



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2020 – 09:14 PM BST

PDB ID : 6VU6
Title : Sialic acid binding region of Streptococcus Sanguinis SK1 adhesin bound to 3'sLn
Authors : Stubbs, H.E.; Iverson, T.M.
Deposited on : 2020-02-14
Resolution : 2.10 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 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 : 2.14.6
buster-report : 1.1.7 (2018)
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) : 2.14.6

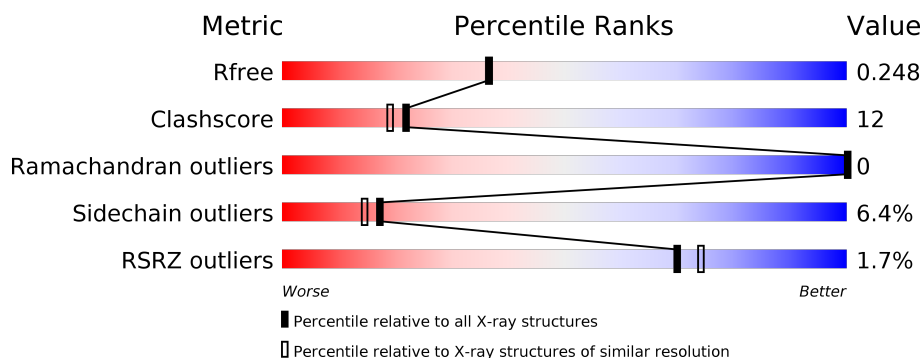
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	409	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>.</div> </div> </div>
1	E	409	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>.</div> </div> </div>
2	B	3	<div> <div></div> <div> <div>33%</div> <div>67%</div> </div> </div>
2	C	3	<div> <div></div> <div> <div>33%</div> <div>33%</div> <div>33%</div> </div> </div>
2	D	3	<div> <div></div> <div> <div>33%</div> <div>67%</div> </div> </div>
2	F	3	<div> <div></div> <div> <div>33%</div> <div>33%</div> <div>33%</div> </div> </div>

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	SIA	D	3	-	-	X	-

2 Entry composition [i](#)

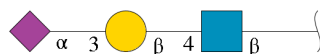
There are 4 unique types of molecules in this entry. The entry contains 6792 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adhesin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	0	0	0
			3136	1947	545	644			
1	E	409	Total	C	N	O	0	1	0
			3147	1953	549	645			

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			46	25	2	19			
2	C	3	Total	C	N	O	0	0	0
			46	25	2	19			
2	D	3	Total	C	N	O	0	0	0
			46	25	2	19			
2	F	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		
3	E	4	Total	Ca	0	0
			4	4		

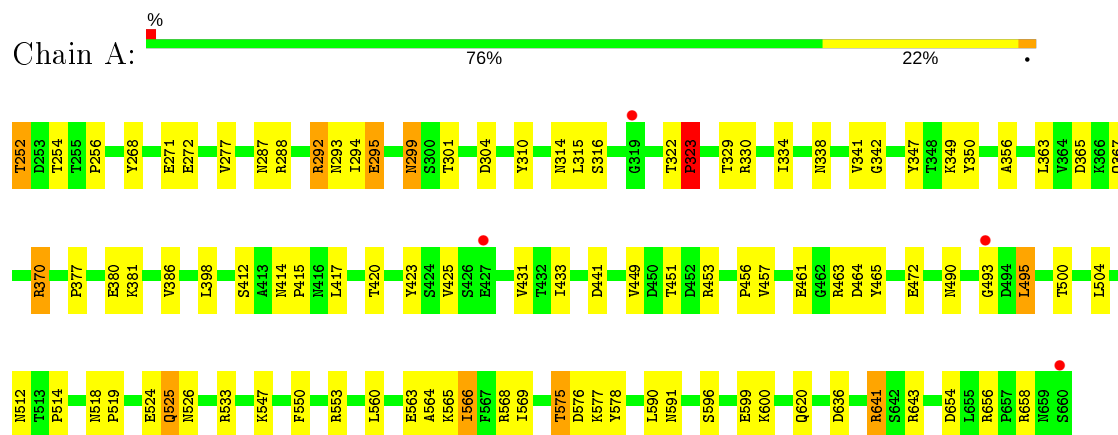
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	174	Total 174	O 174	0	0
4	E	143	Total 143	O 143	0	0

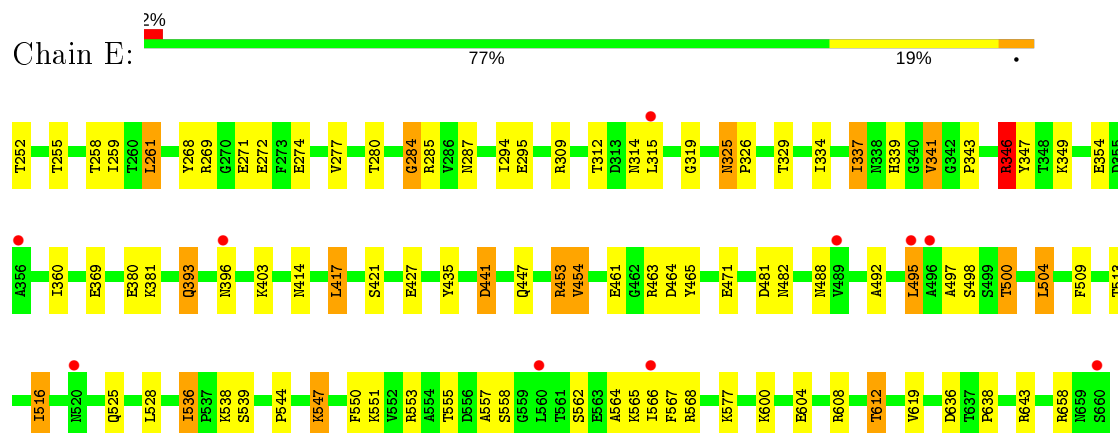
3 Residue-property plots

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: Adhesin




• Molecule 1: Adhesin



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



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

Chain C:  33% 33% 33%

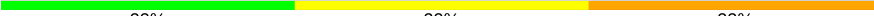


- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  33% 67%



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

Chain F:  33% 33% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.21 Å 269.86 Å 47.51 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.10 – 2.10 45.12 – 2.09	Depositor EDS
% Data completeness (in resolution range)	87.4 (35.10-2.10) 87.4 (45.12-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.08 Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.225 , 0.248 0.225 , 0.248	Depositor DCC
R_{free} test set	2753 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6792	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.72% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GAL, NAG, SIA

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	0.95	9/3199 (0.3%)	0.92	9/4384 (0.2%)
1	E	0.91	7/3210 (0.2%)	0.89	5/4398 (0.1%)
All	All	0.93	16/6409 (0.2%)	0.90	14/8782 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	PRO	N-CA	12.66	1.68	1.47
1	A	575	THR	C-O	-9.09	1.06	1.23
1	A	386	VAL	C-N	8.09	1.49	1.34
1	E	417	LEU	C-N	8.01	1.49	1.34
1	E	255	THR	C-N	7.83	1.49	1.34
1	A	526	ASN	C-N	7.42	1.48	1.34
1	A	342	GLY	C-N	6.93	1.47	1.34
1	A	295	GLU	CD-OE1	-6.25	1.18	1.25
1	E	274	GLU	CD-OE1	-5.92	1.19	1.25
1	E	380	GLU	CD-OE2	-5.70	1.19	1.25
1	A	563	GLU	CD-OE1	-5.50	1.19	1.25
1	A	256	PRO	C-O	-5.30	1.12	1.23
1	A	322	THR	C-N	5.19	1.44	1.34
1	E	295	GLU	CD-OE1	-5.13	1.20	1.25
1	E	284	GLY	C-O	-5.08	1.15	1.23
1	E	343	PRO	C-O	-5.05	1.13	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	342	GLY	O-C-N	-7.39	107.06	121.10
1	A	370	ARG	CG-CD-NE	-6.95	97.20	111.80
1	A	370	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	E	346	ARG	CG-CD-NE	6.38	125.21	111.80
1	E	453	ARG	CB-CG-CD	6.03	127.28	111.60
1	A	620	GLN	CB-CA-C	5.88	122.15	110.40
1	E	658	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	323	PRO	CA-N-CD	-5.59	103.68	111.50
1	A	415	PRO	N-CA-CB	-5.46	96.59	102.60
1	E	325	ASN	CB-CA-C	5.42	121.23	110.40
1	E	284	GLY	C-N-CA	5.28	134.91	121.70
1	A	295	GLU	CB-CA-C	-5.26	99.88	110.40
1	A	453	ARG	CB-CG-CD	-5.12	98.29	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	285	ARG	Mainchain

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	3136	0	3044	74	1
1	E	3147	0	3056	75	1
2	B	46	0	40	2	0
2	C	46	0	40	1	0
2	D	46	0	40	10	0
2	F	46	0	40	1	0
3	A	4	0	0	0	0
3	E	4	0	0	0	0
4	A	174	0	0	26	0
4	E	143	0	0	19	0
All	All	6792	0	6260	150	1

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 12.

All (150) 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:A:323:PRO:CA	1:A:323:PRO:N	1.68	1.37
1:A:338:ASN:HB2	4:A:804:HOH:O	1.25	1.35
1:A:457:VAL:HA	4:A:801:HOH:O	1.29	1.30
1:E:500:THR:HG22	2:D:3:SIA:C9	1.71	1.19
1:E:309:ARG:CG	4:E:803:HOH:O	1.96	1.13
1:A:461:GLU:CD	1:A:565:LYS:HE2	1.71	1.11
1:E:500:THR:HG22	2:D:3:SIA:H91	1.15	1.11
1:A:461:GLU:CG	1:A:565:LYS:HE2	1.83	1.08
1:A:599:GLU:N	4:A:802:HOH:O	1.88	1.06
1:A:512:ASN:ND2	4:A:803:HOH:O	1.90	1.04
1:A:461:GLU:CD	1:A:565:LYS:CE	2.26	1.04
1:A:461:GLU:HG3	1:A:565:LYS:HE2	1.40	1.00
1:A:461:GLU:OE2	1:A:565:LYS:NZ	1.94	1.00
1:E:309:ARG:NE	4:E:803:HOH:O	1.93	1.00
1:E:309:ARG:HB2	4:E:803:HOH:O	1.60	0.99
1:A:457:VAL:CA	4:A:801:HOH:O	1.95	0.98
1:A:456:PRO:O	4:A:801:HOH:O	1.83	0.95
1:E:604:GLU:OE2	4:E:801:HOH:O	1.88	0.91
1:A:599:GLU:HB2	4:A:802:HOH:O	1.70	0.90
1:A:599:GLU:CA	4:A:802:HOH:O	2.18	0.87
1:A:524:GLU:HG2	1:E:525:GLN:NE2	1.89	0.87
1:A:456:PRO:C	4:A:801:HOH:O	2.13	0.85
1:A:658:ARG:O	4:A:806:HOH:O	1.95	0.85
1:E:369:GLU:OE2	4:E:804:HOH:O	1.97	0.83
1:E:500:THR:CG2	2:D:3:SIA:O9	2.28	0.82
1:A:596:SER:O	4:A:802:HOH:O	1.99	0.80
1:E:453:ARG:HG2	4:E:813:HOH:O	1.82	0.79
1:E:309:ARG:HG3	4:E:803:HOH:O	1.69	0.79
1:E:612:THR:OG1	4:E:805:HOH:O	2.01	0.78
1:E:500:THR:CG2	2:D:3:SIA:C9	2.60	0.78
1:A:524:GLU:HG2	1:E:525:GLN:HE21	1.48	0.78
1:A:461:GLU:CD	1:A:565:LYS:HZ1	1.87	0.77
1:E:604:GLU:OE1	4:E:806:HOH:O	2.02	0.77
1:A:338:ASN:ND2	4:A:804:HOH:O	1.93	0.75
1:E:500:THR:HG22	2:D:3:SIA:O9	1.83	0.75
1:E:435:TYR:OH	1:E:441:ASP:OD2	2.02	0.75
1:A:338:ASN:CB	4:A:804:HOH:O	1.97	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLU:CD	1:A:565:LYS:NZ	2.41	0.72
1:A:576:ASP:OD2	4:A:808:HOH:O	2.08	0.71
1:E:309:ARG:CB	4:E:803:HOH:O	2.10	0.70
1:E:403:LYS:NZ	1:E:427:GLU:OE2	2.25	0.70
1:A:600:LYS:N	4:A:802:HOH:O	2.17	0.70
1:A:367:GLN:O	4:A:809:HOH:O	2.10	0.69
1:A:314:ASN:OD1	4:A:810:HOH:O	2.11	0.69
1:A:288:ARG:NH1	4:A:813:HOH:O	2.23	0.66
1:A:457:VAL:N	4:A:801:HOH:O	2.14	0.66
1:E:312:THR:HB	1:E:315:LEU:HD11	1.78	0.66
1:E:481:ASP:O	4:E:807:HOH:O	2.12	0.65
4:E:802:HOH:O	2:F:2:GAL:O2	1.89	0.65
1:E:500:THR:CG2	2:D:3:SIA:H91	2.09	0.65
1:E:612:THR:CB	4:E:805:HOH:O	2.45	0.64
1:A:599:GLU:OE2	4:A:811:HOH:O	2.15	0.64
1:E:553:ARG:HG2	1:E:562:SER:O	1.97	0.64
1:E:414:ASN:HB3	1:E:417:LEU:HG	1.79	0.64
1:E:325:ASN:ND2	4:E:808:HOH:O	2.18	0.63
1:A:575:THR:C	4:A:807:HOH:O	2.34	0.63
1:A:599:GLU:CB	4:A:802:HOH:O	2.28	0.62
1:E:497:ALA:HB2	1:E:551:LYS:HB2	1.81	0.62
1:E:427:GLU:HA	1:E:427:GLU:OE1	2.02	0.60
1:A:323:PRO:C	1:A:323:PRO:N	2.51	0.59
1:E:284:GLY:O	1:E:319:GLY:HA2	2.04	0.58
1:A:287:ASN:ND2	1:A:356:ALA:HA	2.19	0.56
1:E:547:LYS:NZ	2:D:3:SIA:O1A	2.39	0.56
1:E:259:ILE:HB	1:E:369:GLU:HG2	1.85	0.56
1:E:513:THR:HG22	1:E:528:LEU:HD11	1.87	0.56
1:A:553:ARG:HG2	1:A:564:ALA:HA	1.88	0.54
1:E:271:GLU:OE2	1:E:381:LYS:NZ	2.38	0.54
1:E:497:ALA:CB	1:E:551:LYS:HB2	2.37	0.54
1:E:347:TYR:HB3	1:E:349:LYS:HE2	1.90	0.54
1:E:612:THR:HB	4:E:805:HOH:O	2.05	0.54
1:E:492:ALA:HB1	1:E:498:SER:HB2	1.90	0.53
1:E:550:PHE:HB2	1:E:567:PHE:CE2	2.43	0.53
1:A:654:ASP:OD2	1:A:656:ARG:NH1	2.42	0.53
1:E:509:PHE:HZ	1:E:536:ILE:HD12	1.74	0.53
1:A:272:GLU:HG2	1:A:334:ILE:HG12	1.91	0.52
1:E:461:GLU:HG3	1:E:565:LYS:HB3	1.90	0.52
1:A:641:ARG:NH2	4:A:805:HOH:O	1.95	0.52
1:E:268:TYR:CZ	1:E:381:LYS:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:ASN:O	1:E:315:LEU:HD22	2.10	0.51
1:E:600:LYS:NZ	4:E:822:HOH:O	2.42	0.51
1:A:292:ARG:HD3	1:A:293:ASN:O	2.11	0.51
2:D:2:GAL:H3	2:D:3:SIA:H92	1.93	0.51
1:E:252:THR:HG23	1:E:252:THR:O	2.10	0.51
1:A:461:GLU:OE1	1:A:565:LYS:CE	2.59	0.50
1:E:396:ASN:OD1	4:E:809:HOH:O	2.19	0.50
1:A:512:ASN:CG	4:A:803:HOH:O	2.39	0.50
1:E:463:ARG:HD3	1:E:465:TYR:CZ	2.47	0.50
1:E:500:THR:HG21	2:D:3:SIA:O9	2.10	0.50
1:E:346:ARG:HD3	4:E:907:HOH:O	2.12	0.50
1:A:398:LEU:HD21	1:A:449:VAL:HG11	1.95	0.49
1:E:557:ALA:N	4:E:811:HOH:O	2.25	0.49
1:A:294:ILE:HB	1:A:350:TYR:CE1	2.47	0.49
1:E:272:GLU:HG2	1:E:334:ILE:CG1	2.44	0.48
1:E:454:VAL:HG13	1:E:482:ASN:ND2	2.29	0.48
1:E:471:GLU:OE2	1:E:577:LYS:NZ	2.44	0.47
1:A:566:ILE:H	1:A:566:ILE:HD12	1.80	0.47
1:E:354:GLU:HB2	1:E:360:ILE:HG13	1.96	0.47
1:E:464:ASP:OD1	1:E:568:ARG:NE	2.48	0.46
1:E:550:PHE:HB2	1:E:567:PHE:CZ	2.51	0.46
1:A:636:ASP:OD1	1:A:643:ARG:HD2	2.16	0.46
1:A:463:ARG:HD3	1:A:465:TYR:CZ	2.52	0.45
1:E:312:THR:HB	1:E:315:LEU:CD1	2.46	0.45
1:A:577:LYS:HE2	1:A:578:TYR:CZ	2.50	0.45
1:A:495:LEU:HD22	1:A:495:LEU:HA	1.72	0.45
1:E:551:LYS:NZ	1:E:566:ILE:HG12	2.31	0.45
1:A:514:PRO:HD2	4:A:890:HOH:O	2.15	0.45
1:E:608:ARG:NH2	1:E:619:VAL:O	2.49	0.45
1:E:636:ASP:OD1	1:E:643:ARG:HD2	2.17	0.45
1:A:425:VAL:HG22	1:A:431:VAL:HG22	1.99	0.44
1:E:341:VAL:HG13	1:E:341:VAL:O	2.18	0.44
1:E:551:LYS:HB3	1:E:564:ALA:HB1	1.99	0.44
1:A:590:LEU:HD23	1:A:590:LEU:HA	1.74	0.44
1:E:261:LEU:HD23	1:E:261:LEU:O	2.17	0.44
1:E:337:ILE:HD12	1:E:337:ILE:HA	1.84	0.44
1:A:414:ASN:HB3	1:A:417:LEU:HG	1.99	0.43
1:E:269:ARG:HD3	1:E:339:HIS:O	2.18	0.43
1:A:550:PHE:CE1	1:A:569:ILE:HG13	2.54	0.43
1:A:365:ASP:OD1	2:B:2:GAL:H61	2.18	0.43
1:E:325:ASN:HA	1:E:326:PRO:HD3	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:TYR:CE1	1:A:381:LYS:HB2	2.53	0.43
1:A:423:TYR:CD2	1:A:433:ILE:HG12	2.53	0.43
1:A:654:ASP:OD1	1:A:656:ARG:HD3	2.18	0.43
1:E:277:VAL:HB	1:E:329:THR:HB	2.00	0.42
1:A:299:ASN:HD22	1:A:299:ASN:C	2.22	0.42
1:A:472:GLU:CD	1:A:533:ARG:HE	2.23	0.42
1:E:495:LEU:HD22	1:E:495:LEU:HA	1.74	0.42
1:E:393:GLN:HG3	1:E:558:SER:O	2.19	0.42
1:A:252:THR:O	1:A:254:THR:HG23	2.19	0.42
1:A:271:GLU:OE1	1:A:381:LYS:NZ	2.45	0.42
1:A:377:PRO:HG2	1:A:380:GLU:HG3	2.02	0.42
1:A:518:ASN:HA	1:A:519:PRO:HD3	1.83	0.41
1:A:464:ASP:OD2	1:A:568:ARG:NH2	2.52	0.41
1:A:315:LEU:HB2	4:A:867:HOH:O	2.21	0.41
1:A:547:LYS:NZ	2:C:3:SIA:O1B	2.54	0.41
1:E:504:LEU:HD22	1:E:509:PHE:CD1	2.55	0.41
1:E:551:LYS:HD2	1:E:551:LYS:HA	1.94	0.41
1:A:299:ASN:C	1:A:299:ASN:ND2	2.74	0.41
1:E:284:GLY:O	1:E:319:GLY:CA	2.69	0.41
1:A:277:VAL:HB	1:A:329:THR:HB	2.02	0.41
1:E:268:TYR:CE1	1:E:381:LYS:HB2	2.56	0.41
1:A:347:TYR:HB3	1:A:349:LYS:HE2	2.03	0.41
1:E:488:ASN:HA	1:E:516:ILE:HD11	2.03	0.41
1:E:636:ASP:CG	1:E:643:ARG:HH11	2.24	0.41
1:A:310:TYR:HA	1:A:330:ARG:O	2.21	0.41
2:D:3:SIA:H92	2:D:3:SIA:O6	2.21	0.41
1:A:525:GLN:HB3	1:A:525:GLN:HE21	1.69	0.40
1:A:365:ASP:OD2	2:B:1:NAG:H82	2.20	0.40
1:E:495:LEU:N	1:E:495:LEU:CD2	2.82	0.40
1:A:490:ASN:HD21	1:A:493:GLY:HA2	1.85	0.40
1:A:341:VAL:HB	1:A:377:PRO:HD3	2.03	0.40

All (1) 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)
1:A:591:ASN:ND2	1:E:638:PRO:O[2_765]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	407/409 (100%)	395 (97%)	12 (3%)	0	100	100
1	E	408/409 (100%)	398 (98%)	10 (2%)	0	100	100
All	All	815/818 (100%)	793 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/349 (100%)	328 (94%)	21 (6%)	19	16
1	E	350/349 (100%)	326 (93%)	24 (7%)	15	12
All	All	699/698 (100%)	654 (94%)	45 (6%)	17	14

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	THR
1	A	292	ARG
1	A	295	GLU
1	A	299	ASN
1	A	301	THR
1	A	304	ASP
1	A	316	SER
1	A	323	PRO

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Mol	Chain	Res	Type
1	A	363	LEU
1	A	370	ARG
1	A	412	SER
1	A	420	THR
1	A	441	ASP
1	A	451	THR
1	A	495	LEU
1	A	500	THR
1	A	504	LEU
1	A	525	GLN
1	A	560	LEU
1	A	566	ILE
1	A	641	ARG
1	E	258	THR
1	E	261	LEU
1	E	280	THR
1	E	294	ILE
1	E	314	ASN
1	E	337	ILE
1	E	341	VAL
1	E	346	ARG
1	E	393	GLN
1	E	421	SER
1	E	441	ASP
1	E	447	GLN
1	E	454	VAL
1	E	495	LEU
1	E	500	THR
1	E	504	LEU
1	E	516	ILE
1	E	536	ILE
1	E	538	LYS
1	E	539	SER
1	E	544	PRO
1	E	547	LYS
1	E	555	THR
1	E	612	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	ASN

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Mol	Chain	Res	Type
1	A	490	ASN
1	A	525	GLN
1	E	490	ASN
1	E	525	GLN
1	E	526	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

12 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	NAG	B	1	2	15,15,15	0.58	0	21,21,21	0.77	1 (4%)
2	GAL	B	2	2	11,11,12	1.40	1 (9%)	15,15,17	1.65	2 (13%)
2	SIA	B	3	2	17,20,21	0.87	0	21,28,31	1.57	3 (14%)
2	NAG	C	1	2	15,15,15	0.20	0	21,21,21	0.39	0
2	GAL	C	2	2	11,11,12	1.02	1 (9%)	15,15,17	0.98	2 (13%)
2	SIA	C	3	2	17,20,21	0.93	0	21,28,31	1.61	4 (19%)
2	NAG	D	1	2	15,15,15	0.32	0	21,21,21	0.51	0
2	GAL	D	2	2	11,11,12	0.72	0	15,15,17	0.92	1 (6%)
2	SIA	D	3	2	17,20,21	1.29	2 (11%)	21,28,31	1.61	6 (28%)
2	NAG	F	1	2	15,15,15	0.30	0	21,21,21	0.56	0
2	GAL	F	2	2	11,11,12	0.90	0	15,15,17	1.48	3 (20%)
2	SIA	F	3	2	17,20,21	1.08	0	21,28,31	1.57	4 (19%)

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	NAG	B	1	2	-	4/6/26/26	0/1/1/1
2	GAL	B	2	2	-	1/2/19/22	0/1/1/1
2	SIA	B	3	2	-	2/14/34/38	0/1/1/1
2	NAG	C	1	2	-	2/6/26/26	0/1/1/1
2	GAL	C	2	2	-	2/2/19/22	0/1/1/1
2	SIA	C	3	2	-	2/14/34/38	0/1/1/1
2	NAG	D	1	2	-	2/6/26/26	0/1/1/1
2	GAL	D	2	2	-	2/2/19/22	0/1/1/1
2	SIA	D	3	2	-	8/14/34/38	0/1/1/1
2	NAG	F	1	2	-	0/6/26/26	0/1/1/1
2	GAL	F	2	2	-	1/2/19/22	0/1/1/1
2	SIA	F	3	2	-	2/14/34/38	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	GAL	O5-C1	-3.68	1.37	1.43
2	D	3	SIA	C7-C6	3.64	1.57	1.53
2	D	3	SIA	C8-C7	2.64	1.58	1.53
2	C	2	GAL	O5-C1	-2.31	1.40	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	GAL	C1-O5-C5	3.77	117.30	112.19
2	B	2	GAL	O5-C5-C6	-3.75	101.33	107.20
2	B	3	SIA	O6-C2-C3	-3.63	103.51	109.87
2	B	2	GAL	C1-O5-C5	3.54	116.99	112.19
2	D	3	SIA	C4-C5-N5	-3.43	103.59	110.38
2	C	3	SIA	O6-C2-C3	-3.37	103.96	109.87
2	F	3	SIA	O6-C2-C3	-3.08	104.47	109.87
2	B	3	SIA	C3-C2-C1	2.95	118.36	111.93
2	F	3	SIA	C3-C2-C1	2.78	118.00	111.93
2	C	3	SIA	C5-N5-C10	2.75	129.86	123.18
2	C	3	SIA	C4-C5-N5	-2.67	105.10	110.38
2	D	3	SIA	O8-C8-C7	2.66	115.56	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	2.63	118.62	113.66
2	F	3	SIA	O9-C9-C8	-2.63	105.35	111.07
2	D	3	SIA	O6-C2-C3	-2.47	105.54	109.87
2	D	3	SIA	C5-N5-C10	2.42	129.07	123.18
2	F	3	SIA	C4-C3-C2	2.41	114.13	109.81
2	C	2	GAL	O2-C2-C3	-2.38	105.37	110.14
2	D	3	SIA	C6-O6-C2	2.38	116.42	111.34
2	C	3	SIA	C6-O6-C2	2.21	116.07	111.34
2	D	3	SIA	O7-C7-C8	2.20	114.12	108.81
2	D	2	GAL	C1-O5-C5	2.19	115.16	112.19
2	B	3	SIA	C4-C3-C2	2.16	113.68	109.81
2	F	2	GAL	O5-C5-C6	-2.14	103.84	107.20
2	F	2	GAL	C1-C2-C3	2.07	112.20	109.67
2	C	2	GAL	C1-C2-C3	2.02	112.15	109.67

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	SIA	O8-C8-C9-O9
2	D	3	SIA	C6-C7-C8-C9
2	D	3	SIA	O7-C7-C8-C9
2	D	3	SIA	O7-C7-C8-O8
2	D	2	GAL	O5-C5-C6-O6
2	D	3	SIA	O8-C8-C9-O9
2	B	3	SIA	C7-C8-C9-O9
2	B	1	NAG	C4-C5-C6-O6
2	D	2	GAL	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	C	2	GAL	C4-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	C	3	SIA	C11-C10-N5-C5
2	C	3	SIA	O10-C10-N5-C5
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	3	SIA	C11-C10-N5-C5
2	D	3	SIA	O10-C10-N5-C5
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	C	2	GAL	O5-C5-C6-O6
2	F	3	SIA	C7-C8-C9-O9

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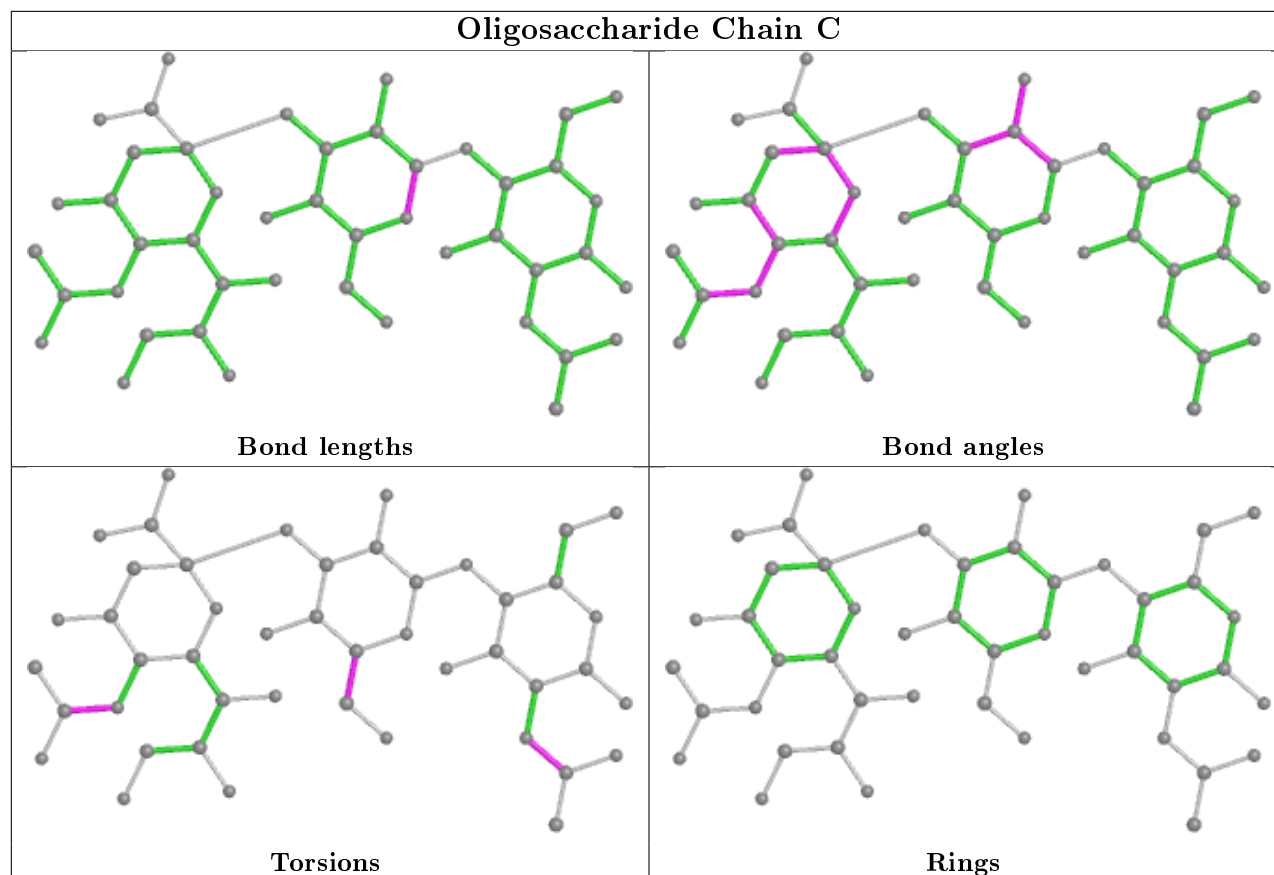
Mol	Chain	Res	Type	Atoms
2	D	3	SIA	C6-C7-C8-O8
2	D	3	SIA	C7-C8-C9-O9
2	B	2	GAL	O5-C5-C6-O6
2	F	3	SIA	O8-C8-C9-O9
2	F	2	GAL	C4-C5-C6-O6

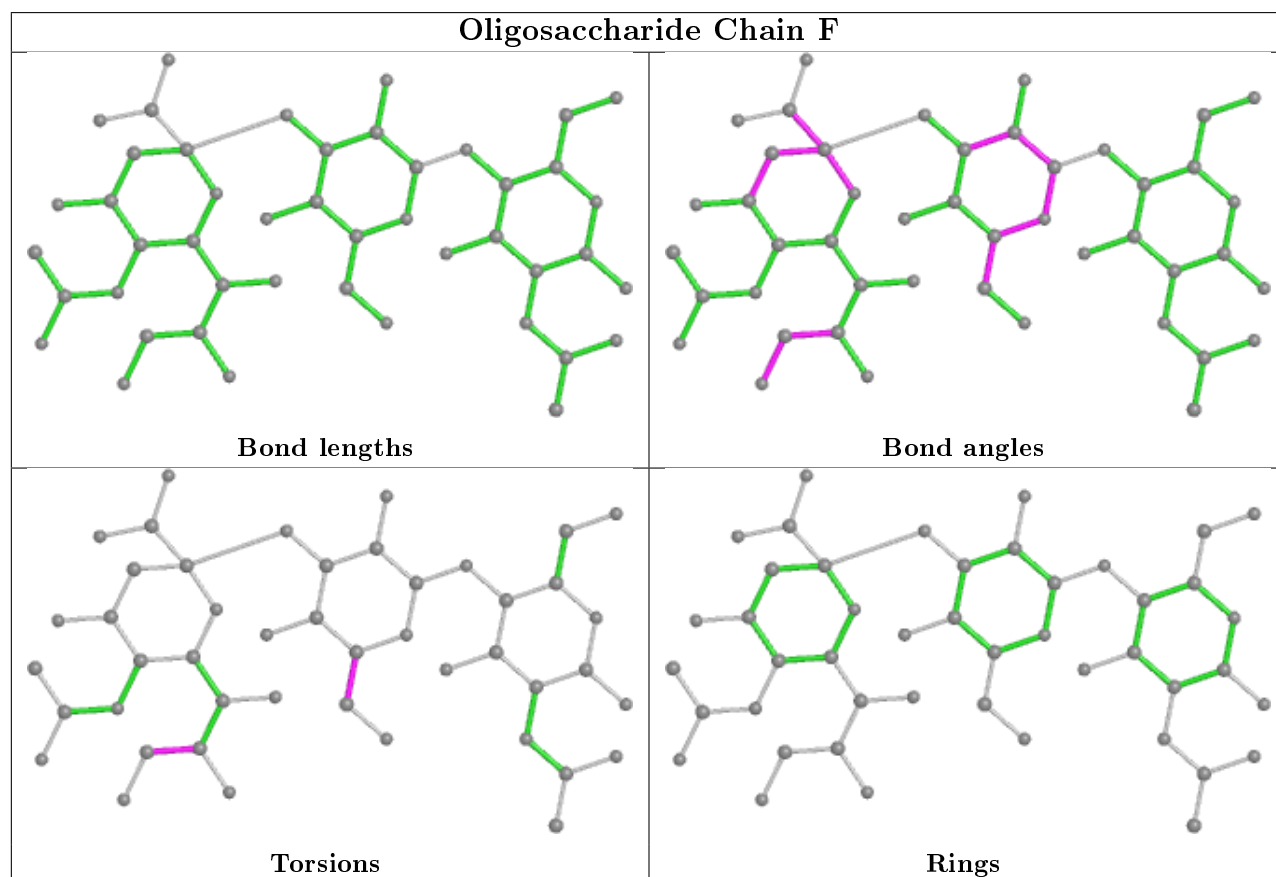
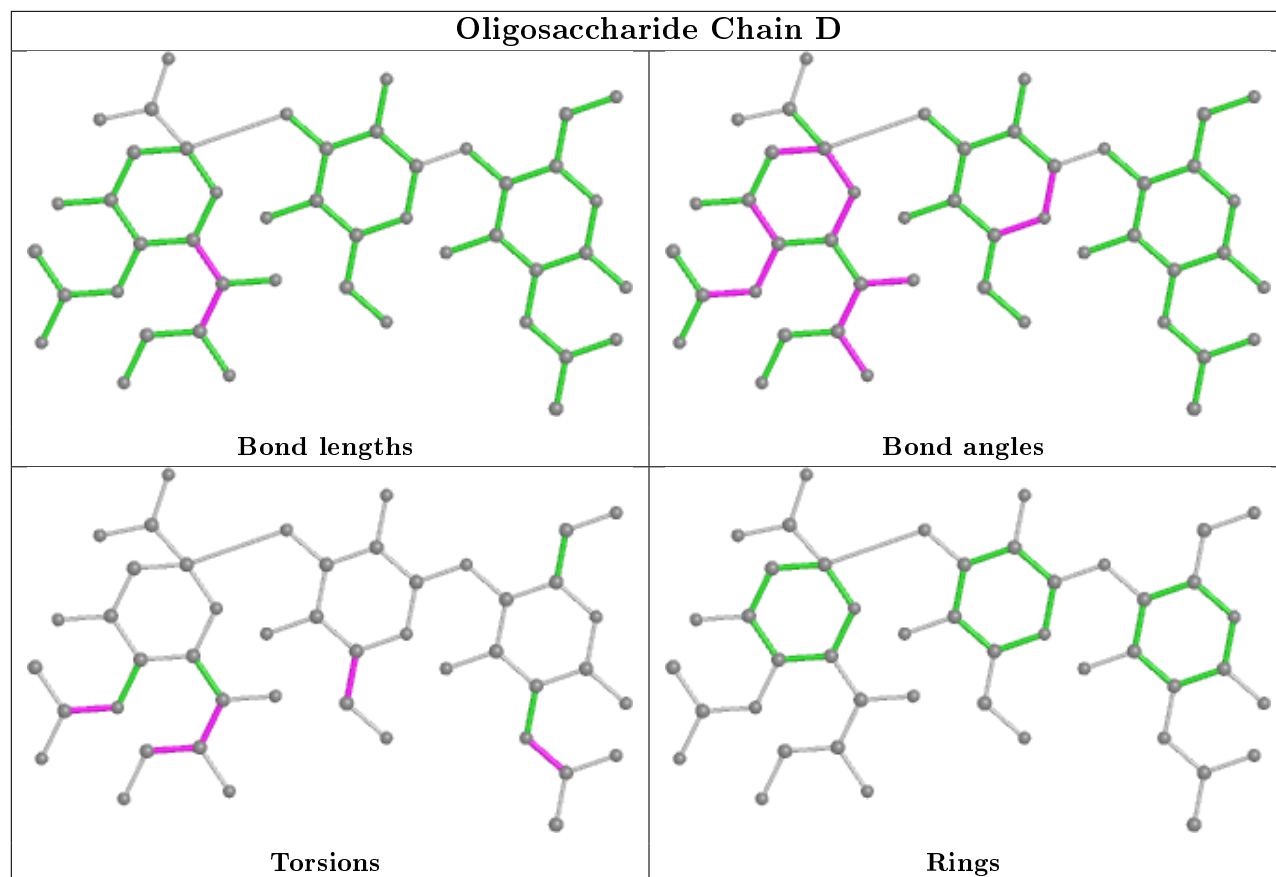
There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	GAL	1	0
2	B	1	NAG	1	0
2	B	2	GAL	1	0
2	C	3	SIA	1	0
2	D	3	SIA	10	0
2	D	2	GAL	1	0

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





5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	409/409 (100%)	0.31	4 (0%) 82 85	21, 35, 50, 65	0
1	E	409/409 (100%)	0.35	10 (2%) 59 64	20, 36, 52, 68	0
All	All	818/818 (100%)	0.33	14 (1%) 70 74	20, 36, 52, 68	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	520	ASN	2.6
1	E	495	LEU	2.5
1	A	493	GLY	2.5
1	E	660	SER	2.4
1	A	319	GLY	2.3
1	E	356	ALA	2.2
1	E	315	LEU	2.1
1	E	396	ASN	2.1
1	E	496	ALA	2.1
1	A	427	GLU	2.1
1	A	660	SER	2.0
1	E	560	LEU	2.0
1	E	566	ILE	2.0
1	E	489	VAL	2.0

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

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

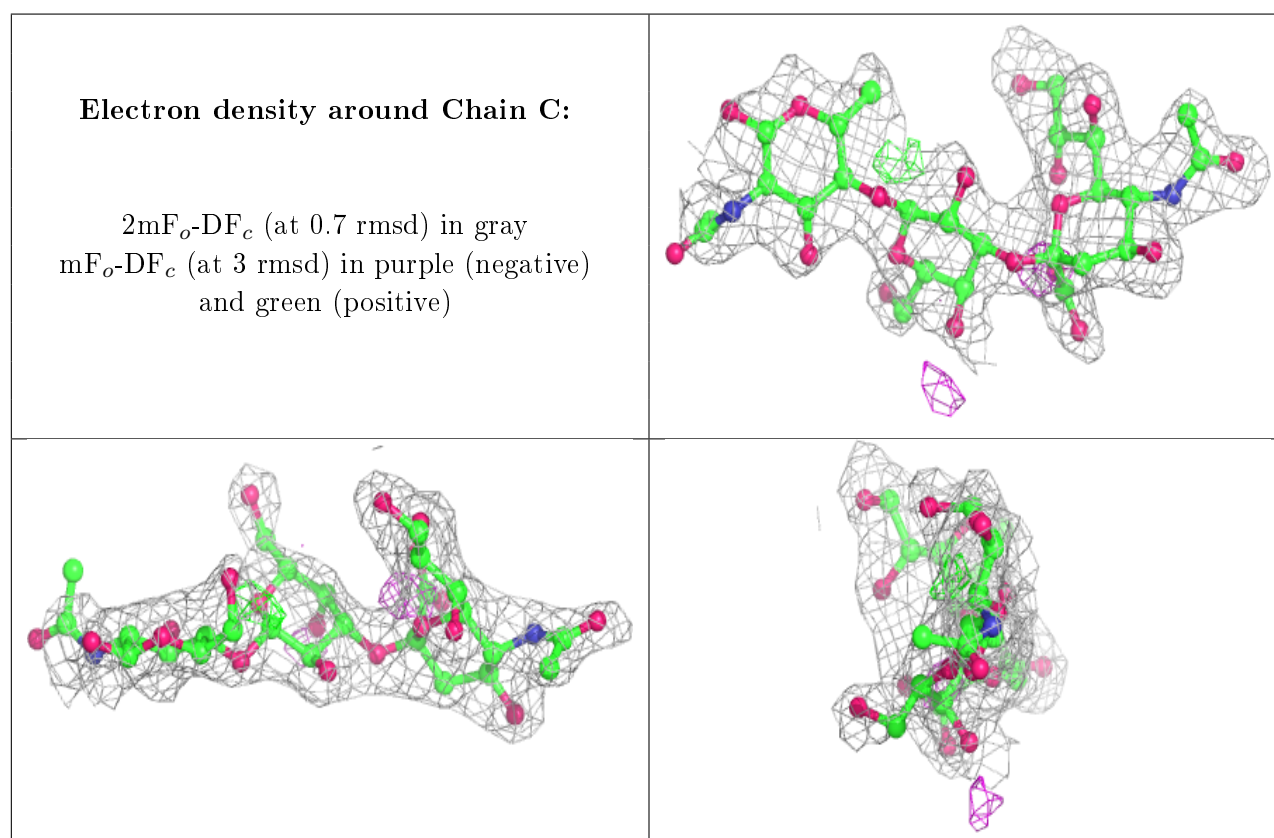
6.3 Carbohydrates ⓘ

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.

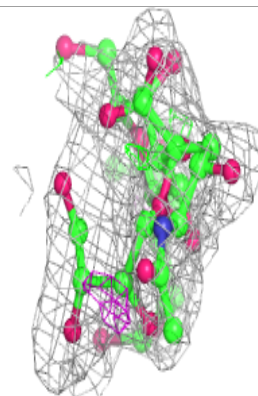
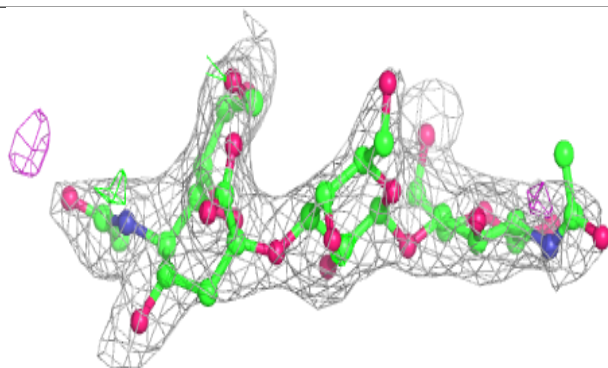
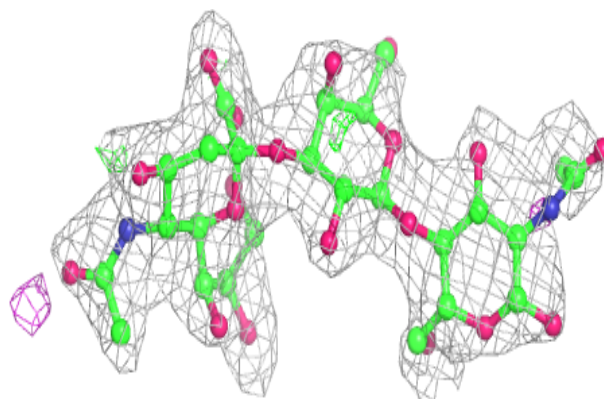
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	1	15/15	0.79	0.22	71,76,79,80	0
2	NAG	C	1	15/15	0.83	0.19	61,70,75,75	0
2	SIA	D	3	20/21	0.84	0.17	47,52,58,59	0
2	GAL	C	2	11/12	0.85	0.18	53,57,60,61	0
2	NAG	B	1	15/15	0.85	0.17	42,57,66,68	0
2	SIA	C	3	20/21	0.86	0.15	42,46,52,55	0
2	NAG	F	1	15/15	0.87	0.18	38,50,59,59	0
2	GAL	D	2	11/12	0.87	0.17	56,66,72,73	0
2	SIA	B	3	20/21	0.92	0.13	23,30,38,42	0
2	GAL	B	2	11/12	0.93	0.14	35,37,41,42	0
2	GAL	F	2	11/12	0.94	0.15	28,33,41,46	0
2	SIA	F	3	20/21	0.94	0.13	21,30,41,48	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.

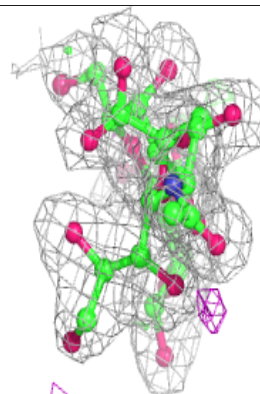
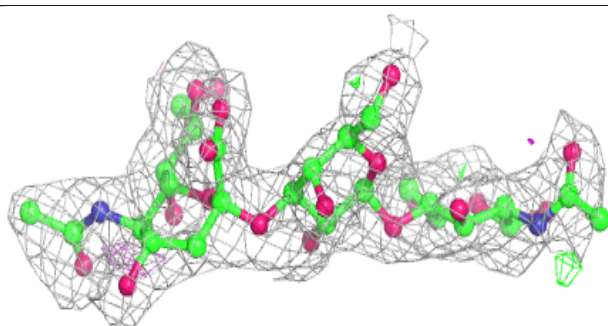
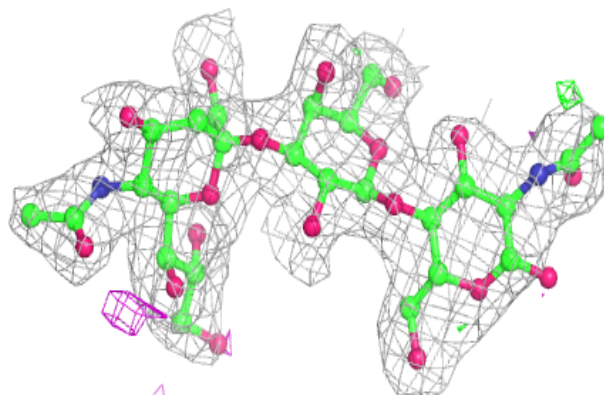


Electron density around Chain D:

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

**Electron density around Chain 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

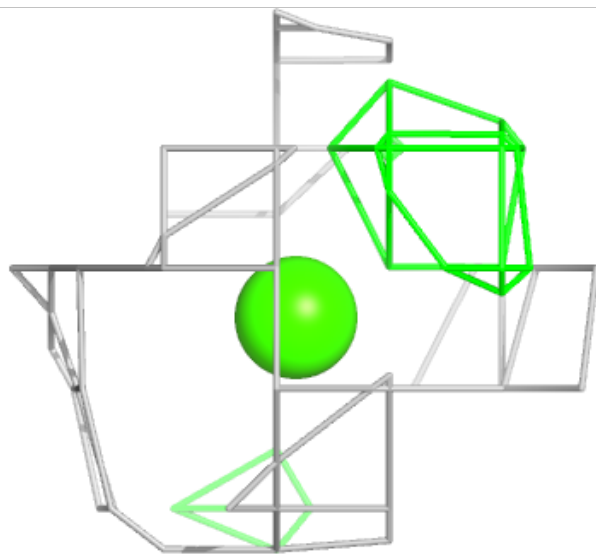
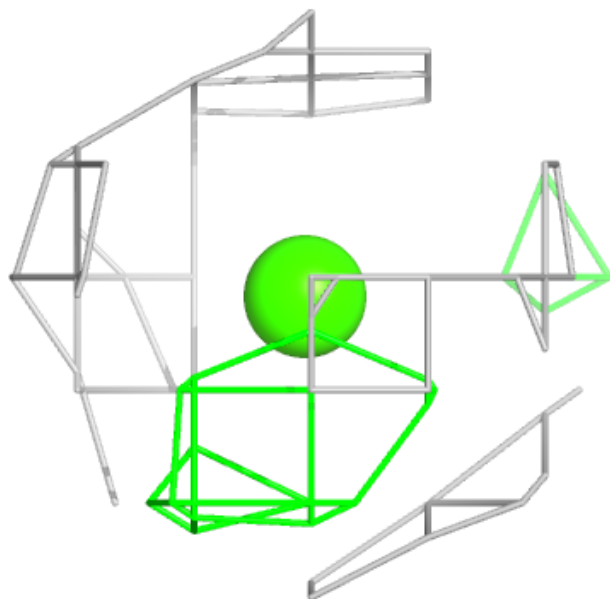
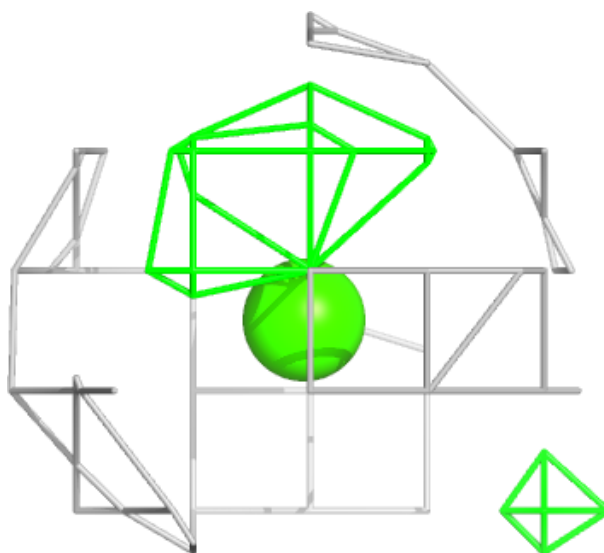
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	A	701	1/1	0.89	0.09	39,39,39,39	0
3	CA	E	702	1/1	0.90	0.10	47,47,47,47	0
3	CA	A	702	1/1	0.93	0.10	49,49,49,49	0
3	CA	E	703	1/1	0.93	0.08	38,38,38,38	0
3	CA	A	703	1/1	0.93	0.14	34,34,34,34	0
3	CA	A	704	1/1	0.97	0.07	40,40,40,40	0
3	CA	E	704	1/1	0.98	0.10	37,37,37,37	0
3	CA	E	701	1/1	0.99	0.08	33,33,33,33	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

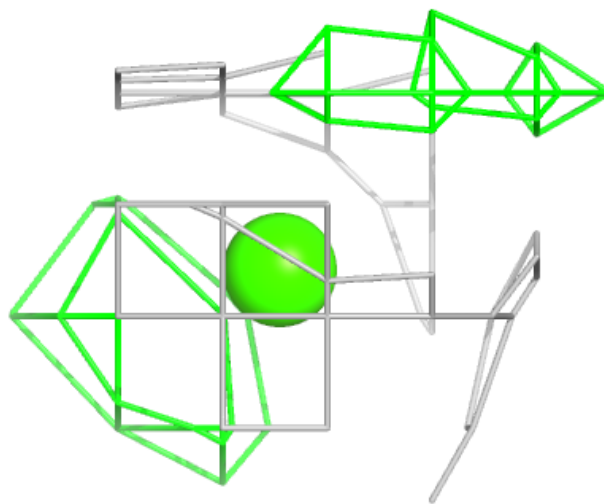
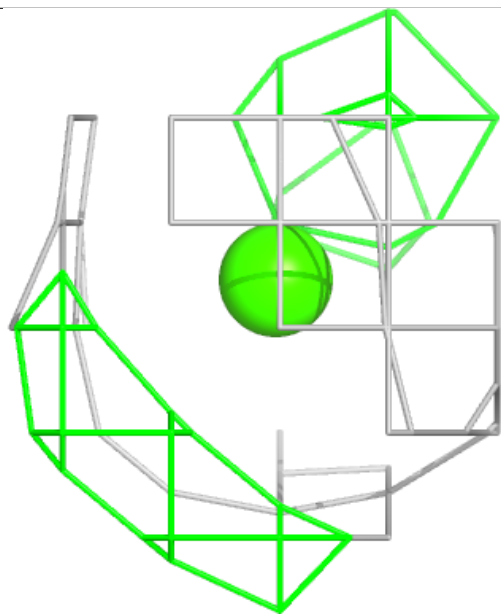
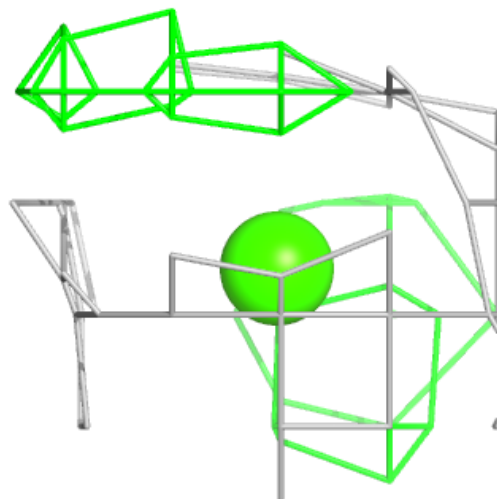
Electron density around CA A 701:

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



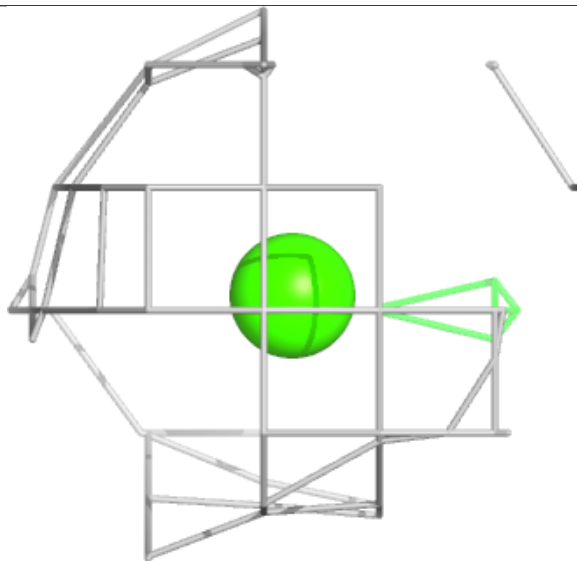
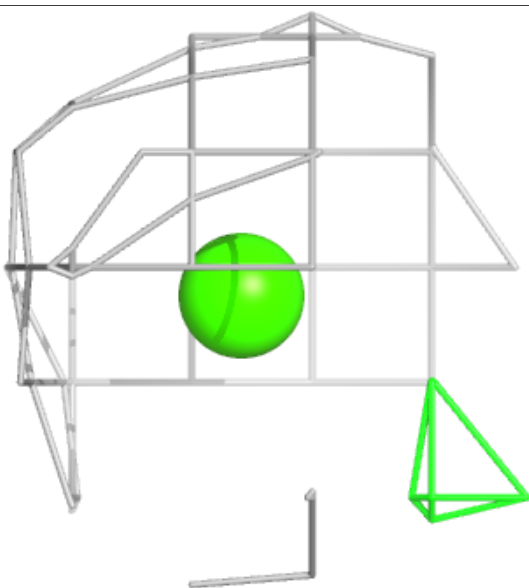
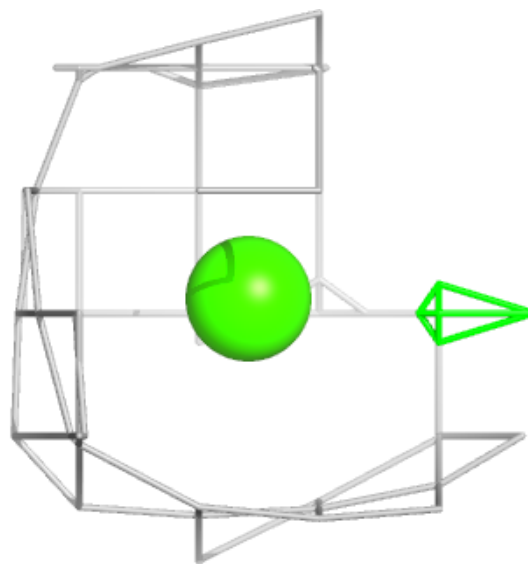
Electron density around CA E 702:

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



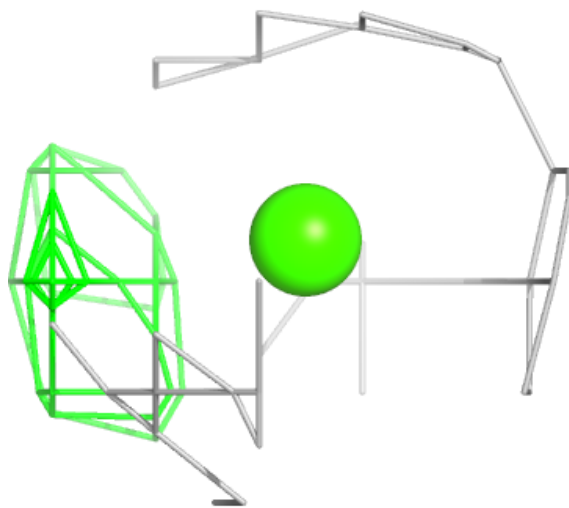
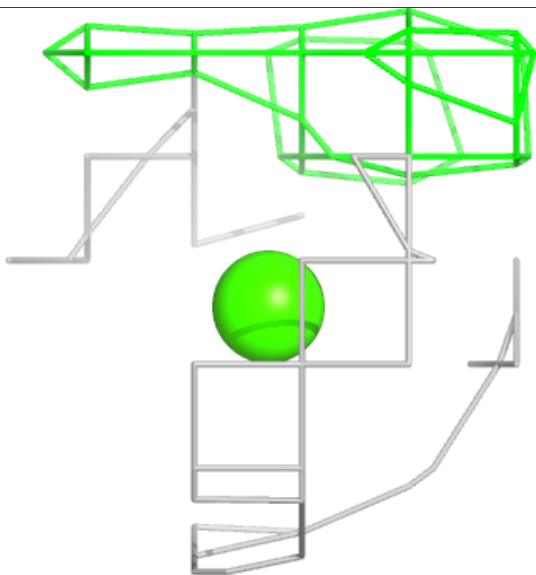
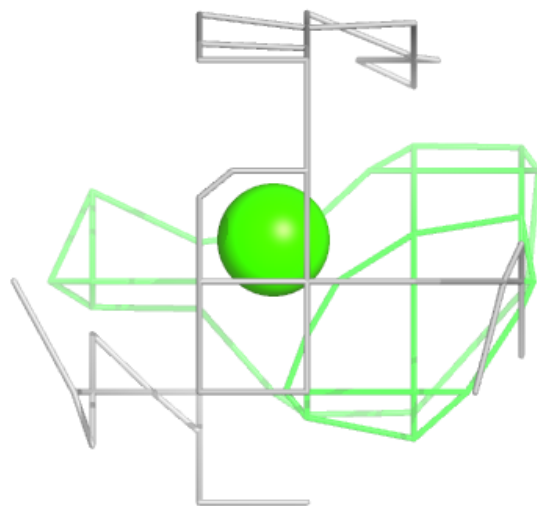
Electron density around CA A 702:

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



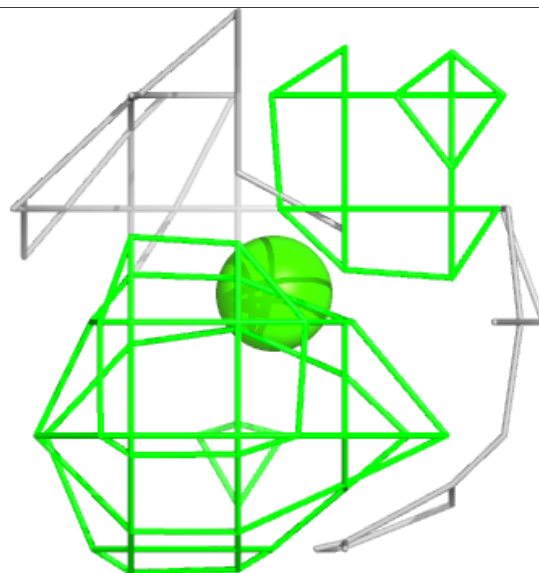
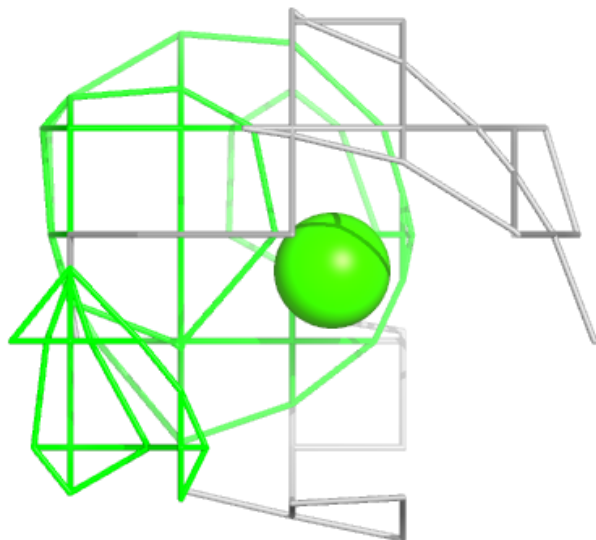
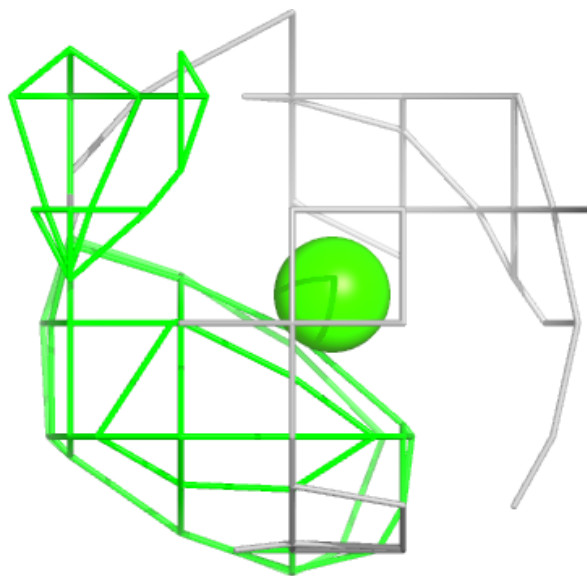
Electron density around CA E 703:

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



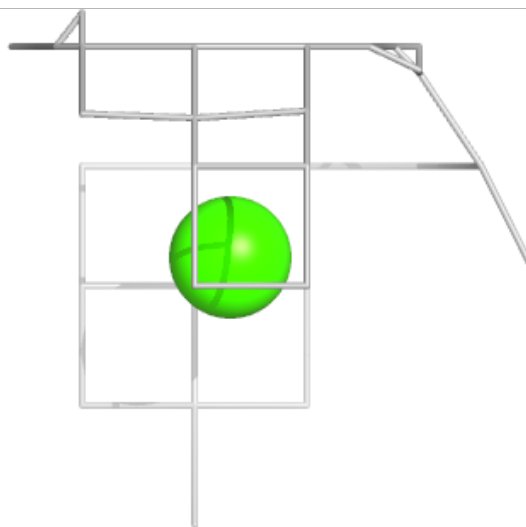
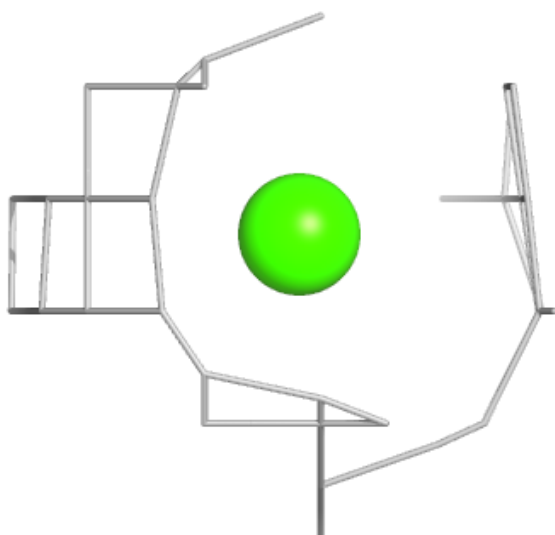
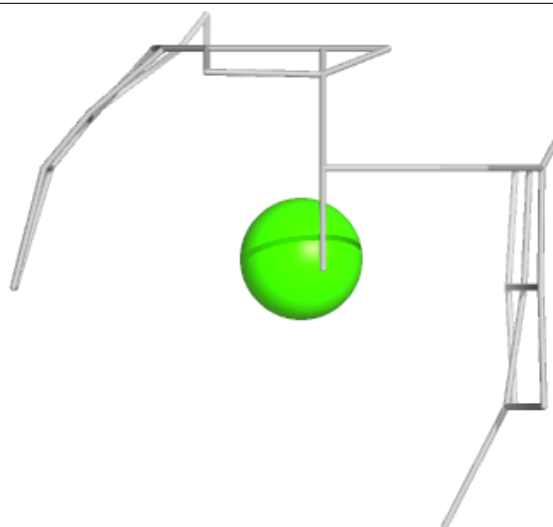
Electron density around CA A 703:

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



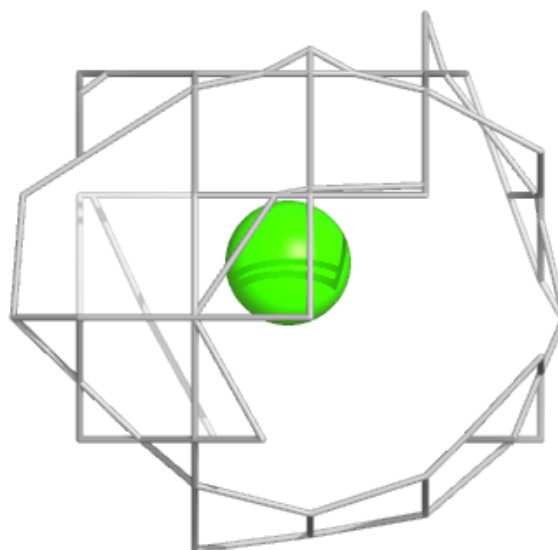
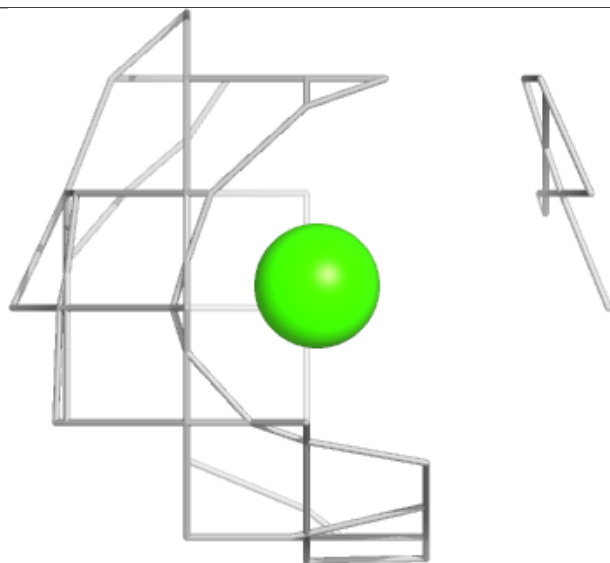
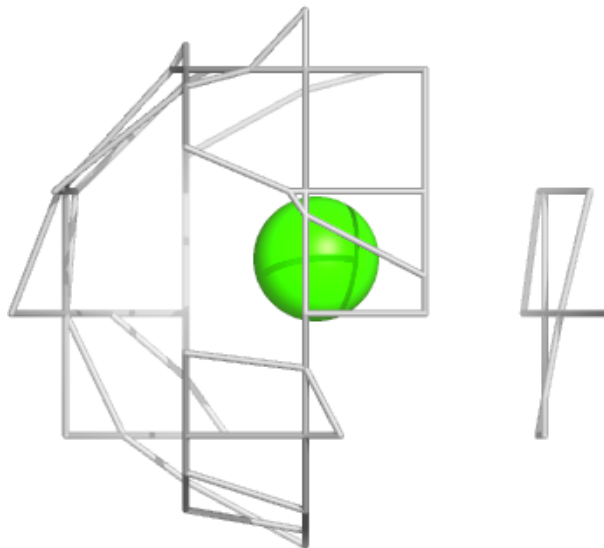
Electron density around CA A 704:

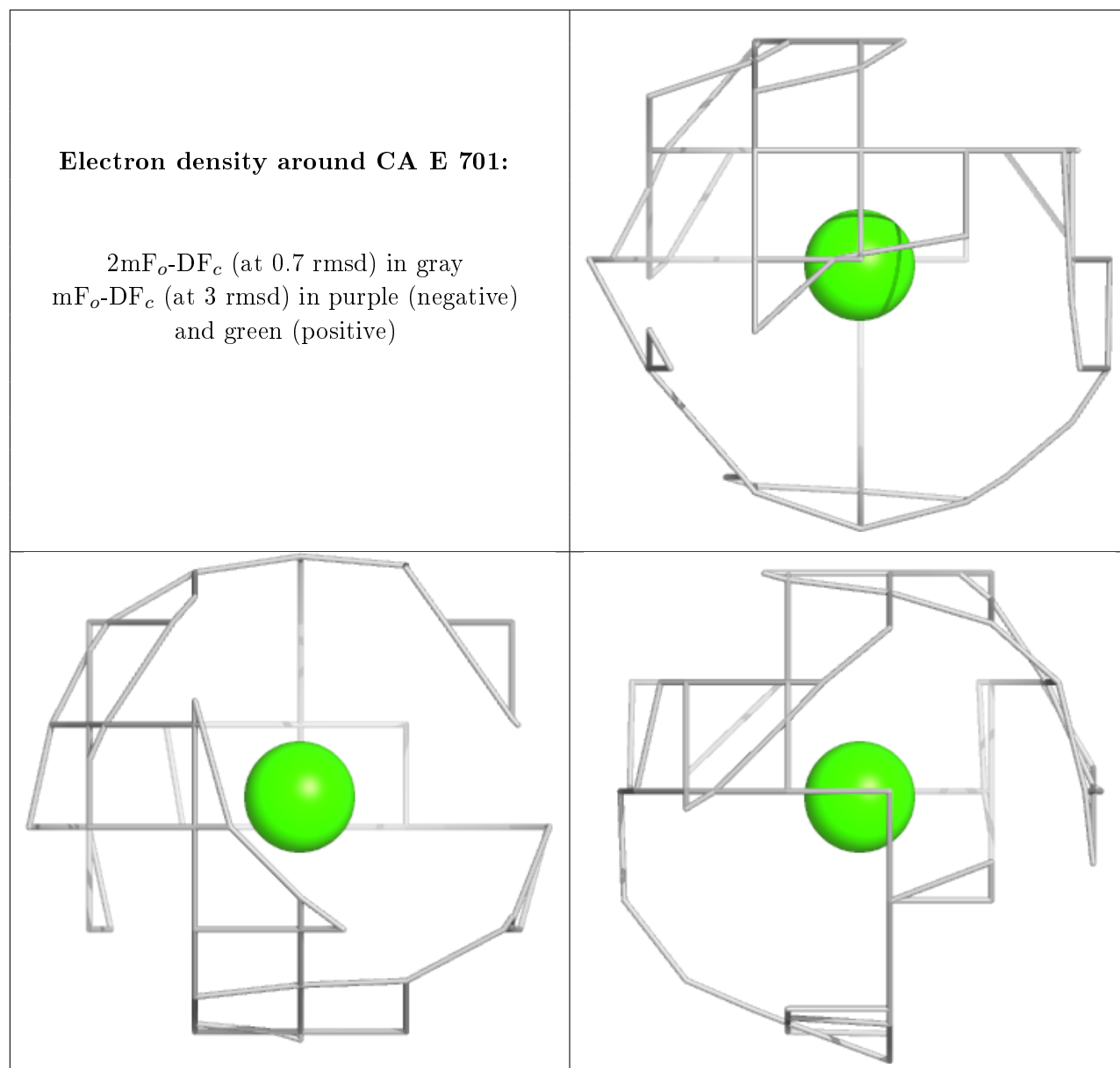
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA E 704:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.