



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:41 AM UTC

PDB ID : 1JZ8 / pdb_00001jz8
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 Full wwPDB X-ray Structure Validation 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

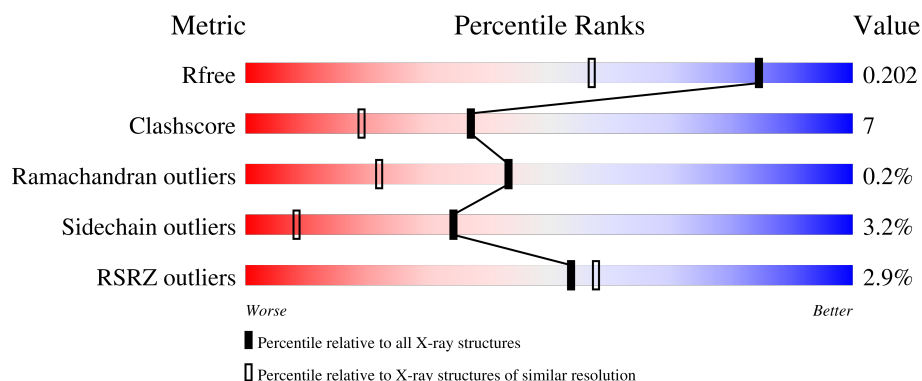
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

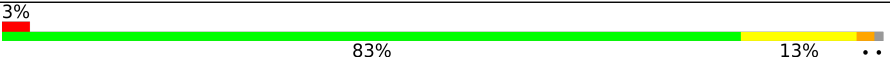
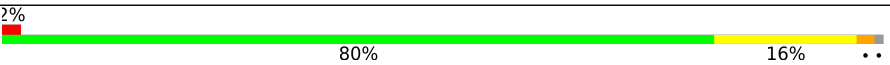
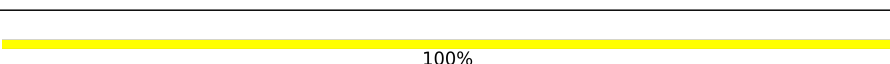
The reported resolution of this entry is 1.50 Å.

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.



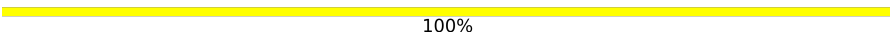
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	
1	B	1023	
1	C	1023	
1	D	1023	
2	E	2	

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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	8412	-	-	X	-
5	DMS	A	8413	-	X	-	-
5	DMS	A	8425	-	X	-	-
5	DMS	A	8428	-	-	X	-
5	DMS	A	8502	-	X	-	-
5	DMS	B	8415	-	-	X	-
5	DMS	B	8418	-	-	X	-
5	DMS	B	8501	-	-	X	-
5	DMS	C	8424	-	-	X	-
5	DMS	D	8701	-	X	-	-
5	DMS	D	8705	-	-	X	-
6	BGC	B	2002[B]	X	-	-	-
7	TAR	B	2003[C]	X	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	THR	cloning artifact	? P00722
C	5	LEU	ASP	cloning artifact	? P00722
C	6	GLU	SER	cloning artifact	? P00722
C	7	ASP	LEU	cloning artifact	? P00722
C	8	PRO	ALA	cloning artifact	? P00722
C	537	GLN	GLU	engineered 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 (CCD ID: 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		

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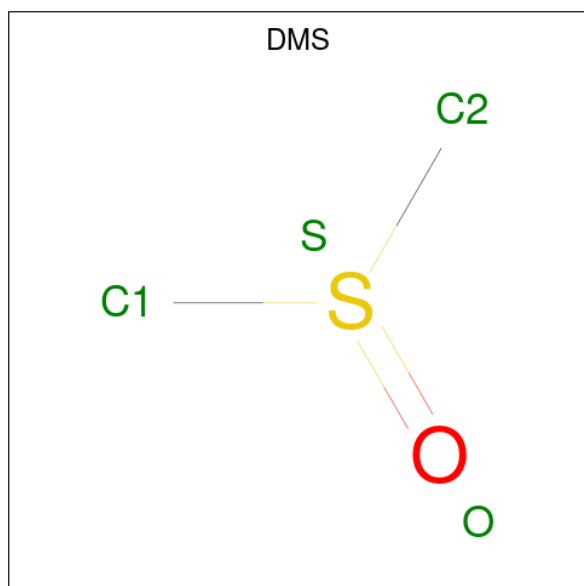
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	4	Total	Mg	0	0
			4	4		

- Molecule 4 is SODIUM ION (CCD ID: 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 (CCD ID: 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		

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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	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	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

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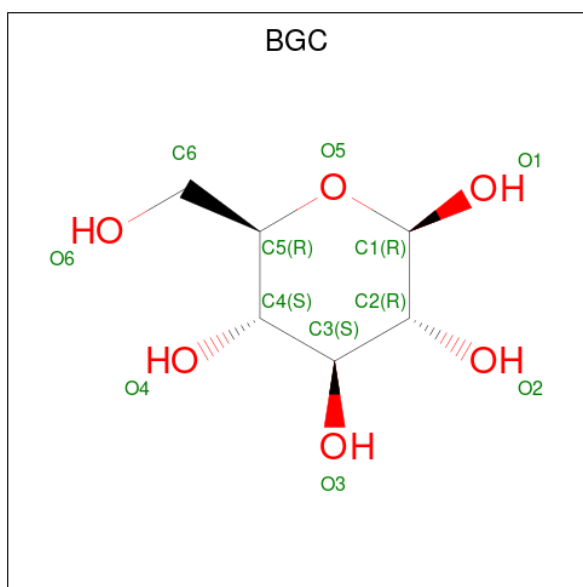
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S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

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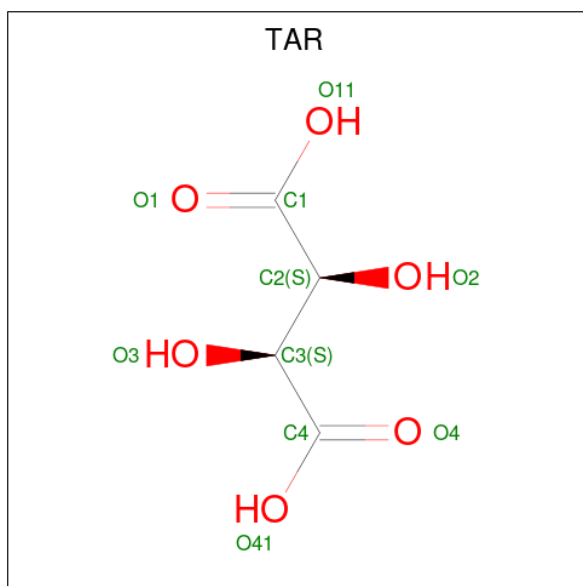
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- Molecule 6 is beta-D-glucopyranose (CCD ID: BGC) (formula: $\text{C}_6\text{H}_{12}\text{O}_6$).



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

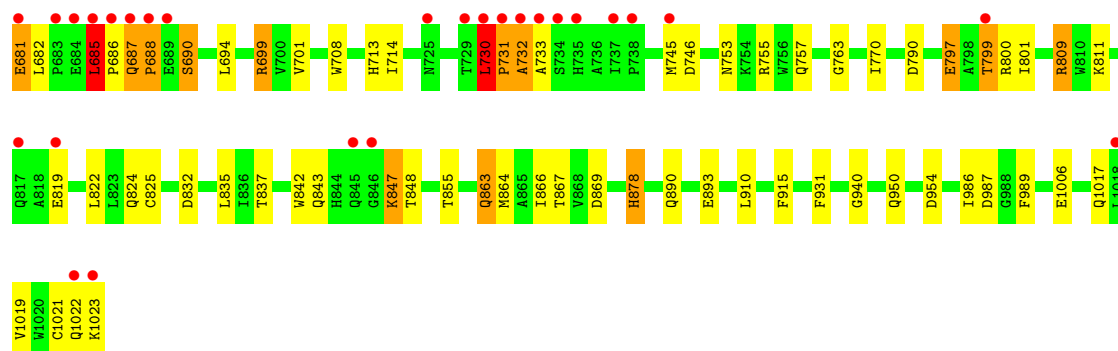
- Molecule 7 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: $C_4H_6O_6$).



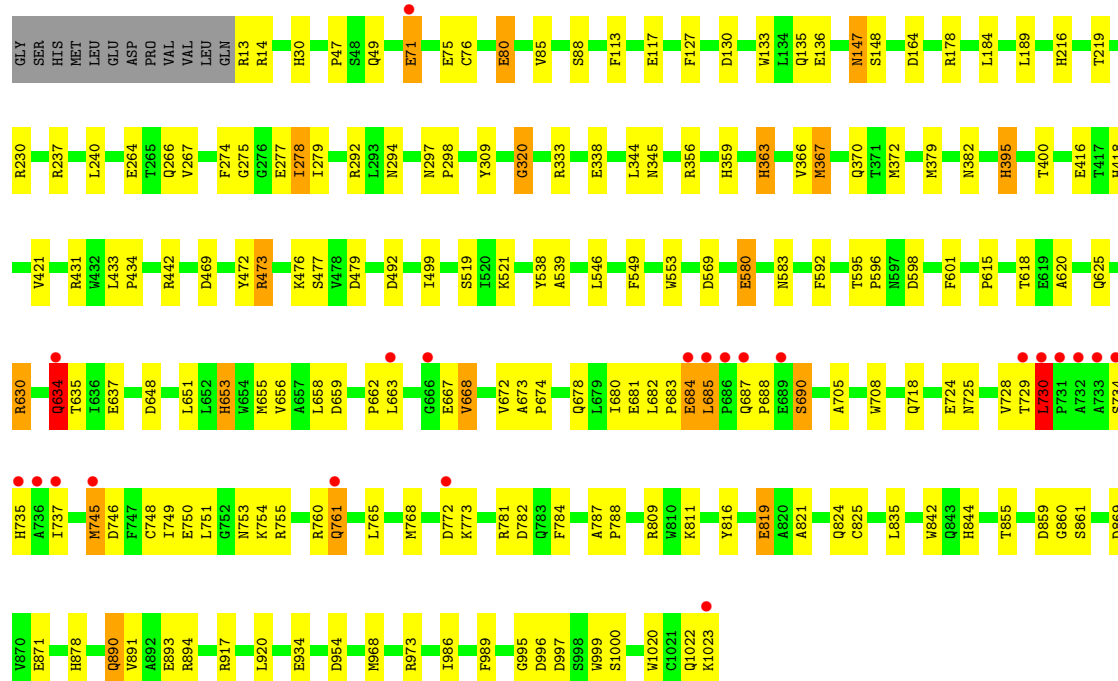
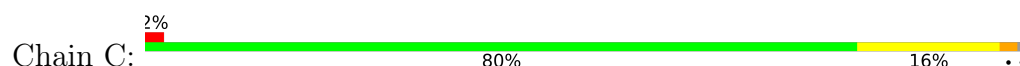
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	1
			9	4	5		

- Molecule 8 is water.

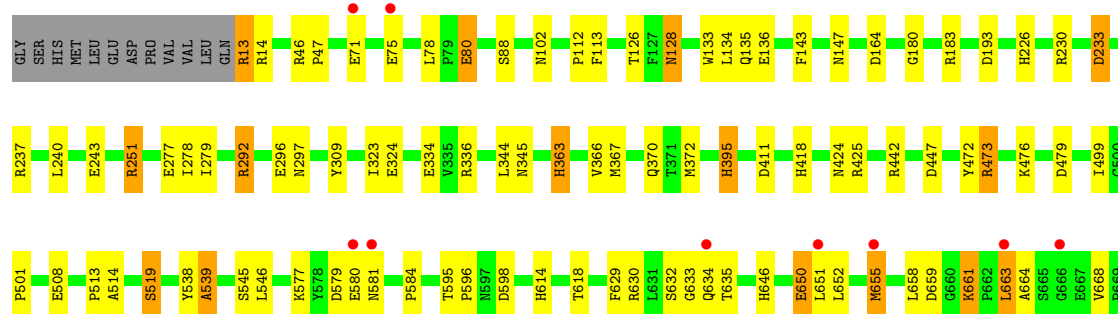
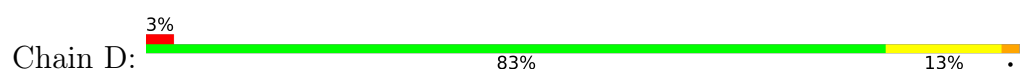
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1144	Total 1144	O 1144	0	0
8	B	1148	Total 1148	O 1148	0	0
8	C	1126	Total 1126	O 1126	0	0
8	D	1105	Total 1105	O 1105	0	0

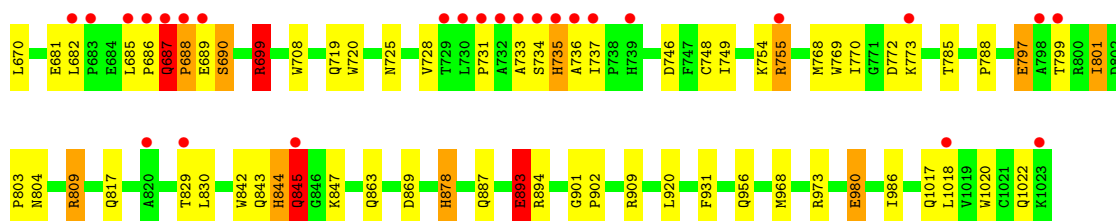


• Molecule 1: Beta-Galactosidase



• Molecule 1: Beta-Galactosidase





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

Chain E: 100%

BGC1
GAL2

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

Chain F: 50% 50%

BGC1
GAL2

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

Chain G: 100%

BGC1
GAL2

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

Chain H: 50% 50%

BGC1
GAL2

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) 97.7 (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 , 0.202	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)	0.39 , 81.9	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, GAL, TAR, DMS, MG, NA

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	1.42	16/8383 (0.2%)	1.60	66/11437 (0.6%)
1	B	1.44	20/8383 (0.2%)	1.58	44/11437 (0.4%)
1	C	1.42	25/8383 (0.3%)	1.61	81/11437 (0.7%)
1	D	1.45	25/8383 (0.3%)	1.60	61/11437 (0.5%)
All	All	1.43	86/33532 (0.3%)	1.60	252/45748 (0.6%)

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	630	ARG	NE-CZ	8.77	1.42	1.33
1	A	479	ASP	C-N	-7.51	1.26	1.33
1	B	540[A]	HIS	ND1-CE1	7.15	1.39	1.32
1	B	540[B]	HIS	ND1-CE1	7.15	1.39	1.32
1	C	442	ARG	CZ-NH1	7.07	1.42	1.32
1	C	479	ASP	C-N	-6.75	1.27	1.33
1	D	893	GLU	CD-OE2	6.74	1.38	1.25
1	C	297	ASN	C-O	-6.60	1.20	1.23
1	A	191	TRP	NE1-CE2	6.57	1.44	1.37
1	D	418	HIS	CE1-NE2	6.43	1.39	1.32
1	A	379	MET	SD-CE	-6.34	1.63	1.79
1	B	391	HIS	ND1-CE1	6.32	1.38	1.32
1	D	71	GLU	CD-OE2	6.31	1.37	1.25
1	D	479	ASP	C-N	-6.28	1.27	1.34
1	B	322	LEU	C-N	6.25	1.39	1.33
1	B	950	GLN	C-O	6.22	1.31	1.23
1	A	442	ARG	CZ-NH1	6.22	1.41	1.32
1	A	296	GLU	CD-OE2	6.17	1.37	1.25
1	A	772	ASP	CG-OD2	6.17	1.37	1.25
1	D	425	ARG	NE-CZ	6.14	1.39	1.33
1	C	30	HIS	ND1-CE1	6.08	1.38	1.32
1	D	442	ARG	NE-CZ	5.96	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	684	GLU	CD-OE2	5.92	1.36	1.25
1	A	909	ARG	NE-CZ	5.92	1.39	1.33
1	B	258	VAL	C-O	5.88	1.30	1.24
1	C	630	ARG	CD-NE	5.86	1.54	1.46
1	B	954	ASP	CG-OD2	5.81	1.36	1.25
1	D	699	ARG	CZ-NH2	5.81	1.41	1.33
1	C	80	GLU	CD-OE2	5.74	1.36	1.25
1	C	705	ALA	C-O	5.73	1.30	1.23
1	A	13	ARG	C-N	-5.71	1.26	1.33
1	B	1006	GLU	CD-OE2	5.70	1.36	1.25
1	D	424	ASN	N-CA	5.70	1.53	1.46
1	B	310	ARG	CZ-NH1	5.70	1.40	1.32
1	D	646	HIS	CE1-NE2	5.70	1.38	1.32
1	B	157	ARG	NE-CZ	5.68	1.39	1.33
1	D	920	LEU	N-CA	-5.59	1.42	1.46
1	D	842	TRP	CA-C	-5.54	1.46	1.52
1	A	1006	GLU	CD-OE2	5.52	1.35	1.25
1	D	650	GLU	CD-OE2	5.51	1.35	1.25
1	B	940	GLY	CA-C	5.49	1.57	1.51
1	A	18	ASN	CA-CB	5.48	1.58	1.53
1	D	243	GLU	CD-OE2	5.48	1.35	1.25
1	D	80	GLU	CD-OE2	5.46	1.35	1.25
1	D	646	HIS	CG-CD2	5.45	1.41	1.35
1	C	934	GLU	CD-OE2	5.44	1.35	1.25
1	B	508	GLU	CA-CB	5.44	1.61	1.53
1	C	216	HIS	CE1-NE2	5.40	1.38	1.32
1	D	233	ASP	CG-OD2	5.40	1.35	1.25
1	A	392	TYR	CA-CB	5.37	1.61	1.53
1	B	418	HIS	CE1-NE2	5.33	1.37	1.32
1	C	333	ARG	CD-NE	5.29	1.53	1.46
1	D	226	HIS	ND1-CE1	5.27	1.37	1.32
1	B	296	GLU	CD-OE2	5.26	1.35	1.25
1	D	442	ARG	CZ-NH1	5.25	1.40	1.32
1	D	13	ARG	C-N	-5.25	1.26	1.33
1	C	47	PRO	C-O	5.25	1.29	1.23
1	C	920	LEU	C-O	-5.25	1.18	1.24
1	A	450	HIS	ND1-CE1	5.25	1.37	1.32
1	C	954	ASP	CA-CB	5.22	1.59	1.52
1	B	842	TRP	CD2-CE3	-5.21	1.31	1.40
1	A	644	PHE	C-O	-5.20	1.17	1.24
1	A	974	HIS	CE1-NE2	5.20	1.37	1.32
1	B	32	PRO	N-CD	5.20	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	442	ARG	NE-CZ	5.18	1.38	1.33
1	C	842	TRP	CA-C	-5.18	1.46	1.52
1	C	421	VAL	CA-CB	5.18	1.58	1.54
1	C	71	GLU	CD-OE2	5.17	1.35	1.25
1	D	279	ILE	CB-CG1	-5.17	1.43	1.53
1	C	297	ASN	CA-CB	5.17	1.57	1.52
1	A	669	PRO	CA-C	5.14	1.59	1.52
1	B	157	ARG	CD-NE	5.12	1.53	1.46
1	D	292	ARG	N-CA	5.11	1.52	1.46
1	B	650	GLU	CD-OE2	5.10	1.35	1.25
1	C	492	ASP	CG-OD2	5.10	1.35	1.25
1	D	442	ARG	CZ-NH2	5.09	1.40	1.33
1	D	863	GLN	CA-C	-5.09	1.46	1.52
1	A	800	ARG	CZ-NH1	5.09	1.39	1.32
1	B	418	HIS	CG-ND1	5.09	1.43	1.38
1	C	499	ILE	N-CA	5.08	1.51	1.46
1	C	297	ASN	CA-C	-5.08	1.50	1.53
1	D	75	GLU	CD-OE2	5.08	1.34	1.25
1	C	267	VAL	CA-C	-5.08	1.46	1.52
1	D	580	GLU	CD-OE2	5.08	1.34	1.25
1	B	30	HIS	ND1-CE1	5.07	1.37	1.32
1	C	894	ARG	C-N	5.01	1.39	1.33

All (252) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	630	ARG	NE-CZ-NH1	12.04	133.53	121.50
1	C	630	ARG	CD-NE-CZ	11.82	140.95	124.40
1	D	297	ASN	CB-CA-C	-9.56	104.41	111.20
1	B	363	HIS	CA-CB-CG	-8.95	104.85	113.80
1	D	128	ASN	CA-CB-CG	-8.90	103.70	112.60
1	C	725	ASN	CA-CB-CG	-8.68	103.92	112.60
1	C	442	ARG	NE-CZ-NH2	-8.39	111.64	119.20
1	A	431	ARG	NE-CZ-NH2	-8.36	111.67	119.20
1	D	893	GLU	CB-CG-CD	8.22	126.57	112.60
1	A	685	LEU	CA-C-N	7.75	129.53	119.84
1	A	685	LEU	C-N-CA	7.75	129.53	119.84
1	D	733	ALA	N-CA-C	7.61	121.55	110.28
1	D	736	ALA	N-CA-C	7.43	121.36	110.59
1	A	583	ASN	CA-CB-CG	-7.35	105.25	112.60
1	B	479	ASP	CA-CB-CG	-7.35	105.25	112.60
1	A	736	ALA	N-CA-C	7.30	119.68	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	680	ILE	CA-C-N	-7.27	113.10	122.77
1	C	680	ILE	C-N-CA	-7.27	113.10	122.77
1	A	661	LYS	CA-C-O	7.18	124.63	119.32
1	C	71	GLU	CB-CG-CD	7.14	124.74	112.60
1	A	771	GLY	N-CA-C	-7.06	97.87	110.86
1	B	382	ASN	CA-CB-CG	-7.05	105.55	112.60
1	D	843	GLN	OE1-CD-NE2	7.02	129.62	122.60
1	D	687	GLN	CB-CA-C	7.00	120.35	109.15
1	D	878	HIS	CA-CB-CG	-6.96	106.84	113.80
1	D	734	SER	CA-C-O	6.96	128.62	120.69
1	C	76	CYS	N-CA-CB	-6.93	98.63	111.53
1	D	279	ILE	CA-CB-CG2	6.91	122.25	110.50
1	B	878	HIS	CA-CB-CG	-6.90	106.90	113.80
1	D	733	ALA	N-CA-CB	6.85	120.05	109.97
1	A	867	THR	CA-CB-OG1	-6.84	99.34	109.60
1	C	753	ASN	CA-C-N	-6.80	111.38	122.81
1	C	753	ASN	C-N-CA	-6.80	111.38	122.81
1	C	421	VAL	CA-C-O	-6.79	116.41	119.94
1	C	989	PHE	CA-CB-CG	-6.74	107.06	113.80
1	C	634	GLN	N-CA-CB	-6.74	100.72	110.56
1	A	917	ARG	NE-CZ-NH1	-6.73	114.77	121.50
1	C	592	PHE	CA-CB-CG	-6.72	107.08	113.80
1	C	274	PHE	CA-CB-CG	-6.68	107.12	113.80
1	C	668	VAL	N-CA-CB	-6.68	101.86	111.21
1	A	771	GLY	CA-C-N	-6.67	112.02	122.49
1	A	771	GLY	C-N-CA	-6.67	112.02	122.49
1	A	890	GLN	N-CA-CB	-6.64	100.03	110.06
1	C	363	HIS	CA-CB-CG	-6.64	107.16	113.80
1	C	890	GLN	N-CA-CB	-6.62	99.61	110.41
1	B	216	HIS	CA-CB-CG	-6.58	107.22	113.80
1	A	687	GLN	CB-CA-C	6.57	117.71	110.15
1	B	809	ARG	CG-CD-NE	6.57	126.45	112.00
1	D	845	GLN	CA-C-N	-6.55	111.78	122.20
1	D	845	GLN	C-N-CA	-6.55	111.78	122.20
1	A	632	SER	N-CA-CB	6.53	122.24	110.95
1	C	85	VAL	CA-CB-CG2	-6.51	99.33	110.40
1	B	730	LEU	CB-CA-C	6.51	120.36	109.69
1	D	803	PRO	N-CA-CB	6.50	109.52	103.41
1	C	113	PHE	CA-CB-CG	-6.48	107.32	113.80
1	B	790	ASP	CA-CB-CG	-6.46	106.14	112.60
1	B	755	ARG	NE-CZ-NH2	6.45	125.00	119.20
1	D	113	PHE	CA-CB-CG	-6.42	107.38	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	GLU	CB-CA-C	-6.40	96.69	110.45
1	B	519	SER	N-CA-CB	-6.38	99.55	109.69
1	A	235	PHE	CA-CB-CG	-6.37	107.43	113.80
1	A	128	ASN	CA-CB-CG	-6.37	106.23	112.60
1	D	80	GLU	CB-CG-CD	-6.36	101.79	112.60
1	D	817	GLN	CB-CG-CD	-6.35	101.80	112.60
1	D	278	ILE	CA-C-N	-6.35	114.09	121.71
1	D	278	ILE	C-N-CA	-6.35	114.09	121.71
1	A	689	GLU	CA-C-N	6.35	130.57	121.50
1	A	689	GLU	C-N-CA	6.35	130.57	121.50
1	B	279	ILE	N-CA-CB	-6.34	104.44	111.41
1	C	685	LEU	CB-CA-C	6.34	116.95	109.47
1	D	183	ARG	CD-NE-CZ	-6.32	115.55	124.40
1	A	832	ASP	N-CA-CB	-6.32	101.00	111.49
1	C	630	ARG	CA-CB-CG	6.31	126.72	114.10
1	D	183	ARG	NE-CZ-NH1	-6.26	115.24	121.50
1	C	630	ARG	NH1-CZ-NH2	-6.25	111.17	119.30
1	C	869	ASP	CA-CB-CG	-6.23	106.37	112.60
1	B	384	PHE	CA-CB-CG	-6.20	107.60	113.80
1	D	632	SER	N-CA-CB	6.19	120.55	110.90
1	C	729	THR	CA-C-N	6.16	129.02	120.65
1	C	729	THR	C-N-CA	6.16	129.02	120.65
1	D	193	ASP	N-CA-C	-6.14	105.05	112.54
1	A	382	ASN	CA-CB-CG	-6.12	106.48	112.60
1	A	113	PHE	CA-CB-CG	-6.11	107.69	113.80
1	D	731	PRO	N-CA-CB	6.10	108.66	103.35
1	A	682	LEU	CA-C-N	6.10	126.11	119.89
1	A	682	LEU	C-N-CA	6.10	126.11	119.89
1	D	143	PHE	CA-CB-CG	-6.09	107.71	113.80
1	A	598	ASP	CA-CB-CG	-6.09	106.51	112.60
1	A	688	PRO	N-CA-C	6.07	121.52	113.57
1	B	39	SER	CA-CB-OG	-6.07	98.97	111.10
1	D	863	GLN	CA-CB-CG	-6.06	101.98	114.10
1	A	14	ARG	N-CA-CB	-6.05	103.15	110.53
1	C	279	ILE	N-CA-C	-6.05	107.00	111.90
1	B	843	GLN	O-C-N	6.04	131.01	123.15
1	B	634	GLN	N-CA-C	-6.02	105.58	113.17
1	D	14	ARG	N-CA-CB	-6.01	103.62	110.35
1	B	797	GLU	CB-CG-CD	-5.98	102.43	112.60
1	D	689	GLU	N-CA-C	-5.98	105.97	113.20
1	A	442	ARG	NE-CZ-NH2	-5.98	113.82	119.20
1	C	730	LEU	CA-C-O	5.96	125.36	119.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	309	TYR	N-CA-C	-5.93	101.42	110.14
1	A	663	LEU	CB-CA-C	-5.93	99.69	109.65
1	C	473	ARG	NH1-CZ-NH2	-5.92	111.61	119.30
1	D	324	GLU	N-CA-CB	5.91	120.54	111.56
1	C	583	ASN	CA-CB-CG	-5.88	106.72	112.60
1	D	147	ASN	OD1-CG-ND2	5.87	128.47	122.60
1	C	601	PHE	CA-CB-CG	-5.87	107.93	113.80
1	A	735	HIS	CA-CB-CG	-5.87	107.93	113.80
1	C	477	SER	CB-CA-C	-5.86	101.64	110.90
1	A	363	HIS	CA-CB-CG	-5.86	107.94	113.80
1	C	893	GLU	N-CA-C	5.86	117.75	111.36
1	A	871	GLU	CB-CG-CD	-5.85	102.65	112.60
1	D	801	ILE	N-CA-CB	-5.85	101.00	110.13
1	A	477	SER	N-CA-CB	5.84	118.53	110.07
1	D	598	ASP	CA-CB-CG	-5.82	106.78	112.60
1	D	931	PHE	CA-CB-CG	-5.81	107.99	113.80
1	C	598	ASP	CA-CB-CG	-5.78	106.82	112.60
1	D	395	HIS	N-CA-CB	-5.78	101.26	109.75
1	D	844	HIS	CA-CB-CG	-5.77	108.03	113.80
1	A	685	LEU	N-CA-C	5.76	118.62	109.64
1	A	685	LEU	O-C-N	5.75	128.38	121.60
1	C	553	TRP	CA-CB-CG	-5.74	102.69	113.60
1	C	431	ARG	CA-CB-CG	-5.73	102.65	114.10
1	D	297	ASN	O-C-N	-5.72	118.90	121.53
1	C	917	ARG	CD-NE-CZ	-5.71	116.41	124.40
1	B	989	PHE	CA-CB-CG	-5.71	108.09	113.80
1	D	473	ARG	NE-CZ-NH1	5.69	127.19	121.50
1	C	653	HIS	CA-CB-CG	5.67	119.47	113.80
1	D	735	HIS	N-CA-CB	-5.66	101.65	109.91
1	C	294	ASN	CA-CB-CG	-5.65	106.95	112.60
1	B	869	ASP	CA-CB-CG	-5.64	106.95	112.60
1	C	630	ARG	CG-CD-NE	5.64	124.41	112.00
1	D	251	ARG	CG-CD-NE	-5.64	99.59	112.00
1	B	20	GLY	N-CA-C	-5.62	107.95	115.32
1	D	363	HIS	CA-CB-CG	-5.62	108.18	113.80
1	C	761	GLN	CB-CG-CD	5.62	122.14	112.60
1	C	320	GLY	CA-C-N	-5.61	114.28	122.19
1	C	320	GLY	C-N-CA	-5.61	114.28	122.19
1	B	184	LEU	CB-CA-C	-5.60	100.03	109.50
1	B	733	ALA	N-CA-C	5.57	118.39	110.10
1	B	755	ARG	CA-CB-CG	5.56	125.23	114.10
1	B	345	ASN	CA-CB-CG	-5.56	107.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	735	HIS	CA-CB-CG	5.56	119.36	113.80
1	B	753	ASN	N-CA-CB	5.55	118.23	110.56
1	C	809	ARG	CD-NE-CZ	-5.54	116.64	124.40
1	D	869	ASP	CA-CB-CG	-5.53	107.07	112.60
1	B	915	PHE	CA-CB-CG	-5.53	108.27	113.80
1	C	130	ASP	CA-CB-CG	-5.52	107.08	112.60
1	A	116	THR	CA-CB-OG1	-5.50	101.34	109.60
1	A	1000	SER	CA-CB-OG	-5.50	100.09	111.10
1	C	298	PRO	CB-CA-C	-5.50	104.19	111.23
1	C	821	ALA	N-CA-CB	5.49	119.19	110.57
1	C	809	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	C	400	THR	CA-CB-OG1	-5.48	101.38	109.60
1	C	728	VAL	CA-C-N	-5.47	115.17	122.72
1	C	728	VAL	C-N-CA	-5.47	115.17	122.72
1	A	297	ASN	CA-CB-CG	-5.47	107.13	112.60
1	C	338	GLU	CG-CD-OE2	-5.47	105.82	118.40
1	A	519	SER	N-CA-CB	-5.47	101.00	109.69
1	A	725	ASN	CA-CB-CG	-5.46	107.14	112.60
1	A	816	TYR	CA-C-N	-5.46	114.03	122.49
1	A	816	TYR	C-N-CA	-5.46	114.03	122.49
1	A	770	ILE	N-CA-CB	5.46	118.74	111.64
1	D	323	ILE	N-CA-C	-5.44	106.39	111.45
1	A	800	ARG	N-CA-CB	-5.44	101.30	110.49
1	C	395	HIS	ND1-CG-CD2	5.43	111.53	106.10
1	C	782	ASP	CA-CB-CG	-5.43	107.17	112.60
1	C	871	GLU	CB-CA-C	-5.43	100.33	109.72
1	A	93	HIS	N-CA-C	-5.40	106.36	113.17
1	B	931	PHE	CA-C-O	5.39	122.80	119.29
1	B	661	LYS	CA-C-O	5.38	123.30	119.32
1	D	690	SER	N-CA-C	-5.38	101.68	109.59
1	B	893	GLU	CA-CB-CG	5.37	124.84	114.10
1	C	395	HIS	ND1-CE1-NE2	5.37	113.77	108.40
1	A	1004	SER	CA-CB-OG	-5.37	100.37	111.10
1	D	126	THR	CA-CB-OG1	-5.36	101.55	109.60
1	D	279	ILE	CB-CG1-CD1	-5.36	102.55	113.80
1	C	277	GLU	CA-CB-CG	-5.35	103.40	114.10
1	A	917	ARG	CD-NE-CZ	-5.35	116.91	124.40
1	C	469	ASP	CA-CB-CG	-5.35	107.25	112.60
1	B	733	ALA	N-CA-CB	5.34	117.86	109.69
1	C	917	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	477	SER	CB-CA-C	-5.30	102.52	110.90
1	A	593	GLY	CA-C-O	5.30	124.90	119.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	519	SER	N-CA-C	-5.29	102.78	110.24
1	A	356	ARG	NE-CZ-NH2	-5.29	114.44	119.20
1	A	299	LYS	CA-CB-CG	-5.29	103.53	114.10
1	D	728	VAL	CA-C-O	5.28	124.77	119.97
1	B	685	LEU	N-CA-C	5.27	119.17	109.10
1	A	20	GLY	N-CA-C	-5.27	108.42	115.32
1	A	274	PHE	CA-CB-CG	-5.27	108.53	113.80
1	C	382	ASN	CA-CB-CG	-5.27	107.33	112.60
1	D	719	GLN	CB-CA-C	-5.27	98.37	109.38
1	C	1000	SER	CA-CB-OG	-5.27	100.57	111.10
1	C	678	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	C	690	SER	N-CA-C	5.26	117.32	110.53
1	A	78	LEU	CA-C-O	5.25	123.97	119.66
1	C	345	ASN	CA-CB-CG	-5.24	107.36	112.60
1	D	279	ILE	CB-CA-C	5.23	115.77	110.65
1	B	688	PRO	CB-CA-C	-5.22	104.14	110.98
1	D	519	SER	N-CA-C	-5.21	102.89	110.24
1	A	599	ARG	NE-CZ-NH1	-5.21	116.29	121.50
1	A	155	ASN	CA-CB-CG	-5.20	107.40	112.60
1	D	633	GLY	CA-C-N	-5.19	114.50	122.60
1	D	633	GLY	C-N-CA	-5.19	114.50	122.60
1	C	473	ARG	NE-CZ-NH1	5.18	126.68	121.50
1	D	785	THR	CA-CB-OG1	-5.18	101.83	109.60
1	A	82	ASP	CA-CB-CG	-5.18	107.42	112.60
1	D	614	HIS	N-CA-C	-5.18	103.42	110.36
1	D	345	ASN	CA-CB-CG	-5.17	107.43	112.60
1	B	867	THR	CA-CB-OG1	-5.17	101.85	109.60
1	A	788	PRO	N-CA-CB	5.17	107.91	103.31
1	C	519	SER	N-CA-C	-5.16	102.97	110.24
1	B	539[A]	ALA	CB-CA-C	-5.16	100.15	110.42
1	B	539[B]	ALA	CB-CA-C	-5.16	100.15	110.42
1	C	521	LYS	CG-CD-CE	5.14	123.13	111.30
1	C	309	TYR	N-CA-C	-5.14	102.58	110.14
1	B	832	ASP	N-CA-CB	-5.13	102.97	111.49
1	A	19	PRO	N-CA-CB	5.13	108.23	103.41
1	C	809	ARG	CG-CD-NE	5.13	123.29	112.00
1	D	746	ASP	N-CA-C	5.13	116.87	109.07
1	C	147	ASN	N-CA-CB	-5.13	102.55	110.65
1	C	117	GLU	CB-CG-CD	-5.12	103.89	112.60
1	A	147	ASN	N-CA-CB	-5.12	102.67	110.65
1	A	687	GLN	C-N-CD	-5.11	104.03	125.00
1	B	634	GLN	CA-C-N	-5.11	115.66	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	634	GLN	C-N-CA	-5.11	115.66	122.72
1	C	688	PRO	CB-CA-C	-5.11	104.69	111.23
1	B	359	HIS	ND1-CG-CD2	5.11	111.20	106.10
1	A	719	GLN	CB-CA-C	-5.10	99.33	109.79
1	B	648	ASP	N-CA-C	5.10	118.64	112.93
1	C	219	THR	CA-CB-OG1	-5.10	101.95	109.60
1	B	987	ASP	CA-C-N	-5.09	113.76	120.22
1	B	987	ASP	C-N-CA	-5.09	113.76	120.22
1	C	359	HIS	CA-CB-CG	-5.09	108.71	113.80
1	D	1018	LEU	CB-CA-C	-5.08	98.28	109.56
1	D	980	GLU	CA-C-N	-5.08	109.25	120.99
1	D	980	GLU	C-N-CA	-5.08	109.25	120.99
1	D	980	GLU	N-CA-CB	-5.07	102.87	110.17
1	B	699	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	A	878	HIS	CA-CB-CG	-5.05	108.75	113.80
1	B	519	SER	N-CA-C	-5.05	103.12	110.24
1	C	469	ASP	CA-C-O	-5.04	115.21	120.55
1	C	297	ASN	CB-CA-C	-5.03	105.98	110.71
1	D	845	GLN	CB-CA-C	-5.03	103.76	111.66
1	C	745	MET	N-CA-C	5.03	117.87	111.69
1	A	14	ARG	CA-CB-CG	-5.03	104.05	114.10
1	C	784	PHE	CA-CB-CG	-5.02	108.78	113.80
1	A	63	PHE	CA-CB-CG	-5.02	108.78	113.80
1	C	648	ASP	CA-CB-CG	-5.01	107.59	112.60
1	A	553	TRP	CA-CB-CG	-5.01	104.08	113.60
1	B	770	ILE	CA-CB-CG1	-5.01	101.89	110.40

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	112	0
1	B	8128	0	7712	105	0
1	C	8128	0	7712	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	8128	0	7712	93	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	22	0
5	B	128	0	192	27	0
5	C	128	0	192	23	0
5	D	132	0	195	28	0
6	B	9	0	5	3	0
7	B	9	0	5	9	0
8	A	1144	0	0	15	0
8	B	1148	0	0	14	0
8	C	1126	0	0	18	0
8	D	1105	0	0	15	0
All	All	37685	0	31691	458	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (458) 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
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
5:D:8429:DMS:S	5:D:8429:DMS:C2	2.05	1.43
5:D:8704:DMS:C1	5:D:8704:DMS:S	2.05	1.43
5:B:8415:DMS:C2	5:B:8415:DMS:S	2.06	1.42
5:B:8508:DMS:C1	5:B:8508:DMS:S	2.11	1.37
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.47	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:GLN:H	1:A:634:GLN:NE2	1.44	1.12
1:B:655:MET:HE2	1:B:665:SER:HB3	1.43	1.00
1:C:230:ARG:NH1	5:C:8418:DMS:H12	1.79	0.98
1:D:809:ARG:HH11	1:D:809:ARG:HG2	1.27	0.98
1:B:685:LEU:HD23	1:B:686:PRO:HD2	1.45	0.95
1:B:600:GLN:H	1:B:600:GLN:HE21	1.15	0.94
1:C:816:TYR:CE1	1:C:968:MET:HE1	2.02	0.94
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.66	0.93
1:A:809:ARG:HG2	1:A:809:ARG:HH11	1.33	0.93
1:B:730:LEU:HD12	1:B:730:LEU:H	1.34	0.91
1:D:804:ASN:HD22	1:D:809:ARG:HH21	1.17	0.90
1:A:685:LEU:HD23	1:A:686:PRO:HD2	1.56	0.88
1:A:777:LEU:CD1	1:A:980:GLU:HG2	2.04	0.88
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.56	0.87
1:B:655:MET:CE	1:B:665:SER:HB3	2.06	0.85
1:A:634:GLN:H	1:A:634:GLN:HE21	1.23	0.85
1:C:745:MET:HA	1:C:761:GLN:HE22	1.44	0.83
1:B:230:ARG:HH21	5:B:8418:DMS:H12	1.45	0.82
5:A:8420:DMS:H22	8:D:9535:HOH:O	1.77	0.82
1:B:699:ARG:NH2	5:B:8415:DMS:H11	1.94	0.82
1:B:699:ARG:HH21	5:B:8415:DMS:H11	1.44	0.82
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.22	0.81
1:B:811:LYS:HD2	5:B:8424:DMS:H11	1.62	0.81
1:A:292:ARG:HH12	5:A:8412:DMS:C2	1.93	0.81
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.15	0.81
1:C:133:TRP:CD1	5:C:8504:DMS:H21	2.17	0.80
1:B:685:LEU:CD2	1:B:686:PRO:HD2	2.10	0.80
1:A:292:ARG:HH12	5:A:8412:DMS:H23	1.45	0.79
1:A:600:GLN:H	1:A:600:GLN:HE21	1.30	0.79
1:A:777:LEU:HD13	1:A:980:GLU:HG2	1.62	0.79
8:B:9512:HOH:O	5:C:8420:DMS:H22	1.81	0.79
5:C:8417:DMS:H22	8:C:9249:HOH:O	1.82	0.79
1:D:658:LEU:O	1:D:661:LYS:HG3	1.83	0.79
1:A:1023:LYS:HZ2	1:A:1023:LYS:CB	1.94	0.78
1:A:735:HIS:ND1	1:A:735:HIS:N	2.31	0.78
1:B:262:GLN:HE21	1:B:263:GLY:N	1.82	0.78
1:A:230:ARG:NH1	5:A:8418:DMS:H12	2.00	0.77
1:A:685:LEU:CD2	1:A:686:PRO:HD2	2.15	0.76
1:A:737:ILE:HD11	8:A:9656:HOH:O	1.85	0.76
5:D:8703:DMS:H21	8:D:9708:HOH:O	1.85	0.75
1:B:687:GLN:HG3	1:B:688:PRO:HD2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.17	0.75
1:C:367:MET:HB3	1:C:372:MET:HE3	1.69	0.74
1:C:745:MET:HG2	8:C:9490:HOH:O	1.87	0.74
1:A:973:ARG:O	5:A:8423:DMS:H12	1.87	0.74
1:C:367:MET:HE3	1:C:367:MET:HA	1.70	0.74
1:B:745:MET:HA	1:B:745:MET:HE2	1.70	0.73
1:B:863:GLN:HG2	1:B:1019:VAL:CG1	2.18	0.73
1:C:580:GLU:HG2	8:C:9648:HOH:O	1.88	0.73
1:A:634:GLN:NE2	1:A:634:GLN:N	2.29	0.73
1:A:1022:GLN:CG	1:A:1023:LYS:HZ1	2.02	0.73
1:D:292:ARG:HH12	5:D:8412:DMS:C2	2.02	0.73
1:D:655:MET:HE3	8:D:9610:HOH:O	1.89	0.73
1:A:655:MET:HE2	1:A:656:VAL:O	1.89	0.72
1:A:1022:GLN:HG2	1:A:1023:LYS:HE3	1.72	0.72
1:D:663:LEU:HD21	1:D:686:PRO:HG2	1.72	0.72
1:A:277:GLU:H	1:A:277:GLU:CD	1.96	0.72
1:B:651:LEU:O	1:B:651:LEU:HD23	1.90	0.71
1:B:1017:GLN:HB2	8:B:9693:HOH:O	1.89	0.71
1:B:685:LEU:HD23	1:B:686:PRO:CD	2.20	0.71
1:C:653:HIS:ND1	1:C:667:GLU:HG2	2.06	0.71
1:C:788:PRO:HD3	1:C:968:MET:HE3	1.72	0.71
1:B:233:ASP:HA	5:B:8417:DMS:H13	1.71	0.70
5:D:8421:DMS:H12	8:D:9369:HOH:O	1.91	0.70
1:B:863:GLN:HG3	1:B:1021:CYS:HB3	1.71	0.70
1:B:1022:GLN:HG2	1:B:1023:LYS:N	2.05	0.70
1:C:230:ARG:CZ	5:C:8418:DMS:H12	2.20	0.70
1:C:765:LEU:HD21	1:C:768:MET:HE2	1.72	0.69
1:D:685:LEU:HB3	1:D:686:PRO:CD	2.20	0.69
1:A:804:ASN:OD1	1:A:809:ARG:NH2	2.26	0.69
1:B:262:GLN:HE21	1:B:262:GLN:C	2.01	0.69
1:C:788:PRO:HD3	1:C:968:MET:CE	2.22	0.69
1:D:797:GLU:O	1:D:801:ILE:HD13	1.93	0.69
1:A:797:GLU:O	1:A:801:ILE:HD13	1.93	0.68
1:C:630:ARG:HD3	1:C:637:GLU:OE1	1.93	0.67
1:D:135:GLN:C	1:D:136:GLU:HG2	2.19	0.67
1:D:134:LEU:HA	5:D:8705:DMS:H23	1.76	0.66
1:C:133:TRP:NE1	5:C:8504:DMS:H21	2.11	0.66
1:C:278:ILE:HD13	1:C:278:ILE:N	2.11	0.66
1:A:861:SER:OG	1:A:863:GLN:HG3	1.95	0.66
1:C:356:ARG:HD2	1:C:379:MET:CE	2.26	0.65
1:D:809:ARG:HG2	1:D:809:ARG:NH1	2.04	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:ARG:NH1	1:B:477:SER:HB2	2.11	0.65
1:A:770:ILE:O	1:A:773:LYS:HD3	1.97	0.65
5:B:8428:DMS:H13	8:B:9754:HOH:O	1.96	0.65
1:C:754:LYS:NZ	1:C:1022:GLN:OE1	2.29	0.65
1:B:36:TRP:CZ2	5:B:8501:DMS:H11	2.32	0.65
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.77	0.65
1:A:1022:GLN:CD	1:A:1023:LYS:HZ1	2.05	0.64
1:D:237:ARG:NH1	1:D:296:GLU:OE2	2.30	0.64
1:B:878:HIS:HD2	8:B:8805:HOH:O	1.79	0.64
1:D:102:ASN:ND2	5:D:8506:DMS:H11	2.12	0.64
1:A:685:LEU:HD23	1:A:686:PRO:CD	2.26	0.64
1:B:863:GLN:HG2	1:B:1019:VAL:HG11	1.79	0.64
1:C:230:ARG:NH1	8:C:8967:HOH:O	2.30	0.64
1:B:655:MET:HE2	1:B:665:SER:CB	2.26	0.64
1:B:890:GLN:HB2	8:B:9801:HOH:O	1.98	0.63
1:D:687:GLN:N	1:D:687:GLN:OE1	2.31	0.63
1:A:878:HIS:HD2	8:A:8676:HOH:O	1.81	0.63
1:B:1022:GLN:HG2	1:B:1023:LYS:O	1.99	0.63
1:C:292:ARG:HH12	5:C:8412:DMS:H23	1.63	0.62
1:A:251:ARG:HH11	5:A:8416:DMS:H23	1.64	0.62
1:D:708:TRP:CZ2	5:D:8403:DMS:H13	2.34	0.62
1:A:372:MET:HE1	1:A:395:HIS:HB3	1.82	0.62
1:C:708:TRP:CZ2	5:C:8403:DMS:H13	2.35	0.62
1:D:663:LEU:CD2	1:D:686:PRO:HG2	2.29	0.62
1:A:768:MET:HE1	1:A:1020:TRP:CE2	2.34	0.62
1:C:651:LEU:HD12	1:C:651:LEU:C	2.24	0.62
1:A:1022:GLN:HG2	1:A:1023:LYS:CE	2.30	0.62
1:C:768:MET:HE1	1:C:1020:TRP:CH2	2.35	0.62
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.35	0.61
1:B:600:GLN:HE21	1:B:600:GLN:N	1.94	0.61
1:D:230:ARG:HH21	5:D:8418:DMS:H12	1.64	0.61
1:D:134:LEU:CA	5:D:8705:DMS:H23	2.31	0.61
1:D:685:LEU:HB3	1:D:686:PRO:HD2	1.83	0.61
1:B:745:MET:HE2	1:B:745:MET:CA	2.29	0.61
1:D:748:CYS:C	1:D:749:ILE:HD12	2.25	0.61
5:B:8410:DMS:H22	8:B:8992:HOH:O	2.00	0.61
1:D:292:ARG:HH12	5:D:8412:DMS:H23	1.64	0.61
5:D:8429:DMS:C2	5:D:8429:DMS:C1	2.78	0.61
5:C:8415:DMS:H11	8:C:9662:HOH:O	2.00	0.61
1:A:651:LEU:C	1:A:651:LEU:HD12	2.25	0.60
1:D:749:ILE:HD12	1:D:749:ILE:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:878:HIS:HD2	8:C:8701:HOH:O	1.84	0.60
1:A:595:THR:HA	1:A:596:PRO:C	2.25	0.60
1:D:618:THR:HG21	8:D:9060:HOH:O	2.00	0.60
1:A:231:PHE:O	5:A:8417:DMS:H23	2.02	0.60
1:C:595:THR:HG22	5:C:8413:DMS:S	2.41	0.60
1:B:157:ARG:HD3	8:B:9582:HOH:O	2.02	0.59
1:D:508:GLU:OE2	5:D:8407:DMS:H11	2.02	0.59
1:A:367:MET:HB3	1:A:372:MET:HE3	1.82	0.59
1:A:777:LEU:HD11	1:A:980:GLU:HG2	1.83	0.59
1:B:687:GLN:HG3	1:B:688:PRO:CD	2.30	0.59
1:C:178:ARG:HD2	8:C:9579:HOH:O	2.01	0.59
1:D:233:ASP:HA	5:D:8417:DMS:H13	1.85	0.59
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.37	0.59
1:A:102:ASN:ND2	5:A:8506:DMS:H11	2.17	0.59
1:A:773:LYS:HD3	1:A:773:LYS:H	1.67	0.59
1:B:730:LEU:H	1:B:730:LEU:CD1	1.95	0.59
1:D:579:ASP:OD1	1:D:581:ASN:HB2	2.01	0.59
1:A:887:GLN:NE2	1:A:980:GLU:O	2.34	0.59
1:D:878:HIS:HD2	8:D:8818:HOH:O	1.85	0.59
1:D:363:HIS:HD2	8:D:9332:HOH:O	1.84	0.58
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.86	0.58
1:D:973:ARG:O	5:D:8423:DMS:H12	2.03	0.58
1:B:615:PRO:O	1:B:618:THR:HG22	2.03	0.58
1:B:797:GLU:O	1:B:801:ILE:HD13	2.04	0.58
1:D:134:LEU:C	5:D:8705:DMS:H23	2.29	0.58
1:A:1023:LYS:HZ2	1:A:1023:LYS:HB2	1.69	0.58
1:C:237:ARG:NH1	1:C:237:ARG:HB3	2.19	0.58
1:C:367:MET:HE3	1:C:367:MET:CA	2.33	0.57
1:A:688:PRO:C	1:A:690:SER:H	2.11	0.57
1:D:664:ALA:HB3	1:D:685:LEU:CD2	2.34	0.57
1:A:372:MET:HE2	8:A:8795:HOH:O	2.03	0.57
1:C:473:ARG:NH2	8:C:8614:HOH:O	2.37	0.57
1:D:595:THR:HA	1:D:596:PRO:C	2.29	0.57
1:C:749:ILE:N	1:C:749:ILE:HD12	2.20	0.57
1:C:367:MET:HB3	1:C:372:MET:CE	2.34	0.56
5:C:8420:DMS:H21	8:C:9688:HOH:O	2.04	0.56
1:A:387:VAL:HG22	8:A:9694:HOH:O	2.06	0.56
1:B:658:LEU:HB2	1:B:663:LEU:HD11	1.87	0.56
1:B:800:ARG:HD3	8:B:9817:HOH:O	2.06	0.56
1:C:240:LEU:C	1:C:240:LEU:HD23	2.31	0.56
1:C:811:LYS:HD2	5:C:8424:DMS:C1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:LEU:HD23	1:B:651:LEU:C	2.31	0.55
1:D:134:LEU:O	5:D:8705:DMS:H23	2.07	0.55
1:D:473:ARG:NE	8:D:9481:HOH:O	2.31	0.55
1:D:618:THR:HG23	8:D:9077:HOH:O	2.05	0.55
1:A:809:ARG:HH11	1:A:809:ARG:CG	2.12	0.55
1:A:521:LYS:HE2	8:A:9035:HOH:O	2.07	0.55
1:A:646:HIS:ND1	8:A:9463:HOH:O	2.28	0.54
1:B:36:TRP:HZ2	5:B:8501:DMS:C1	2.21	0.54
1:A:797:GLU:HB3	1:A:799:THR:HG23	1.89	0.54
1:B:699:ARG:HH21	5:B:8415:DMS:C1	2.17	0.54
1:D:663:LEU:CD2	1:D:686:PRO:HD2	2.37	0.54
1:A:654:TRP:CZ2	1:A:683:PRO:HG2	2.43	0.54
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.90	0.54
1:B:363:HIS:HD2	8:B:9311:HOH:O	1.90	0.54
1:A:88:SER:HA	1:A:366:VAL:HG21	1.90	0.54
1:B:230:ARG:HH21	5:B:8418:DMS:C1	2.20	0.54
5:D:8428:DMS:H23	8:D:9768:HOH:O	2.07	0.54
1:A:708:TRP:CZ2	5:A:8403:DMS:H13	2.43	0.54
1:B:230:ARG:NH2	5:B:8418:DMS:H12	2.21	0.54
1:B:639:THR:OG1	1:B:677:LYS:HD3	2.08	0.54
1:B:699:ARG:NH1	8:B:9823:HOH:O	2.41	0.53
1:B:797:GLU:HG2	1:B:799:THR:HG23	1.89	0.53
1:C:595:THR:HA	1:C:596:PRO:C	2.33	0.53
1:C:266:GLN:HE21	5:C:8602:DMS:H23	1.75	0.52
1:C:367:MET:HE1	8:C:9665:HOH:O	2.09	0.52
1:B:36:TRP:HZ2	5:B:8501:DMS:H11	1.72	0.52
1:A:292:ARG:NH1	5:A:8412:DMS:H23	2.21	0.52
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.90	0.52
1:C:724:GLU:O	1:D:847:LYS:NZ	2.42	0.51
1:A:764:PHE:CE2	1:A:781:ARG:NH1	2.78	0.51
1:C:653:HIS:CE1	1:C:667:GLU:HG2	2.46	0.51
1:A:251:ARG:HA	5:A:8416:DMS:S	2.51	0.51
1:A:634:GLN:H	1:A:634:GLN:CD	2.07	0.50
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.94	0.50
5:A:8428:DMS:H12	8:A:8812:HOH:O	2.11	0.50
1:B:634:GLN:HG2	1:B:682:LEU:O	2.12	0.50
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.12	0.50
1:C:651:LEU:CD1	1:C:653:HIS:CE1	2.95	0.50
1:A:1022:GLN:CD	1:A:1023:LYS:NZ	2.70	0.50
1:B:713:HIS:ND1	8:B:9513:HOH:O	2.35	0.50
1:D:634:GLN:OE1	1:D:682:LEU:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:LEU:O	1:C:659:ASP:C	2.53	0.50
1:A:46:ARG:HB3	1:A:47:PRO:HD2	1.94	0.49
1:A:688:PRO:O	1:A:690:SER:N	2.45	0.49
5:B:8407:DMS:C2	5:B:8407:DMS:C1	2.89	0.49
5:D:8429:DMS:H21	8:D:9343:HOH:O	2.11	0.49
1:A:668:VAL:HG12	1:A:669:PRO:O	2.12	0.49
1:A:699:ARG:NH2	8:A:9479:HOH:O	2.46	0.49
1:B:595:THR:HA	1:B:596:PRO:C	2.37	0.49
1:B:600:GLN:H	1:B:600:GLN:NE2	1.97	0.49
1:D:664:ALA:CB	1:D:685:LEU:HD23	2.42	0.49
1:A:738:PRO:HD3	1:A:751:LEU:HD13	1.95	0.49
1:A:773:LYS:HD3	1:A:773:LYS:N	2.27	0.49
1:C:835:LEU:HD11	1:C:855:THR:HB	1.93	0.49
1:C:844:HIS:HD2	8:C:9496:HOH:O	1.95	0.49
1:D:133:TRP:NE1	5:D:8703:DMS:H23	2.28	0.49
1:C:824:GLN:HG3	1:C:825:CYS:N	2.28	0.49
1:B:127:PHE:CE1	1:B:184:LEU:HG	2.48	0.49
1:C:634:GLN:OE1	1:C:635:THR:OG1	2.29	0.49
1:A:685:LEU:O	1:A:687:GLN:NE2	2.46	0.49
1:C:667:GLU:C	1:C:668:VAL:HG23	2.37	0.48
1:C:824:GLN:CG	1:C:825:CYS:N	2.74	0.48
1:C:651:LEU:HD12	1:C:651:LEU:O	2.12	0.48
1:C:730:LEU:HD12	1:C:730:LEU:H	1.78	0.48
1:D:663:LEU:HD23	1:D:686:PRO:HD2	1.95	0.48
1:A:292:ARG:HH12	5:A:8412:DMS:H21	1.75	0.48
1:A:738:PRO:HD3	1:A:860:GLY:HA2	1.94	0.48
1:C:127:PHE:CE1	1:C:184:LEU:HG	2.48	0.48
1:A:230:ARG:NH1	5:A:8418:DMS:C1	2.76	0.48
1:C:147:ASN:HA	1:C:148:SER:HA	1.64	0.48
1:A:867:THR:HB	8:A:9360:HOH:O	2.13	0.48
1:A:147:ASN:HA	1:A:148:SER:HA	1.60	0.48
1:C:615:PRO:O	1:C:618:THR:HG22	2.13	0.47
1:D:372:MET:HE1	1:D:395:HIS:HB3	1.96	0.47
1:B:655:MET:SD	1:B:656:VAL:N	2.88	0.47
1:A:742:THR:HG22	1:A:743:SER:N	2.28	0.47
1:D:367:MET:HB3	1:D:372:MET:HE3	1.96	0.47
1:C:748:CYS:C	1:C:749:ILE:HD12	2.39	0.47
1:D:686:PRO:O	1:D:687:GLN:HG3	2.14	0.47
1:C:734:SER:HB3	1:C:860:GLY:HA3	1.96	0.47
1:A:178:ARG:HD2	8:A:9492:HOH:O	2.13	0.47
1:C:655:MET:CE	1:C:662:PRO:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:GLU:HA	1:B:75:GLU:OE1	2.13	0.47
1:B:635:THR:OG1	1:B:681:GLU:OE2	2.28	0.47
1:B:746:ASP:OD1	1:B:757:GLN:NE2	2.45	0.47
5:B:8423:DMS:H11	8:B:9818:HOH:O	2.13	0.47
1:C:730:LEU:H	1:C:730:LEU:CD1	2.04	0.47
1:C:811:LYS:HD2	5:C:8424:DMS:H11	1.96	0.47
1:D:755:ARG:HG3	1:D:769:TRP:HB2	1.97	0.47
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.95	0.47
1:B:687:GLN:CG	1:B:688:PRO:HD2	2.42	0.47
1:B:708:TRP:CZ2	5:B:8403:DMS:H13	2.50	0.47
1:D:88:SER:HA	1:D:366:VAL:HG21	1.97	0.47
1:C:655:MET:SD	1:C:656:VAL:N	2.88	0.46
1:D:251:ARG:NH2	8:D:9800:HOH:O	2.47	0.46
1:B:685:LEU:CG	1:B:686:PRO:HD2	2.45	0.46
1:C:88:SER:HA	1:C:366:VAL:HG21	1.96	0.46
1:C:997:ASP:HB2	1:C:999:TRP:CZ2	2.50	0.46
1:B:230:ARG:NH2	5:B:8418:DMS:C1	2.78	0.46
1:D:708:TRP:CH2	5:D:8403:DMS:H13	2.50	0.46
1:C:968:MET:HE2	5:C:8424:DMS:O	2.16	0.46
1:D:651:LEU:HD12	1:D:668:VAL:O	2.14	0.46
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.41	0.46
1:D:128:ASN:HB3	1:D:180:GLY:O	2.15	0.46
1:D:688:PRO:C	1:D:690:SER:H	2.23	0.46
1:C:653:HIS:CE1	1:C:667:GLU:CG	3.00	0.45
1:D:292:ARG:NH1	5:D:8412:DMS:H23	2.30	0.45
1:C:320:GLY:HA2	5:C:8406:DMS:O	2.16	0.45
1:C:781:ARG:NH1	8:C:9379:HOH:O	2.49	0.45
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.98	0.45
1:B:292:ARG:NH1	5:B:8412:DMS:H23	2.31	0.45
1:B:824:GLN:OE1	1:B:837:THR:HG22	2.16	0.45
1:C:13:ARG:O	1:C:14:ARG:C	2.59	0.45
1:C:237:ARG:NH1	1:C:237:ARG:CB	2.79	0.45
1:A:252:ASP:CG	5:A:8416:DMS:H12	2.41	0.45
1:C:356:ARG:CD	1:C:379:MET:HE1	2.46	0.45
1:C:651:LEU:CD1	1:C:653:HIS:ND1	2.80	0.45
1:C:372:MET:HE1	1:C:395:HIS:HB3	1.99	0.45
1:D:663:LEU:HD23	1:D:686:PRO:CD	2.46	0.45
1:A:1022:GLN:NE2	1:A:1023:LYS:HE2	2.32	0.45
1:C:595:THR:HG23	1:C:595:THR:O	2.15	0.45
1:D:240:LEU:HD23	1:D:240:LEU:C	2.42	0.45
1:B:147:ASN:HA	1:B:148:SER:HA	1.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:787:ALA:HA	1:C:968:MET:HE3	1.99	0.45
1:A:783:GLN:HG2	1:A:881:ARG:HD2	1.99	0.45
1:A:819:GLU:HG3	8:A:9703:HOH:O	2.17	0.45
1:A:997:ASP:HB2	1:A:999:TRP:CZ2	2.52	0.44
1:B:670:LEU:HD23	1:B:670:LEU:HA	1.81	0.44
1:D:725:ASN:HB2	8:D:9591:HOH:O	2.17	0.44
1:B:847:LYS:HG3	1:B:848:THR:N	2.32	0.44
1:C:973:ARG:O	5:C:8423:DMS:H12	2.17	0.44
1:D:887:GLN:OE1	1:D:980:GLU:O	2.36	0.44
1:C:625:GLN:NE2	8:C:8830:HOH:O	2.45	0.44
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.34	0.44
1:C:634:GLN:CD	1:C:634:GLN:H	2.02	0.44
1:A:46:ARG:HB3	1:A:47:PRO:CD	2.47	0.44
1:B:809:ARG:NH2	8:B:9728:HOH:O	2.51	0.44
1:D:829:THR:O	1:D:830:LEU:HD23	2.17	0.44
1:A:239:VAL:HG23	5:A:8418:DMS:H22	1.99	0.44
1:A:600:GLN:HE21	1:A:600:GLN:N	2.07	0.44
1:B:824:GLN:HG2	1:B:825:CYS:N	2.33	0.44
1:C:237:ARG:CB	1:C:237:ARG:HH11	2.31	0.44
1:A:251:ARG:HG3	1:A:253:TYR:CZ	2.52	0.44
1:A:687:GLN:HG3	8:A:9470:HOH:O	2.18	0.44
1:B:13:ARG:O	1:B:14:ARG:C	2.61	0.44
1:B:262:GLN:CA	1:B:262:GLN:NE2	2.80	0.44
1:A:127:PHE:CE1	1:A:184:LEU:HG	2.52	0.43
5:B:8420:DMS:H13	8:C:9240:HOH:O	2.18	0.43
5:B:8501:DMS:H23	8:B:9183:HOH:O	2.18	0.43
1:C:751:LEU:HD21	1:C:860:GLY:O	2.19	0.43
1:A:685:LEU:CB	1:A:686:PRO:HD2	2.48	0.43
1:C:890:GLN:HG3	1:C:891:VAL:N	2.33	0.43
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.54	0.43
1:B:731:PRO:O	1:B:732:ALA:HB2	2.17	0.43
1:A:720:TRP:HA	5:A:8428:DMS:H13	2.00	0.43
1:C:230:ARG:HG3	5:C:8418:DMS:C1	2.49	0.43
1:C:718:GLN:HG2	5:C:8503:DMS:C1	2.48	0.43
1:A:663:LEU:HD22	1:A:663:LEU:HA	1.71	0.43
1:A:756:TRP:CD2	1:A:858:ILE:HD13	2.53	0.43
1:D:128:ASN:HB2	8:D:9726:HOH:O	2.19	0.43
1:B:663:LEU:HD12	1:B:694:LEU:CD2	2.49	0.43
1:D:629:PHE:O	1:D:630:ARG:HD3	2.18	0.43
1:A:844:HIS:O	1:A:845:GLN:C	2.60	0.43
5:A:8406:DMS:H22	8:A:9450:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:LEU:HB3	1:C:434:PRO:HD3	2.00	0.43
1:D:770:ILE:HD13	1:D:770:ILE:HA	1.67	0.43
1:A:654:TRP:HZ2	1:A:683:PRO:HG2	1.83	0.43
5:A:8428:DMS:H21	8:A:8979:HOH:O	2.18	0.43
1:D:658:LEU:O	1:D:659:ASP:C	2.62	0.43
1:D:230:ARG:NH2	5:D:8418:DMS:H12	2.31	0.43
1:D:754:LYS:HG2	1:D:770:ILE:CD1	2.48	0.43
1:B:88:SER:HA	1:B:366:VAL:HG21	2.01	0.43
1:C:275:GLY:O	5:C:8412:DMS:H12	2.19	0.43
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.01	0.43
1:D:664:ALA:HB3	1:D:685:LEU:HD23	2.00	0.43
1:D:720:TRP:NE1	5:D:8503:DMS:O	2.48	0.43
1:D:78:LEU:HD23	1:D:78:LEU:HA	1.89	0.42
1:D:688:PRO:C	1:D:690:SER:N	2.76	0.42
1:A:890:GLN:OE1	1:A:948:PRO:HD3	2.19	0.42
1:B:70:PRO:HG2	1:B:78:LEU:HD21	2.01	0.42
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.19	0.42
1:B:577:LYS:HB3	1:B:577:LYS:HE3	1.87	0.42
1:C:768:MET:HE1	1:C:1020:TRP:CZ2	2.54	0.42
1:D:682:LEU:HD23	1:D:682:LEU:HA	1.76	0.42
5:A:8420:DMS:H23	8:A:9735:HOH:O	2.20	0.42
1:B:262:GLN:NE2	1:B:262:GLN:HA	2.34	0.42
1:C:997:ASP:HB2	1:C:999:TRP:CE2	2.54	0.42
1:D:577:LYS:O	1:D:584:PRO:HA	2.19	0.42
1:A:59:ARG:NH2	1:A:81:ALA:HB3	2.35	0.42
1:A:240:LEU:C	1:A:240:LEU:HD23	2.45	0.42
1:A:538:TYR:C	1:A:539[B]:ALA:O	2.62	0.42
1:B:133:TRP:CD1	5:B:8504:DMS:H12	2.55	0.42
1:D:133:TRP:HE1	5:D:8703:DMS:H23	1.84	0.42
1:A:719:GLN:O	5:A:8428:DMS:H13	2.19	0.42
1:A:859:ASP:OD1	1:A:861:SER:OG	2.27	0.42
5:D:8423:DMS:C1	5:D:8423:DMS:C2	2.96	0.42
1:A:472:TYR:O	1:A:476:LYS:HG2	2.20	0.42
1:B:658:LEU:O	1:B:659:ASP:C	2.61	0.42
1:B:1022:GLN:HG2	1:B:1023:LYS:H	1.83	0.42
1:C:655:MET:SD	1:C:656:VAL:O	2.77	0.42
1:C:472:TYR:OH	1:C:476:LYS:HE2	2.19	0.42
1:C:995:GLY:O	1:C:996:ASP:C	2.62	0.42
1:D:844:HIS:O	1:D:845:GLN:C	2.61	0.42
1:A:658:LEU:O	1:A:659:ASP:C	2.62	0.42
1:A:688:PRO:O	1:A:689:GLU:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:LEU:HD13	1:C:653:HIS:ND1	2.35	0.42
1:C:859:ASP:OD1	1:C:861:SER:OG	2.27	0.42
1:D:650:GLU:HB3	1:D:670:LEU:HD12	2.02	0.42
1:A:986:ILE:HD12	1:A:986:ILE:HG21	1.83	0.42
1:A:1022:GLN:CG	1:A:1023:LYS:NZ	2.80	0.42
1:B:646:HIS:CE1	1:B:673:ALA:HA	2.54	0.42
1:C:127:PHE:HE1	1:C:184:LEU:HG	1.85	0.42
1:D:893:GLU:HG2	1:D:894:ARG:HG2	2.02	0.42
1:D:699:ARG:HE	1:D:699:ARG:HB3	1.51	0.42
1:A:684:GLU:HG2	1:A:685:LEU:N	2.35	0.41
1:A:688:PRO:C	1:A:690:SER:N	2.78	0.41
1:B:651:LEU:HD22	1:B:701:VAL:O	2.20	0.41
1:B:763:GLY:HA3	1:B:822:LEU:HD13	2.01	0.41
1:A:98:PRO:HB2	1:A:203:TRP:CE3	2.55	0.41
1:A:111:PRO:HA	1:A:112:PRO:HA	1.85	0.41
1:A:668:VAL:HG13	1:A:669:PRO:HD2	2.02	0.41
1:D:46:ARG:HB3	1:D:47:PRO:HD2	2.02	0.41
1:A:1022:GLN:NE2	1:A:1023:LYS:CE	2.84	0.41
1:B:114:VAL:HB	1:B:115:PRO:HD2	2.01	0.41
1:C:653:HIS:ND1	1:C:667:GLU:CG	2.78	0.41
1:D:538:TYR:C	1:D:539[B]:ALA:O	2.61	0.41
1:B:730:LEU:HD12	1:B:730:LEU:N	2.17	0.41
5:C:8503:DMS:H13	8:C:9050:HOH:O	2.20	0.41
1:D:788:PRO:HD2	1:D:968:MET:HG3	2.03	0.41
1:A:634:GLN:HE21	1:A:634:GLN:N	2.03	0.41
1:B:699:ARG:HE	1:B:714:ILE:HD13	1.85	0.41
1:B:910:LEU:C	1:B:910:LEU:HD12	2.46	0.41
1:D:545:SER:O	1:D:909:ARG:HD3	2.21	0.41
1:B:240:LEU:C	1:B:240:LEU:HD23	2.46	0.41
1:B:864:MET:HE3	1:B:866:ILE:HD11	2.03	0.41
1:C:749:ILE:O	1:C:755:ARG:HA	2.21	0.41
1:D:844:HIS:O	1:D:845:GLN:HB2	2.20	0.41
1:B:475:ILE:HG21	1:B:475:ILE:HD13	1.86	0.41
1:C:363:HIS:HD2	8:C:9215:HOH:O	2.03	0.41
1:D:230:ARG:NH2	5:D:8418:DMS:C1	2.84	0.41
1:D:635:THR:HG23	1:D:681:GLU:CD	2.45	0.41
1:D:663:LEU:CD2	1:D:686:PRO:CG	2.98	0.41
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.37	0.41
1:C:538:TYR:C	1:C:539[B]:ALA:O	2.63	0.41
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.56	0.41
1:C:788:PRO:CD	1:C:968:MET:HE3	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:513:PRO:O	1:D:514:ALA:HB3	2.21	0.41
8:D:9024:HOH:O	2:H:2:GAL:C4	2.68	0.41
1:B:13:ARG:NH1	8:C:8622:HOH:O	2.54	0.41
1:B:106:PRO:O	5:B:8419:DMS:H21	2.21	0.41
1:B:655:MET:HE2	1:B:655:MET:HB2	1.87	0.41
1:A:460:ASN:O	1:A:461:GLU:C	2.64	0.40
1:A:737:ILE:HD12	1:A:738:PRO:O	2.21	0.40
1:B:663:LEU:CD1	1:B:694:LEU:HD21	2.51	0.40
1:C:278:ILE:HD12	1:C:278:ILE:HA	1.82	0.40
1:C:653:HIS:CE1	1:C:667:GLU:CD	2.99	0.40
1:B:37:ARG:NH1	5:B:8504:DMS:H21	2.36	0.40
1:B:127:PHE:N	1:B:127:PHE:CD1	2.90	0.40
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.50	0.40
1:C:746:ASP:HA	1:C:760:ARG:HG3	2.03	0.40
1:B:360:HIS:HE1	1:B:362:LEU:HD12	1.85	0.40
1:B:646:HIS:ND1	1:B:673:ALA:HA	2.37	0.40
1:B:835:LEU:HD11	1:B:855:THR:HB	2.04	0.40
1:C:811:LYS:HD2	5:C:8424:DMS:S	2.62	0.40
1:C:569:ASP:HB2	8:C:9439:HOH:O	2.22	0.40
1:C:819:GLU:H	1:C:819:GLU:HG2	1.25	0.40
1:D:687:GLN:HA	1:D:688:PRO:HD3	1.48	0.40
1:D:901:GLY:HA3	1:D:902:PRO:HA	1.91	0.40
1:A:427:THR:HG21	1:A:462:SER:HB3	2.02	0.40
1:B:685:LEU:O	1:B:686:PRO:C	2.64	0.40
1:C:416:GLU:OE2	1:C:418:HIS:HB2	2.21	0.40
1:D:472:TYR:O	1:D:476:LYS:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	48 24
1	B	1011/1023 (99%)	976 (96%)	31 (3%)	4 (0%)	30 12
1	C	1011/1023 (99%)	979 (97%)	31 (3%)	1 (0%)	48 24
1	D	1011/1023 (99%)	978 (97%)	29 (3%)	4 (0%)	30 12
All	All	4044/4092 (99%)	3910 (97%)	124 (3%)	10 (0%)	43 22

All (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
1	D	539[B]	ALA
1	C	164	ASP
1	D	164	ASP
1	A	164	ASP
1	B	164	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	865/875 (99%)	837 (97%)	28 (3%)	34 8
1	B	865/875 (99%)	841 (97%)	24 (3%)	38 11
1	C	865/875 (99%)	836 (97%)	29 (3%)	32 7
1	D	865/875 (99%)	837 (97%)	28 (3%)	34 8
All	All	3460/3500 (99%)	3351 (97%)	109 (3%)	34 8

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	GLU

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Mol	Chain	Res	Type
1	A	250	LEU
1	A	262	GLN
1	A	277	GLU
1	A	344	LEU
1	A	519	SER
1	A	546	LEU
1	A	580	GLU
1	A	595	THR
1	A	600	GLN
1	A	634	GLN
1	A	655	MET
1	A	663	LEU
1	A	667	GLU
1	A	672	VAL
1	A	682	LEU
1	A	684	GLU
1	A	689	GLU
1	A	735	HIS
1	A	737	ILE
1	A	773	LYS
1	A	799	THR
1	A	809	ARG
1	A	817	GLN
1	A	885	ASN
1	A	986	ILE
1	A	1017	GLN
1	A	1023	LYS
1	B	71	GLU
1	B	76	CYS
1	B	80	GLU
1	B	237	ARG
1	B	262	GLN
1	B	264	GLU
1	B	344	LEU
1	B	367	MET
1	B	370	GLN
1	B	478	VAL
1	B	546	LEU
1	B	600	GLN
1	B	634	GLN
1	B	651	LEU
1	B	681	GLU

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Mol	Chain	Res	Type
1	B	685	LEU
1	B	687	GLN
1	B	690	SER
1	B	730	LEU
1	B	799	THR
1	B	819	GLU
1	B	847	LYS
1	B	863	GLN
1	B	986	ILE
1	C	49	GLN
1	C	71	GLU
1	C	75	GLU
1	C	80	GLU
1	C	135	GLN
1	C	189	LEU
1	C	264	GLU
1	C	278	ILE
1	C	344	LEU
1	C	367	MET
1	C	370	GLN
1	C	546	LEU
1	C	580	GLU
1	C	634	GLN
1	C	663	LEU
1	C	672	VAL
1	C	681	GLU
1	C	684	GLU
1	C	685	LEU
1	C	687	GLN
1	C	690	SER
1	C	730	LEU
1	C	737	ILE
1	C	750	GLU
1	C	772	ASP
1	C	773	LYS
1	C	819	GLU
1	C	986	ILE
1	C	1023	LYS
1	D	13	ARG
1	D	80	GLU
1	D	112	PRO
1	D	277	GLU

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Mol	Chain	Res	Type
1	D	344	LEU
1	D	370	GLN
1	D	519	SER
1	D	546	LEU
1	D	652	LEU
1	D	655	MET
1	D	661	LYS
1	D	663	LEU
1	D	687	GLN
1	D	699	ARG
1	D	735	HIS
1	D	737	ILE
1	D	755	ARG
1	D	772	ASP
1	D	773	LYS
1	D	797	GLU
1	D	799	THR
1	D	809	ARG
1	D	845	GLN
1	D	893	GLU
1	D	956	GLN
1	D	986	ILE
1	D	1017	GLN
1	D	1022	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	163	GLN
1	A	445	GLN
1	A	485	GLN
1	A	600	GLN
1	A	624	GLN
1	A	634	GLN
1	A	704	ASN
1	A	757	GLN
1	A	817	GLN
1	A	844	HIS
1	A	878	HIS
1	A	977	HIS
1	A	1017	GLN

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Mol	Chain	Res	Type
1	A	1022	GLN
1	B	262	GLN
1	B	294	ASN
1	B	363	HIS
1	B	365	GLN
1	B	485	GLN
1	B	581	ASN
1	B	600	GLN
1	B	624	GLN
1	B	628	GLN
1	B	646	HIS
1	B	675	GLN
1	B	687	GLN
1	B	704	ASN
1	B	843	GLN
1	B	878	HIS
1	B	885	ASN
1	B	945	ASN
1	B	950	GLN
1	B	977	HIS
1	C	163	GLN
1	C	266	GLN
1	C	363	HIS
1	C	445	GLN
1	C	485	GLN
1	C	646	HIS
1	C	704	ASN
1	C	761	GLN
1	C	843	GLN
1	C	844	HIS
1	C	878	HIS
1	C	977	HIS
1	C	1017	GLN
1	D	163	GLN
1	D	262	GLN
1	D	363	HIS
1	D	485	GLN
1	D	624	GLN
1	D	804	ASN
1	D	843	GLN
1	D	878	HIS
1	D	887	GLN

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Mol	Chain	Res	Type
1	D	903	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	0.81	0	17,17,17	1.10	2 (11%)
2	GAL	E	2	2,4	11,11,12	1.62	3 (27%)	15,15,17	1.44	2 (13%)
2	GAL	F	2	2,4	11,11,12	1.48	2 (18%)	15,15,17	1.49	4 (26%)
2	BGC	G	1	2	12,12,12	1.17	1 (8%)	17,17,17	1.32	1 (5%)
2	GAL	G	2	2,4	11,11,12	1.58	2 (18%)	15,15,17	1.10	2 (13%)
2	BGC	H	1	2	12,12,12	1.15	1 (8%)	17,17,17	0.86	0
2	GAL	H	2	2,4	11,11,12	1.55	3 (27%)	15,15,17	1.14	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	E	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	F	1[A]	-	1/1/5/5	-	-
2	GAL	F	2	2,4	-	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	2,4	-	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	2,4	-	1/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	GAL	O4-C4	3.31	1.51	1.43
2	H	2	GAL	O4-C4	3.21	1.50	1.43
2	E	2	GAL	O4-C4	3.12	1.50	1.43
2	G	2	GAL	O4-C4	2.90	1.50	1.43
2	G	1	BGC	O2-C2	2.64	1.49	1.43
2	E	2	GAL	C4-C5	2.48	1.58	1.53
2	H	1	BGC	C1-C2	2.46	1.58	1.52
2	G	2	GAL	O2-C2	2.42	1.48	1.43
2	F	2	GAL	C4-C5	2.29	1.57	1.53
2	E	2	GAL	O2-C2	2.18	1.47	1.43
2	H	2	GAL	O3-C3	2.16	1.48	1.43
2	H	2	GAL	O2-C2	2.13	1.47	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	GAL	O2-C2-C1	-3.05	102.24	109.22
2	E	2	GAL	O3-C3-C2	-3.03	103.88	110.05
2	F	2	GAL	O3-C3-C2	-2.85	104.24	110.05
2	H	2	GAL	O2-C2-C1	-2.78	102.85	109.22
2	G	2	GAL	O2-C2-C1	-2.65	103.16	109.22
2	G	1	BGC	C4-C3-C2	-2.23	106.91	110.83
2	E	1	BGC	C1-O5-C5	-2.18	109.43	113.65
2	F	2	GAL	O2-C2-C3	-2.14	105.72	110.15
2	F	2	GAL	O4-C4-C5	-2.09	104.17	109.32
2	E	2	GAL	O4-C4-C5	-2.07	104.24	109.32
2	G	2	GAL	O2-C2-C3	-2.05	105.91	110.15
2	E	1	BGC	C4-C3-C2	2.01	114.36	110.83

All (1) chirality outliers are listed below:

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

All (6) torsion outliers are listed below:

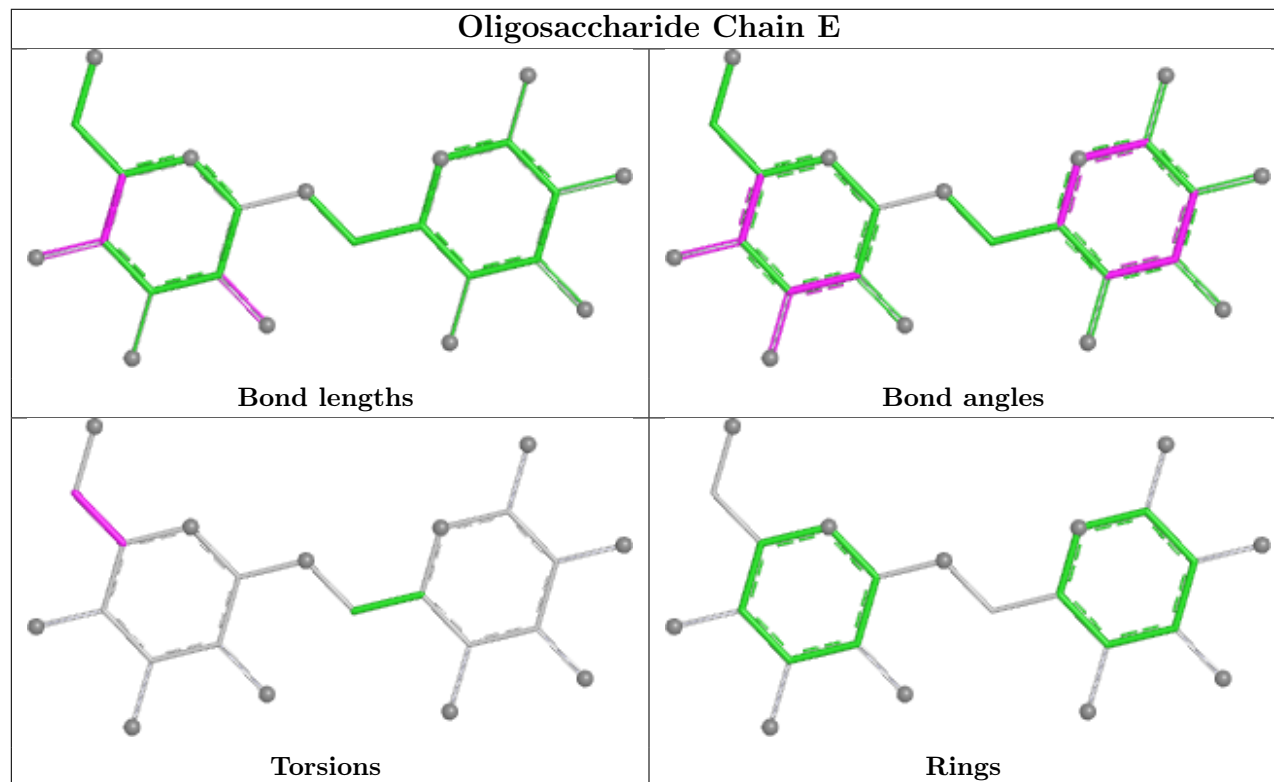
Mol	Chain	Res	Type	Atoms
2	E	2	GAL	O5-C5-C6-O6
2	G	2	GAL	O5-C5-C6-O6
2	H	2	GAL	O5-C5-C6-O6
2	G	1	BGC	C4-C5-C6-O6
2	F	2	GAL	O5-C5-C6-O6
2	G	1	BGC	O5-C5-C6-O6

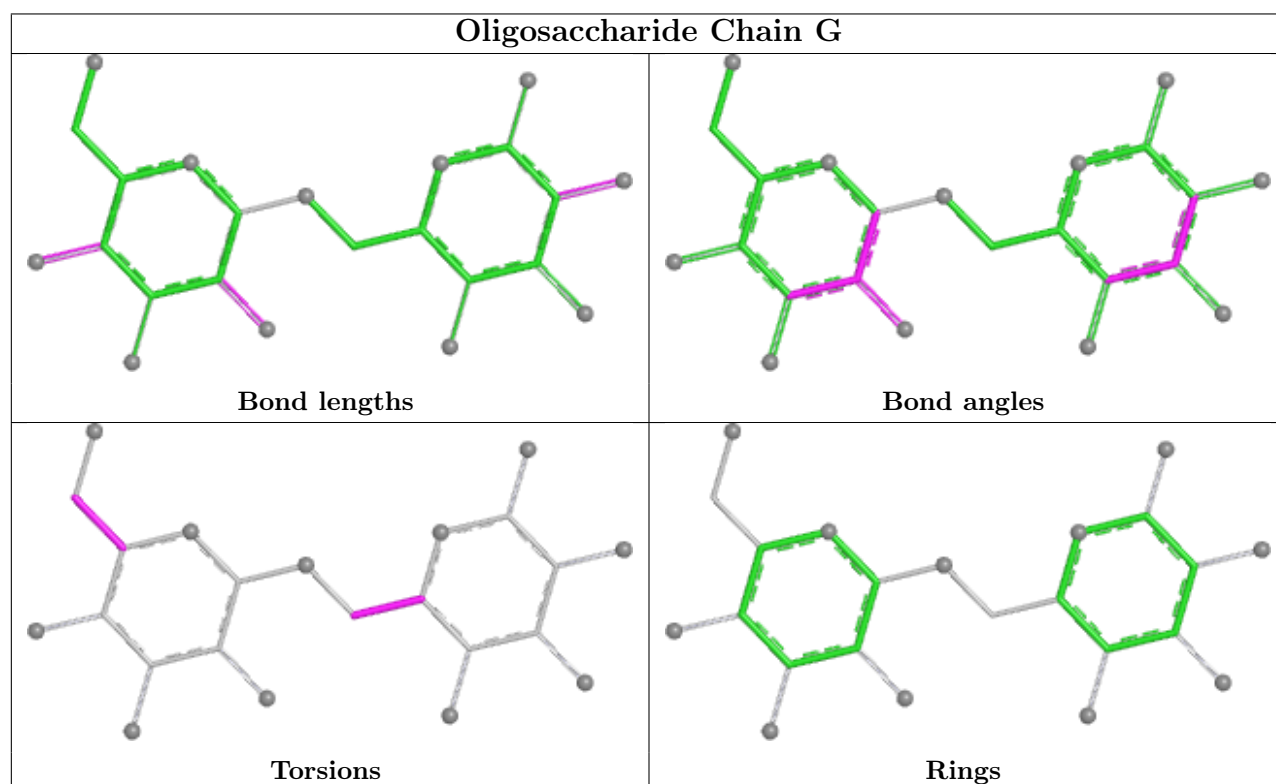
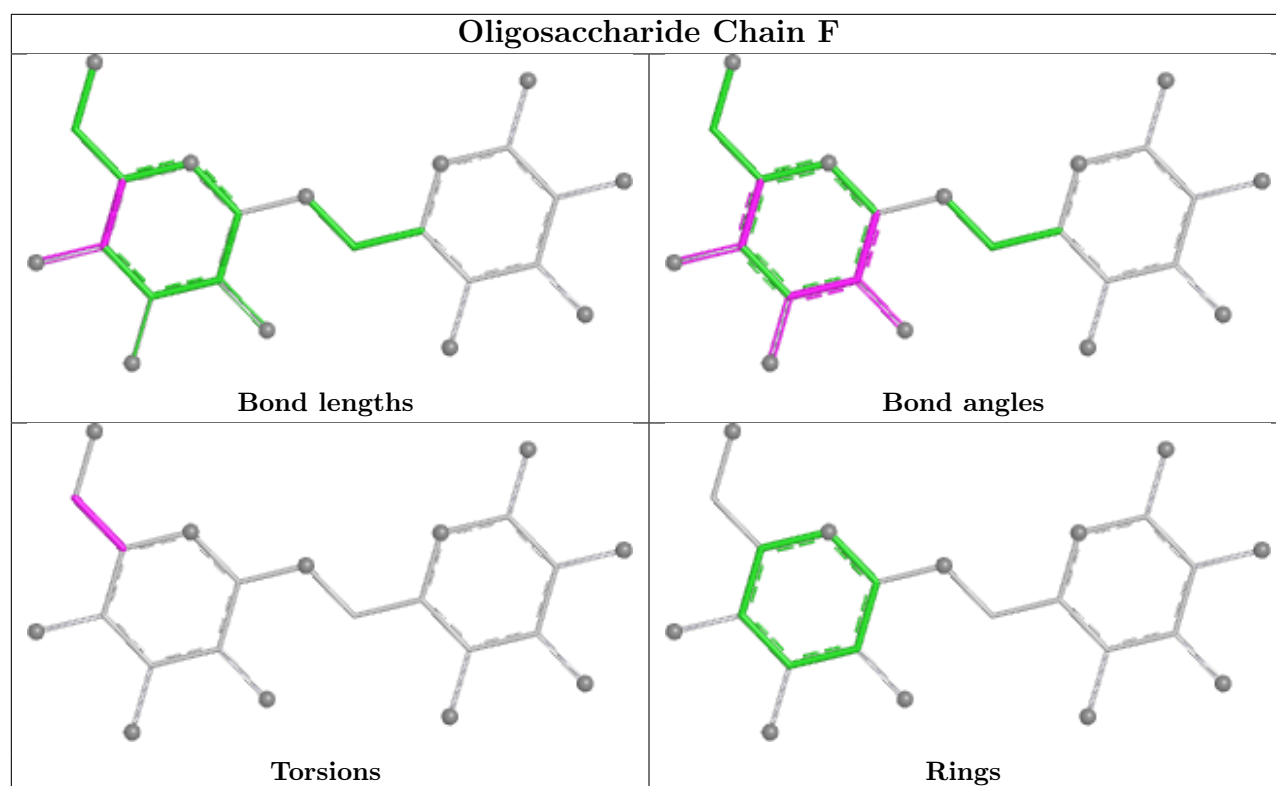
There are no ring outliers.

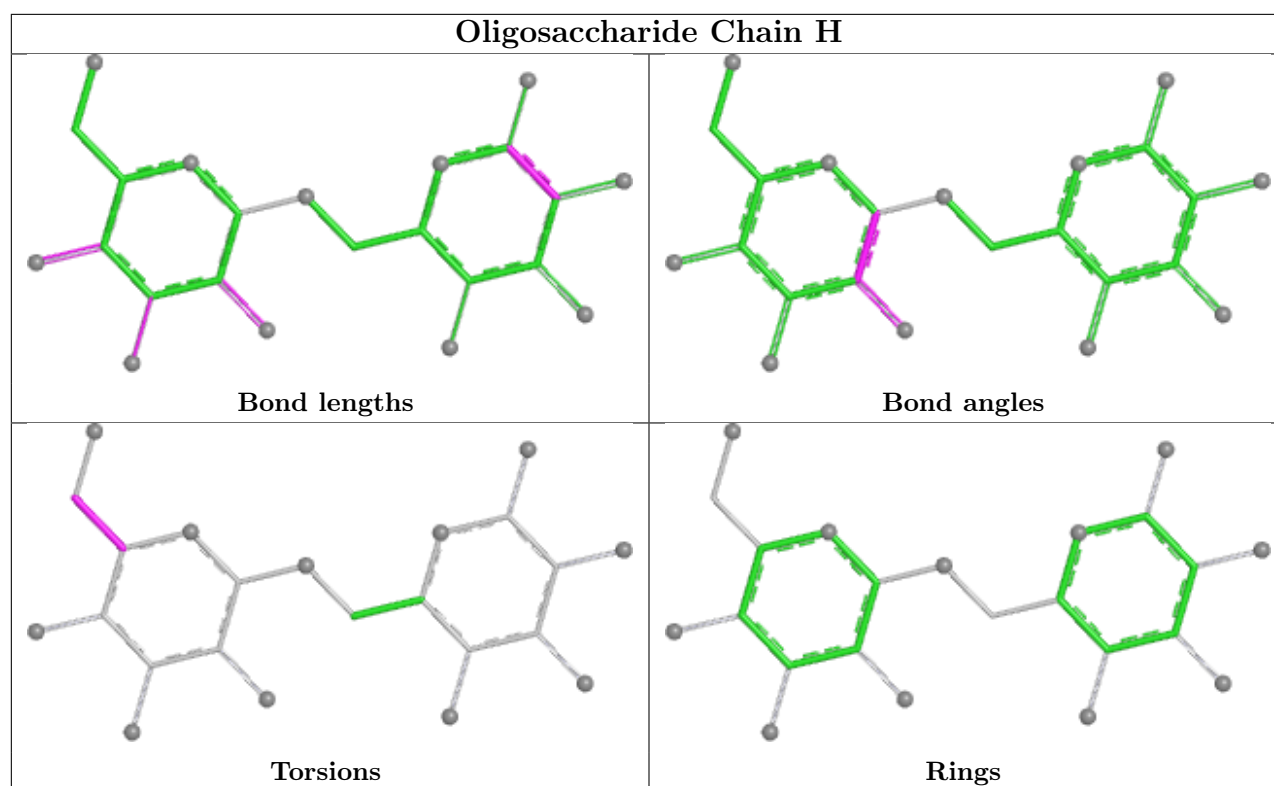
1 monomer is involved in 1 short contact:

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	8421	-	3,3,3	1.22	0	3,3,3	0.88	0
5	DMS	A	8501	-	3,3,3	1.47	1 (33%)	3,3,3	0.58	0
5	DMS	C	8413	-	3,3,3	2.19	2 (66%)	3,3,3	0.56	0
5	DMS	D	8703	-	3,3,3	1.43	0	3,3,3	0.14	0
5	DMS	B	8501	-	3,3,3	1.05	0	3,3,3	0.27	0
5	DMS	A	8403	-	3,3,3	2.39	1 (33%)	3,3,3	0.56	0
5	DMS	C	8429	-	3,3,3	1.43	1 (33%)	3,3,3	0.33	0
5	DMS	A	8407	-	3,3,3	2.48	1 (33%)	3,3,3	1.24	1 (33%)
5	DMS	D	8423	-	3,3,3	2.59	2 (66%)	3,3,3	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	8508	-	3,3,3	2.63	1 (33%)	3,3,3	0.53	0
5	DMS	A	8424	-	3,3,3	1.33	0	3,3,3	0.35	0
5	DMS	D	8428	-	3,3,3	1.22	0	3,3,3	0.40	0
5	DMS	A	8423	-	3,3,3	2.10	2 (66%)	3,3,3	0.46	0
5	DMS	C	8506	-	3,3,3	1.14	0	3,3,3	0.57	0
5	DMS	D	8424	-	3,3,3	1.36	0	3,3,3	0.17	0
5	DMS	C	8407	-	3,3,3	1.80	1 (33%)	3,3,3	0.46	0
5	DMS	D	8417	-	3,3,3	1.59	1 (33%)	3,3,3	0.69	0
5	DMS	C	8421	-	3,3,3	1.24	0	3,3,3	1.16	1 (33%)
5	DMS	C	8403	-	3,3,3	1.27	0	3,3,3	0.51	0
5	DMS	A	8410	-	3,3,3	1.18	0	3,3,3	0.67	0
5	DMS	B	8413	-	3,3,3	3.08	2 (66%)	3,3,3	0.57	0
5	DMS	A	8502	-	3,3,3	2.36	2 (66%)	3,3,3	1.53	1 (33%)
5	DMS	D	8413	-	3,3,3	1.81	1 (33%)	3,3,3	0.50	0
5	DMS	B	8504	-	3,3,3	0.49	0	3,3,3	0.31	0
5	DMS	C	8408	-	3,3,3	0.91	0	3,3,3	0.73	0
5	DMS	C	8424	-	3,3,3	1.19	0	3,3,3	0.59	0
5	DMS	C	8416	-	3,3,3	2.21	2 (66%)	3,3,3	0.57	0
5	DMS	D	8508	-	3,3,3	1.82	1 (33%)	3,3,3	0.81	0
5	DMS	D	8425	4	3,3,3	1.44	1 (33%)	3,3,3	1.18	1 (33%)
5	DMS	A	8428	-	3,3,3	1.31	1 (33%)	3,3,3	0.38	0
5	DMS	C	8410	-	3,3,3	1.23	0	3,3,3	0.25	0
5	DMS	B	8402	-	3,3,3	2.00	2 (66%)	3,3,3	0.54	0
5	DMS	D	8408	-	3,3,3	1.57	0	3,3,3	0.14	0
5	DMS	A	8418	-	3,3,3	1.09	0	3,3,3	0.35	0
5	DMS	B	8407	-	3,3,3	3.04	2 (66%)	3,3,3	0.26	0
5	DMS	D	8402	-	3,3,3	1.30	0	3,3,3	0.29	0
5	DMS	A	8411	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	B	8411	-	3,3,3	1.12	0	3,3,3	0.42	0
5	DMS	B	8601	-	3,3,3	2.37	1 (33%)	3,3,3	0.92	0
5	DMS	D	8704	-	3,3,3	2.38	1 (33%)	3,3,3	0.58	0
5	DMS	A	8408	-	3,3,3	0.30	0	3,3,3	0.74	0
5	DMS	A	8414	-	3,3,3	1.95	2 (66%)	3,3,3	0.21	0
5	DMS	A	8419	-	3,3,3	1.03	0	3,3,3	0.56	0
5	DMS	B	8420	-	3,3,3	1.79	1 (33%)	3,3,3	0.47	0
5	DMS	B	8405	-	3,3,3	1.51	1 (33%)	3,3,3	0.55	0
5	DMS	D	8403	-	3,3,3	1.39	0	3,3,3	0.46	0
5	DMS	A	8412	-	3,3,3	0.82	0	3,3,3	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	8414	-	3,3,3	1.35	0	3,3,3	0.94	0
5	DMS	B	8408	-	3,3,3	0.91	0	3,3,3	0.16	0
5	DMS	D	8405	-	3,3,3	0.97	0	3,3,3	0.51	0
5	DMS	D	8501	-	3,3,3	0.99	0	3,3,3	0.07	0
5	DMS	C	8418	-	3,3,3	2.15	1 (33%)	3,3,3	1.44	1 (33%)
5	DMS	B	8423	-	3,3,3	0.76	0	3,3,3	0.64	0
5	DMS	B	8416	-	3,3,3	1.18	0	3,3,3	0.35	0
5	DMS	A	8503	-	3,3,3	1.11	0	3,3,3	1.19	1 (33%)
5	DMS	C	8405	-	3,3,3	1.85	2 (66%)	3,3,3	0.64	0
5	DMS	D	8416	-	3,3,3	0.84	0	3,3,3	0.29	0
5	DMS	C	8401	-	3,3,3	1.11	0	3,3,3	0.39	0
5	DMS	D	8420	-	3,3,3	2.56	1 (33%)	3,3,3	0.32	0
5	DMS	C	8409	-	3,3,3	2.45	1 (33%)	3,3,3	0.71	0
5	DMS	C	8501	-	3,3,3	1.18	0	3,3,3	1.18	0
5	DMS	C	8504	-	3,3,3	1.24	0	3,3,3	0.29	0
5	DMS	A	8413	-	3,3,3	2.66	3 (100%)	3,3,3	0.68	0
5	DMS	C	8402	-	3,3,3	1.98	1 (33%)	3,3,3	0.43	0
5	DMS	B	8424	-	3,3,3	1.02	0	3,3,3	0.13	0
5	DMS	B	8415	-	3,3,3	2.89	2 (66%)	3,3,3	1.03	0
5	DMS	B	8412	-	3,3,3	0.82	0	3,3,3	0.25	0
5	DMS	D	8406	-	3,3,3	1.12	0	3,3,3	0.60	0
5	DMS	A	8420	-	3,3,3	1.31	0	3,3,3	0.86	0
5	DMS	D	8409	-	3,3,3	2.54	1 (33%)	3,3,3	1.04	0
5	DMS	B	8404	-	3,3,3	1.31	0	3,3,3	0.24	0
5	DMS	D	8412	-	3,3,3	0.83	0	3,3,3	0.60	0
5	DMS	B	8429	-	3,3,3	2.62	2 (66%)	3,3,3	0.77	0
5	DMS	B	8414	-	3,3,3	0.61	0	3,3,3	1.03	0
5	DMS	D	8429	-	3,3,3	2.49	1 (33%)	3,3,3	0.37	0
7	TAR	B	2003[C]	-	8,8,9	3.32	3 (37%)	8,10,12	3.36	2 (25%)
5	DMS	B	8508	-	3,3,3	3.37	2 (66%)	3,3,3	0.72	0
5	DMS	D	8503	-	3,3,3	0.89	0	3,3,3	0.61	0
5	DMS	C	8406	-	3,3,3	0.78	0	3,3,3	0.19	0
5	DMS	B	8401	-	3,3,3	0.91	0	3,3,3	0.39	0
5	DMS	D	8705	-	3,3,3	3.18	1 (33%)	3,3,3	1.65	1 (33%)
5	DMS	D	8701	-	3,3,3	2.51	3 (100%)	3,3,3	0.72	0
5	DMS	A	8506	-	3,3,3	2.45	2 (66%)	3,3,3	0.41	0
5	DMS	D	8401	-	3,3,3	1.27	0	3,3,3	0.43	0
5	DMS	B	8417	-	3,3,3	1.33	0	3,3,3	0.36	0
5	DMS	B	8706	-	3,3,3	1.78	1 (33%)	3,3,3	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	8506	-	3,3,3	1.71	1 (33%)	3,3,3	0.46	0
5	DMS	C	8404	-	3,3,3	0.95	0	3,3,3	0.77	0
5	DMS	C	8423	-	3,3,3	1.11	0	3,3,3	0.39	0
5	DMS	D	8414	-	3,3,3	0.45	0	3,3,3	0.29	0
5	DMS	D	8506	-	3,3,3	1.59	1 (33%)	3,3,3	0.47	0
5	DMS	C	8420	-	3,3,3	2.56	1 (33%)	3,3,3	0.91	0
5	DMS	D	8411	-	3,3,3	0.75	0	3,3,3	0.10	0
5	DMS	A	8409	-	3,3,3	2.82	1 (33%)	3,3,3	0.91	0
5	DMS	A	8504	-	3,3,3	1.44	1 (33%)	3,3,3	0.35	0
6	BGC	B	2002[B]	-	8,8,12	1.13	0	8,10,17	1.48	1 (12%)
5	DMS	A	8602	-	3,3,3	1.17	0	3,3,3	0.44	0
5	DMS	B	8419	-	3,3,3	1.39	0	3,3,3	0.25	0
5	DMS	A	8402	-	3,3,3	1.82	1 (33%)	3,3,3	0.29	0
5	DMS	B	8403	-	3,3,3	1.64	0	3,3,3	0.41	0
5	DMS	C	8412	-	3,3,3	1.73	1 (33%)	3,3,3	0.46	0
5	DMS	D	8419	-	3,3,3	0.45	0	3,3,3	0.13	0
5	DMS	C	8601	-	3,3,3	1.17	0	3,3,3	1.04	0
5	DMS	C	8411	-	3,3,3	1.04	0	3,3,3	0.37	0
5	DMS	B	8428	-	3,3,3	1.64	1 (33%)	3,3,3	0.34	0
5	DMS	C	8425	4	3,3,3	1.68	1 (33%)	3,3,3	0.36	0
5	DMS	B	8410	-	3,3,3	1.78	1 (33%)	3,3,3	0.29	0
5	DMS	C	8419	-	3,3,3	0.89	0	3,3,3	0.22	0
5	DMS	A	8417	-	3,3,3	1.55	1 (33%)	3,3,3	0.62	0
5	DMS	D	8404	-	3,3,3	1.46	1 (33%)	3,3,3	0.15	0
5	DMS	D	8410	-	3,3,3	1.20	0	3,3,3	0.19	0
5	DMS	A	8406	-	3,3,3	0.95	0	3,3,3	0.88	0
5	DMS	D	8407	-	3,3,3	2.97	2 (66%)	3,3,3	0.34	0
5	DMS	C	8503	-	3,3,3	0.98	0	3,3,3	0.79	0
5	DMS	C	8415	-	3,3,3	2.71	2 (66%)	3,3,3	0.95	0
5	DMS	A	8404	-	3,3,3	1.35	1 (33%)	3,3,3	0.22	0
5	DMS	C	8602	-	3,3,3	1.36	1 (33%)	3,3,3	0.17	0
5	DMS	B	8421	-	3,3,3	0.33	0	3,3,3	0.30	0
5	DMS	B	8418	-	3,3,3	0.81	0	3,3,3	0.53	0
5	DMS	A	8425	4	3,3,3	2.66	3 (100%)	3,3,3	1.06	0
5	DMS	A	8405	-	3,3,3	1.35	1 (33%)	3,3,3	0.72	0
5	DMS	D	8421	-	3,3,3	0.95	0	3,3,3	0.35	0
5	DMS	B	8502	-	3,3,3	1.23	0	3,3,3	2.06	1 (33%)
5	DMS	B	8409	-	3,3,3	2.39	2 (66%)	3,3,3	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	D	8418	-	3,3,3	1.43	0	3,3,3	0.93	0
5	DMS	B	8425	4	3,3,3	2.43	2 (66%)	3,3,3	0.30	0
5	DMS	A	8401	-	3,3,3	0.80	0	3,3,3	0.41	0
5	DMS	C	8417	-	3,3,3	0.80	0	3,3,3	0.99	0
5	DMS	A	8416	-	3,3,3	2.47	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
7	TAR	B	2003[C]	-	1/1/3/4	7/10/10/12	-
6	BGC	B	2002[B]	-	1/1/3/5	10/10/10/22	-

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2003[C]	TAR	O1-C1	7.49	1.44	1.22
5	D	8705	DMS	C1-S	-5.43	1.37	1.76
5	B	8508	DMS	C1-S	4.90	2.11	1.76
5	A	8409	DMS	O-S	4.60	1.80	1.50
5	C	8508	DMS	O-S	4.51	1.80	1.50
5	B	8413	DMS	O-S	4.36	1.79	1.50
7	B	2003[C]	TAR	O11-C1	4.27	1.44	1.30
5	B	8415	DMS	C2-S	4.26	2.06	1.76
5	D	8420	DMS	C2-S	-4.22	1.45	1.76
5	C	8420	DMS	O-S	4.17	1.77	1.50
5	B	8407	DMS	C2-S	4.13	2.05	1.76
5	C	8409	DMS	O-S	4.11	1.77	1.50
5	D	8704	DMS	C1-S	4.09	2.05	1.76
5	D	8429	DMS	C2-S	4.05	2.05	1.76
5	D	8407	DMS	O-S	4.03	1.76	1.50
5	D	8409	DMS	O-S	4.02	1.76	1.50
5	B	8601	DMS	C2-S	3.95	2.04	1.76
5	A	8416	DMS	O-S	-3.88	1.24	1.50
5	A	8407	DMS	O-S	3.82	1.75	1.50
5	A	8403	DMS	C2-S	3.67	2.02	1.76
5	C	8415	DMS	C2-S	3.61	2.01	1.76
5	D	8423	DMS	C1-S	3.60	2.01	1.76
5	B	8409	DMS	O-S	3.57	1.73	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	8425	DMS	O-S	3.53	1.73	1.50
5	B	8429	DMS	O-S	3.27	1.71	1.50
5	B	8407	DMS	O-S	3.25	1.71	1.50
5	B	8429	DMS	C2-S	3.04	1.97	1.76
5	A	8502	DMS	C2-S	3.04	1.97	1.76
7	B	2003[C]	TAR	O2-C2	3.02	1.48	1.42
5	A	8506	DMS	C1-S	3.01	1.97	1.76
5	A	8413	DMS	C2-S	3.00	1.97	1.76
5	A	8425	DMS	O-S	2.98	1.69	1.50
5	D	8701	DMS	O-S	2.95	1.69	1.50
5	C	8413	DMS	O-S	2.91	1.69	1.50
5	C	8416	DMS	C2-S	2.88	1.96	1.76
5	B	8706	DMS	O-S	2.86	1.69	1.50
5	C	8402	DMS	C2-S	2.85	1.96	1.76
5	B	8420	DMS	C2-S	2.80	1.96	1.76
5	B	8508	DMS	O-S	2.79	1.68	1.50
5	B	8413	DMS	C2-S	2.76	1.95	1.76
5	D	8506	DMS	O-S	2.76	1.68	1.50
5	D	8413	DMS	O-S	2.73	1.68	1.50
5	B	8410	DMS	C1-S	2.71	1.95	1.76
5	A	8502	DMS	C1-S	2.68	1.95	1.76
5	D	8407	DMS	C2-S	2.68	1.95	1.76
5	D	8417	DMS	C2-S	2.65	1.95	1.76
5	B	8506	DMS	C2-S	2.63	1.94	1.76
5	D	8508	DMS	O-S	2.62	1.67	1.50
5	C	8418	DMS	C1-S	-2.60	1.57	1.76
5	A	8425	DMS	C1-S	2.60	1.94	1.76
5	B	8428	DMS	C1-S	2.59	1.94	1.76
5	A	8413	DMS	O-S	2.52	1.66	1.50
5	D	8404	DMS	C2-S	2.49	1.93	1.76
5	A	8504	DMS	C1-S	-2.48	1.58	1.76
5	C	8429	DMS	O-S	2.48	1.66	1.50
5	C	8416	DMS	O-S	2.46	1.66	1.50
5	C	8407	DMS	O-S	2.45	1.66	1.50
5	A	8414	DMS	O-S	-2.44	1.34	1.50
5	A	8413	DMS	C1-S	2.43	1.93	1.76
5	C	8425	DMS	O-S	2.43	1.66	1.50
5	D	8701	DMS	C1-S	2.42	1.93	1.76
5	C	8415	DMS	C1-S	2.40	1.93	1.76
5	A	8423	DMS	O-S	2.39	1.66	1.50
5	A	8402	DMS	C2-S	2.39	1.93	1.76
5	B	8402	DMS	C2-S	2.37	1.93	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	8425	DMS	C2-S	2.36	1.92	1.76
5	C	8405	DMS	O-S	2.36	1.65	1.50
5	A	8423	DMS	C2-S	2.31	1.92	1.76
5	D	8425	DMS	C2-S	2.29	1.92	1.76
5	B	8425	DMS	C2-S	2.29	1.92	1.76
5	D	8423	DMS	C2-S	2.29	1.92	1.76
5	A	8506	DMS	C2-S	2.29	1.92	1.76
5	C	8412	DMS	O-S	2.19	1.64	1.50
5	B	8402	DMS	O-S	2.18	1.64	1.50
5	A	8417	DMS	O-S	2.17	1.64	1.50
5	A	8428	DMS	C2-S	2.15	1.91	1.76
5	C	8602	DMS	O-S	2.13	1.64	1.50
5	A	8404	DMS	C2-S	2.11	1.91	1.76
5	A	8405	DMS	O-S	2.10	1.64	1.50
5	B	8415	DMS	C1-S	2.08	1.90	1.76
5	D	8701	DMS	C2-S	2.07	1.90	1.76
5	C	8405	DMS	C1-S	2.07	1.90	1.76
5	B	8405	DMS	O-S	2.06	1.63	1.50
5	A	8501	DMS	O-S	2.05	1.63	1.50
5	B	8409	DMS	C1-S	2.04	1.90	1.76
5	C	8413	DMS	C1-S	2.02	1.90	1.76
5	A	8414	DMS	C1-S	-2.00	1.61	1.76

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	2003[C]	TAR	O11-C1-O1	-8.39	105.06	124.08
7	B	2003[C]	TAR	O1-C1-C2	-3.61	111.99	121.62
5	B	8502	DMS	C2-S-C1	3.55	116.60	98.42
5	D	8705	DMS	C2-S-C1	-2.84	83.86	98.42
5	A	8502	DMS	C2-S-C1	2.64	111.93	98.42
5	C	8418	DMS	C2-S-C1	-2.48	85.69	98.42
6	B	2002[B]	BGC	C4-C3-C2	2.32	116.90	112.17
5	A	8407	DMS	C2-S-C1	2.14	109.37	98.42
5	A	8503	DMS	C2-S-C1	-2.05	87.90	98.42
5	D	8425	DMS	C2-S-C1	2.03	108.83	98.42
5	C	8421	DMS	C2-S-C1	-2.00	88.16	98.42

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	2002[B]	BGC	C2

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Mol	Chain	Res	Type	Atom
7	B	2003[C]	TAR	C3

All (17) 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	O1-C1-C2-C3
7	B	2003[C]	TAR	C1-C2-C3-C4
7	B	2003[C]	TAR	O2-C2-C3-C4
7	B	2003[C]	TAR	O3-C3-C4-O41
7	B	2003[C]	TAR	O1-C1-C2-O2
7	B	2003[C]	TAR	C2-C3-C4-O41
6	B	2002[B]	BGC	O5-C1-C2-O2
7	B	2003[C]	TAR	O11-C1-C2-O2
6	B	2002[B]	BGC	O2-C2-C3-C4
6	B	2002[B]	BGC	O1-C1-C2-C3
6	B	2002[B]	BGC	O1-C1-C2-O2
6	B	2002[B]	BGC	O3-C3-C4-O4
6	B	2002[B]	BGC	O5-C1-C2-C3

There are no ring outliers.

55 monomers are involved in 112 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	8413	DMS	1	0
5	D	8703	DMS	3	0
5	B	8501	DMS	4	0
5	A	8403	DMS	2	0
5	D	8423	DMS	3	0
5	D	8428	DMS	1	0
5	A	8423	DMS	1	0
5	D	8417	DMS	1	0
5	C	8403	DMS	1	0
5	B	8504	DMS	2	0
5	C	8424	DMS	4	0
5	A	8428	DMS	4	0
5	A	8418	DMS	3	0
5	B	8407	DMS	2	0
5	B	8601	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	8704	DMS	1	0
5	B	8420	DMS	1	0
5	D	8403	DMS	2	0
5	A	8412	DMS	4	0
5	C	8418	DMS	3	0
5	B	8423	DMS	1	0
5	C	8504	DMS	2	0
5	B	8424	DMS	1	0
5	B	8415	DMS	4	0
5	B	8412	DMS	1	0
5	A	8420	DMS	2	0
5	D	8412	DMS	3	0
5	D	8429	DMS	3	0
7	B	2003[C]	TAR	9	0
5	B	8508	DMS	1	0
5	D	8503	DMS	1	0
5	C	8406	DMS	1	0
5	D	8705	DMS	4	0
5	A	8506	DMS	1	0
5	B	8417	DMS	1	0
5	C	8423	DMS	1	0
5	D	8506	DMS	1	0
5	C	8420	DMS	2	0
6	B	2002[B]	BGC	3	0
5	B	8419	DMS	1	0
5	B	8403	DMS	1	0
5	C	8412	DMS	2	0
5	B	8428	DMS	1	0
5	B	8410	DMS	1	0
5	A	8417	DMS	1	0
5	A	8406	DMS	1	0
5	D	8407	DMS	1	0
5	C	8503	DMS	2	0
5	C	8415	DMS	2	0
5	C	8602	DMS	1	0
5	B	8418	DMS	4	0
5	D	8421	DMS	1	0
5	D	8418	DMS	3	0
5	C	8417	DMS	1	0
5	A	8416	DMS	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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%)	-0.50	32 (3%)	50	54	7, 12, 42, 100	1 (0%)
1	B	1011/1023 (98%)	-0.55	30 (2%)	52	56	6, 12, 39, 100	1 (0%)
1	C	1011/1023 (98%)	-0.48	22 (2%)	62	66	6, 13, 43, 100	1 (0%)
1	D	1011/1023 (98%)	-0.45	35 (3%)	47	51	6, 13, 44, 98	1 (0%)
All	All	4044/4092 (98%)	-0.50	119 (2%)	53	58	6, 13, 43, 100	4 (0%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	685	LEU	5.8
1	A	686	PRO	5.7
1	D	732	ALA	5.5
1	A	685	LEU	5.4
1	D	733	ALA	5.4
1	A	730	LEU	5.3
1	C	730	LEU	5.0
1	B	685	LEU	4.8
1	D	685	LEU	4.7
1	A	688	PRO	4.7
1	A	737	ILE	4.7
1	B	730	LEU	4.7
1	B	732	ALA	4.7
1	C	686	PRO	4.6
1	D	688	PRO	4.5
1	A	735	HIS	4.5
1	C	735	HIS	4.4
1	A	634	GLN	4.4
1	C	733	ALA	4.4
1	B	686	PRO	4.3
1	A	771	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	686	PRO	3.8
1	B	745	MET	3.8
1	D	730	LEU	3.7
1	B	735	HIS	3.7
1	C	734	SER	3.7
1	D	735	HIS	3.7
1	A	736	ALA	3.6
1	A	829	THR	3.5
1	B	725	ASN	3.5
1	A	731	PRO	3.5
1	D	799	THR	3.4
1	C	732	ALA	3.4
1	D	581	ASN	3.3
1	B	1023	LYS	3.3
1	B	663	LEU	3.3
1	D	689	GLU	3.2
1	C	663	LEU	3.2
1	A	1023	LYS	3.2
1	A	729	THR	3.2
1	D	731	PRO	3.2
1	C	737	ILE	3.2
1	B	733	ALA	3.2
1	A	799	THR	3.1
1	B	799	THR	3.1
1	C	731	PRO	3.1
1	B	687	GLN	3.1
1	C	689	GLU	3.0
1	C	736	ALA	3.0
1	C	772	ASP	3.0
1	B	1022	GLN	3.0
1	C	634	GLN	3.0
1	D	729	THR	2.9
1	A	846	GLY	2.9
1	A	687	GLN	2.9
1	C	687	GLN	2.9
1	C	1023	LYS	2.9
1	D	736	ALA	2.8
1	D	737	ILE	2.8
1	B	689	GLU	2.8
1	A	581	ASN	2.7
1	A	733	ALA	2.7
1	B	1018	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	655	MET	2.7
1	D	683	PRO	2.7
1	D	1023	LYS	2.6
1	D	739	HIS	2.6
1	A	664	ALA	2.6
1	C	729	THR	2.6
1	A	773	LYS	2.5
1	D	663	LEU	2.5
1	A	772	ASP	2.5
1	B	737	ILE	2.5
1	B	738	PRO	2.5
1	D	687	GLN	2.5
1	A	580	GLU	2.4
1	B	688	PRO	2.4
1	B	731	PRO	2.4
1	A	689	GLU	2.4
1	B	819	GLU	2.4
1	A	845	GLN	2.4
1	B	684	GLU	2.4
1	A	646	HIS	2.4
1	D	634	GLN	2.4
1	A	798	ALA	2.3
1	A	683	PRO	2.3
1	D	580	GLU	2.3
1	D	666	GLY	2.3
1	D	820	ALA	2.3
1	C	684	GLU	2.3
1	C	666	GLY	2.3
1	A	135	GLN	2.3
1	B	681	GLU	2.3
1	D	829	THR	2.3
1	D	755	ARG	2.3
1	D	773	LYS	2.3
1	D	1018	LEU	2.3
1	D	734	SER	2.3
1	D	845	GLN	2.2
1	B	734	SER	2.2
1	A	663	LEU	2.2
1	A	732	ALA	2.2
1	D	75	GLU	2.2
1	B	845	GLN	2.2
1	D	651	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	682	LEU	2.2
1	B	580	GLU	2.2
1	D	71	GLU	2.2
1	B	683	PRO	2.1
1	B	729	THR	2.1
1	C	761	GLN	2.1
1	B	846	GLY	2.1
1	A	817	GLN	2.1
1	D	798	ALA	2.1
1	C	71	GLU	2.1
1	C	745	MET	2.1
1	B	370	GLN	2.0
1	B	817	GLN	2.0
1	A	725	ASN	2.0

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](#)

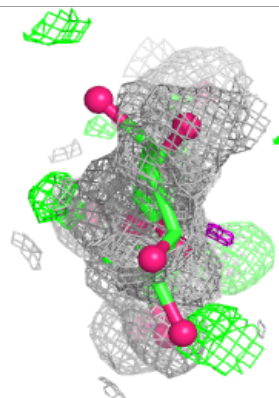
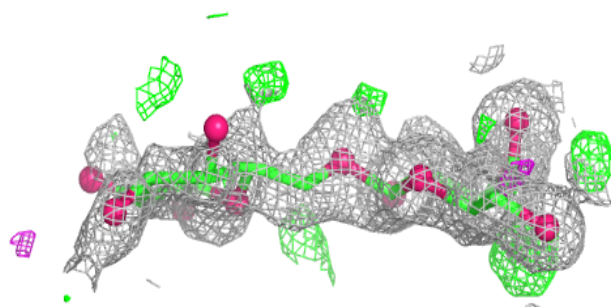
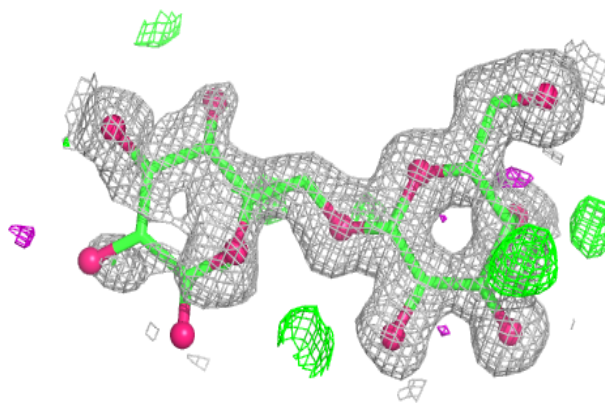
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	G	1	12/12	0.81	0.21	14,85,100,100	0
2	BGC	H	1	12/12	0.82	0.21	18,100,100,100	0
2	BGC	E	1	12/12	0.86	0.17	17,96,100,100	0
2	BGC	F	1[A]	12/12	0.92	0.18	11,32,100,100	9
2	GAL	E	2	11/12	0.96	0.07	12,16,21,21	0
2	GAL	F	2	11/12	0.96	0.10	11,14,19,20	0
2	GAL	G	2	11/12	0.98	0.06	10,14,17,20	0
2	GAL	H	2	11/12	0.98	0.06	13,15,21,24	0

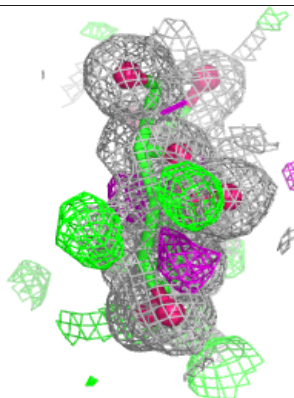
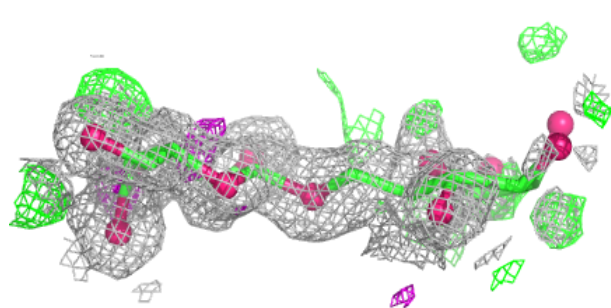
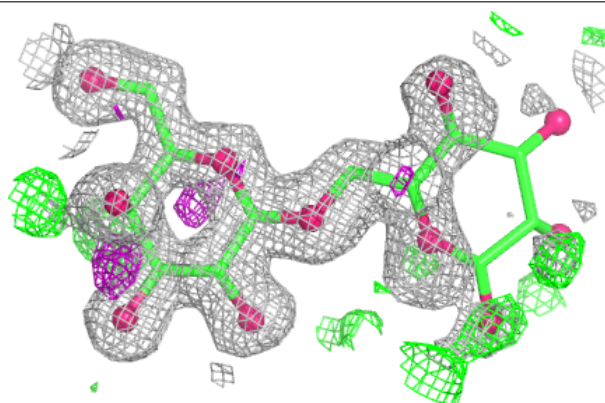
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

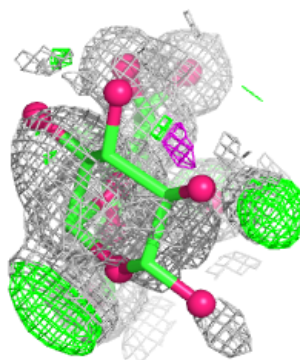
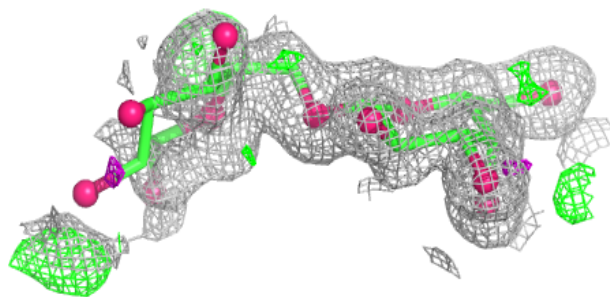
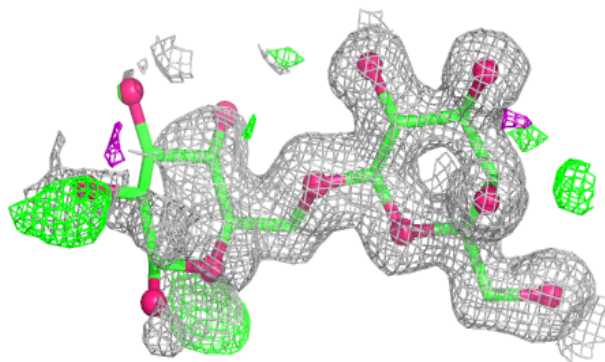
**Electron density around Chain F:**

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

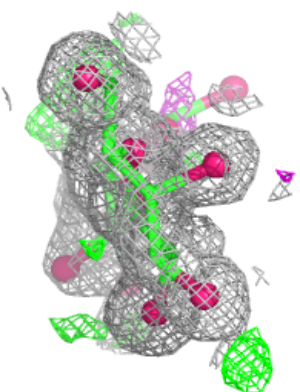
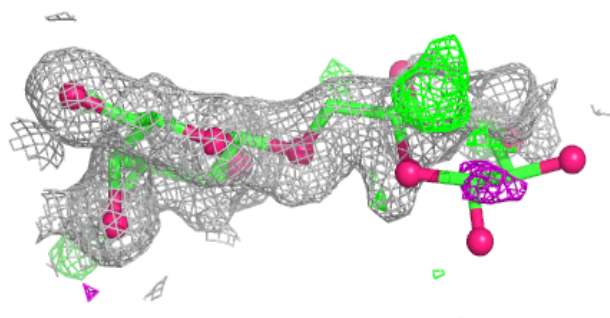
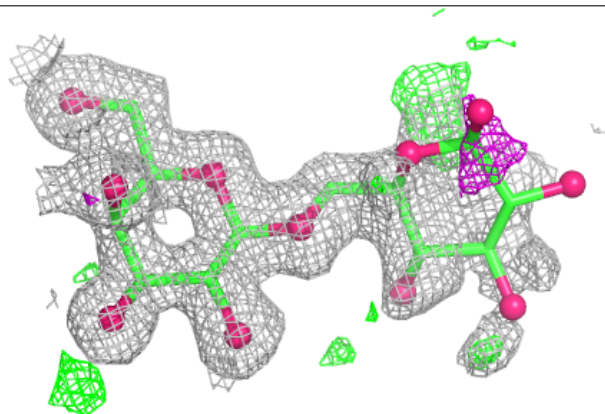


Electron density around Chain G:

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

**Electron density around Chain H:**

$2mF_o-DF_c$ (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
6	BGC	B	2002[B]	9/12	0.44	0.40	6,56,100,100	9
5	DMS	B	8424	4/4	0.72	0.23	50,74,76,77	0
7	TAR	B	2003[C]	9/10	0.75	0.26	13,38,100,100	9
5	DMS	D	8704	4/4	0.79	0.26	31,32,100,100	0
5	DMS	B	8428	4/4	0.80	0.18	34,38,57,61	0
5	DMS	A	8424	4/4	0.80	0.16	34,35,70,100	0
5	DMS	C	8424	4/4	0.81	0.21	41,60,100,100	0
5	DMS	D	8417	4/4	0.82	0.21	26,27,85,92	0
5	DMS	D	8424	4/4	0.82	0.21	47,57,87,100	0
5	DMS	D	8703	4/4	0.82	0.18	25,51,52,58	0
5	DMS	C	8503	4/4	0.83	0.17	23,50,50,52	0
5	DMS	D	8425	4/4	0.83	0.20	35,42,59,100	0
5	DMS	D	8420	4/4	0.83	0.20	18,67,81,83	0
5	DMS	D	8418	4/4	0.85	0.18	25,70,78,100	0
5	DMS	A	8421	4/4	0.85	0.20	34,46,61,63	0
5	DMS	D	8423	4/4	0.85	0.16	30,37,42,50	0
3	MG	A	3105	1/1	0.86	0.23	45,45,45,45	0
5	DMS	A	8418	4/4	0.86	0.15	34,39,76,100	0
5	DMS	C	8406	4/4	0.86	0.26	42,44,99,100	0
5	DMS	D	8429	4/4	0.87	0.19	26,51,82,100	0
5	DMS	D	8501	4/4	0.87	0.12	23,29,37,52	0
5	DMS	D	8503	4/4	0.87	0.19	23,38,49,100	0
5	DMS	A	8602	4/4	0.87	0.20	35,52,100,100	0
5	DMS	A	8417	4/4	0.87	0.20	24,26,73,100	0
5	DMS	A	8502	4/4	0.87	0.15	18,23,49,54	0
5	DMS	D	8428	4/4	0.87	0.16	39,47,61,65	0
5	DMS	A	8423	4/4	0.88	0.17	28,42,51,73	0
5	DMS	A	8406	4/4	0.88	0.20	24,45,69,72	0
5	DMS	B	8416	4/4	0.88	0.14	33,46,47,50	0
5	DMS	C	8417	4/4	0.88	0.14	26,27,50,61	0
5	DMS	C	8418	4/4	0.88	0.13	20,27,56,100	0
5	DMS	B	8417	4/4	0.88	0.18	27,29,70,100	0
5	DMS	B	8420	4/4	0.88	0.17	36,40,43,53	0
5	DMS	A	8503	4/4	0.89	0.22	28,42,100,100	0
5	DMS	A	8428	4/4	0.89	0.20	53,66,100,100	0
5	DMS	B	8419	4/4	0.89	0.20	32,48,65,100	0
5	DMS	C	8423	4/4	0.89	0.13	28,31,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DMS	B	8501	4/4	0.89	0.15	27,44,56,64	0
5	DMS	C	8508	4/4	0.90	0.11	30,35,35,81	0
5	DMS	B	8508	4/4	0.90	0.12	19,40,41,55	0
5	DMS	B	8421	4/4	0.90	0.17	31,49,52,100	0
5	DMS	C	8419	4/4	0.90	0.14	30,32,43,52	0
5	DMS	C	8504	4/4	0.90	0.17	31,37,46,100	0
5	DMS	A	8416	4/4	0.91	0.15	16,31,40,100	0
5	DMS	D	8416	4/4	0.91	0.16	25,32,44,100	0
5	DMS	D	8705	4/4	0.91	0.16	8,44,50,78	0
5	DMS	A	8414	4/4	0.91	0.16	23,24,55,100	0
5	DMS	B	8418	4/4	0.91	0.12	26,30,63,96	0
5	DMS	D	8404	4/4	0.92	0.12	18,19,41,53	0
5	DMS	B	8423	4/4	0.92	0.12	26,28,45,50	0
5	DMS	A	8501	4/4	0.92	0.12	16,27,35,36	0
5	DMS	B	8706	4/4	0.92	0.14	37,41,42,42	0
3	MG	C	3105	1/1	0.92	0.17	35,35,35,35	0
5	DMS	D	8421	4/4	0.92	0.14	32,46,51,66	0
5	DMS	C	8415	4/4	0.93	0.10	19,25,31,38	0
5	DMS	B	8429	4/4	0.93	0.12	29,40,45,51	0
5	DMS	A	8412	4/4	0.93	0.18	29,38,100,100	0
5	DMS	C	8601	4/4	0.93	0.14	39,40,55,57	0
5	DMS	C	8602	4/4	0.93	0.15	43,47,57,68	0
4	NA	D	3104	1/1	0.93	0.12	27,27,27,27	0
5	DMS	D	8407	4/4	0.93	0.15	22,29,31,63	0
5	DMS	D	8409	4/4	0.93	0.13	27,33,36,42	0
5	DMS	D	8508	4/4	0.93	0.10	31,36,41,53	0
5	DMS	A	8419	4/4	0.93	0.13	33,38,46,47	0
5	DMS	A	8409	4/4	0.93	0.13	27,28,41,51	0
5	DMS	C	8429	4/4	0.93	0.17	41,42,51,100	0
5	DMS	D	8419	4/4	0.93	0.12	27,39,41,43	0
5	DMS	C	8501	4/4	0.93	0.12	18,26,37,46	0
5	DMS	B	8504	4/4	0.94	0.10	20,35,38,43	0
5	DMS	B	8415	4/4	0.94	0.11	19,28,30,38	0
5	DMS	D	8414	4/4	0.94	0.19	21,35,76,100	0
5	DMS	A	8408	4/4	0.94	0.10	15,29,31,48	0
3	MG	D	3105	1/1	0.94	0.12	36,36,36,36	0
5	DMS	B	8407	4/4	0.94	0.13	25,29,30,30	0
5	DMS	B	8413	4/4	0.94	0.11	28,28,29,34	0
5	DMS	B	8414	4/4	0.94	0.15	22,38,40,100	0
5	DMS	B	8502	4/4	0.94	0.09	16,22,30,36	0
5	DMS	C	8420	4/4	0.94	0.12	25,32,35,40	0
5	DMS	C	8421	4/4	0.94	0.11	30,37,41,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	A	8425	4/4	0.95	0.11	23,26,30,32	0
5	DMS	B	8404	4/4	0.95	0.08	18,21,28,28	0
5	DMS	B	8601	4/4	0.95	0.11	27,34,36,44	0
5	DMS	A	8420	4/4	0.95	0.12	24,30,31,47	0
5	DMS	A	8413	4/4	0.95	0.10	24,28,29,34	0
5	DMS	C	8407	4/4	0.95	0.10	23,24,30,34	0
4	NA	D	3103	1/1	0.95	0.08	24,24,24,24	0
5	DMS	C	8416	4/4	0.95	0.09	32,43,43,44	0
4	NA	C	3104	1/1	0.95	0.07	22,22,22,22	0
4	NA	B	3104	1/1	0.96	0.08	24,24,24,24	0
5	DMS	A	8407	4/4	0.96	0.09	18,25,28,31	0
5	DMS	A	8504	4/4	0.96	0.12	20,32,35,94	0
5	DMS	A	8506	4/4	0.96	0.12	27,28,46,63	0
3	MG	C	3006	1/1	0.96	0.10	24,24,24,24	0
3	MG	A	3005	1/1	0.96	0.07	25,25,25,25	0
3	MG	C	3004	1/1	0.96	0.12	36,36,36,36	0
5	DMS	C	8404	4/4	0.96	0.07	15,16,21,26	0
5	DMS	B	8408	4/4	0.96	0.09	22,25,31,38	0
5	DMS	B	8409	4/4	0.96	0.08	23,26,28,30	0
5	DMS	C	8409	4/4	0.96	0.11	23,32,33,35	0
5	DMS	C	8412	4/4	0.96	0.12	25,26,29,72	0
5	DMS	C	8413	4/4	0.96	0.10	24,25,27,30	0
5	DMS	D	8506	4/4	0.96	0.11	19,32,44,52	0
5	DMS	C	8414	4/4	0.96	0.11	17,37,46,48	0
5	DMS	D	8406	4/4	0.96	0.11	18,18,21,39	0
5	DMS	B	8410	4/4	0.96	0.10	19,27,33,35	0
5	DMS	D	8408	4/4	0.96	0.07	17,27,27,33	0
5	DMS	B	8425	4/4	0.96	0.08	17,26,26,32	0
5	DMS	A	8404	4/4	0.96	0.08	17,23,23,27	0
5	DMS	B	8506	4/4	0.97	0.14	26,26,29,100	0
5	DMS	D	8403	4/4	0.97	0.08	16,23,25,26	0
5	DMS	C	8410	4/4	0.97	0.08	17,27,28,30	0
5	DMS	B	8412	4/4	0.97	0.08	23,28,28,30	0
5	DMS	A	8410	4/4	0.97	0.09	17,27,32,34	0
5	DMS	C	8425	4/4	0.97	0.09	26,28,29,42	0
4	NA	A	3104	1/1	0.97	0.06	20,20,20,20	0
5	DMS	D	8410	4/4	0.97	0.08	14,27,27,39	0
5	DMS	D	8413	4/4	0.97	0.09	25,26,26,41	0
5	DMS	C	8402	4/4	0.97	0.08	12,22,23,26	0
3	MG	B	3105	1/1	0.97	0.12	35,35,35,35	0
5	DMS	A	8403	4/4	0.97	0.07	19,19,21,24	0
5	DMS	C	8506	4/4	0.97	0.12	26,26,31,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	A	3103	1/1	0.97	0.05	20,20,20,20	0
5	DMS	C	8408	4/4	0.97	0.07	15,28,29,37	0
5	DMS	D	8411	4/4	0.98	0.07	17,17,22,40	0
5	DMS	D	8412	4/4	0.98	0.09	24,26,27,35	0
5	DMS	A	8402	4/4	0.98	0.07	11,18,20,27	0
5	DMS	A	8405	4/4	0.98	0.07	18,22,22,31	0
5	DMS	B	8401	4/4	0.98	0.07	12,16,16,19	0
5	DMS	B	8402	4/4	0.98	0.07	14,14,18,23	0
5	DMS	C	8403	4/4	0.98	0.05	17,19,21,21	0
5	DMS	D	8701	4/4	0.98	0.08	13,14,17,31	0
5	DMS	B	8411	4/4	0.98	0.12	17,20,20,100	0
5	DMS	C	8405	4/4	0.98	0.07	21,23,23,24	0
5	DMS	B	8403	4/4	0.98	0.05	15,15,22,23	0
3	MG	D	3005	1/1	0.98	0.06	21,21,21,21	0
5	DMS	B	8405	4/4	0.98	0.08	22,24,28,34	0
5	DMS	C	8411	4/4	0.99	0.05	15,20,25,25	0
4	NA	B	3103	1/1	0.99	0.04	18,18,18,18	0
5	DMS	C	8401	4/4	0.99	0.05	11,12,16,17	0
3	MG	B	3002	1/1	0.99	0.03	11,11,11,11	0
4	NA	C	3102	1/1	0.99	0.02	10,10,10,10	0
4	NA	C	3103	1/1	0.99	0.06	18,18,18,18	0
3	MG	D	3002	1/1	0.99	0.05	12,12,12,12	0
4	NA	D	3101	1/1	0.99	0.03	11,11,11,11	0
3	MG	A	3002	1/1	0.99	0.04	11,11,11,11	0
4	NA	B	3101	1/1	0.99	0.02	10,10,10,10	0
5	DMS	D	8401	4/4	0.99	0.05	11,12,15,16	0
5	DMS	D	8402	4/4	0.99	0.05	12,15,17,18	0
5	DMS	A	8401	4/4	0.99	0.04	10,11,13,13	0
5	DMS	A	8411	4/4	0.99	0.07	16,21,21,48	0
5	DMS	D	8405	4/4	0.99	0.07	20,20,23,36	0
4	NA	B	3102	1/1	1.00	0.04	9,9,9,9	0
3	MG	A	3001	1/1	1.00	0.03	9,9,9,9	0
3	MG	B	3001	1/1	1.00	0.02	8,8,8,8	0
4	NA	C	3101	1/1	1.00	0.02	9,9,9,9	0
4	NA	A	3101	1/1	1.00	0.03	10,10,10,10	0
4	NA	A	3102	1/1	1.00	0.02	9,9,9,9	0
3	MG	C	3001	1/1	1.00	0.04	8,8,8,8	0
3	MG	D	3001	1/1	1.00	0.03	8,8,8,8	0
4	NA	D	3102	1/1	1.00	0.02	9,9,9,9	0
3	MG	C	3002	1/1	1.00	0.03	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.