



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 01:36 AM EDT

PDB ID : 1TW5
Title : beta1,4-galactosyltransferase mutant M344H-Gal-T1 in complex with Chitobiose
Authors : Ramakrishnan, B.; Boeggeman, E.; Qasba, P.K.
Deposited on : 2004-06-30
Resolution : 2.30 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
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) : 2.23.2

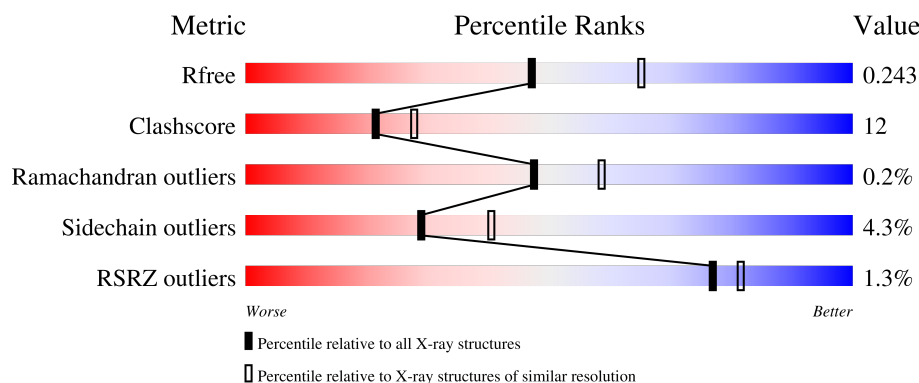
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	286	
1	B	286	
2	C	2	
2	D	2	
2	E	2	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5139 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
1	A	272	Total	C	N	O	S	0	0	0
			2221	1426	384	399	12			
1	B	272	Total	C	N	O	S	0	0	0
			2221	1426	384	399	12			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	ALA	-	SEE REMARK 999	UNP P08037
A	118	SER	-	SEE REMARK 999	UNP P08037
A	119	MET	-	SEE REMARK 999	UNP P08037
A	120	THR	-	SEE REMARK 999	UNP P08037
A	121	GLY	-	SEE REMARK 999	UNP P08037
A	122	GLY	-	SEE REMARK 999	UNP P08037
A	123	GLN	-	SEE REMARK 999	UNP P08037
A	124	GLN	-	SEE REMARK 999	UNP P08037
A	125	MET	-	SEE REMARK 999	UNP P08037
A	126	GLY	-	SEE REMARK 999	UNP P08037
A	127	ARG	-	SEE REMARK 999	UNP P08037
A	128	GLY	-	SEE REMARK 999	UNP P08037
A	129	SER	-	SEE REMARK 999	UNP P08037
A	342	THR	CYS	engineered mutation	UNP P08037
A	344	HIS	MET	engineered mutation	UNP P08037
B	117	ALA	-	SEE REMARK 999	UNP P08037
B	118	SER	-	SEE REMARK 999	UNP P08037
B	119	MET	-	SEE REMARK 999	UNP P08037
B	120	THR	-	SEE REMARK 999	UNP P08037
B	121	GLY	-	SEE REMARK 999	UNP P08037
B	122	GLY	-	SEE REMARK 999	UNP P08037
B	123	GLN	-	SEE REMARK 999	UNP P08037
B	124	GLN	-	SEE REMARK 999	UNP P08037
B	125	MET	-	SEE REMARK 999	UNP P08037
B	126	GLY	-	SEE REMARK 999	UNP P08037

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Chain	Residue	Modelled	Actual	Comment	Reference
B	127	ARG	-	SEE REMARK 999	UNP P08037
B	128	GLY	-	SEE REMARK 999	UNP P08037
B	129	SER	-	SEE REMARK 999	UNP P08037
B	342	THR	CYS	engineered mutation	UNP P08037
B	344	HIS	MET	engineered mutation	UNP P08037

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

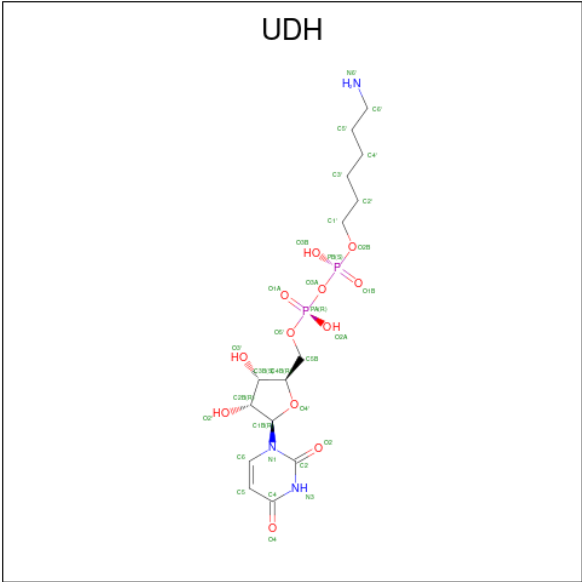


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			29	16	2	11			
2	D	2	Total	C	N	O	0	0	0
			29	16	2	11			
2	E	2	Total	C	N	O	0	0	0
			29	16	2	11			

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

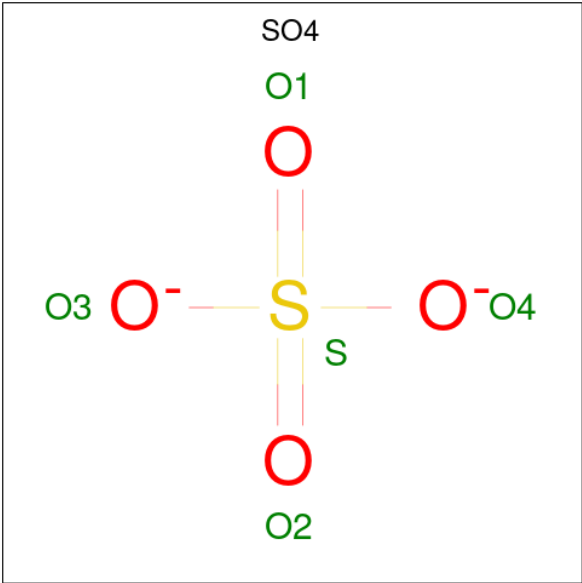
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 6-AMINOHEXYL-URIDINE-C1,5'-DIPHOSPHATE (three-letter code: UDH) (formula: C₁₅H₂₇N₃O₁₂P₂).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



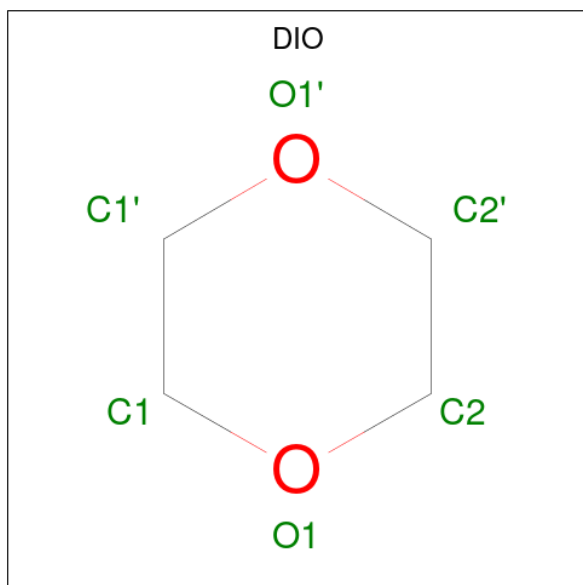
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 6 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



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

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

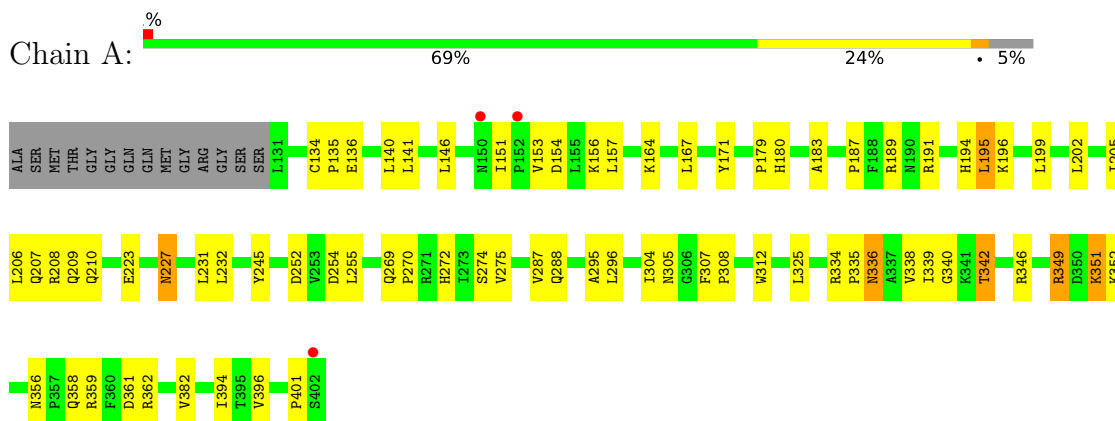
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	248	Total	O	0	0
			248	248		
8	B	247	Total	O	0	0
			247	247		

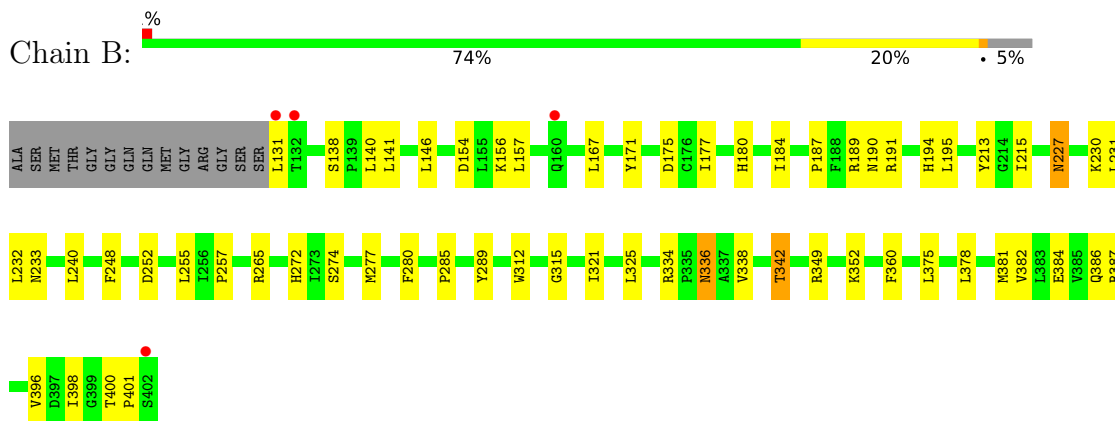
3 Residue-property plots

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

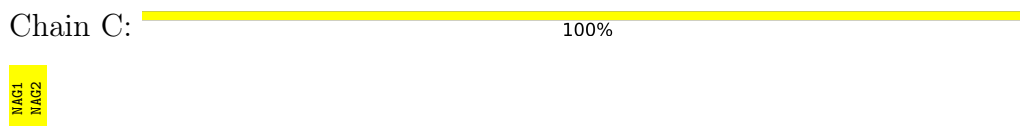
- Molecule 1: Beta-1,4-galactosyltransferase 1



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



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



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

Chain D:  50% 50%

MAG1
MAG2

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

Chain E:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.37Å 92.55Å 143.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.57 – 2.30 19.57 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (19.57-2.30) 89.6 (19.57-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.21Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.195 , 0.257 0.180 , 0.243	Depositor DCC
R_{free} test set	3121 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5139	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: UDH, NAG, DIO, MN, MES, SO4

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	0.49	0/2282	0.75	0/3092
1	B	0.51	0/2282	0.74	1/3092 (0.0%)
All	All	0.50	0/4564	0.74	1/6184 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	GLY	N-CA-C	5.48	126.79	113.10

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	2221	0	2185	64	0
1	B	2221	0	2185	46	0
2	C	29	0	27	0	0
2	D	29	0	27	0	0
2	E	29	0	27	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	32	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	32	0	25	3	0
5	A	20	0	0	0	0
5	B	5	0	0	0	0
6	A	6	0	8	2	0
6	B	6	0	8	3	0
7	A	12	0	13	0	0
8	A	248	0	0	2	0
8	B	247	0	0	3	0
All	All	5139	0	4530	110	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 12.

All (110) 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:349:ARG:H	1:A:349:ARG:CD	1.95	0.80
1:A:151:ILE:HD12	1:A:151:ILE:H	1.47	0.78
1:A:164:LYS:HA	1:A:164:LYS:HE2	1.64	0.77
1:A:154:ASP:HB3	1:A:157:LEU:HD13	1.65	0.77
1:A:349:ARG:H	1:A:349:ARG:HD3	1.51	0.75
1:B:274:SER:O	1:B:277:MET:HE2	1.93	0.69
1:A:336:ASN:HD22	1:A:338:VAL:H	1.41	0.68
1:B:384:GLU:OE2	1:B:386:GLN:NE2	2.27	0.67
1:A:252:ASP:HB2	1:A:255:LEU:HD23	1.77	0.66
1:A:312:TRP:CG	1:A:401:PRO:HB3	2.31	0.66
1:B:175:ASP:H	6:B:861:DIO:H22	1.60	0.64
1:A:287:VAL:HG23	8:A:1193:HOH:O	1.97	0.64
1:A:336:ASN:ND2	1:A:338:VAL:H	1.96	0.64
1:B:191:ARG:HH21	1:B:194:HIS:HD2	1.43	0.64
1:A:287:VAL:HG12	8:A:1272:HOH:O	1.97	0.63
1:A:336:ASN:ND2	1:A:339:ILE:H	1.96	0.63
1:A:154:ASP:CB	1:A:157:LEU:HD13	2.30	0.61
1:A:164:LYS:HA	1:A:164:LYS:CE	2.29	0.61
1:A:349:ARG:HD3	1:A:349:ARG:N	2.16	0.61
1:A:336:ASN:HD21	1:A:339:ILE:H	1.49	0.60
1:A:358:GLN:OE1	1:A:362:ARG:NH1	2.34	0.59
1:A:349:ARG:HG3	4:A:404:UDH:H3'2	1.84	0.59
1:B:349:ARG:HG2	4:B:806:UDH:H4'2	1.84	0.58
1:B:252:ASP:HB3	4:B:806:UDH:O3'	2.03	0.58
1:A:269:GLN:O	1:A:270:PRO:C	2.42	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ALA:C	1:A:296:LEU:HD12	2.24	0.58
1:A:382:VAL:HA	1:A:396:VAL:HG12	1.87	0.57
1:B:175:ASP:HB2	6:B:861:DIO:H22	1.85	0.57
1:A:275:VAL:HG22	1:A:340:GLY:HA3	1.87	0.57
1:B:167:LEU:CD1	1:B:387:ARG:HB3	2.35	0.57
1:B:336:ASN:HD22	1:B:336:ASN:C	2.08	0.57
1:B:277:MET:HE3	1:B:289:TYR:HE2	1.69	0.57
1:A:187:PRO:HD3	1:A:232:LEU:HD21	1.87	0.57
1:A:312:TRP:CD1	1:A:401:PRO:HB3	2.40	0.57
1:B:227:ASN:C	1:B:227:ASN:HD22	2.09	0.56
1:A:336:ASN:HD22	1:A:338:VAL:N	2.02	0.56
1:B:230:LYS:HD3	1:B:398:ILE:HB	1.88	0.55
1:A:351:LYS:O	1:A:352:LYS:HB2	2.06	0.55
1:A:153:VAL:HG13	1:A:196:LYS:HE2	1.89	0.55
1:A:151:ILE:HD12	1:A:151:ILE:N	2.20	0.55
1:A:254:ASP:OD2	1:A:255:LEU:HD22	2.07	0.55
1:A:195:LEU:HD22	1:A:199:LEU:CD1	2.37	0.54
1:A:394:ILE:HG22	1:A:396:VAL:HG13	1.89	0.54
1:B:180:HIS:CE1	1:B:265:ARG:HD2	2.43	0.54
1:A:179:PRO:HG2	1:A:180:HIS:CE1	2.43	0.54
1:A:227:ASN:HD22	1:A:227:ASN:C	2.12	0.53
1:B:138:SER:HB3	1:B:141:LEU:HD13	1.91	0.53
1:A:336:ASN:HD22	1:A:336:ASN:C	2.12	0.53
1:A:135:PRO:HA	6:A:860:DIO:H2'1	1.89	0.52
1:B:382:VAL:HA	1:B:396:VAL:HG12	1.90	0.52
1:A:151:ILE:H	1:A:151:ILE:CD1	2.18	0.52
1:B:349:ARG:HE	4:B:806:UDH:H6'1	1.75	0.52
1:B:233:ASN:HB3	1:B:378:LEU:HD22	1.92	0.51
1:B:277:MET:HE3	1:B:289:TYR:CE2	2.46	0.51
1:A:140:LEU:O	1:A:208:ARG:HD2	2.11	0.50
1:A:205:ILE:O	1:A:209:GLN:HG3	2.12	0.50
1:A:183:ALA:HB2	1:A:245:TYR:CG	2.47	0.49
1:B:156:LYS:HD3	1:B:156:LYS:H	1.76	0.49
1:B:184:ILE:HD12	1:B:215:ILE:CD1	2.42	0.49
1:B:387:ARG:HH11	1:B:387:ARG:HG3	1.77	0.48
1:B:274:SER:HA	1:B:342:THR:HG21	1.96	0.48
1:B:280:PHE:CD1	1:B:285:PRO:HD3	2.49	0.48
1:B:321:ILE:O	1:B:325:LEU:HG	2.14	0.48
1:A:136:GLU:H	6:A:860:DIO:H11	1.79	0.48
1:B:167:LEU:HD13	1:B:387:ARG:HB3	1.96	0.47
1:B:171:TYR:HB3	1:B:213:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ASN:ND2	8:B:910:HOH:O	2.46	0.47
1:A:335:PRO:HB2	1:A:339:ILE:HG13	1.97	0.47
1:B:191:ARG:NH2	1:B:194:HIS:HD2	2.11	0.47
1:A:195:LEU:HD22	1:A:199:LEU:HD11	1.97	0.46
1:B:272:HIS:HB3	1:B:334:ARG:HG2	1.98	0.46
1:A:336:ASN:ND2	1:A:338:VAL:N	2.63	0.45
1:A:351:LYS:NZ	1:A:352:LYS:HE2	2.32	0.45
1:B:187:PRO:HD3	1:B:232:LEU:HD21	1.97	0.45
1:A:154:ASP:CG	1:A:157:LEU:HD13	2.38	0.45
1:A:307:PHE:HB3	1:A:308:PRO:HD2	1.99	0.44
1:A:287:VAL:HG13	1:A:288:GLN:CD	2.38	0.44
1:A:154:ASP:OD1	1:A:156:LYS:HB2	2.17	0.44
1:A:349:ARG:H	1:A:349:ARG:NE	2.15	0.44
1:B:277:MET:CE	1:B:289:TYR:HE2	2.31	0.44
1:B:312:TRP:CG	1:B:401:PRO:HB3	2.53	0.44
1:B:156:LYS:HD3	1:B:156:LYS:N	2.33	0.43
1:A:171:TYR:CE1	1:A:207:GLN:HG2	2.54	0.43
1:A:275:VAL:CG2	1:A:340:GLY:HA3	2.46	0.43
1:A:191:ARG:HD2	1:A:194:HIS:CD2	2.54	0.43
1:B:360:PHE:CD2	2:E:1:NAG:H2	2.53	0.43
1:A:157:LEU:HD12	1:A:157:LEU:N	2.34	0.42
1:B:336:ASN:C	1:B:336:ASN:ND2	2.72	0.42
1:B:375:LEU:HD12	1:B:375:LEU:HA	1.85	0.42
1:A:134:CYS:HB3	1:A:210:GLN:NE2	2.34	0.42
1:A:274:SER:HA	1:A:342:THR:HG21	2.00	0.42
1:B:336:ASN:HD22	1:B:338:VAL:H	1.65	0.42
1:A:191:ARG:HH21	1:A:194:HIS:HD2	1.68	0.42
1:A:346:ARG:HH21	1:A:346:ARG:HG3	1.84	0.42
1:B:189:ARG:HD2	8:B:908:HOH:O	2.19	0.42
1:B:154:ASP:OD1	1:B:157:LEU:HB2	2.20	0.42
1:A:270:PRO:HG2	1:A:325:LEU:HD22	2.01	0.42
1:A:304:ILE:O	1:A:305:ASN:HB3	2.20	0.42
1:B:257:PRO:HA	1:B:342:THR:HB	2.01	0.42
1:B:227:ASN:ND2	1:B:230:LYS:H	2.18	0.42
1:A:356:ASN:O	1:A:359:ARG:HG2	2.20	0.41
1:A:352:LYS:HA	1:A:352:LYS:HD3	1.87	0.41
1:B:131:LEU:HB2	1:B:177:ILE:HG12	2.02	0.41
1:A:272:HIS:HB3	1:A:334:ARG:HG2	2.03	0.41
1:B:140:LEU:HD11	6:B:861:DIO:O1'	2.21	0.41
1:B:194:HIS:HE1	8:B:922:HOH:O	2.03	0.41
1:B:240:LEU:HD21	1:B:248:PHE:HZ	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LEU:O	1:A:206:LEU:HG	2.21	0.40
1:B:400:THR:HB	1:B:401:PRO:HD2	2.03	0.40
1:A:195:LEU:HD22	1:A:199:LEU:HG	2.02	0.40

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	270/286 (94%)	263 (97%)	6 (2%)	1 (0%)	34	42
1	B	270/286 (94%)	263 (97%)	7 (3%)	0	100	100
All	All	540/572 (94%)	526 (97%)	13 (2%)	1 (0%)	47	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	ARG

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	245/254 (96%)	233 (95%)	12 (5%)	25	35
1	B	245/254 (96%)	236 (96%)	9 (4%)	34	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	490/508 (96%)	469 (96%)	21 (4%)	29	40

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	LEU
1	A	146	LEU
1	A	167	LEU
1	A	195	LEU
1	A	223	GLU
1	A	227	ASN
1	A	231	LEU
1	A	336	ASN
1	A	342	THR
1	A	349	ARG
1	A	351	LYS
1	A	361	ASP
1	B	146	LEU
1	B	195	LEU
1	B	227	ASN
1	B	231	LEU
1	B	255	LEU
1	B	336	ASN
1	B	342	THR
1	B	352	LYS
1	B	381	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	194	HIS
1	A	207	GLN
1	A	210	GLN
1	A	227	ASN
1	A	336	ASN
1	B	161	GLN
1	B	190	ASN
1	B	194	HIS
1	B	207	GLN
1	B	227	ASN

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Mol	Chain	Res	Type
1	B	336	ASN
1	B	386	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 ⓘ

6 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	15,15,15	0.87	0	21,21,21	1.34	3 (14%)
2	NAG	C	2	2	14,14,15	0.91	1 (7%)	17,19,21	0.98	0
2	NAG	D	1	2	15,15,15	0.93	0	21,21,21	0.86	0
2	NAG	D	2	2	14,14,15	1.03	1 (7%)	17,19,21	1.06	1 (5%)
2	NAG	E	1	2	15,15,15	0.81	0	21,21,21	1.00	0
2	NAG	E	2	2	14,14,15	1.04	1 (7%)	17,19,21	1.11	2 (11%)

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	-	2/6/26/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2	-	0/6/26/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2	-	0/6/26/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C2-N2	2.22	1.50	1.46
2	E	2	NAG	C4-C5	2.14	1.57	1.53
2	C	2	NAG	C4-C5	2.08	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-O5-C5	2.94	116.18	112.19
2	D	2	NAG	C1-O5-C5	2.85	116.05	112.19
2	C	1	NAG	C4-C3-C2	2.72	114.33	110.34
2	C	1	NAG	O5-C1-C2	-2.47	107.03	109.52
2	E	2	NAG	C8-C7-N2	-2.11	112.52	116.10
2	C	1	NAG	C3-C2-N2	-2.11	106.64	110.62

There are no chirality outliers.

All (5) torsion outliers are listed below:

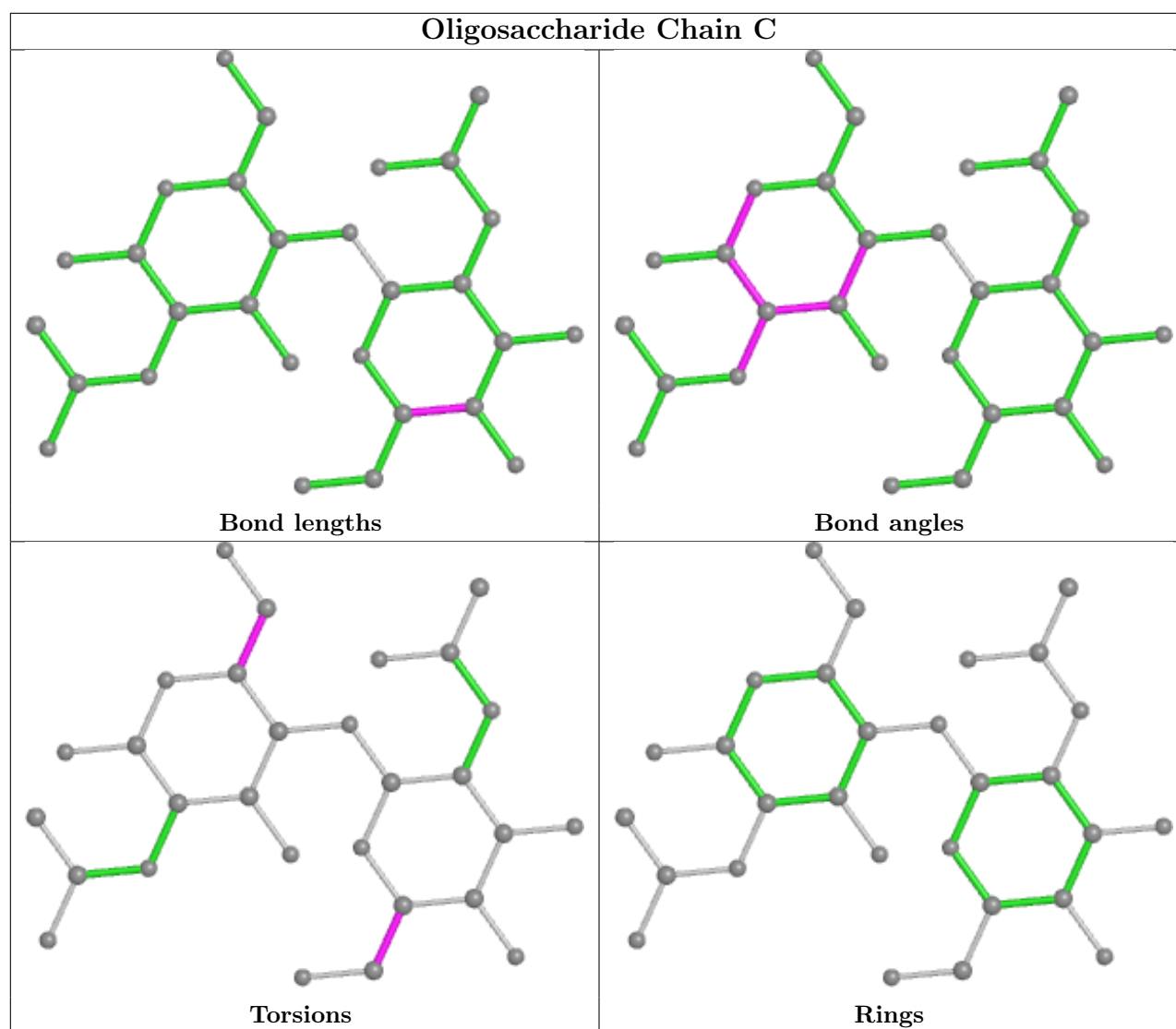
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

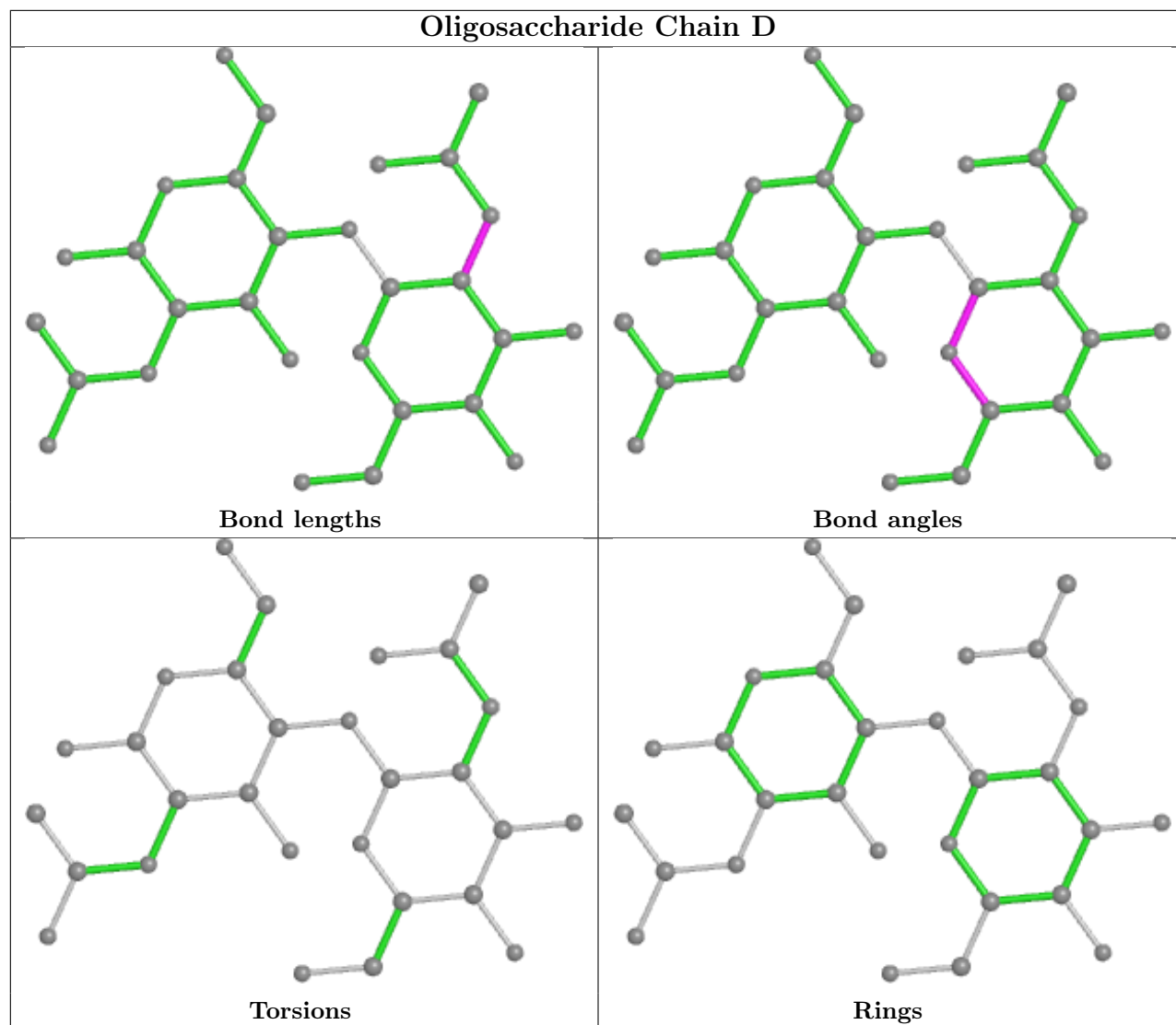
There are no ring outliers.

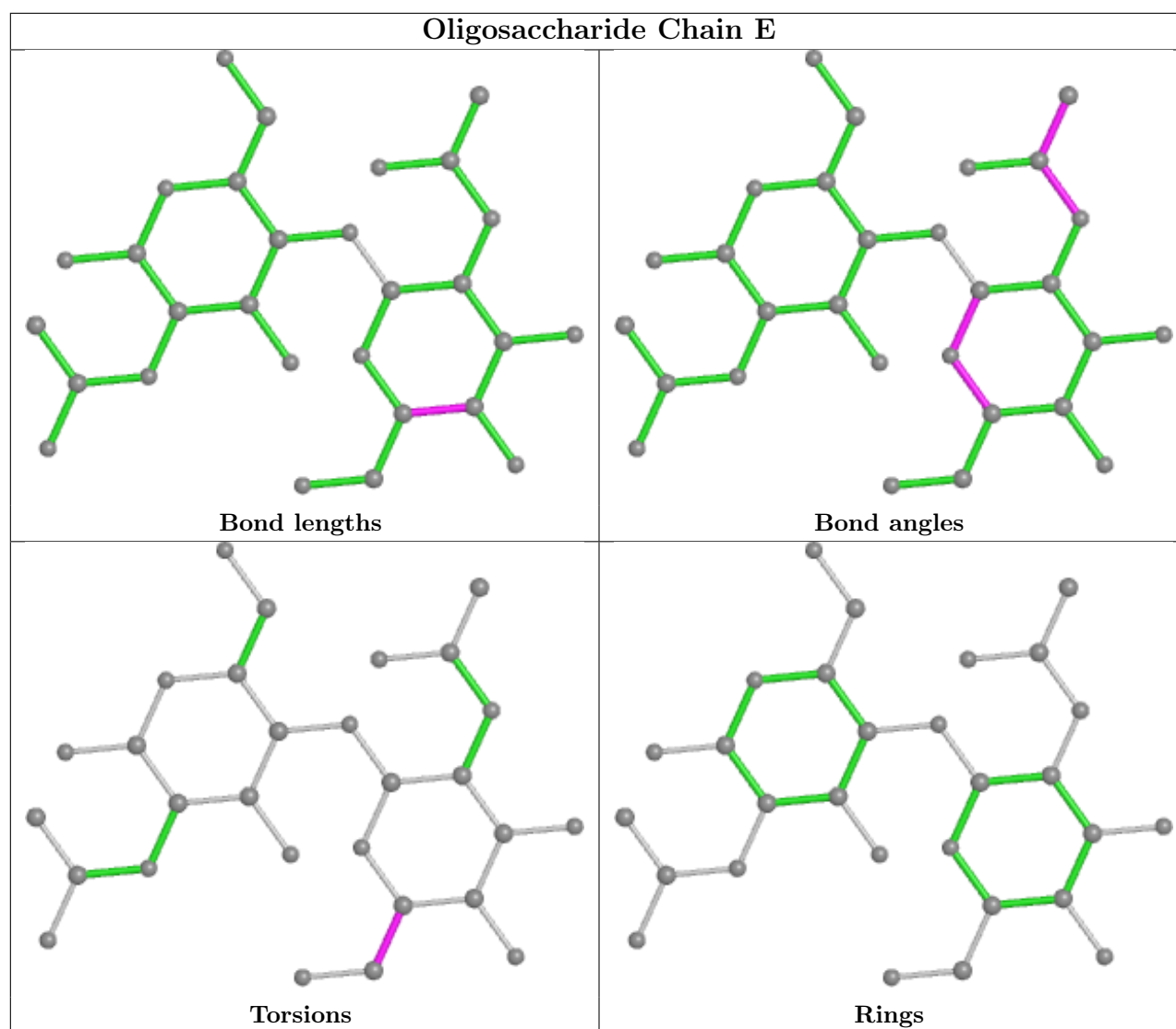
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	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 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z > 2$
5	SO4	B	856	-	4,4,4	1.92	2 (50%)	6,6,6	0.89	0
5	SO4	A	852	-	4,4,4	1.85	1 (25%)	6,6,6	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	UDH	B	806	3	27,33,33	1.65	5 (18%)	29,47,47	1.31	2 (6%)
4	UDH	A	404	3	27,33,33	1.53	4 (14%)	29,47,47	1.27	2 (6%)
5	SO4	A	853	-	4,4,4	1.93	2 (50%)	6,6,6	0.87	0
6	DIO	A	860	-	6,6,6	0.85	0	6,6,6	1.51	2 (33%)
5	SO4	A	854	-	4,4,4	1.92	2 (50%)	6,6,6	0.90	0
7	MES	A	870	-	12,12,12	1.27	2 (16%)	14,16,16	0.88	0
5	SO4	A	855	-	4,4,4	1.87	2 (50%)	6,6,6	0.90	0
6	DIO	B	861	-	6,6,6	0.77	0	6,6,6	1.40	1 (16%)

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
4	UDH	B	806	3	-	4/23/41/41	0/2/2/2
4	UDH	A	404	3	-	5/23/41/41	0/2/2/2
6	DIO	A	860	-	-	-	0/1/1/1
7	MES	A	870	-	-	0/6/14/14	0/1/1/1
6	DIO	B	861	-	-	-	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	806	UDH	C6-N1	4.96	1.42	1.35
4	A	404	UDH	C6-N1	4.34	1.41	1.35
4	B	806	UDH	C4-N3	3.67	1.39	1.33
4	A	404	UDH	C4-N3	3.35	1.38	1.33
5	A	853	SO4	O1-S	3.23	1.63	1.46
5	B	856	SO4	O1-S	3.19	1.63	1.46
5	A	854	SO4	O1-S	3.15	1.63	1.46
5	A	855	SO4	O1-S	3.09	1.62	1.46
5	A	852	SO4	O1-S	3.08	1.62	1.46
4	B	806	UDH	PA-O5'	-2.70	1.48	1.59
7	A	870	MES	C5-N4	2.56	1.54	1.46
4	A	404	UDH	PA-O5'	-2.35	1.49	1.59
4	B	806	UDH	C3B-C2B	-2.30	1.47	1.53
7	A	870	MES	C3-N4	2.28	1.53	1.46
5	A	854	SO4	O3-S	-2.15	1.30	1.47
5	B	856	SO4	O3-S	-2.11	1.30	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	806	UDH	C3B-C4B	-2.10	1.47	1.53
4	A	404	UDH	O4'-C1B	2.08	1.44	1.41
5	A	855	SO4	O3-S	-2.08	1.30	1.47
5	A	853	SO4	O3-S	-2.06	1.31	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	806	UDH	C5-C4-N3	-4.13	114.22	123.31
4	A	404	UDH	C5-C4-N3	-3.68	115.21	123.31
4	B	806	UDH	O5'-PA-O1A	3.61	123.18	109.07
4	A	404	UDH	O5'-PA-O1A	3.14	121.32	109.07
6	A	860	DIO	C2'-O1'-C1'	2.58	118.49	109.89
6	B	861	DIO	C2'-O1'-C1'	2.48	118.16	109.89
6	A	860	DIO	C2-O1-C1	2.14	117.04	109.89

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	UDH	PA-O3A-PB-O2B
4	B	806	UDH	PA-O3A-PB-O2B
4	A	404	UDH	O2B-C1'-C2'-C3'
4	A	404	UDH	C1'-C2'-C3'-C4'
4	B	806	UDH	C1'-C2'-C3'-C4'
4	B	806	UDH	C3'-C4'-C5'-C6'
4	A	404	UDH	C4B-C5B-O5'-PA
4	B	806	UDH	C4B-C5B-O5'-PA
4	A	404	UDH	C2'-C3'-C4'-C5'

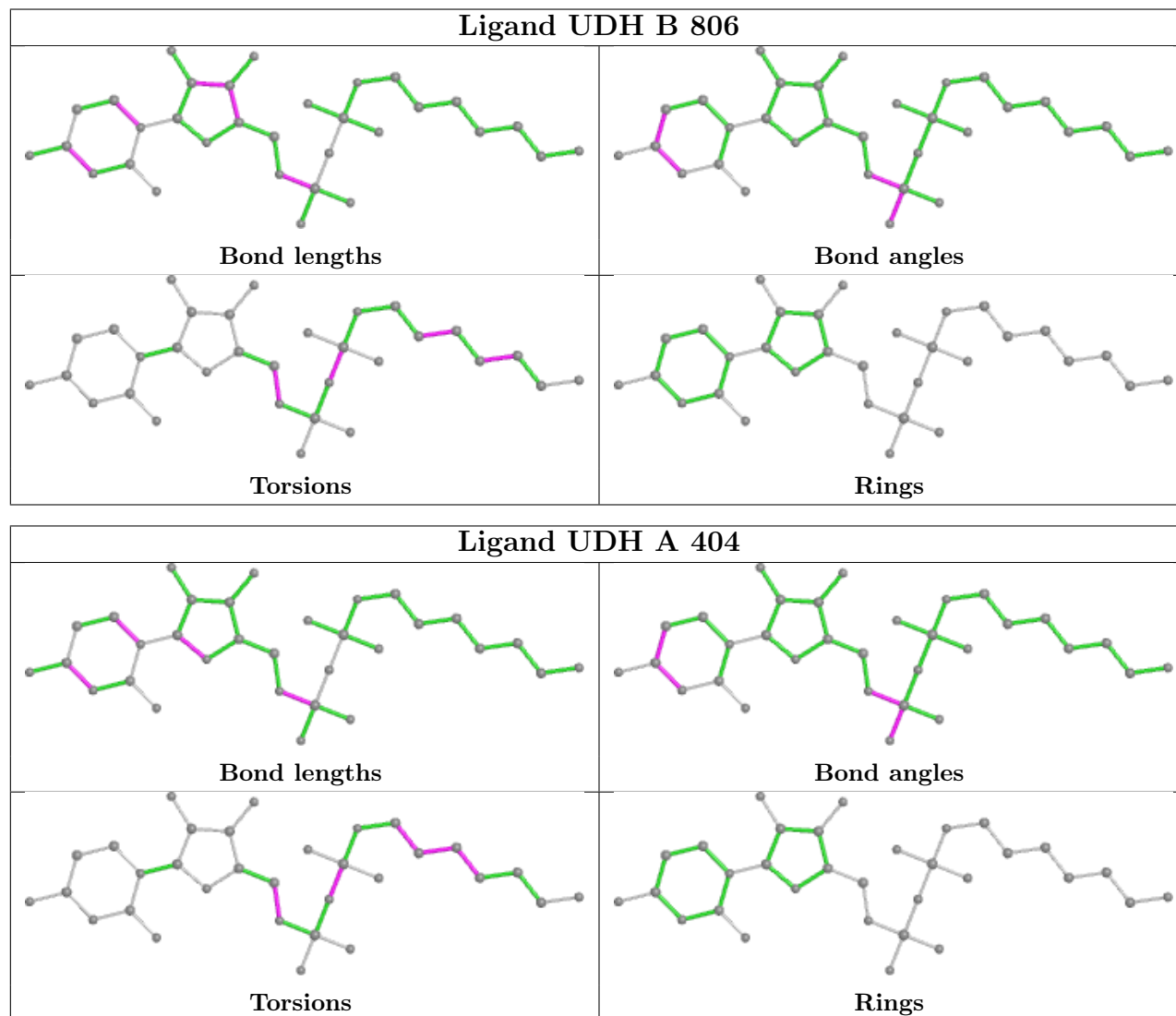
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	806	UDH	3	0
4	A	404	UDH	1	0
6	A	860	DIO	2	0
6	B	861	DIO	3	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 ⓘ

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 [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	272/286 (95%)	-0.27	3 (1%) 80 85	18, 28, 50, 61	0
1	B	272/286 (95%)	-0.40	4 (1%) 73 79	16, 26, 42, 57	0
All	All	544/572 (95%)	-0.33	7 (1%) 77 81	16, 26, 46, 61	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	PRO	4.7
1	A	402	SER	4.0
1	B	402	SER	4.0
1	A	150	ASN	3.0
1	B	132	THR	3.0
1	B	131	LEU	2.6
1	B	160	GLN	2.5

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	2	14/15	0.76	0.34	61,65,68,69	0
2	NAG	E	1	15/15	0.83	0.15	51,52,54,58	0

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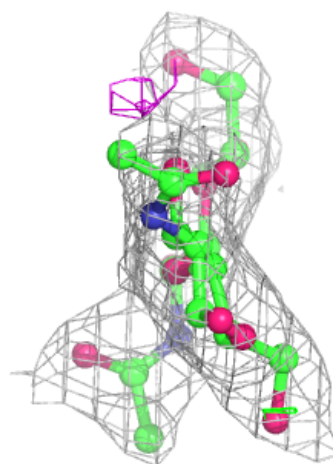
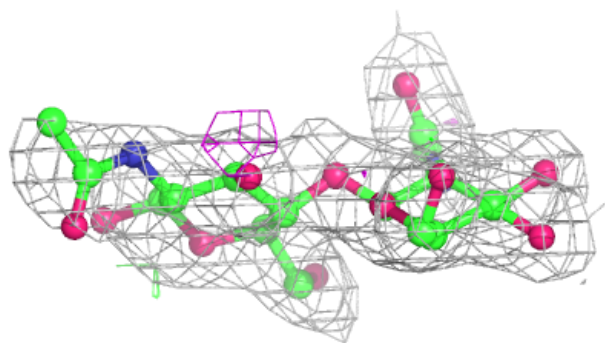
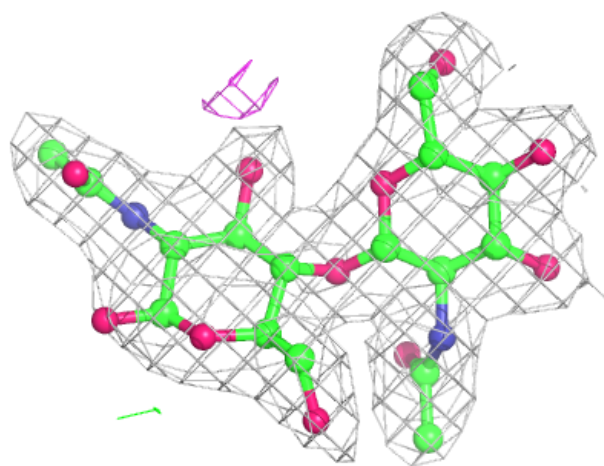
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	C	1	15/15	0.87	0.17	34,45,54,57	0
2	NAG	D	1	15/15	0.92	0.11	26,34,39,40	0
2	NAG	D	2	14/15	0.95	0.10	15,21,23,25	0
2	NAG	C	2	14/15	0.96	0.09	25,27,32,32	0

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

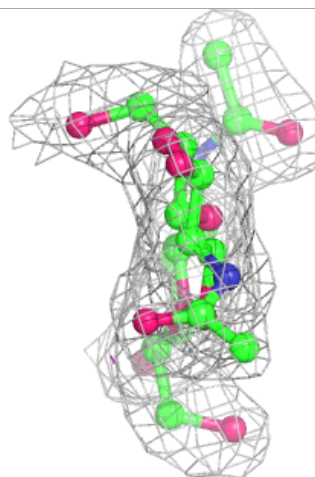
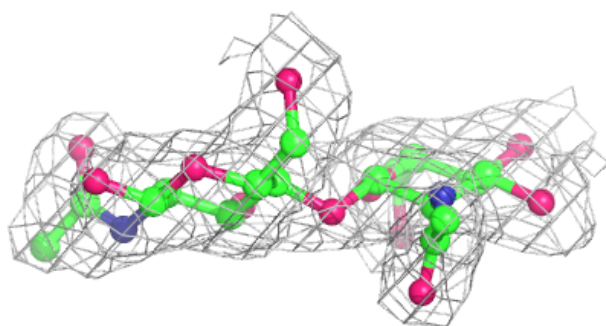
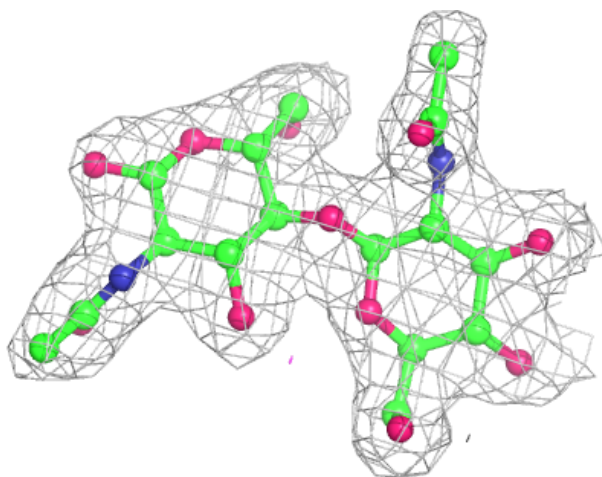
Electron density around Chain C:

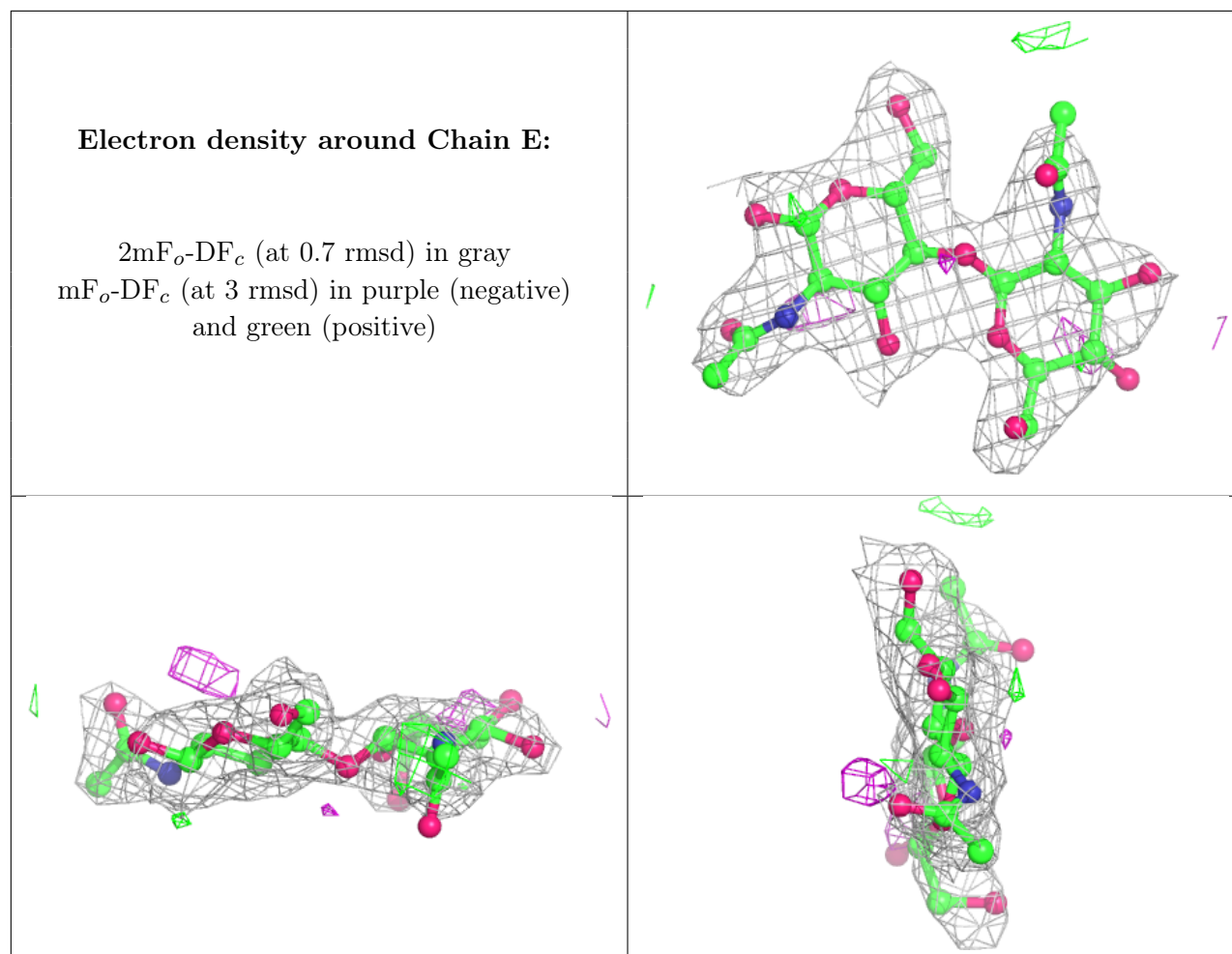
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain D:

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





6.4 Ligands [i](#)

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

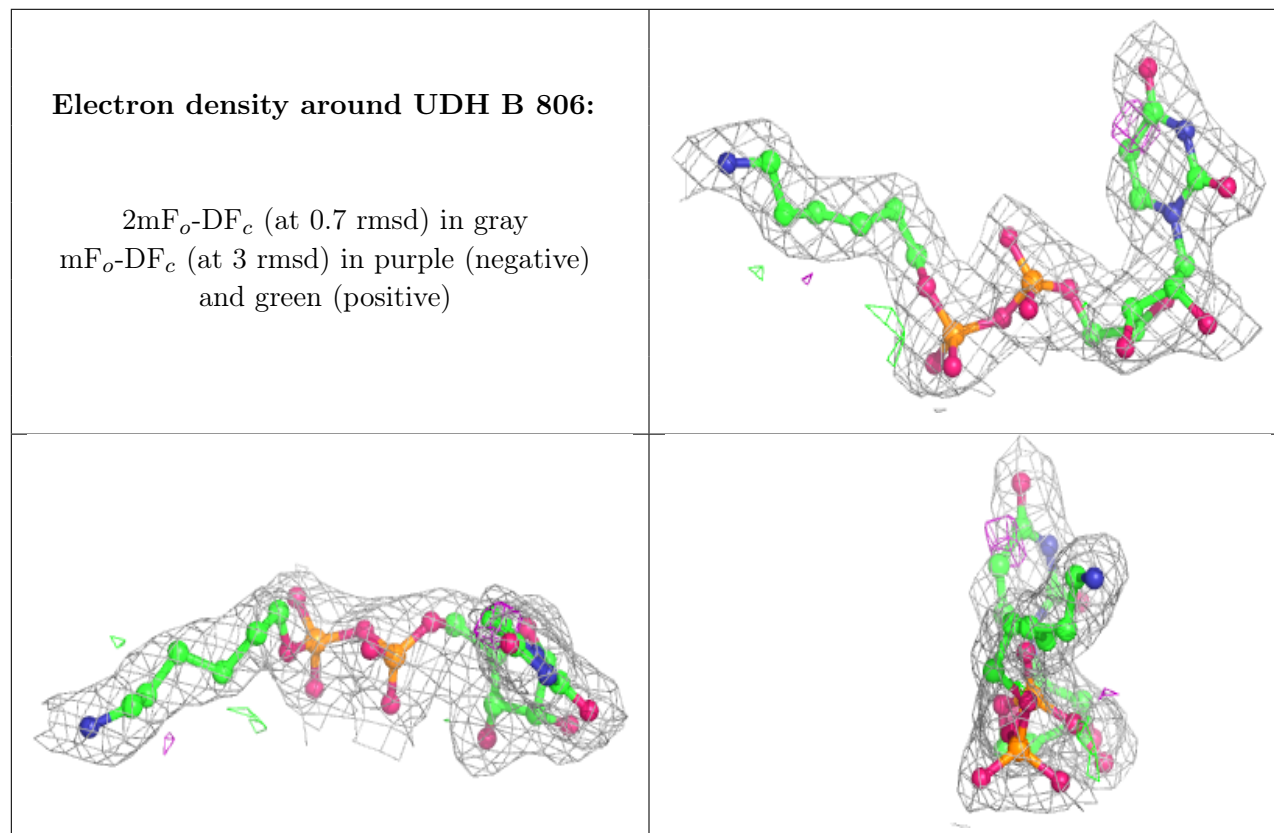
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	DIO	B	861	6/6	0.61	0.32	71,73,73,74	0
5	SO4	A	853	5/5	0.74	0.36	95,95,96,96	0
6	DIO	A	860	6/6	0.78	0.32	75,75,75,76	0
7	MES	A	870	12/12	0.83	0.32	63,66,73,73	0
5	SO4	B	856	5/5	0.92	0.37	87,88,88,88	0
5	SO4	A	854	5/5	0.92	0.21	74,74,75,75	0
5	SO4	A	855	5/5	0.93	0.17	69,70,70,71	0
5	SO4	A	852	5/5	0.96	0.17	71,72,72,73	0
4	UDH	B	806	32/32	0.96	0.10	21,25,35,37	0
4	UDH	A	404	32/32	0.97	0.10	16,20,39,44	0

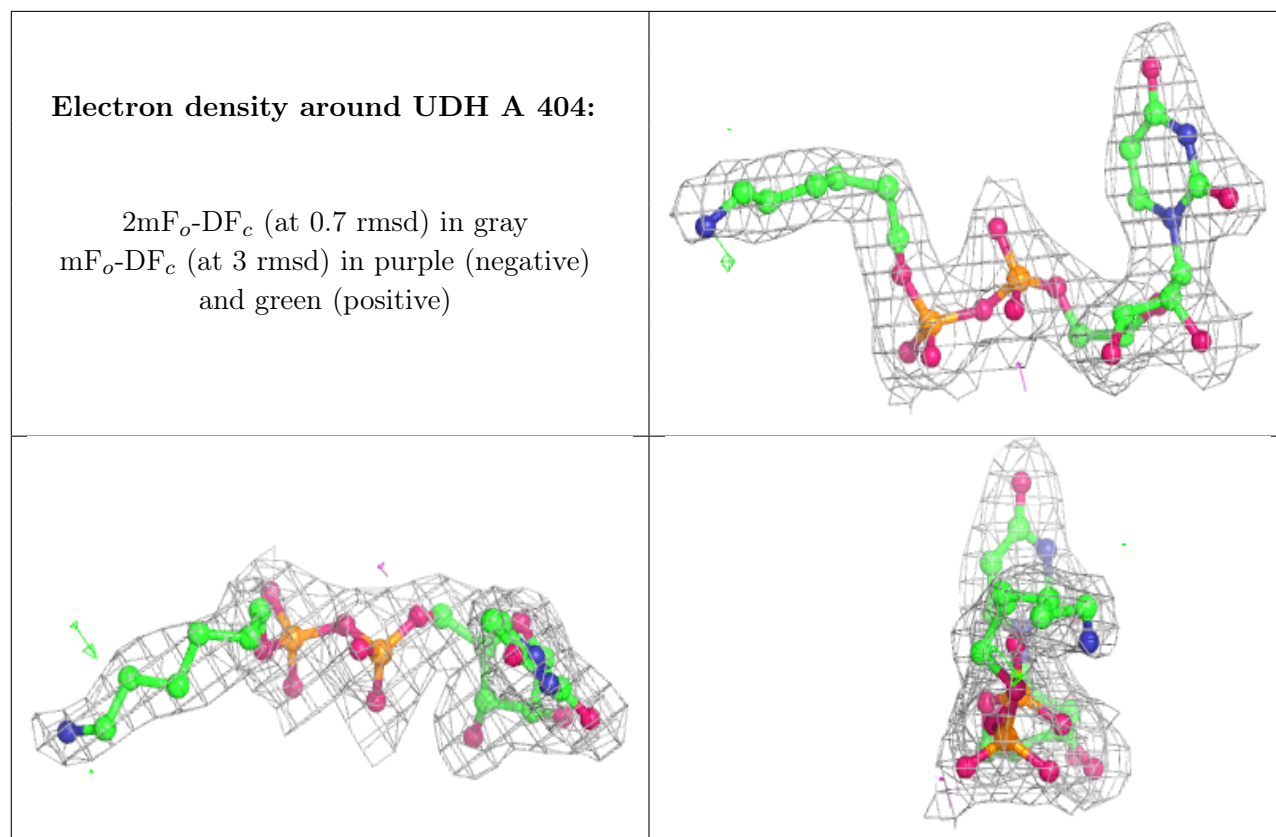
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MN	A	403	1/1	0.99	0.06	24,24,24,24	0
3	MN	B	805	1/1	1.00	0.03	23,23,23,23	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.