



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2023 – 10:24 am BST

PDB ID : 7ZNS
Title : Inactive D62N mutant of BT1760 Endo-acting levanase from *Bacteroides thetaiotaomicron* VPI-5482
Authors : Basle, A.; Bolam, D.
Deposited on : 2022-04-21
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 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.33
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) : 2.33

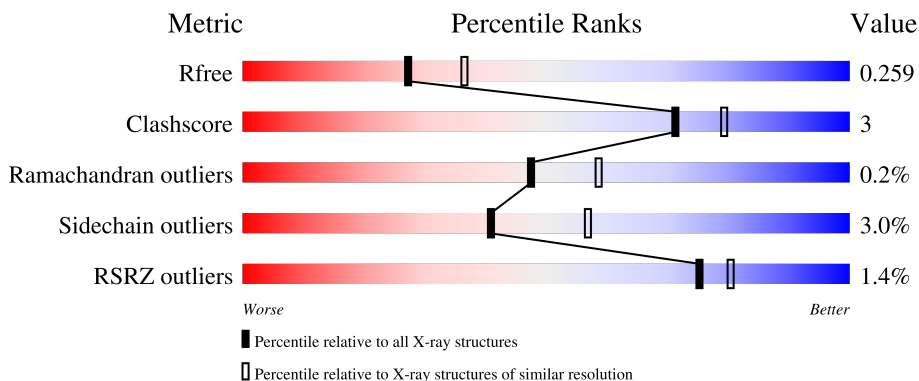
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	523	85% 8% 7%
1	B	523	3% 84% 9% 7%
2	C	3	67% 33%
2	D	3	33% 67%
2	E	3	100%

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Mol	Chain	Length	Quality of chain
3	F	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FRU	E	3	X	-	-	-
4	SO4	A	611	-	-	-	X
4	SO4	B	602	-	-	X	-
4	SO4	B	605	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15180 atoms, of which 6949 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.

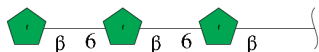
- Molecule 1 is a protein called Glycoside hydrolase family 32.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	487	7327	2476	3427	645	759	20	0	0	0
1	B	487	7327	2476	3427	645	759	20	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

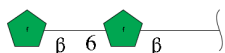
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ASN	ASP	engineered mutation	UNP Q8A6W6
B	42	ASN	ASP	engineered mutation	UNP Q8A6W6

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	H	O			
2	C	3	60	18	26	16	0	0	0
2	D	3	60	18	26	16	0	0	0
2	E	3	60	18	26	16	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-fructofuranose-(2-6)-beta-D-fructofuranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	H	O			
3	F	2	40	12	17	11	0	0	0

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



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

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


- Molecule 5 is water.

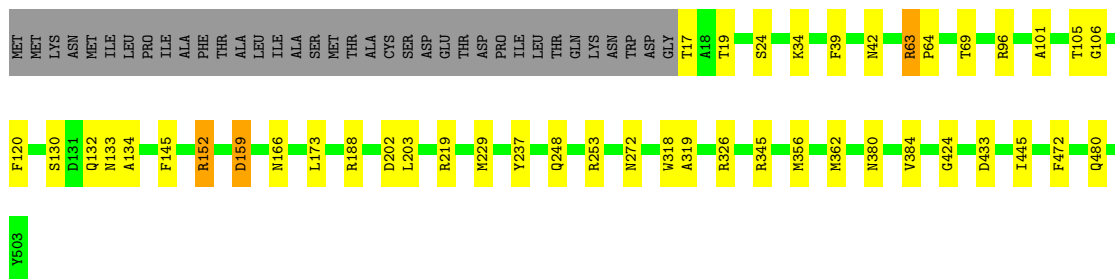
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	145	Total	O	0	0
			145	145		
5	B	56	Total	O	0	0
			56	56		

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.

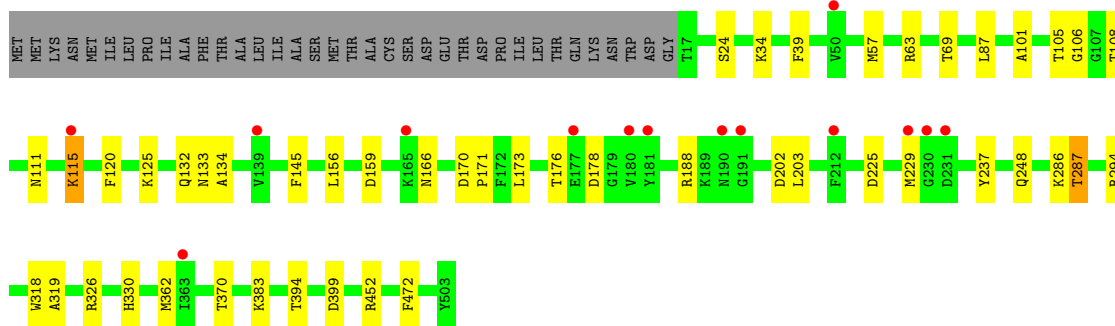
- Molecule 1: Glycoside hydrolase family 32

Chain A: 



- Molecule 1: Glycoside hydrolase family 32

Chain B: 




- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain C: 



- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain D:  33% 67%

FRU1
FRU2
FRU3

- Molecule 2: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain E:  100%

FRU1
FRU2
FRU3

- Molecule 3: beta-D-fructofuranose-(2-6)-beta-D-fructofuranose

Chain F:  50% 50%

FRU1
FRU2

4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	175.50Å 175.50Å 214.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.71 – 2.30 73.71 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (73.71-2.30) 99.6 (73.71-2.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0352, REFMAC 5.8.0352	Depositor
R, R_{free}	0.216 , 0.254 0.223 , 0.259	Depositor DCC
R_{free} test set	3652 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtrriage
Anisotropy	0.724	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15180	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FRU

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	0.39	0/4006	0.74	0/5431
1	B	0.36	0/4006	0.71	1/5431 (0.0%)
All	All	0.38	0/8012	0.72	1/10862 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	383	LYS	CB-CA-C	5.04	120.47	110.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ARG	Sidechain
1	A	326	ARG	Sidechain
1	A	63	ARG	Sidechain
1	B	326	ARG	Sidechain
1	B	63	ARG	Sidechain

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	3900	3427	3665	23	0
1	B	3900	3427	3665	31	0
2	C	34	26	32	2	0
2	D	34	26	32	0	0
2	E	34	26	32	0	0
3	F	23	17	22	1	0
4	A	60	0	0	1	1
4	B	45	0	0	1	2
5	A	145	0	0	2	0
5	B	56	0	0	1	0
All	All	8231	6949	7448	54	3

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

All (54) 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:B:287:THR:CG2	1:B:294:ARG:HH11	1.64	1.10
1:B:225:ASP:OD2	1:B:287:THR:HB	1.69	0.92
1:B:287:THR:HG22	1:B:294:ARG:HH11	1.40	0.83
1:B:287:THR:HG22	1:B:294:ARG:NH1	1.96	0.81
1:B:287:THR:CG2	1:B:294:ARG:NH1	2.42	0.80
1:A:253:ARG:HH11	1:A:253:ARG:HG2	1.53	0.72
1:B:57:MET:HE1	1:B:108:THR:OG1	1.93	0.67
1:B:287:THR:HG21	1:B:294:ARG:HH11	1.56	0.67
1:B:57:MET:CE	1:B:108:THR:OG1	2.50	0.60
1:B:133:ASN:ND2	4:B:602:SO4:O4	2.35	0.60
1:B:394:THR:OG1	1:B:399:ASP:HB2	2.03	0.59
1:B:176:THR:HG23	1:B:178:ASP:OD1	2.02	0.58
1:B:125:LYS:HE3	1:B:132:GLN:NE2	2.21	0.56
1:B:134:ALA:HB3	1:B:166:ASN:HA	1.89	0.54
1:A:132:GLN:HA	4:A:605:SO4:O1	2.08	0.54
1:A:356:MET:HE2	1:A:380:ASN:HB3	1.89	0.53
1:B:287:THR:HG21	1:B:294:ARG:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:THR:HG23	5:B:736:HOH:O	2.08	0.53
1:A:42:ASN:HD21	2:C:1:FRU:H11	1.75	0.52
1:A:17:THR:OG1	1:A:19:THR:HG22	2.13	0.49
1:B:115:LYS:H	1:B:115:LYS:CD	2.27	0.47
1:A:134:ALA:HB3	1:A:166:ASN:HA	1.95	0.47
1:B:237:TYR:CZ	1:B:248:GLN:HB2	2.49	0.47
1:A:237:TYR:CZ	1:A:248:GLN:HB2	2.51	0.46
1:A:356:MET:CE	1:A:380:ASN:HB3	2.46	0.46
1:A:345:ARG:HB2	1:A:345:ARG:NH1	2.31	0.45
1:A:202:ASP:O	1:A:203:LEU:HB2	2.18	0.44
1:B:34:LYS:HE2	1:B:39:PHE:CE1	2.53	0.44
1:B:287:THR:CG2	1:B:294:ARG:HD3	2.47	0.44
1:B:202:ASP:O	1:B:203:LEU:HB2	2.17	0.44
1:A:152:ARG:NH1	5:A:706:HOH:O	2.50	0.43
1:A:106:GLY:HA3	1:A:120:PHE:O	2.19	0.43
1:A:69:THR:HA	1:A:101:ALA:O	2.17	0.43
1:A:219:ARG:HE	3:F:1:FRU:H12	1.84	0.43
1:B:176:THR:CG2	1:B:178:ASP:OD1	2.67	0.43
1:B:69:THR:HA	1:B:101:ALA:O	2.19	0.42
1:A:34:LYS:HE2	1:A:39:PHE:CE2	2.54	0.42
1:A:42:ASN:ND2	2:C:1:FRU:H11	2.34	0.42
1:B:106:GLY:HA3	1:B:120:PHE:O	2.19	0.42
1:B:115:LYS:H	1:B:115:LYS:HD2	1.83	0.42
1:A:272:ASN:ND2	5:A:711:HOH:O	2.53	0.42
1:B:287:THR:HG23	1:B:294:ARG:CG	2.48	0.42
1:B:125:LYS:HE3	1:B:132:GLN:HE22	1.84	0.42
1:B:394:THR:HG1	1:B:399:ASP:HB2	1.82	0.42
1:A:345:ARG:HB2	1:A:345:ARG:CZ	2.51	0.41
1:B:111:ASN:HB2	1:B:203:LEU:HD12	2.03	0.41
1:B:170:ASP:N	1:B:171:PRO:CD	2.83	0.41
1:A:318:TRP:O	1:A:319:ALA:HB3	2.20	0.41
1:B:225:ASP:HB2	1:B:286:LYS:HG2	2.03	0.40
1:A:133:ASN:HD21	1:A:159:ASP:HB2	1.86	0.40
1:B:318:TRP:O	1:B:319:ALA:HB3	2.22	0.40
1:A:63:ARG:HA	1:A:64:PRO:HA	1.89	0.40
1:A:384:VAL:HA	1:A:480:GLN:HB2	2.03	0.40
1:A:424:GLY:HA2	1:A:445:ILE:CG1	2.52	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:605:SO4:O2	4:B:605:SO4:O2[7_455]	1.27	0.93
4:B:602:SO4:O2	4:B:602:SO4:O2[6_555]	1.40	0.80
4:A:611:SO4:O4	4:A:611:SO4:O4[10_555]	1.56	0.64

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	485/523 (93%)	462 (95%)	22 (4%)	1 (0%)	47 58
1	B	485/523 (93%)	459 (95%)	25 (5%)	1 (0%)	47 58
All	All	970/1046 (93%)	921 (95%)	47 (5%)	2 (0%)	47 58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	ASP
1	B	159	ASP

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	413/444 (93%)	402 (97%)	11 (3%)	44 61
1	B	413/444 (93%)	399 (97%)	14 (3%)	37 51
All	All	826/888 (93%)	801 (97%)	25 (3%)	41 57

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	96	ARG
1	A	105	THR
1	A	130	SER
1	A	145	PHE
1	A	173	LEU
1	A	188	ARG
1	A	229	MET
1	A	362	MET
1	A	433	ASP
1	A	472	PHE
1	B	24	SER
1	B	87	LEU
1	B	105	THR
1	B	115	LYS
1	B	145	PHE
1	B	156	LEU
1	B	173	LEU
1	B	188	ARG
1	B	229	MET
1	B	287	THR
1	B	330	HIS
1	B	362	MET
1	B	452	ARG
1	B	472	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	B	132	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

11 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	FRU	C	1	2	11,12,12	1.07	2 (18%)	10,18,18	1.57	2 (20%)
2	FRU	C	2	2	11,11,12	0.75	0	15,15,18	1.83	1 (6%)
2	FRU	C	3	2	11,11,12	0.91	1 (9%)	15,15,18	4.03	6 (40%)
2	FRU	D	1	2	11,12,12	1.18	1 (9%)	10,18,18	1.28	1 (10%)
2	FRU	D	2	2	11,11,12	0.73	0	15,15,18	0.71	0
2	FRU	D	3	2	11,11,12	0.54	0	15,15,18	1.05	1 (6%)
2	FRU	E	1	2	11,12,12	1.03	1 (9%)	10,18,18	1.44	1 (10%)
2	FRU	E	2	2	11,11,12	0.98	0	15,15,18	1.56	2 (13%)
2	FRU	E	3	2	11,11,12	0.87	0	15,15,18	1.77	3 (20%)
3	FRU	F	1	3	11,12,12	1.27	1 (9%)	10,18,18	0.87	0
3	FRU	F	2	3	11,11,12	1.15	0	15,15,18	1.55	4 (26%)

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	FRU	C	1	2	-	1/5/24/24	0/1/1/1
2	FRU	C	2	2	-	2/4/20/24	0/1/1/1
2	FRU	C	3	2	-	1/4/20/24	0/1/1/1
2	FRU	D	1	2	-	2/5/24/24	0/1/1/1
2	FRU	D	2	2	-	0/4/20/24	0/1/1/1
2	FRU	D	3	2	-	1/4/20/24	0/1/1/1
2	FRU	E	1	2	-	1/5/24/24	0/1/1/1
2	FRU	E	2	2	-	2/4/20/24	0/1/1/1
2	FRU	E	3	2	1/1/4/4	2/4/20/24	0/1/1/1
3	FRU	F	1	3	-	5/5/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FRU	F	2	3	-	3/4/20/24	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	FRU	O2-C2	3.26	1.46	1.40
2	E	1	FRU	O2-C2	2.58	1.45	1.40
2	D	1	FRU	O2-C2	2.32	1.44	1.40
2	C	1	FRU	C1-C2	2.26	1.56	1.52
2	C	1	FRU	O2-C2	2.18	1.44	1.40
2	C	3	FRU	O5-C2	-2.06	1.40	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	FRU	O5-C2-C1	-13.23	80.61	109.21
2	C	2	FRU	O6-C6-C5	-6.45	89.18	111.29
2	E	3	FRU	C1-C2-C3	-4.52	104.19	115.09
2	C	3	FRU	O5-C5-C6	-4.16	100.21	109.21
2	C	3	FRU	C6-C5-C4	3.78	124.20	115.09
2	C	3	FRU	O5-C2-C3	-3.66	97.87	105.11
2	C	3	FRU	O6-C6-C5	-3.24	100.17	111.29
2	C	1	FRU	O5-C5-C6	-3.13	100.14	108.85
2	E	2	FRU	C6-C5-C4	3.13	122.62	115.09
2	E	2	FRU	O4-C4-C5	3.01	119.74	111.05
2	E	1	FRU	O2-C2-O5	-2.93	103.84	109.50
2	C	3	FRU	C4-C3-C2	2.81	108.11	102.64
2	E	3	FRU	C4-C3-C2	2.64	107.78	102.64
2	C	1	FRU	O6-C6-C5	2.56	120.06	111.29
3	F	2	FRU	C1-C2-C3	-2.54	108.96	115.09
3	F	2	FRU	O5-C2-C1	2.46	114.53	109.21
2	D	1	FRU	O5-C5-C6	-2.45	102.02	108.85
3	F	2	FRU	C6-C5-C4	2.37	120.79	115.09
2	E	3	FRU	O5-C5-C6	2.28	114.15	109.21
3	F	2	FRU	O5-C5-C6	2.27	114.13	109.21
2	D	3	FRU	O5-C2-C3	-2.04	101.08	105.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	3	FRU	C2

All (20) torsion outliers are listed below:

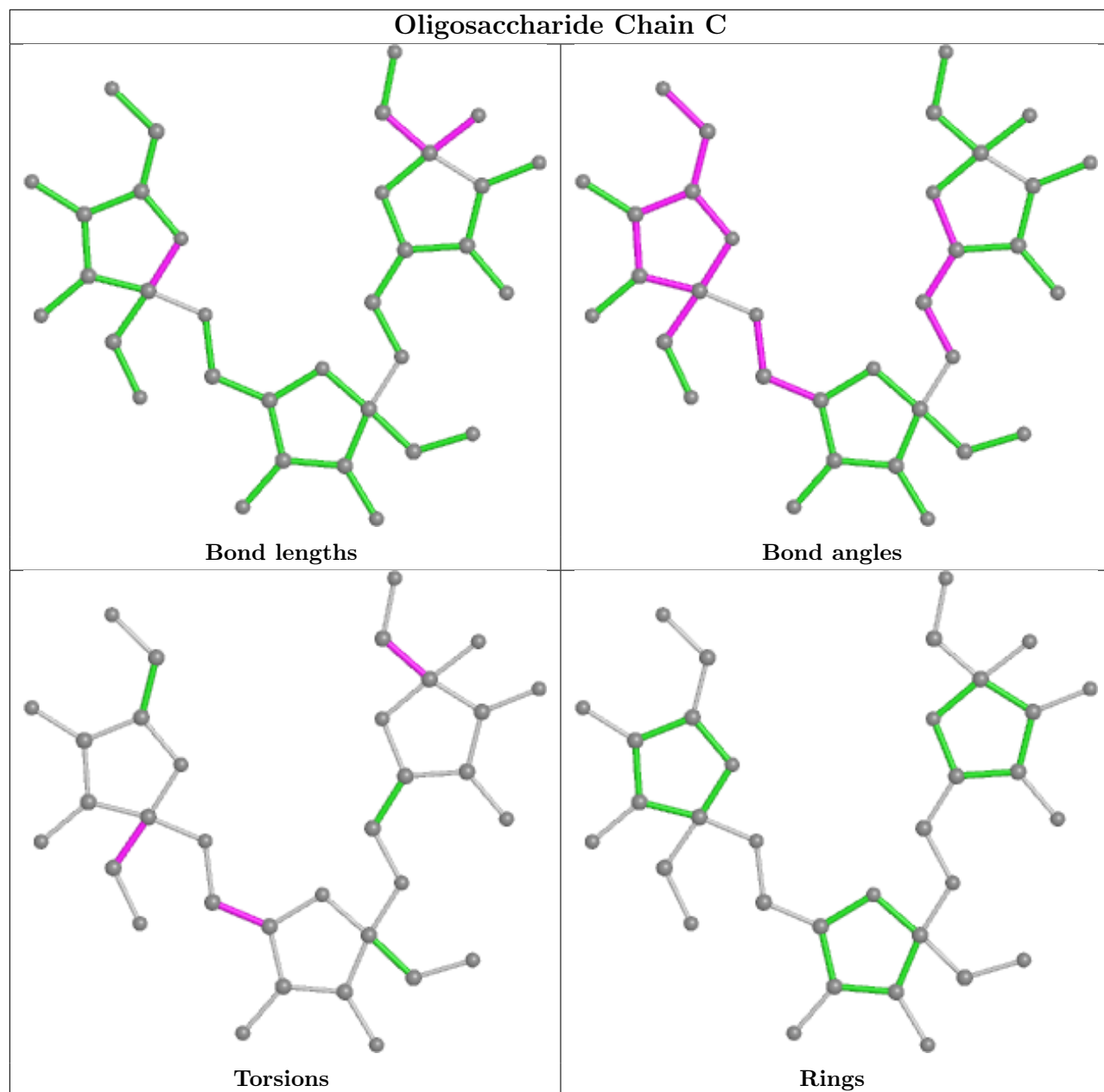
Mol	Chain	Res	Type	Atoms
3	F	1	FRU	O1-C1-C2-C3
3	F	1	FRU	O1-C1-C2-O2
3	F	1	FRU	O1-C1-C2-O5
2	E	2	FRU	O5-C5-C6-O6
2	E	2	FRU	C4-C5-C6-O6
2	C	2	FRU	C4-C5-C6-O6
3	F	1	FRU	C4-C5-C6-O6
3	F	1	FRU	O5-C5-C6-O6
2	C	2	FRU	O5-C5-C6-O6
2	C	3	FRU	O1-C1-C2-C3
2	E	3	FRU	O5-C5-C6-O6
3	F	2	FRU	O5-C5-C6-O6
2	E	3	FRU	C4-C5-C6-O6
2	D	3	FRU	O1-C1-C2-O5
2	E	1	FRU	O5-C5-C6-O6
2	D	1	FRU	O5-C5-C6-O6
2	C	1	FRU	O1-C1-C2-C3
2	D	1	FRU	O1-C1-C2-C3
3	F	2	FRU	O1-C1-C2-O5
3	F	2	FRU	O1-C1-C2-C3

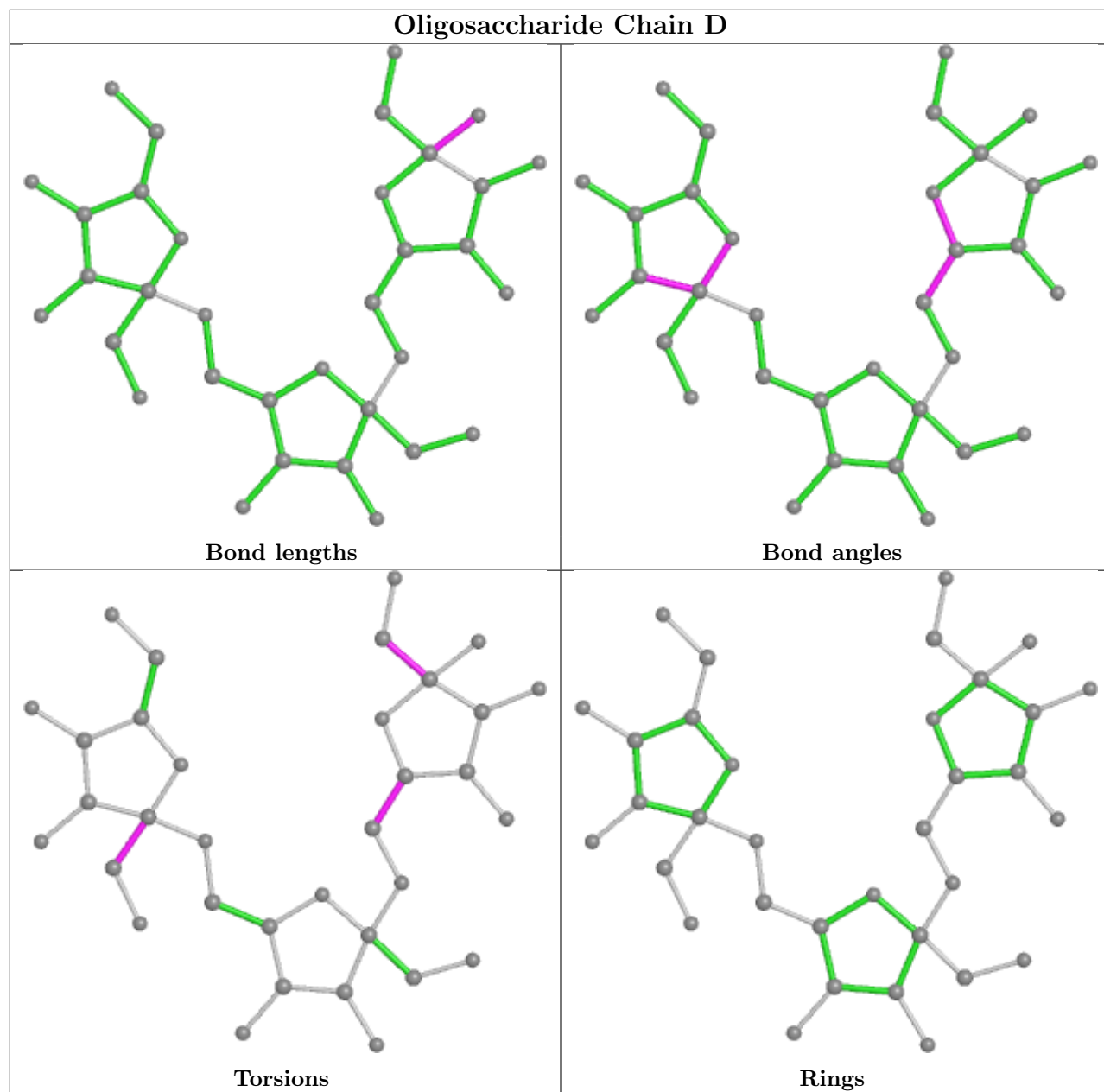
There are no ring outliers.

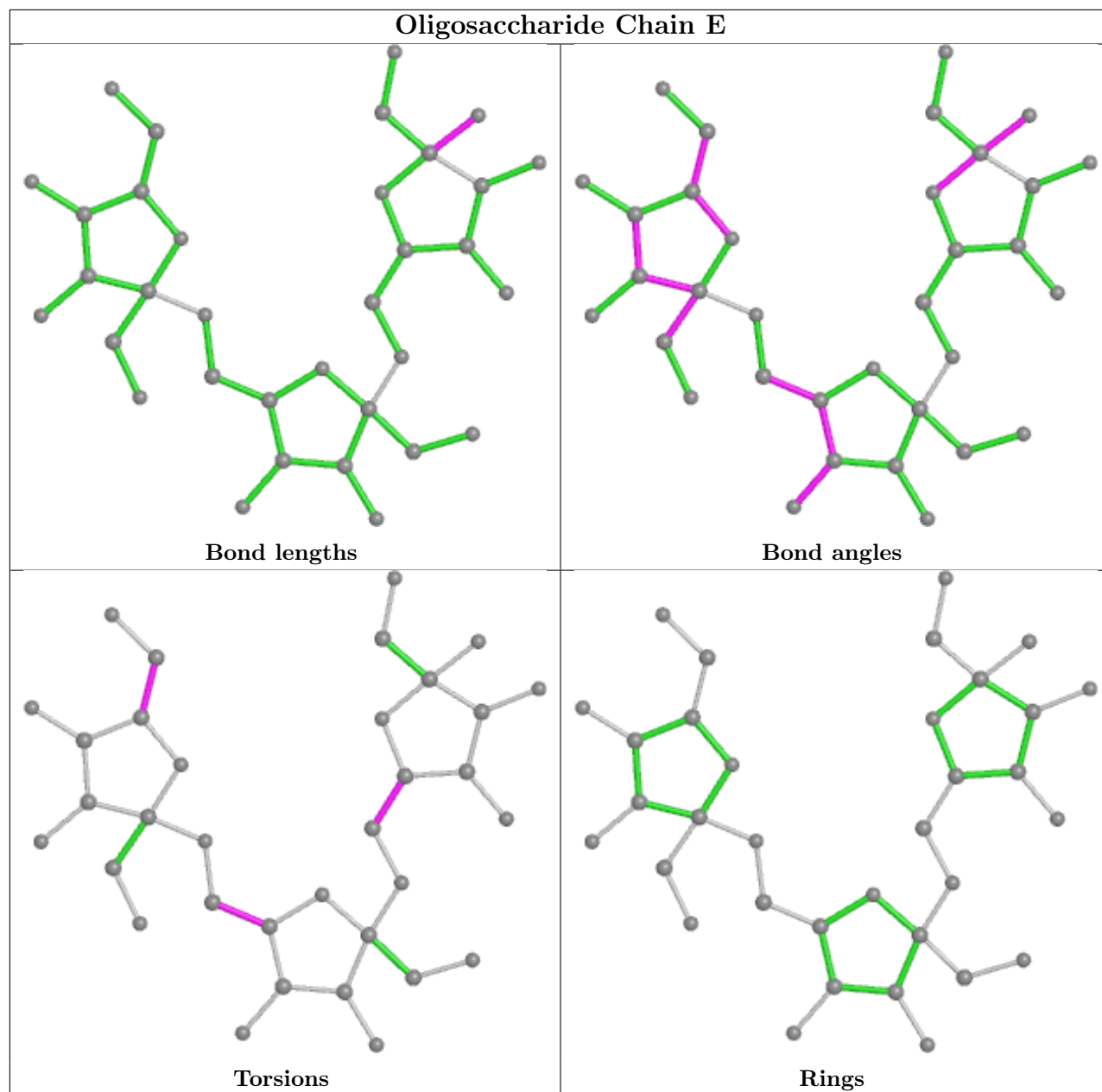
2 monomers are involved in 3 short contacts:

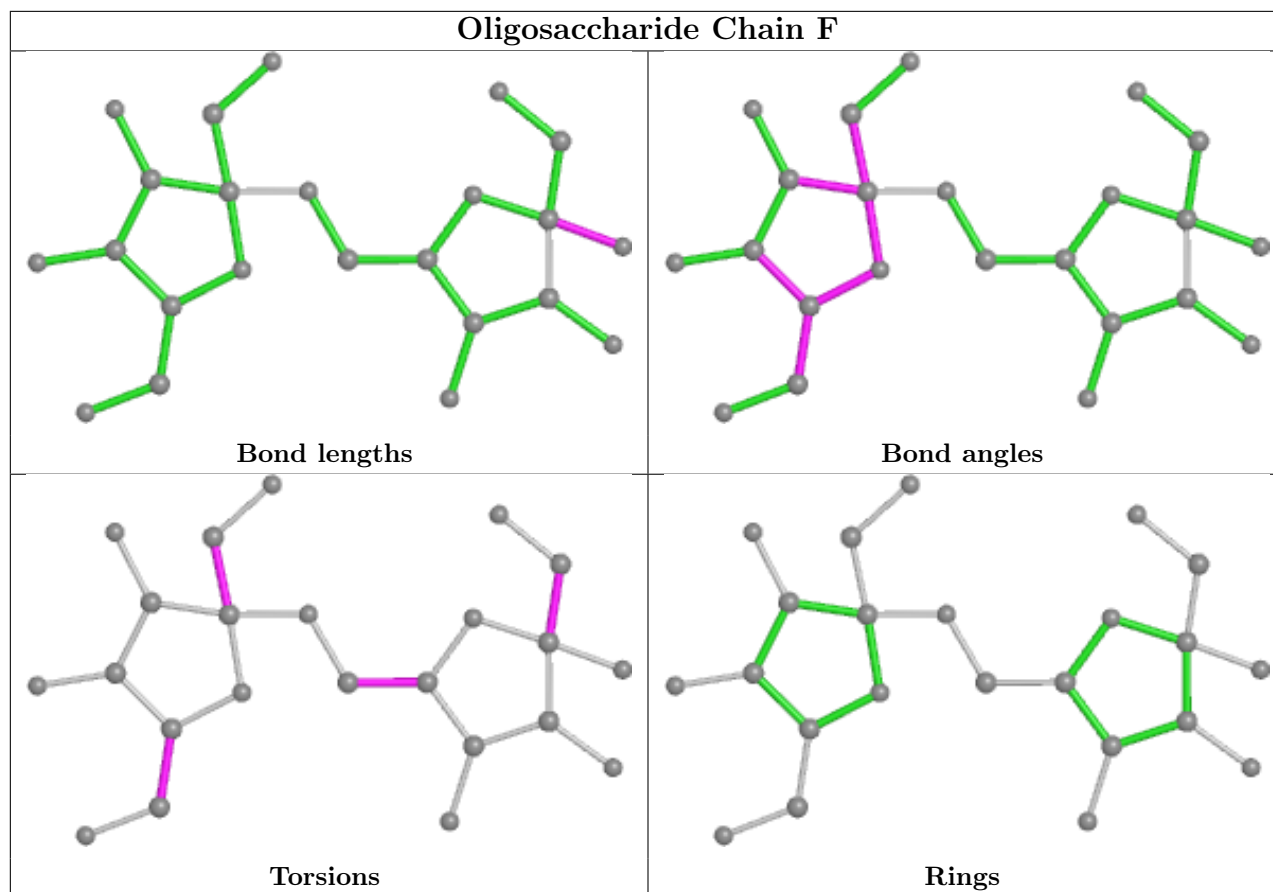
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	FRU	1	0
2	C	1	FRU	2	0

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](#)

21 ligands 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	$\# Z > 2$
4	SO4	A	606	-	4,4,4	0.34	0	6,6,6	0.06	0
4	SO4	A	612	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	B	606	-	4,4,4	0.30	0	6,6,6	0.06	0
4	SO4	B	601	-	4,4,4	0.36	0	6,6,6	0.21	0
4	SO4	A	601	-	4,4,4	0.31	0	6,6,6	0.33	0
4	SO4	B	609	-	4,4,4	0.34	0	6,6,6	0.12	0
4	SO4	B	602	-	4,4,4	0.28	0	6,6,6	0.12	0
4	SO4	B	607	-	4,4,4	0.33	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	608	-	4,4,4	0.34	0	6,6,6	0.10	0
4	SO4	B	603	-	4,4,4	0.33	0	6,6,6	0.16	0
4	SO4	B	604	-	4,4,4	0.31	0	6,6,6	0.13	0
4	SO4	B	608	-	4,4,4	0.29	0	6,6,6	0.05	0
4	SO4	A	609	-	4,4,4	0.30	0	6,6,6	0.10	0
4	SO4	A	610	-	4,4,4	0.33	0	6,6,6	0.13	0
4	SO4	A	607	-	4,4,4	0.29	0	6,6,6	0.10	0
4	SO4	A	602	-	4,4,4	0.27	0	6,6,6	0.12	0
4	SO4	A	603	-	4,4,4	0.22	0	6,6,6	0.10	0
4	SO4	A	604	-	4,4,4	0.29	0	6,6,6	0.08	0
4	SO4	A	611	-	4,4,4	0.22	0	6,6,6	0.15	0
4	SO4	B	605	-	4,4,4	0.26	0	6,6,6	0.16	0
4	SO4	A	605	-	4,4,4	0.40	0	6,6,6	0.16	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	SO4	1	1
4	A	611	SO4	0	1
4	B	605	SO4	0	1
4	A	605	SO4	1	0

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	487/523 (93%)	0.27	0 100 100	23, 35, 54, 66	0
1	B	487/523 (93%)	0.42	14 (2%) 51 58	34, 50, 71, 94	0
All	All	974/1046 (93%)	0.35	14 (1%) 75 80	23, 44, 67, 94	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	177	GLU	3.2
1	B	191	GLY	3.1
1	B	231	ASP	2.7
1	B	229	MET	2.7
1	B	181	TYR	2.5
1	B	212	PHE	2.4
1	B	50	VAL	2.4
1	B	165	LYS	2.3
1	B	115	LYS	2.3
1	B	190	ASN	2.1
1	B	230	GLY	2.1
1	B	363	ILE	2.1
1	B	139	VAL	2.1
1	B	180	VAL	2.0

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

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

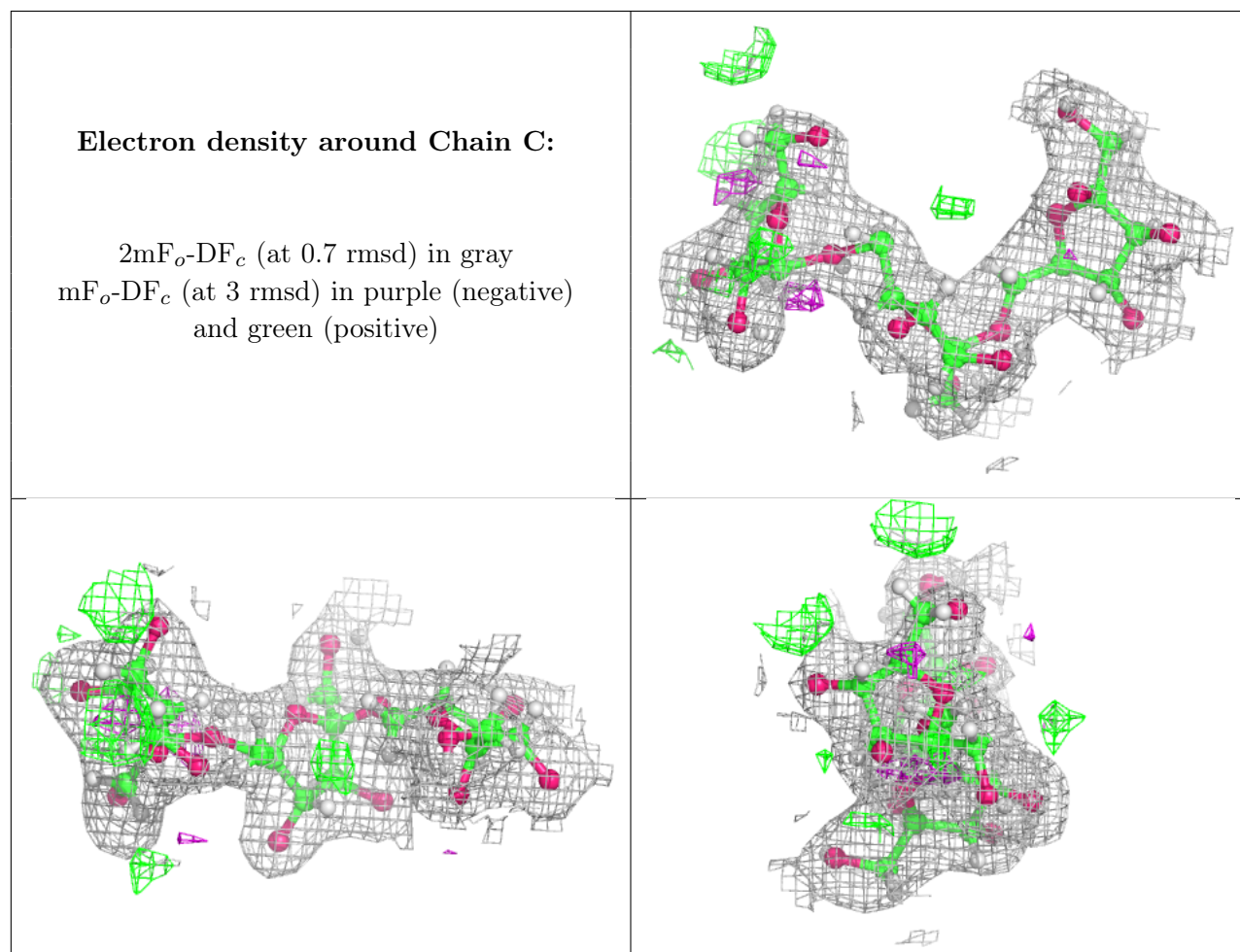
6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

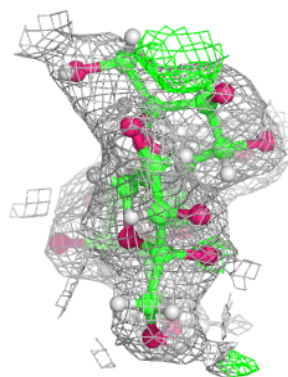
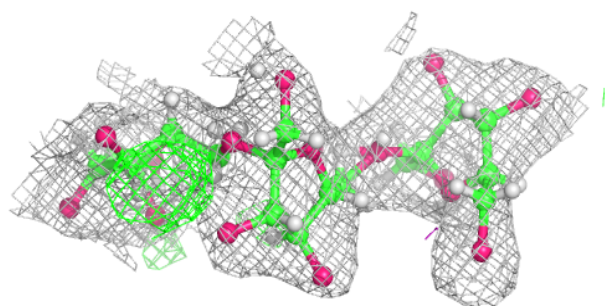
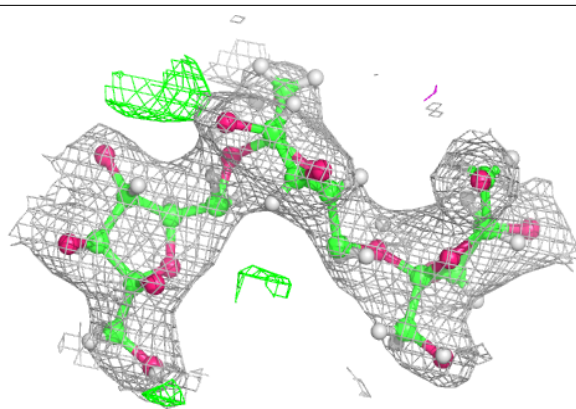
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FRU	F	2	11/12	0.52	0.32	54,94,104,109	0
2	FRU	E	3	11/12	0.78	0.28	66,85,98,99	0
2	FRU	E	1	12/12	0.83	0.26	57,74,95,103	0
3	FRU	F	1	12/12	0.86	0.15	51,61,72,79	0
2	FRU	E	2	11/12	0.86	0.15	48,63,76,83	0
2	FRU	C	3	11/12	0.87	0.22	37,50,55,56	0
2	FRU	D	3	11/12	0.91	0.15	48,56,59,59	0
2	FRU	D	1	12/12	0.95	0.14	46,54,57,68	0
2	FRU	D	2	11/12	0.96	0.13	57,61,67,68	0
2	FRU	C	2	11/12	0.97	0.12	34,38,40,51	0
2	FRU	C	1	12/12	0.98	0.13	30,35,39,40	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.

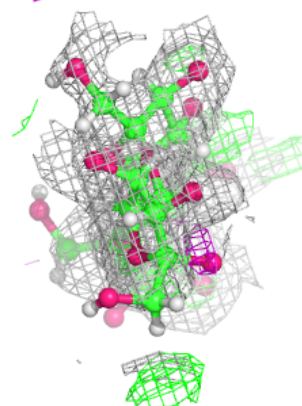
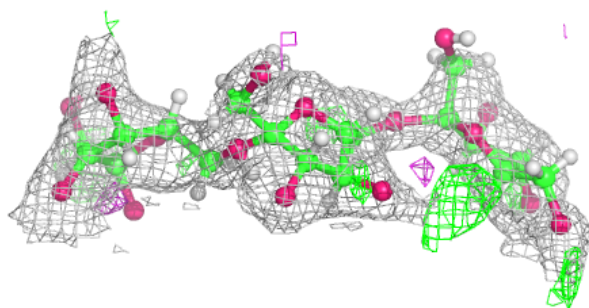
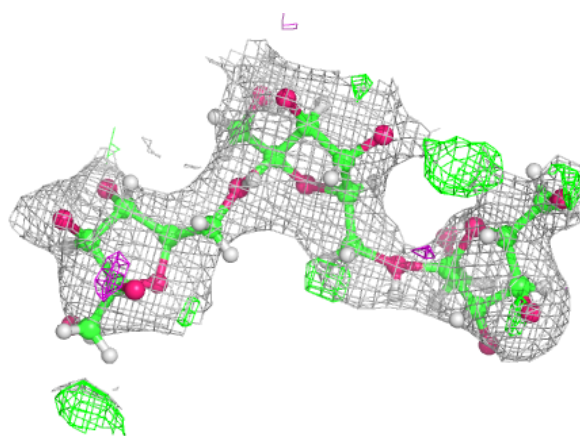


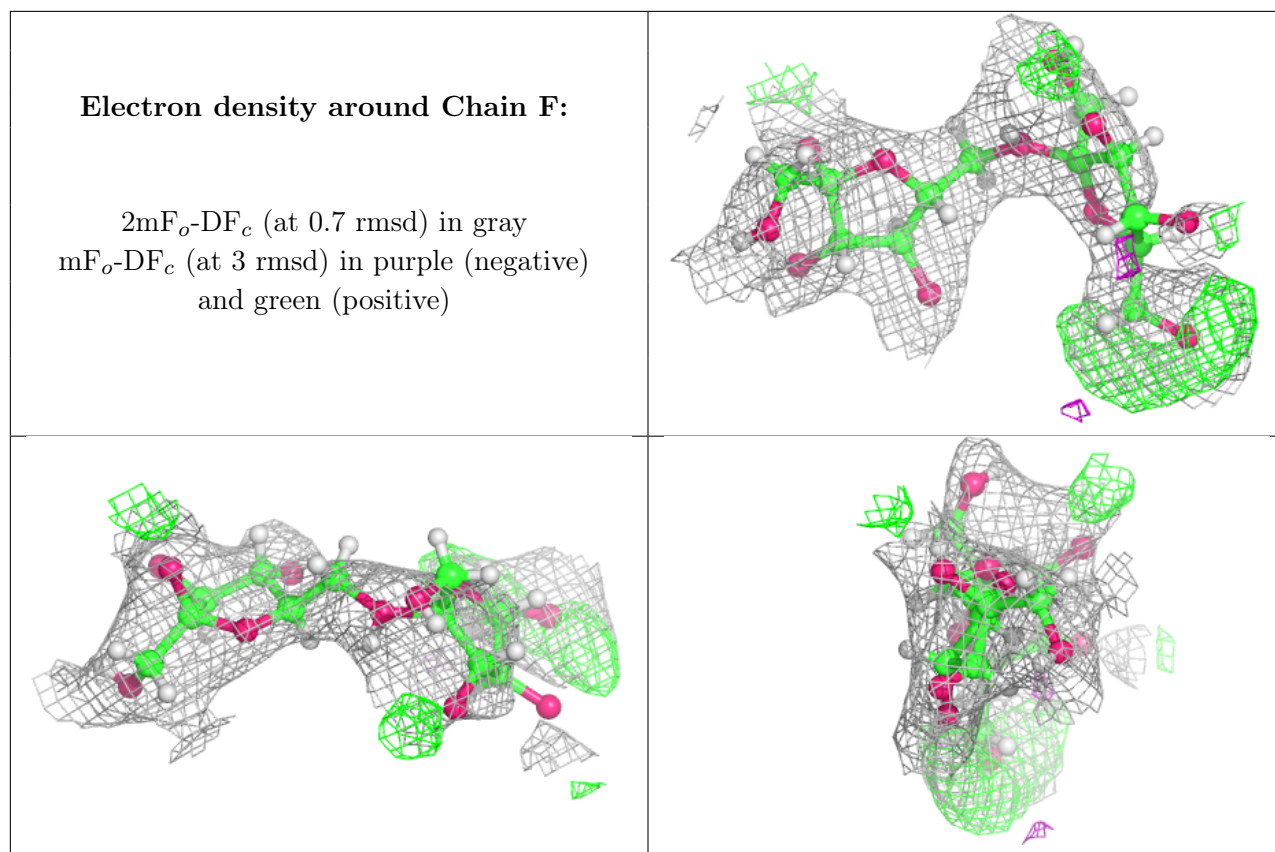
Electron density around Chain D:

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

**Electron density around Chain 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
4	SO4	A	611	5/5	0.69	0.56	78,105,113,116	1
4	SO4	B	605	5/5	0.78	0.43	67,93,103,112	1
4	SO4	B	602	5/5	0.83	0.47	61,93,95,106	1
4	SO4	A	605	5/5	0.83	0.50	78,84,90,101	1
4	SO4	A	610	5/5	0.85	0.17	86,87,100,114	0
4	SO4	B	603	5/5	0.87	0.20	77,89,95,103	0
4	SO4	A	608	5/5	0.88	0.19	78,92,95,107	0
4	SO4	B	608	5/5	0.88	0.14	82,83,97,98	0
4	SO4	B	609	5/5	0.88	0.21	98,103,118,118	0
4	SO4	B	607	5/5	0.91	0.31	77,95,112,113	0
4	SO4	A	609	5/5	0.92	0.21	94,94,97,104	0
4	SO4	A	607	5/5	0.92	0.13	74,78,86,86	0
4	SO4	A	606	5/5	0.92	0.38	52,53,58,60	5
4	SO4	B	606	5/5	0.93	0.25	73,81,92,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	603	5/5	0.93	0.34	64,71,91,104	0
4	SO4	A	602	5/5	0.94	0.17	62,63,70,80	0
4	SO4	A	604	5/5	0.94	0.22	62,80,82,92	0
4	SO4	B	601	5/5	0.95	0.18	64,65,68,71	0
4	SO4	A	612	5/5	0.95	0.19	84,91,93,93	0
4	SO4	A	601	5/5	0.96	0.16	51,54,68,75	0
4	SO4	B	604	5/5	0.98	0.18	71,77,88,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.