



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2023 – 12:20 PM EDT

PDB ID : 2AEC
Title : Crystal Structure of Human M340H-Beta1,4-Galactosyltransferase-I (M340H-B4GAL-T1) in Complex with GlcNAc-beta1,2-Man-alpha1,6-Man-beta-O
R
Authors : Ramasamy, V.; Ramakrishnan, B.; Boeggeman, E.; Ratner, D.M.; Seeberger, P.H.; Qasba, P.K.
Deposited on : 2005-07-22
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

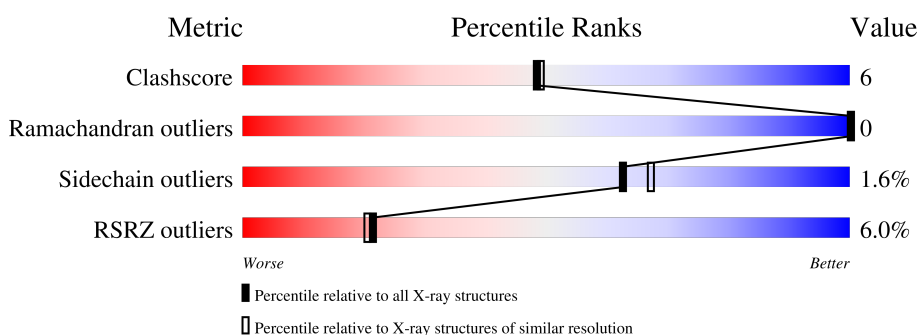
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
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 $\leq 5\%$. 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	287	
1	B	287	
1	C	287	
2	D	3	
2	E	3	
2	F	3	

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 7464 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 Beta-1,4-galactosyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	272	2212	1417	385	399	11	0	0	0
1	B	272	2212	1417	385	399	11	0	0	0
1	C	272	2212	1417	385	399	11	0	0	0

There are 51 discrepancies between the modelled and reference sequences:

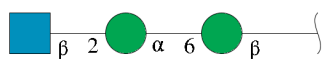
Chain	Residue	Modelled	Actual	Comment	Reference
A	112	ALA	-	SEE REMARK 999	UNP P15291
A	113	SER	-	SEE REMARK 999	UNP P15291
A	114	MET	-	SEE REMARK 999	UNP P15291
A	115	THR	-	SEE REMARK 999	UNP P15291
A	116	GLY	-	SEE REMARK 999	UNP P15291
A	117	GLY	-	SEE REMARK 999	UNP P15291
A	118	GLN	-	SEE REMARK 999	UNP P15291
A	119	GLN	-	SEE REMARK 999	UNP P15291
A	120	MET	-	SEE REMARK 999	UNP P15291
A	121	GLY	-	SEE REMARK 999	UNP P15291
A	122	ARG	-	SEE REMARK 999	UNP P15291
A	123	GLY	-	SEE REMARK 999	UNP P15291
A	124	SER	-	SEE REMARK 999	UNP P15291
A	125	ALA	-	SEE REMARK 999	UNP P15291
A	337	THR	ARG	engineered mutation	UNP P15291
A	338	THR	CYS	engineered mutation	UNP P15291
A	340	HIS	MET	engineered mutation	UNP P15291
B	112	ALA	-	SEE REMARK 999	UNP P15291
B	113	SER	-	SEE REMARK 999	UNP P15291
B	114	MET	-	SEE REMARK 999	UNP P15291
B	115	THR	-	SEE REMARK 999	UNP P15291
B	116	GLY	-	SEE REMARK 999	UNP P15291
B	117	GLY	-	SEE REMARK 999	UNP P15291

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Chain	Residue	Modelled	Actual	Comment	Reference
B	118	GLN	-	SEE REMARK 999	UNP P15291
B	119	GLN	-	SEE REMARK 999	UNP P15291
B	120	MET	-	SEE REMARK 999	UNP P15291
B	121	GLY	-	SEE REMARK 999	UNP P15291
B	122	ARG	-	SEE REMARK 999	UNP P15291
B	123	GLY	-	SEE REMARK 999	UNP P15291
B	124	SER	-	SEE REMARK 999	UNP P15291
B	125	ALA	-	SEE REMARK 999	UNP P15291
B	337	THR	ARG	engineered mutation	UNP P15291
B	338	THR	CYS	engineered mutation	UNP P15291
B	340	HIS	MET	engineered mutation	UNP P15291
C	112	ALA	-	SEE REMARK 999	UNP P15291
C	113	SER	-	SEE REMARK 999	UNP P15291
C	114	MET	-	SEE REMARK 999	UNP P15291
C	115	THR	-	SEE REMARK 999	UNP P15291
C	116	GLY	-	SEE REMARK 999	UNP P15291
C	117	GLY	-	SEE REMARK 999	UNP P15291
C	118	GLN	-	SEE REMARK 999	UNP P15291
C	119	GLN	-	SEE REMARK 999	UNP P15291
C	120	MET	-	SEE REMARK 999	UNP P15291
C	121	GLY	-	SEE REMARK 999	UNP P15291
C	122	ARG	-	SEE REMARK 999	UNP P15291
C	123	GLY	-	SEE REMARK 999	UNP P15291
C	124	SER	-	SEE REMARK 999	UNP P15291
C	125	ALA	-	SEE REMARK 999	UNP P15291
C	337	THR	ARG	engineered mutation	UNP P15291
C	338	THR	CYS	engineered mutation	UNP P15291
C	340	HIS	MET	engineered mutation	UNP P15291

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
2	D	3	Total	C	N	O	0	0	0
			37	20	1	16			
2	E	3	Total	C	N	O	0	0	0
			37	20	1	16			

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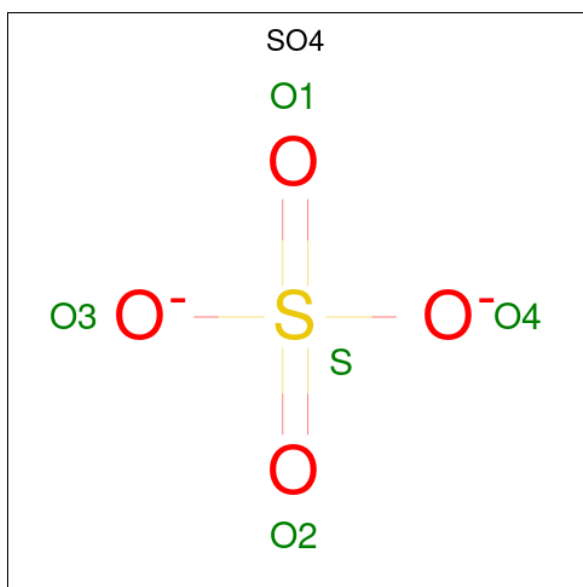
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	3	Total	C	N	O	0	0	0
			37	20	1	16			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



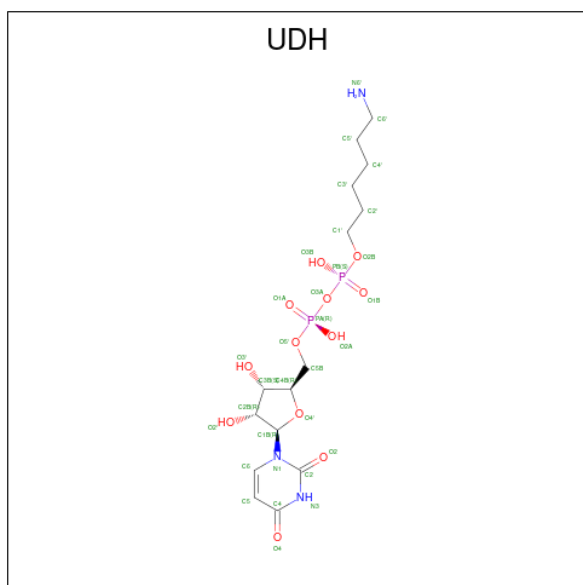
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	C	1	5	4	1	0	0
4	C	1	5	4	1	0	0
4	C	1	5	4	1	0	0
4	C	1	5	4	1	0	0

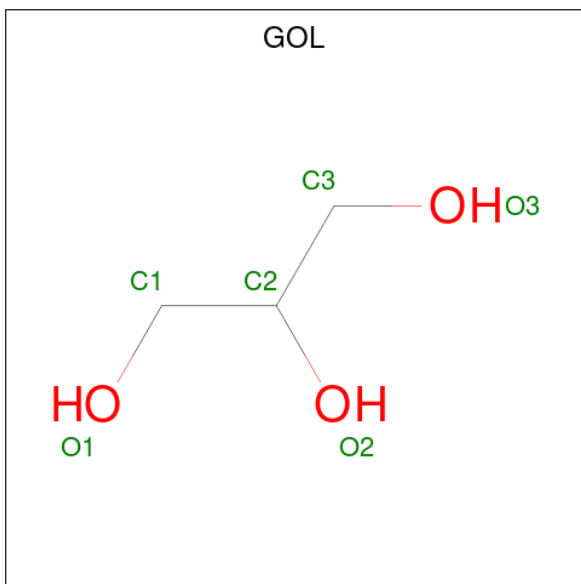
- Molecule 5 is 6-AMINOHEXYL-URIDINE-C1,5'-DIPHOSPHATE (three-letter code: UDH) (formula: $C_{15}H_{27}N_3O_{12}P_2$).



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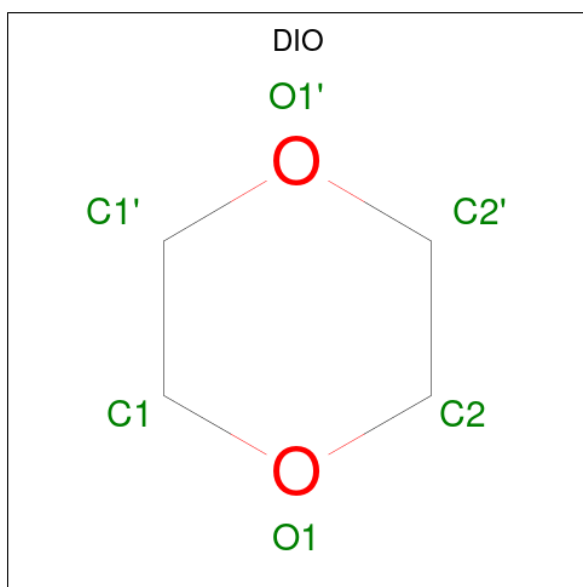
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	C	1	32	15	3	12	2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



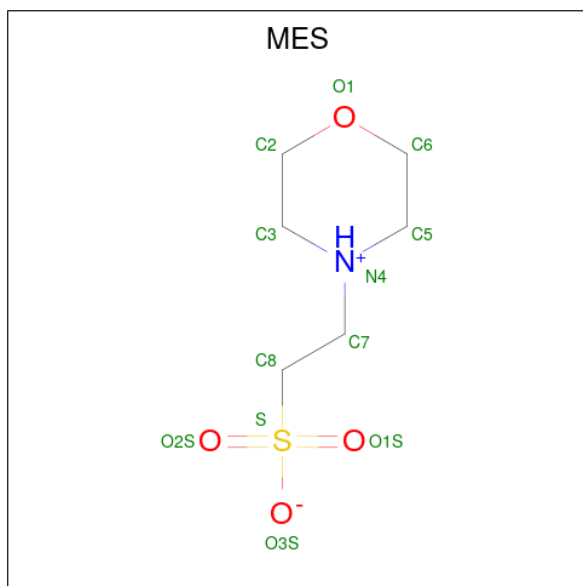
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	6	3	3	0	0
6	A	1	6	3	3	0	0
6	B	1	6	3	3	0	0
6	B	1	6	3	3	0	0
6	B	1	6	3	3	0	0
6	B	1	6	3	3	0	0
6	C	1	6	3	3	0	0

- Molecule 7 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C₄H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			6	4	2		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

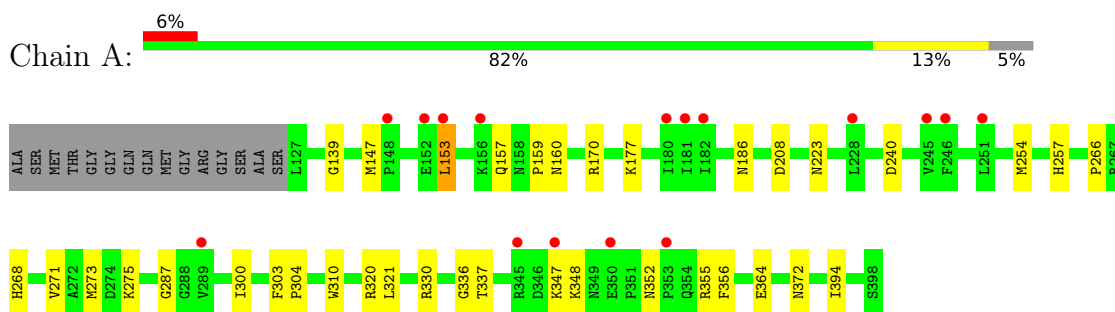
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	171	Total 171	O 171	0	0
9	B	181	Total 181	O 181	0	0
9	C	136	Total 136	O 136	0	0

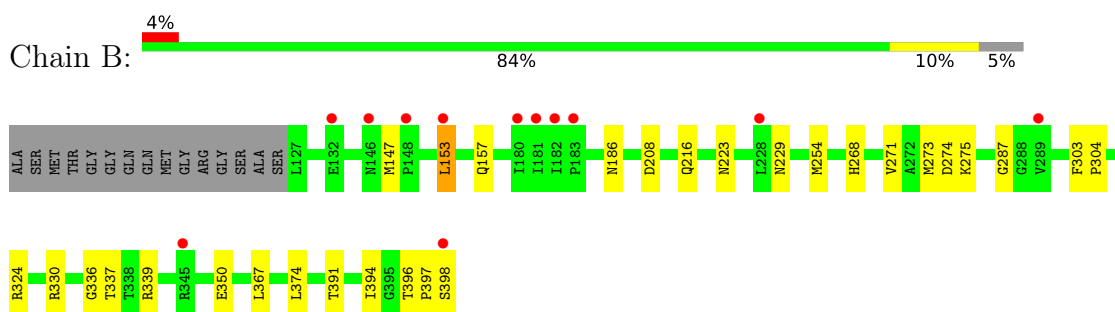
3 Residue-property plots [i](#)

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.

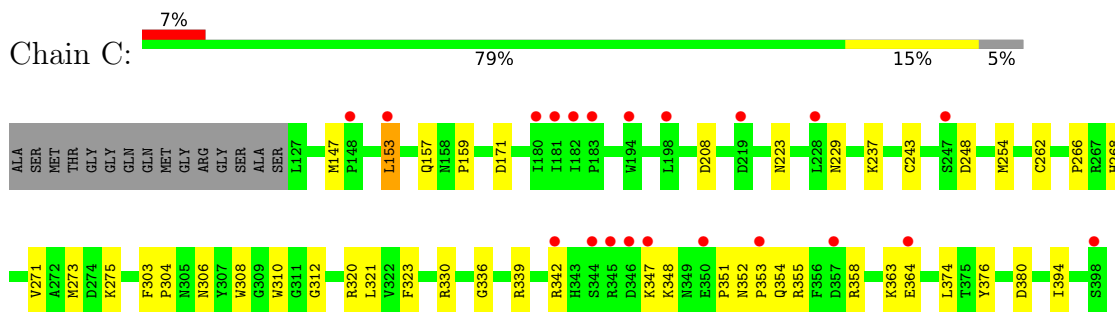
- Molecule 1: Beta-1,4-galactosyltransferase 1



- Molecule 1: Beta-1,4-galactosyltransferase 1



- Molecule 1: Beta-1,4-galactosyltransferase 1



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose



BM11
MAN2
MAG3

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose

Chain E:  100%

BM11
MAN2
MAG3

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose

Chain F:  100%

BM11
MAN2
MAG3

4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	107.23Å 194.99Å 143.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 29.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.00-2.00) 99.4 (29.85-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.05 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.208 , 0.239 0.198 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.775	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.013 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7464	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: MAN, GOL, SO4, BMA, UDH, DIO, NAG, MN, MES

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	0.45	0/2274	0.69	1/3089 (0.0%)
1	B	0.49	0/2274	0.69	1/3089 (0.0%)
1	C	0.41	0/2274	0.66	2/3089 (0.1%)
All	All	0.45	0/6822	0.68	4/9267 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	ASP	N-CA-C	-5.29	96.70	111.00
1	C	208	ASP	N-CA-C	-5.22	96.90	111.00
1	C	312	GLY	N-CA-C	5.18	126.05	113.10
1	A	208	ASP	N-CA-C	-5.15	97.10	111.00

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	2212	0	2157	28	0
1	B	2212	0	2157	22	0
1	C	2212	0	2157	33	0
2	D	37	0	33	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	37	0	33	0	0
2	F	37	0	33	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	20	0	0	0	0
4	B	30	0	0	0	0
4	C	20	0	0	0	0
5	A	32	0	25	0	0
5	B	32	0	25	0	0
5	C	32	0	25	1	0
6	A	12	0	16	3	0
6	B	24	0	32	3	0
6	C	6	0	8	1	0
7	C	6	0	8	2	0
8	C	12	0	13	3	0
9	A	171	0	0	0	0
9	B	181	0	0	1	0
9	C	136	0	0	0	0
All	All	7464	0	6722	82	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 6.

The worst 5 of 82 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:C:268:HIS:HD2	1:C:330:ARG:HE	1.09	0.92
1:A:273:MET:HE1	1:A:275:LYS:HE2	1.52	0.90
1:A:153:LEU:HD22	1:A:157:GLN:HE21	1.36	0.88
1:B:324:ARG:HH11	1:B:367:LEU:HD21	1.41	0.85
1:B:398:SER:H	6:B:419:GOL:H12	1.42	0.84

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	270/287 (94%)	263 (97%)	7 (3%)	0	100	100
1	B	270/287 (94%)	264 (98%)	6 (2%)	0	100	100
1	C	270/287 (94%)	263 (97%)	7 (3%)	0	100	100
All	All	810/861 (94%)	790 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	243/252 (96%)	239 (98%)	4 (2%)	62	67
1	B	243/252 (96%)	240 (99%)	3 (1%)	71	76
1	C	243/252 (96%)	238 (98%)	5 (2%)	53	57
All	All	729/756 (96%)	717 (98%)	12 (2%)	62	67

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	147	MET
1	C	153	LEU
1	C	380	ASP
1	C	342	ARG
1	A	364	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	233	GLN
1	C	268	HIS
1	C	377	GLN
1	A	268	HIS
1	A	377	GLN

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](#)

9 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	BMA	D	1	2	12,12,12	1.66	5 (41%)	17,17,17	0.68	0
2	MAN	D	2	2	11,11,12	2.34	4 (36%)	15,15,17	2.37	4 (26%)
2	NAG	D	3	2	14,14,15	1.70	4 (28%)	17,19,21	0.95	1 (5%)
2	BMA	E	1	2	12,12,12	1.76	5 (41%)	17,17,17	0.69	0
2	MAN	E	2	2	11,11,12	2.35	4 (36%)	15,15,17	2.27	4 (26%)
2	NAG	E	3	2	14,14,15	1.66	4 (28%)	17,19,21	0.95	1 (5%)
2	BMA	F	1	2	12,12,12	1.63	5 (41%)	17,17,17	0.69	0
2	MAN	F	2	2	11,11,12	2.52	4 (36%)	15,15,17	2.39	4 (26%)
2	NAG	F	3	2	14,14,15	2.02	6 (42%)	17,19,21	1.02	1 (5%)

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	BMA	D	1	2	-	1/2/22/22	0/1/1/1
2	MAN	D	2	2	-	2/2/19/22	0/1/1/1
2	NAG	D	3	2	-	0/6/23/26	0/1/1/1
2	BMA	E	1	2	-	2/2/22/22	0/1/1/1
2	MAN	E	2	2	-	1/2/19/22	0/1/1/1
2	NAG	E	3	2	-	0/6/23/26	0/1/1/1
2	BMA	F	1	2	-	2/2/22/22	0/1/1/1
2	MAN	F	2	2	-	2/2/19/22	0/1/1/1
2	NAG	F	3	2	-	0/6/23/26	0/1/1/1

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	MAN	O5-C1	5.32	1.52	1.43
2	E	2	MAN	O5-C1	4.67	1.51	1.43
2	D	2	MAN	O5-C1	4.66	1.51	1.43
2	E	2	MAN	O5-C5	4.18	1.51	1.43
2	F	2	MAN	O5-C5	4.04	1.51	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	MAN	C1-O5-C5	5.16	119.19	112.19
2	F	2	MAN	C1-O5-C5	5.02	119.00	112.19
2	D	2	MAN	O2-C2-C3	-4.98	100.17	110.14
2	F	2	MAN	O2-C2-C3	-4.97	100.19	110.14
2	E	2	MAN	C1-O5-C5	4.67	118.52	112.19

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

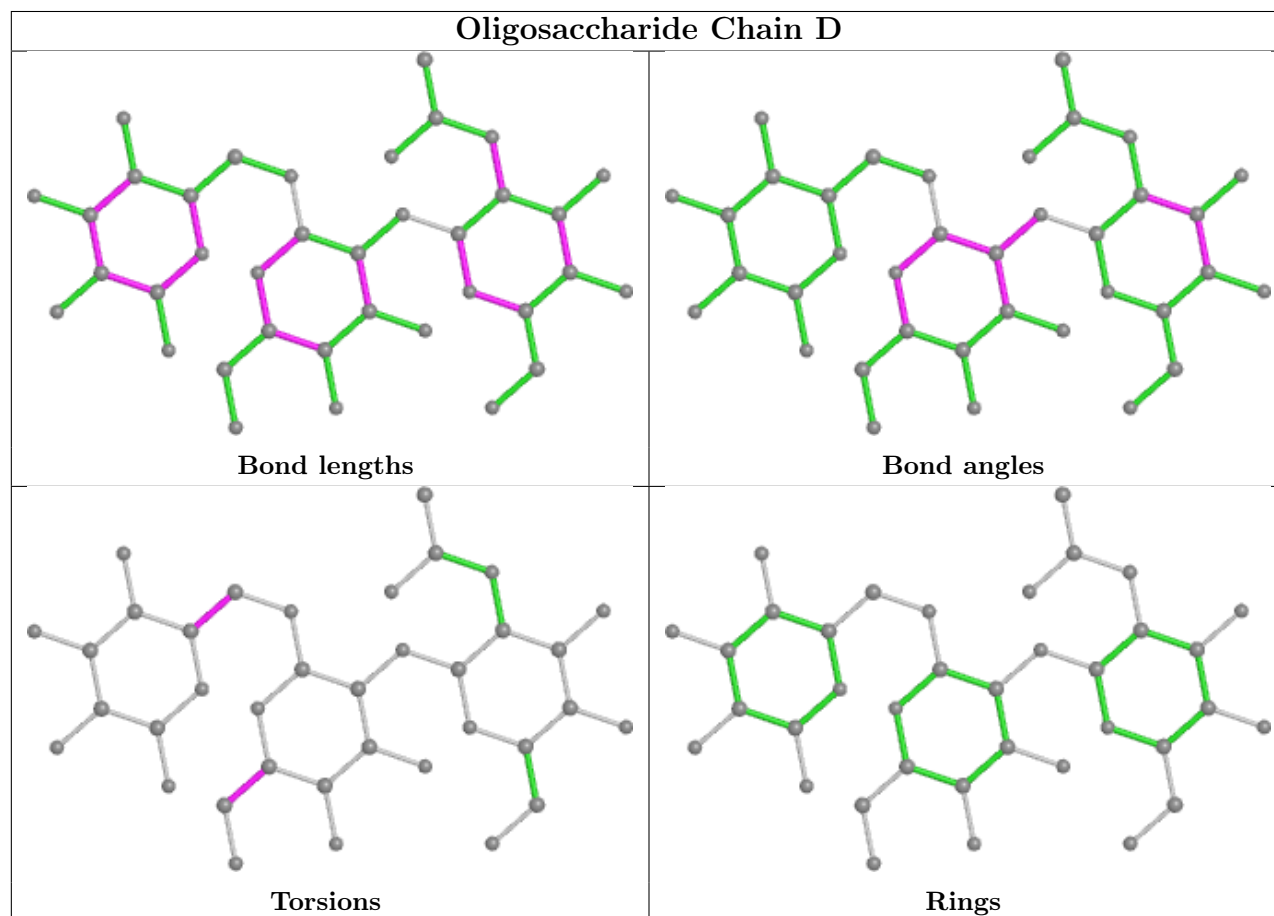
Mol	Chain	Res	Type	Atoms
2	D	2	MAN	O5-C5-C6-O6
2	E	1	BMA	O5-C5-C6-O6
2	D	2	MAN	C4-C5-C6-O6
2	F	1	BMA	O5-C5-C6-O6
2	F	2	MAN	C4-C5-C6-O6

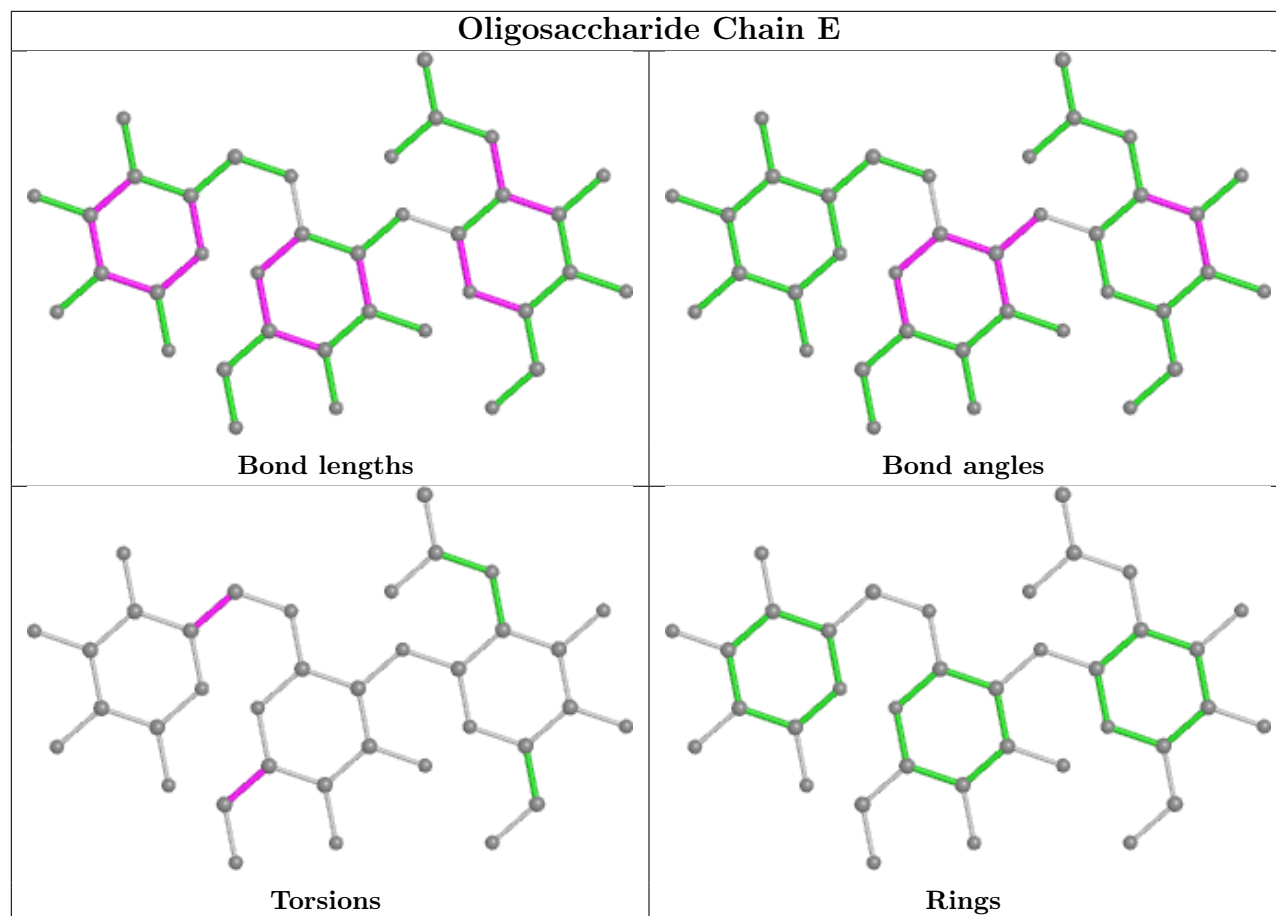
There are no ring outliers.

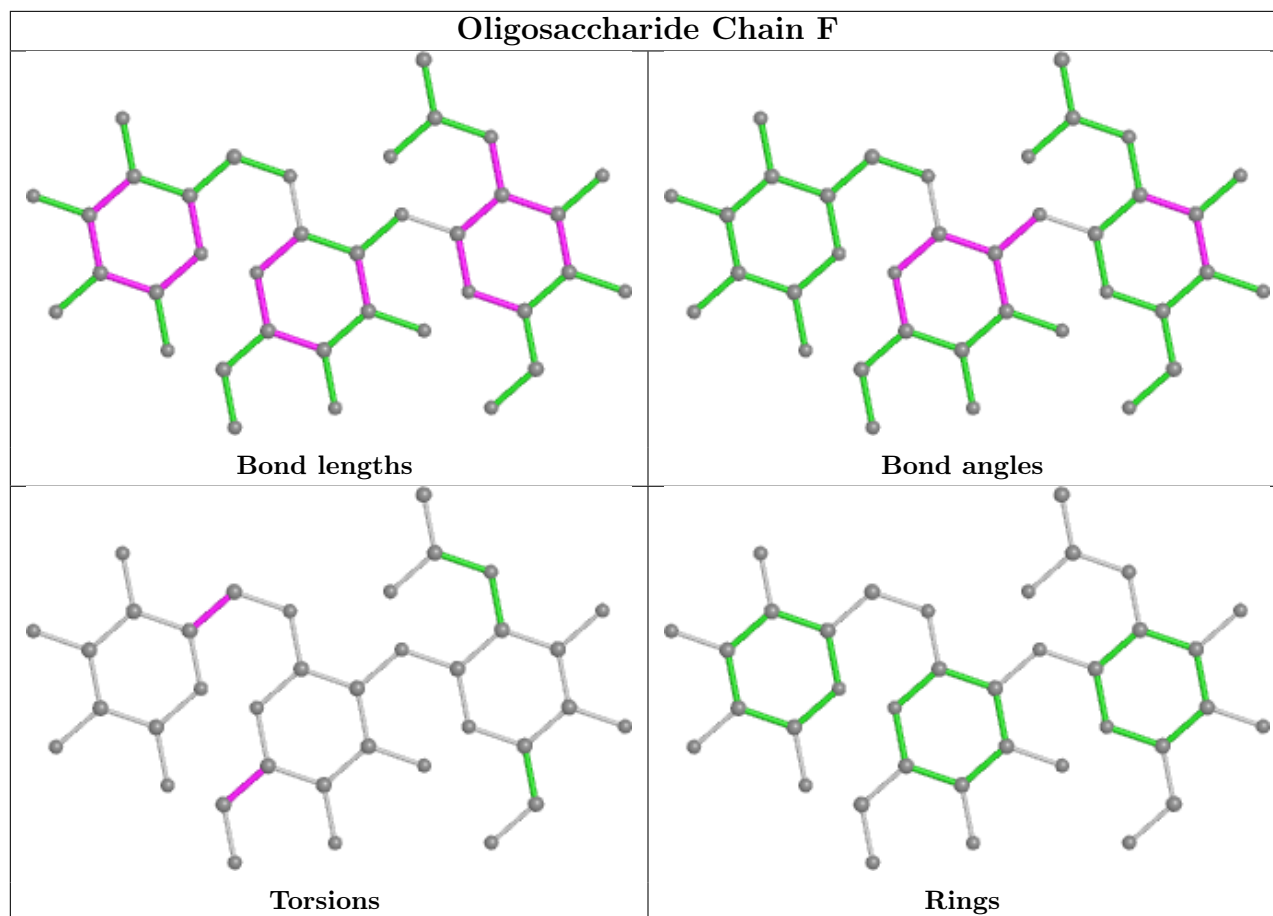
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	MAN	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 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 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$
4	SO4	A	421	-	4,4,4	1.83	1 (25%)	6,6,6	0.95	0
7	DIO	C	435	-	6,6,6	0.95	0	6,6,6	0.70	0
6	GOL	C	418	-	5,5,5	0.35	0	5,5,5	0.65	0
8	MES	C	436	-	12,12,12	1.47	3 (25%)	14,16,16	0.67	0
6	GOL	B	414	-	5,5,5	0.46	0	5,5,5	0.73	0
5	UDH	C	403	3	31,33,33	1.11	3 (9%)	41,47,47	1.43	7 (17%)
6	GOL	B	416	-	5,5,5	0.55	0	5,5,5	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	C	426	-	4,4,4	1.87	1 (25%)	6,6,6	0.90	0
6	GOL	A	417	-	5,5,5	0.20	0	5,5,5	0.65	0
4	SO4	B	425	-	4,4,4	1.90	2 (50%)	6,6,6	0.90	0
4	SO4	A	422	-	4,4,4	1.82	1 (25%)	6,6,6	0.91	0
6	GOL	B	415	-	5,5,5	0.32	0	5,5,5	0.68	0
4	SO4	B	431	-	4,4,4	1.85	2 (50%)	6,6,6	0.91	0
4	SO4	B	428	-	4,4,4	1.82	2 (50%)	6,6,6	0.83	0
4	SO4	C	434	-	4,4,4	1.95	2 (50%)	6,6,6	0.88	0
4	SO4	B	427	-	4,4,4	1.82	1 (25%)	6,6,6	0.94	0
4	SO4	B	424	-	4,4,4	1.86	1 (25%)	6,6,6	0.91	0
6	GOL	B	419	-	5,5,5	0.40	0	5,5,5	0.54	0
5	UDH	B	401	3	31,33,33	1.17	3 (9%)	41,47,47	1.40	8 (19%)
4	SO4	B	433	-	4,4,4	1.92	2 (50%)	6,6,6	0.89	0
6	GOL	A	420	-	5,5,5	0.36	0	5,5,5	0.57	0
4	SO4	C	429	-	4,4,4	1.84	2 (50%)	6,6,6	0.91	0
4	SO4	A	432	-	4,4,4	1.89	2 (50%)	6,6,6	0.90	0
4	SO4	C	430	-	4,4,4	1.91	2 (50%)	6,6,6	0.90	0
5	UDH	A	399	3	31,33,33	1.05	4 (12%)	41,47,47	1.42	8 (19%)
4	SO4	A	423	-	4,4,4	1.89	1 (25%)	6,6,6	0.90	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
6	GOL	A	420	-	-	2/4/4/4	-
6	GOL	B	415	-	-	4/4/4/4	-
6	GOL	A	417	-	-	2/4/4/4	-
7	DIO	C	435	-	-	-	0/1/1/1
6	GOL	C	418	-	-	0/4/4/4	-
8	MES	C	436	-	-	0/6/14/14	0/1/1/1
5	UDH	A	399	3	-	2/25/41/41	0/2/2/2
6	GOL	B	416	-	-	0/4/4/4	-
6	GOL	B	414	-	-	1/4/4/4	-
5	UDH	C	403	3	-	2/25/41/41	0/2/2/2
5	UDH	B	401	3	-	4/25/41/41	0/2/2/2
6	GOL	B	419	-	-	2/4/4/4	-

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	434	SO4	O1-S	3.28	1.63	1.46
4	B	433	SO4	O1-S	3.24	1.63	1.46
4	C	430	SO4	O1-S	3.19	1.63	1.46
4	A	423	SO4	O1-S	3.18	1.63	1.46
4	B	425	SO4	O1-S	3.18	1.63	1.46

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	399	UDH	O4'-C4B-C3B	-3.47	98.24	105.11
5	B	401	UDH	O4'-C4B-C3B	-3.40	98.39	105.11
5	C	403	UDH	O4'-C4B-C3B	-3.11	98.96	105.11
5	C	403	UDH	O3B-PB-O1B	2.95	126.84	112.24
5	B	401	UDH	O2-C2-N1	-2.89	118.95	122.79

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	415	GOL	O1-C1-C2-C3
6	B	415	GOL	O1-C1-C2-O2
6	A	417	GOL	C1-C2-C3-O3
6	A	420	GOL	O1-C1-C2-C3
6	B	414	GOL	O1-C1-C2-C3

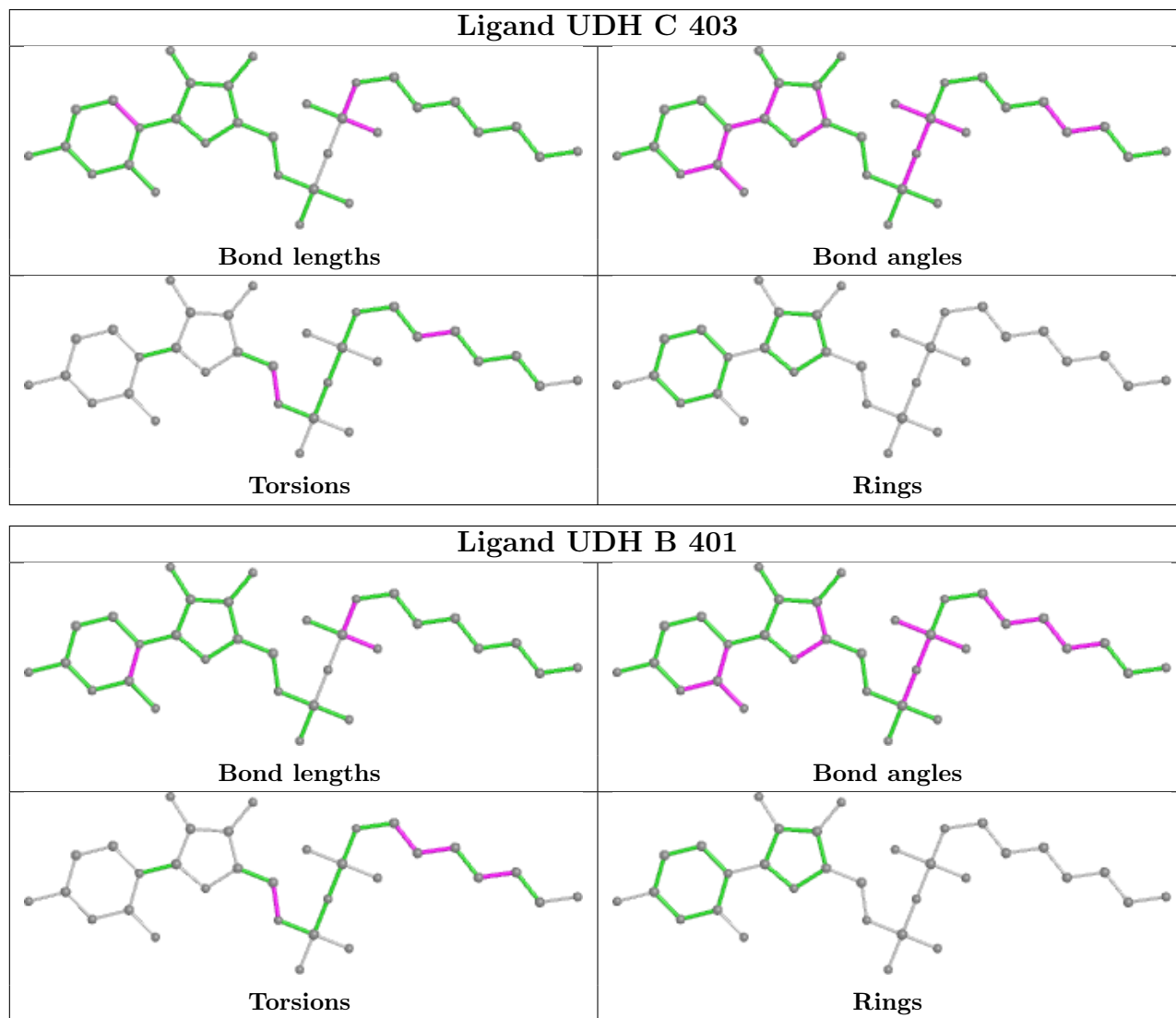
There are no ring outliers.

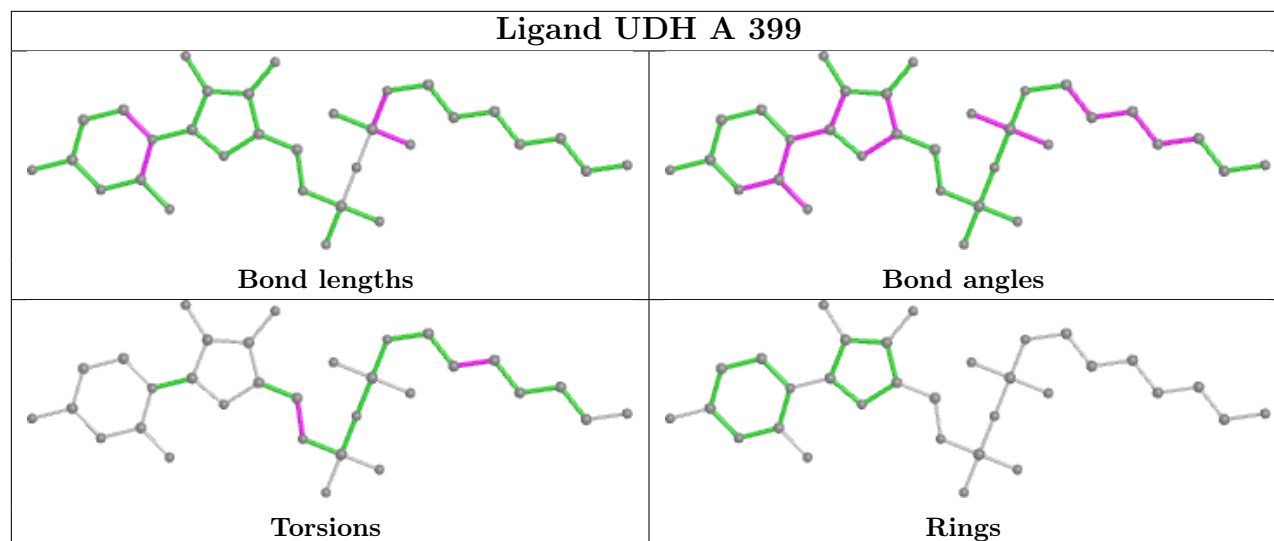
8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	435	DIO	2	0
6	C	418	GOL	1	0
8	C	436	MES	3	0
6	B	414	GOL	1	0
5	C	403	UDH	1	0
6	B	416	GOL	1	0
6	A	417	GOL	3	0
6	B	419	GOL	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 [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	272/287 (94%)	0.11	16 (5%) 22 21	18, 27, 44, 55	0
1	B	272/287 (94%)	-0.02	12 (4%) 34 33	16, 24, 39, 50	0
1	C	272/287 (94%)	0.35	21 (7%) 13 12	22, 33, 52, 61	0
All	All	816/861 (94%)	0.15	49 (6%) 21 20	16, 28, 47, 61	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	347	LYS	4.3
1	C	398	SER	4.1
1	B	398	SER	4.0
1	C	182	ILE	3.7
1	A	347	LYS	3.3

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.

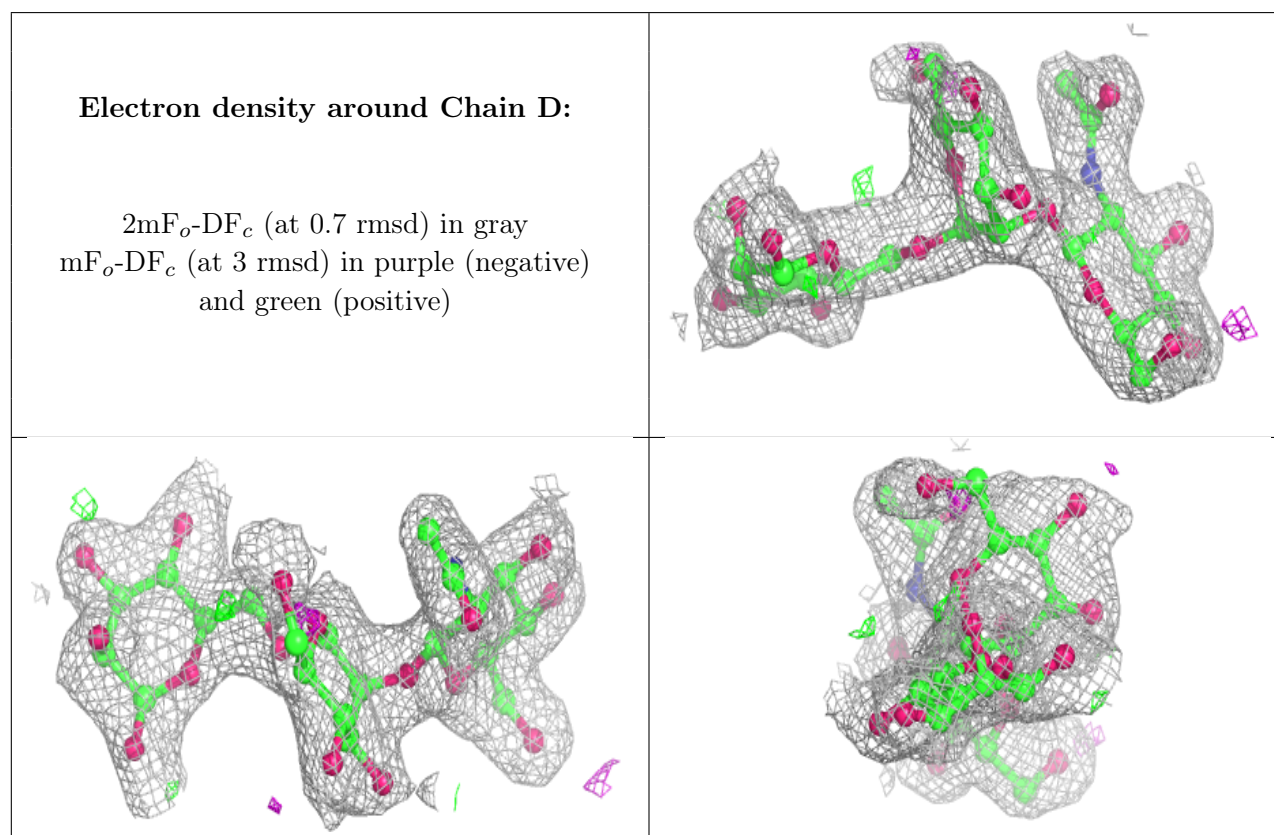
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BMA	F	1	12/12	0.80	0.25	58,60,61,62	0
2	BMA	E	1	12/12	0.87	0.24	40,43,45,47	0
2	BMA	D	1	12/12	0.87	0.24	41,46,48,49	0

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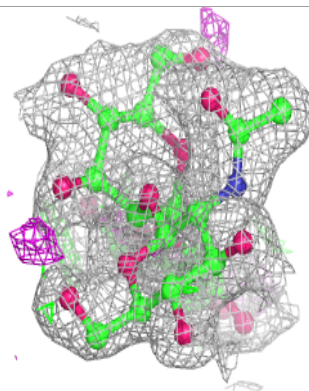
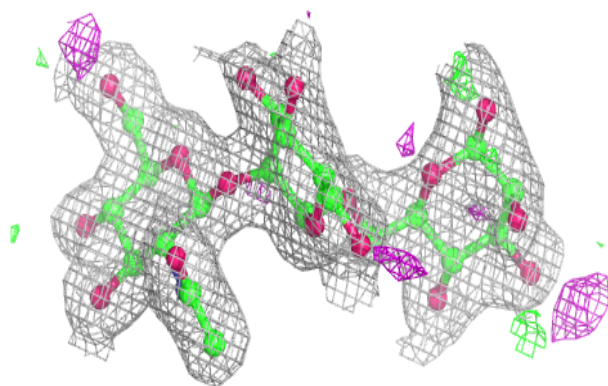
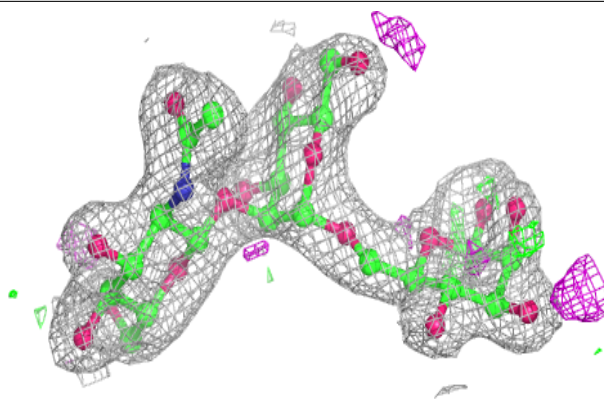
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	D	2	11/12	0.88	0.22	40,47,51,53	0
2	MAN	F	2	11/12	0.88	0.24	56,60,62,64	0
2	NAG	F	3	14/15	0.88	0.13	48,50,52,53	0
2	MAN	E	2	11/12	0.93	0.24	36,45,47,50	0
2	NAG	D	3	14/15	0.94	0.11	30,34,36,37	0
2	NAG	E	3	14/15	0.95	0.09	26,29,30,31	0

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.

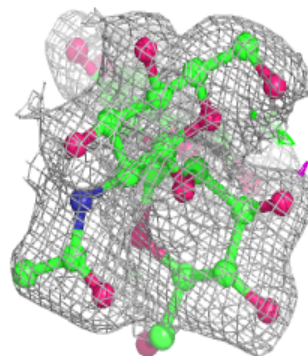
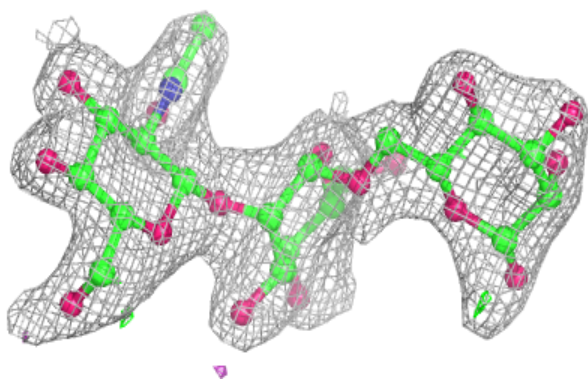
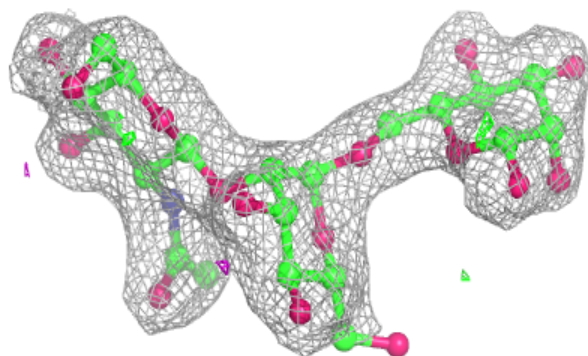


Electron density around Chain E:

$2mF_o-DF_c$ (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 [i](#)

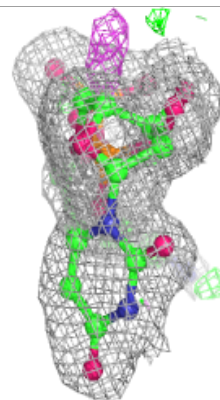
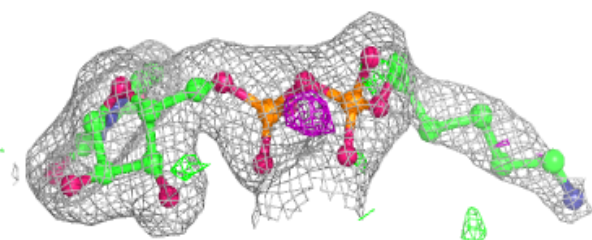
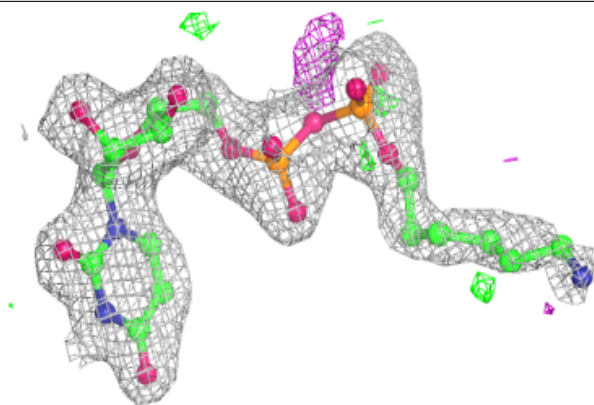
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MES	C	436	12/12	0.43	0.36	79,82,89,90	0
7	DIO	C	435	6/6	0.67	0.21	66,66,67,67	0
6	GOL	B	419	6/6	0.76	0.17	47,49,50,54	0
4	SO4	C	434	5/5	0.83	0.48	107,107,107,108	0
4	SO4	B	433	5/5	0.84	0.34	86,87,87,88	0
4	SO4	A	423	5/5	0.84	0.31	86,87,87,88	0
6	GOL	B	415	6/6	0.84	0.20	44,48,49,52	0
4	SO4	A	432	5/5	0.85	0.35	96,96,96,96	0
6	GOL	A	420	6/6	0.85	0.39	49,55,55,55	0
4	SO4	C	430	5/5	0.85	0.29	100,100,101,101	0
4	SO4	B	425	5/5	0.86	0.48	98,98,98,99	0
4	SO4	B	424	5/5	0.87	0.25	75,75,76,76	0
4	SO4	B	428	5/5	0.89	0.26	58,62,62,62	0
4	SO4	A	422	5/5	0.91	0.19	64,66,67,67	0
4	SO4	A	421	5/5	0.91	0.14	74,74,74,74	0
6	GOL	C	418	6/6	0.92	0.22	45,45,47,47	0
4	SO4	B	431	5/5	0.93	0.28	87,88,88,88	0
4	SO4	B	427	5/5	0.93	0.16	76,76,77,78	0
5	UDH	C	403	32/32	0.93	0.16	31,36,54,57	0
6	GOL	A	417	6/6	0.94	0.14	32,36,37,40	0
4	SO4	C	429	5/5	0.94	0.15	81,81,81,82	0
6	GOL	B	414	6/6	0.94	0.17	28,34,36,38	0
4	SO4	C	426	5/5	0.94	0.16	51,54,54,54	0
5	UDH	A	399	32/32	0.95	0.14	23,28,51,54	0
5	UDH	B	401	32/32	0.96	0.14	17,21,54,59	0
3	MN	C	404	1/1	0.97	0.05	34,34,34,34	0
6	GOL	B	416	6/6	0.97	0.10	20,24,25,26	0
3	MN	A	400	1/1	0.99	0.07	29,29,29,29	0
3	MN	B	402	1/1	1.00	0.07	22,22,22,22	0

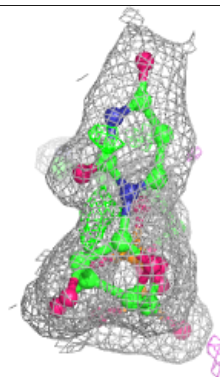
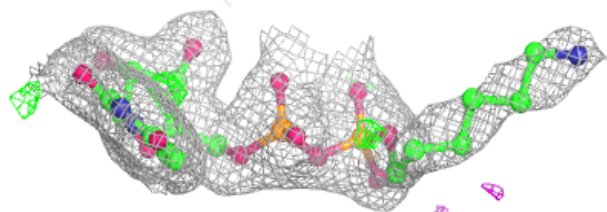
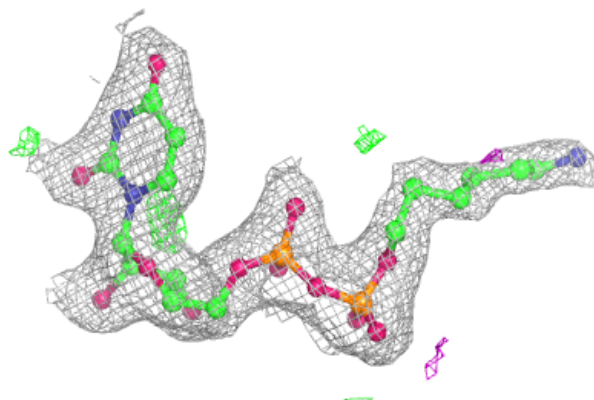
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

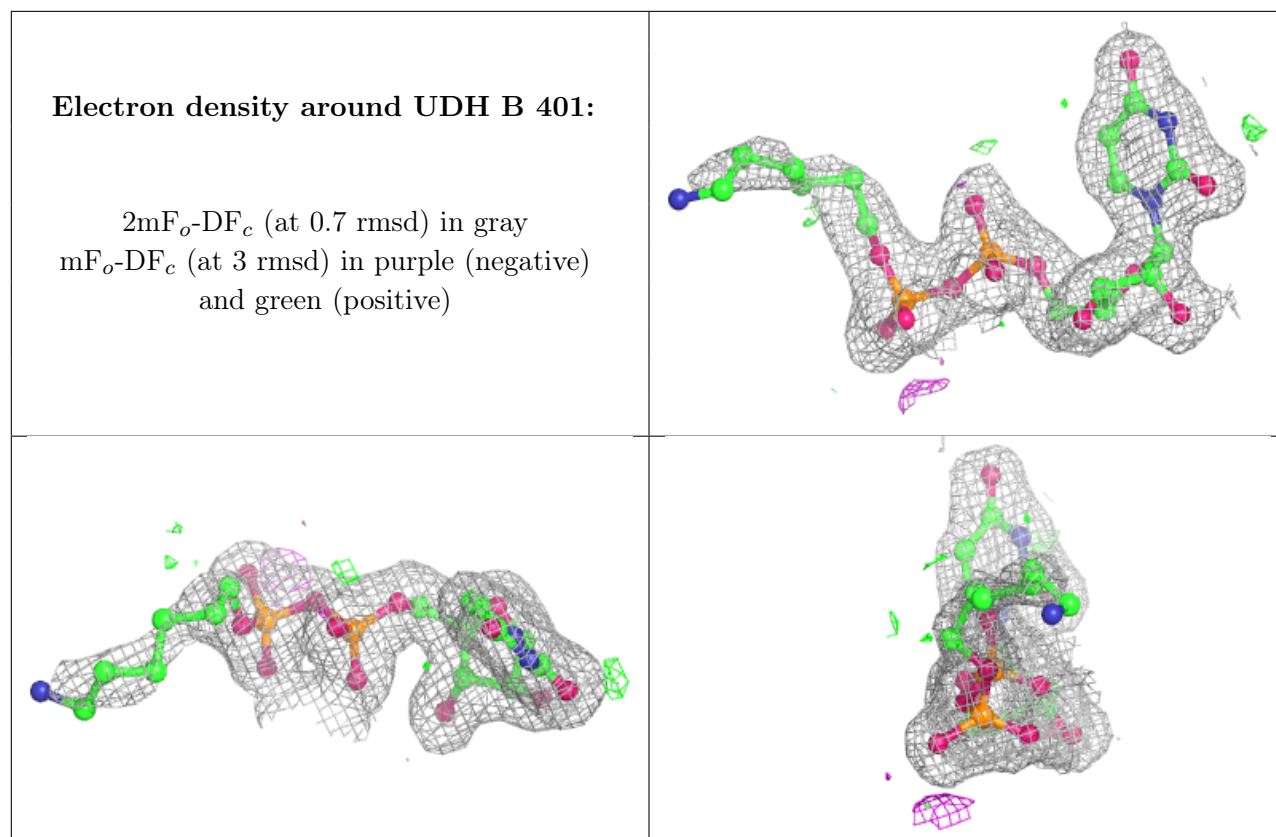
Electron density around UDH C 403:

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

**Electron density around UDH A 399:**

$2mF_o-DF_c$ (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.