Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 01:25 PM EST

PDB ID	:	3S6Z
Title	:	Structure of reovirus attachment protein sigma1 in complex with alpha-2,8-di sialyllactose
Authors	:	Reiter, D.M.; Dermody, T.S.; Stehle, T.
Deposited on	:	2011-05-26
Resolution	:	2.28 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:

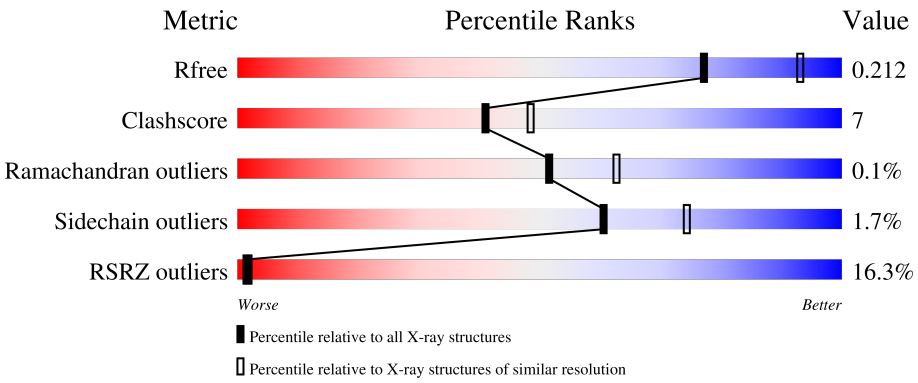
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	325	14% 80% 9% 11%
1	B	325	15% 78% 11% • 9%
1	C	325	15% 76% 14% 10%
2	D	3	33% 67%
2	E	3	67% 33%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GAL	E	1	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7499 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 Outer capsid protein sigma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	290	2203	1381	384	430	8	0	0	0
1	B	295	2243	1407	392	436	8	0	1	0
1	C	292	2234	1402	389	435	8	0	2	0

There are 123 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	GLN	-	expression tag	UNP P03528
A	132	ILE	-	expression tag	UNP P03528
A	133	GLU	-	expression tag	UNP P03528
A	134	ASP	-	expression tag	UNP P03528
A	135	LYS	-	expression tag	UNP P03528
A	136	ILE	-	expression tag	UNP P03528
A	137	GLU	-	expression tag	UNP P03528
A	138	GLU	-	expression tag	UNP P03528
A	139	ILE	-	expression tag	UNP P03528
A	140	LEU	-	expression tag	UNP P03528
A	141	SER	-	expression tag	UNP P03528
A	142	LYS	-	expression tag	UNP P03528
A	143	ILE	-	expression tag	UNP P03528
A	144	TYR	-	expression tag	UNP P03528
A	145	HIS	-	expression tag	UNP P03528
A	146	ILE	-	expression tag	UNP P03528
A	147	GLU	-	expression tag	UNP P03528
A	148	ASN	-	expression tag	UNP P03528
A	149	GLU	-	expression tag	UNP P03528
A	150	ILE	-	expression tag	UNP P03528
A	151	ALA	-	expression tag	UNP P03528
A	152	ARG	-	expression tag	UNP P03528
A	153	ILE	-	expression tag	UNP P03528

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Chain	Residue	Modelled	Actual	Comment	Reference
A	154	LYS	-	expression tag	UNP P03528
A	155	LYS	-	expression tag	UNP P03528
A	156	LEU	-	expression tag	UNP P03528
A	157	ILE	-	expression tag	UNP P03528
A	158	GLY	-	expression tag	UNP P03528
A	159	GLU	-	expression tag	UNP P03528
A	160	GLY	-	expression tag	UNP P03528
A	161	SER	-	expression tag	UNP P03528
A	162	GLY	-	expression tag	UNP P03528
A	163	ARG	-	expression tag	UNP P03528
A	164	PRO	-	expression tag	UNP P03528
A	165	VAL	-	expression tag	UNP P03528
A	166	LEU	-	expression tag	UNP P03528
A	167	ASN	-	expression tag	UNP P03528
A	168	GLN	-	expression tag	UNP P03528
A	169	GLY	-	expression tag	UNP P03528
A	249	ILE	THR	engineered mutation	UNP P03528
A	408	THR	ALA	conflict	UNP P03528
B	131	GLN	-	expression tag	UNP P03528
B	132	ILE	-	expression tag	UNP P03528
B	133	GLU	-	expression tag	UNP P03528
B	134	ASP	-	expression tag	UNP P03528
B	135	LYS	-	expression tag	UNP P03528
B	136	ILE	-	expression tag	UNP P03528
B	137	GLU	-	expression tag	UNP P03528
B	138	GLU	-	expression tag	UNP P03528
B	139	ILE	-	expression tag	UNP P03528
B	140	LEU	-	expression tag	UNP P03528
B	141	SER	-	expression tag	UNP P03528
B	142	LYS	-	expression tag	UNP P03528
B	143	ILE	-	expression tag	UNP P03528
B	144	TYR	-	expression tag	UNP P03528
B	145	HIS	-	expression tag	UNP P03528
B	146	ILE	-	expression tag	UNP P03528
B	147	GLU	-	expression tag	UNP P03528
B	148	ASN	-	expression tag	UNP P03528
B	149	GLU	-	expression tag	UNP P03528
B	150	ILE	-	expression tag	UNP P03528
B	151	ALA	-	expression tag	UNP P03528
B	152	ARG	-	expression tag	UNP P03528
B	153	ILE	-	expression tag	UNP P03528
B	154	LYS	-	expression tag	UNP P03528

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Chain	Residue	Modelled	Actual	Comment	Reference
B	155	LYS	-	expression tag	UNP P03528
B	156	LEU	-	expression tag	UNP P03528
B	157	ILE	-	expression tag	UNP P03528
B	158	GLY	-	expression tag	UNP P03528
B	159	GLU	-	expression tag	UNP P03528
B	160	GLY	-	expression tag	UNP P03528
B	161	SER	-	expression tag	UNP P03528
B	162	GLY	-	expression tag	UNP P03528
B	163	ARG	-	expression tag	UNP P03528
B	164	PRO	-	expression tag	UNP P03528
B	165	VAL	-	expression tag	UNP P03528
B	166	LEU	-	expression tag	UNP P03528
B	167	ASN	-	expression tag	UNP P03528
B	168	GLN	-	expression tag	UNP P03528
B	169	GLY	-	expression tag	UNP P03528
B	249	ILE	THR	engineered mutation	UNP P03528
B	408	THR	ALA	conflict	UNP P03528
C	131	GLN	-	expression tag	UNP P03528
C	132	ILE	-	expression tag	UNP P03528
C	133	GLU	-	expression tag	UNP P03528
C	134	ASP	-	expression tag	UNP P03528
C	135	LYS	-	expression tag	UNP P03528
C	136	ILE	-	expression tag	UNP P03528
C	137	GLU	-	expression tag	UNP P03528
C	138	GLU	-	expression tag	UNP P03528
C	139	ILE	-	expression tag	UNP P03528
C	140	LEU	-	expression tag	UNP P03528
C	141	SER	-	expression tag	UNP P03528
C	142	LYS	-	expression tag	UNP P03528
C	143	ILE	-	expression tag	UNP P03528
C	144	TYR	-	expression tag	UNP P03528
C	145	HIS	-	expression tag	UNP P03528
C	146	ILE	-	expression tag	UNP P03528
C	147	GLU	-	expression tag	UNP P03528
C	148	ASN	-	expression tag	UNP P03528
C	149	GLU	-	expression tag	UNP P03528
C	150	ILE	-	expression tag	UNP P03528
C	151	ALA	-	expression tag	UNP P03528
C	152	ARG	-	expression tag	UNP P03528
C	153	ILE	-	expression tag	UNP P03528
C	154	LYS	-	expression tag	UNP P03528
C	155	LYS	-	expression tag	UNP P03528

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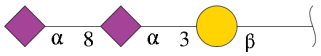
Chain	Residue	Modelled	Actual	Comment	Reference
C	156	LEU	-	expression tag	UNP P03528
C	157	ILE	-	expression tag	UNP P03528
C	158	GLY	-	expression tag	UNP P03528
C	159	GLU	-	expression tag	UNP P03528
C	160	GLY	-	expression tag	UNP P03528
C	161	SER	-	expression tag	UNP P03528
C	162	GLY	-	expression tag	UNP P03528
C	163	ARG	-	expression tag	UNP P03528
C	164	PRO	-	expression tag	UNP P03528
C	165	VAL	-	expression tag	UNP P03528
C	166	LEU	-	expression tag	UNP P03528
C	167	ASN	-	expression tag	UNP P03528
C	168	GLN	-	expression tag	UNP P03528
C	169	GLY	-	expression tag	UNP P03528
C	249	ILE	THR	engineered mutation	UNP P03528
C	408	THR	ALA	conflict	UNP P03528

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha -neuraminic acid-(2-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	3	52	28	2	22	0	0	0
2	E	3	52	28	2	22	0	0	0

- Molecule 3 is water.

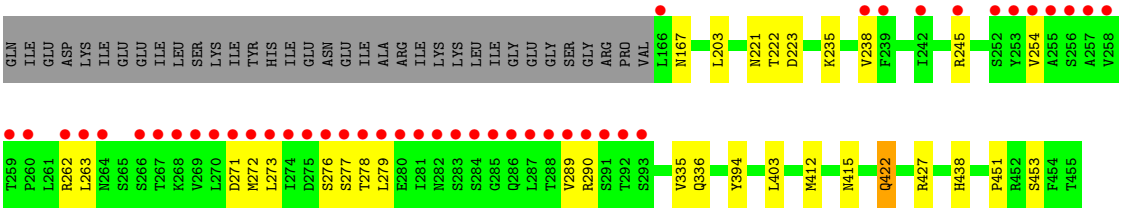
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	251	251	251	0	0
3	B	240	240	240	0	0
3	C	224	224	224	0	0

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.

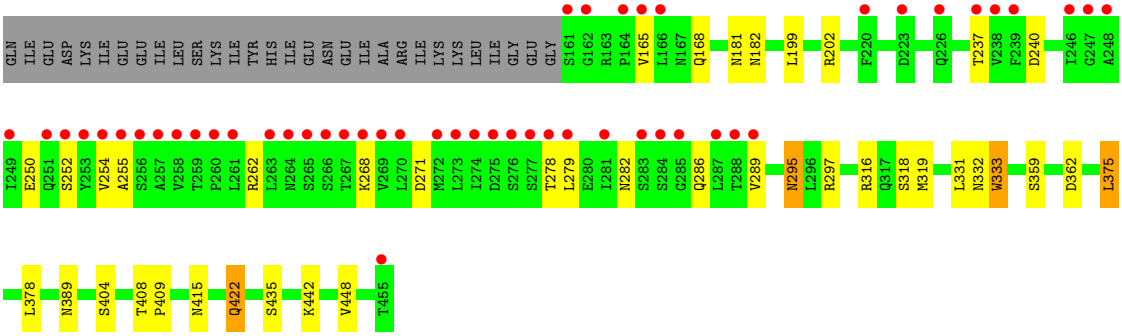
• Molecule 1: Outer capsid protein sigma-1

Chain A:



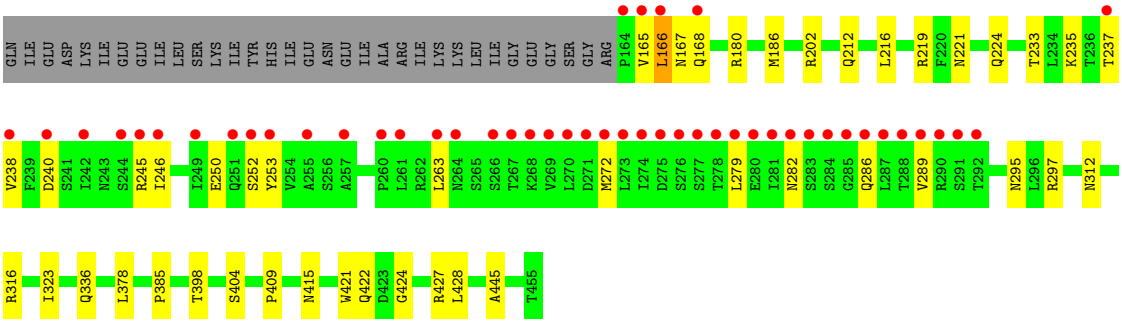
• Molecule 1: Outer capsid protein sigma-1

Chain B:



• Molecule 1: Outer capsid protein sigma-1

Chain C:



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain D:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	87.15Å 333.18Å 58.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.06 – 2.28 48.06 – 2.28	Depositor EDS
% Data completeness (in resolution range)	96.0 (48.06-2.28) 96.0 (48.06-2.28)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.173 , 0.219 0.166 , 0.212	Depositor DCC
R_{free} test set	3829 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 69.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7499	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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: SIA, 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	0.34	0/2247	0.51	0/3059
1	B	0.36	0/2291	0.51	0/3119
1	C	0.33	0/2282	0.51	0/3107
All	All	0.34	0/6820	0.51	0/9285

There are no bond length outliers.

There are no bond angle outliers.

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	2203	0	2162	30	0
1	B	2243	0	2210	30	0
1	C	2234	0	2201	48	1
2	D	52	0	44	6	0
2	E	52	0	44	1	0
3	A	251	0	0	4	3
3	B	240	0	0	6	2
3	C	224	0	0	10	6
All	All	7499	0	6661	95	9

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 7.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ARG:NH1	3:C:515:HOH:O	2.07	0.88
1:A:221:ASN:HB2	1:C:233:THR:HG22	1.56	0.87
1:C:316:ARG:NH1	3:C:785:HOH:O	2.07	0.86
1:A:415:ASN:HD21	1:C:445:ALA:H	1.24	0.86
1:B:319:MET:HB2	1:B:375:LEU:HD22	1.64	0.80
1:A:278:THR:HB	1:C:289:VAL:HG22	1.64	0.79
1:A:245:ARG:NH1	1:C:250:GLU:OE1	2.17	0.78
1:B:389:ASN:HD22	1:B:422:GLN:HE22	1.33	0.76
2:D:1:GAL:O3	2:D:2:SIA:H92	1.89	0.73
1:A:415:ASN:HD21	1:C:445:ALA:N	1.91	0.67
1:B:168:GLN:OE1	3:B:506:HOH:O	2.14	0.65
1:A:289:VAL:HG22	1:B:278:THR:HB	1.78	0.65
1:C:323:ILE:HD13	1:C:336[A]:GLN:HE21	1.62	0.65
1:B:165:VAL:HA	1:C:165:VAL:O	1.98	0.64
1:A:415:ASN:ND2	1:C:445:ALA:H	1.94	0.63
1:A:262:ARG:NH2	1:A:271:ASP:OD2	2.30	0.63
1:A:276:SER:O	1:A:290:ARG:NH1	2.32	0.62
1:B:362:ASP:OD1	1:B:435:SER:HB3	1.99	0.62
1:B:282:ASN:HD21	1:B:286:GLN:HB2	1.64	0.62
1:C:398:THR:OG1	3:C:621:HOH:O	1.77	0.62
1:B:279:LEU:HD23	1:B:289:VAL:HA	1.82	0.60
1:B:332:ASN:O	1:B:333:TRP:HB3	2.03	0.59
1:A:272:MET:HE1	1:C:272:MET:SD	2.43	0.58
2:D:1:GAL:C2	2:D:2:SIA:C1	2.82	0.57
1:C:295:ASN:HD21	1:C:297:ARG:HH22	1.53	0.57
1:C:427:ARG:HD3	3:C:606:HOH:O	2.03	0.57
1:C:312[A]:ASN:HD21	1:C:316:ARG:HD3	1.70	0.56
1:C:323:ILE:HD13	1:C:336[A]:GLN:NE2	2.21	0.56
1:C:295:ASN:CG	1:C:297:ARG:HH12	2.08	0.55
1:C:166:LEU:HD13	1:C:166:LEU:H	1.70	0.55
1:A:277:SER:HA	1:A:290:ARG:HH11	1.72	0.55
1:B:282:ASN:ND2	1:B:286:GLN:HB2	2.21	0.55
1:C:378:LEU:HD12	3:C:617:HOH:O	2.05	0.55
1:C:167:ASN:O	1:C:168:GLN:HB3	2.07	0.55
1:B:442:LYS:HG3	3:B:776:HOH:O	2.07	0.55
1:B:262:ARG:HB3	1:B:271:ASP:OD1	2.08	0.54
1:C:316:ARG:HD3	3:C:512:HOH:O	2.08	0.54
1:B:255:ALA:O	1:C:252:SER:OG	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ARG:NH2	3:B:814:HOH:O	2.42	0.53
1:B:295:ASN:OD1	1:B:297:ARG:NH1	2.31	0.53
1:A:263:LEU:HD13	1:B:254:VAL:HG22	1.91	0.52
2:D:1:GAL:O2	2:D:2:SIA:O1B	2.24	0.52
1:A:245:ARG:HD2	1:C:250:GLU:OE2	2.09	0.52
1:A:427:ARG:HD2	3:A:601:HOH:O	2.11	0.51
1:B:332:ASN:O	1:B:333:TRP:CB	2.57	0.51
1:B:333:TRP:N	3:B:805:HOH:O	2.42	0.51
1:B:254:VAL:O	1:C:253:TYR:HA	2.09	0.51
1:A:422:GLN:HE21	1:A:422:GLN:HA	1.77	0.50
1:C:316:ARG:NH2	3:C:599:HOH:O	2.40	0.50
1:C:427:ARG:NH2	3:C:564:HOH:O	2.18	0.49
1:C:246:ILE:O	1:C:250:GLU:HG3	2.12	0.49
2:D:1:GAL:H2	2:D:2:SIA:C1	2.43	0.49
1:C:279:LEU:HD23	1:C:289:VAL:HA	1.95	0.48
1:C:224:GLN:HA	1:C:238:VAL:HG22	1.95	0.48
1:C:421:TRP:CZ2	1:C:424:GLY:HA2	2.48	0.48
1:B:181:ASN:ND2	3:B:823:HOH:O	2.47	0.48
1:C:282:ASN:HD21	1:C:286:GLN:HB2	1.78	0.48
1:B:237:THR:HA	1:B:240:ASP:OD2	2.14	0.47
1:C:237:THR:HA	1:C:240:ASP:OD2	2.14	0.47
1:C:295:ASN:ND2	1:C:297:ARG:HH12	2.13	0.46
1:B:268:LYS:NZ	1:C:250:GLU:O	2.48	0.46
1:A:453:SER:HB3	3:A:782:HOH:O	2.16	0.46
1:A:262:ARG:HD3	1:A:273:LEU:HD21	1.97	0.46
1:A:336:GLN:OE1	3:A:640:HOH:O	2.21	0.45
2:E:1:GAL:H3	2:E:2:SIA:H32	1.63	0.45
1:A:403:LEU:HD22	1:A:438:HIS:CD2	2.51	0.45
1:B:250:GLU:OE2	1:C:245:ARG:HD2	2.16	0.45
1:A:403:LEU:HD12	1:A:412:MET:HG3	1.99	0.45
1:C:404:SER:HB3	1:C:409:PRO:HA	1.98	0.45
1:B:199:LEU:HD22	1:C:186:MET:CE	2.46	0.45
1:B:318:SER:HB3	1:B:378:LEU:HD22	1.98	0.45
2:D:1:GAL:HO2	2:D:2:SIA:C1	2.28	0.44
1:A:335:VAL:HG23	3:A:94:HOH:O	2.18	0.44
1:C:385:PRO:HD3	1:C:421:TRP:CG	2.53	0.44
1:A:221:ASN:CB	1:C:233:THR:HG22	2.39	0.43
1:A:235:LYS:HB2	1:A:238:VAL:HG23	2.00	0.43
1:A:221:ASN:OD1	1:A:223:ASP:HB2	2.19	0.43
1:C:235:LYS:HB2	1:C:238:VAL:HG23	2.00	0.43
1:C:221:ASN:OD1	1:C:224:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:THR:O	1:A:235:LYS:NZ	2.52	0.43
1:C:212:GLN:OE1	1:C:219:ARG:HD2	2.19	0.42
1:C:224:GLN:HA	1:C:238:VAL:CG2	2.49	0.42
1:A:221:ASN:HB2	1:C:233:THR:CG2	2.40	0.42
1:A:394:TYR:CZ	1:A:451:PRO:HD3	2.54	0.42
2:D:2:SIA:H92	2:D:2:SIA:C2	2.49	0.42
1:A:254:VAL:HG22	1:C:263:LEU:HD13	1.99	0.42
1:B:404:SER:HB3	1:B:409:PRO:HA	2.02	0.42
1:B:331:LEU:HD13	1:B:359[A]:SER:HB3	2.01	0.42
1:B:182:ASN:N	3:B:548:HOH:O	2.30	0.42
1:A:203:LEU:HD23	1:C:216:LEU:HB3	2.02	0.41
1:A:279:LEU:HD23	1:A:289:VAL:HA	2.02	0.41
1:B:331:LEU:HD22	1:B:359[B]:SER:OG	2.20	0.41
1:B:408:THR:HA	1:B:409:PRO:HD3	1.95	0.41
1:C:316:ARG:HD2	3:C:617:HOH:O	2.21	0.41
1:C:422:GLN:NE2	3:C:485:HOH:O	2.54	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:723:HOH:O	3:C:738:HOH:O[3_555]	1.81	0.39
1:C:336[B]:GLN:OE1	3:A:852:HOH:O[3_545]	1.82	0.38
3:A:460:HOH:O	3:B:653:HOH:O[2_665]	1.96	0.24
3:B:582:HOH:O	3:C:468:HOH:O[3_555]	2.00	0.20
3:C:724:HOH:O	3:C:738:HOH:O[3_555]	2.05	0.15
3:C:724:HOH:O	3:C:739:HOH:O[3_555]	2.08	0.12
3:A:741:HOH:O	3:A:758:HOH:O[3_556]	2.10	0.10
3:C:529:HOH:O	3:C:637:HOH:O[2_665]	2.10	0.10
3:C:739:HOH:O	3:C:740:HOH:O[3_545]	2.11	0.09

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	288/325 (89%)	278 (96%)	10 (4%)	0	100	100
1	B	294/325 (90%)	281 (96%)	12 (4%)	1 (0%)	41	49
1	C	292/325 (90%)	279 (96%)	13 (4%)	0	100	100
All	All	874/975 (90%)	838 (96%)	35 (4%)	1 (0%)	51	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	333	TRP

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	246/278 (88%)	244 (99%)	2 (1%)	81	90
1	B	251/278 (90%)	244 (97%)	7 (3%)	43	57
1	C	251/278 (90%)	247 (98%)	4 (2%)	62	76
All	All	748/834 (90%)	735 (98%)	13 (2%)	60	74

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	422	GLN
1	B	252	SER
1	B	295	ASN
1	B	316	ARG
1	B	375	LEU
1	B	415	ASN
1	B	422	GLN
1	B	448	VAL
1	C	166	LEU

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Mol	Chain	Res	Type
1	C	202	ARG
1	C	415	ASN
1	C	428	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	251	GLN
1	A	397	GLN
1	A	415	ASN
1	A	422	GLN
1	B	182	ASN
1	B	422	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)

6 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	GAL	D	1	2	12,12,12	0.68	0	17,17,17	1.32	4 (23%)
2	SIA	D	2	2	20,20,21	0.66	0	24,28,31	1.44	3 (12%)
2	SIA	D	3	2	20,20,21	0.59	0	24,28,31	1.08	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GAL	E	1	2	12,12,12	0.54	0	17,17,17	0.60	0
2	SIA	E	2	2	20,20,21	0.63	0	24,28,31	1.52	3 (12%)
2	SIA	E	3	2	20,20,21	0.61	0	24,28,31	1.10	2 (8%)

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	GAL	D	1	2	-	0/2/22/22	0/1/1/1
2	SIA	D	2	2	-	6/18/34/38	0/1/1/1
2	SIA	D	3	2	-	0/18/34/38	0/1/1/1
2	GAL	E	1	2	-	0/2/22/22	0/1/1/1
2	SIA	E	2	2	-	1/18/34/38	0/1/1/1
2	SIA	E	3	2	-	2/18/34/38	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	SIA	C6-O6-C2	5.58	123.27	111.34
2	D	2	SIA	C6-O6-C2	4.10	120.11	111.34
2	E	3	SIA	C6-O6-C2	3.12	118.02	111.34
2	D	2	SIA	C6-C5-N5	-2.92	106.06	110.91
2	D	1	GAL	C3-C4-C5	2.92	115.45	110.24
2	D	1	GAL	C1-C2-C3	2.90	116.33	110.31
2	D	2	SIA	O6-C2-C1	-2.76	102.28	107.70
2	D	3	SIA	C6-O6-C2	2.42	116.51	111.34
2	D	3	SIA	O1B-C1-C2	2.12	119.09	113.03
2	E	3	SIA	O1B-C1-C2	2.12	119.09	113.03
2	E	2	SIA	C3-C4-C5	-2.09	108.94	111.46
2	D	3	SIA	C4-C3-C2	2.08	113.54	109.81
2	D	1	GAL	C4-C3-C2	2.04	114.39	110.82
2	D	1	GAL	C1-O5-C5	-2.03	109.84	113.66
2	E	2	SIA	O1B-C1-C2	2.03	118.82	113.03

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	SIA	O1A-C1-C2-O6
2	D	2	SIA	C6-C7-C8-O8
2	D	2	SIA	O8-C8-C9-O9
2	D	2	SIA	C7-C8-C9-O9
2	E	3	SIA	C7-C8-C9-O9
2	D	2	SIA	O1B-C1-C2-O6
2	E	2	SIA	O8-C8-C9-O9
2	D	2	SIA	C6-C7-C8-C9
2	E	3	SIA	O1A-C1-C2-C3

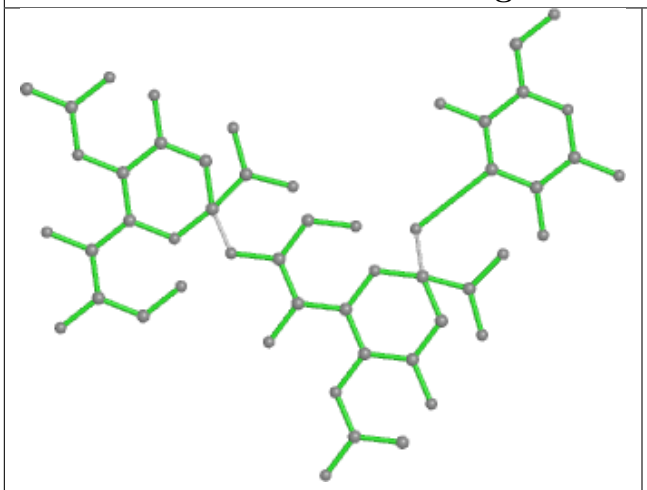
There are no ring outliers.

4 monomers are involved in 7 short contacts:

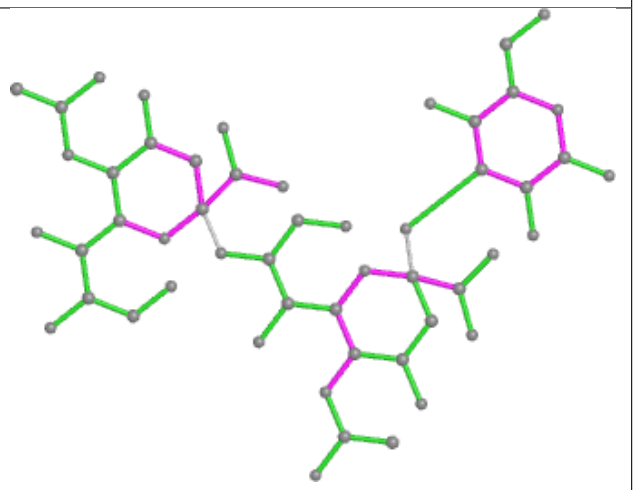
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	GAL	1	0
2	D	2	SIA	6	0
2	D	1	GAL	5	0
2	E	2	SIA	1	0

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

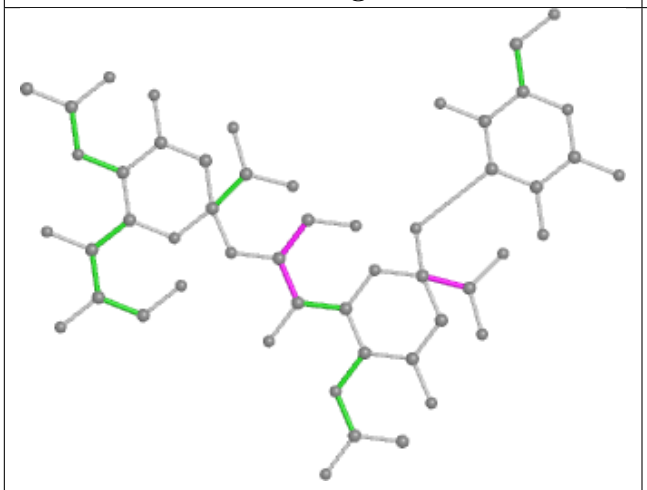
Oligosaccharide Chain D



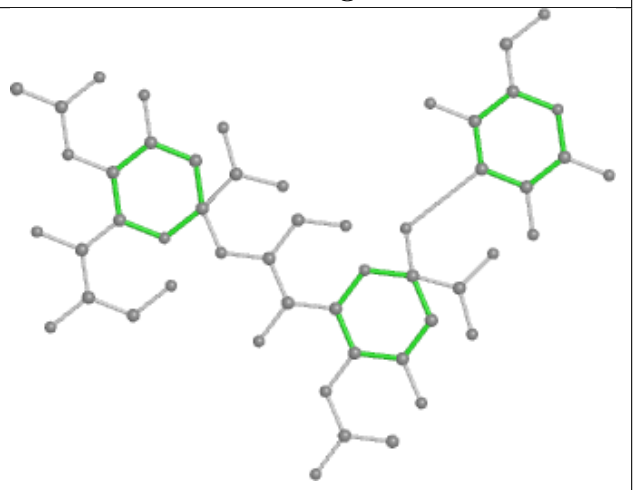
Bond lengths



Bond angles

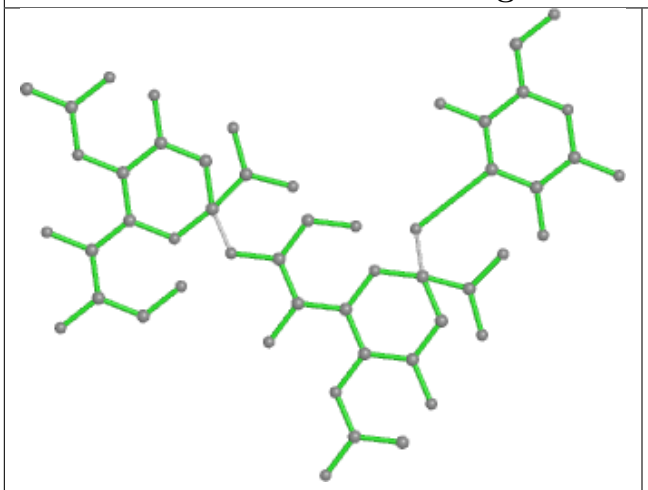


Torsions

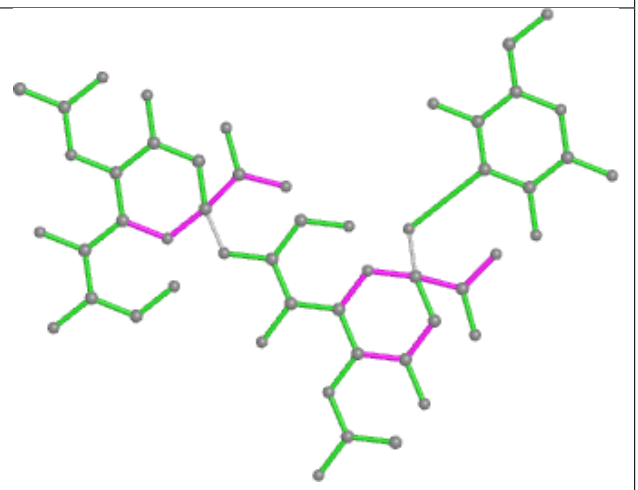


Rings

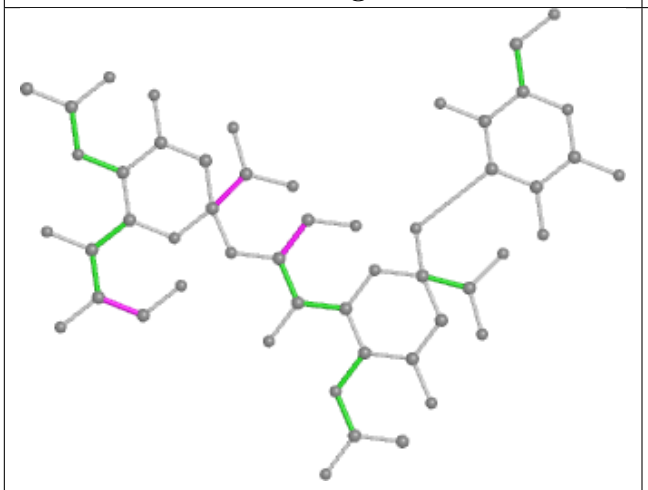
Oligosaccharide Chain E



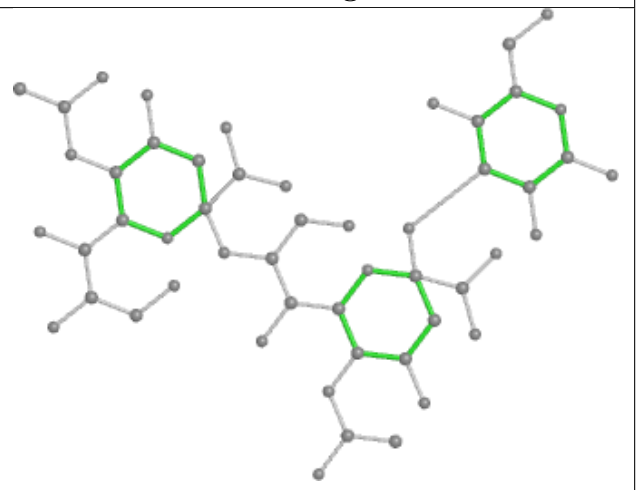
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	290/325 (89%)	0.38	45 (15%)	2	2	18, 37, 112, 141	0
1	B	295/325 (90%)	0.59	50 (16%)	1	2	15, 38, 108, 134	0
1	C	292/325 (89%)	0.43	48 (16%)	1	2	20, 42, 110, 141	1 (0%)
All	All	877/975 (89%)	0.47	143 (16%)	1	2	15, 39, 110, 141	1 (0%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	LEU	8.9
1	A	263	LEU	7.3
1	B	257	ALA	7.1
1	A	257	ALA	6.9
1	A	273	LEU	6.8
1	C	273	LEU	6.0
1	A	281	ILE	5.9
1	C	283	SER	5.8
1	C	289	VAL	5.6
1	B	272	MET	5.5
1	A	276	SER	5.4
1	C	281	ILE	5.4
1	A	272	MET	5.4
1	B	273	LEU	5.3
1	B	256	SER	5.2
1	A	274	ILE	5.1
1	A	283	SER	4.9
1	B	260	PRO	4.9
1	A	288	THR	4.9
1	A	277	SER	4.9
1	A	289	VAL	4.7
1	B	258	VAL	4.7
1	C	285	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	287	LEU	4.6
1	A	278	THR	4.6
1	A	258	VAL	4.6
1	A	290	ARG	4.5
1	A	291	SER	4.5
1	B	261	LEU	4.5
1	B	166	LEU	4.5
1	B	252	SER	4.4
1	C	279	LEU	4.4
1	B	238	VAL	4.4
1	A	269	VAL	4.3
1	C	284	SER	4.3
1	B	263	LEU	4.3
1	C	272	MET	4.3
1	C	269	VAL	4.2
1	A	280	GLU	4.2
1	A	256	SER	4.2
1	B	283	SER	4.1
1	C	291	SER	4.1
1	B	264	ASN	4.1
1	C	276	SER	3.9
1	A	285	GLY	3.9
1	C	164	PRO	3.9
1	C	263	LEU	3.8
1	A	287	LEU	3.8
1	B	266	SER	3.8
1	C	280	GLU	3.7
1	B	239	PHE	3.7
1	C	288	THR	3.7
1	A	270	LEU	3.7
1	A	275	ASP	3.7
1	C	290	ARG	3.6
1	B	287	LEU	3.6
1	C	274	ILE	3.6
1	B	274	ILE	3.6
1	B	247	GLY	3.6
1	C	165	VAL	3.6
1	A	292	THR	3.6
1	B	289	VAL	3.5
1	B	265	SER	3.4
1	C	277	SER	3.4
1	B	161	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	282	ASN	3.4
1	C	252	SER	3.4
1	B	269	VAL	3.3
1	C	166	LEU	3.3
1	A	252	SER	3.3
1	B	164	PRO	3.3
1	C	246	ILE	3.3
1	B	248	ALA	3.2
1	A	271	ASP	3.2
1	B	288	THR	3.2
1	C	260	PRO	3.2
1	C	238	VAL	3.1
1	A	282	ASN	3.1
1	B	285	GLY	3.1
1	B	259	THR	3.1
1	B	277	SER	3.1
1	B	251	GLN	3.1
1	C	251	GLN	3.1
1	A	239	PHE	3.0
1	A	262	ARG	3.0
1	C	264	ASN	3.0
1	A	242	ILE	3.0
1	C	286	GLN	2.9
1	A	260	PRO	2.9
1	C	278	THR	2.9
1	B	253	TYR	2.8
1	B	276	SER	2.8
1	A	259	THR	2.8
1	A	284	SER	2.8
1	A	293	SER	2.8
1	B	278	THR	2.8
1	C	266	SER	2.7
1	C	168	GLN	2.7
1	C	253	TYR	2.7
1	B	268	LYS	2.7
1	B	279	LEU	2.7
1	C	268	LYS	2.6
1	C	267	THR	2.6
1	A	267	THR	2.6
1	C	275	ASP	2.6
1	C	249	ILE	2.6
1	B	165	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	220	PHE	2.6
1	B	226	GLN	2.5
1	C	270	LEU	2.5
1	A	166	LEU	2.5
1	A	254	VAL	2.5
1	B	267	THR	2.5
1	C	240	ASP	2.5
1	B	255	ALA	2.5
1	C	292	THR	2.4
1	C	257	ALA	2.4
1	A	286	GLN	2.4
1	B	254	VAL	2.4
1	C	242	ILE	2.3
1	B	270	LEU	2.3
1	B	455	THR	2.3
1	C	271	ASP	2.3
1	A	253	TYR	2.3
1	A	266	SER	2.3
1	A	238	VAL	2.3
1	C	245	ARG	2.2
1	A	268	LYS	2.2
1	C	255	ALA	2.2
1	C	261	LEU	2.2
1	B	249	ILE	2.2
1	B	284	SER	2.2
1	C	237	THR	2.1
1	A	245	ARG	2.1
1	B	162	GLY	2.1
1	B	281	ILE	2.1
1	B	275	ASP	2.0
1	B	223	ASP	2.0
1	A	255	ALA	2.0
1	A	264	ASN	2.0
1	B	246	ILE	2.0
1	B	237	THR	2.0
1	C	244	SER	2.0

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

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

6.3 Carbohydrates (i)

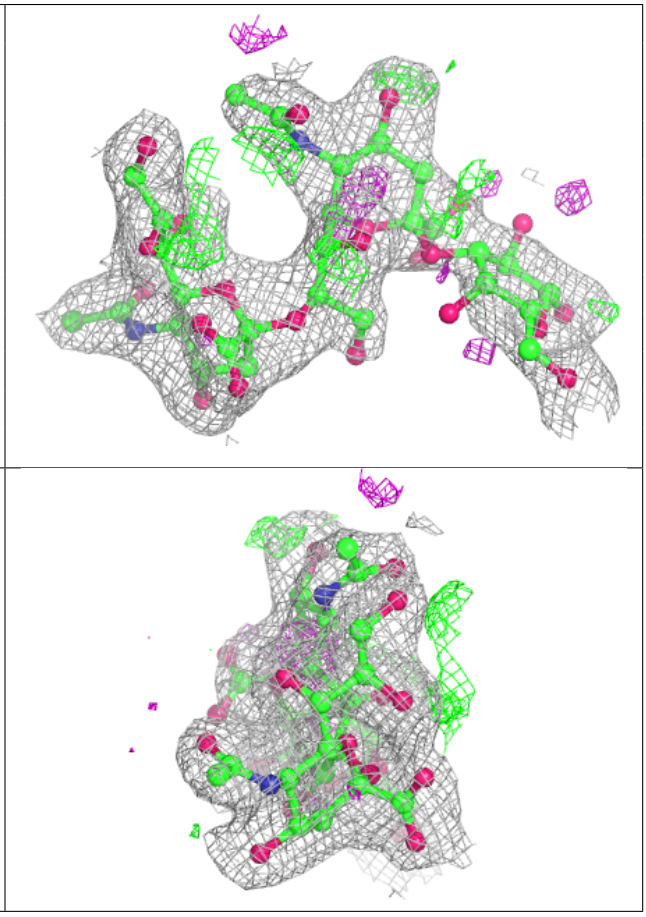
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAL	E	1	12/12	0.68	0.53	115,136,141,143	0
2	GAL	D	1	12/12	0.70	0.29	87,110,117,121	0
2	SIA	D	2	20/21	0.79	0.21	47,73,110,111	0
2	SIA	E	2	20/21	0.88	0.23	35,71,101,104	0
2	SIA	D	3	20/21	0.92	0.10	36,46,67,68	0
2	SIA	E	3	20/21	0.92	0.20	44,59,71,71	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.

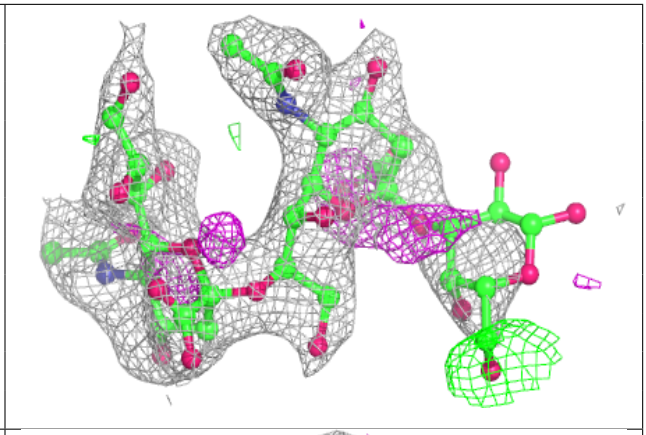
Electron density around Chain D:

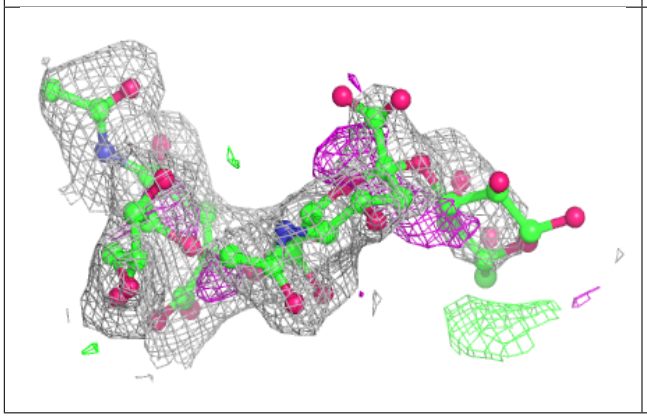
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

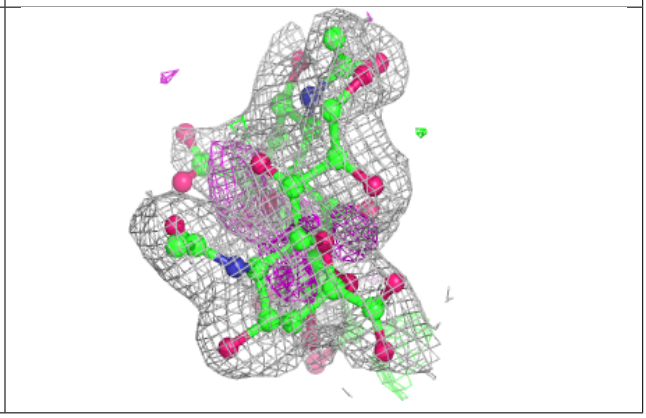


Electron density around Chain E:

$2mF_o$-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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.