Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2024 – 01:47 am BST

PDB ID	:	8RZK
Title	:	The Michaelis complex of ZgGH129 D486N from Zobellia galactanivorans with neo-b/k-oligo-carrageenan tetrasaccharide (beta-kappa neo-oligo-carrageenan DP4).
Authors	:	Roret, T.; Czjzek, M.; Ficko-Blean, E.
Deposited on	:	2024-02-12
Resolution	:	2.29 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:

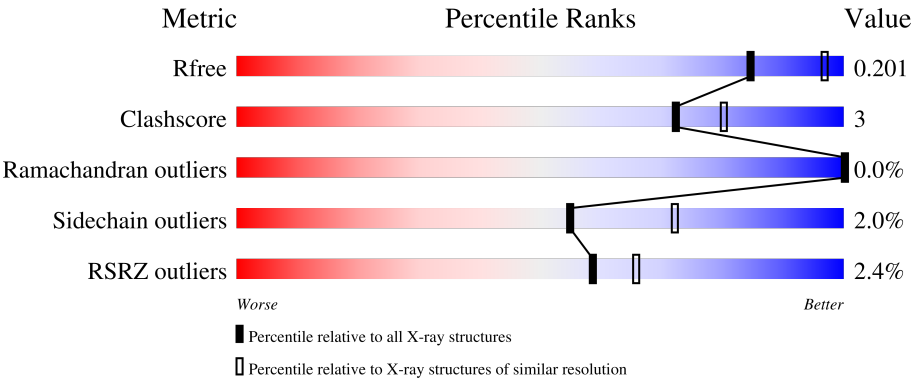
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	676	2% 90% 7%
1	B	676	88% 9%
1	C	676	2% 88% 9%
1	D	676	4% 86% 12%
2	E	4	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	4	50% 50%
2	G	4	75% 25%
2	H	4	75% 25%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 22347 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 Conserved hypothetical periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	659	Total	C	N	O	S	0	0	0
			5238	3347	889	979	23			
1	B	659	Total	C	N	O	S	0	0	0
			5241	3348	889	981	23			
1	C	659	Total	C	N	O	S	0	0	0
			5234	3345	886	980	23			
1	D	659	Total	C	N	O	S	0	0	0
			5238	3347	888	980	23			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	initiating methionine	UNP G0L004
A	19	GLY	-	expression tag	UNP G0L004
A	20	SER	-	expression tag	UNP G0L004
A	21	SER	-	expression tag	UNP G0L004
A	22	HIS	-	expression tag	UNP G0L004
A	23	HIS	-	expression tag	UNP G0L004
A	24	HIS	-	expression tag	UNP G0L004
A	25	HIS	-	expression tag	UNP G0L004
A	26	HIS	-	expression tag	UNP G0L004
A	27	HIS	-	expression tag	UNP G0L004
A	28	GLY	-	expression tag	UNP G0L004
A	29	SER	-	expression tag	UNP G0L004
A	30	LEU	-	expression tag	UNP G0L004
A	31	ASP	-	expression tag	UNP G0L004
A	486	ASN	ASP	engineered mutation	UNP G0L004
B	18	MET	-	initiating methionine	UNP G0L004
B	19	GLY	-	expression tag	UNP G0L004
B	20	SER	-	expression tag	UNP G0L004
B	21	SER	-	expression tag	UNP G0L004
B	22	HIS	-	expression tag	UNP G0L004
B	23	HIS	-	expression tag	UNP G0L004

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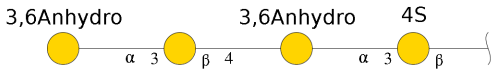
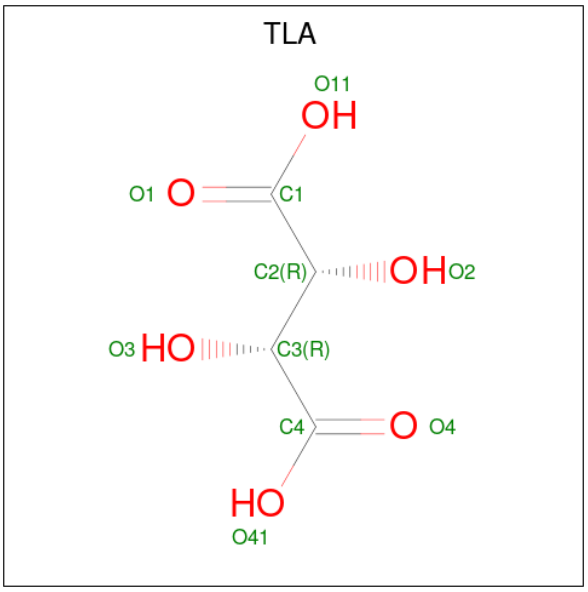
Chain	Residue	Modelled	Actual	Comment	Reference
B	24	HIS	-	expression tag	UNP G0L004
B	25	HIS	-	expression tag	UNP G0L004
B	26	HIS	-	expression tag	UNP G0L004
B	27	HIS	-	expression tag	UNP G0L004
B	28	GLY	-	expression tag	UNP G0L004
B	29	SER	-	expression tag	UNP G0L004
B	30	LEU	-	expression tag	UNP G0L004
B	31	ASP	-	expression tag	UNP G0L004
B	486	ASN	ASP	engineered mutation	UNP G0L004
C	18	MET	-	initiating methionine	UNP G0L004
C	19	GLY	-	expression tag	UNP G0L004
C	20	SER	-	expression tag	UNP G0L004
C	21	SER	-	expression tag	UNP G0L004
C	22	HIS	-	expression tag	UNP G0L004
C	23	HIS	-	expression tag	UNP G0L004
C	24	HIS	-	expression tag	UNP G0L004
C	25	HIS	-	expression tag	UNP G0L004
C	26	HIS	-	expression tag	UNP G0L004
C	27	HIS	-	expression tag	UNP G0L004
C	28	GLY	-	expression tag	UNP G0L004
C	29	SER	-	expression tag	UNP G0L004
C	30	LEU	-	expression tag	UNP G0L004
C	31	ASP	-	expression tag	UNP G0L004
C	486	ASN	ASP	engineered mutation	UNP G0L004
D	18	MET	-	initiating methionine	UNP G0L004
D	19	GLY	-	expression tag	UNP G0L004
D	20	SER	-	expression tag	UNP G0L004
D	21	SER	-	expression tag	UNP G0L004
D	22	HIS	-	expression tag	UNP G0L004
D	23	HIS	-	expression tag	UNP G0L004
D	24	HIS	-	expression tag	UNP G0L004
D	25	HIS	-	expression tag	UNP G0L004
D	26	HIS	-	expression tag	UNP G0L004
D	27	HIS	-	expression tag	UNP G0L004
D	28	GLY	-	expression tag	UNP G0L004
D	29	SER	-	expression tag	UNP G0L004
D	30	LEU	-	expression tag	UNP G0L004
D	31	ASP	-	expression tag	UNP G0L004
D	486	ASN	ASP	engineered mutation	UNP G0L004

- Molecule 2 is an oligosaccharide called 3,6-anhydro-alpha-D-galactopyranose-(1-3)-beta-D-galactopyranose-(1-4)-3,6-anhydro-alpha-D-galactopyranose-(1-3)-4-O-sulfo-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	E	4	Total C O S 47 24 22 1	0	0	0
2	F	4	Total C O S 47 24 22 1	0	0	0
2	G	4	Total C O S 47 24 22 1	0	0	0
2	H	4	Total C O S 47 24 22 1	0	0	0

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



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

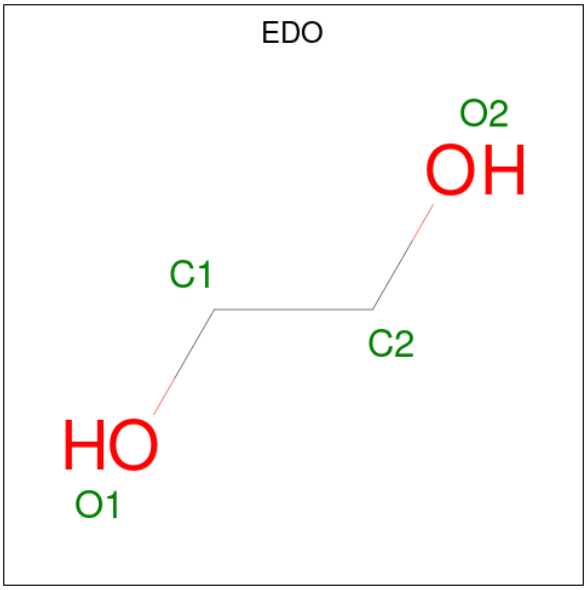
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is water.

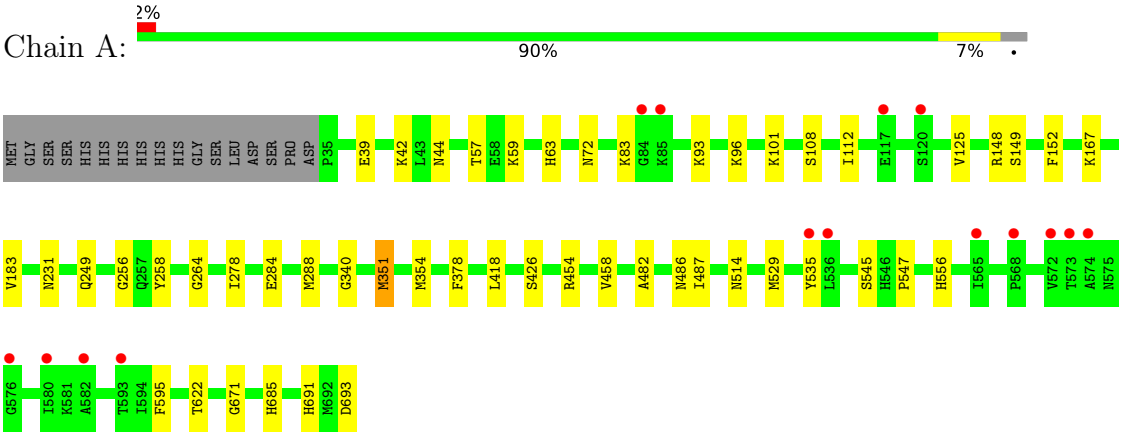
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	310	Total O 310 310	0	0
7	B	290	Total O 290 290	0	0
7	C	281	Total O 281 281	0	0
7	D	265	Total O 265 265	0	0

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.

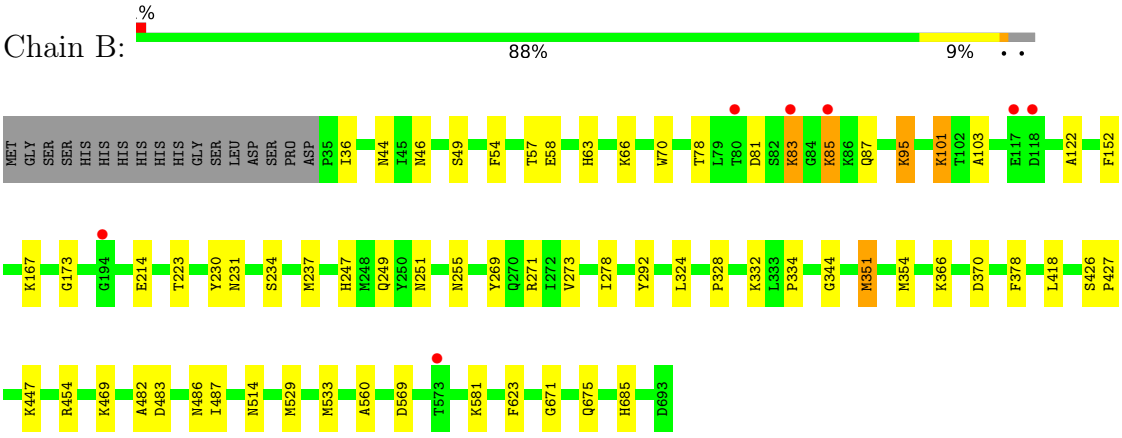
• Molecule 1: Conserved hypothetical periplasmic protein

Chain A:



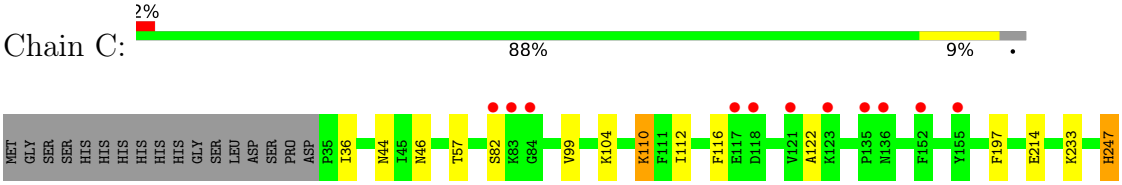
• Molecule 1: Conserved hypothetical periplasmic protein

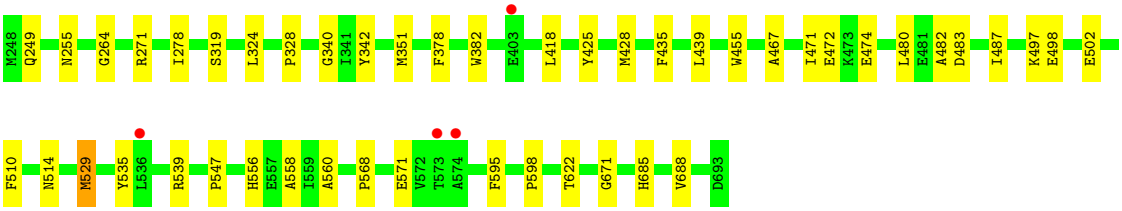
Chain B:



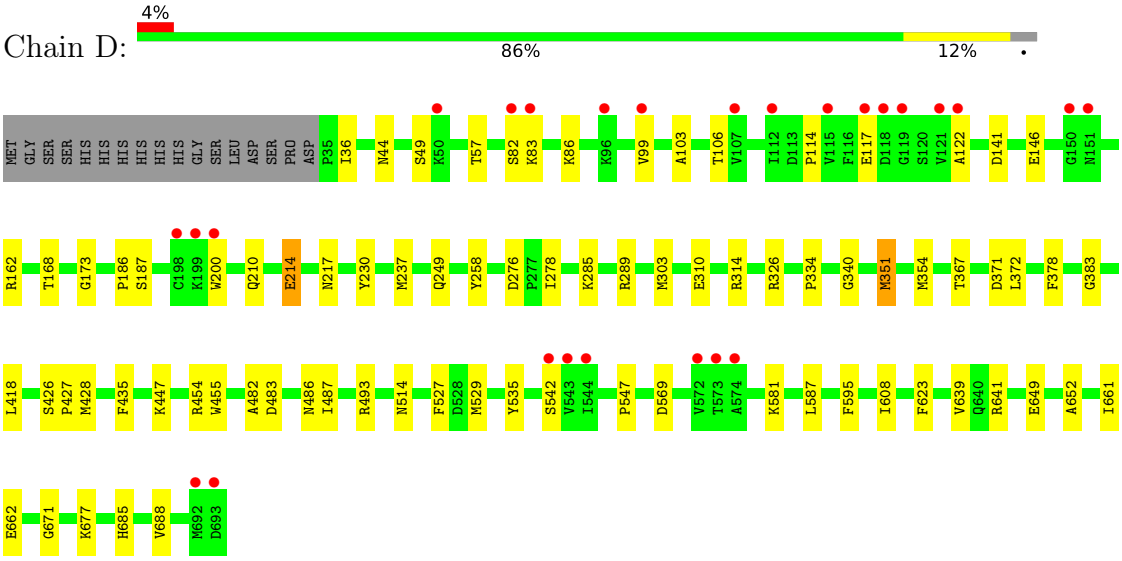
• Molecule 1: Conserved hypothetical periplasmic protein

Chain C:





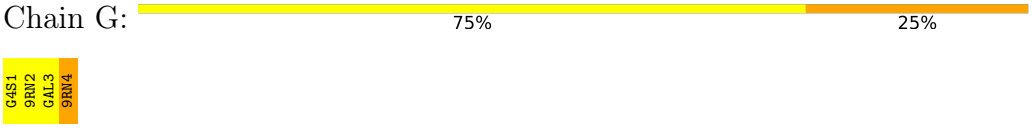
• Molecule 1: Conserved hypothetical periplasmic protein



• Molecule 2: 3,6-anhydro-alpha-D-galactopyranose-(1-3)-beta-D-galactopyranose-(1-4)-3,6-anhydro-alpha-D-galactopyranose-(1-3)-4-O-sulfo-beta-D-galactopyranose

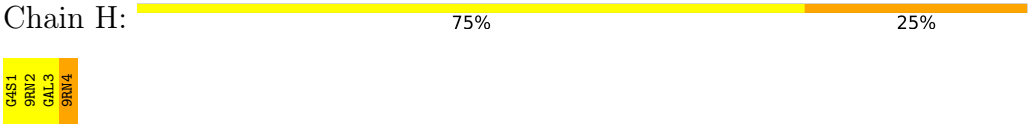
• Molecule 2: 3,6-anhydro-alpha-D-galactopyranose-(1-3)-beta-D-galactopyranose-(1-4)-3,6-anhydro-alpha-D-galactopyranose-(1-3)-4-O-sulfo-beta-D-galactopyranose

• Molecule 2: 3,6-anhydro-alpha-D-galactopyranose-(1-3)-beta-D-galactopyranose-(1-4)-3,6-anhydro-alpha-D-galactopyranose-(1-3)-4-O-sulfo-beta-D-galactopyranose



• Molecule 2: 3,6-anhydro-alpha-D-galactopyranose-(1-3)-beta-D-galactopyranose-(1-4)-3,6-anhydro-alpha-D-galactopyranose-(1-3)-4-O-sulfo-beta-D-galactopyranose

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.73Å 105.94Å 213.66Å 90.00° 111.23° 90.00°	Depositor
Resolution (Å)	47.82 – 2.29 47.82 – 2.29	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.82-2.29) 100.0 (47.82-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.169 , 0.202 0.168 , 0.201	Depositor DCC
R_{free} test set	7610 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.2	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	22347	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9RN, G4S, NA, CL, TLA, EDO, GAL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.33	0/5372	0.54	0/7262
1	B	0.34	0/5375	0.53	1/7266 (0.0%)
1	C	0.33	0/5367	0.54	0/7255
1	D	0.34	0/5372	0.54	0/7262
All	All	0.33	0/21486	0.53	1/29045 (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})
1	B	344	GLY	C-N-CA	5.78	136.15	121.70

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	5238	0	5129	23	0
1	B	5241	0	5131	36	0
1	C	5234	0	5124	35	0
1	D	5238	0	5127	41	0
2	E	47	0	20	3	0
2	F	47	0	20	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	47	0	20	2	0
2	H	47	0	20	2	0
3	A	20	0	8	1	0
3	B	10	0	4	0	0
3	C	10	0	4	0	0
3	D	10	0	4	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	1	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	B	4	0	6	0	0
7	A	310	0	0	3	0
7	B	290	0	0	7	0
7	C	281	0	0	3	0
7	D	265	0	0	3	0
All	All	22347	0	20617	140	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 3.

All (140) 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)
2:G:4:9RN:O5	2:G:4:9RN:C1	1.68	1.42
2:F:4:9RN:C1	2:F:4:9RN:O5	1.68	1.41
2:E:4:9RN:O5	2:E:4:9RN:C1	1.67	1.40
2:H:4:9RN:O5	2:H:4:9RN:C1	1.67	1.39
2:G:4:9RN:C1	2:G:4:9RN:C5	2.57	0.76
1:C:44:ASN:HB3	1:C:57:THR:HB	1.68	0.75
2:F:4:9RN:C1	2:F:4:9RN:C5	2.58	0.74
1:B:351:MET:HG2	1:B:354:MET:HB2	1.73	0.69
5:B:704:CL:CL	7:B:977:HOH:O	2.48	0.69
1:D:114:PRO:HD2	1:D:122:ALA:HB3	1.80	0.64
2:E:4:9RN:C1	2:E:4:9RN:C5	2.57	0.64
2:H:4:9RN:C1	2:H:4:9RN:C5	2.58	0.64
1:C:264:GLY:HA3	1:D:447:LYS:HB3	1.81	0.63
1:B:255:ASN:HB3	1:B:271:ARG:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ASN:HB2	1:A:57:THR:HB	1.84	0.60
1:B:486:ASN:ND2	7:B:803:HOH:O	2.34	0.60
1:A:418:LEU:HD22	1:A:482:ALA:HB2	1.85	0.58
1:C:44:ASN:OD1	1:C:46:ASN:ND2	2.38	0.57
1:A:249:GLN:HB2	1:A:278:ILE:HD11	1.88	0.56
1:B:469:LYS:NZ	7:B:802:HOH:O	2.34	0.56
1:B:487:ILE:HG23	2:F:3:GAL:H62	1.89	0.56
1:A:96:LYS:HB2	1:A:112:ILE:HB	1.89	0.55
1:A:39:GLU:OE1	1:A:59:LYS:NZ	2.29	0.55
1:B:36:ILE:HD13	1:B:49:SER:HB3	1.88	0.54
1:D:367:THR:HG23	1:D:371:ASP:OD2	2.07	0.54
1:A:351:MET:HG2	1:A:354:MET:HB2	1.90	0.53
1:C:539:ARG:NH2	7:C:807:HOH:O	2.41	0.53
1:B:418:LEU:HD22	1:B:482:ALA:HB2	1.91	0.53
1:B:81:ASP:OD2	1:B:85:LYS:HB3	2.09	0.52
1:C:474:GLU:HG2	1:C:480:LEU:HD11	1.91	0.52
1:C:535:TYR:CZ	1:C:547:PRO:HB3	2.44	0.52
1:B:101:LYS:HG2	1:B:103:ALA:O	2.10	0.51
1:C:498:GLU:H	1:C:498:GLU:CD	2.15	0.50
1:C:197:PHE:CZ	1:D:351:MET:HE1	2.46	0.50
1:D:486:ASN:ND2	7:D:807:HOH:O	2.43	0.50
1:C:455:TRP:HB3	1:C:487:ILE:HD13	1.92	0.50
1:A:183:VAL:HB	1:A:545:SER:HB2	1.94	0.49
1:D:514:ASN:ND2	7:D:802:HOH:O	2.29	0.49
1:D:237:MET:HG2	1:D:303:MET:HG2	1.93	0.49
1:A:535:TYR:CZ	1:A:547:PRO:HB3	2.48	0.49
1:C:688:VAL:HG22	1:D:688:VAL:HG22	1.95	0.49
1:A:101:LYS:O	3:A:702:TLA:H2	2.13	0.49
1:D:455:TRP:HB3	1:D:487:ILE:HD13	1.95	0.49
1:C:324:LEU:HD12	1:C:328:PRO:HA	1.94	0.49
1:A:691:HIS:ND1	7:A:803:HOH:O	2.35	0.48
1:C:233:LYS:NZ	7:C:809:HOH:O	2.44	0.48
1:B:249:GLN:HB2	1:B:278:ILE:HD11	1.94	0.48
1:B:483:ASP:O	1:B:514:ASN:HA	2.13	0.48
1:C:418:LEU:HD22	1:C:482:ALA:HB2	1.95	0.48
1:D:514:ASN:OD1	1:D:527:PHE:HA	2.14	0.48
1:B:58:GLU:OE2	1:B:234:SER:HB3	2.14	0.47
1:B:83:LYS:H	1:B:83:LYS:HG3	1.48	0.47
1:B:223:THR:HG21	1:B:533:MET:SD	2.55	0.47
1:D:36:ILE:HD13	1:D:99:VAL:HG12	1.95	0.47
1:B:78:THR:HA	1:B:87:GLN:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:ASP:OD2	1:D:289:ARG:HD2	2.15	0.47
1:D:351:MET:HE3	1:D:351:MET:HB3	1.67	0.47
1:D:671:GLY:HA2	1:D:685:HIS:HA	1.97	0.47
1:D:418:LEU:HD22	1:D:482:ALA:HB2	1.96	0.47
1:A:256:GLY:HA2	1:A:258:TYR:CE1	2.51	0.46
1:B:70:TRP:CD1	1:B:269:TYR:HB3	2.50	0.46
1:C:671:GLY:HA2	1:C:685:HIS:HA	1.97	0.46
1:D:44:ASN:HB3	1:D:57:THR:HB	1.98	0.46
1:D:103:ALA:HB3	1:D:106:THR:HB	1.97	0.46
1:D:535:TYR:CZ	1:D:547:PRO:HB3	2.51	0.46
1:B:95:LYS:HD2	1:B:95:LYS:HA	1.52	0.45
1:D:168:THR:HA	1:D:187:SER:O	2.17	0.45
1:B:324:LEU:HD12	1:B:328:PRO:HA	1.99	0.45
1:C:342:TYR:HA	1:C:382:TRP:HB2	1.98	0.45
1:A:264:GLY:HA3	1:B:447:LYS:HB3	1.98	0.45
1:A:284:GLU:HG2	1:A:288:MET:HG2	1.99	0.45
1:B:66:LYS:HD3	7:B:912:HOH:O	2.16	0.45
1:B:332:LYS:NZ	7:B:805:HOH:O	2.40	0.45
1:D:587:LEU:HD11	1:D:652:ALA:HB3	1.98	0.45
1:C:110:LYS:HG2	1:C:112:ILE:HD11	1.99	0.45
1:D:285:LYS:HD2	1:D:285:LYS:HA	1.78	0.45
1:A:486:ASN:ND2	7:A:818:HOH:O	2.50	0.44
1:C:249:GLN:HB2	1:C:278:ILE:HD11	1.97	0.44
1:D:569:ASP:HA	1:D:581:LYS:HD3	2.00	0.44
1:C:116:PHE:CE2	1:C:122:ALA:HB2	2.53	0.44
1:B:366:LYS:NZ	1:B:370:ASP:OD2	2.26	0.44
1:B:122:ALA:HA	1:B:152:PHE:CZ	2.53	0.44
1:D:186:PRO:HD2	1:D:200:TRP:CZ2	2.53	0.44
1:C:342:TYR:O	1:C:598:PRO:HD3	2.18	0.44
1:C:483:ASP:O	1:C:514:ASN:HA	2.17	0.43
1:C:556:HIS:HE1	1:C:622:THR:O	2.01	0.43
1:C:529:MET:HA	1:C:560:ALA:O	2.18	0.43
1:D:639:VAL:HG11	1:D:661:ILE:HG21	1.99	0.43
1:A:125:VAL:HA	1:A:148:ARG:O	2.18	0.43
1:D:249:GLN:HB2	1:D:278:ILE:HD11	2.01	0.43
1:D:428:MET:HG3	1:D:435:PHE:CE2	2.53	0.43
1:D:334:PRO:HG3	1:D:623:PHE:CD2	2.53	0.43
1:A:671:GLY:HA2	1:A:685:HIS:HA	2.01	0.42
1:D:641:ARG:HD2	1:D:649:GLU:OE2	2.19	0.42
1:B:426:SER:H	1:B:427:PRO:HD3	1.84	0.42
1:C:319:SER:HA	1:C:558:ALA:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:PRO:HG3	1:B:623:PHE:CD1	2.54	0.42
1:D:173:GLY:HA3	1:D:230:TYR:O	2.19	0.42
1:D:186:PRO:HD2	1:D:200:TRP:HZ2	1.83	0.42
1:D:483:ASP:O	1:D:514:ASN:HA	2.19	0.42
1:A:63:HIS:CD2	1:A:231:ASN:HD21	2.38	0.42
1:A:149:SER:HB3	1:A:152:PHE:O	2.19	0.42
1:B:237:MET:O	1:B:292:TYR:HA	2.20	0.42
1:B:251:ASN:O	1:B:273:VAL:HA	2.19	0.42
1:C:247:HIS:HB2	1:C:278:ILE:HB	2.02	0.42
1:B:514:ASN:HB2	7:B:853:HOH:O	2.20	0.42
1:D:310:GLU:O	1:D:314:ARG:HG3	2.20	0.42
1:A:340:GLY:HA3	1:A:595:PHE:CD1	2.55	0.42
1:B:247:HIS:HB2	1:B:278:ILE:HB	2.02	0.42
1:C:36:ILE:HD12	1:C:99:VAL:HG12	2.02	0.42
1:B:569:ASP:HA	1:B:581:LYS:HD3	2.02	0.41
1:D:426:SER:N	1:D:427:PRO:HD3	2.35	0.41
1:D:351:MET:HE3	1:D:354:MET:HB2	2.01	0.41
1:D:214:GLU:HG2	1:D:217:ASN:HD22	1.85	0.41
1:D:340:GLY:HA3	1:D:595:PHE:HD1	1.85	0.41
1:D:493:ARG:HD2	7:D:962:HOH:O	2.20	0.41
1:C:428:MET:HE1	1:C:439:LEU:HD12	2.02	0.41
1:D:372:LEU:HD13	1:D:608:ILE:HG21	2.03	0.41
1:B:44:ASN:HB3	1:B:57:THR:HB	2.03	0.41
1:B:671:GLY:HA2	1:B:685:HIS:HA	2.02	0.41
1:C:428:MET:HG3	1:C:435:PHE:CD2	2.56	0.41
1:B:560:ALA:HB1	7:B:866:HOH:O	2.20	0.41
1:C:340:GLY:HA3	1:C:595:PHE:HD1	1.86	0.41
1:C:471:ILE:HD12	1:C:471:ILE:HA	1.88	0.41
1:D:426:SER:H	1:D:427:PRO:HD3	1.85	0.41
1:C:255:ASN:HB3	1:C:271:ARG:HG3	2.02	0.41
1:D:162:ARG:H	1:D:276:ASP:CG	2.25	0.41
1:B:63:HIS:CD2	1:B:231:ASN:HD21	2.39	0.40
1:C:425:TYR:CE1	1:C:467:ALA:HA	2.56	0.40
1:C:472:GLU:HG2	1:C:510:PHE:CE1	2.56	0.40
1:C:514:ASN:HB2	7:C:854:HOH:O	2.21	0.40
1:B:46:ASN:O	1:B:54:PHE:HA	2.22	0.40
1:D:210:GLN:HG2	1:D:258:TYR:CD1	2.57	0.40
1:A:426:SER:HA	1:A:458:VAL:HB	2.01	0.40
1:C:568:PRO:HD2	1:C:571:GLU:HB2	2.03	0.40
1:A:556:HIS:HE1	1:A:622:THR:O	2.04	0.40
1:C:214:GLU:HG2	1:C:247:HIS:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ILE:HG23	2:E:3:GAL:H62	2.04	0.40
1:A:514:ASN:HB2	7:A:926:HOH:O	2.21	0.40
1:B:173:GLY:HA3	1:B:230:TYR:O	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	657/676 (97%)	627 (95%)	30 (5%)	0	100	100
1	B	657/676 (97%)	629 (96%)	28 (4%)	0	100	100
1	C	657/676 (97%)	629 (96%)	28 (4%)	0	100	100
1	D	657/676 (97%)	629 (96%)	27 (4%)	1 (0%)	47	58
All	All	2628/2704 (97%)	2514 (96%)	113 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	383	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	561/577 (97%)	550 (98%)	11 (2%)	55 72
1	B	562/577 (97%)	551 (98%)	11 (2%)	55 72
1	C	560/577 (97%)	551 (98%)	9 (2%)	62 78
1	D	561/577 (97%)	546 (97%)	15 (3%)	44 61
All	All	2244/2308 (97%)	2198 (98%)	46 (2%)	55 72

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LYS
1	A	72	ASN
1	A	83	LYS
1	A	93	LYS
1	A	108	SER
1	A	167	LYS
1	A	351	MET
1	A	378	PHE
1	A	454	ARG
1	A	529	MET
1	A	693	ASP
1	B	83	LYS
1	B	85	LYS
1	B	95	LYS
1	B	101	LYS
1	B	167	LYS
1	B	214	GLU
1	B	351	MET
1	B	378	PHE
1	B	454	ARG
1	B	529	MET
1	B	675	GLN
1	C	82	SER
1	C	104	LYS
1	C	110	LYS
1	C	247	HIS
1	C	351	MET
1	C	378	PHE
1	C	497	LYS
1	C	502	GLU
1	C	529	MET
1	D	49	SER
1	D	82	SER

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Mol	Chain	Res	Type
1	D	83	LYS
1	D	86	LYS
1	D	117	GLU
1	D	146	GLU
1	D	214	GLU
1	D	326	ARG
1	D	351	MET
1	D	378	PHE
1	D	454	ARG
1	D	529	MET
1	D	542	SER
1	D	662	GLU
1	D	677	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	640	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

16 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	G4S	E	1	2	16,16,16	1.68	4 (25%)	19,24,24	1.15	2 (10%)
2	9RN	E	2	2	11,11,12	5.67	7 (63%)	15,16,18	2.59	5 (33%)
2	GAL	E	3	2	11,11,12	1.40	2 (18%)	15,15,17	1.25	1 (6%)
2	9RN	E	4	2	11,11,12	6.94	7 (63%)	15,16,18	3.10	7 (46%)
2	G4S	F	1	2	16,16,16	1.66	4 (25%)	19,24,24	0.99	0
2	9RN	F	2	2	11,11,12	5.70	7 (63%)	15,16,18	2.34	6 (40%)
2	GAL	F	3	2	11,11,12	1.44	3 (27%)	15,15,17	1.28	2 (13%)
2	9RN	F	4	2	11,11,12	7.11	7 (63%)	15,16,18	3.24	7 (46%)
2	G4S	G	1	2	16,16,16	1.66	4 (25%)	19,24,24	0.82	0
2	9RN	G	2	2	11,11,12	5.71	7 (63%)	15,16,18	2.61	7 (46%)
2	GAL	G	3	2	11,11,12	1.37	2 (18%)	15,15,17	1.16	1 (6%)
2	9RN	G	4	2	11,11,12	7.15	7 (63%)	15,16,18	3.03	7 (46%)
2	G4S	H	1	2	16,16,16	1.62	4 (25%)	19,24,24	1.24	2 (10%)
2	9RN	H	2	2	11,11,12	5.66	7 (63%)	15,16,18	2.54	7 (46%)
2	GAL	H	3	2	11,11,12	1.41	2 (18%)	15,15,17	1.10	2 (13%)
2	9RN	H	4	2	11,11,12	6.97	7 (63%)	15,16,18	3.26	7 (46%)

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	G4S	E	1	2	-	5/7/27/27	0/1/1/1
2	9RN	E	2	2	-	-	0/3/2/2
2	GAL	E	3	2	-	0/2/19/22	0/1/1/1
2	9RN	E	4	2	-	-	0/3/2/2
2	G4S	F	1	2	-	5/7/27/27	0/1/1/1
2	9RN	F	2	2	-	-	0/3/2/2
2	GAL	F	3	2	-	0/2/19/22	0/1/1/1
2	9RN	F	4	2	-	-	0/3/2/2
2	G4S	G	1	2	-	4/7/27/27	0/1/1/1
2	9RN	G	2	2	-	-	0/3/2/2
2	GAL	G	3	2	-	0/2/19/22	0/1/1/1
2	9RN	G	4	2	-	-	0/3/2/2
2	G4S	H	1	2	-	4/7/27/27	0/1/1/1
2	9RN	H	2	2	-	-	0/3/2/2
2	GAL	H	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9RN	H	4	2	-	-	0/3/2/2

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	9RN	O5-C1	15.70	1.68	1.43
2	G	4	9RN	O5-C1	15.55	1.68	1.43
2	H	4	9RN	O5-C1	15.11	1.67	1.43
2	E	4	9RN	O5-C1	15.07	1.67	1.43
2	F	2	9RN	O5-C1	10.22	1.60	1.43
2	G	2	9RN	O5-C1	10.14	1.59	1.43
2	H	2	9RN	O5-C1	10.07	1.59	1.43
2	E	2	9RN	O5-C1	9.95	1.59	1.43
2	G	4	9RN	O3-C6	-9.67	1.22	1.43
2	H	4	9RN	O3-C6	-9.50	1.22	1.43
2	E	4	9RN	O3-C6	-9.44	1.23	1.43
2	F	4	9RN	O3-C6	-9.33	1.23	1.43
2	E	2	9RN	C4-C3	-9.30	1.32	1.52
2	H	2	9RN	C4-C3	-9.28	1.32	1.52
2	F	2	9RN	C4-C3	-9.22	1.32	1.52
2	G	4	9RN	C1-C2	9.15	1.73	1.52
2	G	2	9RN	C4-C3	-9.10	1.32	1.52
2	F	4	9RN	C1-C2	9.03	1.72	1.52
2	E	4	9RN	C1-C2	9.00	1.72	1.52
2	H	4	9RN	C1-C2	8.78	1.72	1.52
2	G	2	9RN	C4-C5	-8.36	1.31	1.53
2	E	2	9RN	C4-C5	-8.24	1.31	1.53
2	F	2	9RN	C4-C5	-8.19	1.32	1.53
2	H	2	9RN	C4-C5	-8.04	1.32	1.53
2	G	2	9RN	O3-C6	6.80	1.58	1.43
2	H	2	9RN	O3-C6	6.72	1.58	1.43
2	F	2	9RN	O3-C6	6.56	1.58	1.43
2	E	2	9RN	O3-C6	6.54	1.58	1.43
2	G	4	9RN	C4-C3	-6.45	1.38	1.52
2	H	4	9RN	C4-C3	-6.39	1.38	1.52
2	F	4	9RN	C4-C3	-6.33	1.38	1.52
2	H	4	9RN	C4-C5	-6.30	1.36	1.53
2	G	4	9RN	C4-C5	-6.25	1.37	1.53
2	F	4	9RN	C4-C5	-6.23	1.37	1.53
2	E	4	9RN	C4-C3	-6.22	1.39	1.52
2	E	4	9RN	C4-C5	-6.12	1.37	1.53
2	E	2	9RN	C1-C2	6.12	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	9RN	C1-C2	5.92	1.65	1.52
2	F	2	9RN	C1-C2	5.89	1.65	1.52
2	G	4	9RN	C6-C5	-5.80	1.41	1.52
2	F	4	9RN	C6-C5	-5.79	1.41	1.52
2	H	4	9RN	C6-C5	-5.62	1.41	1.52
2	E	4	9RN	C6-C5	-5.61	1.41	1.52
2	H	2	9RN	C1-C2	5.59	1.65	1.52
2	G	4	9RN	C2-C3	-4.85	1.41	1.52
2	F	4	9RN	C2-C3	-4.77	1.41	1.52
2	H	4	9RN	C2-C3	-4.66	1.41	1.52
2	E	4	9RN	C2-C3	-4.62	1.41	1.52
2	H	1	G4S	O4-S	3.46	1.67	1.57
2	G	2	9RN	O3-C3	3.40	1.51	1.43
2	E	2	9RN	O3-C3	3.33	1.51	1.43
2	H	2	9RN	O3-C3	3.32	1.51	1.43
2	G	1	G4S	O4-C4	-3.31	1.39	1.46
2	F	1	G4S	O4-S	3.30	1.67	1.57
2	F	2	9RN	O3-C3	3.28	1.51	1.43
2	E	1	G4S	O4-C4	-3.18	1.39	1.46
2	F	2	9RN	C2-C3	-3.15	1.45	1.52
2	H	2	9RN	C2-C3	-3.12	1.45	1.52
2	G	1	G4S	O4-S	3.06	1.66	1.57
2	F	1	G4S	O4-C4	-3.00	1.40	1.46
2	G	2	9RN	C2-C3	-2.98	1.45	1.52
2	E	1	G4S	O4-S	2.97	1.66	1.57
2	E	3	GAL	O5-C5	2.83	1.49	1.43
2	E	2	9RN	C2-C3	-2.78	1.45	1.52
2	H	1	G4S	O4-C4	-2.74	1.40	1.46
2	F	3	GAL	O5-C5	2.65	1.48	1.43
2	H	3	GAL	O5-C5	2.51	1.48	1.43
2	H	3	GAL	C2-C3	-2.45	1.48	1.52
2	H	1	G4S	O5-C1	2.43	1.49	1.42
2	F	1	G4S	O5-C1	2.39	1.48	1.42
2	E	1	G4S	O5-C1	2.38	1.48	1.42
2	G	3	GAL	O5-C5	2.35	1.48	1.43
2	G	3	GAL	C2-C3	-2.34	1.49	1.52
2	F	3	GAL	C2-C3	-2.33	1.49	1.52
2	F	1	G4S	C3-C2	-2.31	1.46	1.52
2	E	1	G4S	C3-C2	-2.27	1.46	1.52
2	G	1	G4S	C3-C2	-2.21	1.46	1.52
2	E	3	GAL	C2-C3	-2.20	1.49	1.52
2	H	1	G4S	C3-C2	-2.09	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	G4S	O5-C1	2.08	1.48	1.42
2	F	3	GAL	O5-C1	2.07	1.47	1.43

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	4	9RN	O3-C3-C4	-6.82	91.39	103.59
2	F	4	9RN	O3-C3-C4	-6.73	91.55	103.59
2	E	4	9RN	O3-C3-C4	-6.49	91.99	103.59
2	G	4	9RN	O3-C3-C4	-6.30	92.32	103.59
2	F	4	9RN	C6-C5-C4	-5.71	92.29	102.28
2	E	4	9RN	C6-C5-C4	-5.63	92.44	102.28
2	H	4	9RN	C6-C5-C4	-5.40	92.83	102.28
2	G	4	9RN	C6-C5-C4	-5.18	93.22	102.28
2	E	2	9RN	O3-C3-C2	5.16	119.86	108.07
2	G	2	9RN	C3-C4-C5	4.89	112.62	101.99
2	E	2	9RN	C3-C4-C5	4.81	112.44	101.99
2	H	2	9RN	C3-C4-C5	4.80	112.42	101.99
2	F	2	9RN	C3-C4-C5	4.68	112.15	101.99
2	F	4	9RN	C3-C4-C5	4.48	111.73	101.99
2	G	4	9RN	C3-C4-C5	4.31	111.36	101.99
2	G	4	9RN	O3-C6-C5	4.29	112.19	104.52
2	H	4	9RN	O3-C6-C5	4.23	112.09	104.52
2	E	4	9RN	O3-C6-C5	4.23	112.08	104.52
2	H	4	9RN	O5-C5-C6	4.22	119.59	113.33
2	H	4	9RN	C3-C4-C5	4.18	111.06	101.99
2	G	2	9RN	O3-C3-C2	4.16	117.58	108.07
2	H	2	9RN	O3-C3-C2	4.15	117.56	108.07
2	E	4	9RN	C3-C4-C5	4.14	111.00	101.99
2	F	4	9RN	O3-C6-C5	4.08	111.81	104.52
2	E	2	9RN	O3-C3-C4	-4.05	96.34	103.59
2	H	4	9RN	O3-C3-C2	4.04	117.32	108.07
2	G	4	9RN	O3-C3-C2	3.95	117.10	108.07
2	F	4	9RN	O3-C3-C2	3.89	116.97	108.07
2	G	2	9RN	C6-O3-C3	-3.88	99.92	107.84
2	E	4	9RN	O3-C3-C2	3.88	116.94	108.07
2	F	4	9RN	O5-C5-C6	3.83	119.01	113.33
2	F	2	9RN	O3-C3-C2	3.78	116.71	108.07
2	H	2	9RN	O3-C3-C4	-3.77	96.84	103.59
2	F	2	9RN	C6-O3-C3	-3.62	100.46	107.84
2	E	2	9RN	C6-O3-C3	-3.55	100.60	107.84
2	G	2	9RN	C1-O5-C5	-3.47	107.50	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	2	9RN	C1-O5-C5	-3.46	107.51	112.19
2	G	2	9RN	O3-C3-C4	-3.39	97.52	103.59
2	H	2	9RN	C6-O3-C3	-3.27	101.16	107.84
2	G	2	9RN	O5-C5-C6	3.24	118.14	113.33
2	E	3	GAL	C1-C2-C3	3.19	113.59	109.67
2	F	2	9RN	C1-O5-C5	-3.17	107.90	112.19
2	F	3	GAL	C1-C2-C3	3.15	113.54	109.67
2	E	4	9RN	O5-C5-C6	3.09	117.92	113.33
2	G	3	GAL	C1-C2-C3	3.03	113.39	109.67
2	F	2	9RN	O3-C3-C4	-2.96	98.29	103.59
2	H	3	GAL	C1-C2-C3	2.87	113.19	109.67
2	E	2	9RN	O5-C5-C6	2.83	117.52	113.33
2	G	4	9RN	O5-C5-C6	2.74	117.39	113.33
2	E	1	G4S	O5-C1-C2	2.64	115.00	110.28
2	H	1	G4S	O5-C1-C2	2.50	114.74	110.28
2	H	4	9RN	C1-C2-C3	2.48	112.17	109.17
2	H	2	9RN	O5-C5-C6	2.46	116.98	113.33
2	F	2	9RN	O5-C5-C6	2.45	116.96	113.33
2	E	1	G4S	O8-S-O7	-2.31	102.96	112.22
2	F	3	GAL	C6-C5-C4	-2.20	107.85	113.00
2	G	4	9RN	C1-C2-C3	2.18	111.81	109.17
2	H	1	G4S	O9-S-O8	-2.13	101.08	108.49
2	E	4	9RN	C1-C2-C3	2.13	111.74	109.17
2	G	2	9RN	O4-C4-C5	-2.06	105.09	111.05
2	H	2	9RN	C6-C5-C4	-2.03	98.73	102.28
2	F	4	9RN	C6-O3-C3	2.03	111.98	107.84
2	H	3	GAL	O3-C3-C2	-2.01	106.15	109.99

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	G4S	C4-O4-S-O7
2	E	1	G4S	C4-O4-S-O9
2	F	1	G4S	C4-O4-S-O7
2	F	1	G4S	C4-O4-S-O8
2	F	1	G4S	C4-O4-S-O9
2	H	1	G4S	C4-O4-S-O8
2	F	1	G4S	O5-C5-C6-O6
2	E	1	G4S	O5-C5-C6-O6
2	F	1	G4S	C4-C5-C6-O6
2	E	1	G4S	C4-O4-S-O8

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Mol	Chain	Res	Type	Atoms
2	G	1	G4S	C4-O4-S-O7
2	G	1	G4S	C4-O4-S-O8
2	H	1	G4S	O5-C5-C6-O6
2	G	1	G4S	O5-C5-C6-O6
2	G	1	G4S	C4-O4-S-O9
2	H	1	G4S	C4-O4-S-O7
2	E	1	G4S	C4-C5-C6-O6
2	H	1	G4S	C4-O4-S-O9

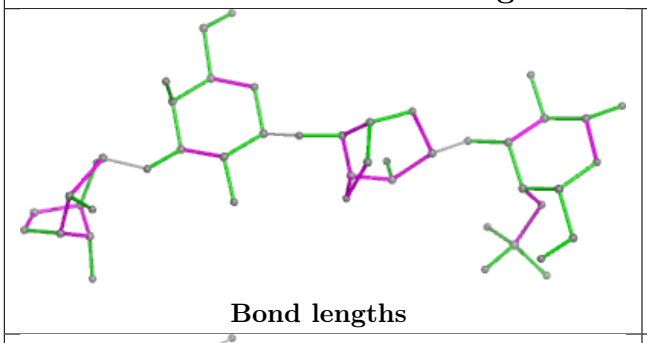
There are no ring outliers.

6 monomers are involved in 10 short contacts:

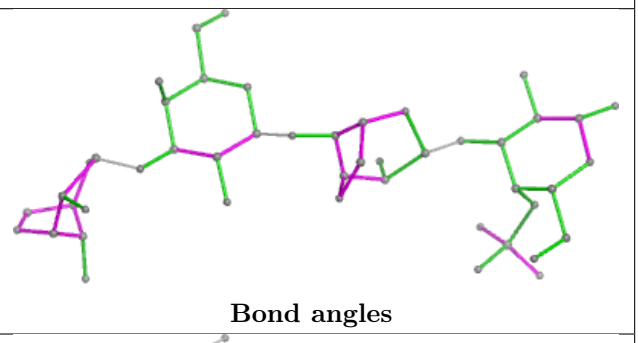
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	4	9RN	2	0
2	E	4	9RN	2	0
2	H	4	9RN	2	0
2	E	3	GAL	1	0
2	F	3	GAL	1	0
2	G	4	9RN	2	0

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

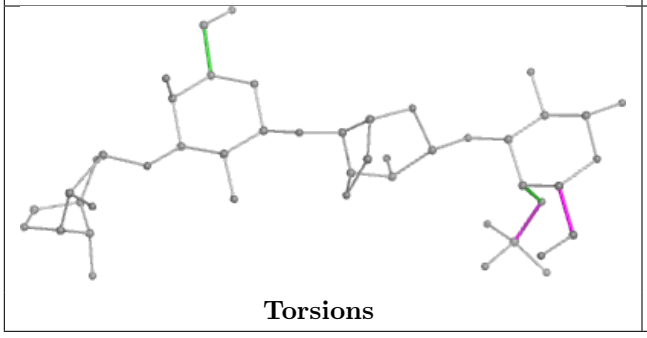
Oligosaccharide Chain E



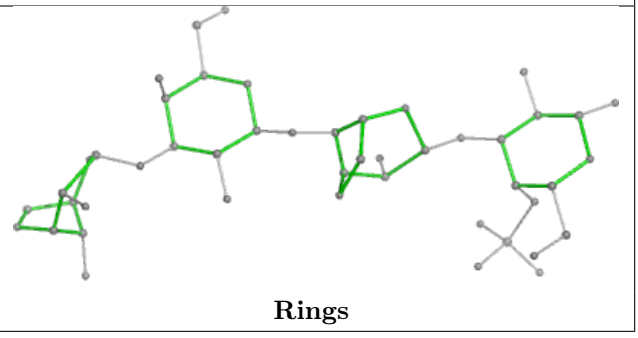
Bond lengths



Bond angles

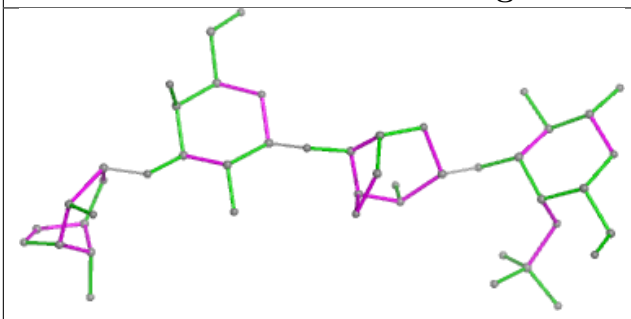


Torsions

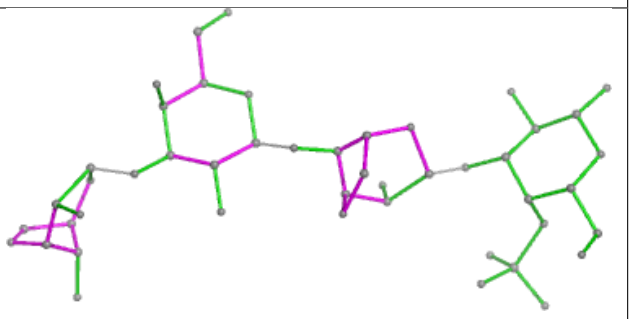


Rings

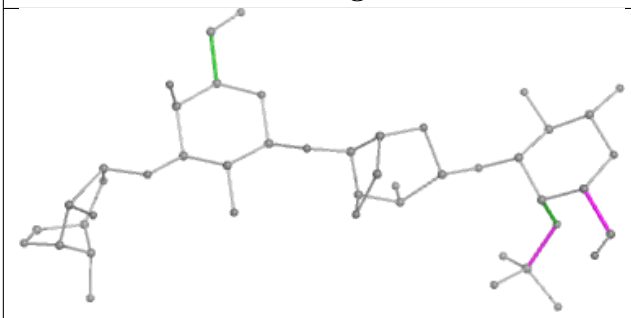
Oligosaccharide Chain F



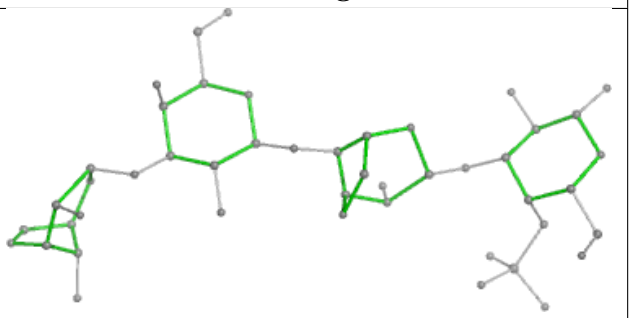
Bond lengths



Bond angles

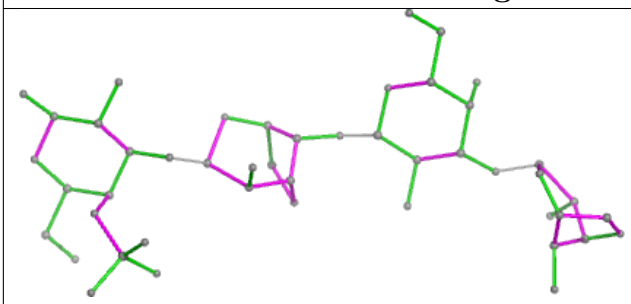


Torsions

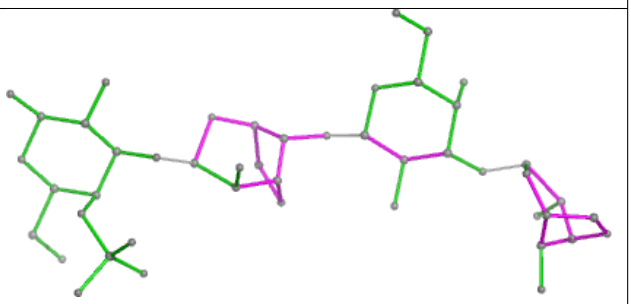


Rings

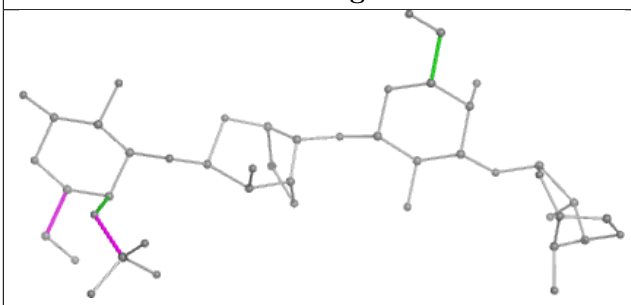
Oligosaccharide Chain G



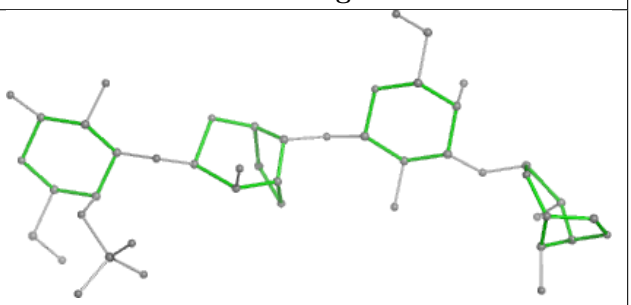
Bond lengths



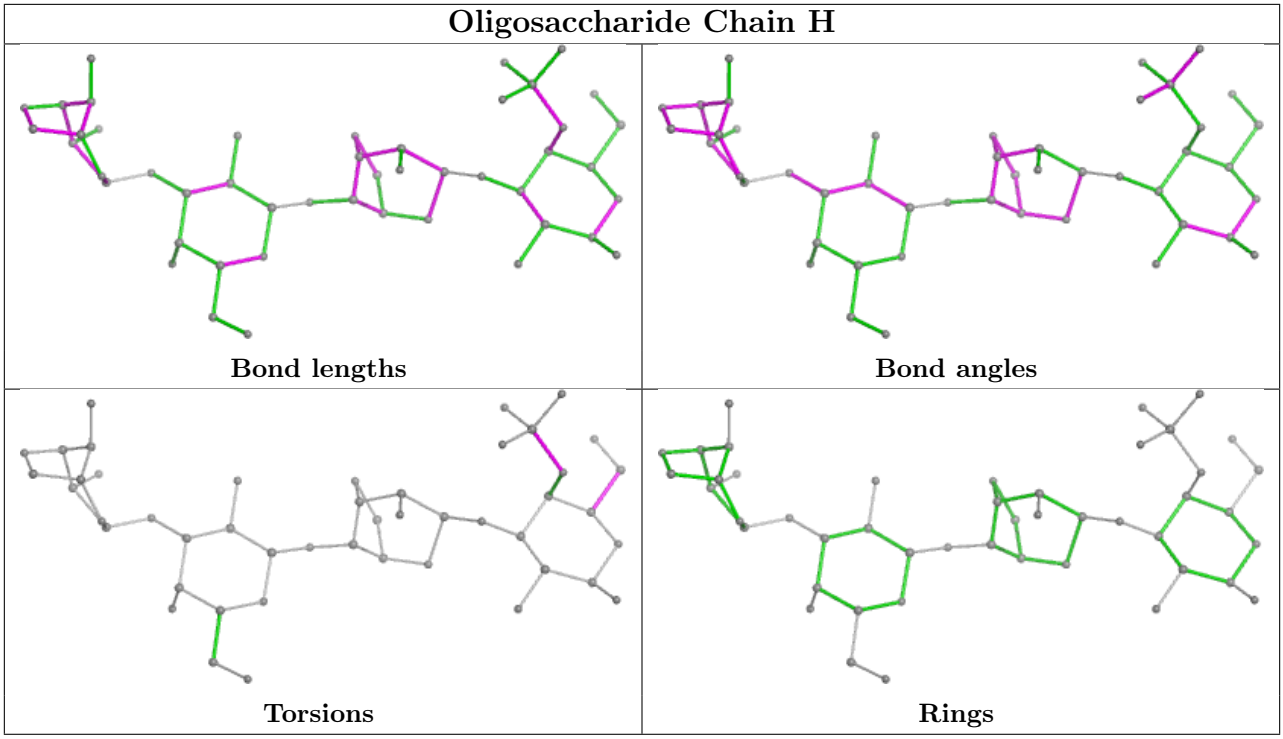
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	TLA	D	701	-	9,9,9	0.99	0	12,12,12	1.45	2 (16%)
3	TLA	A	702	-	9,9,9	1.08	0	12,12,12	2.20	5 (41%)
3	TLA	B	701	-	9,9,9	1.00	0	12,12,12	1.24	1 (8%)
3	TLA	C	701	-	9,9,9	1.00	0	12,12,12	1.33	2 (16%)
6	EDO	B	702	-	3,3,3	0.43	0	2,2,2	0.35	0
3	TLA	A	701	-	9,9,9	1.08	0	12,12,12	1.31	2 (16%)

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
3	TLA	D	701	-	-	0/12/12/12	-
3	TLA	A	702	-	-	5/12/12/12	-
3	TLA	B	701	-	-	2/12/12/12	-
3	TLA	C	701	-	-	4/12/12/12	-
6	EDO	B	702	-	-	1/1/1/1	-
3	TLA	A	701	-	-	3/12/12/12	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	TLA	C3-C2-C1	3.60	117.90	109.87
3	A	702	TLA	O11-C1-C2	3.24	122.03	113.27
3	A	702	TLA	C2-C3-C4	3.22	117.06	109.87
3	A	702	TLA	O41-C4-C3	3.15	121.78	113.27
3	D	701	TLA	O11-C1-C2	2.77	120.75	113.27
3	C	701	TLA	O11-C1-C2	2.75	120.70	113.27
3	A	701	TLA	O41-C4-C3	2.74	120.67	113.27
3	B	701	TLA	O11-C1-C2	2.73	120.66	113.27
3	D	701	TLA	O41-C4-C3	2.69	120.54	113.27
3	A	701	TLA	O11-C1-C2	2.15	119.08	113.27
3	C	701	TLA	O41-C4-C3	2.12	119.01	113.27
3	A	702	TLA	O11-C1-O1	-2.07	119.38	124.09

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	TLA	C1-C2-C3-C4
3	A	702	TLA	O3-C3-C4-O4
3	A	702	TLA	O3-C3-C4-O41
3	A	702	TLA	C1-C2-C3-O3
3	A	702	TLA	O2-C2-C3-C4
6	B	702	EDO	O1-C1-C2-O2
3	C	701	TLA	O11-C1-C2-C3
3	C	701	TLA	O1-C1-C2-C3
3	A	701	TLA	C2-C3-C4-O4
3	B	701	TLA	O1-C1-C2-C3
3	C	701	TLA	O1-C1-C2-O2
3	A	701	TLA	O3-C3-C4-O4
3	C	701	TLA	O11-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	701	TLA	C2-C3-C4-O41
3	B	701	TLA	O11-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	TLA	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

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, 95^{th} 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	659/676 (97%)	-0.06	15 (2%) 60 67	30, 40, 58, 83	0
1	B	659/676 (97%)	-0.12	7 (1%) 80 85	32, 42, 61, 83	0
1	C	659/676 (97%)	-0.05	15 (2%) 60 67	33, 44, 62, 87	0
1	D	659/676 (97%)	0.03	26 (3%) 39 46	34, 44, 63, 83	0
All	All	2636/2704 (97%)	-0.05	63 (2%) 59 66	30, 43, 61, 87	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	83	LYS	3.4
1	D	574	ALA	3.3
1	C	123	LYS	3.3
1	C	83	LYS	3.3
1	D	151	ASN	3.3
1	D	115	VAL	3.2
1	A	573	THR	3.1
1	D	99	VAL	3.1
1	D	543	VAL	3.0
1	C	152	PHE	2.9
1	B	85	LYS	2.8
1	D	573	THR	2.8
1	A	576	GLY	2.8
1	D	121	VAL	2.8
1	D	118	ASP	2.8
1	A	117	GLU	2.7
1	D	112	ILE	2.7
1	B	117	GLU	2.7
1	A	85	LYS	2.7
1	D	119	GLY	2.7
1	D	82	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	122	ALA	2.7
1	A	568	PRO	2.6
1	D	542	SER	2.6
1	C	117	GLU	2.6
1	C	121	VAL	2.5
1	D	544	ILE	2.5
1	D	117	GLU	2.5
1	C	136	ASN	2.5
1	A	535	TYR	2.5
1	A	84	GLY	2.5
1	D	198	CYS	2.4
1	C	155	TYR	2.4
1	B	118	ASP	2.4
1	A	536	LEU	2.3
1	B	573	THR	2.3
1	D	200	TRP	2.3
1	A	574	ALA	2.3
1	A	582	ALA	2.3
1	C	536	LEU	2.3
1	A	572	VAL	2.2
1	D	150	GLY	2.2
1	B	83	LYS	2.2
1	D	199	LYS	2.2
1	D	692	MET	2.2
1	C	573	THR	2.2
1	C	135	PRO	2.2
1	A	593	THR	2.1
1	D	96	LYS	2.1
1	C	84	GLY	2.1
1	D	107	VAL	2.1
1	A	565	ILE	2.1
1	C	403	GLU	2.1
1	D	693	ASP	2.1
1	C	574	ALA	2.1
1	A	120	SER	2.1
1	C	118	ASP	2.0
1	A	580	ILE	2.0
1	C	82	SER	2.0
1	B	80	THR	2.0
1	D	50	LYS	2.0
1	D	572	VAL	2.0
1	B	194	GLY	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)

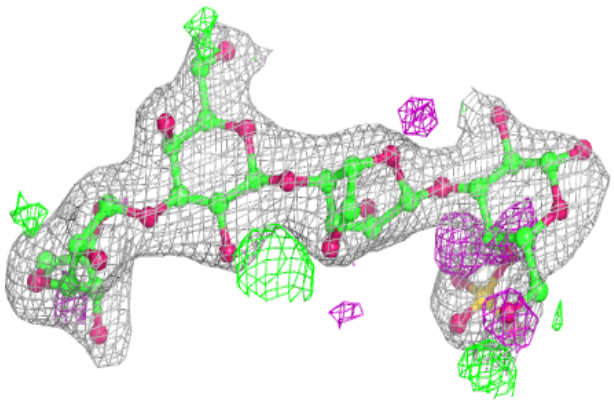
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

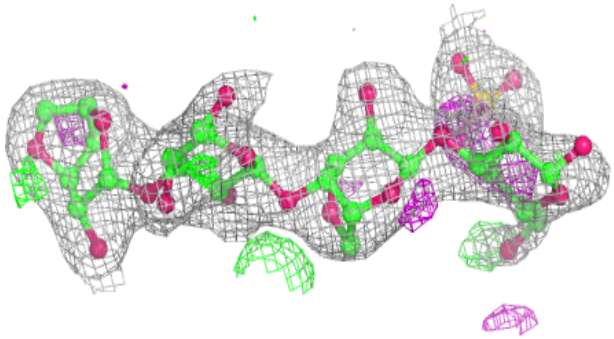
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	G4S	F	1	16/16	0.77	0.23	76,86,92,93	0
2	G4S	H	1	16/16	0.87	0.18	74,79,86,90	0
2	G4S	G	1	16/16	0.88	0.21	74,82,85,85	0
2	G4S	E	1	16/16	0.89	0.18	69,79,86,89	0
2	9RN	G	2	10/11	0.93	0.18	57,60,62,66	0
2	9RN	F	2	10/11	0.93	0.13	53,59,64,68	0
2	9RN	H	2	10/11	0.93	0.13	54,61,65,66	0
2	9RN	H	4	10/11	0.93	0.14	45,50,51,53	0
2	GAL	H	3	11/12	0.94	0.14	48,50,53,57	0
2	9RN	E	2	10/11	0.95	0.14	49,52,59,59	0
2	GAL	G	3	11/12	0.95	0.17	43,47,51,53	0
2	GAL	E	3	11/12	0.95	0.17	39,47,51,55	0
2	GAL	F	3	11/12	0.95	0.12	46,50,55,60	0
2	9RN	F	4	10/11	0.95	0.11	46,51,54,54	0
2	9RN	E	4	10/11	0.95	0.15	37,46,47,47	0
2	9RN	G	4	10/11	0.96	0.14	49,52,54,55	0

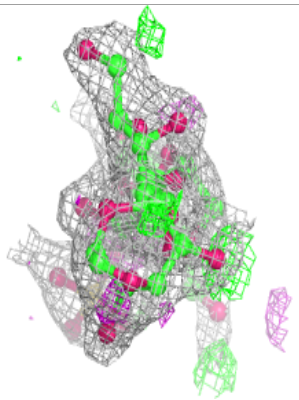
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

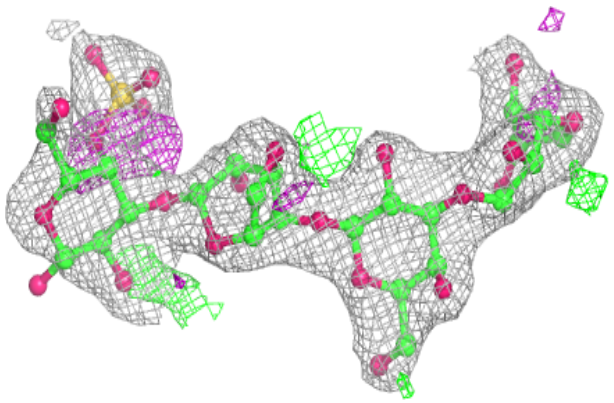


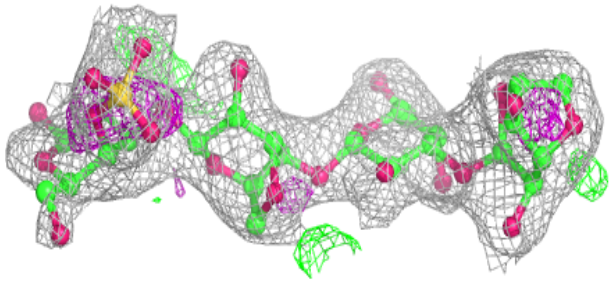


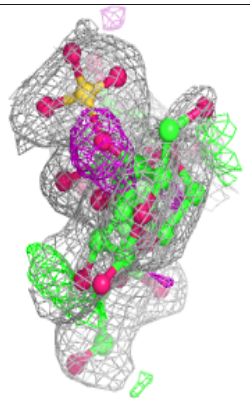


Electron density around Chain F:

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

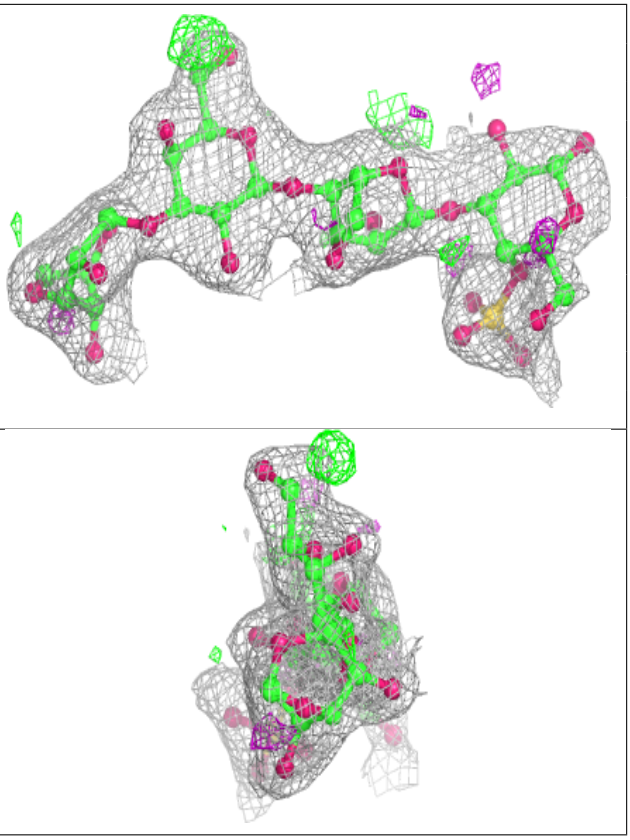






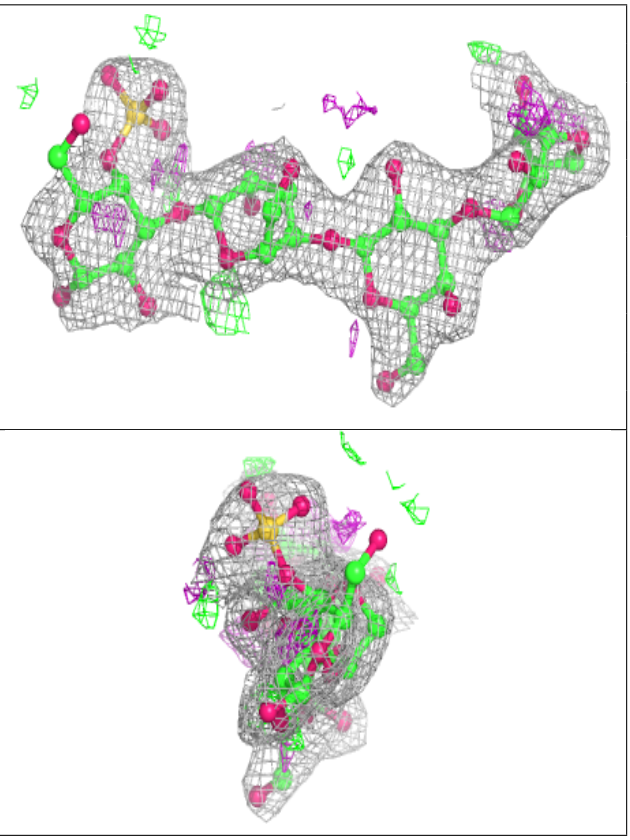
Electron density around Chain G:

$2mF_o$-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 (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, 95^{th} 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
4	NA	C	702	1/1	0.62	0.12	79,79,79,79	0
4	NA	A	703	1/1	0.67	0.20	80,80,80,80	0
4	NA	B	703	1/1	0.77	0.20	78,78,78,78	0
3	TLA	A	702	10/10	0.79	0.18	66,69,72,72	0
3	TLA	A	701	10/10	0.94	0.17	40,45,50,52	0
4	NA	D	702	1/1	0.94	0.13	68,68,68,68	0
3	TLA	C	701	10/10	0.95	0.25	47,51,58,58	0
3	TLA	D	701	10/10	0.96	0.13	46,52,60,62	0
6	EDO	B	702	4/4	0.96	0.12	53,55,55,56	0
3	TLA	B	701	10/10	0.97	0.14	46,52,59,60	0
5	CL	B	704	1/1	0.98	0.13	57,57,57,57	0
5	CL	C	703	1/1	0.98	0.21	58,58,58,58	0
5	CL	D	703	1/1	0.98	0.20	61,61,61,61	0
5	CL	A	704	1/1	0.98	0.26	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.