



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:51 PM UTC

PDB ID : 6K55 / pdb_00006k55
Title : Inactivated mutant (D140A) of Hyperthermophilic GH6 cellobiohydrolase II (HmCel6A) in complex with hexasaccharide
Authors : Baba, S.; Takeda, M.; Okuma, J.; Hirose, Y.; Nishimura, A.; Takata, M.; Oda, K.; Shibata, D.; Kondo, Y.; Kumasaka, T.
Deposited on : 2019-05-28
Resolution : 2.88 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

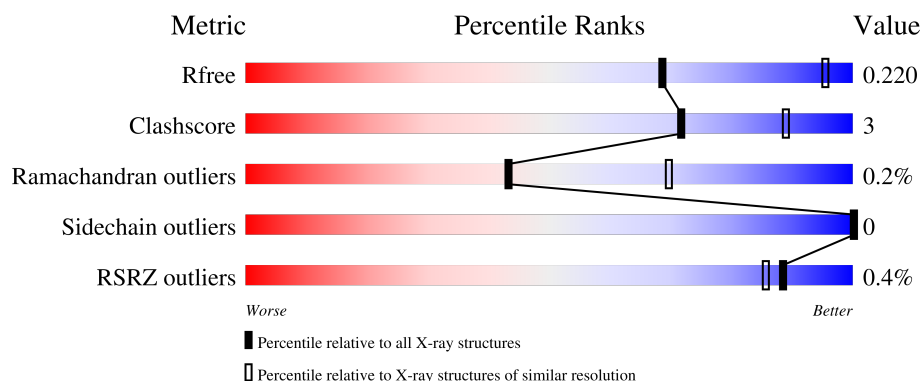
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	428	% 90% 10%
1	B	428	93% 7%
1	C	428	90% 10%
2	D	7	43% 57%
2	E	7	43% 57%

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Mol	Chain	Length	Quality of chain
2	F	7	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (57%), yellow (29%), and orange (14%).

2 Entry composition [i](#)

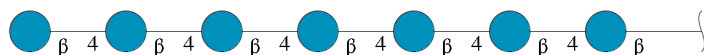
There are 4 unique types of molecules in this entry. The entry contains 10273 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	3	0
			3322	2097	585	628	12			
1	B	428	Total	C	N	O	S	0	1	0
			3311	2090	583	626	12			
1	C	428	Total	C	N	O	S	0	1	0
			3308	2089	582	625	12			

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	7	Total	C	O	0	0	0
			78	42	36			
2	E	7	Total	C	O	0	0	0
			78	42	36			
2	F	7	Total	C	O	0	0	0
			78	42	36			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		

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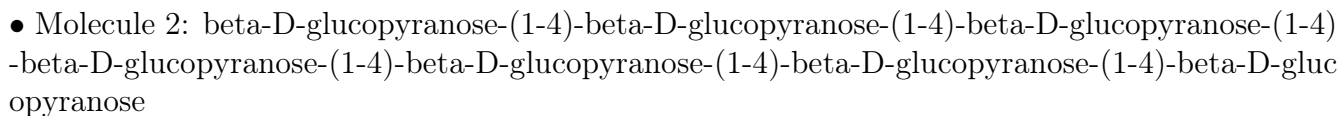
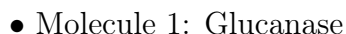
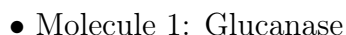
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total 2	Mg 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total 50	O 50	0	0
4	B	12	Total 12	O 12	0	0
4	C	30	Total 30	O 30	0	0

- Molecule 1: Glucanase





- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain E: 43% 57%



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain F: 57% 29% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.95Å 140.01Å 110.58Å 90.00° 101.06° 90.00°	Depositor
Resolution (Å)	42.35 – 2.88 42.35 – 2.88	Depositor EDS
% Data completeness (in resolution range)	96.1 (42.35-2.88) 96.0 (42.35-2.88)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.179 , 0.218 0.181 , 0.220	Depositor DCC
R_{free} test set	2856 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for $-1/2^*h+1/2^*k+1, 1/2^*h-1/2^*k+1, 1/2^*h+1/2^*k$ 0.045 for $-1/2^*h-1/2^*k+1, -1/2^*h-1/2^*k-1, 1/2^*h-1/2^*k$	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10273	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: MG, BGC

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	0.13	0/3422	0.37	1/4685 (0.0%)
1	B	0.11	0/3405	0.34	0/4661
1	C	0.14	0/3402	0.38	0/4658
All	All	0.13	0/10229	0.36	1/14004 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ALA	CB-CA-C	-5.92	108.06	116.34

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	3322	0	3194	26	0
1	B	3311	0	3180	18	0
1	C	3308	0	3179	22	0
2	D	78	0	65	0	0
2	E	78	0	65	0	0
2	F	78	0	65	1	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	50	0	0	0	0
4	B	12	0	0	0	0
4	C	30	0	0	0	0
All	All	10273	0	9748	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (66) 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:149:LEU:HD23	1:A:149:LEU:O	1.76	0.84
1:A:32:LEU:HD21	1:A:415:GLU:HG3	1.72	0.71
1:C:248:ARG:HG2	1:C:255:TRP:HA	1.80	0.64
1:A:124:SER:HB3	1:A:175:ILE:HD12	1.81	0.62
1:A:230:LEU:HD21	1:A:352:TYR:CZ	2.36	0.61
1:C:173:ARG:HD3	1:C:216:SER:HA	1.87	0.56
1:C:146:VAL:HG23	1:C:147:THR:HG23	1.89	0.55
1:A:25:ASN:ND2	1:A:37:ARG:HH21	2.06	0.54
1:C:187:SER:OG	1:C:228:THR:HG21	2.08	0.54
1:C:48:LEU:HD11	1:C:60:LEU:HD13	1.90	0.52
1:C:92:CYS:HB2	1:C:161:TYR:OH	2.11	0.51
1:C:250:ALA:HB2	1:C:312:VAL:HG12	1.92	0.51
1:A:25:ASN:HD22	1:A:37:ARG:HH21	1.59	0.50
1:A:336:GLY:HA2	1:A:417:LEU:HA	1.94	0.49
1:B:204:THR:O	1:B:208:GLN:HB2	2.12	0.49
1:C:141:SER:OG	1:C:142:LEU:N	2.45	0.49
1:B:291:GLY:O	1:B:301:ARG:NH1	2.46	0.48
1:C:169:VAL:HG13	1:C:180:ILE:HD13	1.94	0.48
1:B:252:PHE:CZ	1:B:327:ARG:HG3	2.47	0.48
1:B:292:TRP:CZ2	1:B:324:ARG:HD3	2.49	0.48
1:C:311:SER:HB2	1:C:314:ALA:H	1.79	0.48
1:C:144:ASN:HB3	1:C:154:CYS:SG	2.54	0.47
1:C:239:ASN:OD1	1:C:248:ARG:NH1	2.47	0.47
1:B:200:VAL:O	1:B:204:THR:OG1	2.25	0.47
1:C:136:ILE:HG23	1:C:221:ILE:HG21	1.97	0.47
1:A:149:LEU:HD23	1:A:149:LEU:C	2.39	0.46
1:B:136:ILE:HG23	1:B:221:ILE:HG21	1.98	0.46
1:B:340:ARG:NH2	1:B:425:ILE:HD13	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASN:OD1	1:A:275:ARG:NH2	2.49	0.46
1:B:32:LEU:HD21	1:B:415:GLU:HG3	1.98	0.46
1:A:191:GLY:HA3	1:A:256:ASN:HD21	1.80	0.46
1:B:264:TYR:CZ	1:B:268:LEU:HD11	2.50	0.45
1:B:31:THR:O	1:B:35:GLN:HG3	2.16	0.45
1:B:240:LEU:O	1:B:247:VAL:HG13	2.16	0.45
1:B:324:ARG:NH1	1:B:329:ASN:O	2.50	0.45
1:A:133:ILE:O	1:A:178:VAL:HA	2.18	0.44
1:B:293:GLY:O	1:B:323:ARG:NH2	2.35	0.44
1:B:371:ASP:OD1	1:B:408:ARG:NH1	2.50	0.44
1:C:143:PRO:O	1:C:146:VAL:HG22	2.18	0.44
1:A:138:GLU:O	1:A:141:SER:OG	2.33	0.44
1:B:269:ARG:O	1:B:273:ILE:HG13	2.18	0.44
1:C:340:ARG:NH2	1:C:425:ILE:HD13	2.33	0.43
1:A:87:LEU:HD13	1:A:161:TYR:CD1	2.54	0.43
1:A:379:PHE:HZ	1:A:384:ASP:HB2	1.82	0.43
1:C:65:ASP:OD1	1:C:127:ARG:NH2	2.52	0.43
1:C:204:THR:O	1:C:208:GLN:HB2	2.19	0.43
1:A:108:LEU:HD22	1:A:160:ALA:HA	2.01	0.42
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.91	0.42
1:A:79:VAL:HA	1:A:132:ARG:O	2.19	0.42
1:A:367:PRO:HB2	1:B:202:LEU:HD13	2.02	0.42
1:B:299:ARG:NH2	1:B:317:ASP:HB3	2.34	0.42
1:C:382:MET:HG2	1:C:390:ARG:HD3	2.01	0.42
1:A:275:ARG:HE	1:A:275:ARG:HB3	1.69	0.41
1:A:340:ARG:N	1:A:340:ARG:HD3	2.34	0.41
1:A:402:ASN:HB2	1:A:412:GLN:HE22	1.84	0.41
1:A:111:TYR:CZ	1:A:116:ILE:HD11	2.56	0.41
1:B:247:VAL:HA	1:B:312:VAL:CG2	2.51	0.41
1:C:247:VAL:HA	1:C:312:VAL:HG13	2.02	0.41
2:F:7:BGC:O6	2:F:7:BGC:O4	2.34	0.41
1:C:97:SER:HA	1:C:377:LYS:HG2	2.02	0.41
1:A:58:ARG:HD2	1:A:63:HIS:CE1	2.55	0.41
1:A:228:THR:HA	1:A:229:PRO:HD3	1.91	0.41
1:A:0:MET:SD	1:A:173:ARG:NH1	2.94	0.41
1:C:46:VAL:HB	1:C:82:LEU:HD23	2.02	0.40
1:A:423:PRO:HA	1:A:424:PRO:HD3	1.91	0.40
1:C:223:ASN:O	1:C:286:ASP:HB3	2.20	0.40

There are no symmetry-related clashes.

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	429/428 (100%)	411 (96%)	17 (4%)	1 (0%)	43	70
1	B	427/428 (100%)	408 (96%)	19 (4%)	0	100	100
1	C	427/428 (100%)	407 (95%)	18 (4%)	2 (0%)	24	51
All	All	1283/1284 (100%)	1226 (96%)	54 (4%)	3 (0%)	43	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	92	CYS
1	C	329	ASN
1	A	86	ASP

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	349/346 (101%)	349 (100%)	0	100	100
1	B	347/346 (100%)	347 (100%)	0	100	100
1	C	347/346 (100%)	347 (100%)	0	100	100
All	All	1043/1038 (100%)	1043 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	105	GLN
1	A	159	ASN
1	A	342	GLN
1	A	376	ASN
1	B	105	GLN
1	B	205	GLN
1	B	342	GLN
1	C	73	GLN
1	C	148	ASN
1	C	392	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 ⓘ

21 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	0.46	0	17,17,17	0.55	0
2	BGC	D	2	2	11,11,12	0.22	0	15,15,17	0.80	1 (6%)
2	BGC	D	3	2	11,11,12	0.23	0	15,15,17	0.56	0
2	BGC	D	4	2	11,11,12	0.23	0	15,15,17	0.50	0
2	BGC	D	5	2	11,11,12	0.34	0	15,15,17	1.96	2 (13%)
2	BGC	D	6	2	11,11,12	0.27	0	15,15,17	1.30	2 (13%)
2	BGC	D	7	2	11,11,12	0.28	0	15,15,17	1.17	1 (6%)
2	BGC	E	1	2	12,12,12	0.47	0	17,17,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	E	2	2	11,11,12	0.28	0	15,15,17	0.95	1 (6%)
2	BGC	E	3	2	11,11,12	0.22	0	15,15,17	0.55	0
2	BGC	E	4	2	11,11,12	0.26	0	15,15,17	0.65	0
2	BGC	E	5	2	11,11,12	0.38	0	15,15,17	2.00	3 (20%)
2	BGC	E	6	2	11,11,12	0.24	0	15,15,17	1.13	2 (13%)
2	BGC	E	7	2	11,11,12	0.34	0	15,15,17	1.45	2 (13%)
2	BGC	F	1	2	12,12,12	0.46	0	17,17,17	0.50	0
2	BGC	F	2	2	11,11,12	0.22	0	15,15,17	0.67	0
2	BGC	F	3	2	11,11,12	0.23	0	15,15,17	0.45	0
2	BGC	F	4	2	11,11,12	0.23	0	15,15,17	0.62	0
2	BGC	F	5	2	11,11,12	0.31	0	15,15,17	1.93	2 (13%)
2	BGC	F	6	2	11,11,12	0.24	0	15,15,17	1.25	2 (13%)
2	BGC	F	7	2	11,11,12	0.32	0	15,15,17	1.14	1 (6%)

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	BGC	D	2	2	-	2/2/19/22	0/1/1/1
2	BGC	D	3	2	-	0/2/19/22	0/1/1/1
2	BGC	D	4	2	-	0/2/19/22	0/1/1/1
2	BGC	D	5	2	-	0/2/19/22	0/1/1/1
2	BGC	D	6	2	-	2/2/19/22	0/1/1/1
2	BGC	D	7	2	-	0/2/19/22	0/1/1/1
2	BGC	E	1	2	-	1/2/22/22	0/1/1/1
2	BGC	E	2	2	-	2/2/19/22	0/1/1/1
2	BGC	E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	E	4	2	-	0/2/19/22	0/1/1/1
2	BGC	E	5	2	-	2/2/19/22	0/1/1/1
2	BGC	E	6	2	-	2/2/19/22	0/1/1/1
2	BGC	E	7	2	-	0/2/19/22	0/1/1/1
2	BGC	F	1	2	-	0/2/22/22	0/1/1/1
2	BGC	F	2	2	-	0/2/19/22	0/1/1/1
2	BGC	F	3	2	-	2/2/19/22	0/1/1/1
2	BGC	F	4	2	-	0/2/19/22	0/1/1/1
2	BGC	F	5	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	F	6	2	-	2/2/19/22	0/1/1/1
2	BGC	F	7	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5	BGC	C1-O5-C5	6.66	121.11	112.19
2	F	5	BGC	C1-O5-C5	6.54	120.96	112.19
2	E	5	BGC	C1-O5-C5	6.32	120.65	112.19
2	E	7	BGC	C1-C2-C3	3.89	115.31	109.64
2	F	6	BGC	C1-O5-C5	3.81	117.29	112.19
2	D	6	BGC	C1-O5-C5	3.79	117.26	112.19
2	E	6	BGC	C1-O5-C5	3.34	116.66	112.19
2	D	7	BGC	C1-C2-C3	3.19	114.30	109.64
2	F	7	BGC	C1-C2-C3	3.04	114.07	109.64
2	E	2	BGC	C1-C2-C3	2.78	113.69	109.64
2	E	5	BGC	C3-C4-C5	2.66	115.06	110.23
2	E	5	BGC	O5-C5-C4	2.66	117.29	110.83
2	E	7	BGC	C2-C3-C4	2.40	115.08	110.86
2	D	6	BGC	C2-C3-C4	-2.35	106.73	110.86
2	F	6	BGC	C2-C3-C4	-2.30	106.82	110.86
2	D	5	BGC	O5-C5-C4	2.22	116.24	110.83
2	F	5	BGC	O5-C5-C4	2.15	116.06	110.83
2	E	6	BGC	C2-C3-C4	-2.12	107.14	110.86
2	D	2	BGC	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	BGC	O5-C5-C6-O6
2	F	3	BGC	O5-C5-C6-O6
2	D	2	BGC	C4-C5-C6-O6
2	E	5	BGC	C4-C5-C6-O6
2	E	5	BGC	O5-C5-C6-O6
2	F	3	BGC	C4-C5-C6-O6
2	F	6	BGC	C4-C5-C6-O6
2	E	6	BGC	C4-C5-C6-O6
2	F	6	BGC	O5-C5-C6-O6
2	E	6	BGC	O5-C5-C6-O6

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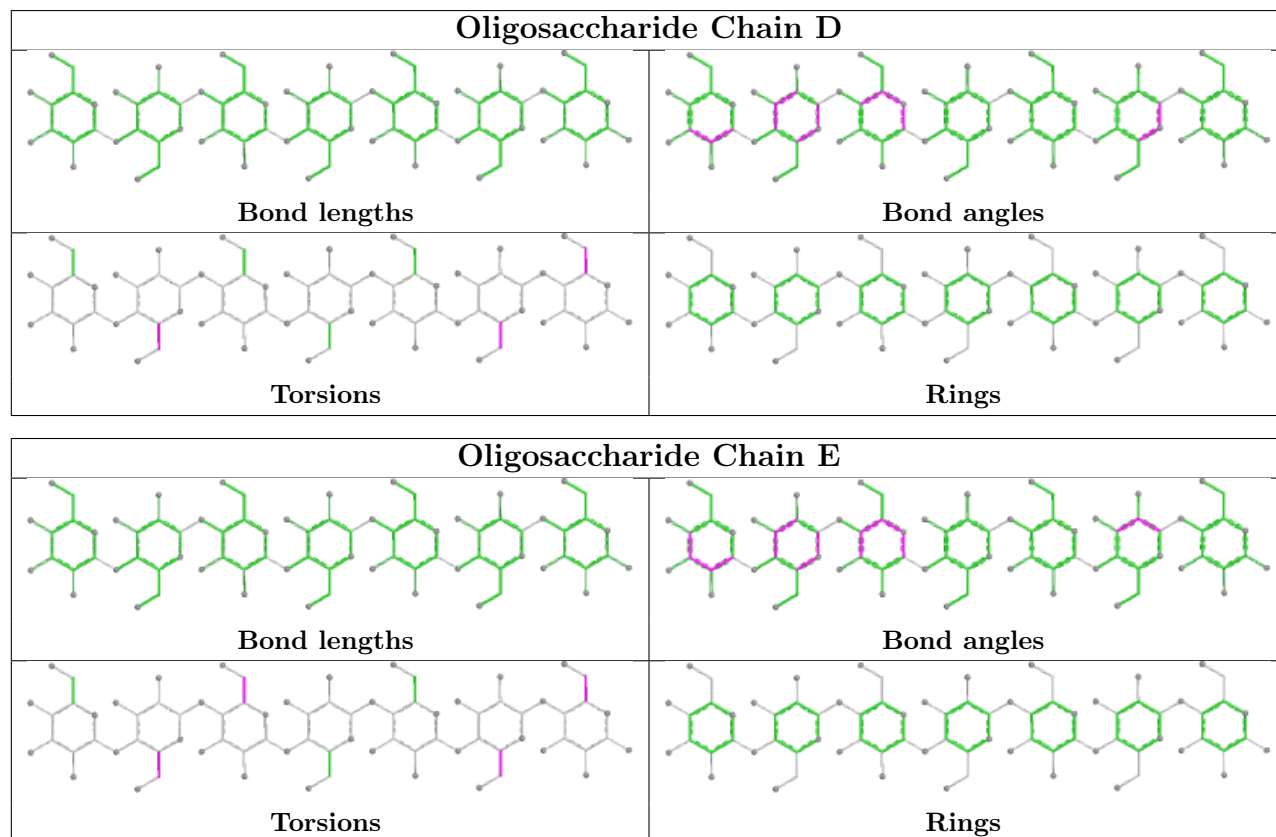
Mol	Chain	Res	Type	Atoms
2	F	7	BGC	O5-C5-C6-O6
2	D	1	BGC	C4-C5-C6-O6
2	E	2	BGC	C4-C5-C6-O6
2	D	6	BGC	C4-C5-C6-O6
2	E	2	BGC	O5-C5-C6-O6
2	E	1	BGC	C4-C5-C6-O6
2	D	6	BGC	O5-C5-C6-O6

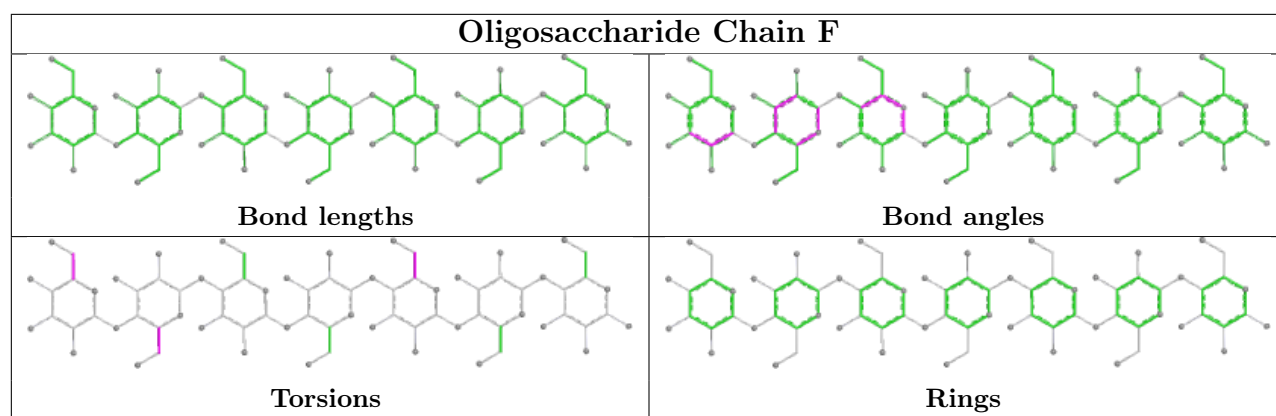
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	7	BGC	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 6 ligands modelled in this entry, 6 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	428/428 (100%)	-0.44	3 (0%) 84 80	33, 56, 74, 90	3 (0%)
1	B	428/428 (100%)	-0.45	1 (0%) 91 89	36, 56, 72, 98	1 (0%)
1	C	428/428 (100%)	-0.43	1 (0%) 91 89	41, 58, 76, 87	1 (0%)
All	All	1284/1284 (100%)	-0.44	5 (0%) 88 86	33, 57, 75, 98	5 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	366	GLN	3.4
1	A	149	LEU	2.4
1	A	0	MET	2.1
1	C	150	SER	2.0
1	A	106[A]	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.

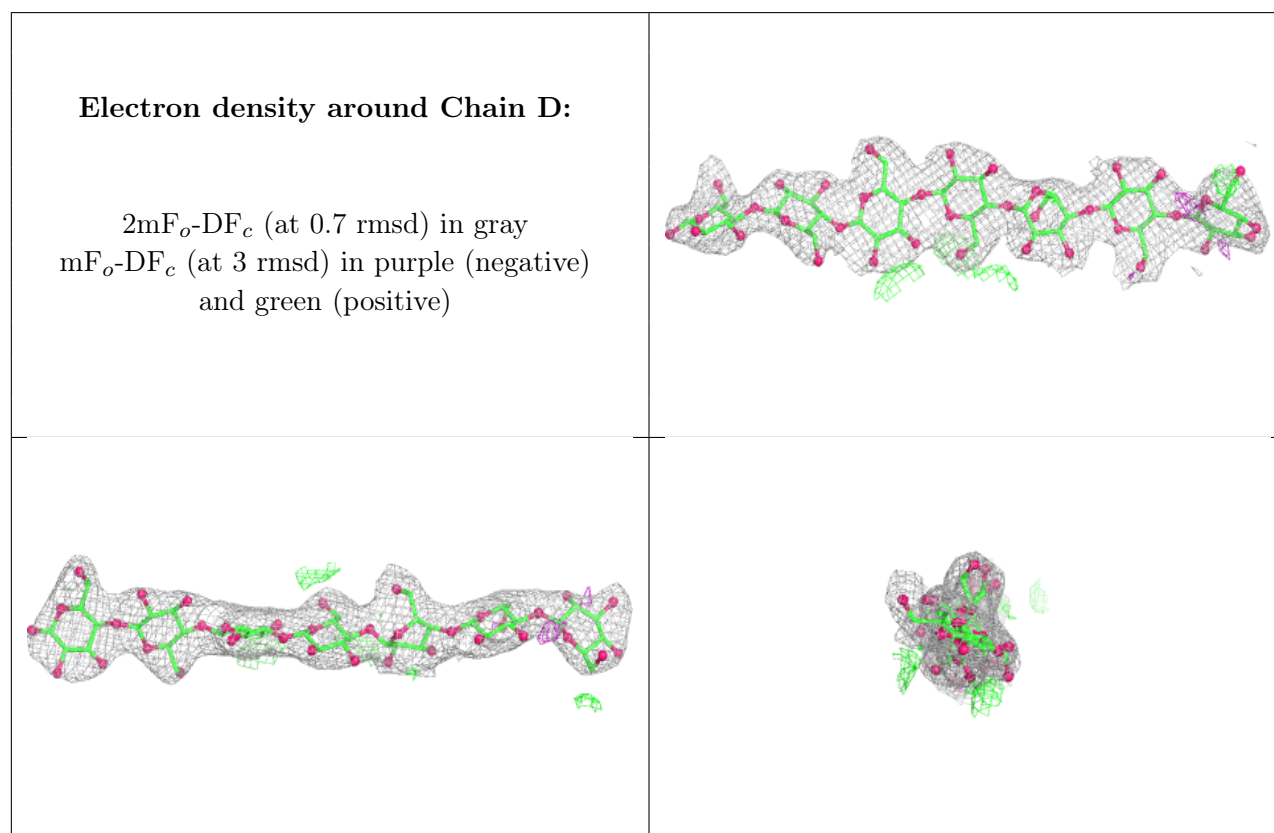
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	F	7	11/12	0.79	0.21	60,80,89,91	0
2	BGC	E	7	11/12	0.87	0.18	68,83,88,88	11
2	BGC	F	1	12/12	0.89	0.13	53,74,82,90	12

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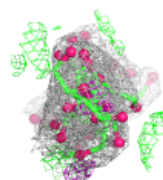
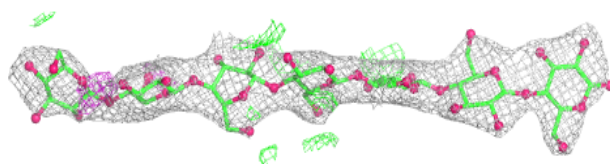
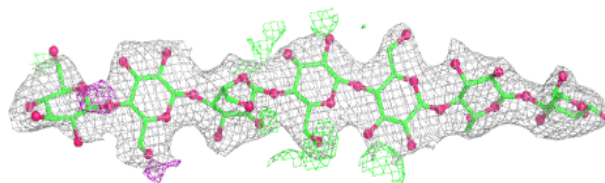
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	D	7	11/12	0.89	0.15	59,66,73,76	0
2	BGC	D	1	12/12	0.92	0.11	50,58,66,66	12
2	BGC	E	1	12/12	0.93	0.10	54,65,78,78	12
2	BGC	F	6	11/12	0.94	0.10	56,61,74,74	0
2	BGC	F	3	11/12	0.94	0.08	50,54,60,70	0
2	BGC	E	6	11/12	0.95	0.09	55,59,70,76	0
2	BGC	F	2	11/12	0.96	0.08	51,54,66,69	0
2	BGC	D	4	11/12	0.96	0.08	41,47,51,55	0
2	BGC	F	5	11/12	0.96	0.07	51,57,63,70	0
2	BGC	D	2	11/12	0.96	0.09	46,52,57,64	0
2	BGC	D	3	11/12	0.96	0.07	42,47,53,54	0
2	BGC	E	2	11/12	0.97	0.07	52,55,64,68	0
2	BGC	E	3	11/12	0.97	0.07	45,49,57,58	0
2	BGC	E	4	11/12	0.97	0.08	48,50,57,59	0
2	BGC	F	4	11/12	0.97	0.08	49,52,57,65	0
2	BGC	E	5	11/12	0.97	0.07	49,57,70,74	0
2	BGC	D	5	11/12	0.97	0.08	50,53,60,63	0
2	BGC	D	6	11/12	0.97	0.08	49,54,68,69	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.

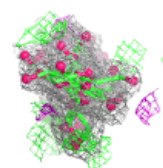
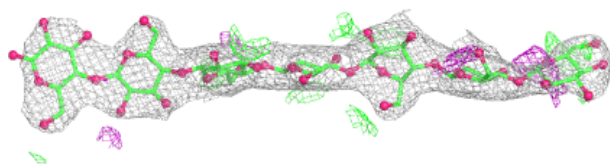
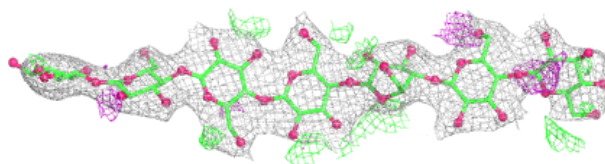


Electron density around Chain E:

$2mF_o-DF_c$ (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

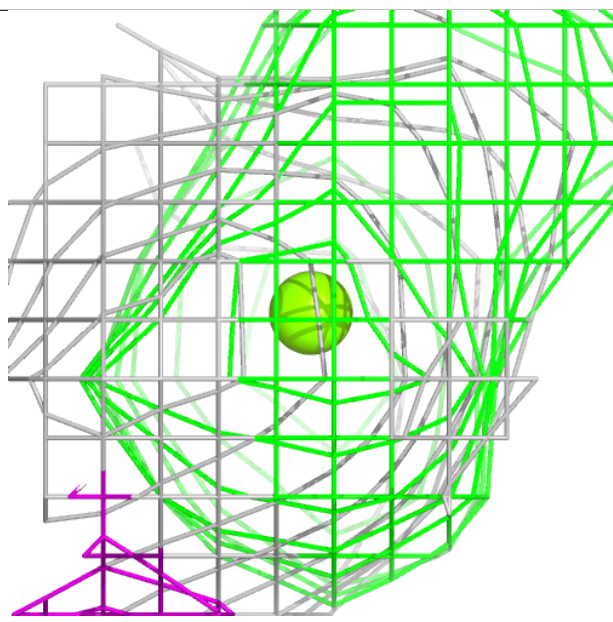
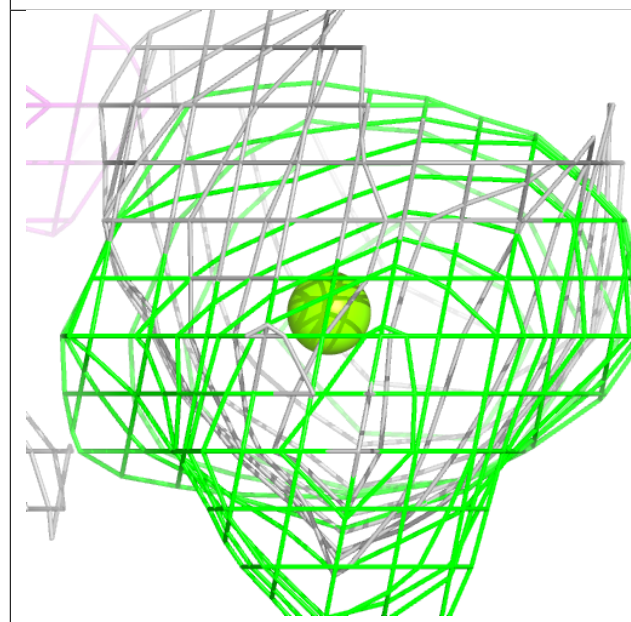
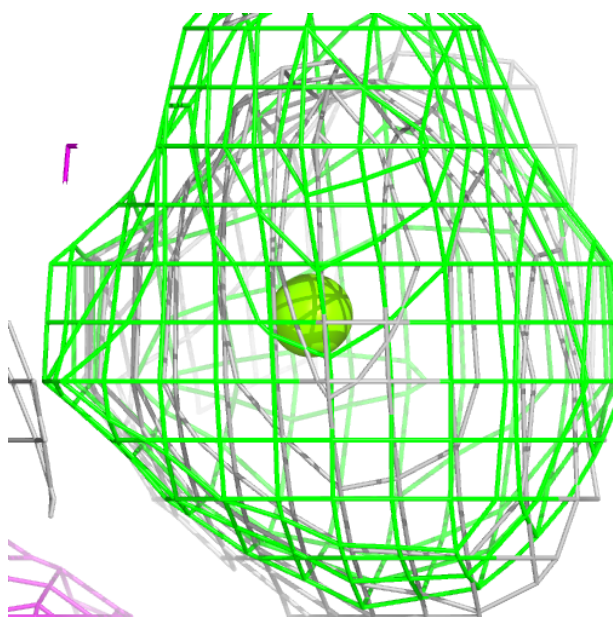
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	B	501	1/1	0.89	0.34	47,47,47,47	0
3	MG	B	502	1/1	0.91	0.19	49,49,49,49	0
3	MG	C	501	1/1	0.93	0.21	44,44,44,44	0
3	MG	A	502	1/1	0.95	0.17	50,50,50,50	0
3	MG	A	501	1/1	0.95	0.23	44,44,44,44	0
3	MG	C	502	1/1	0.99	0.05	53,53,53,53	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.

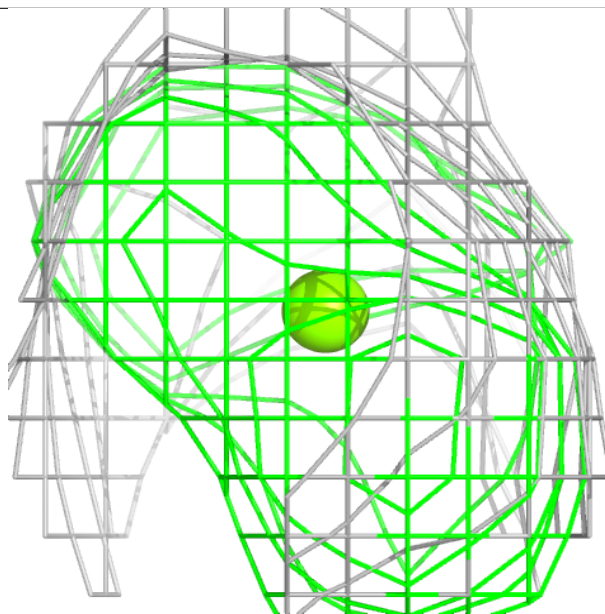
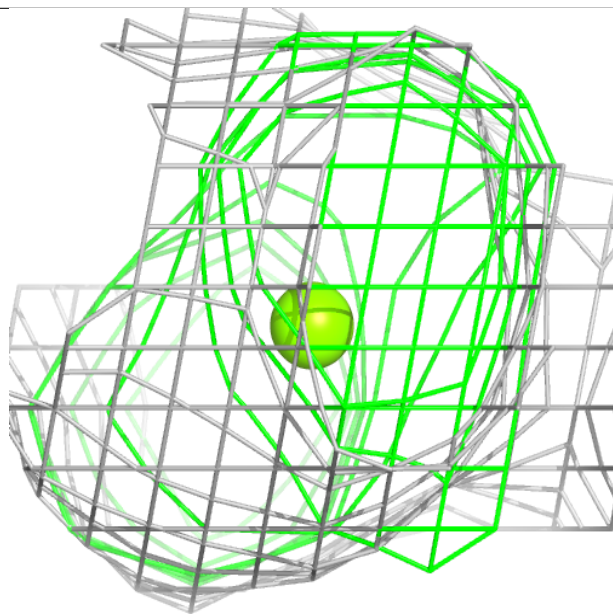
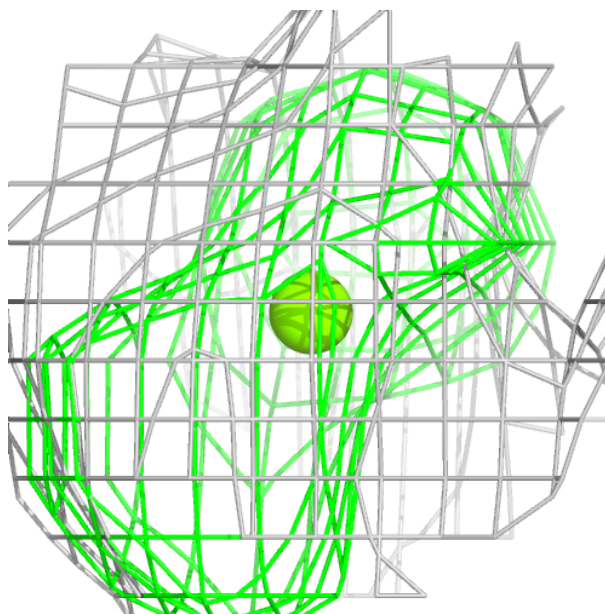
Electron density around MG B 501:

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



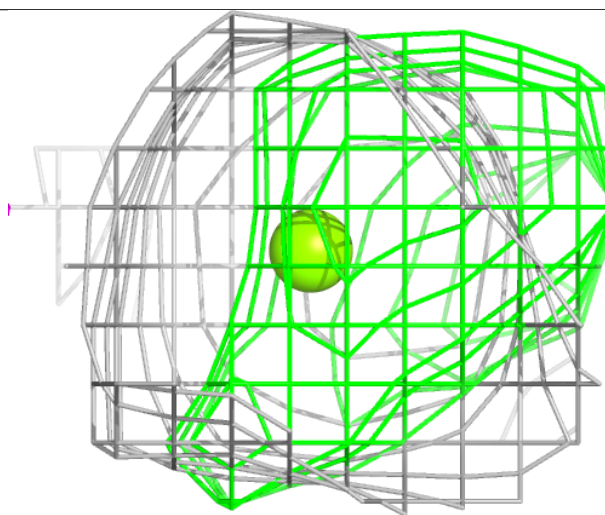
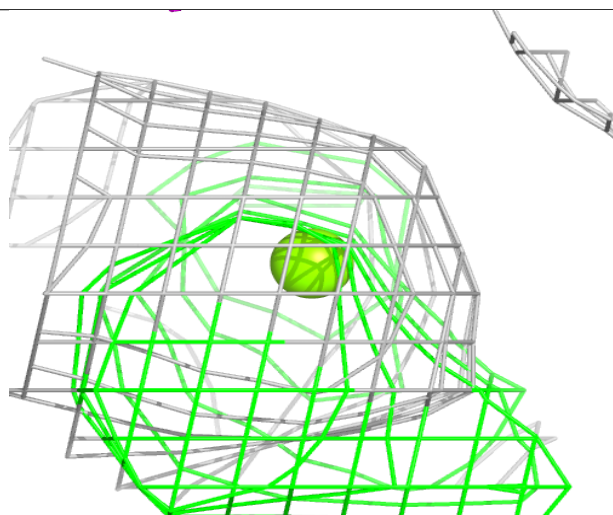
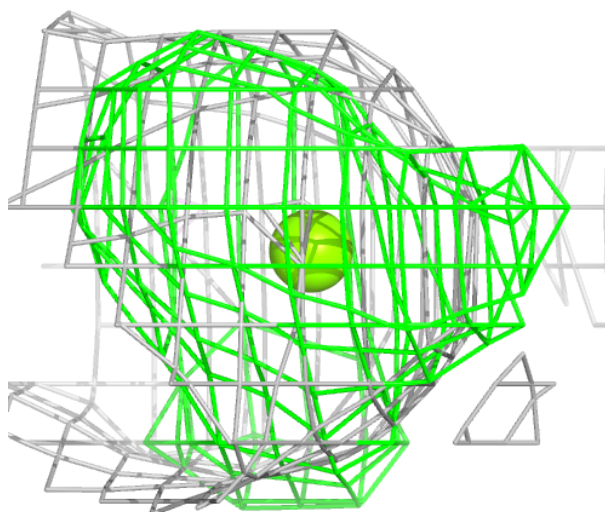
Electron density around MG B 502:

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



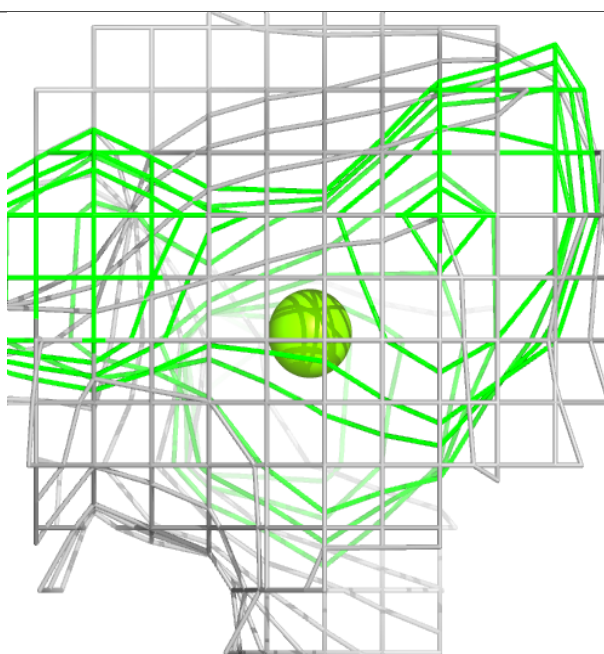
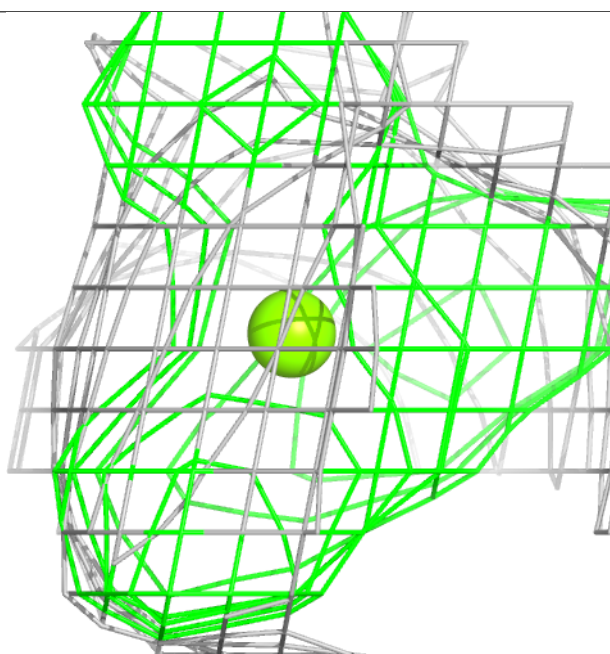
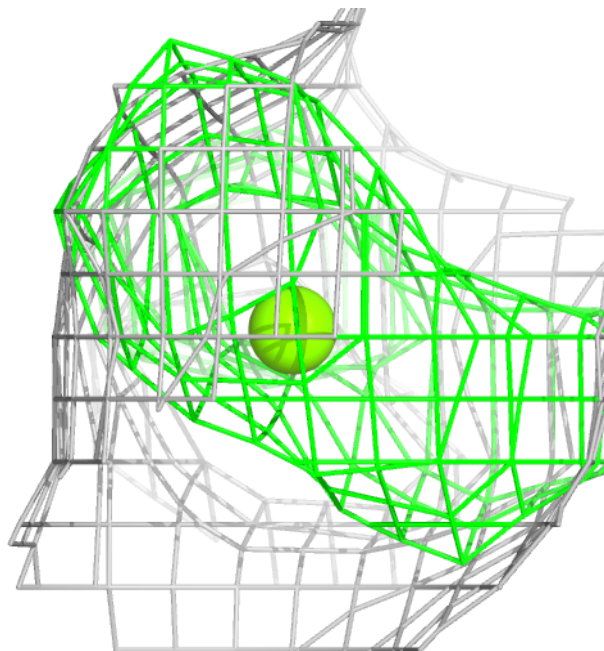
Electron density around MG C 501:

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



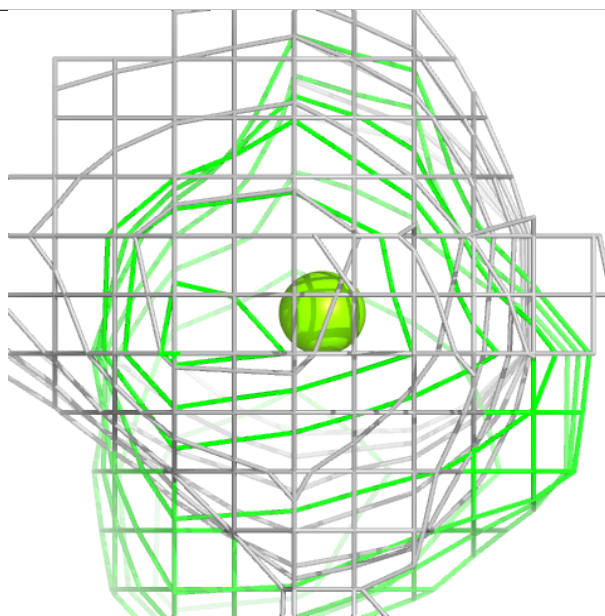
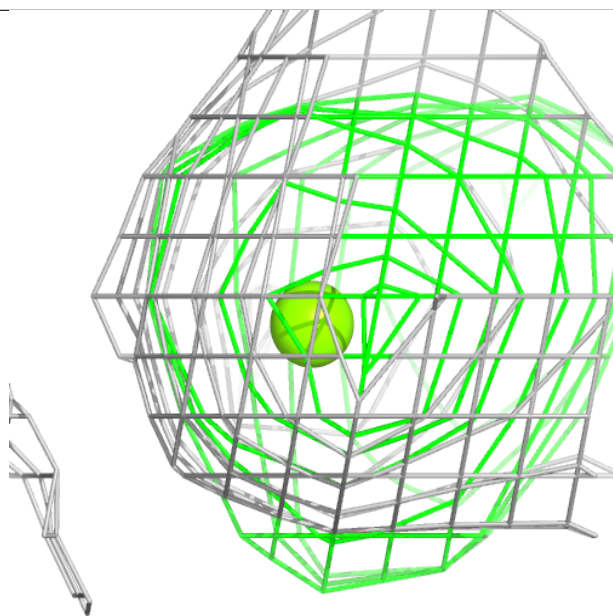
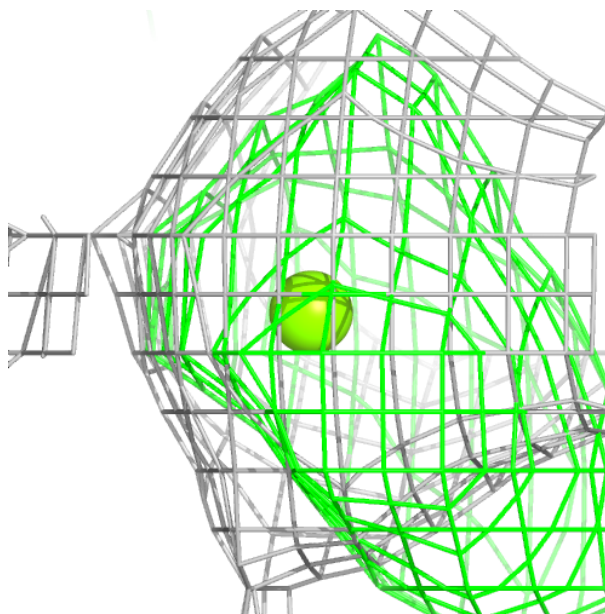
Electron density around MG A 502:

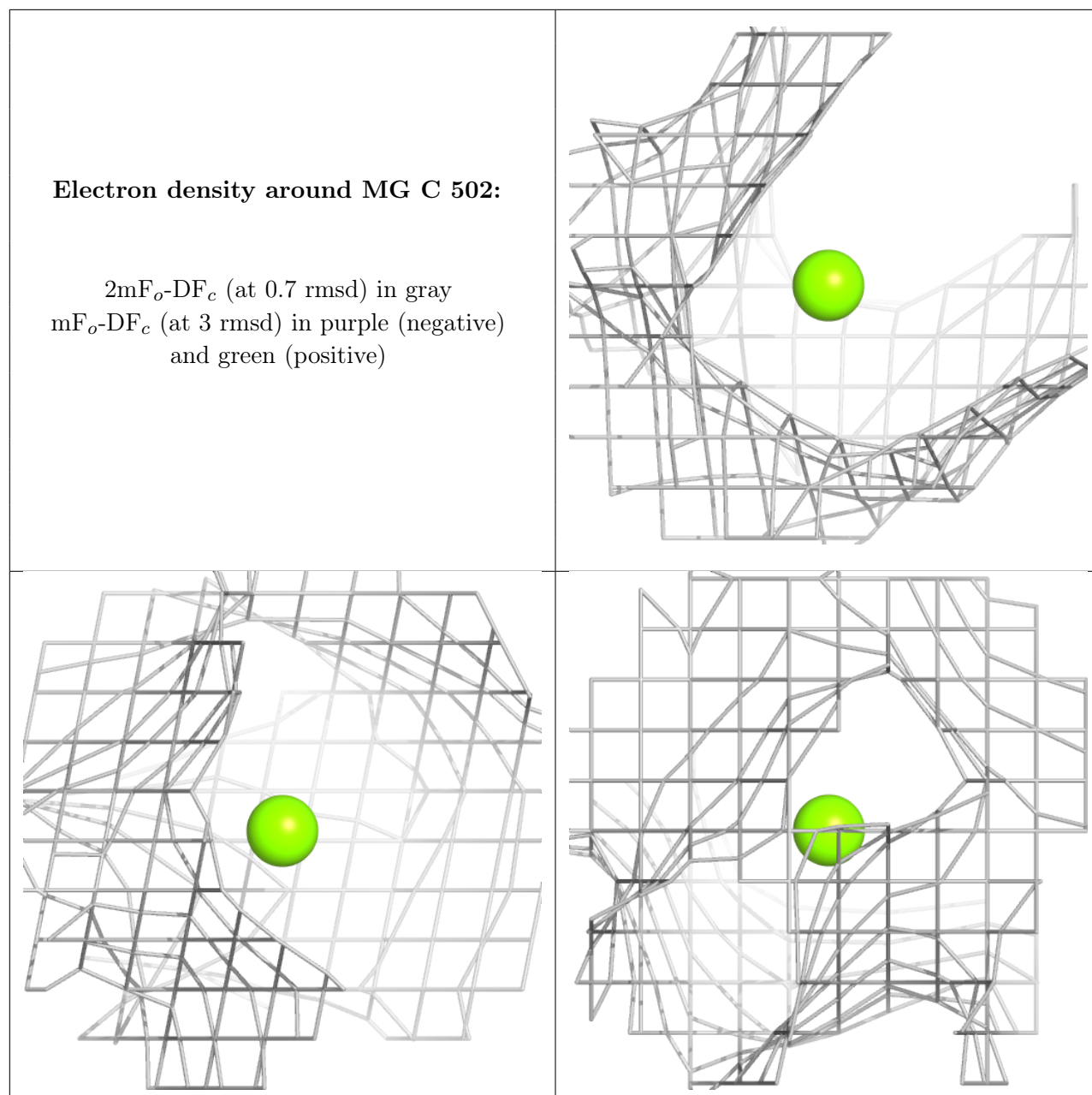
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG A 501:

$2mF_o-DF_c$ (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.