



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:05 AM UTC

PDB ID : 6VU6 / pdb_00006vu6
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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

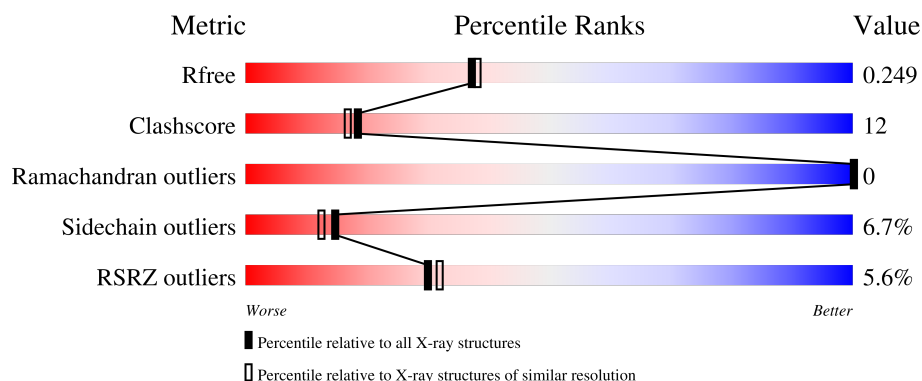
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	409	4% 68% 28% .
1	E	409	7% 71% 23% 6%
2	B	3	33% 67%
2	C	3	33% 33% 33%
2	D	3	33% 67%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	3	

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](#)

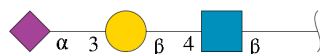
There are 4 unique types of molecules in this entry. The entry contains 6792 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

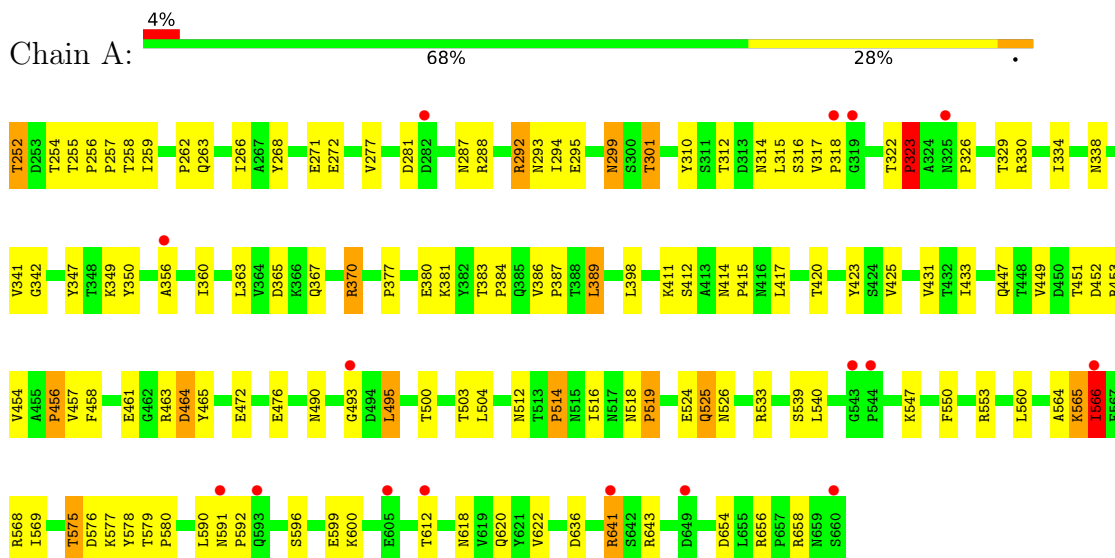
- Molecule 4 is water.

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

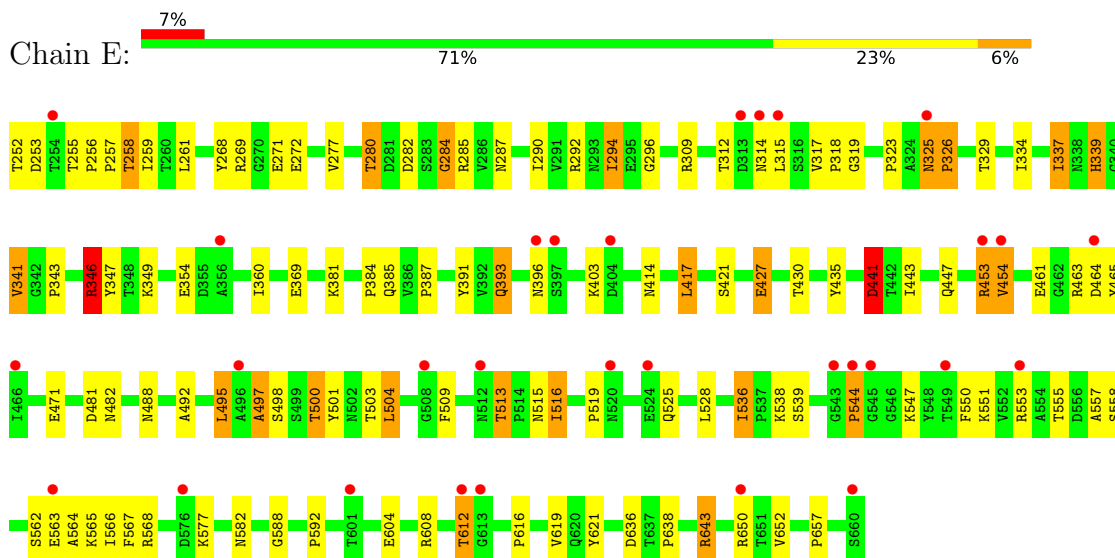
3 Residue-property plots

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

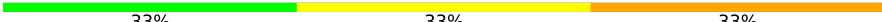


• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  33% 67%

HA01
GAL2
SIA3

- 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%

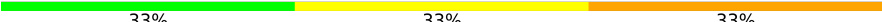
HA01
GAL2
SIA3

- 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%

HA01
GAL2
SIA3

- 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%

HA01
GAL2
SIA3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.21Å 269.86Å 47.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.10 – 2.10 35.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.4 (35.10-2.10) 88.6 (35.10-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.225 , 0.248 0.226 , 0.249	Depositor DCC
R_{free} test set	2753 reflections (3.74%)	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)	0.36 , 43.7	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: SIA, GAL, CA, NAG

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	1.37	40/3199 (1.3%)	1.28	29/4384 (0.7%)
1	E	1.30	34/3210 (1.1%)	1.22	20/4398 (0.5%)
All	All	1.34	74/6409 (1.2%)	1.25	49/8782 (0.6%)

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 (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	PRO	N-CA	16.75	1.68	1.47
1	A	575	THR	C-O	-15.42	1.06	1.24
1	E	255	THR	C-N	13.35	1.49	1.33
1	A	386	VAL	C-N	13.09	1.49	1.33
1	E	417	LEU	C-N	12.20	1.49	1.33
1	A	342	GLY	C-N	11.35	1.47	1.33
1	A	526	ASN	C-N	11.34	1.48	1.33
1	A	256	PRO	C-O	-10.57	1.12	1.24
1	A	454	VAL	C-O	-9.24	1.14	1.24
1	A	592	PRO	C-O	-8.67	1.13	1.24
1	E	343	PRO	C-O	-8.36	1.13	1.24
1	E	657	PRO	C-O	-8.09	1.14	1.23
1	A	580	PRO	C-O	-8.07	1.14	1.23
1	E	257	PRO	C-O	-7.99	1.14	1.23
1	A	318	PRO	C-O	-7.96	1.14	1.23
1	A	456	PRO	C-O	-7.92	1.14	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	THR	C-O	-7.62	1.15	1.24
1	A	383	THR	C-O	-7.40	1.17	1.24
1	A	326	PRO	C-O	-7.37	1.15	1.23
1	E	256	PRO	C-O	-7.29	1.16	1.24
1	E	430	THR	C-O	-7.25	1.15	1.24
1	E	280	THR	C-O	-7.21	1.14	1.23
1	E	294	ILE	C-O	-7.10	1.15	1.24
1	E	592	PRO	C-O	-7.02	1.14	1.24
1	A	476	GLU	C-N	-6.95	1.23	1.33
1	A	281	ASP	C-O	-6.80	1.15	1.23
1	A	262	PRO	C-O	-6.70	1.16	1.23
1	E	284	GLY	C-O	-6.58	1.15	1.24
1	E	497	ALA	C-O	-6.43	1.16	1.24
1	E	339	HIS	C-O	-6.33	1.16	1.23
1	A	257	PRO	C-O	-6.21	1.15	1.23
1	E	519	PRO	C-O	-6.20	1.16	1.23
1	E	616	PRO	C-O	-6.17	1.16	1.23
1	A	618	ASN	C-O	-6.12	1.15	1.24
1	A	312	THR	C-O	-6.03	1.17	1.24
1	E	282	ASP	C-O	-5.94	1.16	1.24
1	A	384	PRO	C-O	-5.93	1.16	1.23
1	E	588	GLY	C-O	-5.92	1.18	1.24
1	A	411	LYS	C-O	-5.89	1.17	1.24
1	E	326	PRO	C-O	-5.84	1.17	1.23
1	E	391	TYR	C-O	-5.79	1.16	1.23
1	A	452	ASP	C-O	-5.78	1.17	1.24
1	A	259	ILE	C-O	-5.66	1.18	1.24
1	A	360	ILE	C-O	-5.66	1.17	1.24
1	A	258	THR	C-O	-5.62	1.17	1.24
1	E	323	PRO	C-O	-5.61	1.17	1.24
1	E	501	TYR	C-O	-5.57	1.17	1.24
1	E	393	GLN	C-O	-5.55	1.17	1.24
1	A	540	LEU	C-O	-5.52	1.17	1.24
1	E	515	ASN	C-O	-5.45	1.16	1.24
1	E	384	PRO	C-O	-5.44	1.17	1.23
1	A	539	SER	C-O	-5.41	1.17	1.24
1	A	622	VAL	C-O	-5.41	1.18	1.24
1	E	255	THR	C-O	-5.39	1.18	1.24
1	A	514	PRO	C-O	-5.36	1.17	1.24
1	A	458	PHE	C-O	-5.35	1.17	1.24
1	E	513	THR	C-O	-5.33	1.18	1.24
1	A	301	THR	C-O	-5.32	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	292	ARG	C-O	-5.25	1.17	1.23
1	E	253	ASP	C-O	-5.20	1.17	1.24
1	E	318	PRO	C-O	-5.20	1.17	1.23
1	A	389	LEU	C-O	-5.18	1.17	1.23
1	E	258	THR	C-O	-5.15	1.17	1.24
1	A	387	PRO	C-O	-5.14	1.17	1.23
1	E	387	PRO	C-O	-5.13	1.17	1.24
1	A	565	LYS	C-O	-5.12	1.17	1.23
1	A	415	PRO	C-O	-5.10	1.18	1.23
1	A	263	GLN	C-O	-5.08	1.17	1.24
1	A	516	ILE	C-O	-5.06	1.17	1.24
1	E	443	ILE	C-O	-5.06	1.18	1.24
1	E	427	GLU	C-O	-5.05	1.17	1.24
1	E	503	THR	C-O	-5.05	1.18	1.24
1	A	266	ILE	C-O	-5.03	1.18	1.24
1	A	519	PRO	C-O	-5.02	1.18	1.23

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	GLY	O-C-N	-14.71	107.06	121.77
1	A	322	THR	CA-C-N	12.81	135.86	119.84
1	A	322	THR	C-N-CA	12.81	135.86	119.84
1	A	526	ASN	CA-C-N	12.51	132.48	119.85
1	A	526	ASN	C-N-CA	12.51	132.48	119.85
1	E	255	THR	O-C-N	-9.63	112.82	121.39
1	E	255	THR	CA-C-N	9.35	130.01	120.38
1	E	255	THR	C-N-CA	9.35	130.01	120.38
1	A	386	VAL	CA-C-N	8.57	130.10	120.85
1	A	386	VAL	C-N-CA	8.57	130.10	120.85
1	E	255	THR	CB-CA-C	-8.35	98.15	109.42
1	A	342	GLY	CA-C-N	8.26	127.98	119.56
1	A	342	GLY	C-N-CA	8.26	127.98	119.56
1	A	452	ASP	CA-CB-CG	-8.12	104.48	112.60
1	E	417	LEU	CA-C-N	7.96	127.96	119.76
1	E	417	LEU	C-N-CA	7.96	127.96	119.76
1	E	284	GLY	CA-C-N	7.90	134.91	122.74
1	E	284	GLY	C-N-CA	7.90	134.91	122.74
1	A	620	GLN	CB-CA-C	7.52	122.15	109.75
1	E	294	ILE	CB-CA-C	-7.52	101.99	112.14
1	E	417	LEU	O-C-N	-7.36	113.28	121.53
1	E	453	ARG	CB-CG-CD	6.95	127.28	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	325	ASN	CB-CA-C	6.88	121.23	110.71
1	A	370	ARG	CG-CD-NE	-6.73	97.20	112.00
1	A	386	VAL	CB-CA-C	-6.47	104.66	111.00
1	E	385	GLN	CB-CA-C	6.44	120.38	109.50
1	A	281	ASP	CA-C-N	6.24	128.93	120.38
1	A	281	ASP	C-N-CA	6.24	128.93	120.38
1	A	386	VAL	O-C-N	-6.22	114.42	121.14
1	E	441	ASP	CA-CB-CG	-6.09	106.51	112.60
1	A	301	THR	CB-CA-C	6.04	120.59	110.44
1	E	346	ARG	CG-CD-NE	6.00	125.21	112.00
1	A	503	THR	CA-C-O	-6.00	114.52	120.82
1	A	301	THR	N-CA-CB	-5.99	101.33	111.27
1	A	323	PRO	CA-N-CD	-5.94	103.68	112.00
1	A	464	ASP	CB-CA-C	-5.80	100.53	110.16
1	E	563	GLU	CB-CA-C	5.72	119.29	109.51
1	E	519	PRO	CB-CA-C	-5.70	103.52	110.98
1	E	294	ILE	N-CA-CB	5.68	118.26	110.54
1	A	453	ARG	CB-CG-CD	-5.66	98.29	111.30
1	A	255	THR	CA-CB-OG1	-5.53	101.30	109.60
1	E	296	GLY	CA-C-O	-5.47	118.51	122.45
1	E	544	PRO	CB-CA-C	-5.40	104.47	113.06
1	A	526	ASN	O-C-N	-5.37	116.54	121.37
1	A	415	PRO	N-CA-CB	-5.32	96.59	102.17
1	A	566	ILE	N-CA-C	5.29	116.20	108.53
1	A	322	THR	O-C-N	-5.24	115.29	121.32
1	A	447	GLN	CB-CA-C	-5.23	100.59	110.01
1	A	612	THR	CB-CA-C	5.13	118.21	109.84

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	75	1
1	E	3147	0	3056	76	1
2	B	46	0	40	2	0
2	C	46	0	40	1	0
2	D	46	0	40	11	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	27	0
4	E	143	0	0	19	0
All	All	6792	0	6260	153	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 (153) 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:N	1:A:323:PRO:CA	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:A:461:GLU:CD	1:A:565:LYS:HE2	1.71	1.16
1:E:309:ARG:CG	4:E:803:HOH:O	1.96	1.13
1:E:500:THR:HG22	2:D:3:SIA:H91	1.15	1.11
1:A:461:GLU:CD	1:A:565:LYS:CE	2.26	1.08
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: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
4:E:802:HOH:O	2:F:2:GAL:O2	1.89	0.90
1:A:599:GLU:HB2	4:A:802:HOH:O	1.70	0.90
1:A:456:PRO:C	4:A:801:HOH:O	2.13	0.88
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:658:ARG:O	4:A:806:HOH:O	1.95	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:GLU:OE2	4:E:804:HOH:O	1.97	0.83
1:A:461:GLU:CD	1:A:565:LYS:HZ1	1.87	0.82
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:E:604:GLU:OE1	4:E:806:HOH:O	2.02	0.77
1:A:461:GLU:CD	1:A:565:LYS:NZ	2.41	0.76
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
1:A:576:ASP:OD2	4:A:808:HOH:O	2.08	0.71
1:A:575:THR:C	4:A:807:HOH:O	2.34	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:323:PRO:N	1:A:323:PRO:C	2.51	0.69
1:A:288:ARG:NH1	4:A:813:HOH:O	2.23	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
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: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:E:284:GLY:O	1:E:319:GLY:HA2	2.04	0.58
1:A:512:ASN:CG	4:A:803:HOH:O	2.39	0.57
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:658:ARG:C	4:A:806:HOH:O	2.50	0.52
1:E:287:ASN:O	1:E:315:LEU:HD22	2.10	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:E:463:ARG:HD3	1:E:465:TYR:CZ	2.47	0.50
1:E:346:ARG:HD3	4:E:907:HOH:O	2.12	0.50
1:E:500:THR:HG21	2:D:3:SIA:O9	2.10	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:471:GLU:OE2	1:E:577:LYS:NZ	2.44	0.48
2:D:3:SIA:O9	2:D:3:SIA:O1B	2.23	0.48
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:A:472:GLU:CD	1:A:533:ARG:HE	2.23	0.47
1:A:299:ASN:C	1:A:299:ASN:HD22	2.22	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:299:ASN:C	1:A:299:ASN:ND2	2.74	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:E:636:ASP:CG	1:E:643:ARG:HH11	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:341:VAL:O	1:E:341:VAL:HG13	2.18	0.44
1:E:261:LEU:O	1:E:261:LEU:HD23	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:E:621:TYR:OH	4:E:810:HOH:O	2.21	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
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:E:393:GLN:HG3	1:E:558:SER:O	2.19	0.42
1:E:495:LEU:HD22	1:E:495:LEU:HA	1.74	0.42
1:E:582:ASN:CG	1:E:650[B]:ARG:HD3	2.45	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:HA	1:E:551:LYS:HD2	1.94	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:A:347:TYR:HB3	1:A:349:LYS:HE2	2.03	0.41
1:A:596:SER:C	4:A:802:HOH:O	2.53	0.41
1:E:268:TYR:CE1	1:E:381:LYS:HB2	2.56	0.41
1:E:488:ASN:HA	1:E:516:ILE:HD11	2.03	0.41
1:A:310:TYR:HA	1:A:330:ARG:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:SIA:H92	2:D:3:SIA:O6	2.21	0.41
1:A:525:GLN:HE21	1:A:525:GLN:HB3	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 [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	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 [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	349/349 (100%)	327 (94%)	22 (6%)	16	14
1	E	350/349 (100%)	325 (93%)	25 (7%)	13	11
All	All	699/698 (100%)	652 (93%)	47 (7%)	15	12

All (47) 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	316	SER
1	A	317	VAL
1	A	323	PRO
1	A	363	LEU
1	A	370	ARG
1	A	389	LEU
1	A	412	SER
1	A	420	THR
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	579	THR
1	A	641	ARG
1	E	258	THR
1	E	280	THR
1	E	290	ILE
1	E	294	ILE
1	E	314	ASN
1	E	317	VAL
1	E	337	ILE
1	E	341	VAL
1	E	346	ARG
1	E	421	SER
1	E	441	ASP
1	E	447	GLN
1	E	454	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	555	THR
1	E	612	THR
1	E	643	ARG
1	E	652	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	ASN
1	A	447	GLN
1	A	490	ASN
1	A	525	GLN
1	E	490	ASN
1	E	515	ASN
1	E	525	GLN
1	E	526	ASN
1	E	617	ASN
1	E	624	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](#)

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	0.59	0	21,21,21	0.76	1 (4%)
2	GAL	B	2	2	11,11,12	1.36	1 (9%)	15,15,17	1.52	2 (13%)
2	SIA	B	3	2	20,20,21	2.28	2 (10%)	21,28,31	1.78	3 (14%)
2	NAG	C	1	2	15,15,15	0.20	0	21,21,21	0.38	0
2	GAL	C	2	2	11,11,12	0.99	1 (9%)	15,15,17	0.92	1 (6%)
2	SIA	C	3	2	20,20,21	1.99	4 (20%)	21,28,31	1.91	4 (19%)
2	NAG	D	1	2	15,15,15	0.31	0	21,21,21	0.51	0
2	GAL	D	2	2	11,11,12	0.71	0	15,15,17	0.88	1 (6%)
2	SIA	D	3	2	20,20,21	2.00	4 (20%)	21,28,31	1.89	7 (33%)
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	0.86	0	15,15,17	1.38	1 (6%)
2	SIA	F	3	2	20,20,21	2.06	3 (15%)	21,28,31	1.60	2 (9%)

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	-	2/18/34/38	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	-	3/18/34/38	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	-	8/18/34/38	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	-	4/18/34/38	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	SIA	C2-C1	9.23	1.63	1.52
2	F	3	SIA	C2-C1	7.53	1.61	1.52
2	C	3	SIA	C2-C1	7.40	1.61	1.52
2	D	3	SIA	C2-C1	6.66	1.60	1.52
2	D	3	SIA	C7-C6	3.74	1.57	1.52
2	B	2	GAL	O5-C1	-3.49	1.37	1.43
2	D	3	SIA	C8-C7	2.87	1.58	1.53
2	F	3	SIA	O6-C2	2.35	1.48	1.43
2	D	3	SIA	O6-C2	2.28	1.48	1.43
2	C	3	SIA	O6-C2	2.25	1.47	1.43
2	B	3	SIA	O6-C2	2.23	1.47	1.43
2	C	2	GAL	O5-C1	-2.19	1.40	1.43
2	F	3	SIA	O1A-C1	2.15	1.28	1.22
2	C	3	SIA	C7-C6	2.05	1.55	1.52
2	C	3	SIA	O1A-C1	2.04	1.28	1.22

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	SIA	O6-C2-C3	-5.24	103.51	110.56
2	C	3	SIA	O6-C2-C3	-4.91	103.96	110.56
2	F	3	SIA	O6-C2-C3	-4.53	104.47	110.56
2	F	2	GAL	C1-O5-C5	3.82	117.30	112.19
2	D	3	SIA	O6-C2-C3	-3.73	105.54	110.56
2	B	2	GAL	C1-O5-C5	3.59	116.99	112.19
2	C	3	SIA	O1A-C1-C2	-3.57	115.13	122.85
2	D	3	SIA	C4-C5-N5	-3.47	103.59	110.44
2	B	2	GAL	O5-C5-C6	-3.25	101.33	107.66
2	C	3	SIA	C5-N5-C10	2.88	129.86	123.11
2	D	3	SIA	O1A-C1-C2	-2.88	116.62	122.85
2	F	3	SIA	O9-C9-C8	-2.76	105.35	111.16
2	C	3	SIA	C4-C5-N5	-2.71	105.10	110.44
2	D	3	SIA	O8-C8-C7	2.70	115.56	109.25
2	B	3	SIA	O6-C2-C1	2.61	112.64	107.72
2	B	1	NAG	C1-O5-C5	2.57	118.62	113.65
2	D	3	SIA	C5-N5-C10	2.55	129.07	123.11
2	D	3	SIA	O6-C2-C1	2.36	112.16	107.72
2	C	2	GAL	O2-C2-C3	-2.31	105.37	110.15
2	D	3	SIA	O7-C7-C8	2.29	114.12	108.93
2	B	3	SIA	O1A-C1-C2	-2.26	117.96	122.85
2	D	2	GAL	C1-O5-C5	2.22	115.16	112.19

There are no chirality outliers.

All (31) 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	3	SIA	O8-C8-C9-O9
2	D	2	GAL	O5-C5-C6-O6
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	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	3	SIA	C11-C10-N5-C5
2	C	3	SIA	O10-C10-N5-C5
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	3	SIA	C11-C10-N5-C5
2	D	3	SIA	O10-C10-N5-C5
2	C	2	GAL	O5-C5-C6-O6
2	F	3	SIA	C7-C8-C9-O9
2	D	3	SIA	C6-C7-C8-O8
2	B	2	GAL	O5-C5-C6-O6
2	D	3	SIA	C7-C8-C9-O9
2	F	3	SIA	O8-C8-C9-O9
2	C	3	SIA	O1A-C1-C2-O6
2	F	3	SIA	O1A-C1-C2-O6
2	F	2	GAL	C4-C5-C6-O6
2	F	3	SIA	C6-C7-C8-O8

There are no ring outliers.

6 monomers are involved in 15 short contacts:

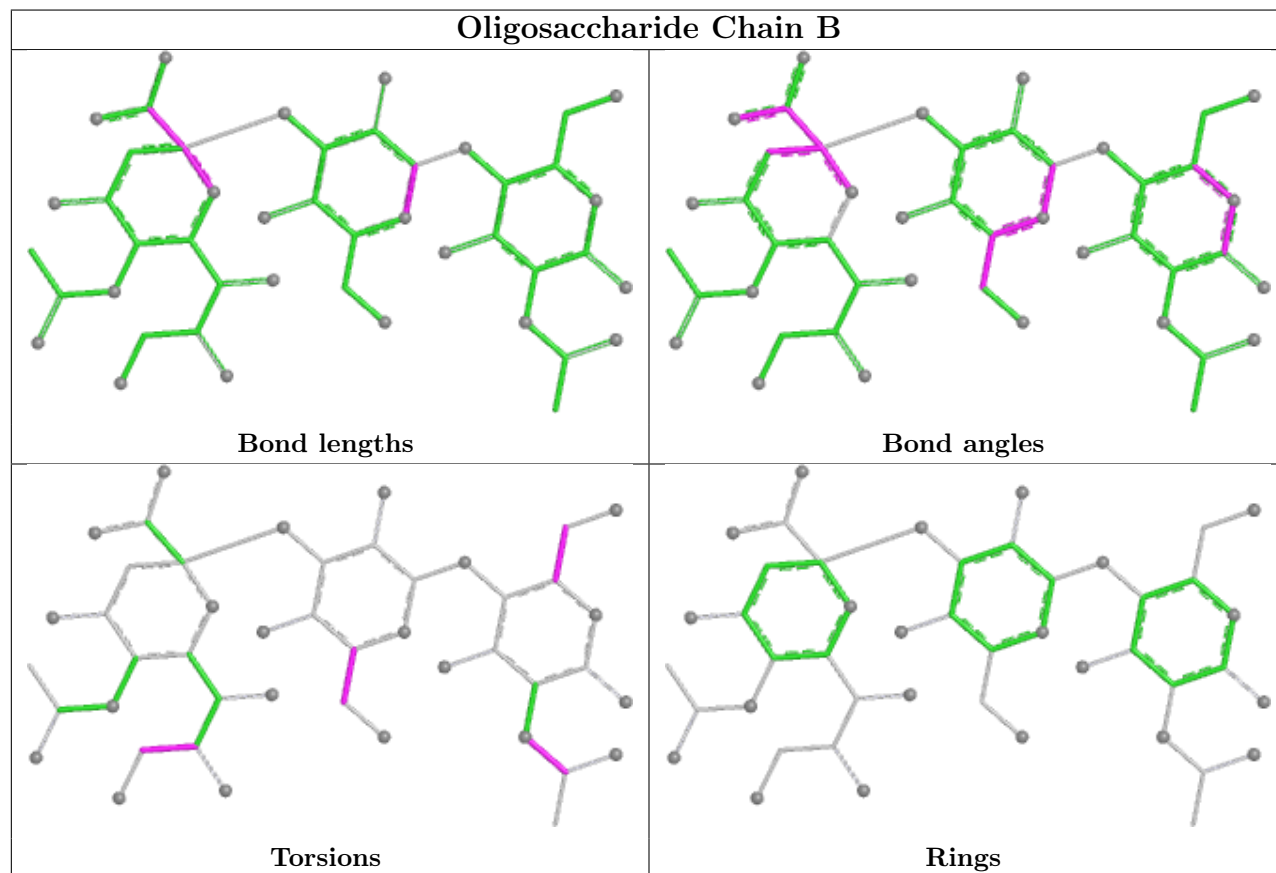
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	GAL	1	0
2	C	3	SIA	1	0
2	B	1	NAG	1	0
2	D	2	GAL	1	0

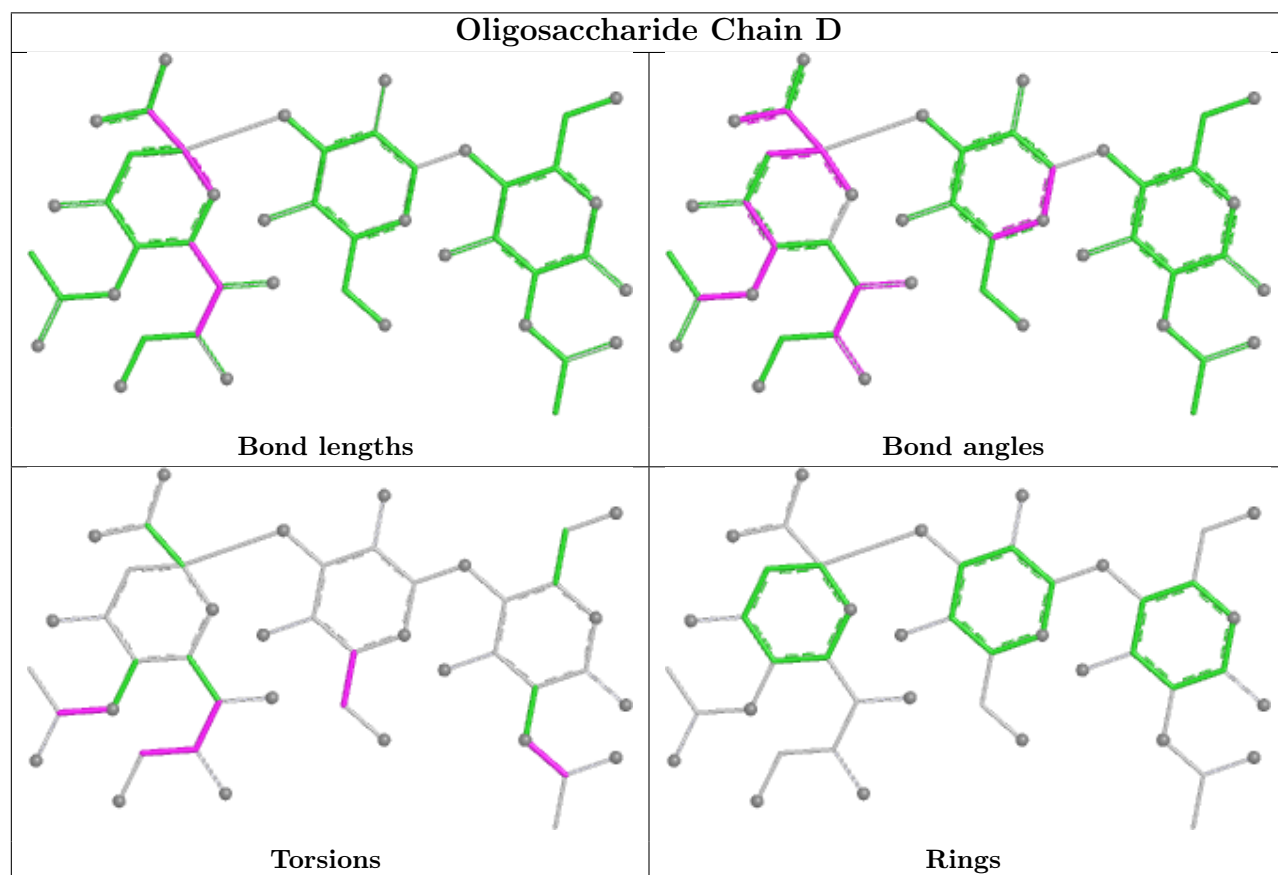
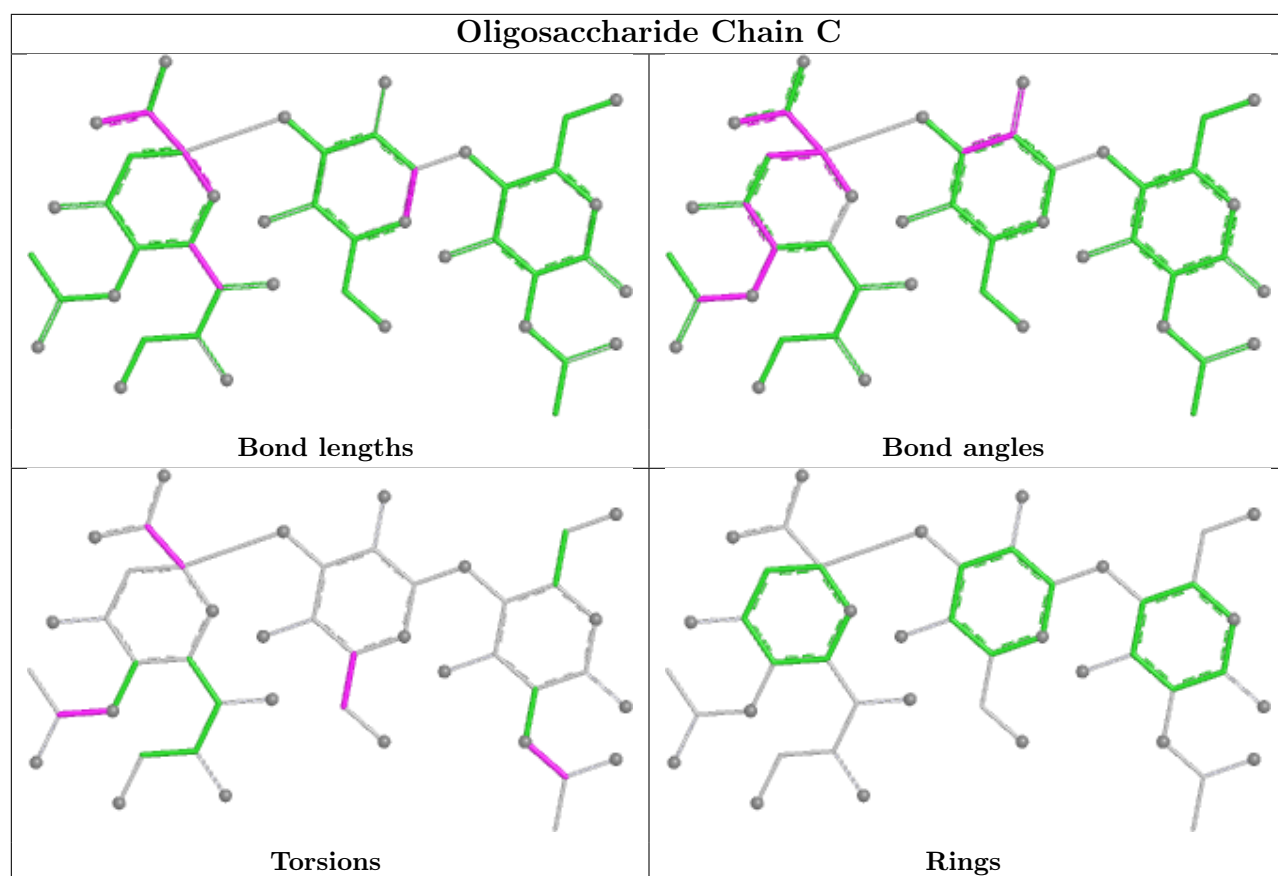
Continued on next page...

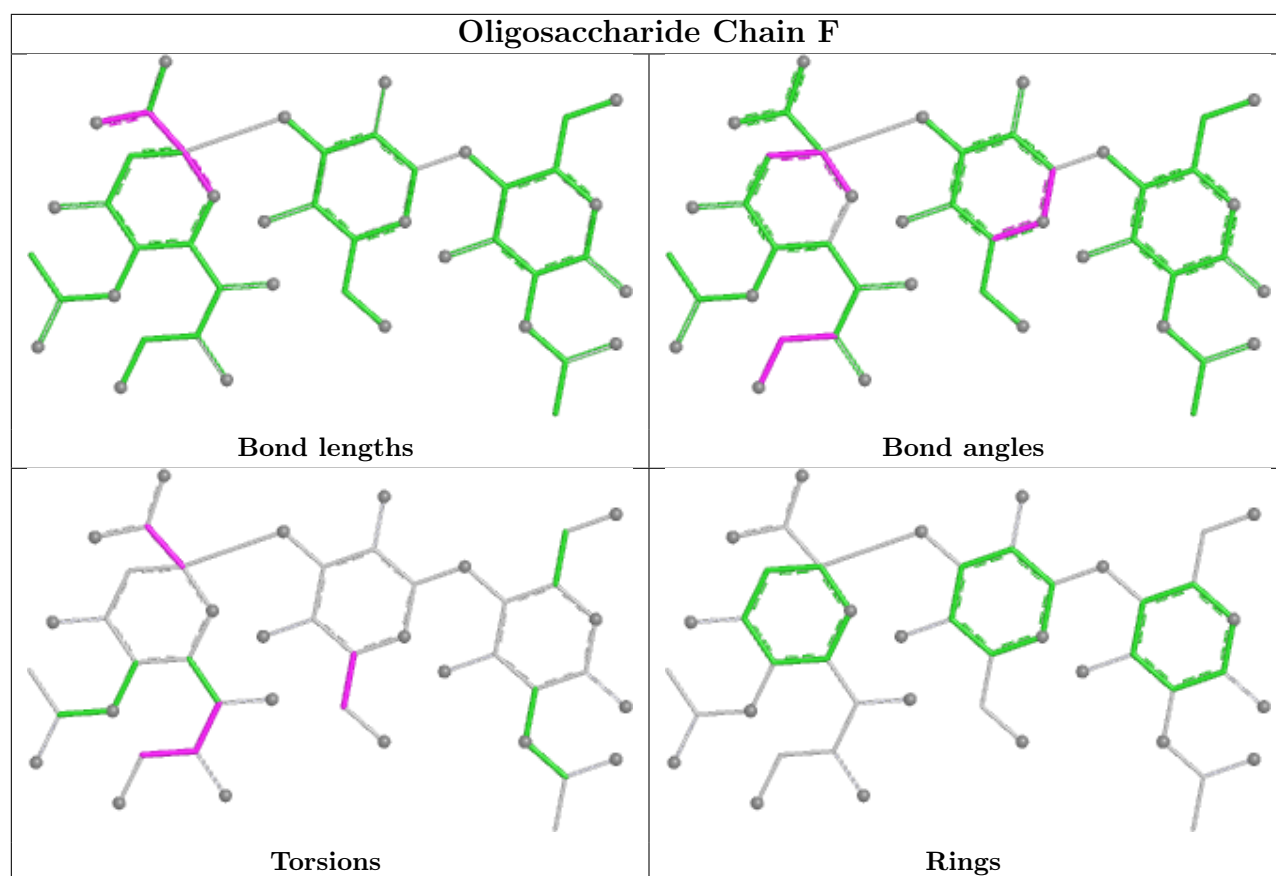
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	SIA	11	0
2	B	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 [i](#)

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 [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	409/409 (100%)	0.53	16 (3%) 43 45	21, 35, 50, 65	0
1	E	409/409 (100%)	0.64	30 (7%) 21 22	18, 36, 52, 68	1 (0%)
All	All	818/818 (100%)	0.59	46 (5%) 30 32	18, 36, 52, 68	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	496	ALA	4.2
1	E	314	ASN	3.9
1	E	544	PRO	3.9
1	E	524	GLU	3.6
1	E	660	SER	3.6
1	A	566	ILE	3.3
1	E	553	ARG	3.3
1	E	325	ASN	3.3
1	A	319	GLY	3.2
1	E	601	THR	3.0
1	E	356	ALA	2.9
1	A	641	ARG	2.9
1	A	660	SER	2.8
1	E	512	ASN	2.7
1	E	650[A]	ARG	2.7
1	E	549	THR	2.7
1	E	613	GLY	2.6
1	A	282	ASP	2.6
1	E	313	ASP	2.6
1	E	404	ASP	2.5
1	E	454	VAL	2.4
1	E	397	SER	2.4
1	E	520	ASN	2.4
1	A	493	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	543	GLY	2.4
1	E	396	ASN	2.4
1	E	464	ASP	2.4
1	E	612	THR	2.4
1	E	453	ARG	2.3
1	E	545	GLY	2.3
1	E	254	THR	2.2
1	A	318	PRO	2.2
1	E	315	LEU	2.2
1	E	466	ILE	2.2
1	A	544	PRO	2.1
1	A	356	ALA	2.1
1	A	325	ASN	2.1
1	A	591	ASN	2.1
1	E	563	GLU	2.1
1	A	593	GLN	2.1
1	A	605	GLU	2.0
1	E	576	ASP	2.0
1	E	543	GLY	2.0
1	A	649	ASP	2.0
1	A	612	THR	2.0
1	E	508	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

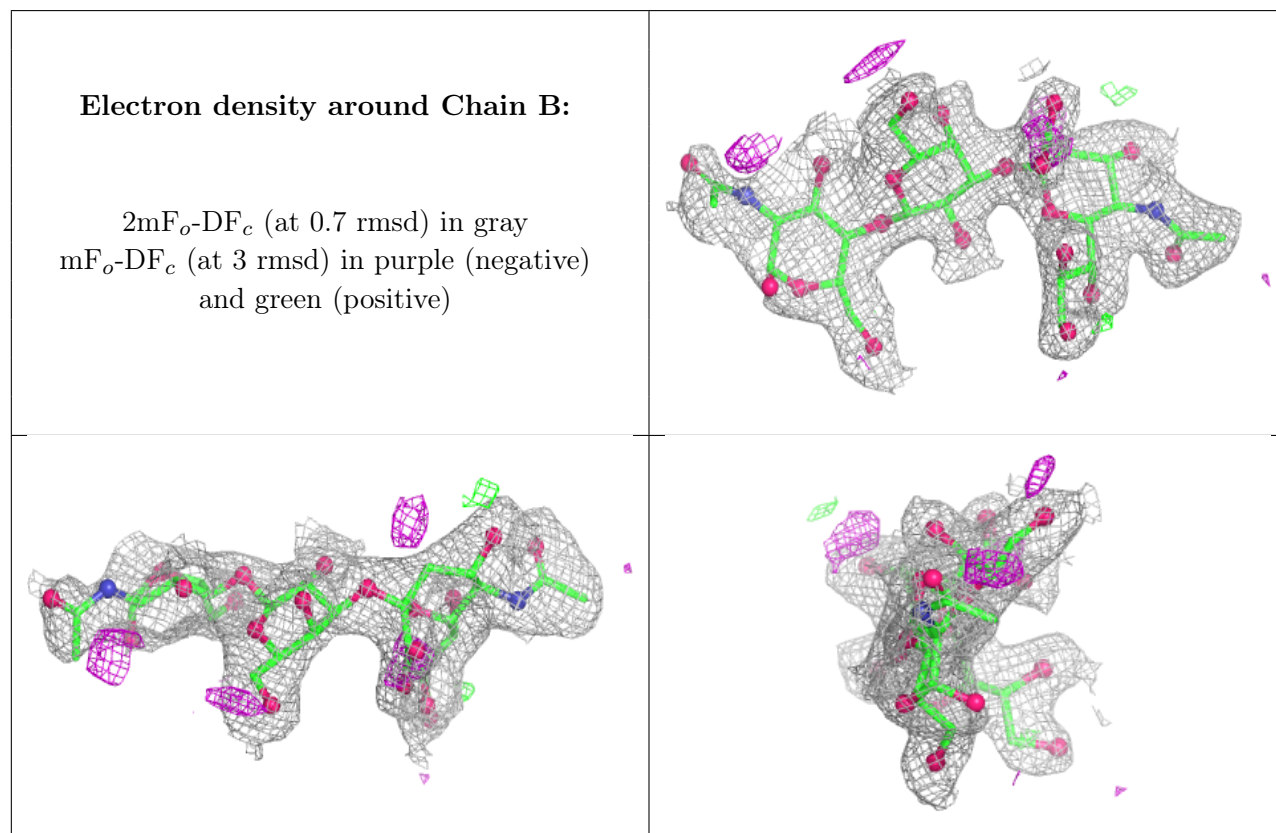
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	1	15/15	-	-	42,57,66,68	0
2	GAL	B	2	11/12	-	-	35,37,41,42	0
2	SIA	B	3	20/21	-	-	23,30,38,42	0
2	NAG	D	1	15/15	0.73	0.14	71,76,79,80	0
2	NAG	C	1	15/15	0.77	0.14	61,70,75,75	0
2	NAG	F	1	15/15	0.78	0.14	38,50,59,59	0

Continued on next page...

Continued from previous page...

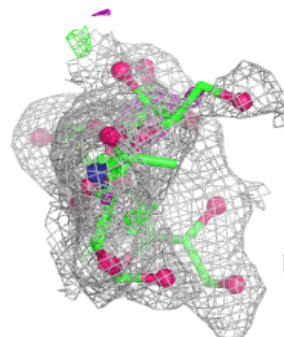
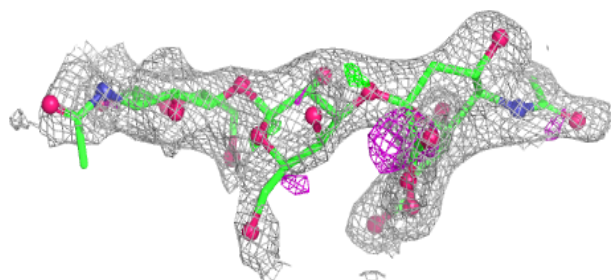
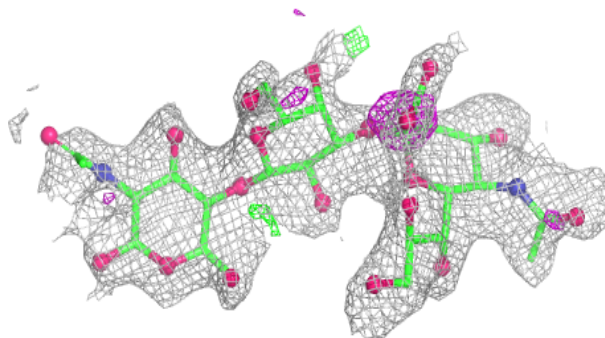
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GAL	D	2	11/12	0.80	0.15	56,66,72,73	0
2	SIA	D	3	20/21	0.81	0.14	47,52,58,59	0
2	SIA	F	3	20/21	0.90	0.10	21,30,41,48	0
2	SIA	C	3	20/21	0.91	0.10	42,46,52,55	0
2	GAL	C	2	11/12	0.91	0.09	53,57,60,61	0
2	GAL	F	2	11/12	0.93	0.08	28,33,41,46	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.

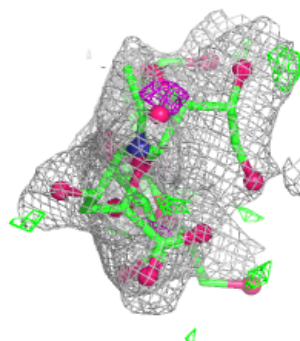
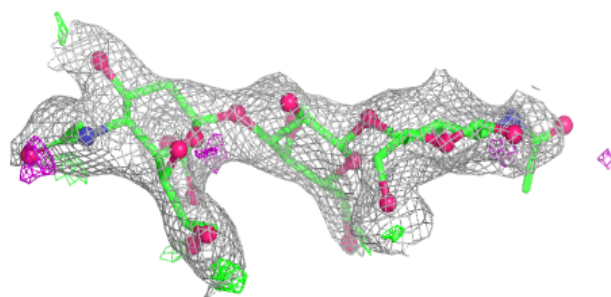
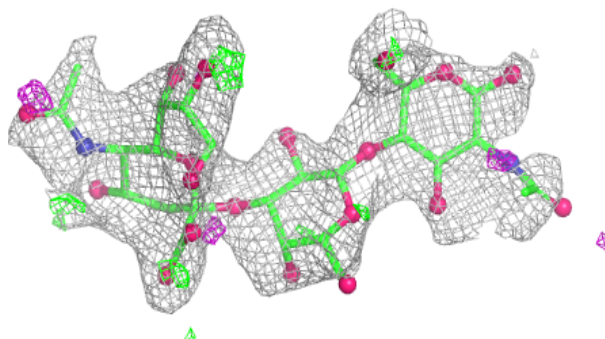


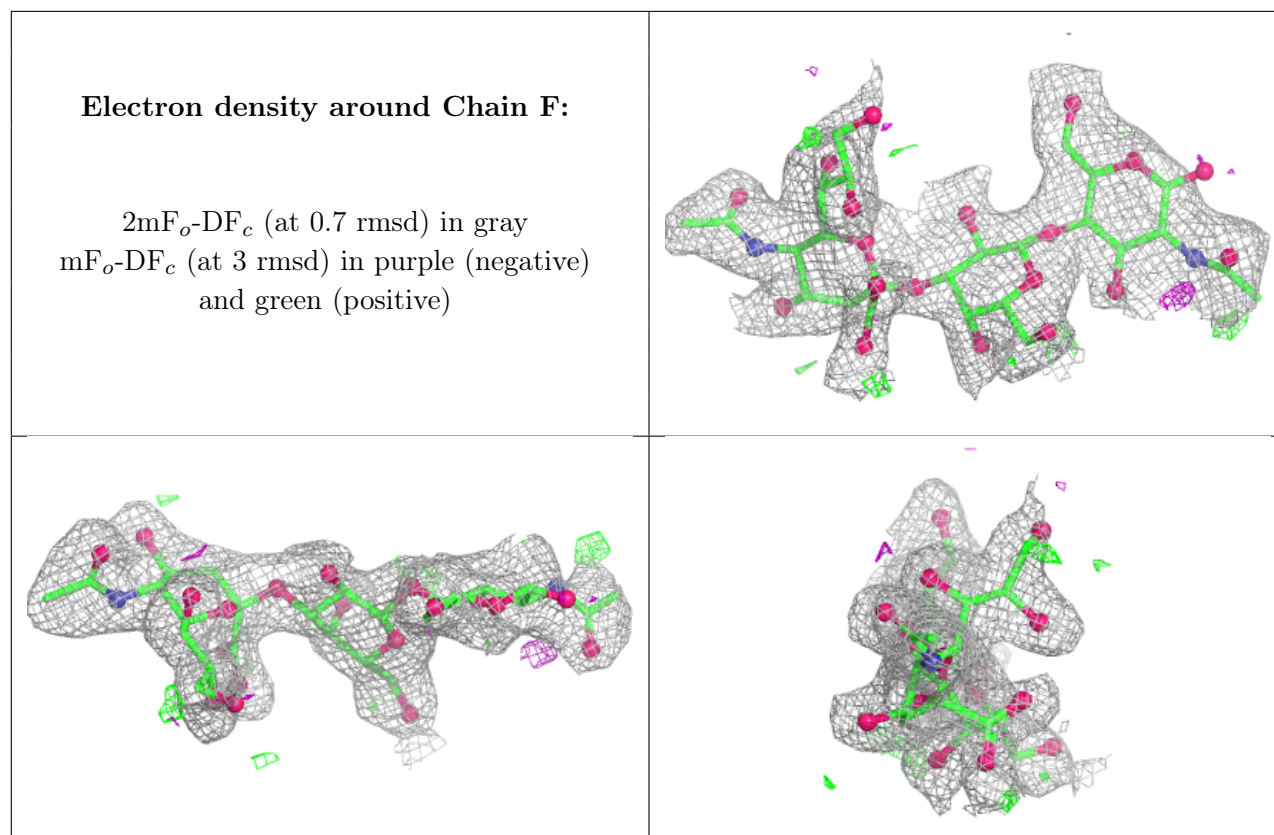
Electron density around Chain C:

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

**Electron density around Chain D:**

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





6.4 Ligands [i](#)

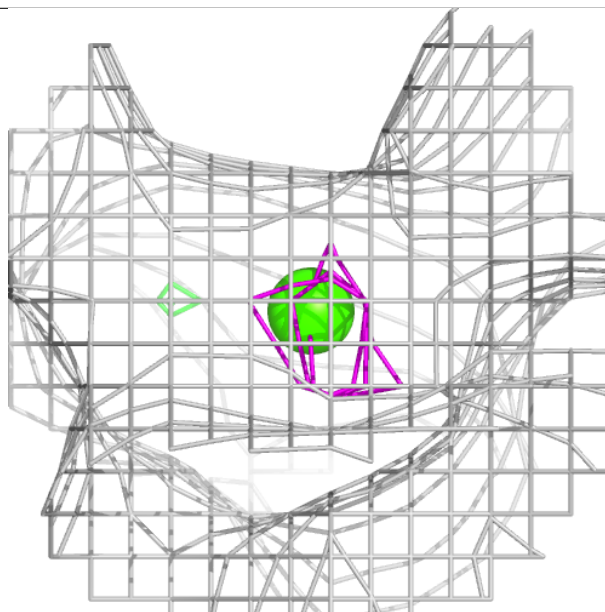
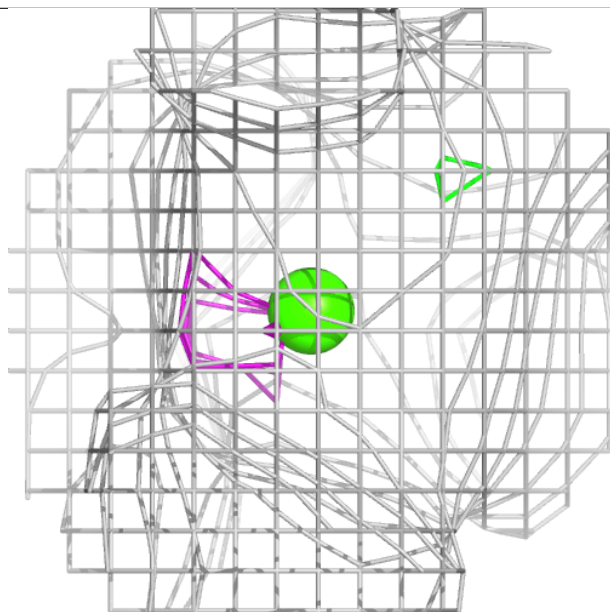
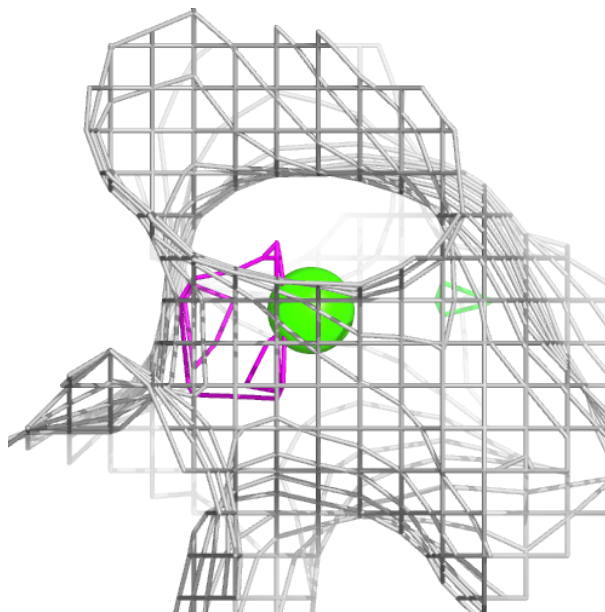
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	A	702	1/1	0.85	0.11	49,49,49,49	0
3	CA	E	702	1/1	0.88	0.10	47,47,47,47	0
3	CA	A	703	1/1	0.92	0.07	34,34,34,34	0
3	CA	A	701	1/1	0.93	0.06	39,39,39,39	0
3	CA	E	703	1/1	0.94	0.06	38,38,38,38	0
3	CA	E	704	1/1	0.97	0.04	37,37,37,37	0
3	CA	A	704	1/1	0.98	0.05	40,40,40,40	0
3	CA	E	701	1/1	0.99	0.02	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.

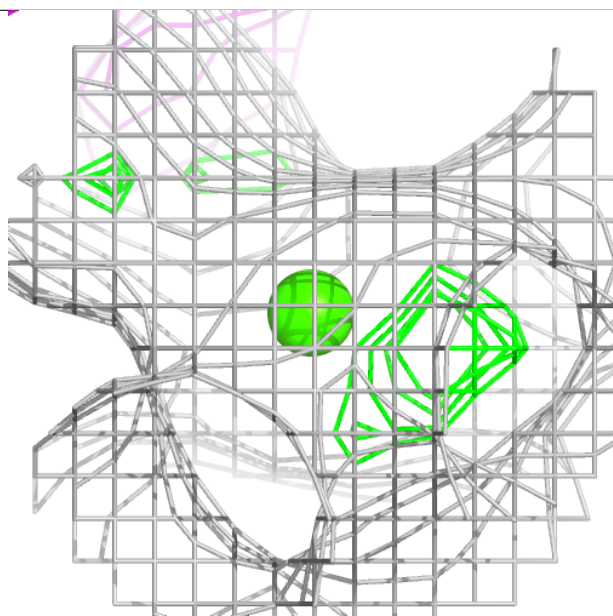
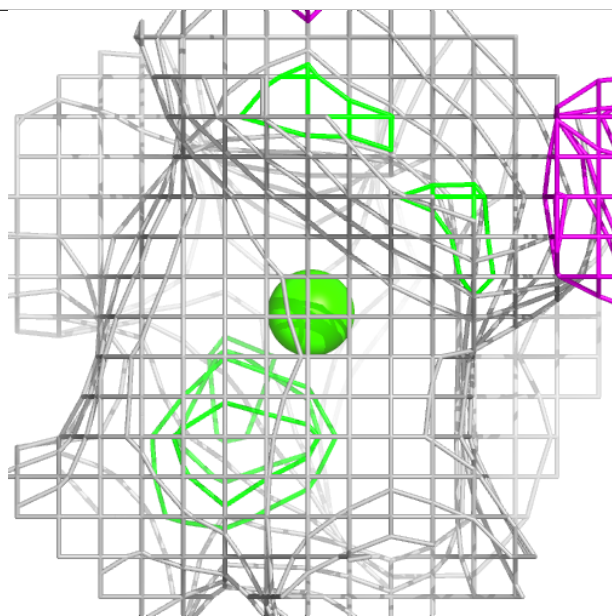
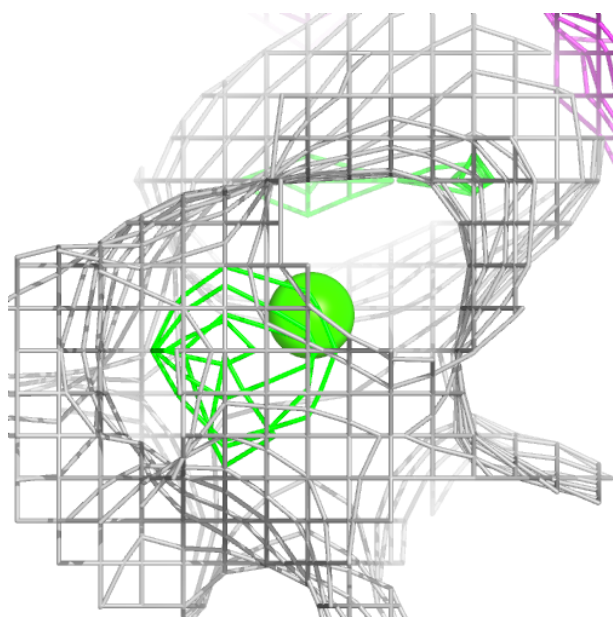
Electron density around CA A 702:

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



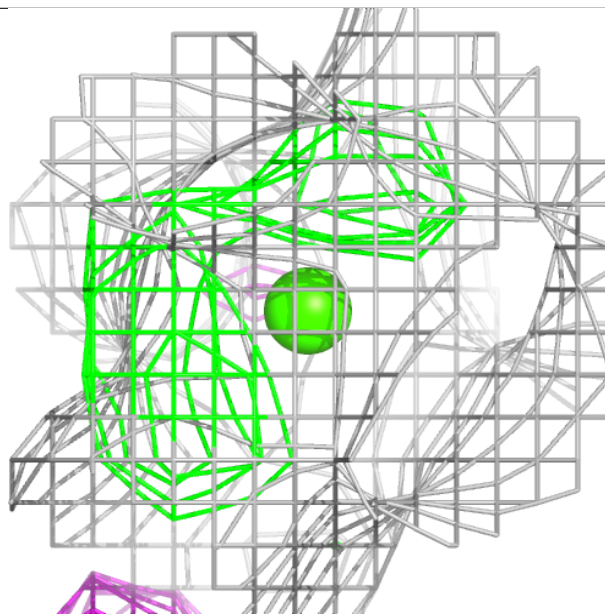
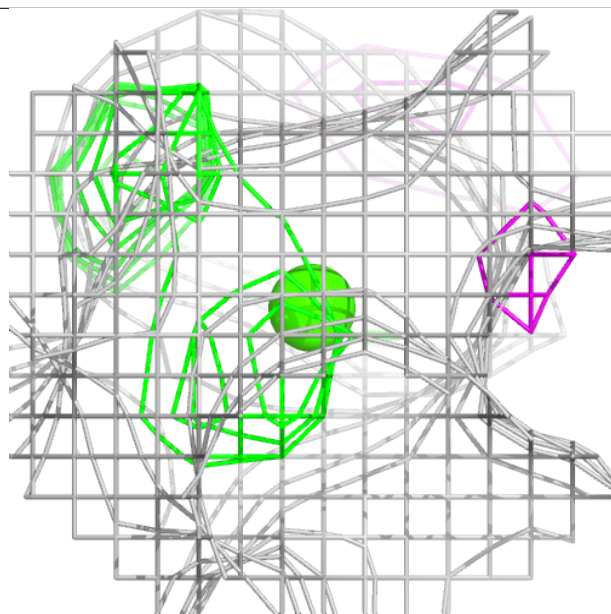
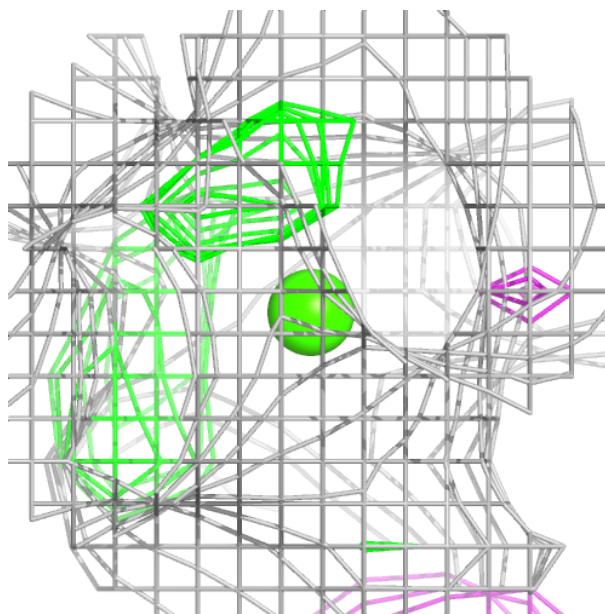
Electron density around CA E 702:

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



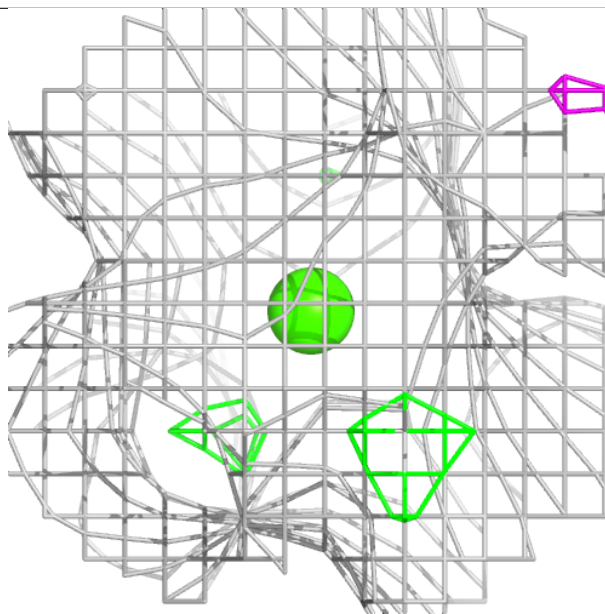
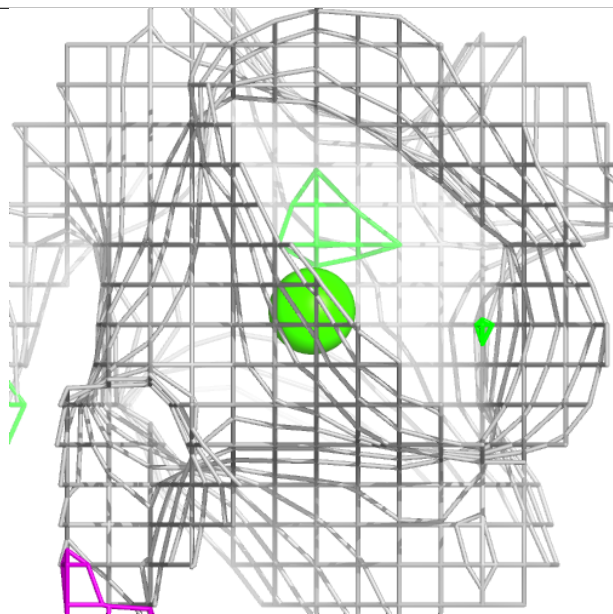
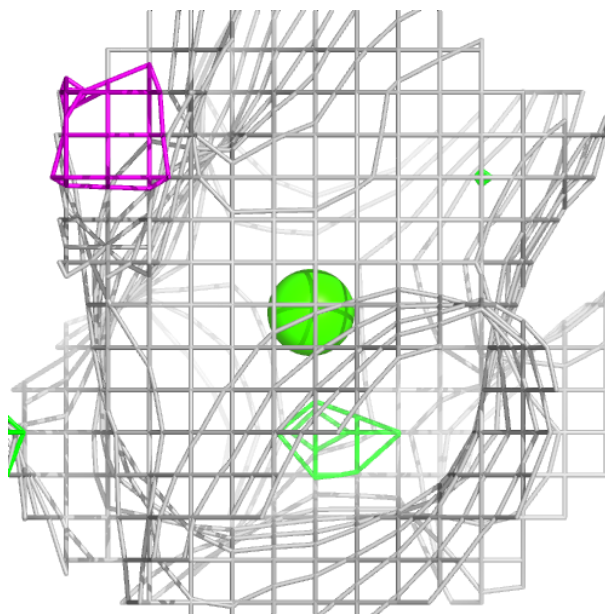
Electron density around CA A 703:

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



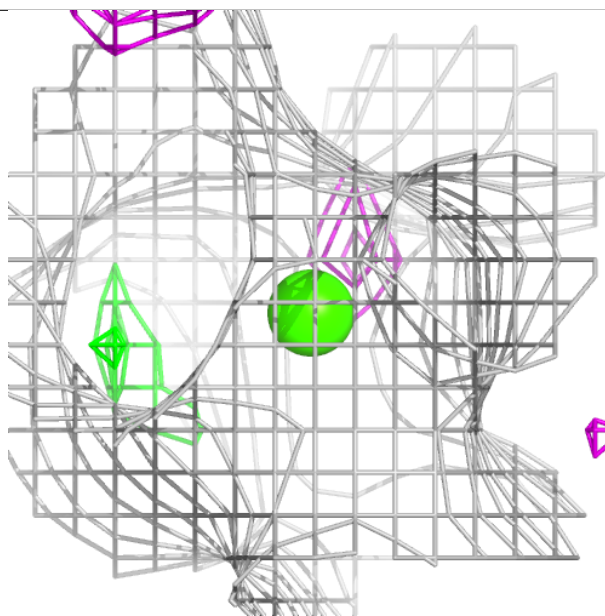
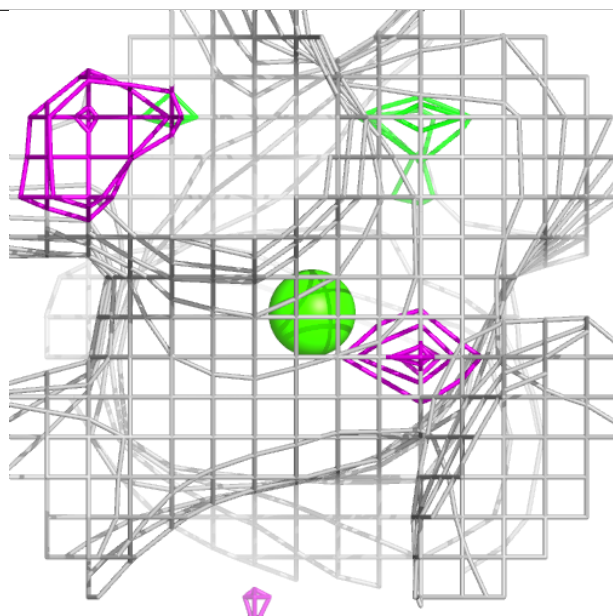
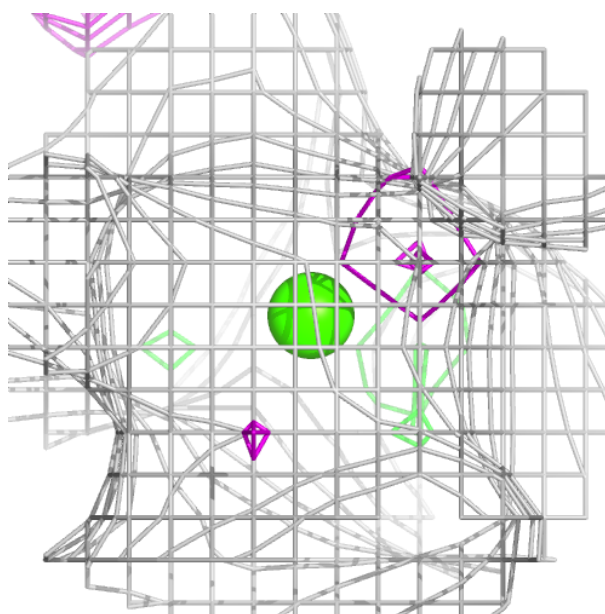
Electron density around CA A 701:

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



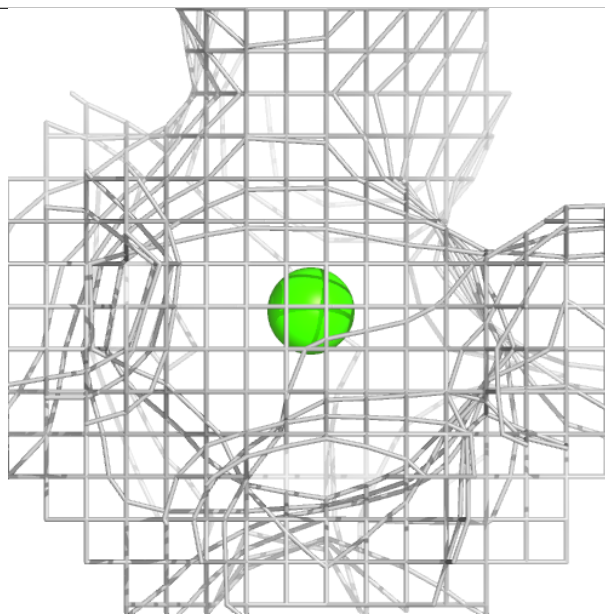
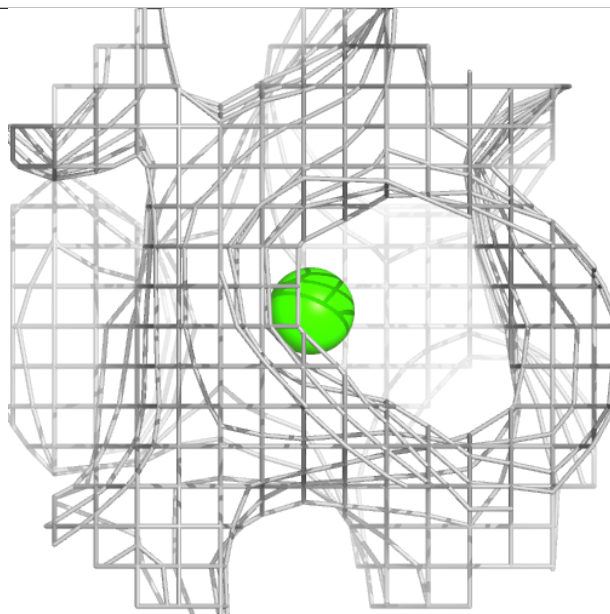
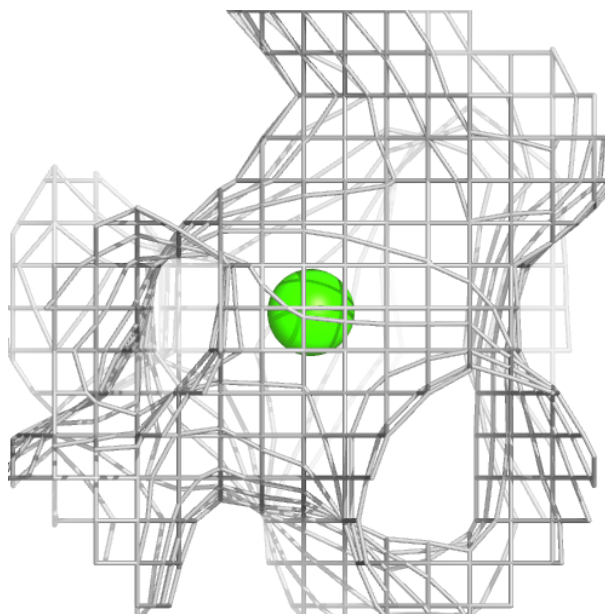
Electron density around CA E 703:

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



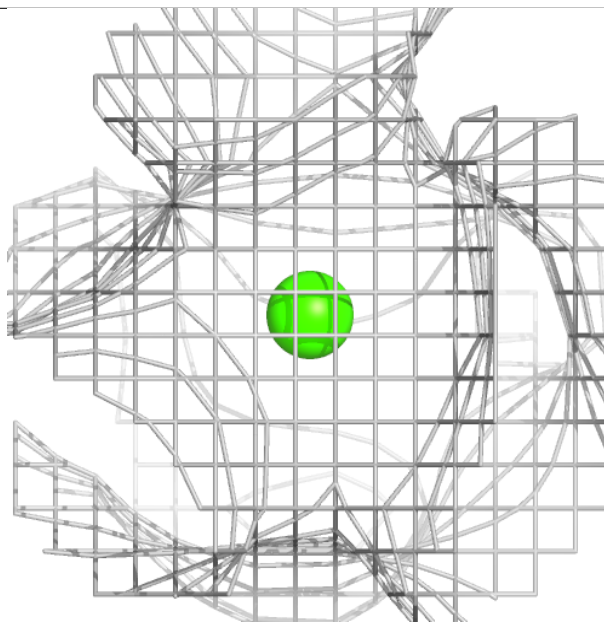
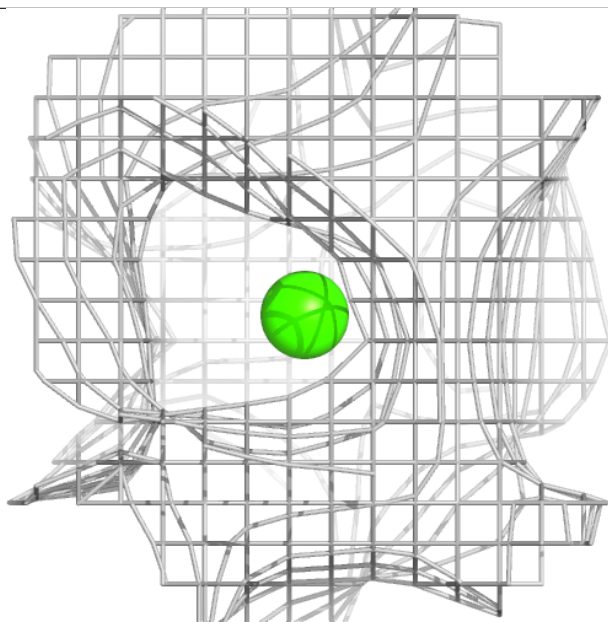
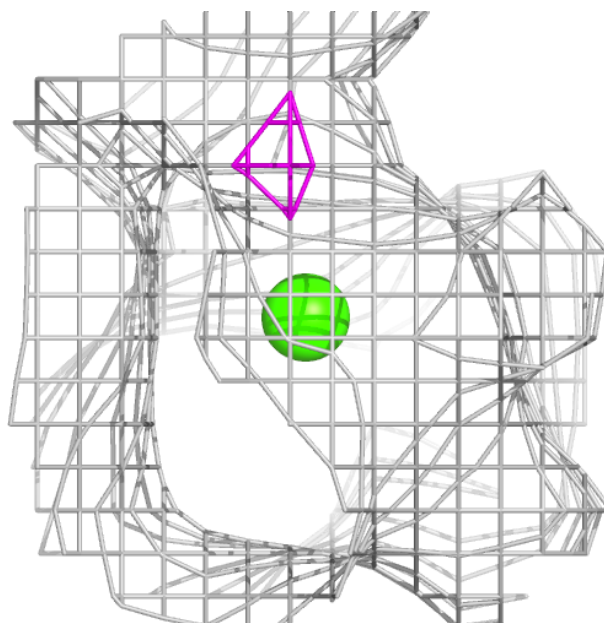
Electron density around CA E 704:

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



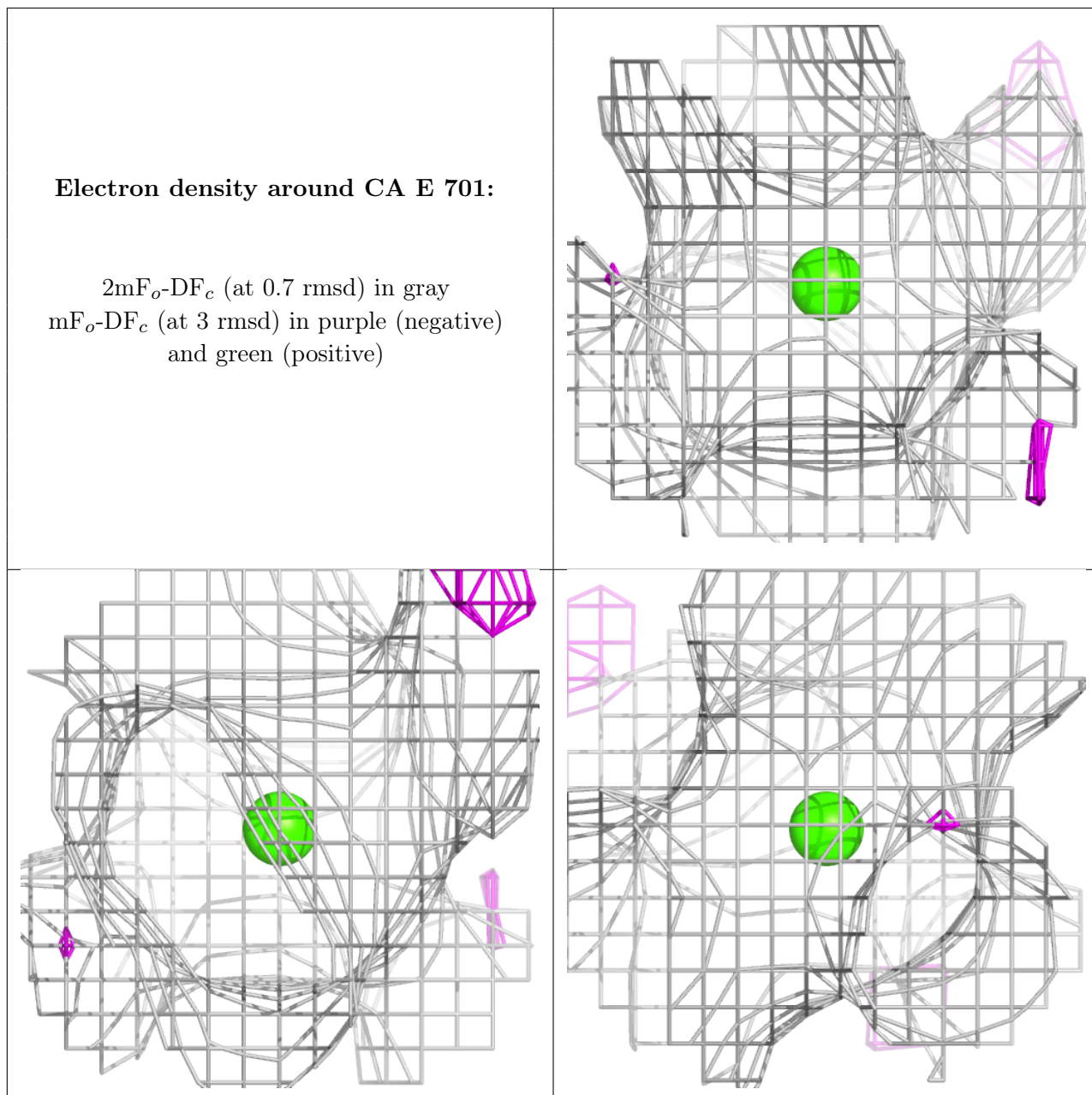
Electron density around CA A 704:

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



Electron density around CA E 701:

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

**6.5 Other polymers** [i](#)

There are no such residues in this entry.