



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 07:57 AM EST

PDB ID : 3S6X
Title : Structure of reovirus attachment protein sigma1 in complex with alpha-2,3-sialyllactose
Authors : Reiter, D.M.; Dermody, T.S.; Stehle, T.
Deposited on : 2011-05-26
Resolution : 2.25 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 : 1.8.5 (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

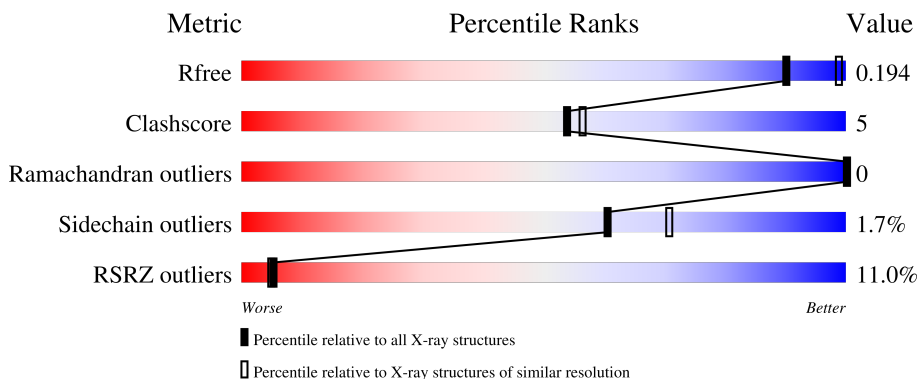
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	325	 11% 78% 11% 11%
1	B	325	 10% 79% 11% 9%
1	C	325	 9% 79% 10% 10%
2	D	3	 33% 67%
2	E	3	 33% 67%

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Mol	Chain	Length	Quality of chain
2	F	3	 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7624 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	Total 2210	C 1386	N 385	O 431	S 8	0	1	0
1	B	295	Total 2262	C 1417	N 396	O 441	S 8	0	3	0
1	C	291	Total 2211	C 1387	N 385	O 431	S 8	1	0	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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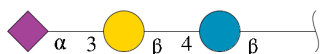
Chain	Residue	Modelled	Actual	Comment	Reference
B	155	LYS	-	expression tag	UNP P03528
B	156	LEU	-	expression tag	UNP P03528
B	157	ILE	-	expression tag	UNP P03528
B	158	GLY	-	expression tag	UNP P03528
B	159	GLU	-	expression tag	UNP P03528
B	160	GLY	-	expression tag	UNP P03528
B	161	SER	-	expression tag	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-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	3	43	23	1	19	0	0	0
2	E	3	43	23	1	19	0	0	0
2	F	3	43	23	1	19	0	0	0

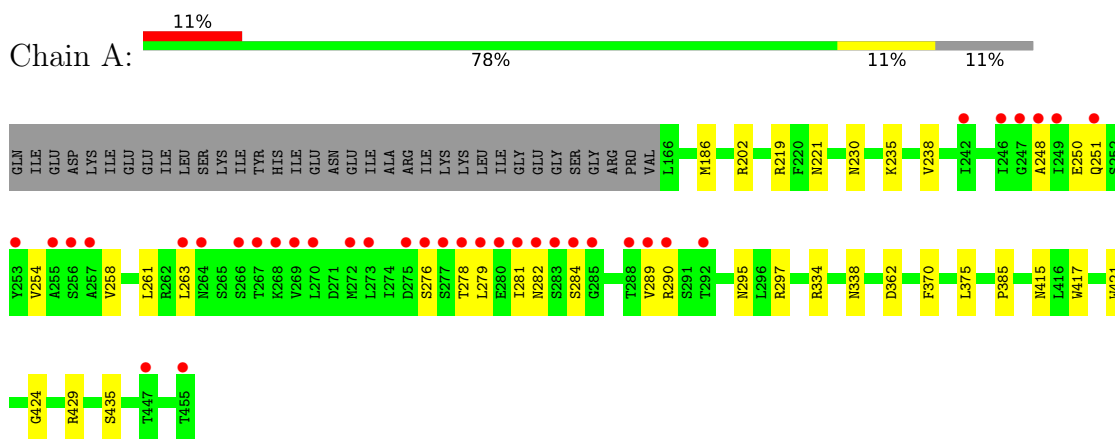
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	326	326	326	0	0
3	B	253	253	253	0	0
3	C	233	233	233	0	0

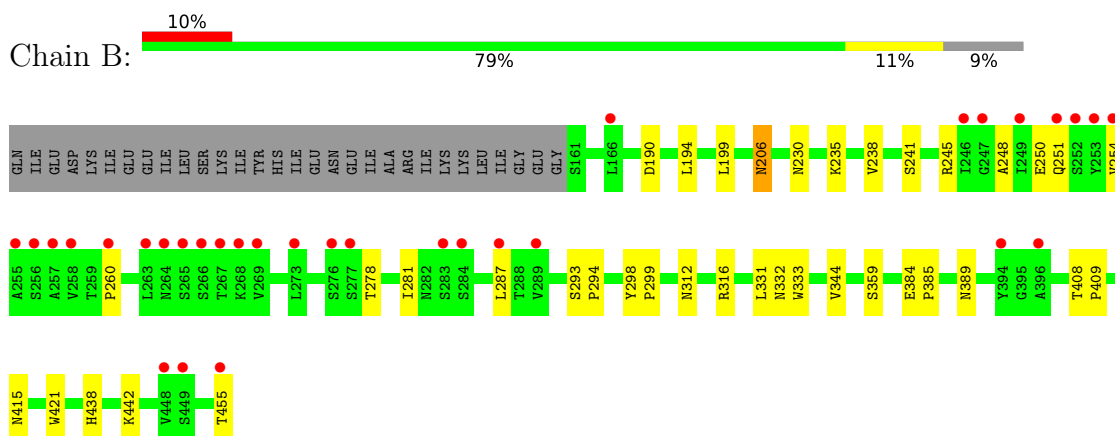
3 Residue-property plots [i](#)

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.

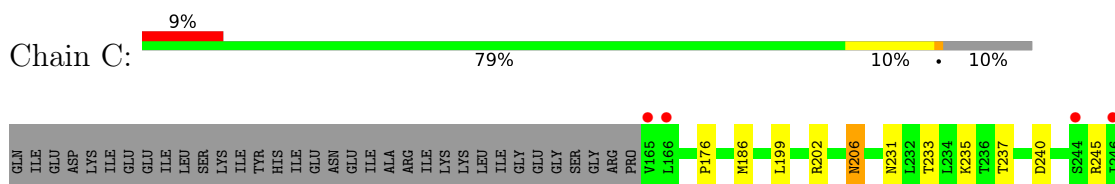
- Molecule 1: Outer capsid protein sigma-1

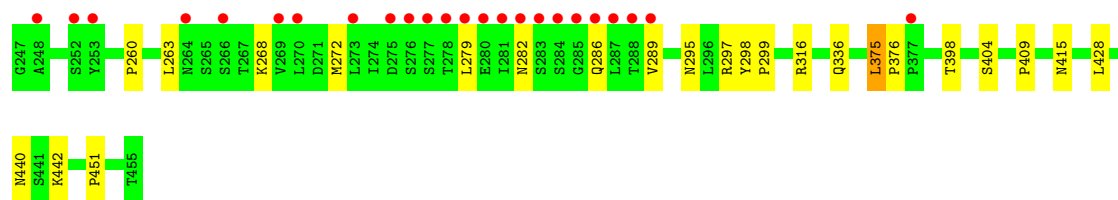


- Molecule 1: Outer capsid protein sigma-1



- Molecule 1: Outer capsid protein sigma-1





- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



4 Data and refinement statistics

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)	38.61 – 2.25 38.61 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.4 (38.61-2.25) 95.4 (38.61-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.24Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.158 , 0.199 0.152 , 0.194	Depositor DCC
R_{free} test set	3956 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtrriage
Anisotropy	0.374	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 67.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7624	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, 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	0.32	0/2254	0.49	0/3069
1	B	0.33	0/2307	0.50	0/3141
1	C	0.32	0/2255	0.50	0/3070
All	All	0.32	0/6816	0.50	0/9280

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	2210	0	2170	25	0
1	B	2262	0	2225	31	0
1	C	2211	0	2173	32	0
2	D	43	0	37	1	0
2	E	43	0	37	0	0
2	F	43	0	37	3	0
3	A	326	0	0	2	5
3	B	253	0	0	9	6
3	C	233	0	0	6	2
All	All	7624	0	6679	72	8

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 5.

All (72) 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:B:332:ASN:HB3	3:B:693:HOH:O	1.83	0.77
1:B:250:GLU:OE2	1:C:245:ARG:HD2	1.87	0.74
1:A:221:ASN:HB2	1:C:233:THR:HG22	1.67	0.74
1:A:278:THR:HB	1:C:289:VAL:HG22	1.68	0.73
1:A:334:ARG:NE	3:A:707:HOH:O	2.22	0.72
1:C:440:ASN:ND2	3:C:818:HOH:O	2.24	0.70
1:B:389:ASN:HB3	3:B:814:HOH:O	1.94	0.67
2:F:2:GAL:H4	2:F:3:SIA:C1	2.24	0.66
1:B:190:ASP:OD1	3:B:530:HOH:O	2.14	0.65
1:B:316:ARG:NH1	3:B:890:HOH:O	1.98	0.65
1:C:336:GLN:NE2	3:C:498:HOH:O	2.30	0.63
1:A:289:VAL:HG22	1:B:278:THR:HB	1.80	0.62
1:A:186:MET:CE	1:C:199:LEU:HD22	2.30	0.62
1:C:375:LEU:HD13	1:C:376:PRO:HD2	1.81	0.62
1:A:282:ASN:OD1	1:A:284:SER:OG	2.09	0.61
1:A:254:VAL:HG22	1:C:263:LEU:HD13	1.83	0.60
1:A:276:SER:O	1:A:290:ARG:NH2	2.35	0.60
1:A:338:ASN:HB2	3:A:805:HOH:O	2.02	0.58
1:C:237:THR:HA	1:C:240:ASP:OD2	2.04	0.57
1:B:199:LEU:HD22	1:C:186:MET:CE	2.35	0.55
1:B:331:LEU:HD22	1:B:359[B]:SER:OG	2.07	0.54
1:C:282:ASN:HD21	1:C:286:GLN:HB2	1.72	0.54
1:B:235:LYS:O	1:B:238:VAL:HG12	2.09	0.53
1:B:442:LYS:HE2	3:B:527:HOH:O	2.08	0.52
1:A:295:ASN:HD21	1:A:297:ARG:HH22	1.57	0.52
1:B:281:ILE:HD12	1:C:260:PRO:HD3	1.92	0.51
1:C:282:ASN:ND2	1:C:286:GLN:HB2	2.26	0.51
1:C:398:THR:OG1	3:C:571:HOH:O	1.99	0.51
1:A:230:ASN:HB2	1:B:206:ASN:OD1	2.10	0.50
1:B:287:LEU:HB2	1:C:260:PRO:HG3	1.94	0.50
1:C:235:LYS:HG2	1:C:237:THR:HG23	1.94	0.49
1:C:442:LYS:HB2	1:C:442:LYS:NZ	2.28	0.48
1:B:230:ASN:HB2	1:C:206:ASN:OD1	2.14	0.48
1:B:194:LEU:HD21	1:C:176:PRO:HD3	1.95	0.47
1:C:316:ARG:HD3	3:C:515:HOH:O	2.14	0.47
1:A:279:LEU:HD23	1:A:289:VAL:HA	1.96	0.47
1:A:219:ARG:HB3	1:C:231:ASN:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:HD21	1:C:272:MET:HB3	1.97	0.46
1:B:333:TRP:CA	3:B:803:HOH:O	2.63	0.46
1:B:248:ALA:O	1:B:251:GLN:HG2	2.17	0.45
1:A:258:VAL:O	1:A:261:LEU:HB2	2.16	0.45
1:A:186:MET:HE2	1:C:199:LEU:HD22	1.97	0.44
1:A:235:LYS:O	1:A:238:VAL:HG12	2.16	0.44
3:C:817:HOH:O	2:F:2:GAL:O2	2.05	0.44
1:C:231:ASN:O	1:C:233:THR:HG23	2.16	0.44
1:A:421:TRP:CZ2	1:A:424:GLY:HA2	2.53	0.44
1:B:333:TRP:HA	3:B:803:HOH:O	2.16	0.44
1:B:199:LEU:HD22	1:C:186:MET:HE3	1.99	0.43
1:B:359[A]:SER:OG	1:B:438:HIS:O	2.35	0.43
1:B:293:SER:HA	1:B:294:PRO:HD3	1.87	0.43
1:B:333:TRP:N	3:B:803:HOH:O	2.51	0.43
1:B:298:TYR:CG	1:B:299:PRO:HA	2.54	0.43
1:C:295:ASN:HD21	1:C:297:ARG:HH22	1.67	0.42
1:B:385:PRO:HD3	1:B:421:TRP:CG	2.54	0.42
3:C:817:HOH:O	2:F:1:BGC:H6C1	2.20	0.42
1:A:250:GLU:O	1:C:268:LYS:NZ	2.37	0.42
1:A:263:LEU:HD13	1:B:254:VAL:HG22	2.02	0.42
1:A:385:PRO:HD3	1:A:421:TRP:CG	2.55	0.42
1:B:344:VAL:HG21	1:C:451:PRO:HB3	2.01	0.42
1:B:384:GLU:HA	1:B:385:PRO:HD3	1.92	0.42
1:C:298:TYR:CG	1:C:299:PRO:HA	2.55	0.41
1:C:298:TYR:CD1	1:C:299:PRO:HA	2.56	0.41
1:A:370:PHE:HB2	1:A:424:GLY:O	2.21	0.41
1:A:417:TRP:CZ2	1:A:429:ARG:HG2	2.56	0.41
1:C:279:LEU:HD23	1:C:289:VAL:HA	2.03	0.41
1:A:248:ALA:O	1:A:251:GLN:HG2	2.21	0.41
1:A:281:ILE:HD11	1:B:260:PRO:HD3	2.02	0.40
1:B:408:THR:HA	1:B:409:PRO:HD3	1.97	0.40
1:C:404:SER:HB3	1:C:409:PRO:HA	2.03	0.40
1:B:241:SER:O	1:B:245:ARG:HG3	2.21	0.40
1:B:312[A]:ASN:ND2	3:B:551:HOH:O	2.55	0.40
2:D:2:GAL:H3	2:D:3:SIA:H32	1.80	0.40

All (8) 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:A:572:HOH:O	3:A:823:HOH:O[3_555]	1.95	0.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:579:HOH:O	3:B:803:HOH:O[4_455]	1.97	0.23
3:B:530:HOH:O	3:C:497:HOH:O[2_655]	2.03	0.17
3:B:631:HOH:O	3:B:834:HOH:O[3_555]	2.03	0.17
3:A:557:HOH:O	3:B:752:HOH:O[4_455]	2.09	0.11
3:C:537:HOH:O	3:C:811:HOH:O[3_556]	2.11	0.09
3:A:778:HOH:O	3:B:533:HOH:O[4_455]	2.12	0.08
3:A:571:HOH:O	3:B:597:HOH:O[4_455]	2.18	0.02

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	289/325 (89%)	279 (96%)	10 (4%)	0	100	100
1	B	296/325 (91%)	288 (97%)	8 (3%)	0	100	100
1	C	289/325 (89%)	279 (96%)	10 (4%)	0	100	100
All	All	874/975 (90%)	846 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	247/278 (89%)	242 (98%)	5 (2%)	55	64
1	B	254/278 (91%)	251 (99%)	3 (1%)	71	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	247/278 (89%)	242 (98%)	5 (2%)	55	64
All	All	748/834 (90%)	735 (98%)	13 (2%)	60	71

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

Mol	Chain	Res	Type
1	A	202	ARG
1	A	362	ASP
1	A	375	LEU
1	A	415	ASN
1	A	435	SER
1	B	206	ASN
1	B	415	ASN
1	B	455	THR
1	C	202	ARG
1	C	206	ASN
1	C	375	LEU
1	C	415	ASN
1	C	428	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	ASN
1	B	422	GLN
1	C	168	GLN
1	C	264	ASN
1	C	312	ASN

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

9 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	D	1	2	12,12,12	0.58	0	17,17,17	0.98	1 (5%)
2	GAL	D	2	2	11,11,12	0.61	0	15,15,17	1.04	1 (6%)
2	SIA	D	3	2	20,20,21	0.55	0	24,28,31	1.06	2 (8%)
2	BGC	E	1	2	12,12,12	0.56	0	17,17,17	1.12	1 (5%)
2	GAL	E	2	2	11,11,12	0.71	0	15,15,17	1.31	1 (6%)
2	SIA	E	3	2	20,20,21	0.55	0	24,28,31	0.78	0
2	BGC	F	1	2	12,12,12	0.55	0	17,17,17	0.97	1 (5%)
2	GAL	F	2	2	11,11,12	0.61	0	15,15,17	0.97	1 (6%)
2	SIA	F	3	2	20,20,21	0.67	0	24,28,31	1.04	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	D	1	2	-	1/2/22/22	0/1/1/1
2	GAL	D	2	2	-	0/2/19/22	0/1/1/1
2	SIA	D	3	2	-	0/18/34/38	0/1/1/1
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	GAL	E	2	2	-	0/2/19/22	0/1/1/1
2	SIA	E	3	2	-	0/18/34/38	0/1/1/1
2	BGC	F	1	2	-	0/2/22/22	0/1/1/1
2	GAL	F	2	2	-	0/2/19/22	0/1/1/1
2	SIA	F	3	2	-	0/18/34/38	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	GAL	C1-C2-C3	3.52	113.99	109.67
2	D	3	SIA	C6-O6-C2	2.86	117.47	111.34
2	F	2	GAL	O5-C5-C6	2.74	111.50	107.20
2	E	1	BGC	C3-C4-C5	2.65	114.97	110.24
2	F	1	BGC	C3-C4-C5	2.52	114.73	110.24
2	D	3	SIA	C8-C7-C6	-2.45	108.39	113.03
2	D	2	GAL	O5-C1-C2	-2.42	107.03	110.77
2	F	3	SIA	C4-C3-C2	2.35	114.03	109.81
2	D	1	BGC	C3-C4-C5	2.21	114.17	110.24

There are no chirality outliers.

All (1) torsion outliers are listed below:

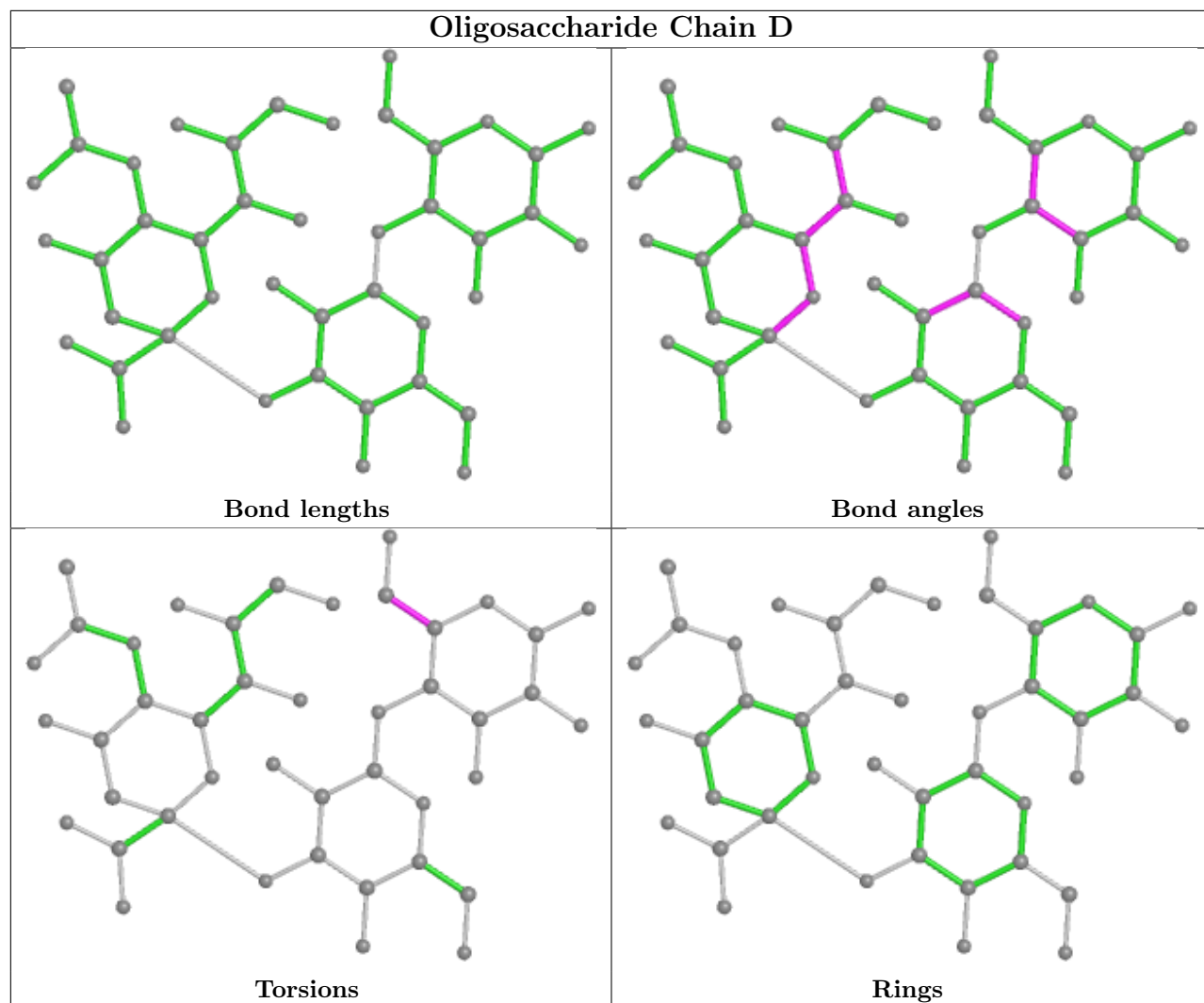
Mol	Chain	Res	Type	Atoms
2	D	1	BGC	O5-C5-C6-O6

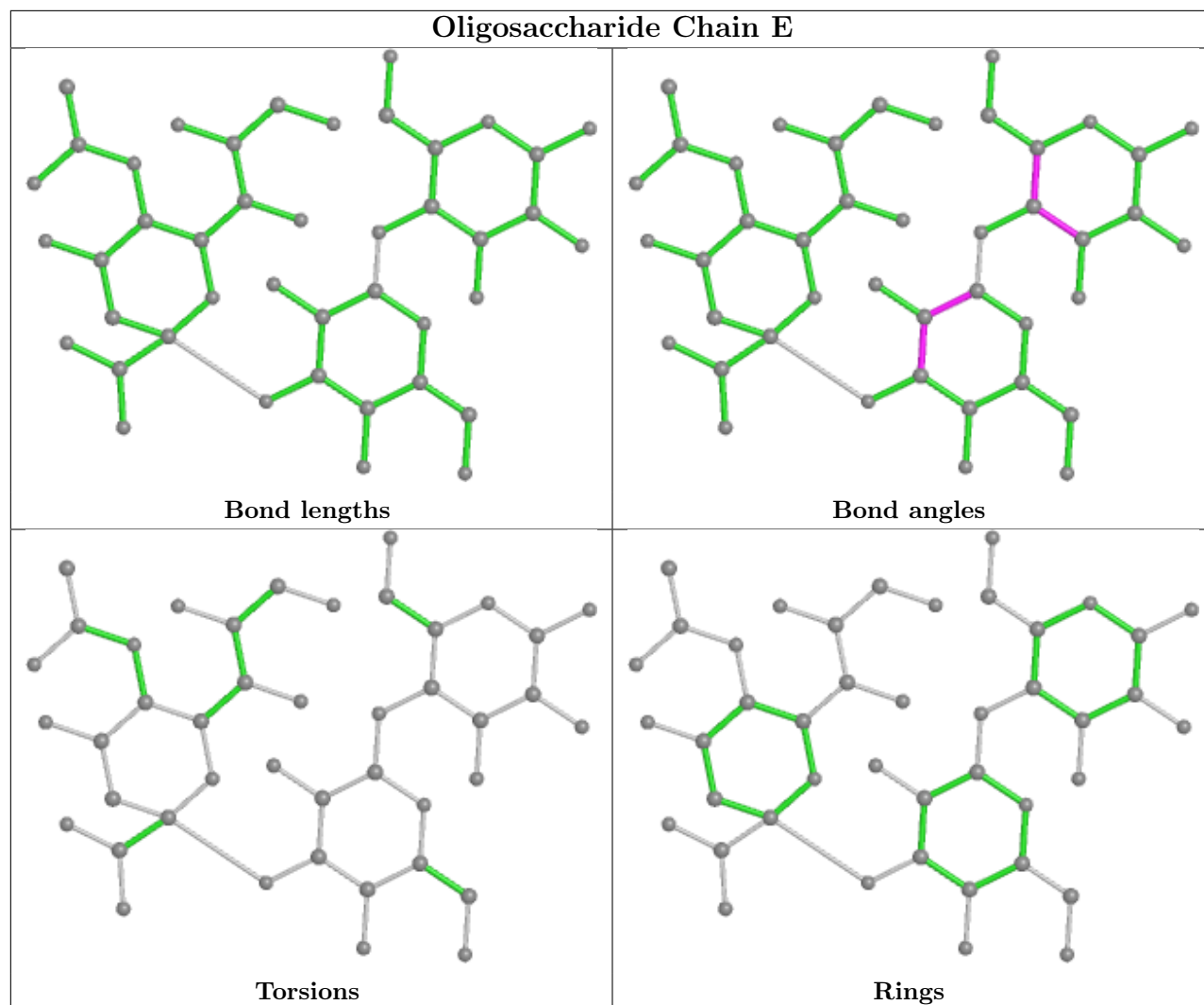
There are no ring outliers.

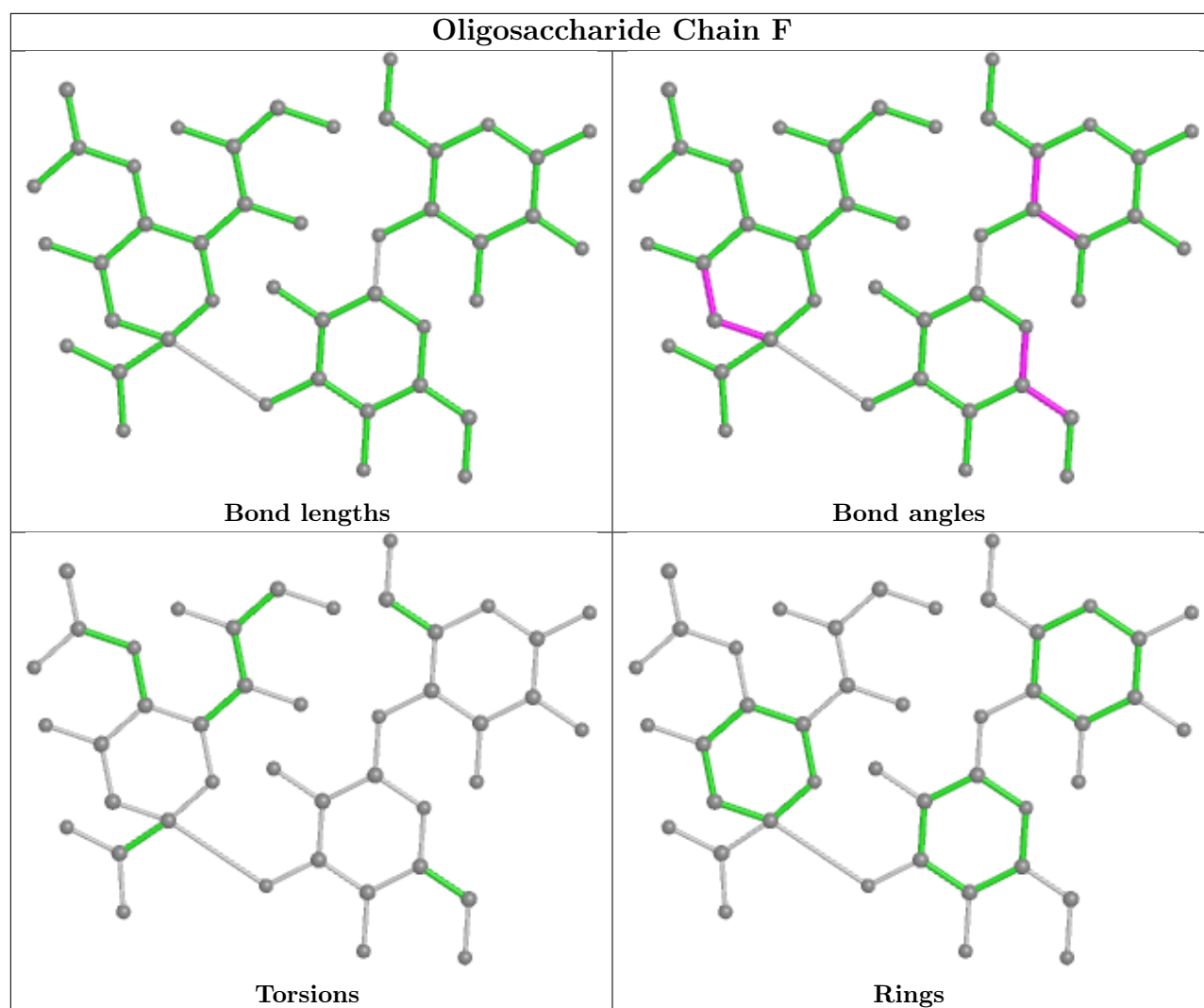
5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	BGC	1	0
2	F	3	SIA	1	0
2	F	2	GAL	2	0
2	D	2	GAL	1	0
2	D	3	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.







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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	290/325 (89%)	0.14	36 (12%) 4 3	21, 39, 119, 149	0
1	B	295/325 (90%)	0.24	32 (10%) 5 5	20, 39, 116, 137	2 (0%)
1	C	291/325 (89%)	0.11	28 (9%) 8 8	23, 44, 116, 144	3 (1%)
All	All	876/975 (89%)	0.17	96 (10%) 5 5	20, 41, 118, 149	5 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	283	SER	6.0
1	B	257	ALA	5.8
1	A	263	LEU	4.8
1	B	256	SER	4.6
1	B	252	SER	4.5
1	C	166	LEU	4.4
1	B	283	SER	4.4
1	A	257	ALA	4.3
1	B	263	LEU	4.3
1	B	269	VAL	4.0
1	B	455	THR	3.9
1	B	265	SER	3.8
1	A	277	SER	3.6
1	A	289	VAL	3.6
1	A	267	THR	3.5
1	C	266	SER	3.5
1	C	285	GLY	3.5
1	B	287	LEU	3.4
1	A	288	THR	3.4
1	A	248	ALA	3.4
1	C	281	ILE	3.4
1	A	269	VAL	3.3
1	A	270	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	285	GLY	3.3
1	A	246	ILE	3.3
1	B	166	LEU	3.2
1	A	276	SER	3.2
1	A	290	ARG	3.2
1	A	242	ILE	3.2
1	C	273	LEU	3.2
1	C	277	SER	3.1
1	B	284	SER	3.0
1	A	284	SER	2.9
1	A	273	LEU	2.9
1	B	249	ILE	2.8
1	A	256	SER	2.8
1	C	269	VAL	2.8
1	A	251	GLN	2.8
1	A	283	SER	2.8
1	B	247	GLY	2.8
1	B	251	GLN	2.7
1	C	253	TYR	2.7
1	A	292	THR	2.6
1	B	273	LEU	2.6
1	C	287	LEU	2.6
1	C	246	ILE	2.6
1	A	249	ILE	2.6
1	A	447	THR	2.6
1	B	255	ALA	2.6
1	A	266	SER	2.5
1	C	284	SER	2.5
1	C	282	ASN	2.5
1	A	281	ILE	2.5
1	B	276	SER	2.5
1	C	279	LEU	2.5
1	C	252	SER	2.4
1	A	280	GLU	2.4
1	A	272	MET	2.4
1	B	254	VAL	2.4
1	B	258	VAL	2.4
1	A	279	LEU	2.4
1	B	260	PRO	2.4
1	A	282	ASN	2.4
1	C	377	PRO	2.4
1	C	289	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	268	LYS	2.3
1	A	253	TYR	2.3
1	A	268	LYS	2.3
1	A	264	ASN	2.3
1	B	267	THR	2.3
1	C	264	ASN	2.3
1	B	289	VAL	2.2
1	B	448	VAL	2.2
1	C	276	SER	2.2
1	A	275	ASP	2.2
1	A	247	GLY	2.2
1	C	278	THR	2.2
1	C	288	THR	2.2
1	B	266	SER	2.2
1	B	449	SER	2.2
1	C	244	SER	2.2
1	B	246	ILE	2.2
1	A	255	ALA	2.2
1	C	248	ALA	2.2
1	B	253	TYR	2.1
1	A	455	THR	2.1
1	B	277	SER	2.1
1	C	280	GLU	2.1
1	C	270	LEU	2.1
1	A	278	THR	2.1
1	C	286	GLN	2.1
1	B	396	ALA	2.1
1	C	275	ASP	2.0
1	C	165	VAL	2.0
1	B	394	TYR	2.0
1	B	264	ASN	2.0

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

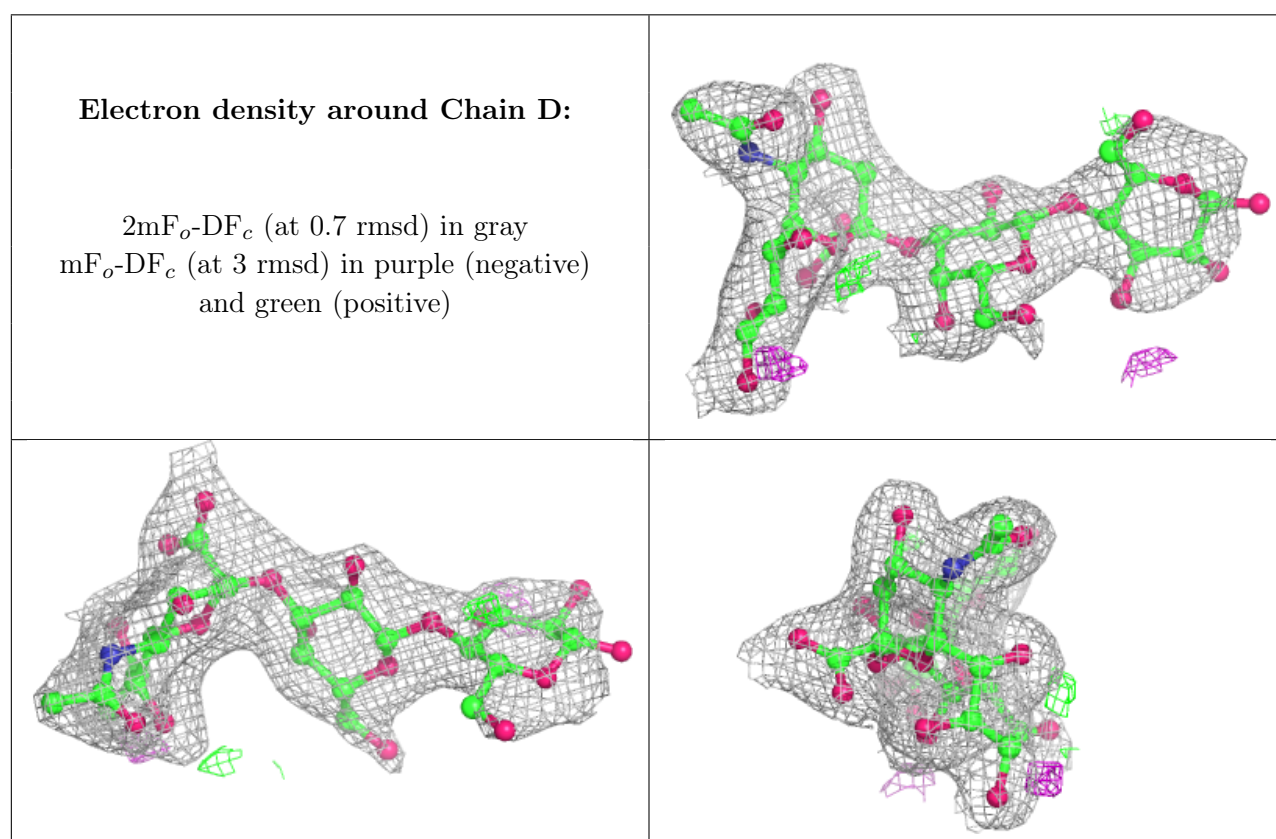
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

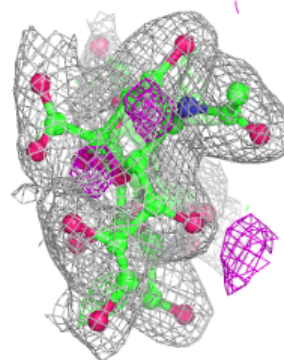
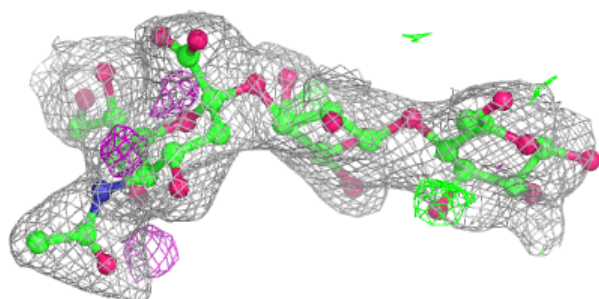
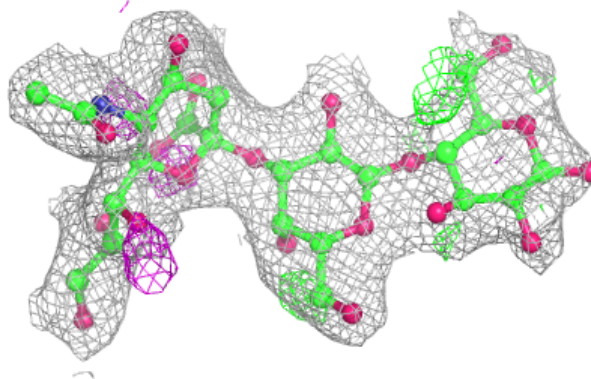
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BGC	E	1	12/12	0.84	0.23	95,113,120,121	0
2	BGC	D	1	12/12	0.86	0.34	95,111,120,124	0
2	BGC	F	1	12/12	0.89	0.33	80,94,104,108	0
2	GAL	D	2	11/12	0.90	0.14	54,72,83,85	0
2	SIA	E	3	20/21	0.93	0.10	39,51,68,74	0
2	GAL	F	2	11/12	0.93	0.17	50,73,83,85	0
2	SIA	F	3	20/21	0.94	0.12	37,55,65,66	0
2	SIA	D	3	20/21	0.95	0.09	33,50,65,67	0
2	GAL	E	2	11/12	0.96	0.10	59,60,69,71	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.

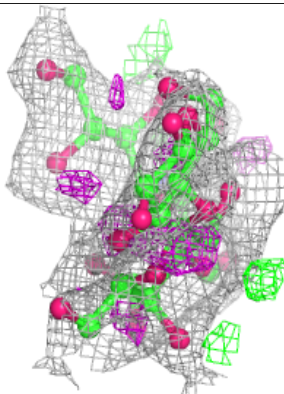
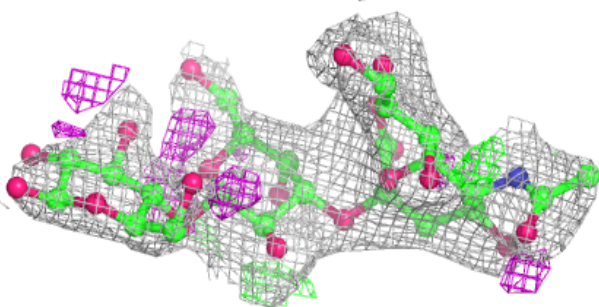
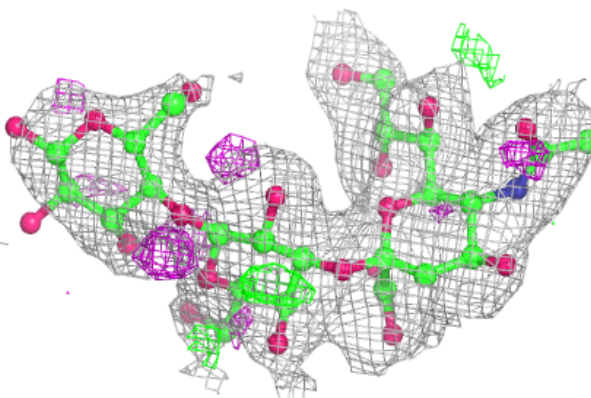


Electron density around Chain E:

$2mF_o-DF_c$ (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)



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.