DMS	C	8406	-	3,3,3	0.77	0	3,3,3	0.19	0
5	DMS	C	8421	-	3,3,3	1.21	0	3,3,3	1.16	0
5	DMS	C	8424	-	3,3,3	1.16	0	3,3,3	0.59	0
5	DMS	B	8415	-	3,3,3	2.81	2 (66%)	3,3,3	1.03	0
7	TAR	B	2003[C]	-	5,8,9	1.52	1 (20%)	6,10,12	1.51	1 (16%)
5	DMS	A	8403	-	3,3,3	2.33	1 (33%)	3,3,3	0.56	0
5	DMS	B	8410	-	3,3,3	1.73	1 (33%)	3,3,3	0.28	0
5	DMS	D	8506	-	3,3,3	1.56	1 (33%)	3,3,3	0.47	0
5	DMS	B	8420	-	3,3,3	1.74	1 (33%)	3,3,3	0.47	0
5	DMS	C	8414	-	3,3,3	1.30	0	3,3,3	0.93	0
5	DMS	B	8601	-	3,3,3	2.30	1 (33%)	3,3,3	0.92	0
5	DMS	C	8412	-	3,3,3	1.69	1 (33%)	3,3,3	0.46	0
5	DMS	D	8417	-	3,3,3	1.55	1 (33%)	3,3,3	0.69	0
5	DMS	C	8429	-	3,3,3	1.40	1 (33%)	3,3,3	0.33	0
5	DMS	C	8501	-	3,3,3	1.13	0	3,3,3	1.18	0
5	DMS	B	8706	-	3,3,3	1.74	1 (33%)	3,3,3	0.42	0
5	DMS	A	8407	-	3,3,3	2.42	1 (33%)	3,3,3	1.23	1 (33%)
5	DMS	D	8428	-	3,3,3	1.19	0	3,3,3	0.40	0
5	DMS	A	8504	-	3,3,3	1.38	1 (33%)	3,3,3	0.35	0
5	DMS	C	8417	-	3,3,3	0.79	0	3,3,3	0.98	0
5	DMS	A	8418	-	3,3,3	1.04	0	3,3,3	0.35	0
5	DMS	A	8401	-	3,3,3	0.79	0	3,3,3	0.42	0
5	DMS	C	8504	-	3,3,3	1.22	0	3,3,3	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	D	8413	-	3,3,3	1.77	1 (33%)	3,3,3	0.50	0
5	DMS	B	8508	-	3,3,3	3.27	2 (66%)	3,3,3	0.71	0
5	DMS	C	8405	-	3,3,3	1.80	2 (66%)	3,3,3	0.63	0
5	DMS	D	8410	-	3,3,3	1.17	0	3,3,3	0.18	0
5	DMS	B	8413	-	3,3,3	3.00	2 (66%)	3,3,3	0.57	0
5	DMS	A	8424	-	3,3,3	1.28	0	3,3,3	0.35	0
5	DMS	A	8413	-	3,3,3	2.59	3 (100%)	3,3,3	0.68	0
5	DMS	D	8416	-	3,3,3	0.79	0	3,3,3	0.29	0
5	DMS	B	8412	-	3,3,3	0.81	0	3,3,3	0.26	0
5	DMS	A	8425	4	3,3,3	2.59	3 (100%)	3,3,3	1.05	0
5	DMS	A	8412	-	3,3,3	0.81	0	3,3,3	0.38	0
5	DMS	B	8504	-	3,3,3	0.46	0	3,3,3	0.31	0
5	DMS	B	8417	-	3,3,3	1.31	0	3,3,3	0.36	0
5	DMS	A	8503	-	3,3,3	1.09	0	3,3,3	1.19	1 (33%)
5	DMS	A	8402	-	3,3,3	1.78	1 (33%)	3,3,3	0.29	0
5	DMS	A	8421	-	3,3,3	1.19	0	3,3,3	0.87	0
5	DMS	D	8419	-	3,3,3	0.44	0	3,3,3	0.14	0
5	DMS	C	8413	-	3,3,3	2.14	1 (33%)	3,3,3	0.55	0
5	DMS	C	8410	-	3,3,3	1.21	0	3,3,3	0.25	0
5	DMS	C	8601	-	3,3,3	1.14	0	3,3,3	1.04	0
5	DMS	A	8502	-	3,3,3	2.29	2 (66%)	3,3,3	1.52	1 (33%)
5	DMS	A	8602	-	3,3,3	1.14	0	3,3,3	0.43	0
5	DMS	D	8404	-	3,3,3	1.42	1 (33%)	3,3,3	0.16	0
5	DMS	C	8506	-	3,3,3	1.11	0	3,3,3	0.57	0
5	DMS	D	8429	-	3,3,3	2.42	1 (33%)	3,3,3	0.37	0
5	DMS	B	8501	-	3,3,3	1.02	0	3,3,3	0.27	0
5	DMS	B	8416	-	3,3,3	1.16	0	3,3,3	0.35	0
5	DMS	C	8409	-	3,3,3	2.40	1 (33%)	3,3,3	0.70	0
5	DMS	A	8428	-	3,3,3	1.28	1 (33%)	3,3,3	0.38	0
5	DMS	C	8508	-	3,3,3	2.57	1 (33%)	3,3,3	0.53	0
5	DMS	D	8424	-	3,3,3	1.32	0	3,3,3	0.17	0
5	DMS	C	8419	-	3,3,3	0.88	0	3,3,3	0.22	0
5	DMS	D	8408	-	3,3,3	1.52	0	3,3,3	0.13	0
5	DMS	D	8705	-	3,3,3	3.07	1 (33%)	3,3,3	1.64	1 (33%)
5	DMS	D	8411	-	3,3,3	0.74	0	3,3,3	0.10	0
5	DMS	A	8405	-	3,3,3	1.32	1 (33%)	3,3,3	0.72	0
5	DMS	D	8503	-	3,3,3	0.87	0	3,3,3	0.61	0
5	DMS	C	8402	-	3,3,3	1.93	1 (33%)	3,3,3	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	8425	4	3,3,3	1.64	1 (33%)	3,3,3	0.36	0
5	DMS	B	8425	4	3,3,3	2.37	2 (66%)	3,3,3	0.30	0
5	DMS	D	8403	-	3,3,3	1.36	0	3,3,3	0.46	0
5	DMS	C	8418	-	3,3,3	2.06	1 (33%)	3,3,3	1.43	1 (33%)
5	DMS	B	8418	-	3,3,3	0.76	0	3,3,3	0.53	0
5	DMS	B	8429	-	3,3,3	2.55	2 (66%)	3,3,3	0.77	0
5	DMS	D	8701	-	3,3,3	2.44	3 (100%)	3,3,3	0.71	0
5	DMS	D	8407	-	3,3,3	2.89	2 (66%)	3,3,3	0.34	0
5	DMS	B	8424	-	3,3,3	1.00	0	3,3,3	0.13	0
5	DMS	B	8419	-	3,3,3	1.34	0	3,3,3	0.26	0
5	DMS	D	8704	-	3,3,3	2.31	1 (33%)	3,3,3	0.57	0
5	DMS	C	8407	-	3,3,3	1.75	1 (33%)	3,3,3	0.45	0
5	DMS	A	8419	-	3,3,3	0.98	0	3,3,3	0.57	0
5	DMS	D	8425	4	3,3,3	1.41	1 (33%)	3,3,3	1.17	1 (33%)
5	DMS	C	8403	-	3,3,3	1.25	0	3,3,3	0.50	0
5	DMS	A	8506	-	3,3,3	2.39	2 (66%)	3,3,3	0.41	0
5	DMS	B	8404	-	3,3,3	1.29	0	3,3,3	0.23	0
5	DMS	D	8405	-	3,3,3	0.95	0	3,3,3	0.51	0
5	DMS	A	8409	-	3,3,3	2.75	1 (33%)	3,3,3	0.90	0
5	DMS	C	8401	-	3,3,3	1.09	0	3,3,3	0.38	0
5	DMS	A	8414	-	3,3,3	1.89	1 (33%)	3,3,3	0.21	0
5	DMS	B	8403	-	3,3,3	1.60	0	3,3,3	0.41	0
5	DMS	C	8503	-	3,3,3	0.96	0	3,3,3	0.78	0
5	DMS	C	8423	-	3,3,3	1.09	0	3,3,3	0.39	0
5	DMS	D	8421	-	3,3,3	0.92	0	3,3,3	0.35	0
5	DMS	B	8411	-	3,3,3	1.10	0	3,3,3	0.42	0
6	BGC	B	2002[B]	-	8,8,12	1.10	0	8,10,17	1.41	1 (12%)
5	DMS	D	8423	-	3,3,3	2.52	2 (66%)	3,3,3	0.41	0
5	DMS	A	8411	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	D	8418	-	3,3,3	1.41	0	3,3,3	0.92	0
5	DMS	A	8408	-	3,3,3	0.28	0	3,3,3	0.74	0
5	DMS	B	8401	-	3,3,3	0.89	0	3,3,3	0.39	0
5	DMS	D	8501	-	3,3,3	0.97	0	3,3,3	0.08	0
5	DMS	D	8703	-	3,3,3	1.39	0	3,3,3	0.14	0
5	DMS	A	8416	-	3,3,3	2.39	1 (33%)	3,3,3	0.42	0
5	DMS	C	8602	-	3,3,3	1.33	1 (33%)	3,3,3	0.17	0
5	DMS	B	8405	-	3,3,3	1.48	1 (33%)	3,3,3	0.55	0
5	DMS	D	8409	-	3,3,3	2.48	1 (33%)	3,3,3	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	D	8420	-	3,3,3	2.47	1 (33%)	3,3,3	0.31	0
5	DMS	A	8501	-	3,3,3	1.43	1 (33%)	3,3,3	0.58	0
5	DMS	C	8416	-	3,3,3	2.16	2 (66%)	3,3,3	0.57	0
5	DMS	C	8408	-	3,3,3	0.90	0	3,3,3	0.72	0
5	DMS	C	8415	-	3,3,3	2.64	2 (66%)	3,3,3	0.94	0
5	DMS	A	8417	-	3,3,3	1.51	1 (33%)	3,3,3	0.61	0
5	DMS	C	8404	-	3,3,3	0.93	0	3,3,3	0.76	0
5	DMS	B	8407	-	3,3,3	2.95	2 (66%)	3,3,3	0.26	0
5	DMS	B	8506	-	3,3,3	1.67	1 (33%)	3,3,3	0.45	0
5	DMS	A	8420	-	3,3,3	1.27	0	3,3,3	0.85	0
5	DMS	D	8402	-	3,3,3	1.27	0	3,3,3	0.29	0
5	DMS	C	8411	-	3,3,3	1.02	0	3,3,3	0.37	0
5	DMS	B	8421	-	3,3,3	0.33	0	3,3,3	0.30	0
5	DMS	D	8401	-	3,3,3	1.24	0	3,3,3	0.43	0
5	DMS	B	8423	-	3,3,3	0.74	0	3,3,3	0.64	0
5	DMS	C	8420	-	3,3,3	2.49	1 (33%)	3,3,3	0.91	0
5	DMS	A	8404	-	3,3,3	1.31	1 (33%)	3,3,3	0.22	0
5	DMS	B	8414	-	3,3,3	0.58	0	3,3,3	1.03	0
5	DMS	D	8406	-	3,3,3	1.10	0	3,3,3	0.60	0
5	DMS	A	8410	-	3,3,3	1.15	0	3,3,3	0.67	0
5	DMS	B	8408	-	3,3,3	0.89	0	3,3,3	0.15	0
5	DMS	B	8409	-	3,3,3	2.33	1 (33%)	3,3,3	0.42	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
6	BGC	B	2002[B]	-	1/1/3/5	10/10/10/22	-
7	TAR	B	2003[C]	-	1/1/3/4	4/6/10/12	-

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	8705	DMS	C1-S	-5.23	1.37	1.75
5	B	8508	DMS	C1-S	4.74	2.11	1.75
5	A	8409	DMS	O-S	4.49	1.80	1.50
5	C	8508	DMS	O-S	4.40	1.80	1.50
5	B	8413	DMS	O-S	4.26	1.79	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	8502	DMS	C2-S-C1	3.53	116.60	98.44
5	D	8705	DMS	C2-S-C1	-2.83	83.86	98.44
5	A	8502	DMS	C2-S-C1	2.62	111.93	98.44
5	C	8418	DMS	C2-S-C1	-2.48	85.69	98.44
7	B	2003[C]	TAR	C4-C3-C2	2.43	116.17	111.95

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	2002[B]	BGC	C2
7	B	2003[C]	TAR	C3

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	2002[B]	BGC	C1-C2-C3-C4
6	B	2002[B]	BGC	C1-C2-C3-O3
6	B	2002[B]	BGC	O2-C2-C3-O3
6	B	2002[B]	BGC	C2-C3-C4-O4
7	B	2003[C]	TAR	O2-C2-C3-C4

There are no ring outliers.

38 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	8412	DMS	2	0
5	B	8428	DMS	1	0
5	C	8406	DMS	2	0
5	C	8424	DMS	2	0
5	B	8415	DMS	4	0
7	B	2003[C]	TAR	9	0
5	A	8403	DMS	1	0
5	D	8506	DMS	1	0
5	B	8601	DMS	1	0
5	D	8428	DMS	1	0
5	A	8418	DMS	2	0
5	B	8508	DMS	1	0
5	B	8412	DMS	1	0
5	A	8412	DMS	3	0
5	C	8413	DMS	1	0
5	A	8502	DMS	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	8429	DMS	2	0
5	B	8501	DMS	6	0
5	A	8428	DMS	1	0
5	D	8705	DMS	5	0
5	D	8503	DMS	1	0
5	D	8403	DMS	1	0
5	C	8418	DMS	5	0
5	B	8418	DMS	4	0
5	B	8424	DMS	1	0
5	D	8704	DMS	1	0
5	C	8503	DMS	1	0
6	B	2002[B]	BGC	3	0
5	D	8423	DMS	2	0
5	D	8418	DMS	2	0
5	D	8703	DMS	2	0
5	A	8416	DMS	3	0
5	C	8602	DMS	1	0
5	C	8415	DMS	1	0
5	B	8407	DMS	2	0
5	A	8420	DMS	1	0
5	B	8423	DMS	1	0
5	C	8420	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%)	-0.71	15 (1%) 73 78	7, 12, 42, 100	0
1	B	1011/1023 (98%)	-0.73	12 (1%) 79 82	6, 12, 39, 100	0
1	C	1011/1023 (98%)	-0.68	11 (1%) 80 84	6, 13, 43, 100	0
1	D	1011/1023 (98%)	-0.66	19 (1%) 66 71	6, 13, 44, 98	0
All	All	4044/4092 (98%)	-0.70	57 (1%) 75 79	6, 13, 43, 100	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	686	PRO	9.9
1	A	735	HIS	8.9
1	C	732	ALA	8.1
1	D	732	ALA	7.6
1	C	730	LEU	7.5

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](#)

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.

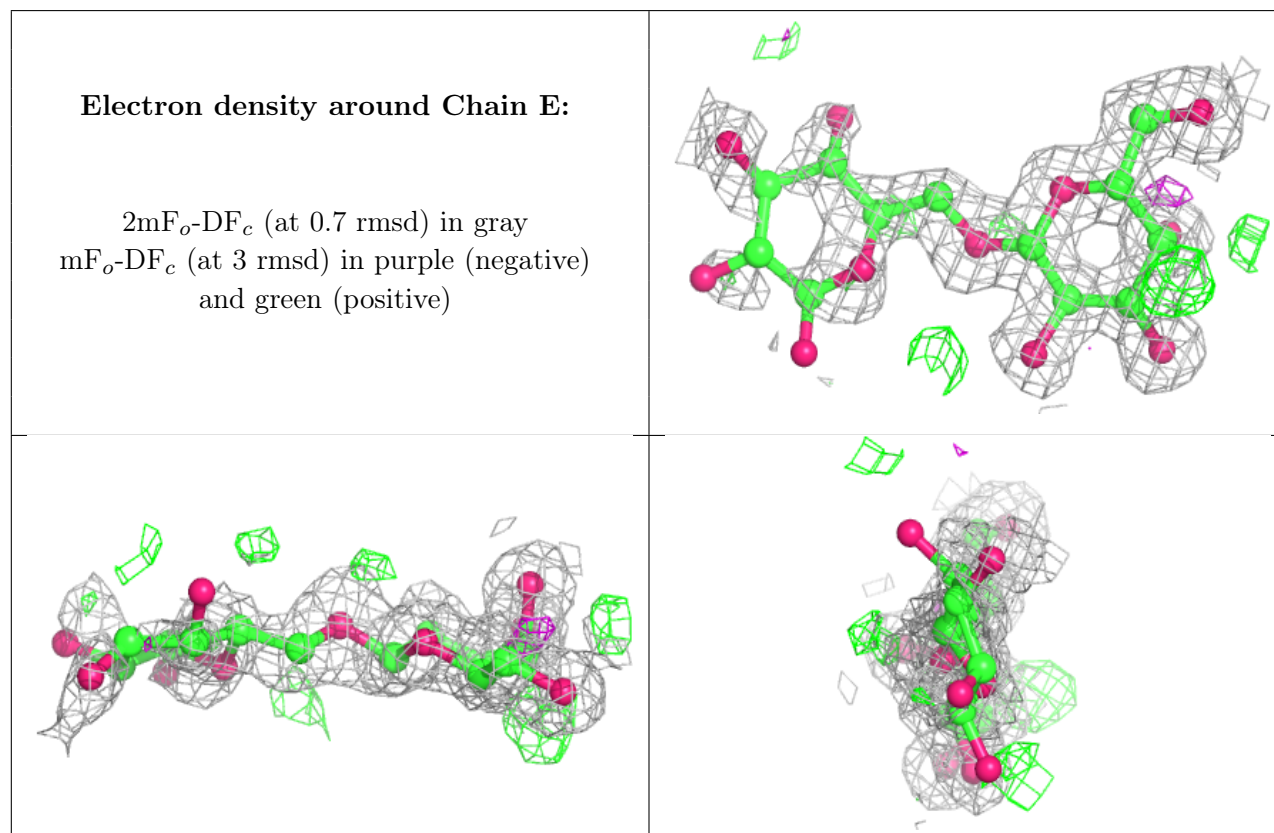
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	H	1	12/12	0.85	0.26	18,100,100,100	0
2	BGC	F	1[A]	12/12	0.91	0.17	11,32,100,100	9

Continued on next page...

Continued from previous page...

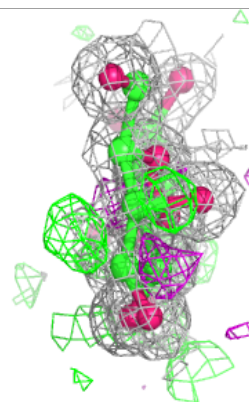
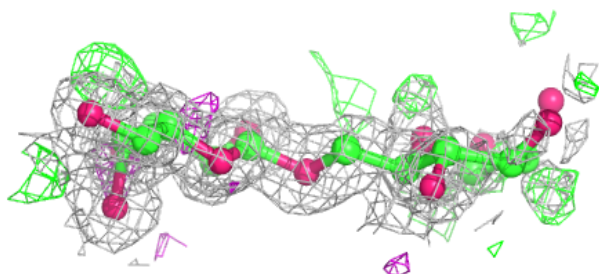
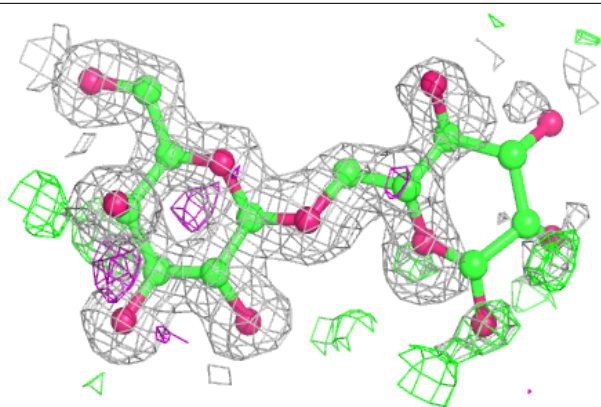
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BGC	E	1	12/12	0.91	0.17	17,96,100,100	0
2	BGC	G	1	12/12	0.92	0.20	14,85,100,100	0
2	GAL	E	2	11/12	0.96	0.07	12,16,21,21	0
2	GAL	F	2	11/12	0.96	0.09	11,14,19,20	0
2	GAL	H	2	11/12	0.97	0.07	13,15,21,24	0
2	GAL	G	2	11/12	0.98	0.07	10,14,17,20	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

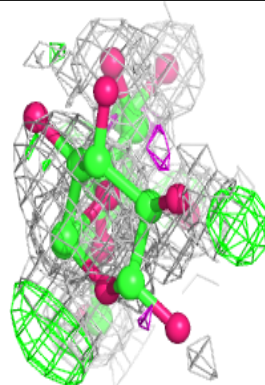
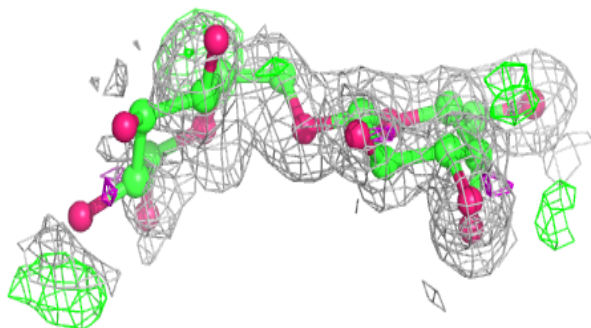
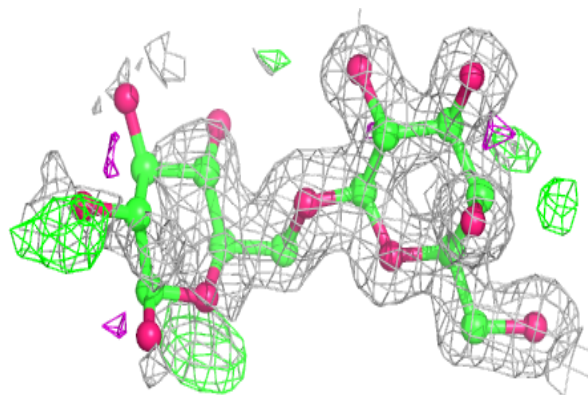


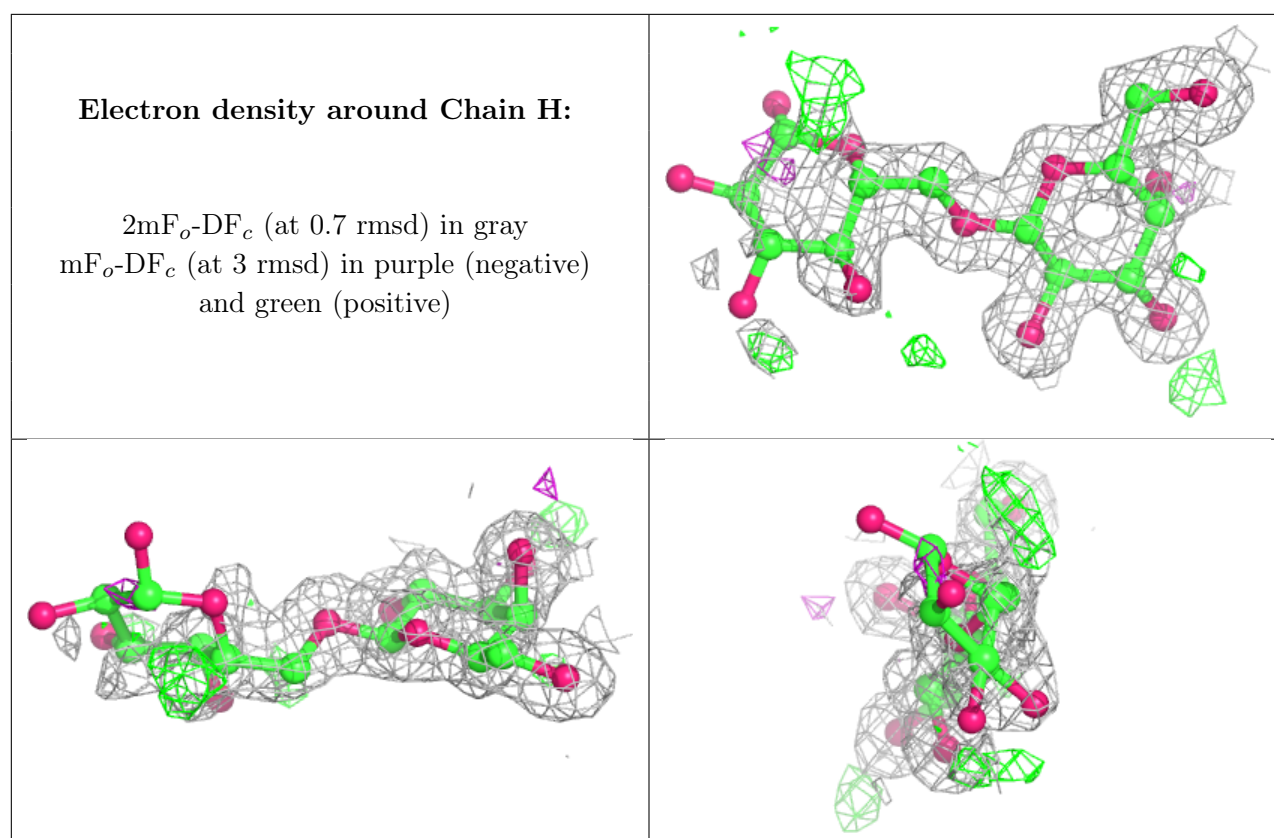
Electron density around Chain F:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain G:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
7	TAR	B	2003[C]	9/10	0.71	0.31	13,38,100,100	9
6	BGC	B	2002[B]	9/12	0.79	0.36	6,56,100,100	9
5	DMS	B	8424	4/4	0.80	0.19	50,74,76,77	0
5	DMS	D	8704	4/4	0.82	0.21	31,32,100,100	0
5	DMS	D	8425	4/4	0.83	0.18	35,42,59,100	0
5	DMS	D	8424	4/4	0.83	0.20	47,57,87,100	0
5	DMS	C	8508	4/4	0.84	0.11	30,35,35,81	0
5	DMS	C	8503	4/4	0.85	0.17	23,50,50,52	0
5	DMS	B	8428	4/4	0.85	0.13	34,38,57,61	0
5	DMS	D	8703	4/4	0.85	0.16	25,51,52,58	0
5	DMS	D	8429	4/4	0.87	0.19	26,51,82,100	0
5	DMS	D	8501	4/4	0.88	0.10	23,29,37,52	0
5	DMS	D	8417	4/4	0.88	0.14	26,27,85,92	0
5	DMS	A	8418	4/4	0.88	0.16	34,39,76,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	DMS	A	8421	4/4	0.88	0.19	34,46,61,63	0
3	MG	A	3105	1/1	0.88	0.16	45,45,45,45	0
5	DMS	B	8508	4/4	0.89	0.10	19,40,41,55	0
5	DMS	B	8420	4/4	0.89	0.15	36,40,43,53	0
5	DMS	D	8423	4/4	0.90	0.14	30,37,42,50	0
5	DMS	D	8503	4/4	0.90	0.17	23,38,49,100	0
5	DMS	D	8418	4/4	0.90	0.14	25,70,78,100	0
5	DMS	A	8419	4/4	0.91	0.11	33,38,46,47	0
5	DMS	C	8417	4/4	0.91	0.10	26,27,50,61	0
5	DMS	A	8428	4/4	0.91	0.20	53,66,100,100	0
5	DMS	B	8418	4/4	0.91	0.09	26,30,63,96	0
5	DMS	D	8428	4/4	0.91	0.19	39,47,61,65	0
5	DMS	B	8501	4/4	0.91	0.13	27,44,56,64	0
5	DMS	B	8417	4/4	0.92	0.11	27,29,70,100	0
5	DMS	C	8424	4/4	0.92	0.17	41,60,100,100	0
5	DMS	A	8406	4/4	0.92	0.15	24,45,69,72	0
5	DMS	C	8504	4/4	0.92	0.14	31,37,46,100	0
5	DMS	B	8419	4/4	0.92	0.12	32,48,65,100	0
5	DMS	A	8502	4/4	0.92	0.12	18,23,49,54	0
4	NA	D	3104	1/1	0.93	0.09	27,27,27,27	0
5	DMS	C	8501	4/4	0.93	0.12	18,26,37,46	0
5	DMS	A	8424	4/4	0.93	0.15	34,35,70,100	0
5	DMS	B	8421	4/4	0.93	0.13	31,49,52,100	0
5	DMS	C	8406	4/4	0.93	0.18	42,44,99,100	0
5	DMS	D	8404	4/4	0.93	0.10	18,19,41,53	0
5	DMS	D	8416	4/4	0.93	0.14	25,32,44,100	0
3	MG	C	3105	1/1	0.93	0.11	35,35,35,35	0
5	DMS	C	8418	4/4	0.93	0.15	20,27,56,100	0
5	DMS	C	8419	4/4	0.93	0.13	30,32,43,52	0
5	DMS	B	8706	4/4	0.94	0.12	37,41,42,42	0
5	DMS	D	8419	4/4	0.94	0.10	27,39,41,43	0
5	DMS	D	8420	4/4	0.94	0.13	18,67,81,83	0
5	DMS	D	8508	4/4	0.94	0.09	31,36,41,53	0
5	DMS	C	8423	4/4	0.94	0.09	28,31,48,48	0
5	DMS	A	8501	4/4	0.94	0.11	16,27,35,36	0
5	DMS	A	8417	4/4	0.94	0.13	24,26,73,100	0
5	DMS	B	8416	4/4	0.94	0.10	33,46,47,50	0
5	DMS	A	8423	4/4	0.95	0.10	28,42,51,73	0
5	DMS	B	8423	4/4	0.95	0.09	26,28,45,50	0
5	DMS	C	8415	4/4	0.95	0.11	19,25,31,38	0
5	DMS	C	8602	4/4	0.95	0.11	43,47,57,68	0
3	MG	C	3006	1/1	0.95	0.14	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DMS	A	8409	4/4	0.95	0.12	27,28,41,51	0
5	DMS	B	8429	4/4	0.95	0.12	29,40,45,51	0
5	DMS	A	8414	4/4	0.95	0.13	23,24,55,100	0
5	DMS	B	8504	4/4	0.95	0.09	20,35,38,43	0
5	DMS	D	8705	4/4	0.95	0.12	8,44,50,78	0
5	DMS	C	8429	4/4	0.95	0.11	41,42,51,100	0
5	DMS	A	8416	4/4	0.95	0.16	16,31,40,100	0
5	DMS	A	8413	4/4	0.96	0.12	24,28,29,34	0
5	DMS	B	8502	4/4	0.96	0.07	16,22,30,36	0
5	DMS	D	8421	4/4	0.96	0.12	32,46,51,66	0
5	DMS	A	8408	4/4	0.96	0.08	15,29,31,48	0
5	DMS	A	8420	4/4	0.96	0.12	24,30,31,47	0
4	NA	D	3103	1/1	0.96	0.08	24,24,24,24	0
5	DMS	A	8503	4/4	0.96	0.13	28,42,100,100	0
5	DMS	B	8407	4/4	0.96	0.11	25,29,30,30	0
5	DMS	C	8601	4/4	0.96	0.12	39,40,55,57	0
5	DMS	C	8416	4/4	0.96	0.17	32,43,43,44	0
5	DMS	D	8403	4/4	0.96	0.08	16,23,25,26	0
5	DMS	B	8414	4/4	0.96	0.12	22,38,40,100	0
5	DMS	D	8407	4/4	0.96	0.10	22,29,31,63	0
5	DMS	B	8415	4/4	0.96	0.11	19,28,30,38	0
5	DMS	A	8412	4/4	0.96	0.11	29,38,100,100	0
5	DMS	C	8420	4/4	0.96	0.09	25,32,35,40	0
5	DMS	C	8412	4/4	0.97	0.08	25,26,29,72	0
5	DMS	D	8409	4/4	0.97	0.09	27,33,36,42	0
5	DMS	D	8414	4/4	0.97	0.11	21,35,76,100	0
3	MG	A	3005	1/1	0.97	0.09	25,25,25,25	0
5	DMS	A	8504	4/4	0.97	0.10	20,32,35,94	0
5	DMS	A	8602	4/4	0.97	0.17	35,52,100,100	0
5	DMS	B	8404	4/4	0.97	0.07	18,21,28,28	0
5	DMS	B	8425	4/4	0.97	0.09	17,26,26,32	0
3	MG	C	3004	1/1	0.97	0.17	36,36,36,36	0
5	DMS	C	8421	4/4	0.97	0.11	30,37,41,49	0
5	DMS	B	8413	4/4	0.97	0.10	28,28,29,34	0
5	DMS	A	8404	4/4	0.97	0.07	17,23,23,27	0
3	MG	D	3105	1/1	0.97	0.10	36,36,36,36	0
5	DMS	A	8425	4/4	0.97	0.08	23,26,30,32	0
5	DMS	A	8407	4/4	0.97	0.09	18,25,28,31	0
4	NA	A	3104	1/1	0.97	0.06	20,20,20,20	0
5	DMS	C	8404	4/4	0.97	0.07	15,16,21,26	0
4	NA	B	3104	1/1	0.97	0.08	24,24,24,24	0
5	DMS	C	8407	4/4	0.97	0.08	23,24,30,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	DMS	C	8408	4/4	0.97	0.07	15,28,29,37	0
5	DMS	C	8409	4/4	0.97	0.11	23,32,33,35	0
5	DMS	D	8406	4/4	0.97	0.09	18,18,21,39	0
5	DMS	C	8402	4/4	0.98	0.06	12,22,23,26	0
5	DMS	B	8412	4/4	0.98	0.08	23,28,28,30	0
5	DMS	C	8405	4/4	0.98	0.09	21,23,23,24	0
4	NA	C	3104	1/1	0.98	0.08	22,22,22,22	0
5	DMS	A	8402	4/4	0.98	0.06	11,18,20,27	0
5	DMS	A	8506	4/4	0.98	0.09	27,28,46,63	0
5	DMS	A	8403	4/4	0.98	0.06	19,19,21,24	0
5	DMS	C	8506	4/4	0.98	0.08	26,26,31,74	0
4	NA	A	3103	1/1	0.98	0.04	20,20,20,20	0
5	DMS	C	8413	4/4	0.98	0.12	24,25,27,30	0
5	DMS	C	8414	4/4	0.98	0.08	17,37,46,48	0
5	DMS	A	8410	4/4	0.98	0.07	17,27,32,34	0
5	DMS	B	8408	4/4	0.98	0.10	22,25,31,38	0
5	DMS	D	8506	4/4	0.98	0.09	19,32,44,52	0
5	DMS	B	8506	4/4	0.98	0.11	26,26,29,100	0
5	DMS	D	8701	4/4	0.98	0.07	13,14,17,31	0
5	DMS	B	8409	4/4	0.98	0.08	23,26,28,30	0
5	DMS	D	8408	4/4	0.98	0.07	17,27,27,33	0
5	DMS	B	8601	4/4	0.98	0.08	27,34,36,44	0
5	DMS	D	8410	4/4	0.98	0.06	14,27,27,39	0
5	DMS	B	8410	4/4	0.98	0.06	19,27,33,35	0
5	DMS	B	8402	4/4	0.99	0.06	14,14,18,23	0
5	DMS	D	8411	4/4	0.99	0.05	17,17,22,40	0
5	DMS	D	8412	4/4	0.99	0.09	24,26,27,35	0
5	DMS	D	8413	4/4	0.99	0.10	25,26,26,41	0
5	DMS	C	8401	4/4	0.99	0.04	11,12,16,17	0
5	DMS	B	8403	4/4	0.99	0.05	15,15,22,23	0
5	DMS	C	8403	4/4	0.99	0.05	17,19,21,21	0
5	DMS	A	8411	4/4	0.99	0.05	16,21,21,48	0
5	DMS	C	8425	4/4	0.99	0.10	26,28,29,42	0
5	DMS	B	8405	4/4	0.99	0.09	22,24,28,34	0
3	MG	B	3105	1/1	0.99	0.11	35,35,35,35	0
4	NA	B	3103	1/1	0.99	0.04	18,18,18,18	0
3	MG	D	3002	1/1	0.99	0.03	12,12,12,12	0
5	DMS	A	8405	4/4	0.99	0.06	18,22,22,31	0
5	DMS	C	8410	4/4	0.99	0.06	17,27,28,30	0
5	DMS	C	8411	4/4	0.99	0.06	15,20,25,25	0
5	DMS	B	8411	4/4	0.99	0.06	17,20,20,100	0
5	DMS	D	8401	4/4	0.99	0.04	11,12,15,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	DMS	D	8402	4/4	0.99	0.04	12,15,17,18	0
4	NA	C	3103	1/1	0.99	0.04	18,18,18,18	0
3	MG	D	3005	1/1	0.99	0.10	21,21,21,21	0
5	DMS	D	8405	4/4	0.99	0.08	20,20,23,36	0
3	MG	A	3002	1/1	0.99	0.03	11,11,11,11	0
3	MG	B	3002	1/1	0.99	0.03	11,11,11,11	0
5	DMS	A	8401	4/4	0.99	0.04	10,11,13,13	0
5	DMS	B	8401	4/4	0.99	0.05	12,16,16,19	0
3	MG	C	3001	1/1	1.00	0.03	8,8,8,8	0
3	MG	D	3001	1/1	1.00	0.02	8,8,8,8	0
4	NA	B	3101	1/1	1.00	0.03	10,10,10,10	0
4	NA	B	3102	1/1	1.00	0.04	9,9,9,9	0
3	MG	C	3002	1/1	1.00	0.01	10,10,10,10	0
3	MG	A	3001	1/1	1.00	0.02	9,9,9,9	0
4	NA	C	3101	1/1	1.00	0.02	9,9,9,9	0
4	NA	C	3102	1/1	1.00	0.03	10,10,10,10	0
3	MG	B	3001	1/1	1.00	0.02	8,8,8,8	0
4	NA	A	3101	1/1	1.00	0.03	10,10,10,10	0
4	NA	D	3101	1/1	1.00	0.02	11,11,11,11	0
4	NA	D	3102	1/1	1.00	0.04	9,9,9,9	0
4	NA	A	3102	1/1	1.00	0.02	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.