



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:09 PM UTC

PDB ID : 7Q24 / pdb_00007q24
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 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:

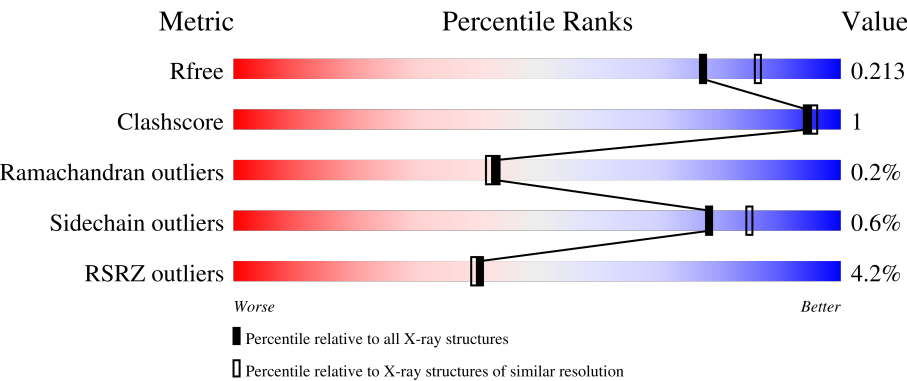
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	629	2% 93% 5% 2%
1	B	629	6% 93% 5% 2%
2	C	2	50% 50%
3	D	4	100%
3	F	4	75% 25%

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Mol	Chain	Length	Quality of chain
4	E	2	 100%
4	G	2	 50%50%

2 Entry composition

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:

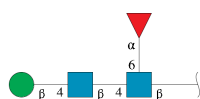
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	engineered mutation	UNP P12821
A	25	GLN	ASN	engineered mutation	UNP P12821
A	82	GLN	ASN	engineered mutation	UNP P12821
A	117	GLN	ASN	engineered mutation	UNP P12821
A	131	GLN	ASN	engineered mutation	UNP P12821
A	289	GLN	ASN	engineered mutation	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.



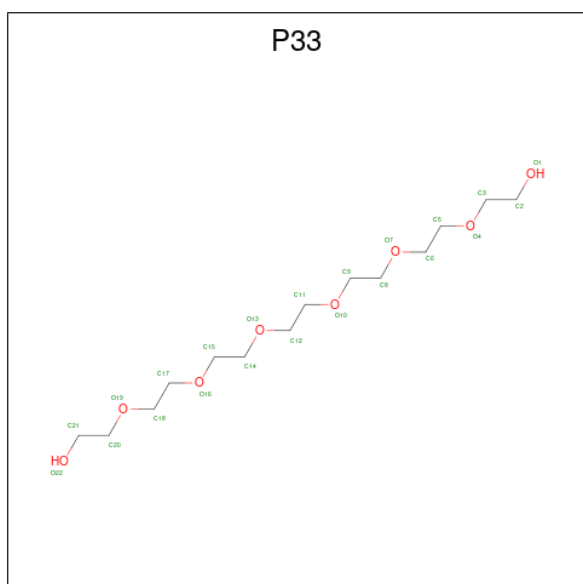
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	2	Total	C	H	N	O	0	0	0
			46	14	22	1	9			
4	G	2	Total	C	H	N	O	0	0	0
			46	14	22	1	9			

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



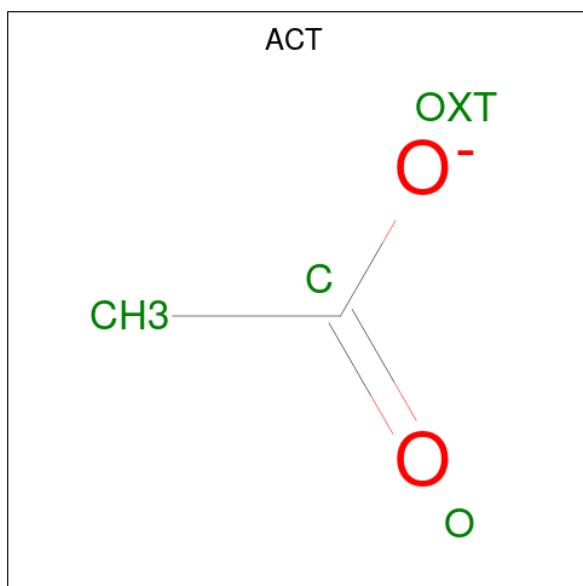
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is 3,6,9,12,15,18-HEXAOXAIICOSANE-1,20-DIOL (CCD ID: P33) (formula: $C_{14}H_{30}O_8$).



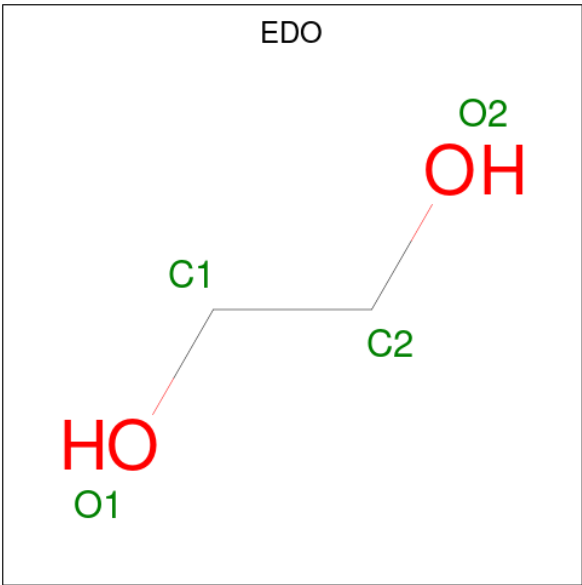
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			52	14	30	8		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



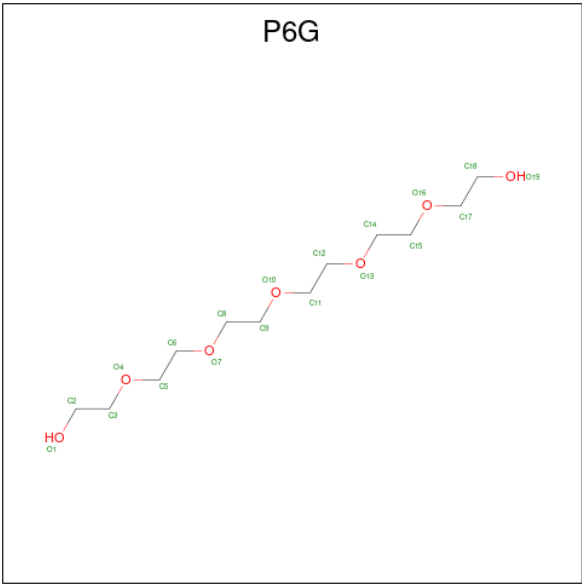
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			7	2	3	2		
7	B	1	Total	C	H	O	0	0
			7	2	3	2		
7	B	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 9 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



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

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

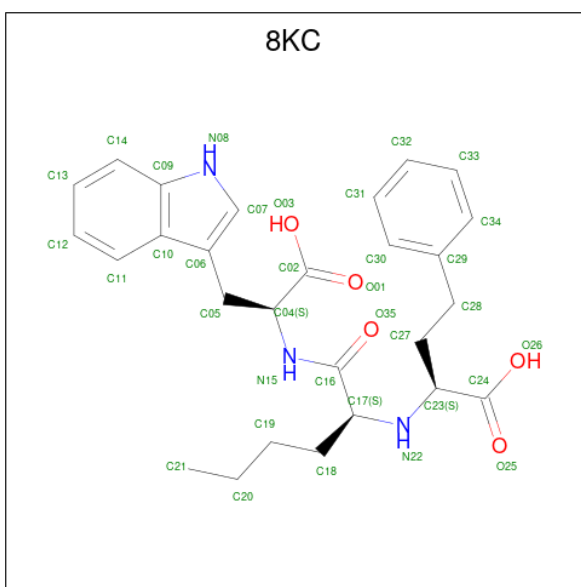
- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

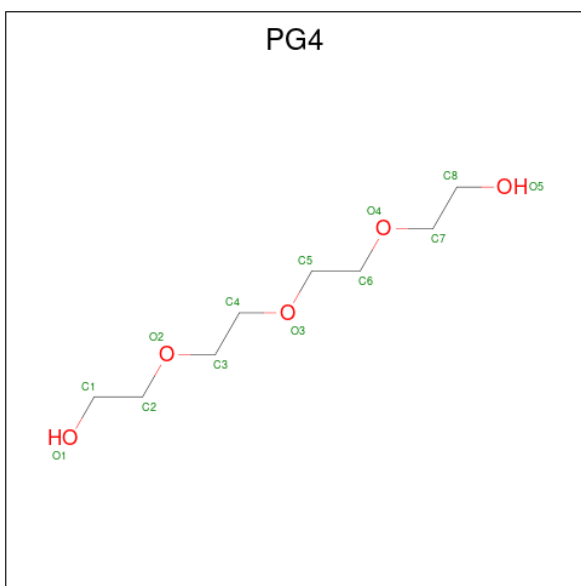
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total	Mg	0	0
			1	1		
12	B	1	Total	Mg	0	0
			1	1		

- 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 (CCD ID: 8KC) (formula: C₂₇H₃₃N₃O₅) (labeled as "Ligand of Interest" by depositor).



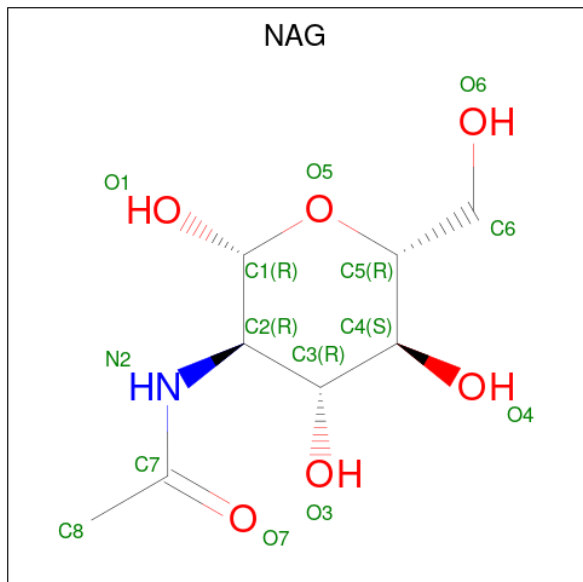
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	H	N	O	0	0
			66	27	31	3	5		
13	B	1	Total	C	H	N	O	0	0
			66	27	31	3	5		

- Molecule 14 is TETRAETHYLENE GLYCOL (CCD ID: 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 (CCD ID: 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		

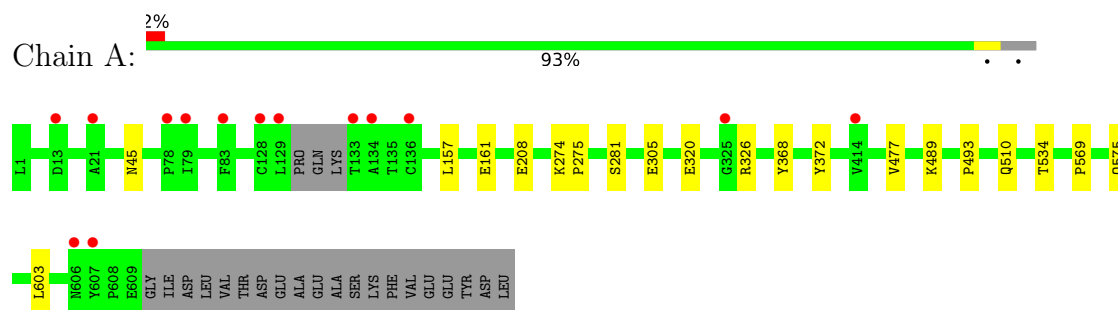
- Molecule 16 is water.

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

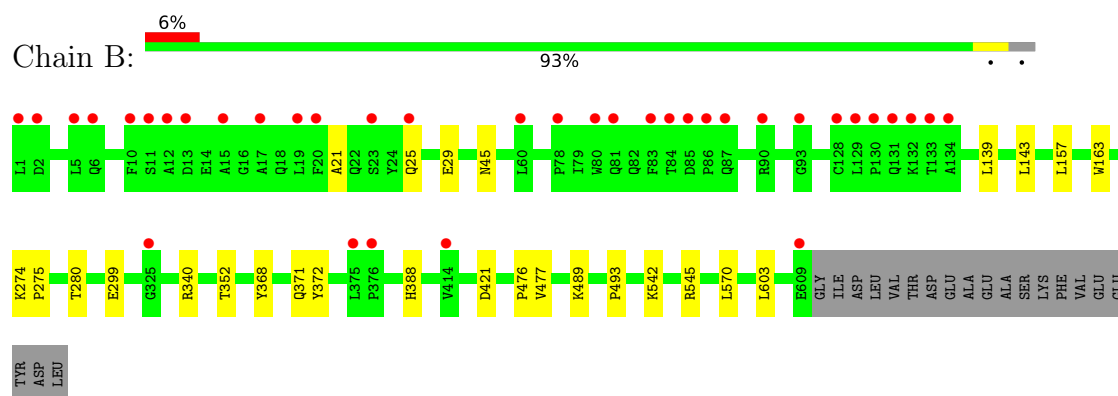
3 Residue-property plots [i](#)

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



- Molecule 1: Angiotensin-converting enzyme



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



- 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





- 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:  75% 25%



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

Chain E:  100%



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

Chain G:  50% 50%



4 Data and refinement statistics

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 63.12 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.4 (63.12-2.00) 97.5 (63.12-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.185 , 0.214 0.183 , 0.213	Depositor DCC
R_{free} test set	1964 reflections (1.88%)	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)	0.43 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.*

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: NAG, ZN, ACT, 8KC, P6G, MG, PEG, P33, BMA, FUC, EDO, PG4, CL

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	0.10	0/5191	0.28	0/7068
1	B	0.10	0/5188	0.27	0/7066
All	All	0.10	0/10379	0.27	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	14	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

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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	27	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 (27) 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:B:570:LEU:C	1:B:570:LEU:HD23	2.42	0.45
1:A:477:VAL:HG12	1:A:603:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LYS:O	1:A:493:PRO:HD2	2.16	0.44
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%)	43	42
1	B	614/629 (98%)	603 (98%)	10 (2%)	1 (0%)	43	42
All	All	1226/1258 (98%)	1204 (98%)	20 (2%)	2 (0%)	43	42

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%)	529 (100%)	2 (0%)	84	89
1	B	531/541 (98%)	527 (99%)	4 (1%)	73	80
All	All	1062/1082 (98%)	1056 (99%)	6 (1%)	78	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	TYR
1	A	372	TYR
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. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	GLN
1	A	371	GLN
1	B	42	HIS
1	B	234	HIS
1	B	582	GLN
1	B	588	ASN
1	B	598	GLN

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 ⓘ

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	1,2	14,14,15	0.23	0	17,19,21	0.60	0
2	NAG	C	2	2	14,14,15	0.23	0	17,19,21	0.48	0
3	NAG	D	1	1,3	14,14,15	0.33	0	17,19,21	0.40	0
3	NAG	D	2	3	14,14,15	0.24	0	17,19,21	0.45	0
3	BMA	D	3	3	11,11,12	0.53	0	15,15,17	0.72	0
3	FUC	D	4	3	10,10,11	0.66	0	14,14,16	0.70	0
4	NAG	E	1	1,4	14,14,15	0.49	0	17,19,21	0.45	0
4	FUC	E	2	4	10,10,11	0.85	0	14,14,16	0.70	0
3	NAG	F	1	1,3	14,14,15	0.38	0	17,19,21	0.40	0
3	NAG	F	2	3	14,14,15	0.38	0	17,19,21	0.56	0
3	BMA	F	3	3	11,11,12	0.50	0	15,15,17	1.01	1 (6%)
3	FUC	F	4	3	10,10,11	0.58	0	14,14,16	0.86	0
4	NAG	G	1	1,4	14,14,15	0.34	0	17,19,21	0.40	0
4	FUC	G	2	4	10,10,11	0.70	0	14,14,16	0.87	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	1,2	-	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	1,4	-	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	1,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUC	G	2	4	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	BMA	C1-O5-C5	2.62	115.70	112.19
4	G	2	FUC	C1-C2-C3	2.07	112.66	109.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

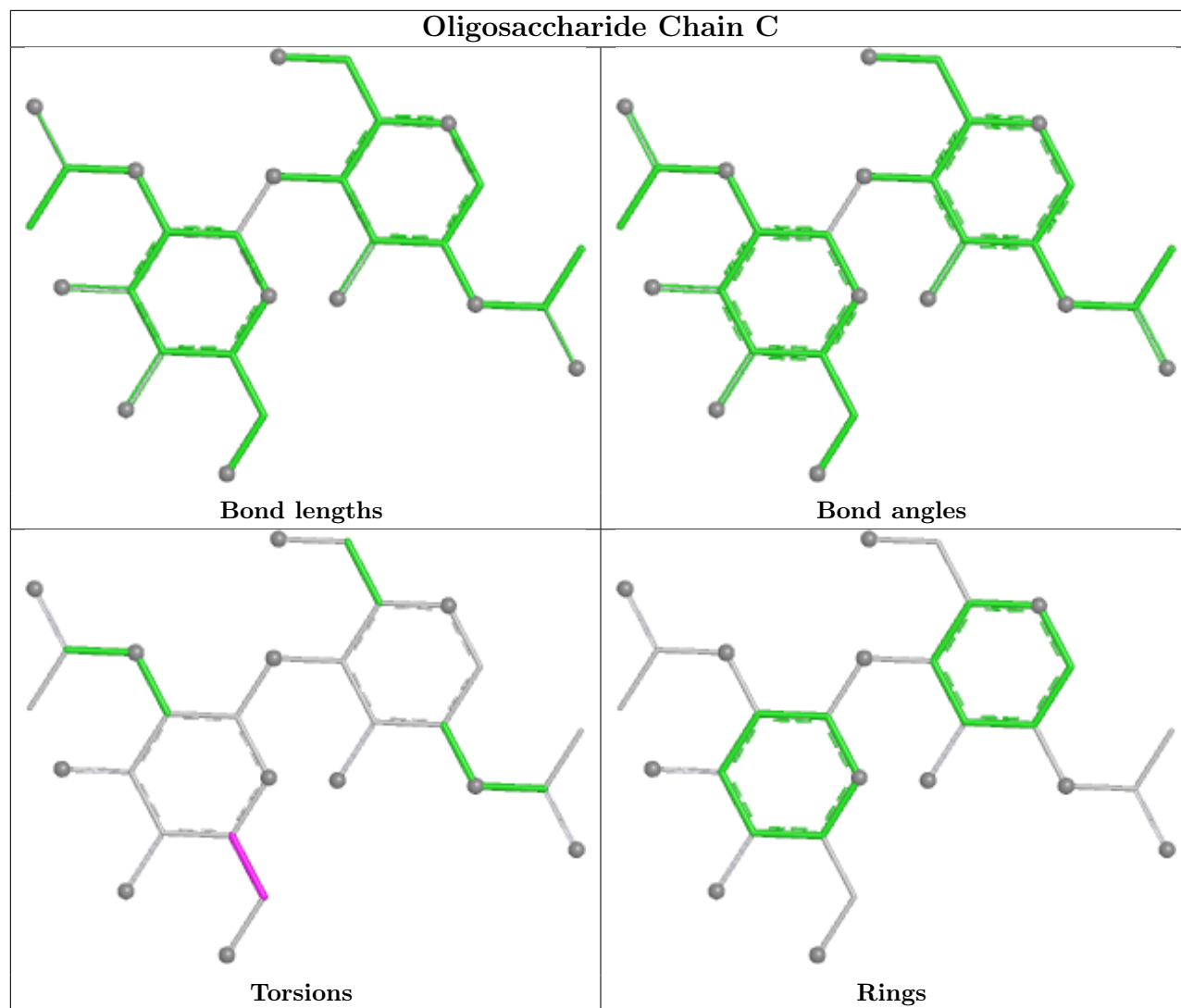
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6

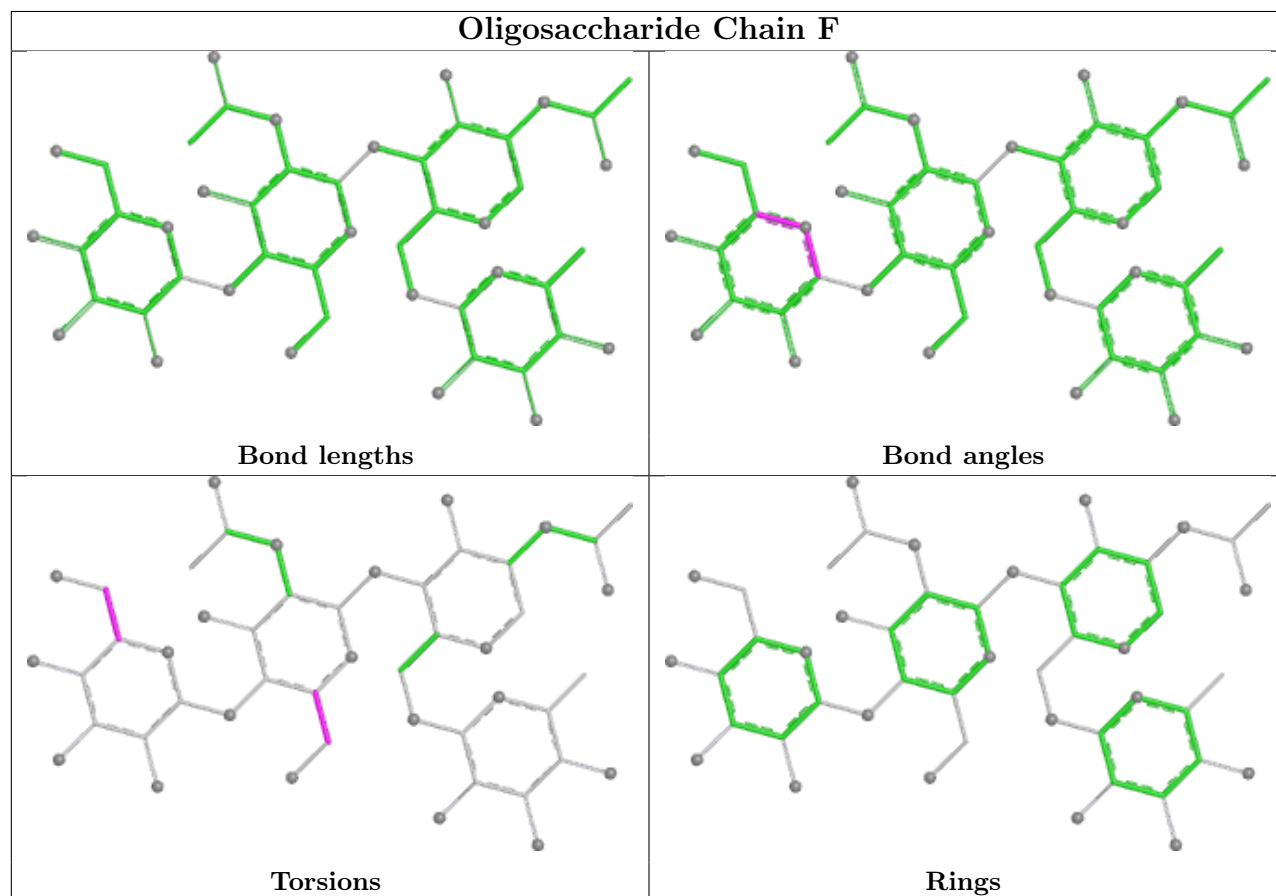
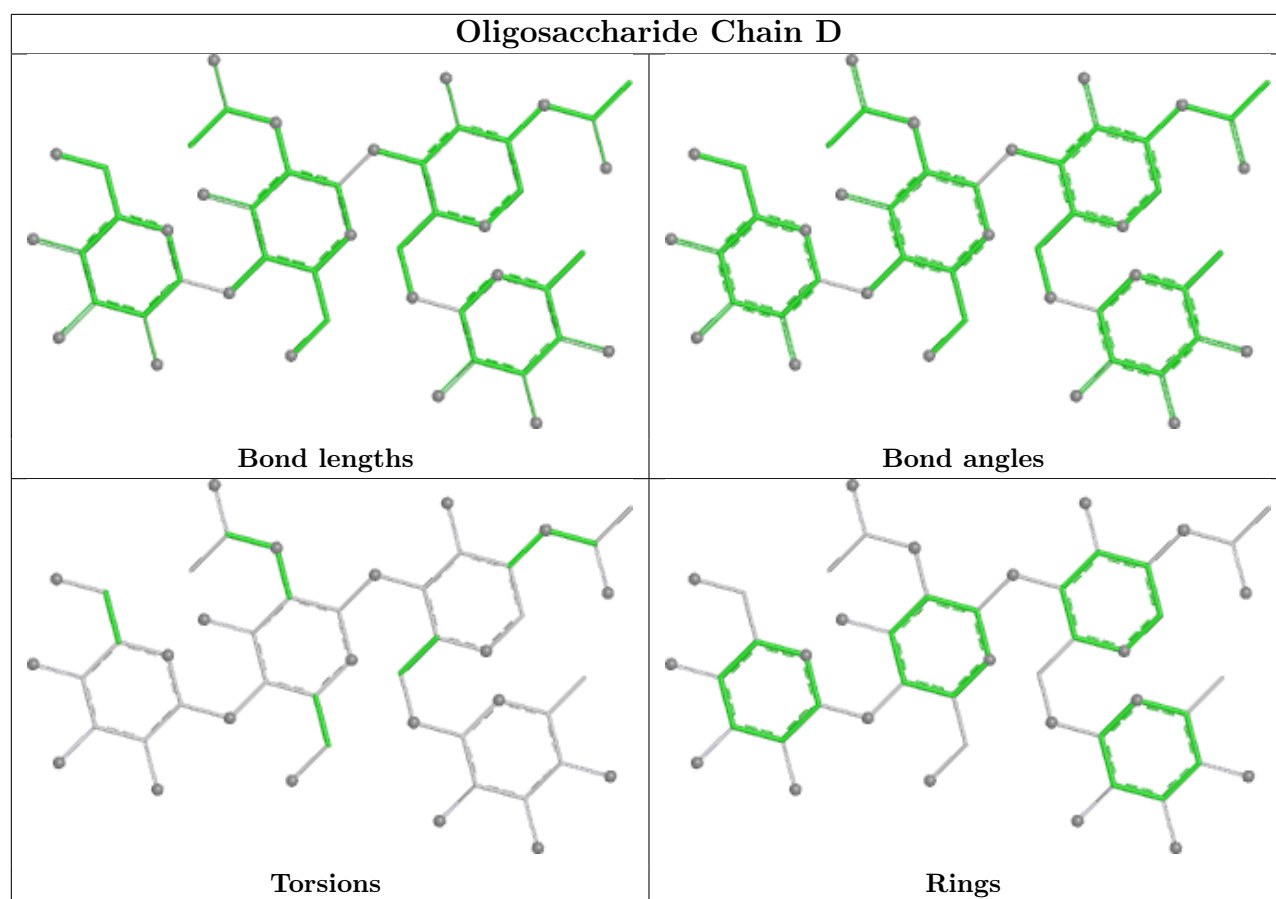
There are no ring outliers.

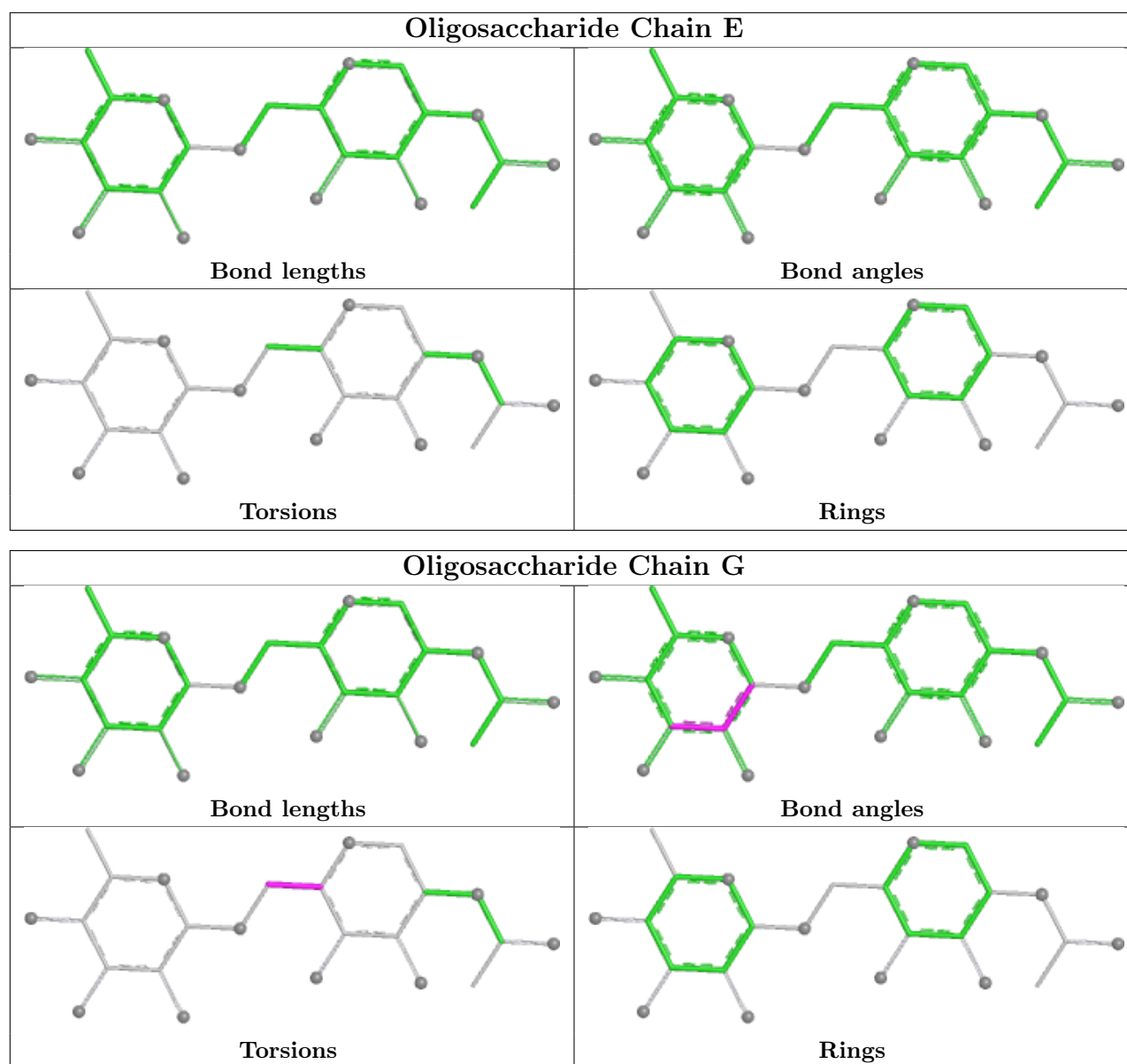
1 monomer is involved in 1 short contact:

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.







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
14	PG4	B	704	-	12,12,12	0.13	0	11,11,11	0.51	0
13	8KC	B	712	10	37,37,37	1.75	7 (18%)	49,49,49	0.99	3 (6%)
5	PEG	A	702	-	6,6,6	0.11	0	5,5,5	0.13	0
5	PEG	A	704	-	6,6,6	0.12	0	5,5,5	0.11	0
8	EDO	A	708	-	3,3,3	0.43	0	2,2,2	0.35	0
7	ACT	A	705	-	3,3,3	1.36	0	3,3,3	1.51	0
14	PG4	B	701	-	12,12,12	0.12	0	11,11,11	0.60	0
5	PEG	A	701	-	6,6,6	0.11	0	5,5,5	0.09	0
8	EDO	B	703	-	3,3,3	0.44	0	2,2,2	0.31	0
5	PEG	B	708	-	6,6,6	0.11	0	5,5,5	0.10	0
7	ACT	B	705	-	3,3,3	1.35	0	3,3,3	1.37	0
6	P33	A	703	-	21,21,21	0.55	0	20,20,20	0.24	0
15	NAG	B	702	1	14,14,15	0.31	0	17,19,21	0.56	0
8	EDO	A	706	-	3,3,3	0.44	0	2,2,2	0.34	0
7	ACT	B	707	-	3,3,3	1.35	0	3,3,3	1.38	0
13	8KC	A	712	10	37,37,37	1.76	7 (18%)	49,49,49	1.02	3 (6%)
8	EDO	B	706	-	3,3,3	0.43	0	2,2,2	0.35	0
9	P6G	A	707	-	18,18,18	0.11	0	17,17,17	0.13	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
14	PG4	B	704	-	-	4/10/10/10	-
13	8KC	B	712	10	-	4/33/42/42	0/3/3/3
5	PEG	A	702	-	-	1/4/4/4	-
5	PEG	A	704	-	-	2/4/4/4	-
8	EDO	A	708	-	-	1/1/1/1	-
14	PG4	B	701	-	-	4/10/10/10	-
5	PEG	A	701	-	-	1/4/4/4	-
8	EDO	B	703	-	-	0/1/1/1	-
5	PEG	B	708	-	-	0/4/4/4	-
6	P33	A	703	-	-	10/19/19/19	-
15	NAG	B	702	1	-	0/6/23/26	0/1/1/1
8	EDO	A	706	-	-	0/1/1/1	-
13	8KC	A	712	10	-	4/33/42/42	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	EDO	B	706	-	-	0/1/1/1	-
9	P6G	A	707	-	-	6/16/16/16	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	712	8KC	C16-N15	6.77	1.48	1.34
13	B	712	8KC	C16-N15	6.74	1.48	1.34
13	B	712	8KC	C05-C06	3.61	1.57	1.50
13	A	712	8KC	C05-C06	3.55	1.56	1.50
13	A	712	8KC	C07-N08	-2.67	1.32	1.37
13	B	712	8KC	C07-N08	-2.64	1.32	1.37
13	A	712	8KC	C10-C09	-2.49	1.38	1.41
13	B	712	8KC	C10-C09	-2.45	1.38	1.41
13	B	712	8KC	C07-C06	2.34	1.40	1.36
13	A	712	8KC	C28-C29	2.25	1.58	1.51
13	B	712	8KC	C28-C29	2.21	1.58	1.51
13	B	712	8KC	O35-C16	-2.19	1.19	1.23
13	A	712	8KC	C07-C06	2.19	1.40	1.36
13	A	712	8KC	O35-C16	-2.15	1.19	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	712	8KC	C04-C05-C06	2.47	118.13	113.44
13	B	712	8KC	C14-C09-C10	-2.39	119.88	122.19
13	A	712	8KC	C14-C09-C10	-2.22	120.04	122.19
13	B	712	8KC	O03-C02-C04	2.15	120.78	113.51
13	B	712	8KC	O26-C24-C23	2.08	120.56	113.51
13	A	712	8KC	O03-C02-C04	2.01	120.30	113.51

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	712	8KC	N22-C23-C27-C28
13	B	712	8KC	N22-C23-C27-C28
6	A	703	P33	O16-C17-C18-O19
14	B	701	PG4	O4-C7-C8-O5
9	A	707	P6G	O7-C8-C9-O10
6	A	703	P33	O4-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
13	A	712	8KC	C24-C23-C27-C28
13	B	712	8KC	C24-C23-C27-C28
6	A	703	P33	O7-C8-C9-O10
13	A	712	8KC	C02-C04-C05-C06
6	A	703	P33	O13-C14-C15-O16
14	B	704	PG4	O4-C7-C8-O5
9	A	707	P6G	O16-C17-C18-O19
14	B	701	PG4	O1-C1-C2-O2
13	A	712	8KC	N15-C04-C05-C06
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
9	A	707	P6G	C18-C17-O16-C15
6	A	703	P33	C17-C18-O19-C20
6	A	703	P33	O1-C2-C3-O4
14	B	704	PG4	O3-C5-C6-O4
8	A	708	EDO	O1-C1-C2-O2
5	A	701	PEG	O2-C3-C4-O4
6	A	703	P33	C5-C6-O7-C8
14	B	701	PG4	C4-C3-O2-C2
9	A	707	P6G	C11-C12-O13-C14
6	A	703	P33	C18-C17-O16-C15
13	B	712	8KC	N15-C04-C05-C06
14	B	701	PG4	O3-C5-C6-O4
9	A	707	P6G	C6-C5-O4-C3
6	A	703	P33	C8-C9-O10-C11
5	A	704	PEG	O1-C1-C2-O2
5	A	704	PEG	C1-C2-O2-C3
9	A	707	P6G	C12-C11-O10-C9

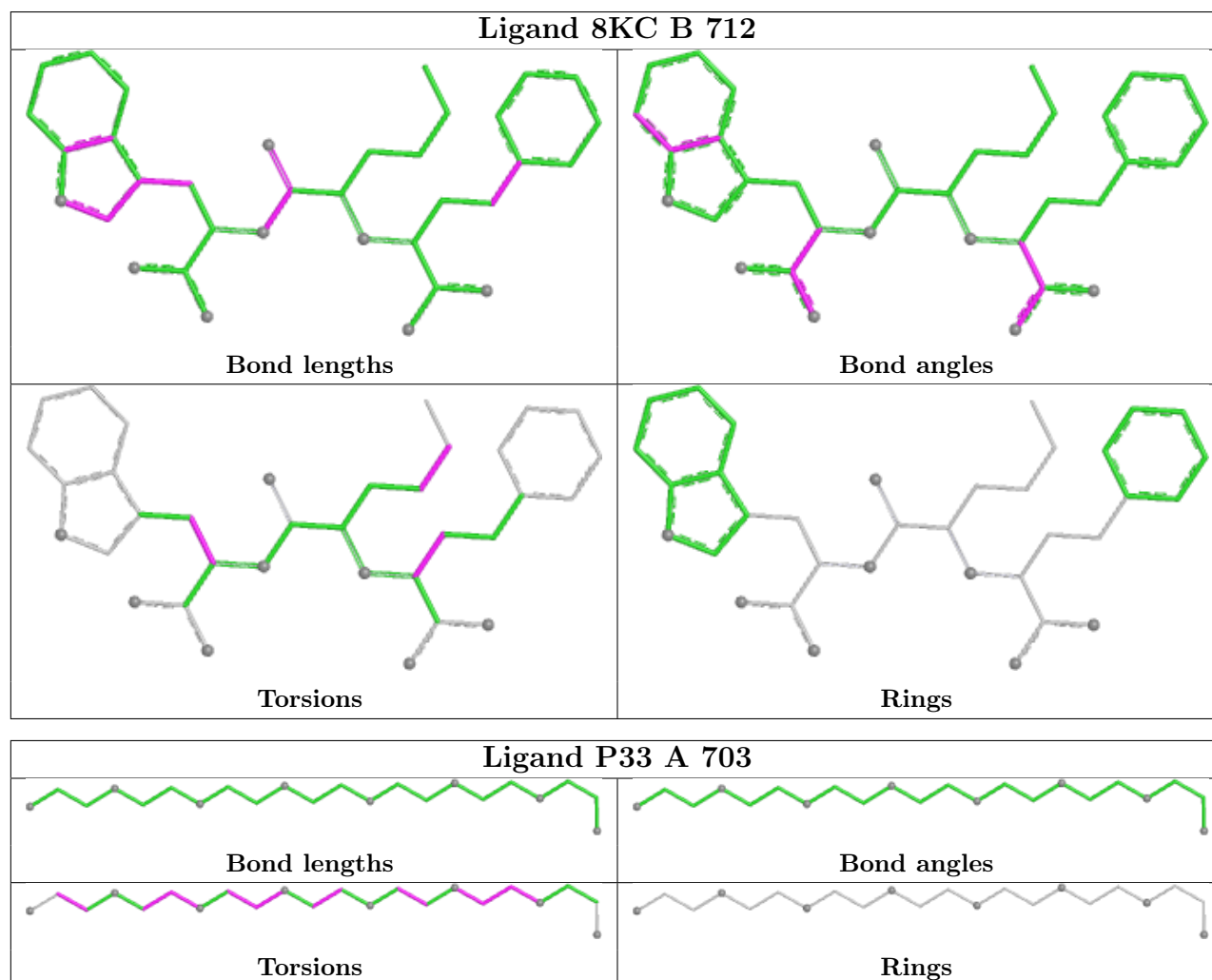
There are no ring outliers.

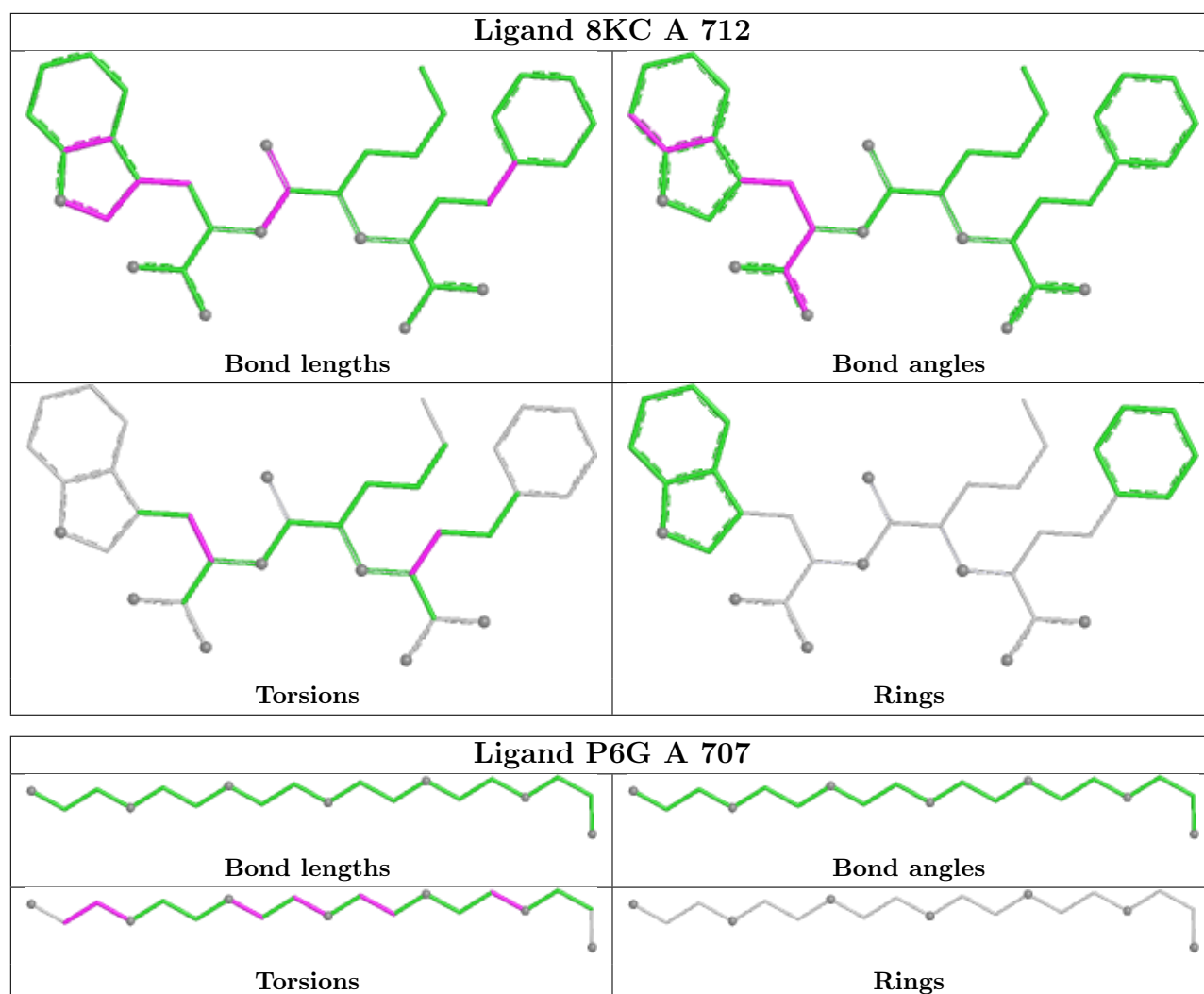
2 monomers are involved in 2 short contacts:

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 than 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.





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	606/629 (96%)	-0.16	14 (2%) 61 60	13, 38, 67, 114	10 (1%)
1	B	609/629 (96%)	0.15	37 (6%) 27 26	16, 47, 87, 135	7 (1%)
All	All	1215/1258 (96%)	-0.00	51 (4%) 40 39	13, 42, 80, 135	17 (1%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	607	TYR	4.9
1	A	133	THR	4.3
1	A	129	LEU	4.1
1	B	130	PRO	3.9
1	B	325	GLY	3.8
1	B	376	PRO	3.5
1	A	325	GLY	3.4
1	B	81	GLN	3.4
1	B	17	ALA	3.3
1	A	79	ILE	3.3
1	A	606	ASN	3.2
1	B	19	LEU	3.2
1	B	133	THR	3.1
1	B	132	LYS	3.1
1	B	83	PHE	3.0
1	B	86	PRO	3.0
1	B	78	PRO	2.9
1	B	1	LEU	2.8
1	B	15	ALA	2.7
1	B	25	GLN	2.7
1	A	83	PHE	2.6
1	B	128	CYS	2.6
1	B	131	GLN	2.5
1	A	134	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	84	THR	2.4
1	B	85	ASP	2.4
1	A	136	CYS	2.4
1	B	13	ASP	2.3
1	A	78	PRO	2.3
1	B	60	LEU	2.3
1	B	20	PHE	2.3
1	A	128	CYS	2.3
1	B	134	ALA	2.3
1	B	129	LEU	2.3
1	B	414	VAL	2.2
1	A	13	ASP	2.2
1	A	21	ALA	2.2
1	B	2	ASP	2.2
1	B	12	ALA	2.2
1	B	375	LEU	2.2
1	B	80	TRP	2.2
1	B	87	GLN	2.2
1	B	6	GLN	2.1
1	B	93	GLY	2.1
1	B	90	ARG	2.1
1	B	5	LEU	2.1
1	B	23[A]	SER	2.1
1	A	414	VAL	2.1
1	B	10	PHE	2.1
1	B	11	SER	2.1
1	B	609	GLU	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.

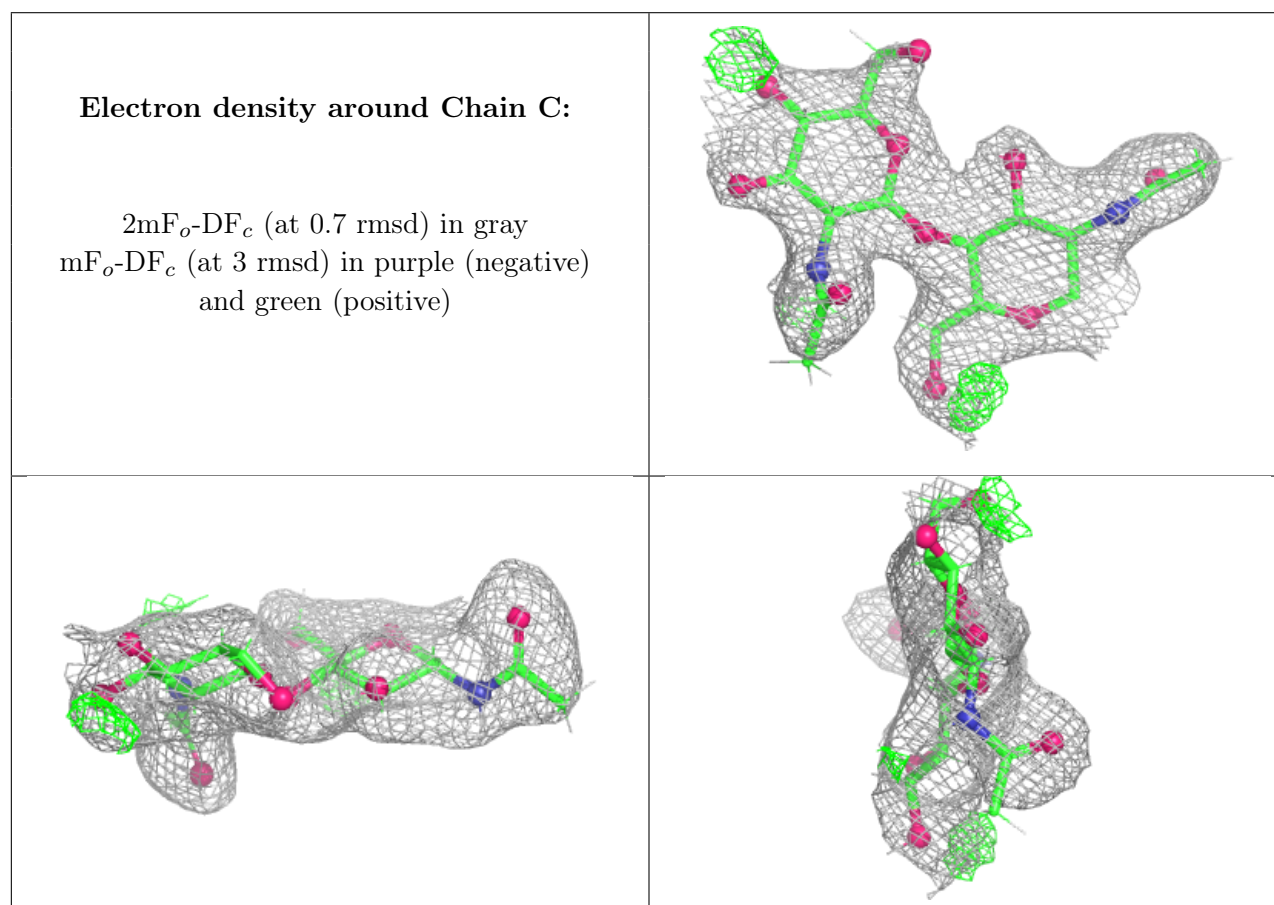
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FUC	G	2	10/11	0.53	0.20	71,85,96,101	0

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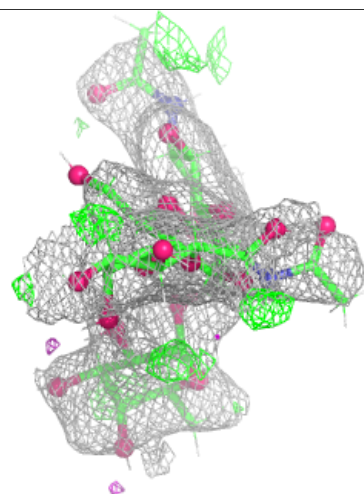
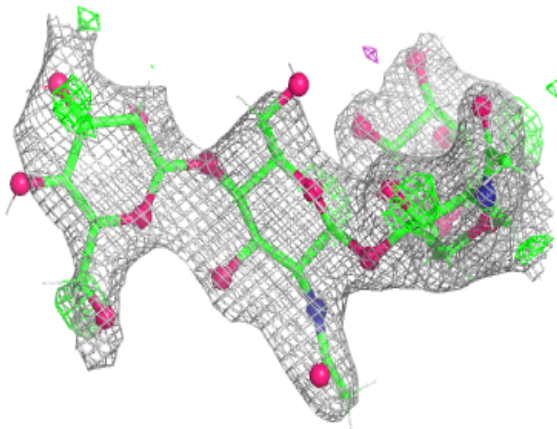
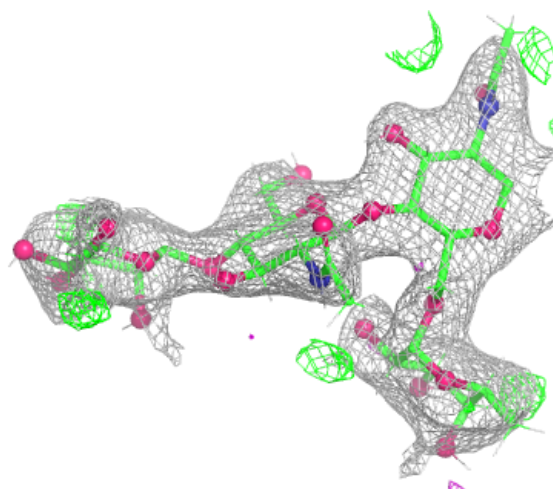
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FUC	F	4	10/11	0.59	0.20	75,95,114,125	0
3	BMA	F	3	11/12	0.63	0.13	107,120,142,145	0
3	BMA	D	3	11/12	0.70	0.13	74,89,105,111	0
4	FUC	E	2	10/11	0.71	0.19	61,80,92,97	0
4	NAG	G	1	14/15	0.76	0.15	45,62,78,90	0
3	NAG	F	1	14/15	0.82	0.11	70,77,92,98	0
2	NAG	C	2	14/15	0.82	0.12	59,83,102,104	0
3	FUC	D	4	10/11	0.83	0.13	59,71,84,86	0
3	NAG	F	2	14/15	0.84	0.12	77,90,104,108	0
4	NAG	E	1	14/15	0.86	0.13	41,57,69,77	0
3	NAG	D	2	14/15	0.88	0.11	53,71,83,90	0
2	NAG	C	1	14/15	0.90	0.10	51,60,71,73	0
3	NAG	D	1	14/15	0.93	0.09	44,57,71,71	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



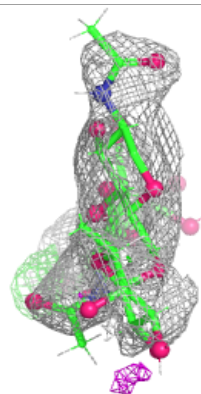
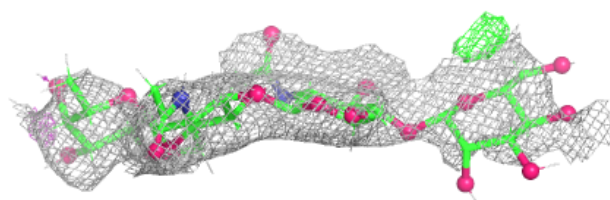
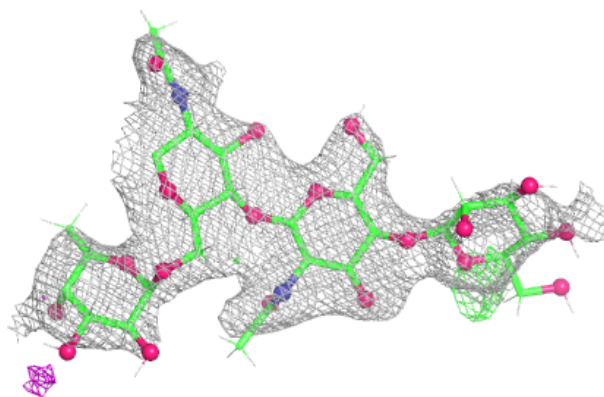
Electron density around Chain D:

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

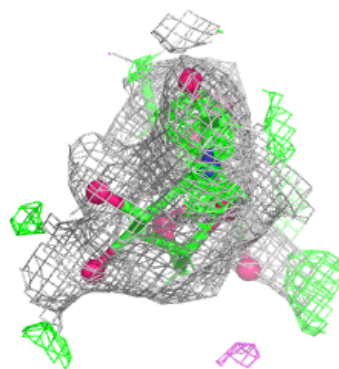
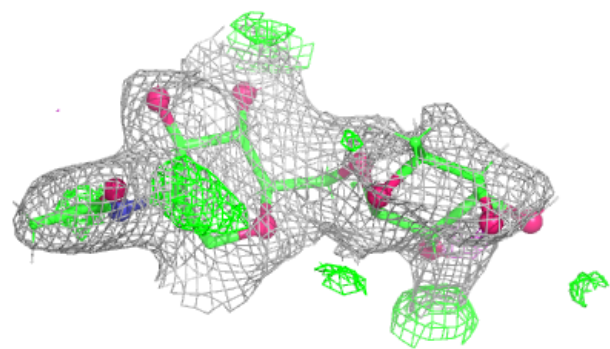
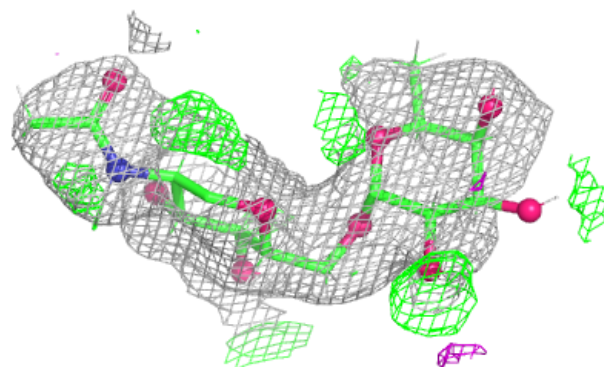


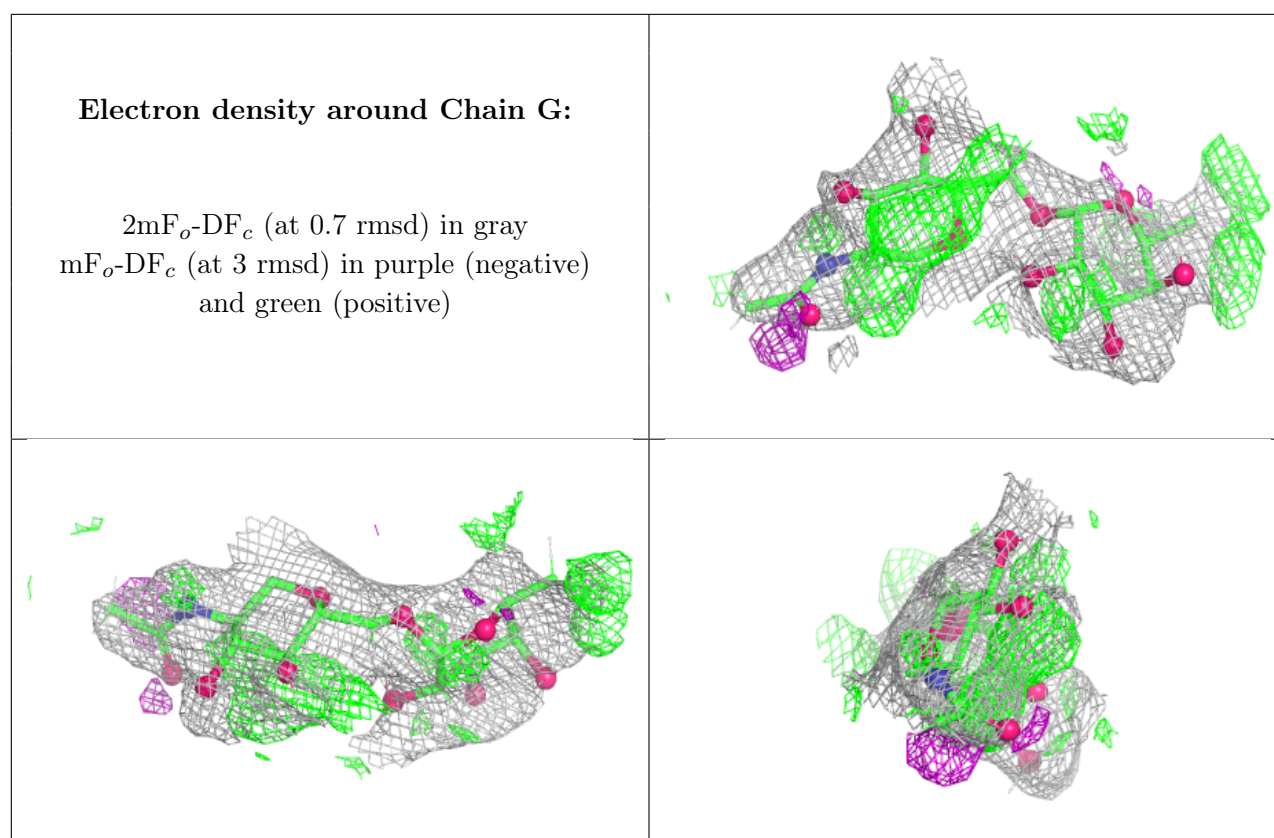
Electron density around Chain F:

$2mF_o-DF_c$ (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)





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
8	EDO	A	708	4/4	0.74	0.16	50,60,65,76	0
8	EDO	B	706	4/4	0.77	0.17	55,66,70,70	0
7	ACT	B	707	4/4	0.78	0.17	59,64,71,71	0
15	NAG	B	702	14/15	0.81	0.12	66,78,94,95	0
6	P33	A	703	22/22	0.83	0.15	43,59,72,82	0
7	ACT	A	705	4/4	0.84	0.18	41,49,54,57	0
5	PEG	A	704	7/7	0.85	0.12	53,63,70,76	0
7	ACT	B	705	4/4	0.85	0.16	48,58,59,61	0
14	PG4	B	701	13/13	0.86	0.12	39,50,68,77	0
8	EDO	A	706	4/4	0.86	0.16	40,50,60,72	0
8	EDO	B	703	4/4	0.88	0.12	51,61,69,76	0
5	PEG	B	708	7/7	0.88	0.12	58,71,86,94	0
5	PEG	A	701	7/7	0.89	0.10	43,54,67,73	0
9	P6G	A	707	19/19	0.90	0.12	33,47,69,78	0

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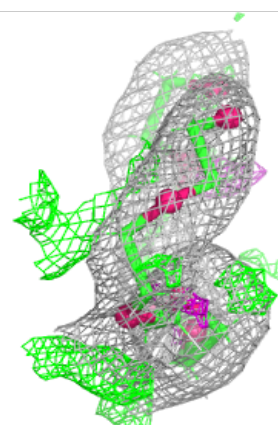
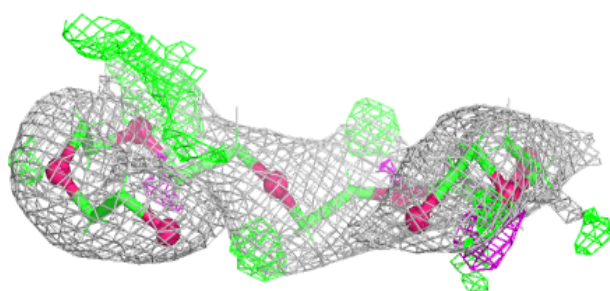
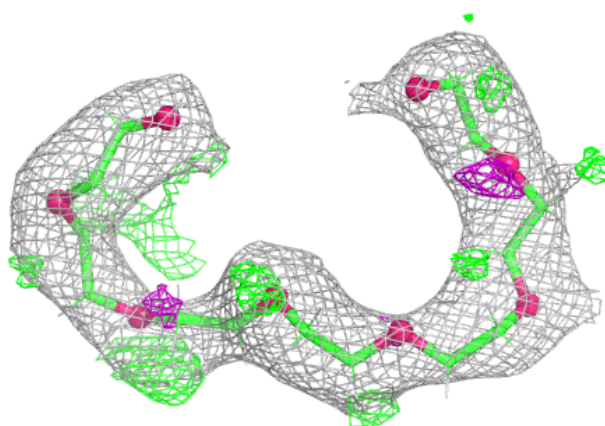
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	PG4	B	704	13/13	0.91	0.10	35,47,59,70	0
5	PEG	A	702	7/7	0.91	0.09	37,48,60,64	0
13	8KC	B	712	35/35	0.92	0.10	26,42,52,62	0
13	8KC	A	712	35/35	0.93	0.10	23,38,53,61	0
12	MG	A	711	1/1	0.94	0.07	52,52,52,52	0
12	MG	B	711	1/1	0.95	0.10	51,51,51,51	0
11	CL	B	710	1/1	0.98	0.05	33,33,33,33	0
10	ZN	A	709	1/1	0.98	0.04	21,21,21,21	0
10	ZN	B	709	1/1	0.99	0.03	23,23,23,23	0
11	CL	A	710	1/1	1.00	0.03	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.

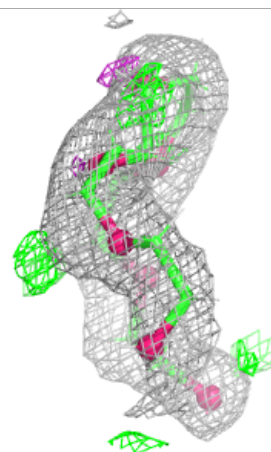
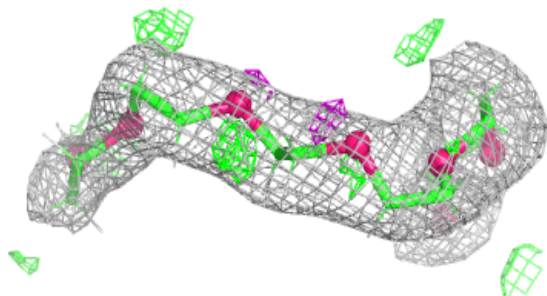
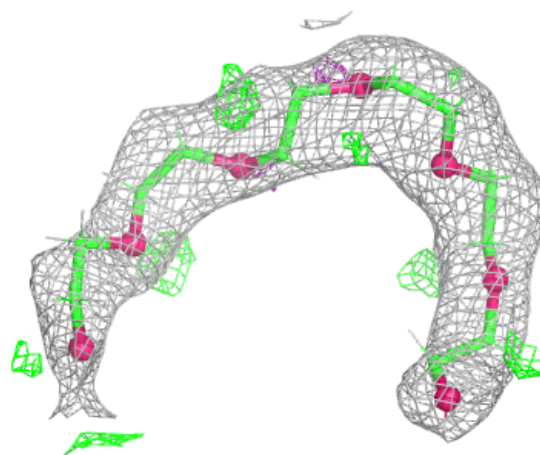
Electron density around P33 A 703:

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



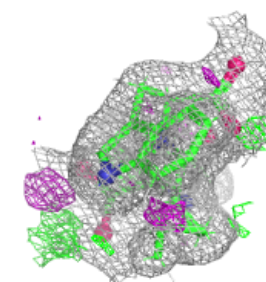
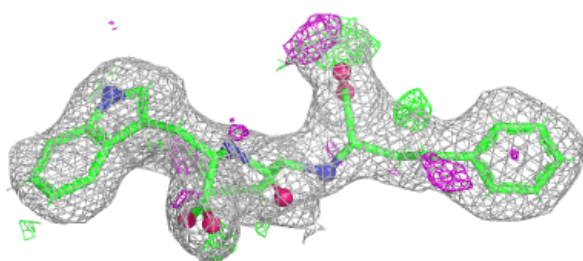
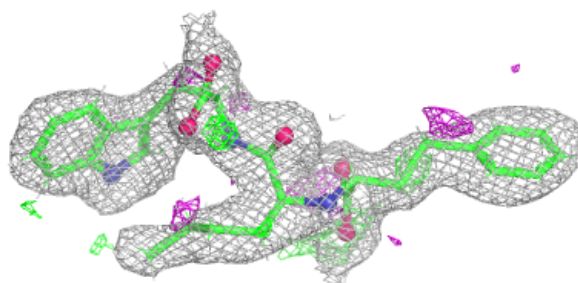
Electron density around P6G A 707:

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

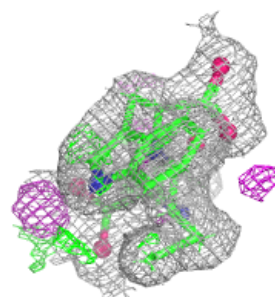
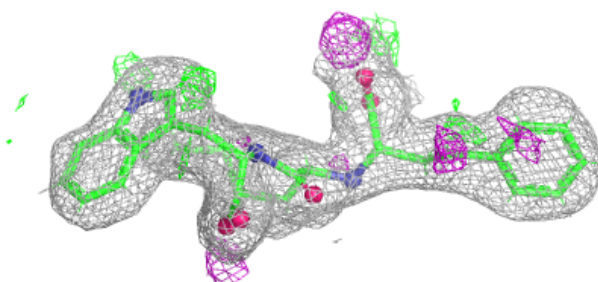
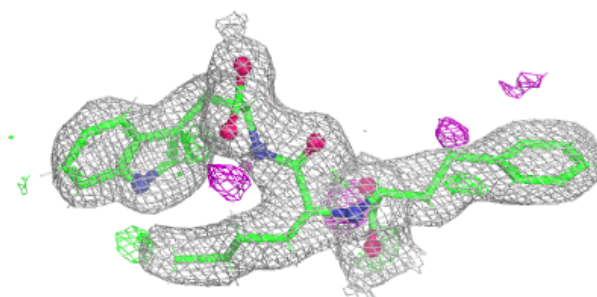


Electron density around 8KC B 712:

$2mF_o-DF_c$ (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.