Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 07:07 AM EDT

PDB ID	:	5E24
Title	:	Structure of the Su(H)-Hairless-DNA Repressor Complex
Authors	:	Kovall, R.A.; Yuan, Z.
Deposited on	:	2015-09-30
Resolution	:	2.14 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 (i) 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 (i)) were used in the production of this report:

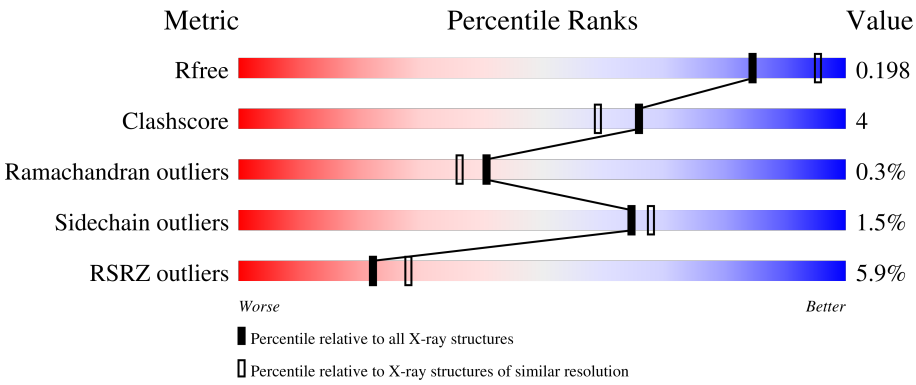
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 <=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	370	92% 8%
1	C	370	5% 94% 6%
2	B	38	18% 79% 21%
2	D	38	16% 76% 21% •
3	E	424	5% 92% 7%

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Mol	Chain	Length	Quality of chain
3	F	424	11% 89% 10%
4	G	15	87% 13%
5	H	15	100%
6	I	4	50% 50%
6	J	4	100%

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
7	EDO	A	418	-	-	-	X
7	EDO	A	444	-	-	-	X
7	EDO	A	445	-	-	-	X
7	EDO	A	446	-	-	-	X
7	EDO	A	447	-	-	-	X
7	EDO	C	411	-	-	-	X
7	EDO	C	414	-	-	-	X
7	EDO	E	609	-	-	-	X
7	EDO	E	611	-	-	-	X
7	EDO	E	623	-	-	X	-
7	EDO	F	614	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14968 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 Maltose-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	370	2876	1849	470	551	6	0	5	0
1	C	370	2851	1835	466	544	6	0	2	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ALA	ASP	engineered mutation	UNP P0AEY0
A	83	ALA	LYS	engineered mutation	UNP P0AEY0
A	172	ALA	GLU	engineered mutation	UNP P0AEY0
A	173	ALA	ASN	engineered mutation	UNP P0AEY0
A	239	ALA	LYS	engineered mutation	UNP P0AEY0
A	367	ASN	ARG	engineered mutation	UNP P0AEY0
C	82	ALA	ASP	engineered mutation	UNP P0AEY0
C	83	ALA	LYS	engineered mutation	UNP P0AEY0
C	172	ALA	GLU	engineered mutation	UNP P0AEY0
C	173	ALA	ASN	engineered mutation	UNP P0AEY0
C	239	ALA	LYS	engineered mutation	UNP P0AEY0
C	367	ASN	ARG	engineered mutation	UNP P0AEY0

- Molecule 2 is a protein called Protein hairless.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	38	292	189	55	48	0	0	0
2	D	38	292	189	55	48	0	0	0

- Molecule 3 is a protein called Suppressor of hairless protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	424	3445	2180	595	641	29	0	11	0
3	F	422	3392	2146	583	634	29	0	5	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	155	THR	ARG	engineered mutation	UNP P28159
E	281	GLY	ASN	engineered mutation	UNP P28159
F	155	THR	ARG	engineered mutation	UNP P28159
F	281	GLY	ASN	engineered mutation	UNP P28159

- Molecule 4 is a DNA chain called DNA (5'-D(*AP*AP*TP*CP*TP*TP*TP*CP*CP*CP*AP*CP*AP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	G	15	298	145	50	89	14	0	0	0

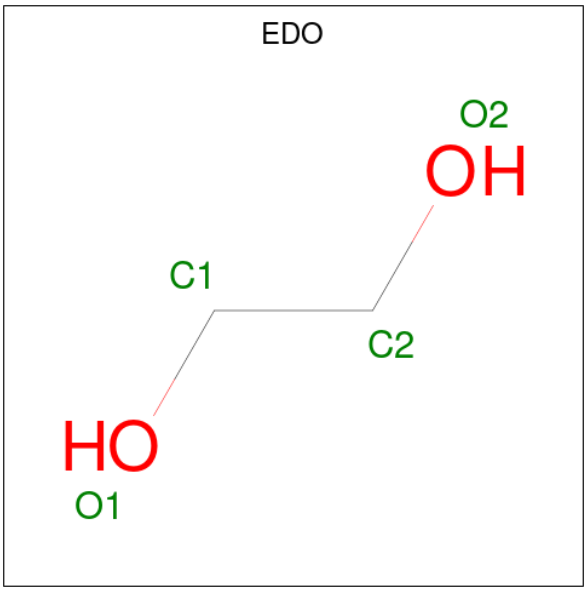
- Molecule 5 is a DNA chain called DNA (5'-D(*TP*TP*AP*CP*TP*GP*TP*GP*GP*GP*AP*AP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	H	15	311	149	61	87	14	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
6	I	4	45	24	21	0	0	0
6	J	4	45	24	21	0	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	C	1	4	2	2	0	0
7	C	1	4	2	2	0	0
7	C	1	4	2	2	0	0
7	C	1	4	2	2	0	0
7	C	1	4	2	2	0	0
7	C	1	4	2	2	0	0
7	D	1	4	2	2	0	0
7	D	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	E	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	F	1	4	2	2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	283	283	283	0	0
8	B	8	8	8	0	0
8	C	96	96	96	0	0
8	D	9	9	9	0	0

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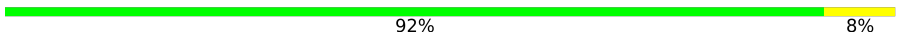
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	E	174	174	174	0	0
			Total	O		
8	F	80	80	80	0	0
			Total	O		
8	G	6	6	6	0	0
			Total	O		
8	H	13	13	13	0	0

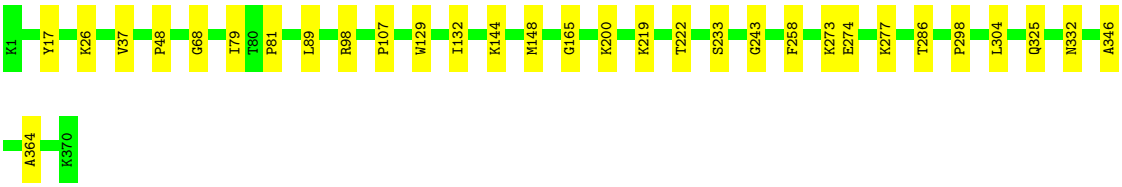
3 Residue-property plots (i)

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: Maltose-binding periplasmic protein

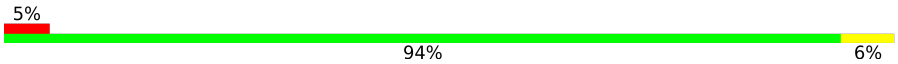
Chain A:

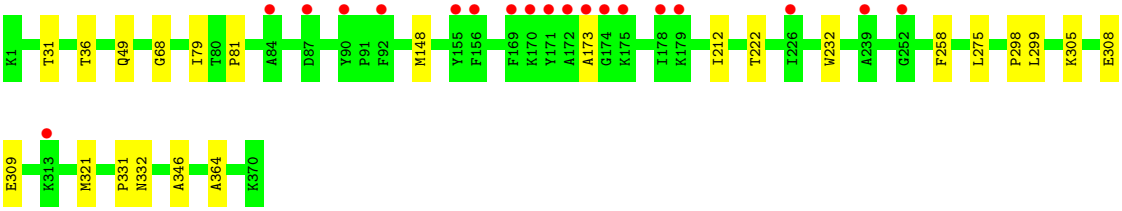




• Molecule 1: Maltose-binding periplasmic protein

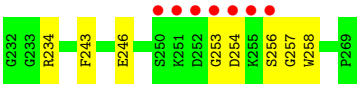
Chain C:





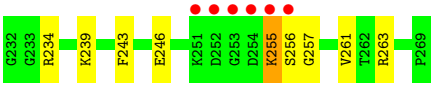
• Molecule 2: Protein hairless

Chain B:



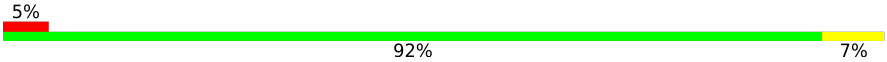
• Molecule 2: Protein hairless

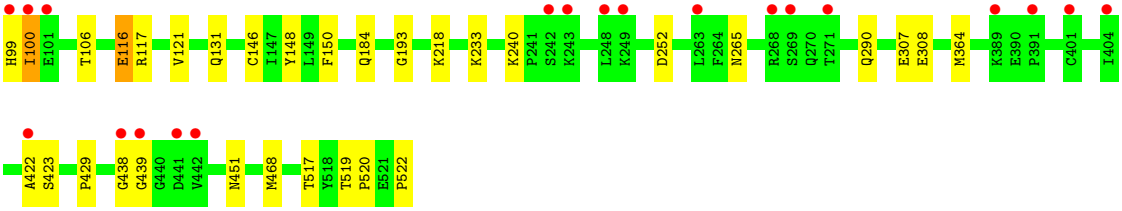
Chain D:



• Molecule 3: Suppressor of hairless protein

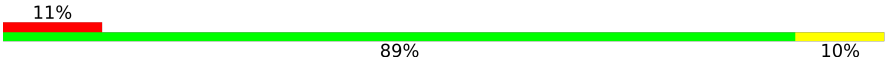
Chain E:

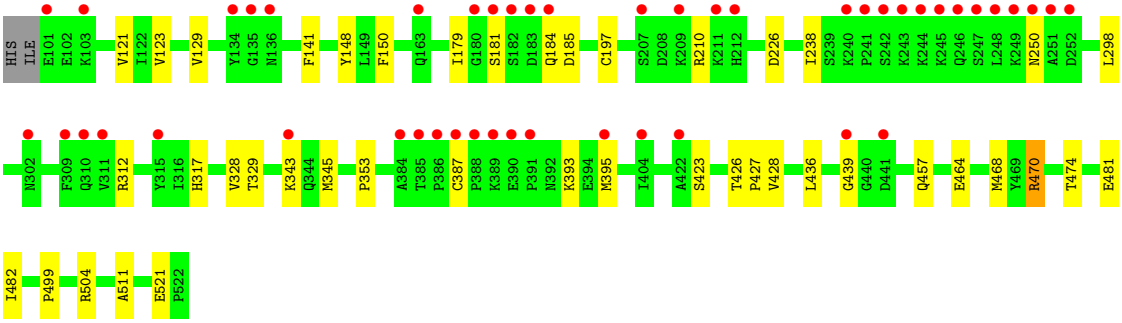




• Molecule 3: Suppressor of hairless protein

Chain F:



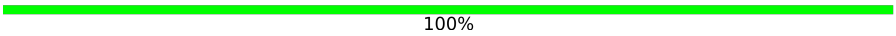


• Molecule 4: DNA (5'-D(*AP*AP*TP*CP*TP*TP*TP*CP*CP*CP*AP*CP*AP*GP*T)-3')

Chain G:

• Molecule 5: DNA (5'-D(*TP*TP*AP*CP*TP*GP*TP*GP*GP*GP*AP*AP*AP*GP*A)-3')

Chain H:



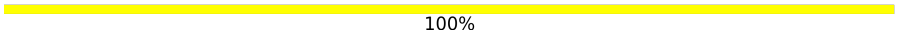
There are no outlier residues recorded for this chain.

• Molecule 6: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I:

• Molecule 6: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J:



GLC1
GLC2
GLC3
GLC4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	177.71Å 93.89Å 154.39Å 90.00° 109.83° 90.00°	Depositor
Resolution (Å)	31.30 – 2.14 31.32 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.6 (31.30-2.14) 100.0 (31.32-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.14Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.173 , 0.193 0.175 , 0.198	Depositor DCC
R_{free} test set	6595 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14968	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, EDO

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	0.57	0/2945	0.59	0/4004
1	C	0.48	0/2920	0.59	0/3971
2	B	0.46	0/299	0.69	0/400
2	D	0.49	0/299	0.77	1/400 (0.2%)
3	E	0.47	0/3525	0.63	0/4763
3	F	0.45	0/3467	0.64	0/4684
4	G	1.11	0/332	0.97	0/509
5	H	1.11	0/350	0.91	0/540
All	All	0.54	0/14137	0.64	1/19271 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	255	LYS	C-N-CA	5.39	135.17	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2876	0	2819	26	0
1	C	2851	0	2797	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	292	0	287	5	0
2	D	292	0	287	7	0
3	E	3445	0	3383	26	0
3	F	3392	0	3342	26	0
4	G	298	0	172	3	0
5	H	311	0	171	0	0
6	I	45	0	39	2	0
6	J	45	0	39	0	0
7	A	192	0	288	22	0
7	C	56	0	84	10	0
7	D	8	0	12	1	0
7	E	96	0	144	18	0
7	F	100	0	150	10	0
8	A	283	0	0	0	0
8	B	8	0	0	0	0
8	C	96	0	0	0	0
8	D	9	0	0	0	0
8	E	174	0	0	0	0
8	F	80	0	0	1	0
8	G	6	0	0	0	0
8	H	13	0	0	0	0
All	All	14968	0	14014	112	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 4.

All (112) 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)
3:E:290:GLN:HA	7:E:623:EDO:H12	1.42	0.99
4:G:1:DA:H2"	4:G:2:DA:H5"	1.46	0.95
3:E:146[B]:CYS:SG	7:E:623:EDO:H11	2.18	0.84
1:C:299:LEU:HD23	7:C:403:EDO:H22	1.60	0.83
3:E:193:GLY:H	7:E:602:EDO:H21	1.45	0.80
3:E:106:THR:HB	7:E:607:EDO:H12	1.64	0.80
7:A:433:EDO:H12	3:F:464:GLU:H	1.50	0.74
3:E:517[A]:THR:HG22	3:E:519:THR:HG23	1.75	0.68
7:A:404:EDO:H22	7:A:434:EDO:H12	1.75	0.68
3:E:520:PRO:HD3	7:E:608:EDO:H21	1.76	0.67
3:F:457:GLN:HG3	7:F:609:EDO:H22	1.79	0.64
3:E:520:PRO:CD	7:E:608:EDO:H21	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:HD11	7:A:430:EDO:H21	1.81	0.63
1:A:219:LYS:HE2	7:A:442:EDO:H21	1.79	0.63
3:F:345:MET:HE1	3:F:393:LYS:HB3	1.81	0.62
1:A:98:ARG:O	7:A:434:EDO:H21	1.98	0.62
1:A:274:GLU:HB3	7:A:448:EDO:H12	1.81	0.61
3:F:141:PHE:HB3	7:F:610:EDO:H11	1.83	0.61
3:E:146[B]:CYS:SG	7:E:623:EDO:C1	2.89	0.60
1:A:144:LYS:NZ	7:A:425:EDO:H22	2.16	0.60
3:E:290:GLN:HA	7:E:623:EDO:C1	2.26	0.59
3:E:233:LYS:HE3	7:E:605:EDO:H22	1.84	0.59
2:D:239:LYS:HG3	7:D:302:EDO:H12	1.84	0.58
1:A:165:GLY:HA3	7:A:421:EDO:H11	1.85	0.58
1:A:48:PRO:HB3	7:A:429:EDO:H11	1.86	0.58
1:C:299:LEU:CD2	7:C:403:EDO:H22	2.34	0.56
3:E:148:TYR:OH	7:E:623:EDO:H22	2.06	0.56
1:A:325:GLN:O	7:A:412:EDO:H12	2.05	0.56
1:A:286:THR:HA	7:A:430:EDO:H22	1.87	0.56
3:E:117:ARG:HH11	7:E:609:EDO:H22	1.73	0.54
3:F:197:CYS:HA	7:F:622:EDO:H11	1.88	0.54
3:E:438:GLY:N	3:E:439:GLY:HA2	2.23	0.53
3:F:179:ILE:HG22	3:F:210:ARG:HH22	1.73	0.53
3:F:470[B]:ARG:HB3	3:F:474:THR:OG1	2.09	0.53
1:C:31:THR:HB	7:C:409:EDO:H12	1.91	0.52
1:A:273:LYS:HB2	7:A:438:EDO:H22	1.92	0.52
3:F:427:PRO:HA	7:F:607:EDO:H12	1.92	0.51
7:E:604:EDO:H12	7:E:617:EDO:H21	1.93	0.50
3:F:298:LEU:O	3:F:312:ARG:HB3	2.11	0.50
3:F:345:MET:HE3	3:F:387:CYS:HB2	1.94	0.50
3:F:499:PRO:HB2	7:F:611:EDO:H11	1.93	0.50
3:F:328:VAL:HG23	3:F:329:THR:HG23	1.94	0.50
4:G:1:DA:C2'	4:G:2:DA:H5"	2.29	0.49
2:D:263:ARG:HH21	3:E:522:PRO:HD2	1.77	0.49
7:A:404:EDO:C2	7:A:434:EDO:H12	2.42	0.49
1:C:212:ILE:HG12	7:C:402:EDO:H12	1.93	0.49
1:C:305:LYS:O	1:C:309:GLU:HG2	2.12	0.49
1:A:144:LYS:CE	7:A:425:EDO:H22	2.42	0.49
1:A:26:LYS:HD2	7:A:401:EDO:H21	1.95	0.49
1:C:79:ILE:HG22	1:C:81:PRO:HD3	1.95	0.48
3:E:364:MET:HB3	7:E:612:EDO:H22	1.93	0.48
3:F:504:ARG:HD3	7:F:616:EDO:H12	1.96	0.48
3:F:345:MET:CE	3:F:387:CYS:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:HG22	1:A:81:PRO:HD3	1.95	0.48
3:F:317:HIS:HA	3:F:353:PRO:HA	1.96	0.48
1:A:148:MET:HB2	1:A:222:THR:HG21	1.96	0.47
1:A:89:LEU:HD23	1:A:107:PRO:HG2	1.95	0.47
2:D:256:SER:HB3	2:D:257:GLY:HA3	1.97	0.47
3:E:218:LYS:HD3	7:E:613:EDO:H11	1.97	0.47
1:C:148:MET:HB2	1:C:222:THR:HG21	1.97	0.47
3:F:482:ILE:HG13	7:F:624:EDO:H11	1.97	0.47
1:C:49:GLN:HE22	7:C:404:EDO:H12	1.79	0.46
3:F:426:THR:HG22	3:F:428:VAL:HG23	1.97	0.46
2:D:243:PHE:HZ	2:D:246:GLU:HB2	1.81	0.46
3:E:438:GLY:H	3:E:439:GLY:HA2	1.80	0.46
2:D:256:SER:HB3	2:D:257:GLY:CA	2.46	0.46
2:D:261:VAL:HG11	2:D:263:ARG:NH1	2.31	0.45
3:E:265:ASN:HA	7:E:620:EDO:H12	1.98	0.45
4:G:1:DA:H2"	4:G:2:DA:C5'	2.33	0.45
1:A:68:GLY:HA3	1:A:332:ASN:O	2.17	0.45
7:A:405:EDO:H22	6:I:3:GLC:H3	1.99	0.45
2:B:243:PHE:HZ	2:B:246:GLU:HB2	1.81	0.45
2:B:256:SER:HA	2:B:257:GLY:HA3	1.72	0.45
3:E:429:PRO:HA	3:E:451:ASN:HB2	1.98	0.45
3:E:307:GLU:HG3	7:E:619:EDO:H21	1.99	0.44
1:A:48:PRO:HB2	3:F:481:GLU:HG2	2.00	0.44
2:B:258:TRP:HZ2	7:F:624:EDO:H12	1.83	0.44
3:F:345:MET:HE3	3:F:395:MET:HG3	1.99	0.44
1:A:277:LYS:HE3	7:A:437:EDO:H12	2.00	0.43
1:C:331:PRO:HA	7:C:407:EDO:H21	1.99	0.43
3:F:121:VAL:HB	3:F:150:PHE:HB2	1.99	0.43
1:C:298:PRO:O	7:C:403:EDO:H11	2.18	0.43
1:C:232:TRP:HB2	1:C:298:PRO:HG2	2.00	0.43
3:E:131:GLN:HB3	7:E:618:EDO:H21	2.00	0.43
3:E:148:TYR:OH	7:E:623:EDO:C2	2.66	0.43
1:A:274:GLU:O	7:A:448:EDO:H21	2.19	0.43
1:C:68:GLY:HA3	1:C:332:ASN:O	2.17	0.43
1:A:200:LYS:O	7:A:447:EDO:H11	2.18	0.43
1:A:243:GLY:HA2	7:A:436:EDO:H12	2.00	0.42
1:A:17:TYR:HD1	7:A:428:EDO:H21	1.84	0.42
3:E:116:GLU:H	3:E:116:GLU:HG2	1.71	0.42
2:D:255:LYS:CB	2:D:256:SER:HA	2.49	0.42
3:F:179:ILE:HG22	3:F:210:ARG:NH2	2.34	0.42
3:F:511:ALA:HB1	7:F:611:EDO:H21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:470[A]:ARG:HH11	3:F:470[A]:ARG:HB3	1.83	0.42
3:E:99:HIS:HA	3:E:100:ILE:HA	1.92	0.42
2:B:253:GLY:HA2	2:B:254:ASP:HA	1.84	0.42
3:F:129:VAL:HB	3:F:238:ILE:HG12	2.02	0.42
1:A:346:ALA:HB2	1:A:364:ALA:HB2	2.01	0.42
1:C:346:ALA:HB2	1:C:364:ALA:HB2	2.02	0.42
1:A:37:VAL:HB	7:A:428:EDO:H22	2.02	0.41
1:A:233[A]:SER:OG	1:A:298:PRO:HD3	2.20	0.41
3:E:100:ILE:HA	3:E:422:ALA:HB2	2.01	0.41
3:E:121:VAL:HB	3:E:150:PHE:HB2	2.02	0.41
1:A:129:TRP:HA	1:A:132:ILE:HD12	2.03	0.41
1:C:332:ASN:H	7:C:407:EDO:H21	1.86	0.41
1:C:321:MET:HG3	7:C:408:EDO:H21	2.03	0.41
6:I:3:GLC:H62	6:I:4:GLC:H5	2.03	0.40
7:F:609:EDO:H12	8:F:716:HOH:O	2.21	0.40
1:C:275:LEU:H	7:C:406:EDO:H11	1.85	0.40
3:F:123:VAL:HB	3:F:148:TYR:HB2	2.03	0.40
2:B:258:TRP:O	3:F:436:LEU:HD21	2.21	0.40

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	373/370 (101%)	369 (99%)	4 (1%)	0	100 100
1	C	370/370 (100%)	362 (98%)	7 (2%)	1 (0%)	41 36
2	B	36/38 (95%)	33 (92%)	3 (8%)	0	100 100
2	D	36/38 (95%)	31 (86%)	5 (14%)	0	100 100
3	E	433/424 (102%)	422 (98%)	10 (2%)	1 (0%)	47 45
3	F	425/424 (100%)	415 (98%)	7 (2%)	3 (1%)	22 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1673/1664 (100%)	1632 (98%)	36 (2%)	5 (0%)	41	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	185	ASP
1	C	173	ALA
3	E	100	ILE
3	F	343	LYS
3	F	439	GLY

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	291/292 (100%)	290 (100%)	1 (0%)	92	94
1	C	287/292 (98%)	284 (99%)	3 (1%)	76	79
2	B	28/32 (88%)	27 (96%)	1 (4%)	35	32
2	D	28/32 (88%)	27 (96%)	1 (4%)	35	32
3	E	378/370 (102%)	371 (98%)	7 (2%)	57	59
3	F	373/370 (101%)	364 (98%)	9 (2%)	49	49
All	All	1385/1388 (100%)	1363 (98%)	22 (2%)	65	65

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	PHE
2	B	234	ARG
1	C	36	THR
1	C	258	PHE
1	C	308	GLU
2	D	234	ARG
3	E	116	GLU

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Mol	Chain	Res	Type
3	E	184	GLN
3	E	240	LYS
3	E	252	ASP
3	E	308	GLU
3	E	423	SER
3	E	468	MET
3	F	181	SER
3	F	184	GLN
3	F	226	ASP
3	F	250	ASN
3	F	423	SER
3	F	468	MET
3	F	470[A]	ARG
3	F	470[B]	ARG
3	F	521	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

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	$\#\|Z\| > 2$
6	GLC	I	1	6	12,12,12	0.70	0	17,17,17	1.02	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GLC	I	2	6	11,11,12	1.16	1 (9%)	15,15,17	1.18	2 (13%)
6	GLC	I	3	6	11,11,12	0.73	0	15,15,17	1.37	1 (6%)
6	GLC	I	4	6	11,11,12	0.64	0	15,15,17	1.36	3 (20%)
6	GLC	J	1	6	12,12,12	0.60	0	17,17,17	1.02	1 (5%)
6	GLC	J	2	6	11,11,12	1.00	0	15,15,17	1.23	2 (13%)
6	GLC	J	3	6	11,11,12	0.72	0	15,15,17	1.28	1 (6%)
6	GLC	J	4	6	11,11,12	0.55	0	15,15,17	1.28	2 (13%)

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	GLC	I	1	6	-	0/2/22/22	0/1/1/1
6	GLC	I	2	6	-	0/2/19/22	0/1/1/1
6	GLC	I	3	6	-	0/2/19/22	0/1/1/1
6	GLC	I	4	6	-	2/2/19/22	0/1/1/1
6	GLC	J	1	6	-	0/2/22/22	0/1/1/1
6	GLC	J	2	6	-	0/2/19/22	0/1/1/1
6	GLC	J	3	6	-	0/2/19/22	0/1/1/1
6	GLC	J	4	6	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	2	GLC	C2-C3	2.07	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	3	GLC	C6-C5-C4	-3.04	105.88	113.00
6	I	4	GLC	O5-C5-C6	-2.94	102.60	107.20
6	J	4	GLC	O5-C5-C6	-2.88	102.69	107.20
6	J	3	GLC	C6-C5-C4	-2.83	106.37	113.00
6	J	4	GLC	C2-C3-C4	-2.74	106.16	110.89
6	J	2	GLC	C6-C5-C4	-2.53	107.08	113.00
6	I	1	GLC	C6-C5-C4	-2.52	107.11	113.00
6	I	2	GLC	C6-C5-C4	-2.43	107.32	113.00
6	I	4	GLC	C2-C3-C4	-2.34	106.84	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	2	GLC	C1-C2-C3	-2.15	107.03	109.67
6	I	2	GLC	C2-C3-C4	-2.08	107.29	110.89
6	I	4	GLC	O4-C4-C3	-2.03	105.67	110.35
6	J	1	GLC	C3-C4-C5	-2.02	106.63	110.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	4	GLC	C4-C5-C6-O6
6	J	4	GLC	C4-C5-C6-O6
6	J	4	GLC	O5-C5-C6-O6
6	I	4	GLC	O5-C5-C6-O6

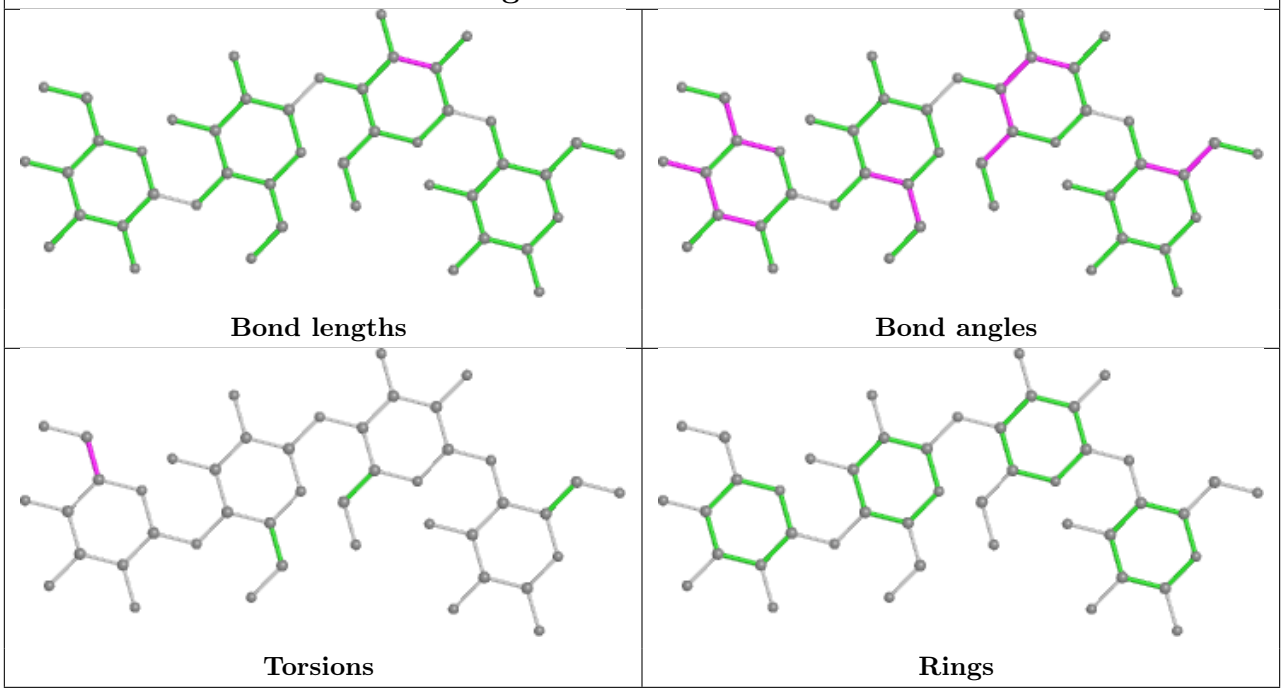
There are no ring outliers.

2 monomers are involved in 2 short contacts:

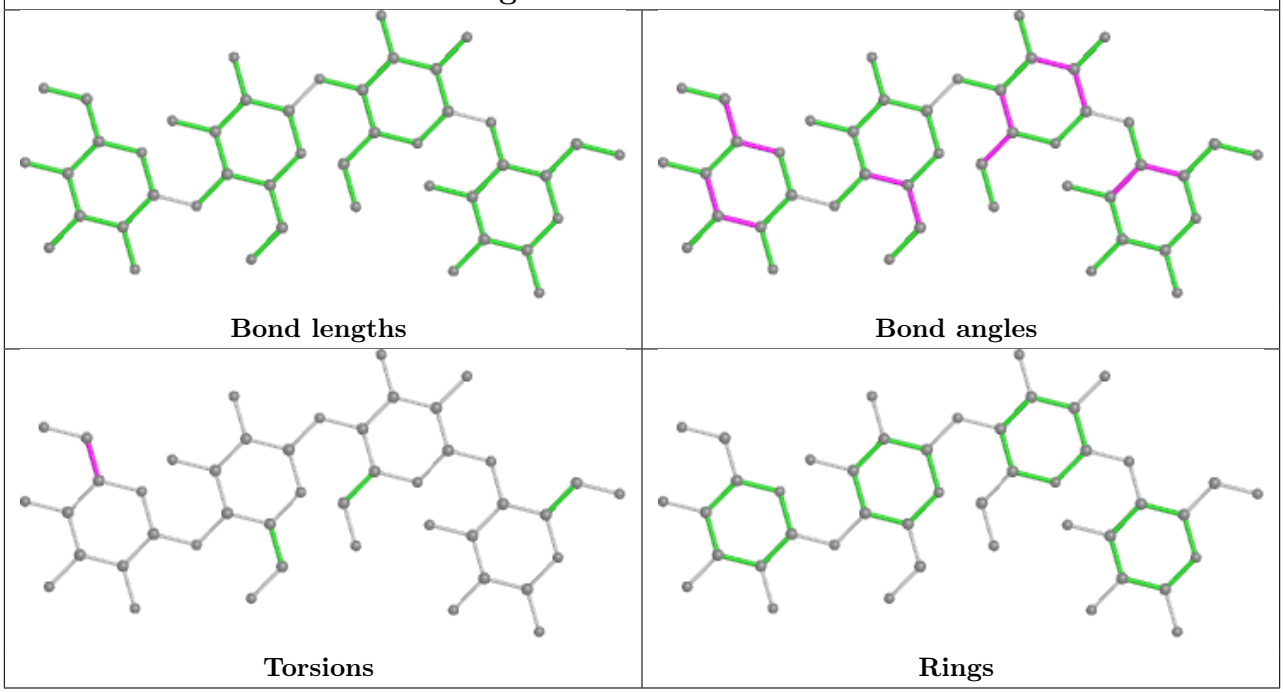
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	3	GLC	2	0
6	I	4	GLC	1	0

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

Oligosaccharide Chain I



Oligosaccharide Chain J



5.6 Ligand geometry (i)

113 ligands 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	$\#\|Z\| > 2$
7	EDO	A	418	-	3,3,3	0.55	0	2,2,2	0.40	0
7	EDO	E	609	-	3,3,3	0.54	0	2,2,2	0.32	0
7	EDO	E	604	-	3,3,3	0.49	0	2,2,2	0.34	0
7	EDO	F	614	-	3,3,3	0.59	0	2,2,2	0.12	0
7	EDO	F	603	-	3,3,3	0.58	0	2,2,2	0.28	0
7	EDO	E	610	-	3,3,3	0.46	0	2,2,2	0.41	0
7	EDO	A	448	-	3,3,3	0.54	0	2,2,2	0.34	0
7	EDO	C	402	-	3,3,3	0.62	0	2,2,2	0.31	0
7	EDO	C	411	-	3,3,3	0.64	0	2,2,2	0.28	0
7	EDO	A	434	-	3,3,3	0.61	0	2,2,2	0.59	0
7	EDO	A	427	-	3,3,3	0.46	0	2,2,2	0.50	0
7	EDO	A	446	-	3,3,3	0.62	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	EDO	C	405	-	3,3,3	0.48	0	2,2,2	0.50	0
7	EDO	A	442	-	3,3,3	0.63	0	2,2,2	0.33	0
7	EDO	A	436	-	3,3,3	0.35	0	2,2,2	0.45	0
7	EDO	F	623	-	3,3,3	0.56	0	2,2,2	0.31	0
7	EDO	E	608	-	3,3,3	0.58	0	2,2,2	0.48	0
7	EDO	A	414	-	3,3,3	0.63	0	2,2,2	0.14	0
7	EDO	A	417	-	3,3,3	0.87	0	2,2,2	0.19	0
7	EDO	E	622	-	3,3,3	0.50	0	2,2,2	0.36	0
7	EDO	A	413	-	3,3,3	0.48	0	2,2,2	0.29	0
7	EDO	E	606	-	3,3,3	0.53	0	2,2,2	0.42	0
7	EDO	E	602	-	3,3,3	0.56	0	2,2,2	0.41	0
7	EDO	F	622	-	3,3,3	0.72	0	2,2,2	0.11	0
7	EDO	F	604	-	3,3,3	0.55	0	2,2,2	0.34	0
7	EDO	A	429	-	3,3,3	0.73	0	2,2,2	0.30	0
7	EDO	F	618	-	3,3,3	0.58	0	2,2,2	0.24	0
7	EDO	F	619	-	3,3,3	0.57	0	2,2,2	0.23	0
7	EDO	A	408	-	3,3,3	0.50	0	2,2,2	0.71	0
7	EDO	C	401	-	3,3,3	0.52	0	2,2,2	0.29	0
7	EDO	A	437	-	3,3,3	0.42	0	2,2,2	0.42	0
7	EDO	E	621	-	3,3,3	0.56	0	2,2,2	0.51	0
7	EDO	E	623	-	3,3,3	0.67	0	2,2,2	0.05	0
7	EDO	F	612	-	3,3,3	0.50	0	2,2,2	0.46	0
7	EDO	E	607	-	3,3,3	0.58	0	2,2,2	0.24	0
7	EDO	A	421	-	3,3,3	0.55	0	2,2,2	0.42	0
7	EDO	F	601	-	3,3,3	0.58	0	2,2,2	0.34	0
7	EDO	A	411	-	3,3,3	0.57	0	2,2,2	0.27	0
7	EDO	A	428	-	3,3,3	0.59	0	2,2,2	0.22	0
7	EDO	C	410	-	3,3,3	0.60	0	2,2,2	0.13	0
7	EDO	A	439	-	3,3,3	0.64	0	2,2,2	0.14	0
7	EDO	F	609	-	3,3,3	0.65	0	2,2,2	0.23	0
7	EDO	E	611	-	3,3,3	0.67	0	2,2,2	0.16	0
7	EDO	A	420	-	3,3,3	0.50	0	2,2,2	0.46	0
7	EDO	C	409	-	3,3,3	0.61	0	2,2,2	0.31	0
7	EDO	A	407	-	3,3,3	0.65	0	2,2,2	0.25	0
7	EDO	C	403	-	3,3,3	0.39	0	2,2,2	0.39	0
7	EDO	A	444	-	3,3,3	0.66	0	2,2,2	0.14	0
7	EDO	A	416	-	3,3,3	0.67	0	2,2,2	0.18	0
7	EDO	E	618	-	3,3,3	0.46	0	2,2,2	0.22	0
7	EDO	A	405	-	3,3,3	0.62	0	2,2,2	0.12	0
7	EDO	C	414	-	3,3,3	0.57	0	2,2,2	0.37	0
7	EDO	A	445	-	3,3,3	0.59	0	2,2,2	0.34	0
7	EDO	F	608	-	3,3,3	0.58	0	2,2,2	0.42	0
7	EDO	F	616	-	3,3,3	0.47	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	EDO	E	601	-	3,3,3	0.67	0	2,2,2	0.32	0
7	EDO	A	402	-	3,3,3	0.41	0	2,2,2	0.57	0
7	EDO	E	614	-	3,3,3	0.58	0	2,2,2	0.38	0
7	EDO	A	443	-	3,3,3	0.52	0	2,2,2	0.42	0
7	EDO	F	607	-	3,3,3	0.48	0	2,2,2	0.62	0
7	EDO	D	302	-	3,3,3	0.57	0	2,2,2	0.29	0
7	EDO	F	611	-	3,3,3	0.64	0	2,2,2	0.29	0
7	EDO	F	605	-	3,3,3	0.65	0	2,2,2	0.10	0
7	EDO	A	410	-	3,3,3	0.56	0	2,2,2	0.22	0
7	EDO	A	431	-	3,3,3	0.52	0	2,2,2	0.25	0
7	EDO	A	404	-	3,3,3	0.44	0	2,2,2	0.52	0
7	EDO	A	440	-	3,3,3	0.56	0	2,2,2	0.28	0
7	EDO	A	412	-	3,3,3	0.52	0	2,2,2	0.47	0
7	EDO	A	425	-	3,3,3	0.66	0	2,2,2	0.48	0
7	EDO	C	404	-	3,3,3	0.47	0	2,2,2	0.49	0
7	EDO	F	615	-	3,3,3	0.58	0	2,2,2	0.29	0
7	EDO	A	424	-	3,3,3	0.70	0	2,2,2	0.05	0
7	EDO	A	447	-	3,3,3	0.52	0	2,2,2	0.38	0
7	EDO	C	412	-	3,3,3	0.61	0	2,2,2	0.25	0
7	EDO	A	441	-	3,3,3	0.53	0	2,2,2	0.20	0
7	EDO	C	407	-	3,3,3	0.66	0	2,2,2	0.23	0
7	EDO	E	616	-	3,3,3	0.49	0	2,2,2	0.48	0
7	EDO	A	415	-	3,3,3	0.55	0	2,2,2	0.36	0
7	EDO	A	406	-	3,3,3	0.41	0	2,2,2	0.41	0
7	EDO	E	603	-	3,3,3	0.58	0	2,2,2	0.24	0
7	EDO	A	430	-	3,3,3	0.35	0	2,2,2	0.57	0
7	EDO	D	301	-	3,3,3	0.55	0	2,2,2	0.32	0
7	EDO	C	408	-	3,3,3	0.66	0	2,2,2	0.21	0
7	EDO	A	435	-	3,3,3	0.51	0	2,2,2	0.23	0
7	EDO	E	605	-	3,3,3	0.45	0	2,2,2	0.50	0
7	EDO	F	613	-	3,3,3	0.60	0	2,2,2	0.19	0
7	EDO	F	602	-	3,3,3	0.64	0	2,2,2	0.41	0
7	EDO	E	615	-	3,3,3	0.68	0	2,2,2	0.21	0
7	EDO	E	617	-	3,3,3	0.60	0	2,2,2	0.21	0
7	EDO	E	624	-	3,3,3	0.64	0	2,2,2	0.24	0
7	EDO	F	606	-	3,3,3	0.56	0	2,2,2	0.32	0
7	EDO	E	620	-	3,3,3	0.46	0	2,2,2	0.53	0
7	EDO	A	426	-	3,3,3	0.68	0	2,2,2	0.24	0
7	EDO	F	625	-	3,3,3	0.56	0	2,2,2	0.36	0
7	EDO	A	423	-	3,3,3	0.54	0	2,2,2	0.15	0
7	EDO	C	406	-	3,3,3	0.64	0	2,2,2	0.26	0
7	EDO	A	403	-	3,3,3	0.54	0	2,2,2	0.82	0
7	EDO	F	624	-	3,3,3	0.46	0	2,2,2	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	EDO	F	610	-	3,3,3	0.69	0	2,2,2	0.42	0
7	EDO	A	401	-	3,3,3	0.50	0	2,2,2	0.20	0
7	EDO	F	617	-	3,3,3	0.52	0	2,2,2	0.31	0
7	EDO	A	433	-	3,3,3	0.55	0	2,2,2	0.25	0
7	EDO	A	422	-	3,3,3	0.70	0	2,2,2	0.14	0
7	EDO	F	620	-	3,3,3	0.56	0	2,2,2	0.32	0
7	EDO	A	438	-	3,3,3	0.76	0	2,2,2	0.12	0
7	EDO	F	621	-	3,3,3	0.60	0	2,2,2	0.23	0
7	EDO	A	432	-	3,3,3	0.59	0	2,2,2	0.11	0
7	EDO	C	413	-	3,3,3	0.56	0	2,2,2	0.59	0
7	EDO	E	613	-	3,3,3	0.47	0	2,2,2	0.44	0
7	EDO	A	409	-	3,3,3	0.52	0	2,2,2	0.29	0
7	EDO	E	619	-	3,3,3	0.57	0	2,2,2	0.30	0
7	EDO	E	612	-	3,3,3	0.61	0	2,2,2	0.24	0
7	EDO	A	419	-	3,3,3	0.62	0	2,2,2	0.21	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	418	-	-	0/1/1/1	-
7	EDO	E	609	-	-	1/1/1/1	-
7	EDO	E	604	-	-	0/1/1/1	-
7	EDO	F	614	-	-	1/1/1/1	-
7	EDO	F	603	-	-	0/1/1/1	-
7	EDO	E	610	-	-	0/1/1/1	-
7	EDO	A	448	-	-	0/1/1/1	-
7	EDO	C	402	-	-	0/1/1/1	-
7	EDO	C	411	-	-	1/1/1/1	-
7	EDO	A	434	-	-	0/1/1/1	-
7	EDO	A	427	-	-	1/1/1/1	-
7	EDO	A	446	-	-	1/1/1/1	-
7	EDO	C	405	-	-	0/1/1/1	-
7	EDO	A	442	-	-	0/1/1/1	-
7	EDO	A	436	-	-	1/1/1/1	-
7	EDO	F	623	-	-	1/1/1/1	-
7	EDO	E	608	-	-	0/1/1/1	-
7	EDO	A	414	-	-	1/1/1/1	-
7	EDO	A	417	-	-	1/1/1/1	-
7	EDO	E	622	-	-	1/1/1/1	-
7	EDO	A	413	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	E	606	-	-	0/1/1/1	-
7	EDO	E	602	-	-	1/1/1/1	-
7	EDO	F	622	-	-	1/1/1/1	-
7	EDO	F	604	-	-	0/1/1/1	-
7	EDO	A	429	-	-	1/1/1/1	-
7	EDO	F	618	-	-	0/1/1/1	-
7	EDO	F	619	-	-	0/1/1/1	-
7	EDO	A	408	-	-	0/1/1/1	-
7	EDO	C	401	-	-	0/1/1/1	-
7	EDO	A	437	-	-	1/1/1/1	-
7	EDO	E	621	-	-	0/1/1/1	-
7	EDO	E	623	-	-	1/1/1/1	-
7	EDO	F	612	-	-	0/1/1/1	-
7	EDO	E	607	-	-	1/1/1/1	-
7	EDO	A	421	-	-	0/1/1/1	-
7	EDO	F	601	-	-	0/1/1/1	-
7	EDO	A	411	-	-	0/1/1/1	-
7	EDO	A	428	-	-	0/1/1/1	-
7	EDO	C	410	-	-	1/1/1/1	-
7	EDO	A	439	-	-	0/1/1/1	-
7	EDO	F	609	-	-	0/1/1/1	-
7	EDO	E	611	-	-	1/1/1/1	-
7	EDO	A	420	-	-	0/1/1/1	-
7	EDO	C	409	-	-	0/1/1/1	-
7	EDO	A	407	-	-	0/1/1/1	-
7	EDO	C	403	-	-	0/1/1/1	-
7	EDO	A	444	-	-	0/1/1/1	-
7	EDO	A	416	-	-	1/1/1/1	-
7	EDO	E	618	-	-	0/1/1/1	-
7	EDO	A	405	-	-	0/1/1/1	-
7	EDO	C	414	-	-	0/1/1/1	-
7	EDO	A	445	-	-	0/1/1/1	-
7	EDO	F	608	-	-	0/1/1/1	-
7	EDO	F	616	-	-	0/1/1/1	-
7	EDO	E	601	-	-	0/1/1/1	-
7	EDO	A	402	-	-	0/1/1/1	-
7	EDO	E	614	-	-	0/1/1/1	-
7	EDO	A	443	-	-	0/1/1/1	-
7	EDO	F	607	-	-	0/1/1/1	-
7	EDO	D	302	-	-	1/1/1/1	-
7	EDO	F	611	-	-	0/1/1/1	-
7	EDO	F	605	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	410	-	-	1/1/1/1	-
7	EDO	A	431	-	-	0/1/1/1	-
7	EDO	A	404	-	-	1/1/1/1	-
7	EDO	A	440	-	-	0/1/1/1	-
7	EDO	A	412	-	-	0/1/1/1	-
7	EDO	A	425	-	-	1/1/1/1	-
7	EDO	C	404	-	-	0/1/1/1	-
7	EDO	F	615	-	-	1/1/1/1	-
7	EDO	A	424	-	-	1/1/1/1	-
7	EDO	A	447	-	-	0/1/1/1	-
7	EDO	C	412	-	-	0/1/1/1	-
7	EDO	A	441	-	-	0/1/1/1	-
7	EDO	C	407	-	-	0/1/1/1	-
7	EDO	E	616	-	-	1/1/1/1	-
7	EDO	A	415	-	-	0/1/1/1	-
7	EDO	A	406	-	-	1/1/1/1	-
7	EDO	E	603	-	-	0/1/1/1	-
7	EDO	A	430	-	-	1/1/1/1	-
7	EDO	D	301	-	-	0/1/1/1	-
7	EDO	C	408	-	-	0/1/1/1	-
7	EDO	A	435	-	-	0/1/1/1	-
7	EDO	E	605	-	-	0/1/1/1	-
7	EDO	F	613	-	-	0/1/1/1	-
7	EDO	F	602	-	-	0/1/1/1	-
7	EDO	E	615	-	-	0/1/1/1	-
7	EDO	E	617	-	-	0/1/1/1	-
7	EDO	E	624	-	-	1/1/1/1	-
7	EDO	F	606	-	-	0/1/1/1	-
7	EDO	E	620	-	-	0/1/1/1	-
7	EDO	A	426	-	-	0/1/1/1	-
7	EDO	F	625	-	-	0/1/1/1	-
7	EDO	A	423	-	-	0/1/1/1	-
7	EDO	C	406	-	-	1/1/1/1	-
7	EDO	A	403	-	-	0/1/1/1	-
7	EDO	F	624	-	-	0/1/1/1	-
7	EDO	F	610	-	-	1/1/1/1	-
7	EDO	A	401	-	-	0/1/1/1	-
7	EDO	F	617	-	-	1/1/1/1	-
7	EDO	A	433	-	-	0/1/1/1	-
7	EDO	A	422	-	-	0/1/1/1	-
7	EDO	F	620	-	-	0/1/1/1	-
7	EDO	A	438	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	F	621	-	-	0/1/1/1	-
7	EDO	A	432	-	-	1/1/1/1	-
7	EDO	C	413	-	-	0/1/1/1	-
7	EDO	E	613	-	-	0/1/1/1	-
7	EDO	A	409	-	-	1/1/1/1	-
7	EDO	E	619	-	-	0/1/1/1	-
7	EDO	E	612	-	-	1/1/1/1	-
7	EDO	A	419	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	410	EDO	O1-C1-C2-O2
7	A	413	EDO	O1-C1-C2-O2
7	A	425	EDO	O1-C1-C2-O2
7	A	429	EDO	O1-C1-C2-O2
7	A	436	EDO	O1-C1-C2-O2
7	E	607	EDO	O1-C1-C2-O2
7	E	622	EDO	O1-C1-C2-O2
7	F	617	EDO	O1-C1-C2-O2
7	A	409	EDO	O1-C1-C2-O2
7	A	432	EDO	O1-C1-C2-O2
7	E	611	EDO	O1-C1-C2-O2
7	E	623	EDO	O1-C1-C2-O2
7	E	624	EDO	O1-C1-C2-O2
7	D	302	EDO	O1-C1-C2-O2
7	A	404	EDO	O1-C1-C2-O2
7	A	406	EDO	O1-C1-C2-O2
7	A	427	EDO	O1-C1-C2-O2
7	A	438	EDO	O1-C1-C2-O2
7	C	411	EDO	O1-C1-C2-O2
7	E	602	EDO	O1-C1-C2-O2
7	F	614	EDO	O1-C1-C2-O2
7	F	623	EDO	O1-C1-C2-O2
7	A	417	EDO	O1-C1-C2-O2
7	A	424	EDO	O1-C1-C2-O2
7	C	410	EDO	O1-C1-C2-O2
7	E	609	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	E	616	EDO	O1-C1-C2-O2
7	A	414	EDO	O1-C1-C2-O2
7	A	419	EDO	O1-C1-C2-O2
7	A	430	EDO	O1-C1-C2-O2
7	A	437	EDO	O1-C1-C2-O2
7	A	446	EDO	O1-C1-C2-O2
7	E	612	EDO	O1-C1-C2-O2
7	F	615	EDO	O1-C1-C2-O2
7	F	622	EDO	O1-C1-C2-O2
7	A	416	EDO	O1-C1-C2-O2
7	C	406	EDO	O1-C1-C2-O2
7	F	610	EDO	O1-C1-C2-O2

There are no ring outliers.

45 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	609	EDO	1	0
7	E	604	EDO	1	0
7	A	448	EDO	2	0
7	C	402	EDO	1	0
7	A	434	EDO	3	0
7	A	442	EDO	1	0
7	A	436	EDO	1	0
7	E	608	EDO	2	0
7	E	602	EDO	1	0
7	F	622	EDO	1	0
7	A	429	EDO	1	0
7	A	437	EDO	1	0
7	E	623	EDO	6	0
7	E	607	EDO	1	0
7	A	421	EDO	1	0
7	A	428	EDO	2	0
7	F	609	EDO	2	0
7	C	409	EDO	1	0
7	C	403	EDO	3	0
7	E	618	EDO	1	0
7	A	405	EDO	1	0
7	F	616	EDO	1	0
7	F	607	EDO	1	0
7	D	302	EDO	1	0
7	F	611	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	404	EDO	2	0
7	A	412	EDO	1	0
7	A	425	EDO	2	0
7	C	404	EDO	1	0
7	A	447	EDO	1	0
7	C	407	EDO	2	0
7	A	430	EDO	2	0
7	C	408	EDO	1	0
7	E	605	EDO	1	0
7	E	617	EDO	1	0
7	E	620	EDO	1	0
7	C	406	EDO	1	0
7	F	624	EDO	2	0
7	F	610	EDO	1	0
7	A	401	EDO	1	0
7	A	433	EDO	1	0
7	A	438	EDO	1	0
7	E	613	EDO	1	0
7	E	619	EDO	1	0
7	E	612	EDO	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	370/370 (100%)	-0.20	0 100 100	19, 30, 51, 82	0
1	C	370/370 (100%)	0.23	19 (5%) 28 34	36, 59, 99, 123	0
2	B	38/38 (100%)	0.98	7 (18%) 1 1	36, 58, 118, 122	0
2	D	38/38 (100%)	0.93	6 (15%) 2 2	38, 56, 114, 116	0
3	E	424/424 (100%)	0.09	20 (4%) 31 38	25, 44, 83, 122	0
3	F	422/424 (99%)	0.55	47 (11%) 5 6	28, 60, 115, 161	0
4	G	15/15 (100%)	-0.14	0 100 100	47, 60, 72, 75	0
5	H	15/15 (100%)	-0.42	0 100 100	38, 57, 70, 73	0
All	All	1692/1694 (99%)	0.20	99 (5%) 22 28	19, 49, 98, 161	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	311	VAL	8.5
3	F	181	SER	8.5
2	D	252	ASP	8.2
3	F	247	SER	8.1
2	B	253	GLY	7.9
1	C	172	ALA	7.1
2	B	252	ASP	7.1
3	E	100	ILE	6.8
3	F	134	TYR	6.4
2	D	256	SER	6.3
2	D	254	ASP	6.3
2	B	254	ASP	6.1
3	F	251	ALA	6.0
3	E	438	GLY	5.9
1	C	174	GLY	5.9
3	E	439	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	173	ALA	5.5
3	E	99	HIS	5.5
2	D	255	LYS	5.5
2	D	253	GLY	5.3
3	F	439	GLY	5.0
3	F	135	GLY	4.9
3	E	271	THR	4.9
3	F	184	GLN	4.7
3	F	391	PRO	4.6
3	F	249	LYS	4.6
3	F	248	LEU	4.4
3	E	243	LYS	4.4
3	F	244	LYS	4.4
1	C	84	ALA	4.3
3	F	441	ASP	4.3
3	F	246	GLN	4.2
3	F	209	LYS	4.2
3	F	252	ASP	4.2
3	F	243	LYS	4.2
3	F	241	PRO	4.1
2	D	251	LYS	4.1
3	F	183	ASP	4.0
1	C	239	ALA	4.0
3	F	387	CYS	3.8
1	C	313	LYS	3.8
3	F	245	LYS	3.8
3	E	441	ASP	3.8
1	C	92	PHE	3.7
1	C	171	TYR	3.7
3	F	250	ASN	3.7
3	F	136	ASN	3.6
1	C	175	LYS	3.5
2	B	250	SER	3.4
1	C	178	ILE	3.3
3	F	101	GLU	3.2
3	F	240	LYS	3.2
3	F	302	ASN	3.1
1	C	87	ASP	3.1
1	C	90	TYR	3.1
3	E	442	VAL	3.1
3	F	309	PHE	3.1
3	F	388	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	180	GLY	2.9
3	F	163	GLN	2.9
3	F	385	THR	2.9
1	C	169	PHE	2.8
1	C	226	ILE	2.8
2	B	251	LYS	2.8
3	F	310	GLN	2.8
3	F	404	ILE	2.7
2	B	256	SER	2.7
1	C	252	GLY	2.7
3	F	242	SER	2.7
3	E	263	LEU	2.6
3	F	103	LYS	2.6
2	B	255	LYS	2.6
3	E	391	PRO	2.6
3	F	211	LYS	2.5
3	F	315	TYR	2.5
3	F	207	SER	2.5
3	F	390	GLU	2.5
3	E	422	ALA	2.5
3	E	249	LYS	2.5
1	C	179	LYS	2.5
3	E	269	SER	2.5
3	F	395	MET	2.4
3	F	212	HIS	2.4
3	F	384	ALA	2.4
1	C	170	LYS	2.4
3	F	182	SER	2.3
3	E	404	ILE	2.3
3	F	386	PRO	2.3
3	E	242	SER	2.3
3	E	101	GLU	2.3
3	F	343	LYS	2.3
3	E	401[A]	CYS	2.2
3	E	268	ARG	2.2
1	C	156	PHE	2.1
1	C	155	TYR	2.1
3	E	389	LYS	2.1
3	F	389	LYS	2.1
3	F	422	ALA	2.0
3	E	248	LEU	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)

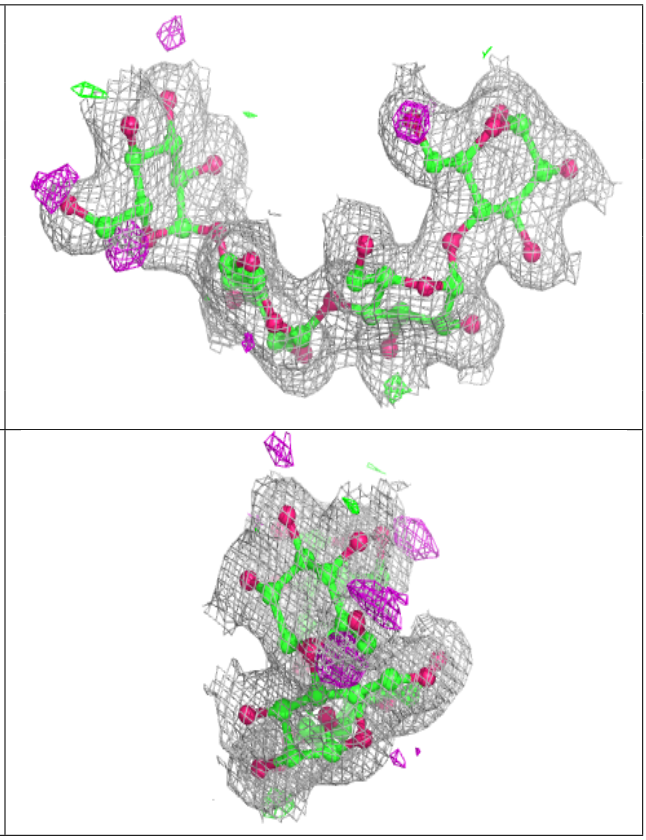
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GLC	I	4	11/12	0.96	0.10	29,32,40,42	0
6	GLC	J	1	12/12	0.96	0.17	33,39,41,42	0
6	GLC	J	4	11/12	0.96	0.11	34,36,38,42	0
6	GLC	J	2	11/12	0.97	0.18	33,36,37,37	0
6	GLC	I	3	11/12	0.97	0.15	23,25,29,34	0
6	GLC	I	2	11/12	0.98	0.17	18,21,22,24	0
6	GLC	J	3	11/12	0.98	0.15	34,36,42,45	0
6	GLC	I	1	12/12	0.98	0.14	20,22,25,26	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.

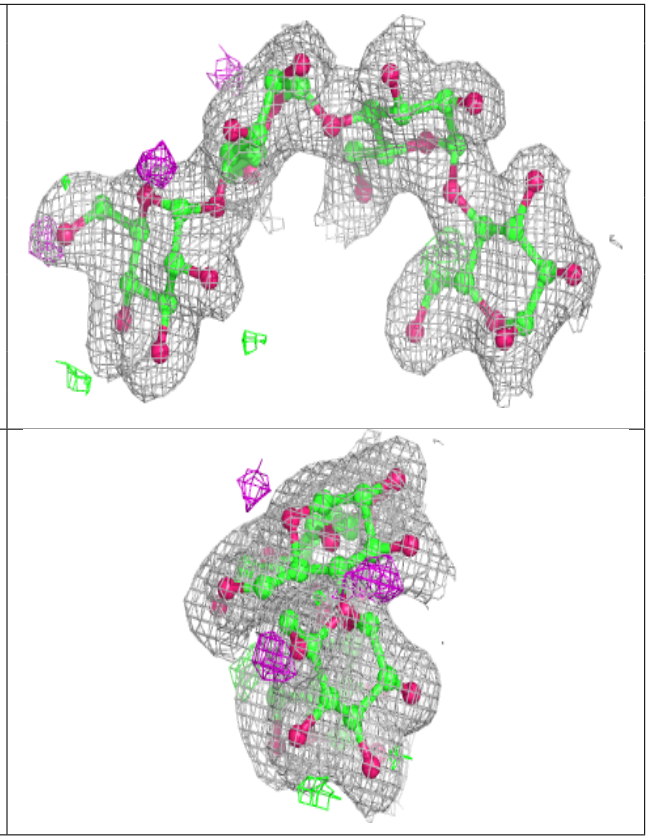
Electron density around Chain I:

$2mF_o$-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 J:

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



6.4 Ligands (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
7	EDO	E	609	4/4	0.60	0.40	79,81,83,84	0
7	EDO	E	617	4/4	0.63	0.34	89,89,90,90	0
7	EDO	A	416	4/4	0.65	0.30	65,67,70,73	0
7	EDO	F	621	4/4	0.65	0.39	83,84,84,84	0
7	EDO	C	408	4/4	0.66	0.33	77,77,78,79	0
7	EDO	F	614	4/4	0.67	0.51	76,77,78,78	0
7	EDO	C	409	4/4	0.68	0.30	68,69,69,69	0
7	EDO	A	424	4/4	0.71	0.29	59,63,66,66	0
7	EDO	A	445	4/4	0.71	0.41	71,72,72,73	0
7	EDO	A	418	4/4	0.72	0.47	73,73,73,74	0
7	EDO	A	446	4/4	0.72	0.45	66,67,68,68	0
7	EDO	A	436	4/4	0.74	0.24	53,56,60,61	0
7	EDO	A	439	4/4	0.74	0.38	68,69,69,70	0
7	EDO	A	422	4/4	0.74	0.16	68,70,73,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	C	414	4/4	0.74	0.60	79,80,81,82	0
7	EDO	E	611	4/4	0.75	0.45	65,67,68,68	0
7	EDO	C	406	4/4	0.75	0.34	69,69,69,69	0
7	EDO	C	407	4/4	0.75	0.20	70,72,73,74	0
7	EDO	A	423	4/4	0.75	0.29	73,74,75,77	0
7	EDO	A	444	4/4	0.76	0.47	57,62,65,68	0
7	EDO	A	407	4/4	0.76	0.23	63,64,65,65	0
7	EDO	E	612	4/4	0.76	0.32	51,55,58,59	0
7	EDO	A	447	4/4	0.77	0.45	63,65,68,71	0
7	EDO	A	437	4/4	0.77	0.29	82,82,82,82	0
7	EDO	E	615	4/4	0.78	0.29	69,71,71,71	0
7	EDO	C	411	4/4	0.78	0.53	76,76,77,77	0
7	EDO	A	413	4/4	0.78	0.26	79,80,80,81	0
7	EDO	E	607	4/4	0.78	0.25	66,67,67,68	0
7	EDO	E	613	4/4	0.79	0.16	59,60,63,66	0
7	EDO	D	301	4/4	0.80	0.24	84,85,86,86	0
7	EDO	A	420	4/4	0.80	0.27	72,73,76,78	0
7	EDO	F	622	4/4	0.80	0.42	64,66,66,67	0
7	EDO	F	619	4/4	0.81	0.32	79,80,81,81	0
7	EDO	C	410	4/4	0.82	0.39	64,67,68,69	0
7	EDO	E	623	4/4	0.82	0.32	47,52,59,63	0
7	EDO	C	412	4/4	0.82	0.27	75,76,77,77	0
7	EDO	A	417	4/4	0.83	0.25	50,51,52,53	0
7	EDO	A	429	4/4	0.83	0.25	37,45,47,52	0
7	EDO	E	624	4/4	0.83	0.31	68,69,69,70	0
7	EDO	F	613	4/4	0.83	0.38	67,70,72,74	0
7	EDO	F	608	4/4	0.84	0.19	61,64,67,69	0
7	EDO	D	302	4/4	0.84	0.43	79,80,81,81	0
7	EDO	F	624	4/4	0.84	0.25	47,51,54,56	0
7	EDO	E	619	4/4	0.85	0.43	73,74,74,74	0
7	EDO	C	402	4/4	0.85	0.44	62,63,63,64	0
7	EDO	A	441	4/4	0.85	0.22	67,68,68,69	0
7	EDO	F	617	4/4	0.85	0.39	76,77,77,77	0
7	EDO	A	448	4/4	0.86	0.23	42,48,51,57	0
7	EDO	F	604	4/4	0.86	0.18	73,74,75,76	0
7	EDO	E	610	4/4	0.86	0.21	72,72,73,73	0
7	EDO	A	442	4/4	0.86	0.42	66,66,66,67	0
7	EDO	C	404	4/4	0.86	0.25	59,63,66,70	0
7	EDO	A	433	4/4	0.86	0.33	54,58,58,59	0
7	EDO	F	618	4/4	0.86	0.32	52,53,57,59	0
7	EDO	A	434	4/4	0.86	0.41	42,47,52,54	0
7	EDO	A	440	4/4	0.86	0.38	77,77,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	E	603	4/4	0.86	0.13	63,63,64,65	0
7	EDO	A	427	4/4	0.86	0.30	75,75,77,77	0
7	EDO	F	625	4/4	0.86	0.17	78,78,78,79	0
7	EDO	A	428	4/4	0.87	0.27	62,63,64,64	0
7	EDO	A	426	4/4	0.87	0.29	45,51,53,54	0
7	EDO	F	610	4/4	0.87	0.21	56,58,59,59	0
7	EDO	F	611	4/4	0.87	0.33	57,57,57,58	0
7	EDO	A	438	4/4	0.87	0.27	38,41,43,45	0
7	EDO	A	435	4/4	0.87	0.20	40,45,46,47	0
7	EDO	F	615	4/4	0.87	0.42	65,65,65,67	0
7	EDO	A	414	4/4	0.88	0.30	52,56,61,63	0
7	EDO	F	612	4/4	0.88	0.16	64,64,65,65	0
7	EDO	F	603	4/4	0.88	0.13	72,73,74,74	0
7	EDO	A	409	4/4	0.88	0.26	63,65,66,67	0
7	EDO	E	608	4/4	0.88	0.39	55,56,56,60	0
7	EDO	A	432	4/4	0.88	0.41	55,57,58,60	0
7	EDO	A	431	4/4	0.89	0.30	58,59,60,60	0
7	EDO	E	622	4/4	0.89	0.29	65,65,66,68	0
7	EDO	E	616	4/4	0.89	0.29	69,70,72,73	0
7	EDO	C	405	4/4	0.89	0.42	75,76,77,78	0
7	EDO	A	425	4/4	0.90	0.26	43,43,46,49	0
7	EDO	A	408	4/4	0.90	0.17	43,43,47,47	0
7	EDO	F	620	4/4	0.90	0.31	68,69,71,72	0
7	EDO	C	401	4/4	0.90	0.39	80,80,81,81	0
7	EDO	A	419	4/4	0.90	0.28	46,53,58,62	0
7	EDO	F	623	4/4	0.90	0.21	71,71,71,71	0
7	EDO	F	609	4/4	0.90	0.22	51,56,57,59	0
7	EDO	A	406	4/4	0.90	0.14	56,58,61,63	0
7	EDO	A	411	4/4	0.91	0.39	65,67,68,69	0
7	EDO	A	410	4/4	0.91	0.14	46,51,54,57	0
7	EDO	E	604	4/4	0.91	0.12	64,64,65,66	0
7	EDO	E	620	4/4	0.92	0.22	50,55,58,62	0
7	EDO	E	606	4/4	0.92	0.14	64,65,66,68	0
7	EDO	F	607	4/4	0.92	0.22	70,70,71,71	0
7	EDO	C	413	4/4	0.92	0.21	56,60,63,64	0
7	EDO	A	403	4/4	0.92	0.19	38,41,41,45	0
7	EDO	E	602	4/4	0.93	0.15	55,57,58,59	0
7	EDO	E	621	4/4	0.93	0.17	63,63,64,64	0
7	EDO	F	605	4/4	0.93	0.25	64,65,66,66	0
7	EDO	F	606	4/4	0.93	0.31	58,59,60,62	0
7	EDO	A	412	4/4	0.93	0.32	50,50,52,54	0
7	EDO	E	618	4/4	0.93	0.24	46,51,52,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	F	616	4/4	0.93	0.19	73,73,73,73	0
7	EDO	A	443	4/4	0.93	0.32	60,61,62,64	0
7	EDO	A	421	4/4	0.94	0.25	57,61,65,69	0
7	EDO	F	601	4/4	0.94	0.21	67,67,68,68	0
7	EDO	A	430	4/4	0.94	0.43	58,58,61,62	0
7	EDO	E	614	4/4	0.94	0.15	60,61,61,62	0
7	EDO	E	605	4/4	0.94	0.19	50,50,52,54	0
7	EDO	E	601	4/4	0.95	0.09	34,37,37,38	0
7	EDO	C	403	4/4	0.95	0.36	45,47,48,51	0
7	EDO	A	415	4/4	0.96	0.12	43,45,48,49	0
7	EDO	A	401	4/4	0.96	0.15	50,51,51,54	0
7	EDO	F	602	4/4	0.97	0.09	29,30,31,31	0
7	EDO	A	405	4/4	0.97	0.11	45,48,49,50	0
7	EDO	A	404	4/4	0.98	0.09	35,36,37,40	0
7	EDO	A	402	4/4	0.98	0.19	47,48,49,53	0

6.5 Other polymers (i)

There are no such residues in this entry.