Full wwPDB X-ray Structure Validation Report ⓘ

Feb 7, 2022 – 03:27 pm GMT

PDB ID	:	7Q24
Title	:	Crystal structure of Angiotensin-1 converting enzyme N-domain in complex with dual ACE/NEP inhibitor AD011
Authors	:	Cozier, G.E.; Acharya, K.R.
Deposited on	:	2021-10-23
Resolution	:	2.00 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:

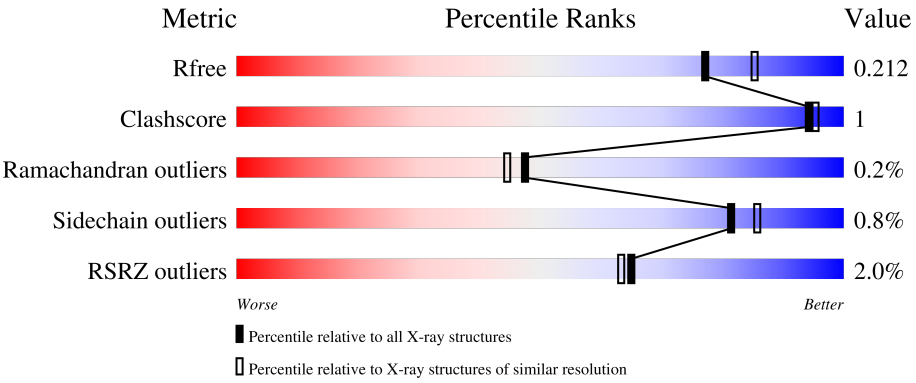
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



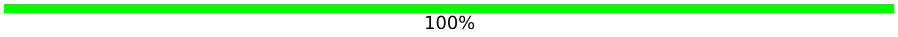
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	629	93%
1	B	629	93%
2	C	2	50% 50%
3	D	4	100%
3	F	4	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	2	
4	G	2	

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 20940 atoms, of which 9976 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 Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	606	Total	C	H	N	O	S	0	10	0
			9822	3227	4787	869	920	19			
1	B	609	Total	C	H	N	O	S	0	7	0
			9825	3227	4794	865	920	19			

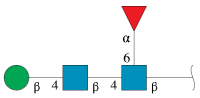
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	engineered mutation	UNP P12821
A	25	GLN	ASN	engineered mutation	UNP P12821
A	82	GLN	ASN	engineered mutation	UNP P12821
A	117	GLN	ASN	engineered mutation	UNP P12821
A	131	GLN	ASN	engineered mutation	UNP P12821
A	289	GLN	ASN	engineered mutation	UNP P12821
A	545	ARG	GLN	engineered mutation	UNP P12821
A	576	LEU	PRO	engineered mutation	UNP P12821
A	629	LEU	-	expression tag	UNP P12821
B	9	GLN	ASN	engineered mutation	UNP P12821
B	25	GLN	ASN	engineered mutation	UNP P12821
B	82	GLN	ASN	engineered mutation	UNP P12821
B	117	GLN	ASN	engineered mutation	UNP P12821
B	131	GLN	ASN	engineered mutation	UNP P12821
B	289	GLN	ASN	engineered mutation	UNP P12821
B	545	ARG	GLN	engineered mutation	UNP P12821
B	576	LEU	PRO	engineered mutation	UNP P12821
B	629	LEU	-	expression tag	UNP P12821

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

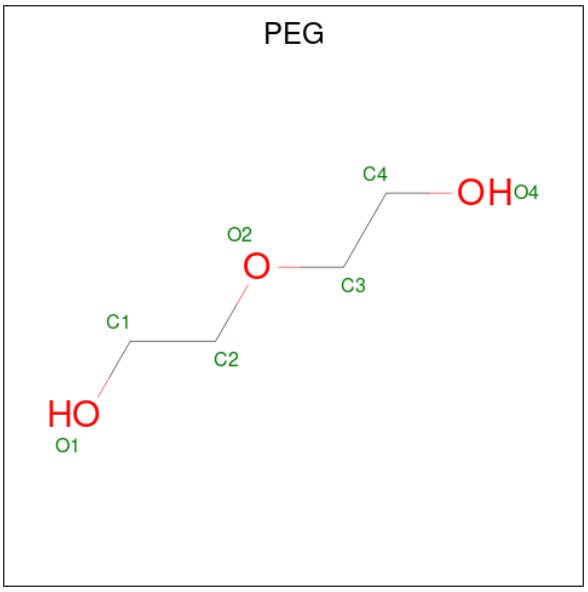


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	4	Total	C	H	N	O	0	0	0
			92	28	43	2	19			
3	F	4	Total	C	H	N	O	0	0	0
			92	28	43	2	19			

- Molecule 4 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

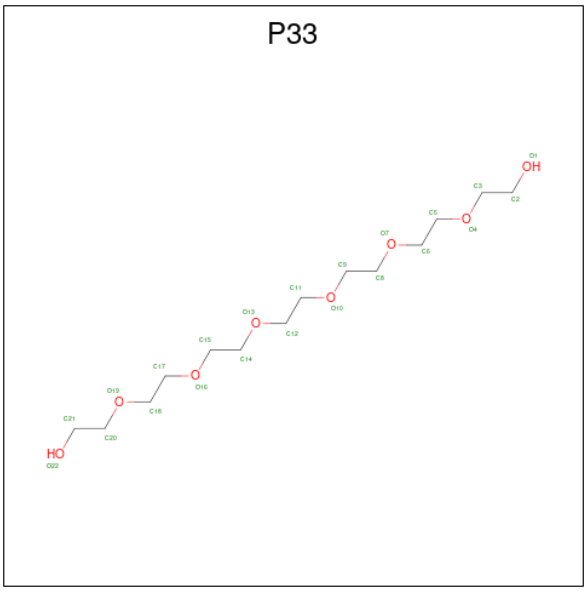
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	2	Total	C	H	N	O	0	0	0
			46	14	22	1	9			
4	G	2	Total	C	H	N	O	0	0	0
			46	14	22	1	9			

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



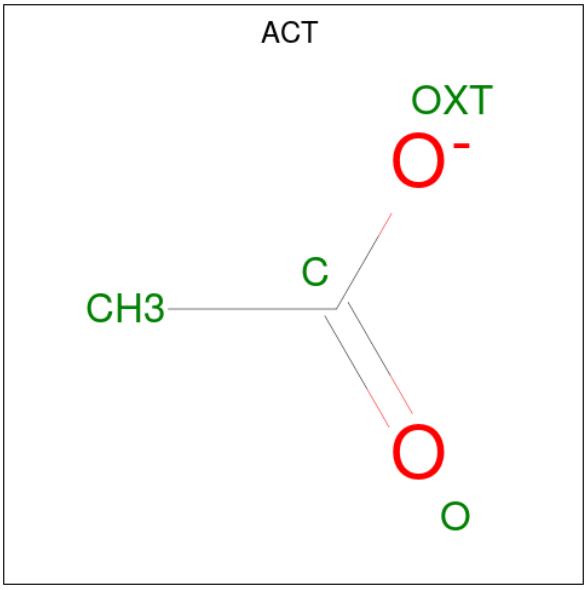
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 17 4 10 3	0	0
5	A	1	Total C H O 17 4 10 3	0	0
5	A	1	Total C H O 17 4 10 3	0	0
5	B	1	Total C H O 17 4 10 3	0	0

- Molecule 6 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (three-letter code: P33) (formula: $C_{14}H_{30}O_8$).



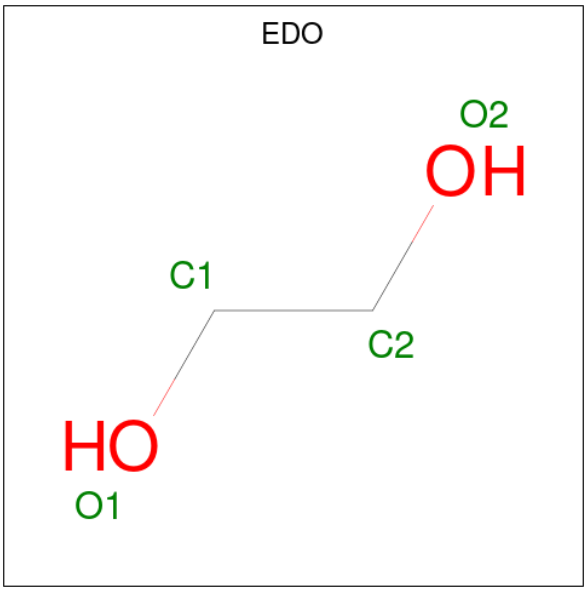
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			52	14	30	8		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



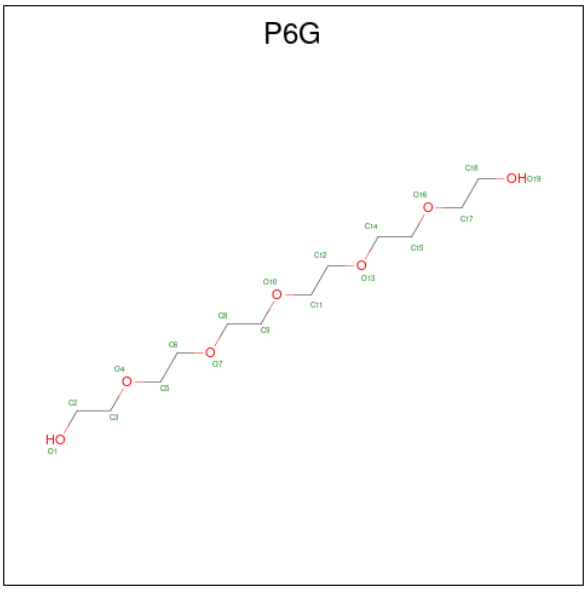
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			7	2	3	2		
7	B	1	Total	C	H	O	0	0
			7	2	3	2		
7	B	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H O 10 2 6 2	0	0
8	A	1	Total C H O 10 2 6 2	0	0
8	B	1	Total C H O 10 2 6 2	0	0
8	B	1	Total C H O 10 2 6 2	0	0

- Molecule 9 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C H O 45 12 26 7	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Zn 1 1	0	0
10	B	1	Total Zn 1 1	0	0

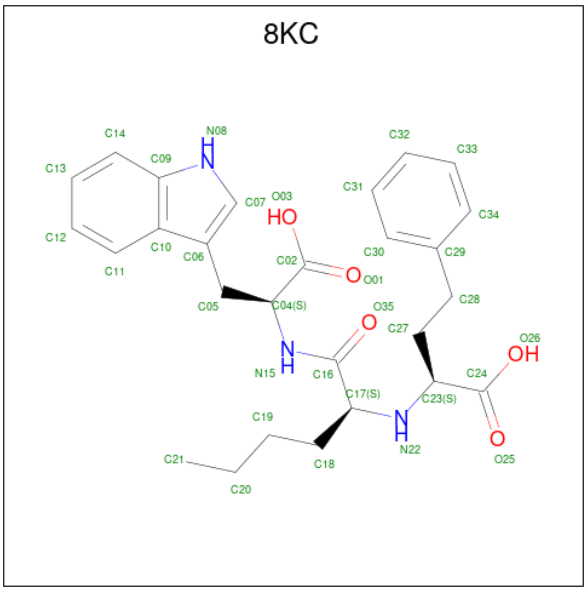
- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total Cl 1 1	0	0
11	B	1	Total Cl 1 1	0	0

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

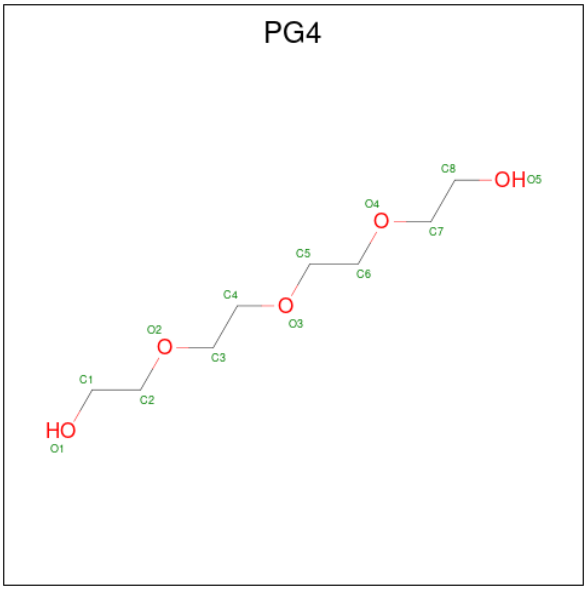
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total Mg 1 1	0	0
12	B	1	Total Mg 1 1	0	0

- Molecule 13 is (2 {S})-2-[[(2 {S})-1-[[(2 {S})-3-(1 {H}-indol-3-yl)-1-oxidanyl-1-oxidanylidene-propan-2-yl]amino]-1-oxidanylidene-hexan-2-yl]amino]-4-phenyl-butanoic acid (three-letter code: 8KC) (formula: $C_{27}H_{33}N_3O_5$) (labeled as "Ligand of Interest" by depositor).



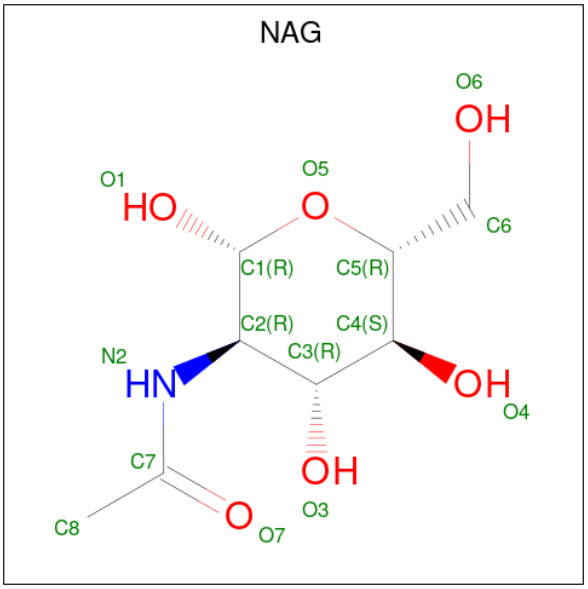
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	H	N	O	0	0
			66	27	31	3	5		
13	B	1	Total	C	H	N	O	0	0
			66	27	31	3	5		

- Molecule 14 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B	1	Total	C	H	O		0	0
			31	8	18	5			
14	B	1	Total	C	H	O		0	0
			31	8	18	5			

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 16 is water.

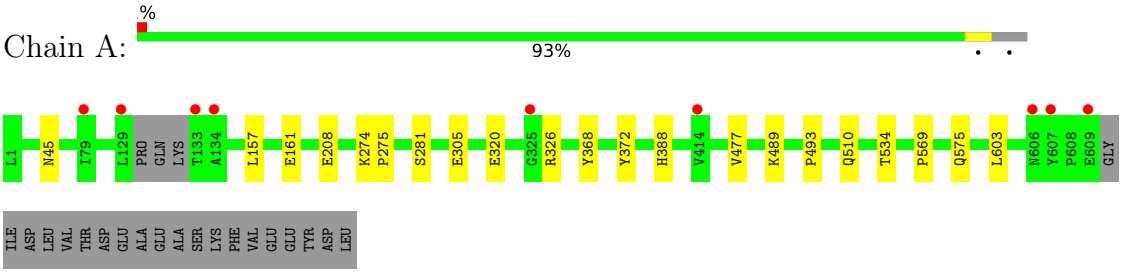
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	294	Total	O	0	1
			295	295		
16	B	216	Total	O	0	0
			216	216		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

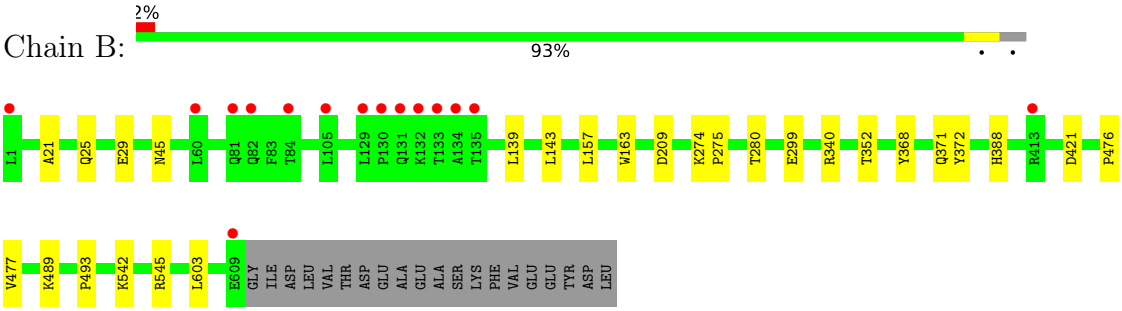
• Molecule 1: Angiotensin-converting enzyme

Chain A:



• Molecule 1: Angiotensin-converting enzyme

Chain B:

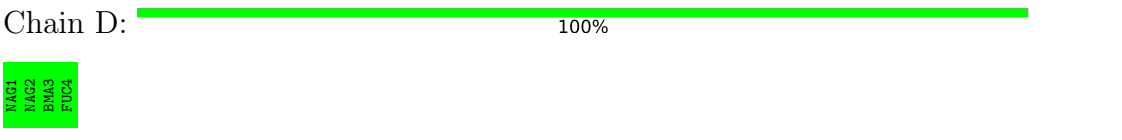


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

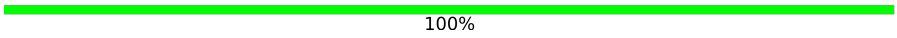


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• Molecule 4: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.77Å 77.61Å 81.65Å 88.93° 64.55° 75.01°	Depositor
Resolution (Å)	63.12 – 2.00 73.31 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (63.12-2.00) 97.5 (73.31-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.185 , 0.214 0.182 , 0.212	Depositor DCC
R_{free} test set	1964 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20940	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P33, CL, P6G, MG, ZN, BMA, FUC, NAG, PG4, PEG, 8KC, ACT, EDO

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	0.25	0/5191	0.47	0/7068
1	B	0.25	0/5188	0.47	0/7066
All	All	0.25	0/10379	0.47	0/14134

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5035	4787	4799	12	0
1	B	5031	4794	4805	13	0
2	C	28	25	25	1	0
3	D	49	43	43	0	0
3	F	49	43	43	0	0
4	E	24	22	22	0	0
4	G	24	22	22	0	0
5	A	21	30	30	0	0
5	B	7	10	10	0	0
6	A	22	30	30	0	0
7	A	4	3	3	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	8	6	6	1	0
8	A	8	12	12	0	0
8	B	8	12	12	0	0
9	A	19	26	26	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
13	A	35	31	0	0	0
13	B	35	31	0	0	0
14	B	26	36	36	0	0
15	B	14	13	13	0	0
16	A	295	0	0	4	0
16	B	216	0	0	3	0
All	All	10964	9976	9937	26	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 1.

All (26) 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:161:GLU:OE2	16:A:801:HOH:O	2.11	0.68
1:A:320:GLU:OE2	16:A:802:HOH:O	2.14	0.65
1:B:371:GLN:OE1	1:B:545:ARG:NH1	2.30	0.64
1:A:281:SER:OG	16:A:803:HOH:O	2.15	0.63
1:A:208:GLU:OE2	7:A:705:ACT:H1	2.07	0.54
1:B:477:VAL:HG12	1:B:603:LEU:HD21	1.89	0.54
1:A:274:LYS:HB3	1:A:275:PRO:HD2	1.95	0.48
1:B:542:LYS:NZ	16:B:812:HOH:O	2.47	0.48
1:A:575:GLN:NE2	16:A:810:HOH:O	2.42	0.48
1:B:489:LYS:O	1:B:493:PRO:HD2	2.14	0.48
1:B:280:THR:HG23	1:B:352:THR:HA	1.96	0.47
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.95	0.47
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.97	0.47
1:B:139:LEU:HA	1:B:143:LEU:HD12	1.98	0.45
1:B:21:ALA:O	1:B:25:GLN:HG2	2.17	0.45
1:A:477:VAL:HG12	1:A:603:LEU:HD21	1.98	0.44
1:A:489:LYS:O	1:A:493:PRO:HD2	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LEU:HD22	1:B:163:TRP:CZ2	2.53	0.44
1:A:326:ARG:HD3	2:C:1:NAG:H82	2.00	0.43
1:B:299:GLU:OE2	16:B:801:HOH:O	2.21	0.43
7:B:705:ACT:H1	16:B:836:HOH:O	2.18	0.43
1:B:157:LEU:HD13	1:B:476:PRO:HB2	2.01	0.42
1:A:305:GLU:HG3	1:A:534:THR:HG22	2.01	0.42
1:A:510:GLN:HG2	1:A:569:PRO:HG2	2.02	0.41
1:B:29:GLU:OE2	1:B:340:ARG:NH1	2.54	0.41
1:B:274:LYS:HB3	1:B:275:PRO:HD2	2.02	0.41

There are no symmetry-related clashes.

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	612/629 (97%)	601 (98%)	10 (2%)	1 (0%)	47	44
1	B	614/629 (98%)	603 (98%)	10 (2%)	1 (0%)	47	44
All	All	1226/1258 (98%)	1204 (98%)	20 (2%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	B	45	ASN

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	531/541 (98%)	528 (99%)	3 (1%)	86 90
1	B	531/541 (98%)	526 (99%)	5 (1%)	78 83
All	All	1062/1082 (98%)	1054 (99%)	8 (1%)	81 86

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	B	209	ASP
1	B	368	TYR
1	B	372	TYR
1	B	388	HIS
1	B	421	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

14 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	C	1	2,1	14,14,15	0.23	0	17,19,21	0.58	0
2	NAG	C	2	2	14,14,15	0.22	0	17,19,21	0.47	0
3	NAG	D	1	1,3	14,14,15	0.33	0	17,19,21	0.38	0
3	NAG	D	2	3	14,14,15	0.24	0	17,19,21	0.43	0
3	BMA	D	3	3	11,11,12	0.55	0	15,15,17	0.74	0
3	FUC	D	4	3	10,10,11	0.68	0	14,14,16	0.75	0
4	NAG	E	1	4,1	14,14,15	0.45	0	17,19,21	0.46	0
4	FUC	E	2	4	10,10,11	0.89	0	14,14,16	0.77	0
3	NAG	F	1	1,3	14,14,15	0.37	0	17,19,21	0.39	0
3	NAG	F	2	3	14,14,15	0.40	0	17,19,21	0.54	0
3	BMA	F	3	3	11,11,12	0.52	0	15,15,17	1.08	1 (6%)
3	FUC	F	4	3	10,10,11	0.59	0	14,14,16	0.91	1 (7%)
4	NAG	G	1	4,1	14,14,15	0.32	0	17,19,21	0.39	0
4	FUC	G	2	4	10,10,11	0.73	0	14,14,16	1.00	1 (7%)

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	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	FUC	D	4	3	-	-	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	FUC	E	2	4	-	-	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
3	FUC	F	4	3	-	-	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	FUC	G	2	4	-	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	3	BMA	C1-O5-C5	2.59	115.70	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	2	FUC	C1-C2-C3	2.44	112.66	109.67
3	F	4	FUC	C1-O5-C5	2.03	117.39	112.78

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6

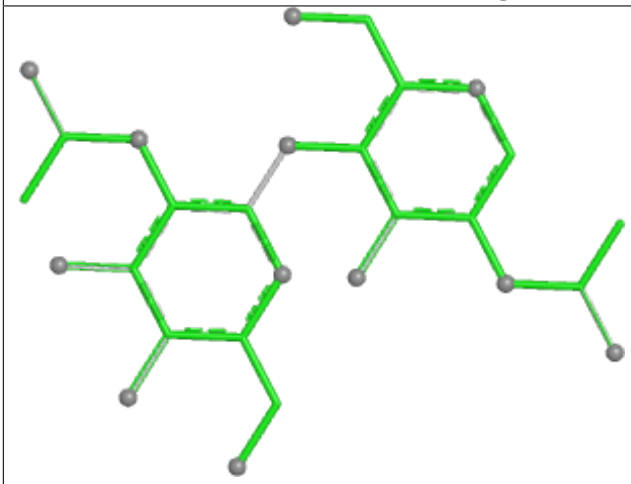
There are no ring outliers.

1 monomer is involved in 1 short contact:

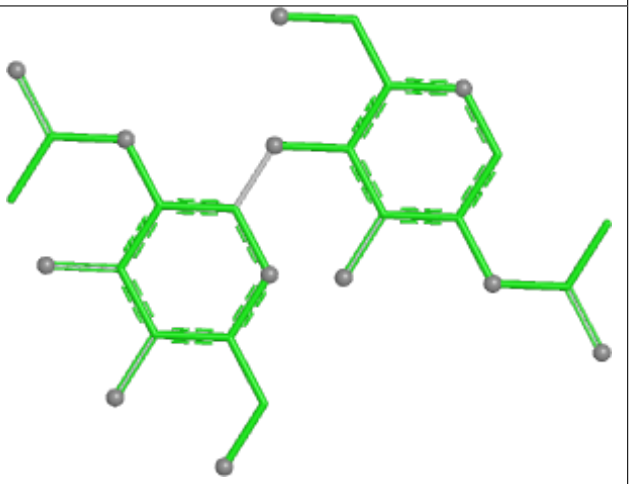
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0

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

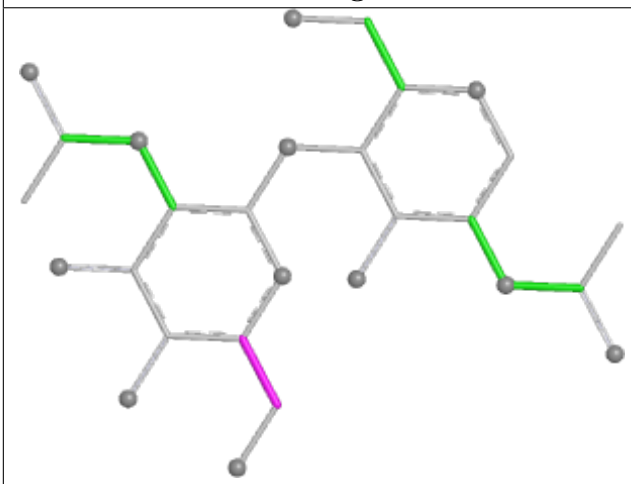
Oligosaccharide Chain C



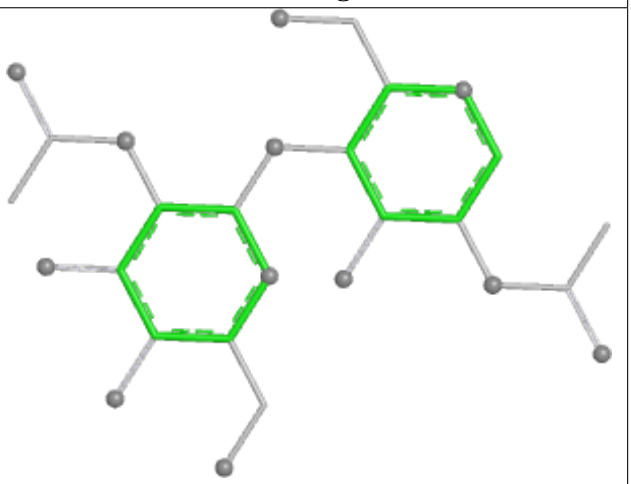
Bond lengths



Bond angles

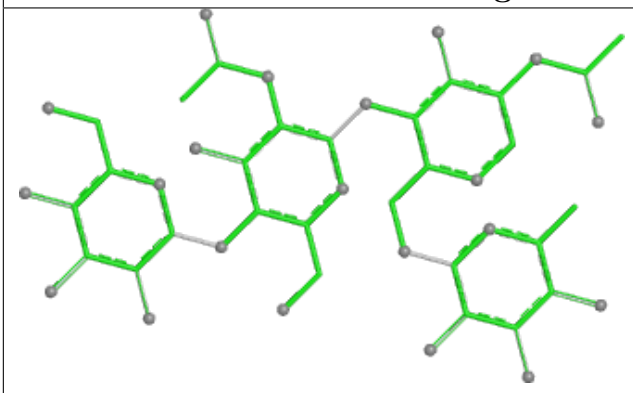


Torsions

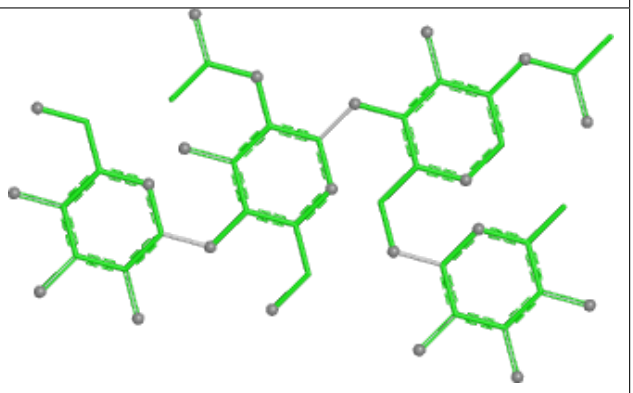


Rings

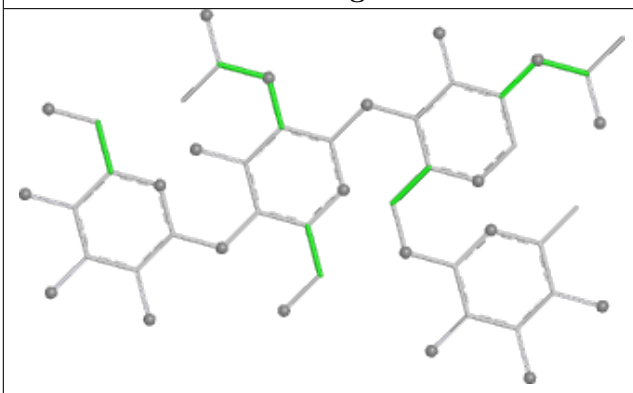
Oligosaccharide Chain D



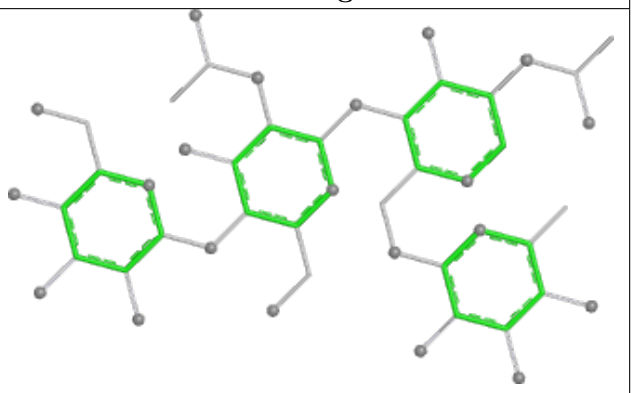
Bond lengths



Bond angles

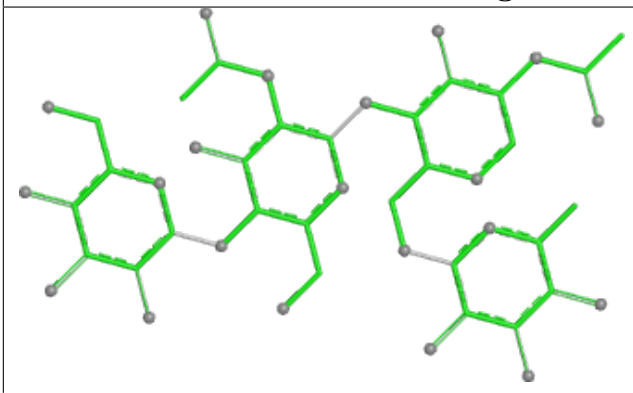


Torsions

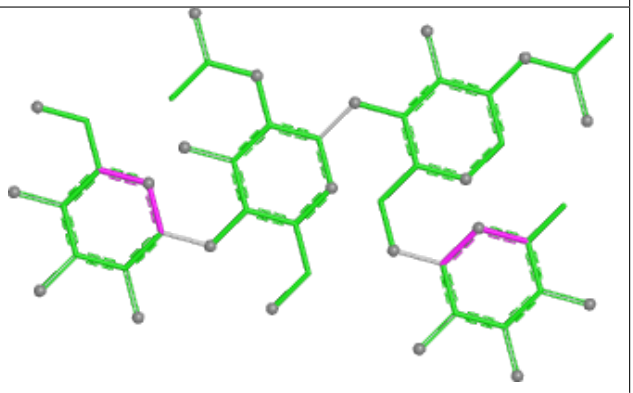


Rings

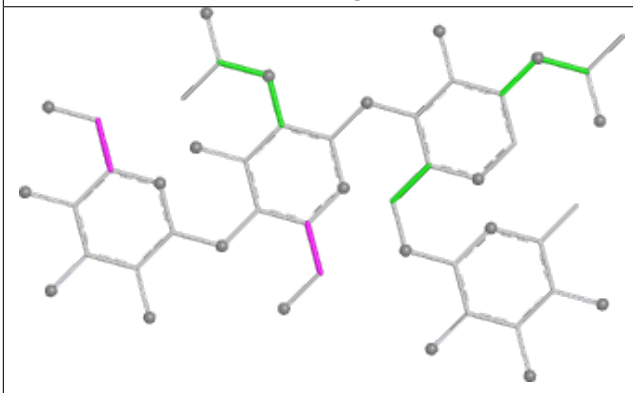
Oligosaccharide Chain F



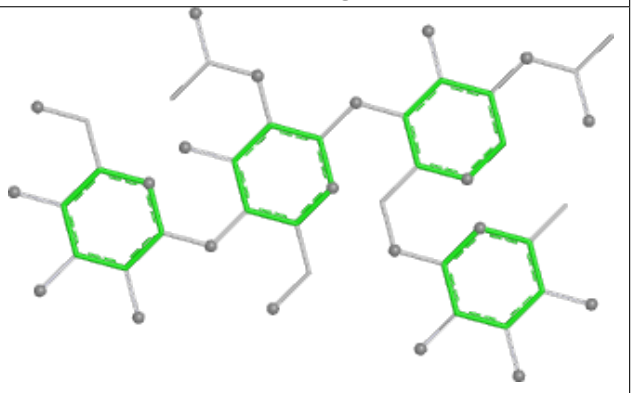
Bond lengths



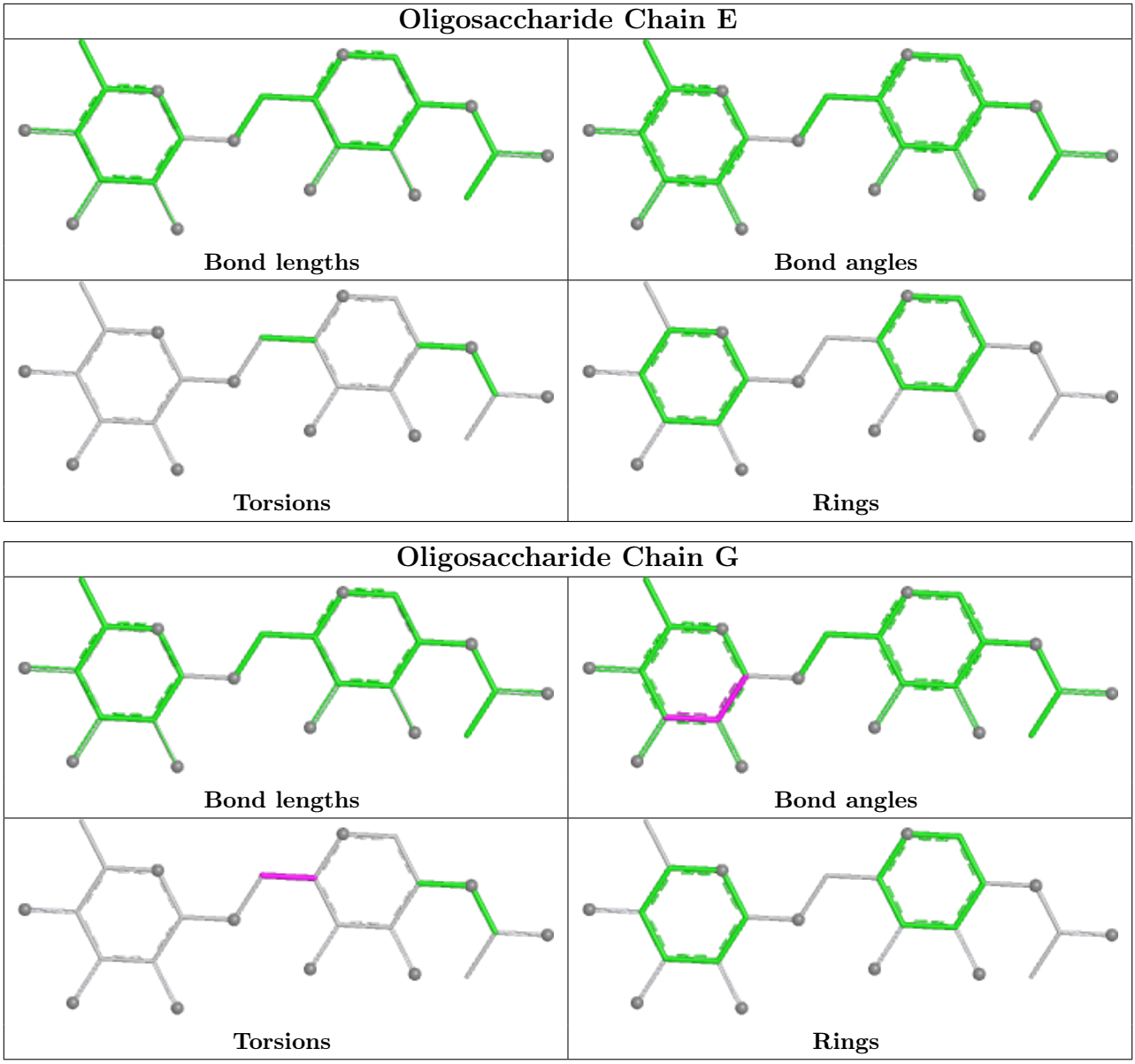
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 for Mogul analysis.

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	$\#\|Z\|>2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PEG	A	704	-	6,6,6	0.11	0	5,5,5	0.11	0
9	P6G	A	707	-	18,18,18	0.11	0	17,17,17	0.14	0
5	PEG	A	702	-	6,6,6	0.10	0	5,5,5	0.13	0
13	8KC	A	712	10	30,37,37	1.72	5 (16%)	34,49,49	0.90	2 (5%)
6	P33	A	703	-	21,21,21	0.54	0	20,20,20	0.24	0
8	EDO	B	706	-	3,3,3	0.47	0	2,2,2	0.30	0
7	ACT	A	705	-	1,3,3	6.20	1 (100%)	0,3,3	-	-
7	ACT	B	705	-	1,3,3	6.24	1 (100%)	0,3,3	-	-
8	EDO	A	706	-	3,3,3	0.47	0	2,2,2	0.29	0
8	EDO	B	703	-	3,3,3	0.47	0	2,2,2	0.26	0
14	PG4	B	701	-	12,12,12	0.12	0	11,11,11	0.61	0
15	NAG	B	702	1	14,14,15	0.29	0	17,19,21	0.54	0
7	ACT	B	707	-	1,3,3	6.24	1 (100%)	0,3,3	-	-
14	PG4	B	704	-	12,12,12	0.13	0	11,11,11	0.52	0
8	EDO	A	708	-	3,3,3	0.46	0	2,2,2	0.31	0
13	8KC	B	712	10	30,37,37	1.71	5 (16%)	34,49,49	0.76	1 (2%)
5	PEG	B	708	-	6,6,6	0.11	0	5,5,5	0.10	0
5	PEG	A	701	-	6,6,6	0.10	0	5,5,5	0.09	0

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
5	PEG	A	704	-	-	2/4/4/4	-
9	P6G	A	707	-	-	6/16/16/16	-
5	PEG	A	702	-	-	1/4/4/4	-
13	8KC	A	712	10	-	6/24/42/42	0/3/3/3
6	P33	A	703	-	-	10/19/19/19	-
8	EDO	B	706	-	-	0/1/1/1	-
14	PG4	B	701	-	-	4/10/10/10	-
15	NAG	B	702	1	-	0/6/23/26	0/1/1/1
8	EDO	A	706	-	-	0/1/1/1	-
8	EDO	B	703	-	-	0/1/1/1	-
14	PG4	B	704	-	-	4/10/10/10	-
8	EDO	A	708	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	8KC	B	712	10	-	6/24/42/42	0/3/3/3
5	PEG	B	708	-	-	0/4/4/4	-
5	PEG	A	701	-	-	1/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	712	8KC	C16-N15	6.59	1.48	1.34
13	B	712	8KC	C16-N15	6.56	1.48	1.34
7	B	705	ACT	CH3-C	6.24	1.56	1.48
7	B	707	ACT	CH3-C	6.24	1.56	1.48
7	A	705	ACT	CH3-C	6.20	1.56	1.48
13	A	712	8KC	C27-C23	3.19	1.57	1.53
13	B	712	8KC	C27-C23	3.13	1.57	1.53
13	A	712	8KC	C28-C29	2.20	1.58	1.51
13	B	712	8KC	C28-C29	2.16	1.58	1.51
13	B	712	8KC	O35-C16	-2.12	1.19	1.23
13	A	712	8KC	O35-C16	-2.07	1.19	1.23
13	B	712	8KC	C05-C06	2.06	1.57	1.51
13	A	712	8KC	C05-C06	2.02	1.56	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	712	8KC	C04-N15-C16	-2.93	118.79	123.19
13	A	712	8KC	C05-C04-N15	2.06	112.75	109.01
13	B	712	8KC	C04-N15-C16	-2.01	120.18	123.19

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	712	8KC	C24-C23-C27-C28
13	A	712	8KC	N22-C23-C27-C28
13	A	712	8KC	C02-C04-C05-C06
13	B	712	8KC	C24-C23-C27-C28
13	B	712	8KC	N22-C23-C27-C28
13	B	712	8KC	C05-C04-N15-C16
14	B	701	PG4	O4-C7-C8-O5
6	A	703	P33	O16-C17-C18-O19
9	A	707	P6G	O7-C8-C9-O10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	703	P33	O4-C5-C6-O7
6	A	703	P33	O7-C8-C9-O10
14	B	704	PG4	O4-C7-C8-O5
6	A	703	P33	O13-C14-C15-O16
9	A	707	P6G	O16-C17-C18-O19
14	B	701	PG4	O1-C1-C2-O2
13	A	712	8KC	C05-C04-N15-C16
13	B	712	8KC	C02-C04-N15-C16
5	A	702	PEG	O2-C3-C4-O4
13	B	712	8KC	C18-C19-C20-C21
14	B	704	PG4	O2-C3-C4-O3
14	B	704	PG4	C1-C2-O2-C3
6	A	703	P33	O10-C11-C12-O13
13	A	712	8KC	N15-C04-C05-C06
13	B	712	8KC	N15-C04-C05-C06
9	A	707	P6G	C18-C17-O16-C15
13	A	712	8KC	C02-C04-N15-C16
6	A	703	P33	C17-C18-O19-C20
14	B	704	PG4	O3-C5-C6-O4
5	A	701	PEG	O2-C3-C4-O4
6	A	703	P33	O1-C2-C3-O4
8	A	708	EDO	O1-C1-C2-O2
6	A	703	P33	C5-C6-O7-C8
14	B	701	PG4	O3-C5-C6-O4
9	A	707	P6G	C11-C12-O13-C14
14	B	701	PG4	C4-C3-O2-C2
6	A	703	P33	C18-C17-O16-C15
9	A	707	P6G	C6-C5-O4-C3
5	A	704	PEG	C1-C2-O2-C3
9	A	707	P6G	C12-C11-O10-C9
6	A	703	P33	C8-C9-O10-C11
5	A	704	PEG	O1-C1-C2-O2

There are no ring outliers.

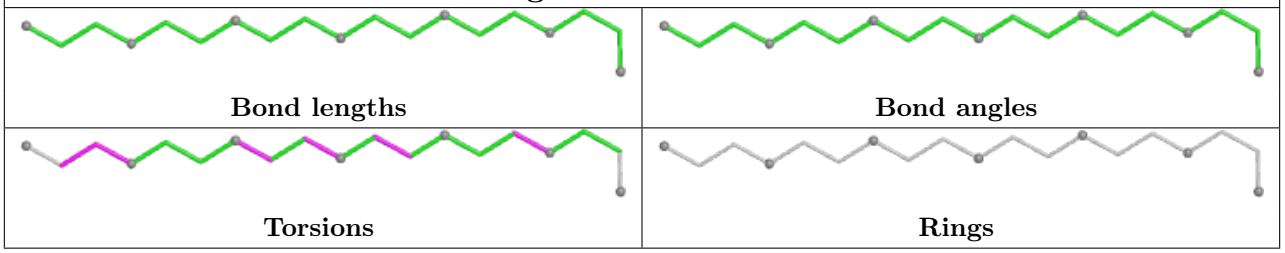
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	705	ACT	1	0
7	B	705	ACT	1	0

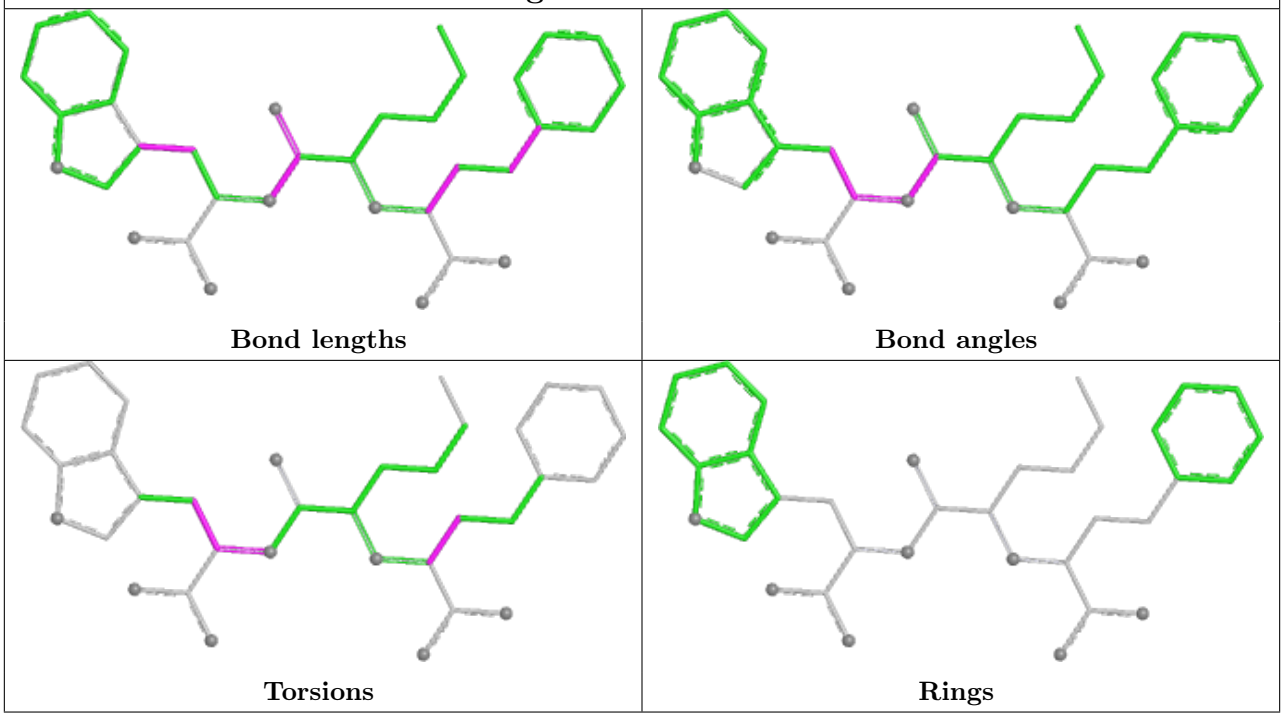
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

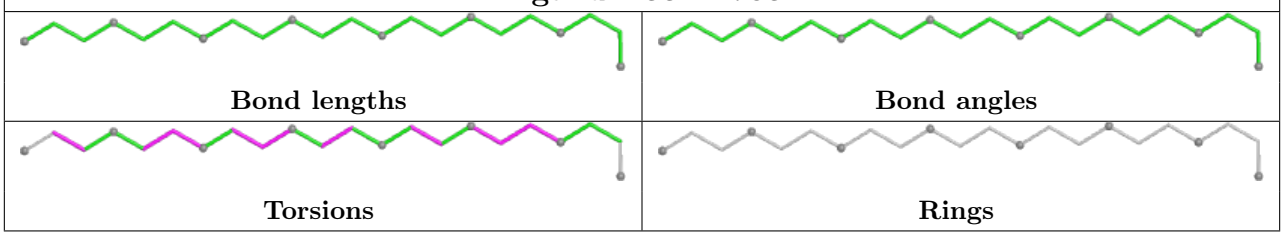
Ligand P6G A 707

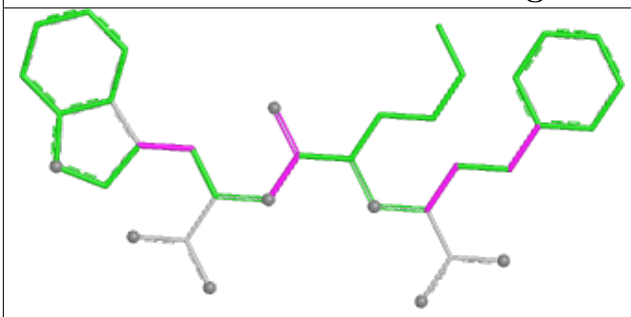
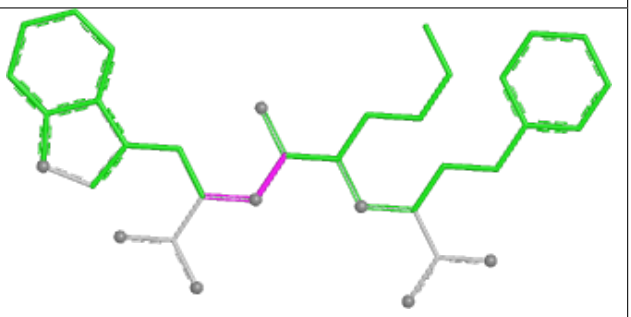
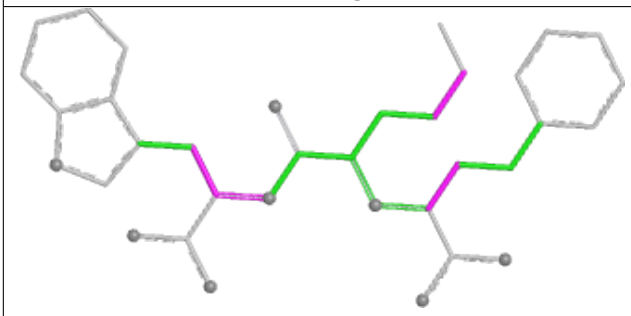
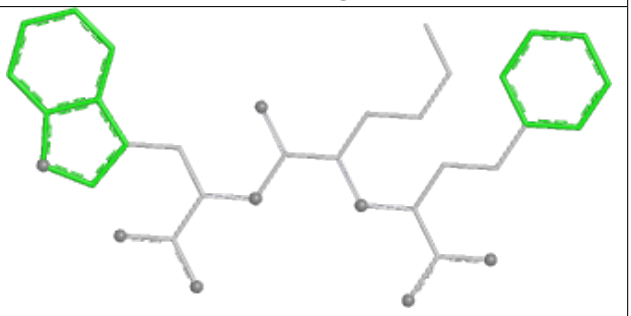


Ligand 8KC A 712



Ligand P33 A 703



Ligand 8KC B 712	
	
Bond lengths	Bond angles
	
Torsions	Rings

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, 95^{th} 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	606/629 (96%)	-0.12	9 (1%)	73	72	21, 35, 61, 106	0
1	B	609/629 (96%)	0.04	15 (2%)	57	56	23, 43, 80, 124	0
All	All	1215/1258 (96%)	-0.04	24 (1%)	65	63	21, 38, 72, 124	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	130	PRO	5.2
1	A	325	GLY	5.1
1	B	134	ALA	5.0
1	B	133	THR	4.1
1	B	132	LYS	4.0
1	B	131	GLN	3.8
1	A	129	LEU	3.5
1	B	1	LEU	3.5
1	A	133	THR	3.4
1	A	607	TYR	3.4
1	B	81	GLN	3.3
1	A	609	GLU	3.1
1	B	609	GLU	3.0
1	B	129	LEU	3.0
1	B	60	LEU	2.7
1	B	84	THR	2.4
1	A	606	ASN	2.4
1	A	134	ALA	2.2
1	A	414	VAL	2.2
1	B	82	GLN	2.1
1	B	135	THR	2.1
1	B	413	ARG	2.1
1	A	79	ILE	2.1
1	B	105	LEU	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)

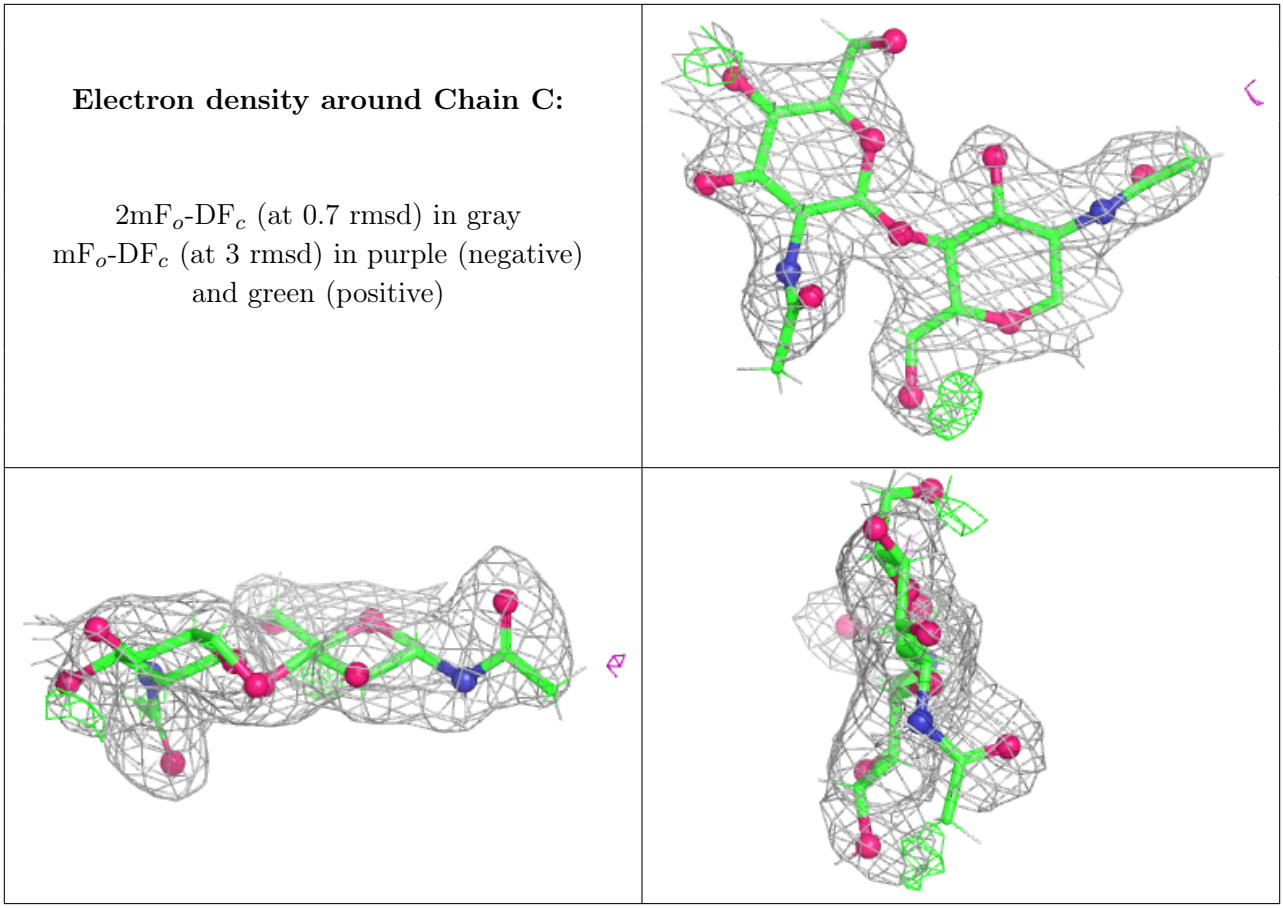
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	FUC	G	2	10/11	0.71	0.20	71,85,96,101	0
3	BMA	F	3	11/12	0.74	0.28	107,120,142,145	0
3	FUC	F	4	10/11	0.80	0.31	75,95,114,125	0
4	FUC	E	2	10/11	0.82	0.20	61,80,92,97	0
3	BMA	D	3	11/12	0.82	0.15	74,89,105,111	0
2	NAG	C	2	14/15	0.83	0.18	59,83,102,104	0
4	NAG	G	1	14/15	0.84	0.15	45,62,78,90	0
4	NAG	E	1	14/15	0.88	0.13	41,57,69,77	0
2	NAG	C	1	14/15	0.89	0.11	51,60,71,73	0
3	FUC	D	4	10/11	0.89	0.19	59,71,84,86	0
3	NAG	F	2	14/15	0.89	0.17	77,90,104,108	0
3	NAG	F	1	14/15	0.92	0.18	70,77,92,98	0
3	NAG	D	1	14/15	0.93	0.12	44,57,71,71	0
3	NAG	D	2	14/15	0.95	0.17	53,71,83,90	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.

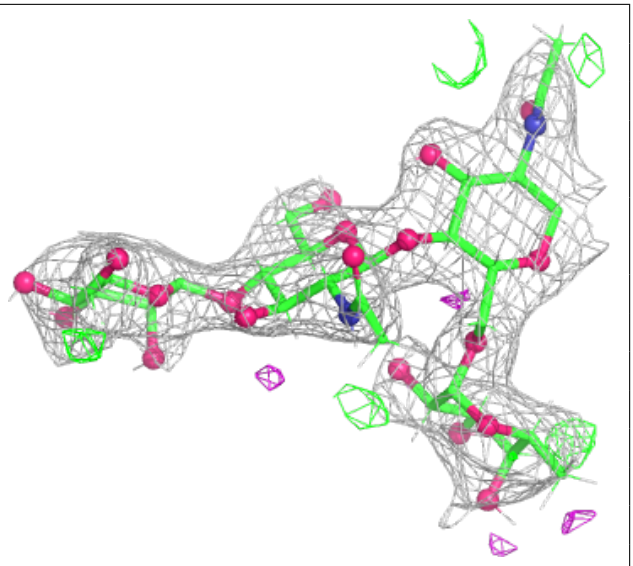
Electron density around Chain C:

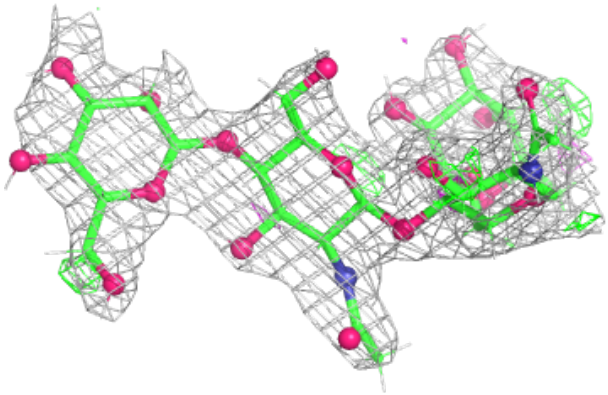
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

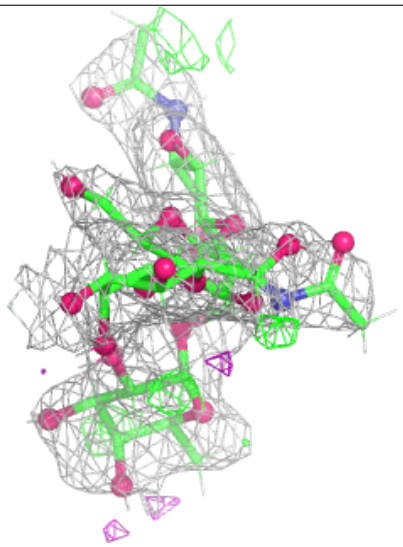


Electron density around Chain D:

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

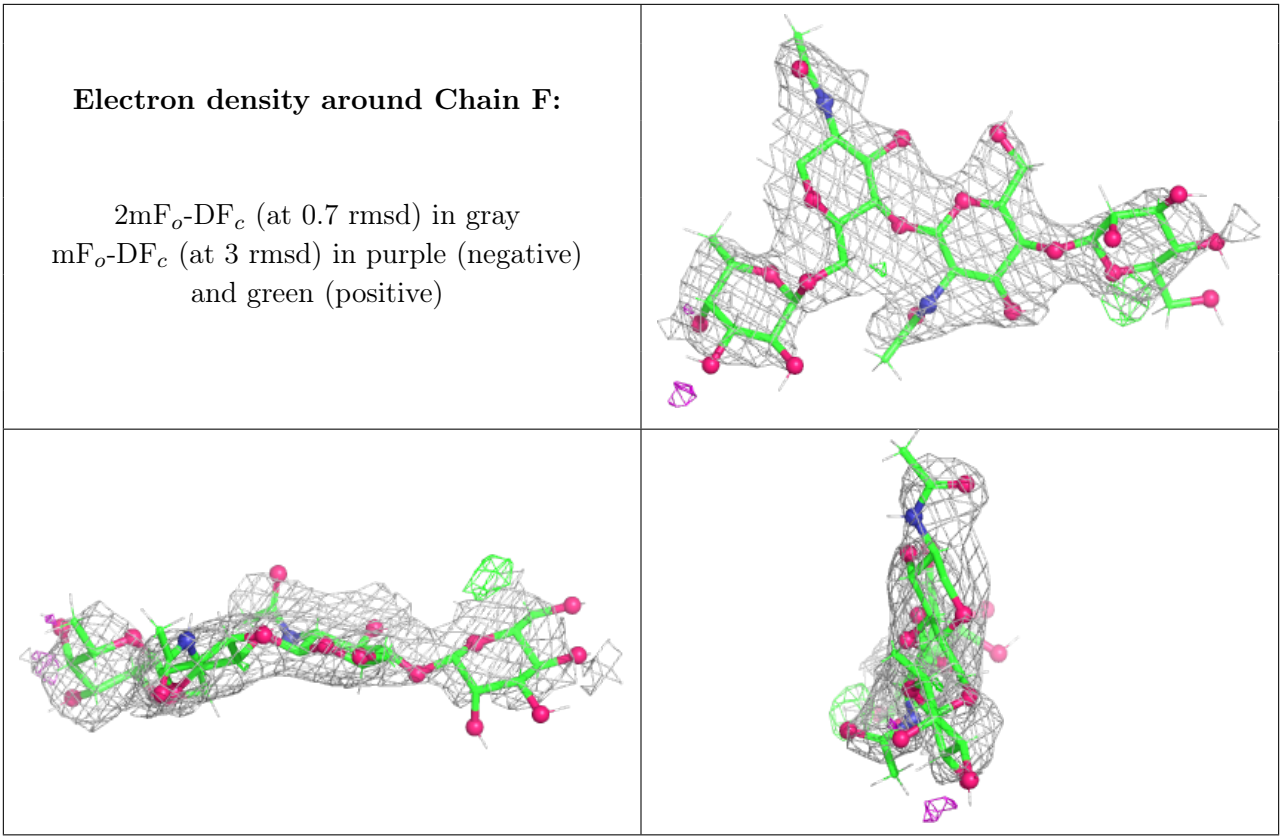






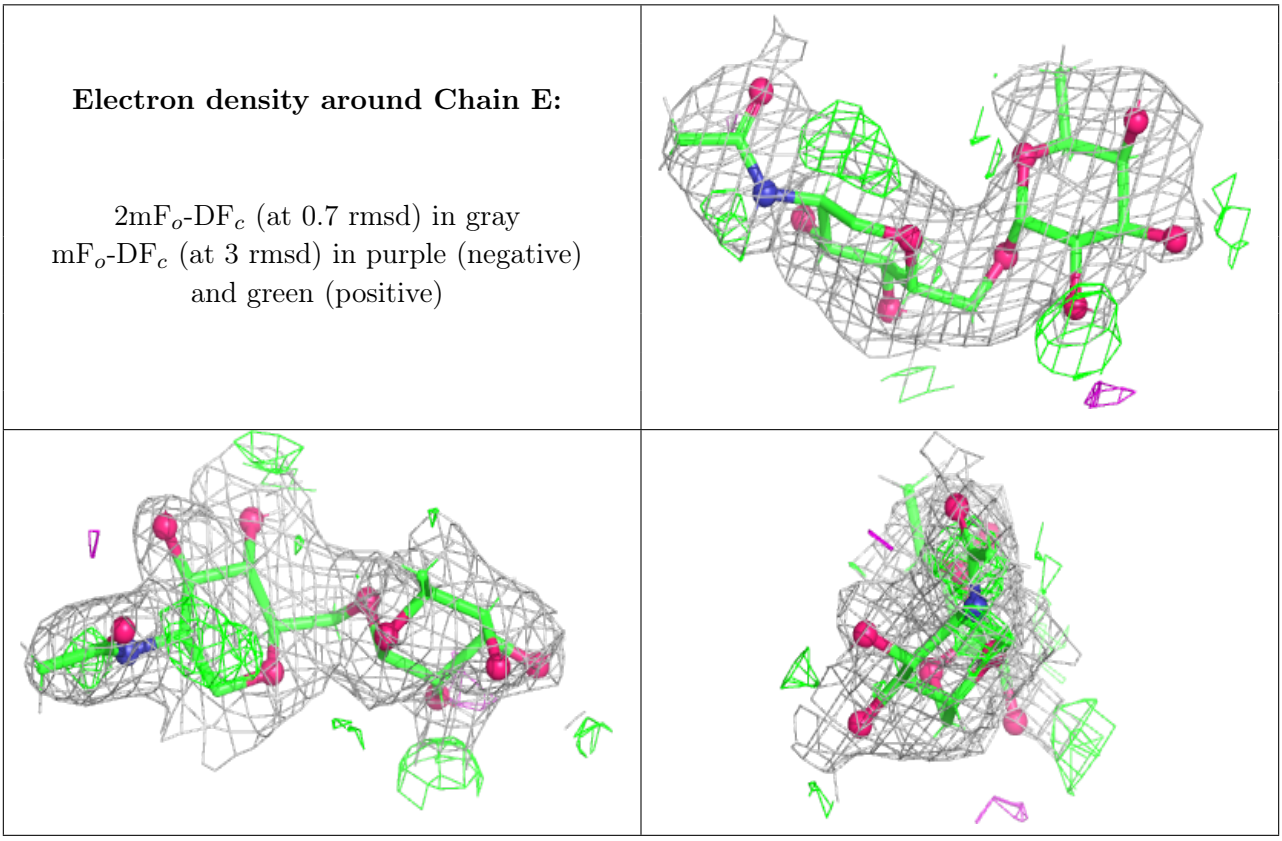
Electron density around Chain F:

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



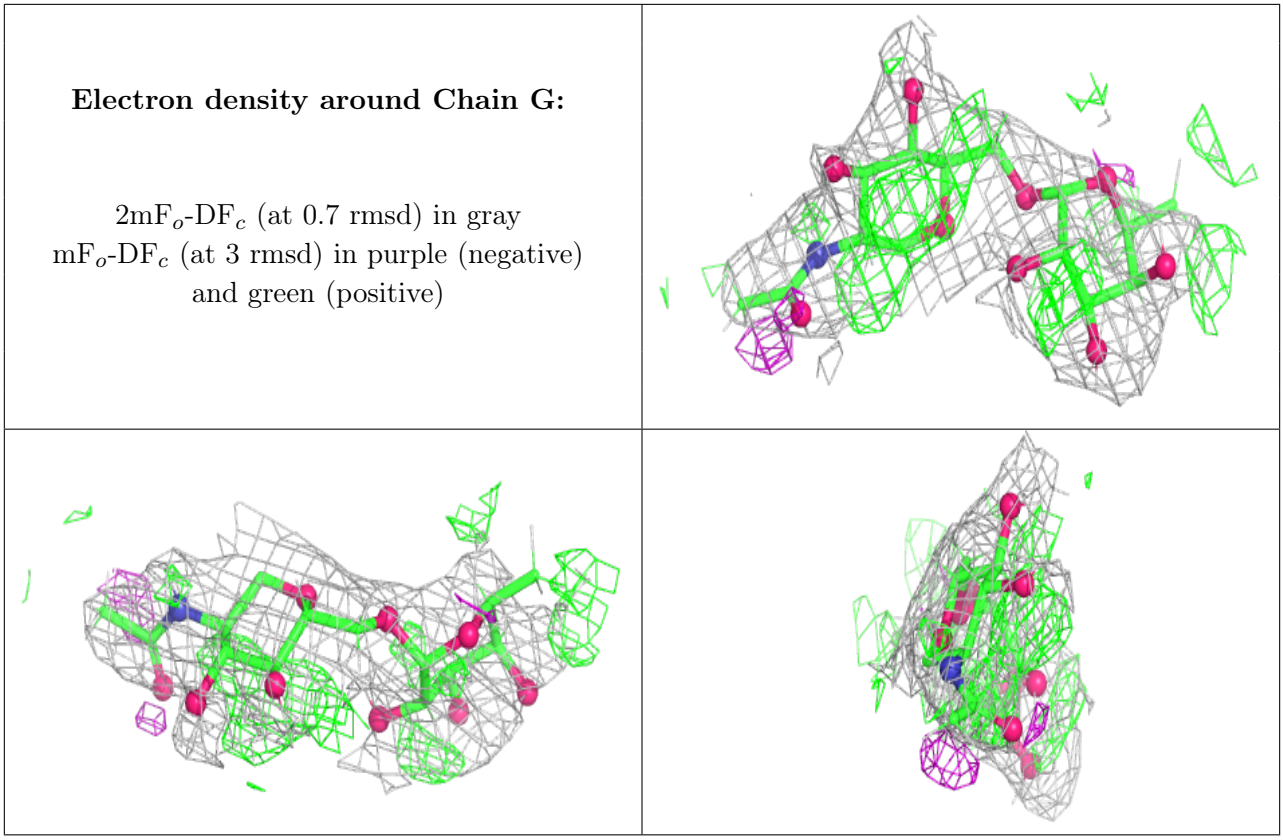
Electron density around Chain E:

$2mF_o$-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 G:

$2mF_o$-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, 95^{th} 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
6	P33	A	703	22/22	0.77	0.16	43,59,72,82	0
15	NAG	B	702	14/15	0.80	0.18	66,78,94,95	0
7	ACT	B	707	4/4	0.83	0.15	59,64,71,71	0
7	ACT	B	705	4/4	0.84	0.15	48,58,59,61	0
7	ACT	A	705	4/4	0.85	0.18	41,49,54,57	0
8	EDO	B	706	4/4	0.86	0.15	55,66,70,70	0
8	EDO	A	708	4/4	0.86	0.10	50,60,65,76	0
8	EDO	B	703	4/4	0.88	0.11	51,61,69,76	0
5	PEG	B	708	7/7	0.88	0.21	58,71,86,94	0
5	PEG	A	704	7/7	0.88	0.18	53,63,70,76	0
12	MG	A	711	1/1	0.89	0.12	52,52,52,52	0
8	EDO	A	706	4/4	0.89	0.29	40,50,60,72	0
5	PEG	A	701	7/7	0.90	0.10	43,54,67,73	0
14	PG4	B	701	13/13	0.90	0.18	39,50,68,77	0

Continued on next page...

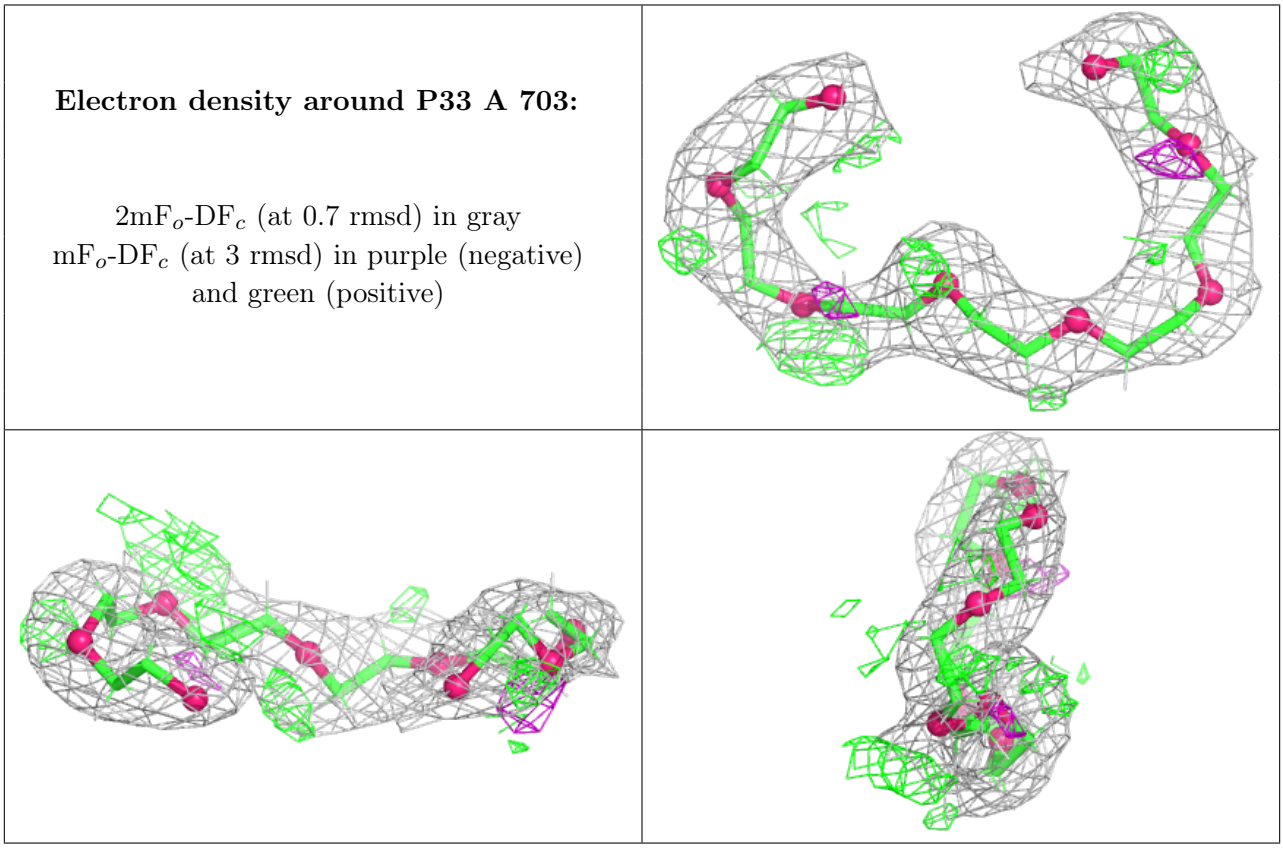
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	P6G	A	707	19/19	0.90	0.17	33,47,69,78	0
5	PEG	A	702	7/7	0.92	0.11	37,48,60,64	0
14	PG4	B	704	13/13	0.93	0.10	35,47,59,70	0
13	8KC	B	712	35/35	0.93	0.14	26,42,52,62	0
13	8KC	A	712	35/35	0.94	0.13	23,38,53,61	0
12	MG	B	711	1/1	0.95	0.06	51,51,51,51	0
11	CL	B	710	1/1	0.98	0.16	33,33,33,33	0
10	ZN	A	709	1/1	0.99	0.13	21,21,21,21	0
10	ZN	B	709	1/1	0.99	0.14	23,23,23,23	0
11	CL	A	710	1/1	1.00	0.11	24,24,24,24	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.

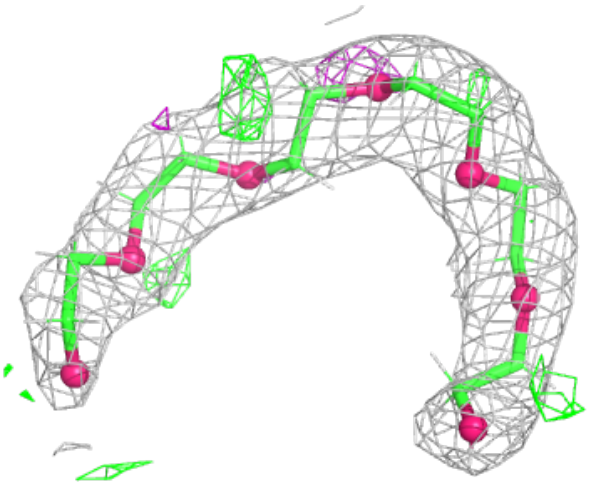
Electron density around P33 A 703:

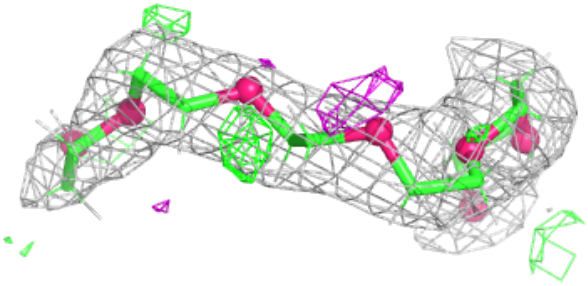
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

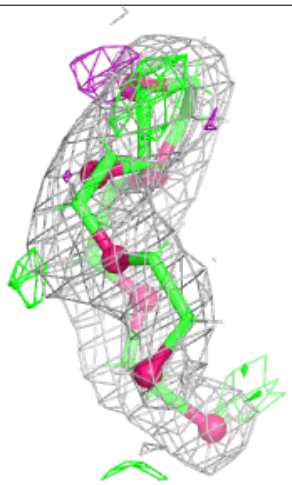


Electron density around P6G A 707:

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

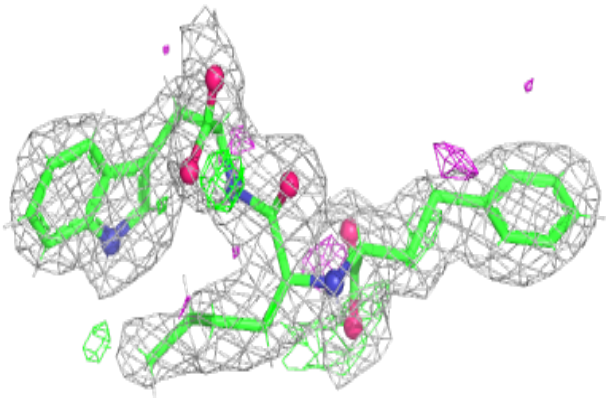


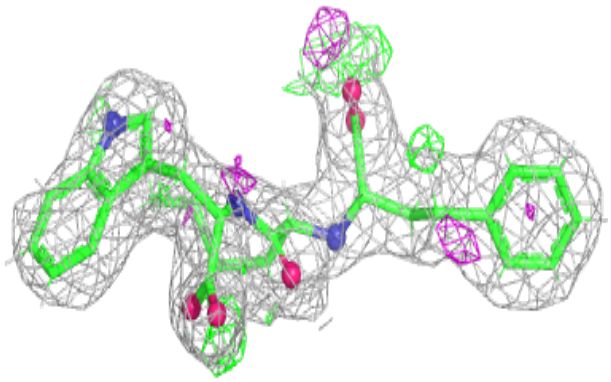




Electron density around 8KC B 712:

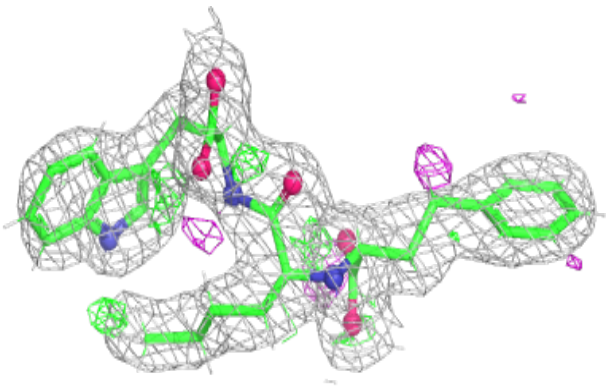
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

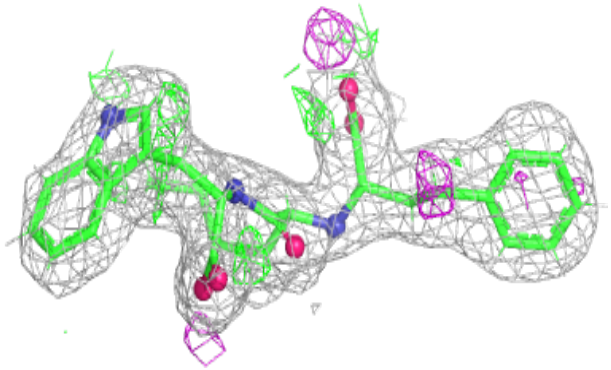


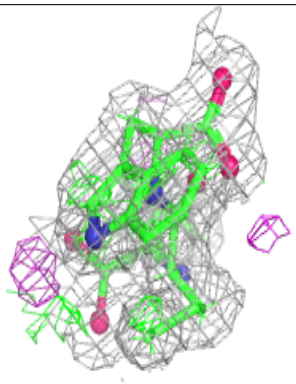


Electron density around 8KC A 712:

$2mF_o$-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.