



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 08:39 PM BST

PDB ID : 3Q7A
Title : Cryptococcus neoformans protein farnesyltransferase in complex with FPP and L-778,123
Authors : Hast, M.A.; Beese, L.S.
Deposited on : 2011-01-04
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

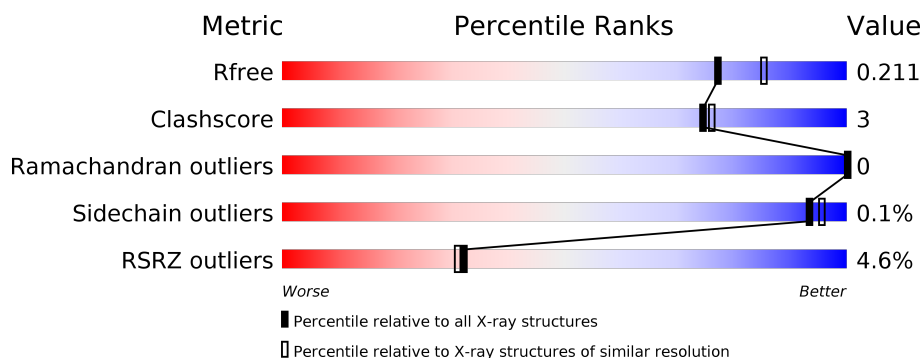
1 Overall quality at a glance

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))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	349	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>10%</div> </div> </div>
2	B	520	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>7%</div> </div> </div>
3	C	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
3	D	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
3	E	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7245 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.

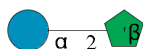
- Molecule 1 is a protein called Farnesyltransferase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2621	1691	446	473	11			

- Molecule 2 is a protein called Farnesyltransferase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	485	Total	C	N	O	S	0	1	0
			3730	2366	649	700	15			

- Molecule 3 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.

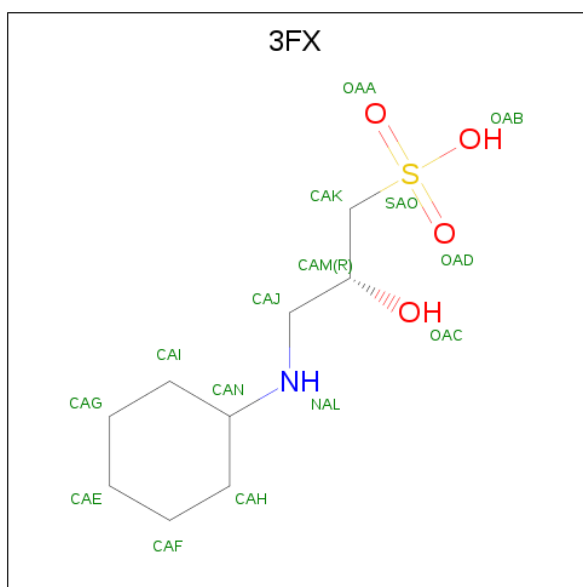


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	0	0	0
			23	12	11			
3	D	2	Total	C	O	0	0	0
			23	12	11			
3	E	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is (2R)-3-(cyclohexylamino)-2-hydroxypropane-1-sulfonic acid (three-letter code: 3FX) (formula: C₉H₁₉NO₄S).



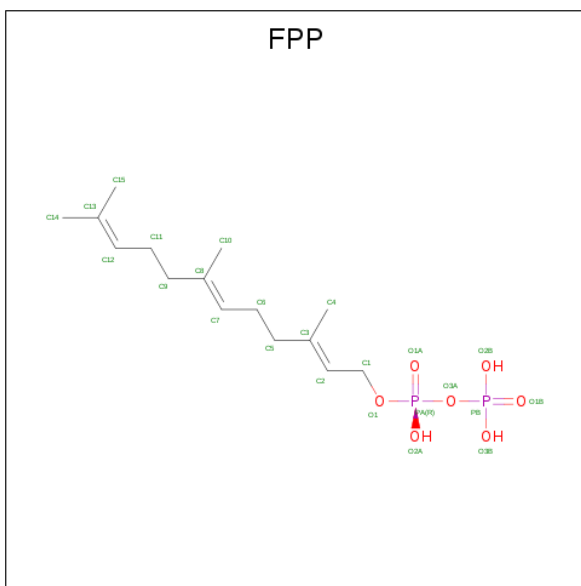
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	9	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	9	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	9	1	4	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



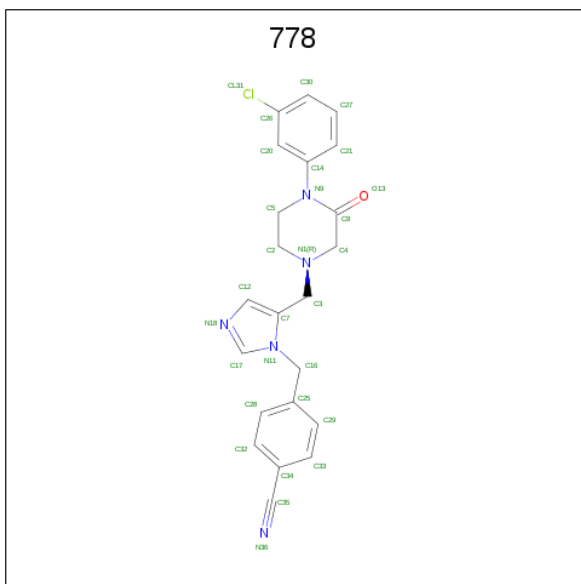
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is FARNESYL DIPHOSPHATE (three-letter code: FPP) (formula: $C_{15}H_{28}O_7P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	O	P	0	0
			24	15	7	2		

- Molecule 8 is 4-[(5-{[4-(3-CHLOROPHENYL)-3-OXOPIPERAZIN-1-YL]METHYL}-1H-IMIDAZOL-1-YL)METHYL]BENZONITRILE (three-letter code: 778) (formula: $C_{22}H_{20}ClN_5O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	Cl	N	O	0	0
			29	22	1	5	1		

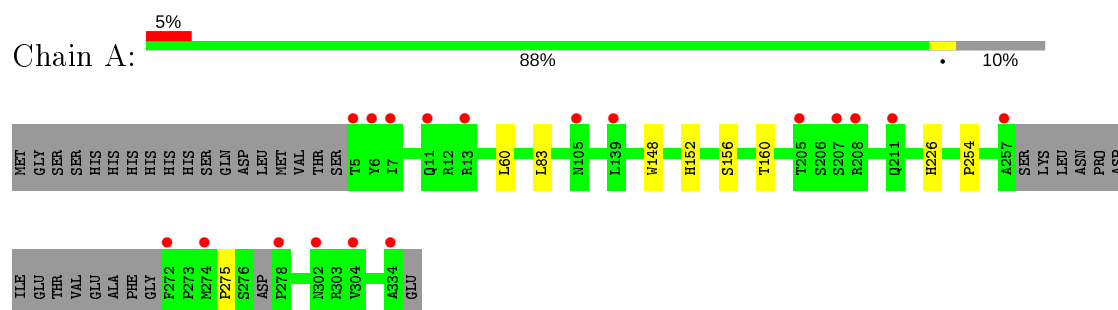
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	253	Total 253	O 253	0	0
9	B	468	Total 468	O 468	0	0

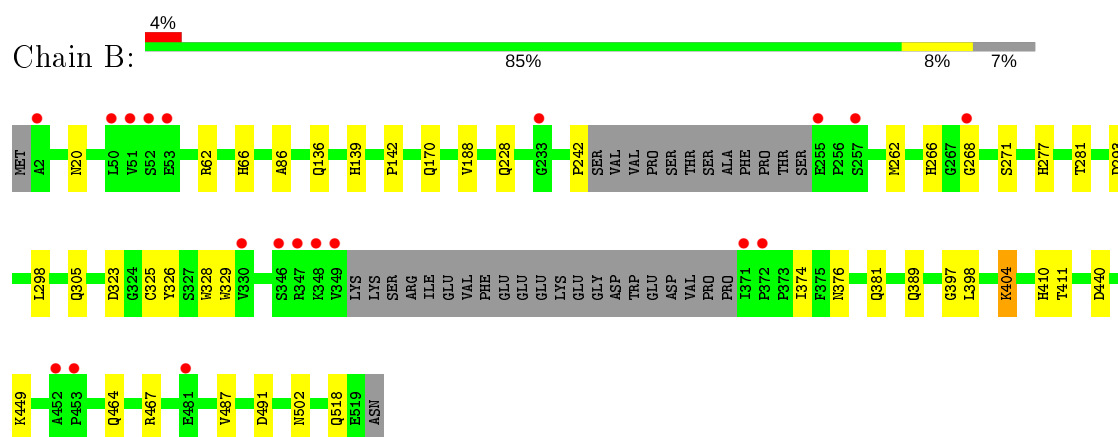
3 Residue-property plots [i](#)

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: Farnesyltransferase alpha subunit



- Molecule 2: Farnesyltransferase beta subunit



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain E:



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	142.71Å 142.71Å 130.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 2.00 48.14 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.14-2.00) 98.7 (48.14-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.203 0.193 , 0.211	Depositor DCC
R_{free} test set	4510 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7245	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: ZN, 3FX, GLC, 778, SO4, FRU, FPP

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	0.33	0/2703	0.44	0/3680
2	B	0.35	0/3827	0.48	1/5198 (0.0%)
All	All	0.34	0/6530	0.46	1/8878 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	242	PRO	CA-N-CD	-8.53	99.56	111.50

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	2621	0	2544	6	0
2	B	3730	0	3657	35	0
3	C	23	0	21	0	0
3	D	23	0	21	0	0
3	E	23	0	21	0	0
4	B	1	0	0	0	0
5	B	45	0	56	2	0
6	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	24	0	25	3	0
8	B	29	0	20	1	0
9	A	253	0	0	0	0
9	B	468	0	0	1	0
All	All	7245	0	6365	41	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 3.

All (41) 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)
2:B:464:GLN:HE22	2:B:467:ARG:HH11	1.21	0.84
2:B:440:ASP:H	2:B:518:GLN:HE22	1.24	0.82
2:B:305:GLN:HE22	2:B:376:ASN:H	1.30	0.79
2:B:62:ARG:H	2:B:389:GLN:HE22	1.29	0.78
2:B:228:GLN:HE22	2:B:293:ASP:H	1.28	0.78
2:B:66:HIS:HD1	2:B:397:GLY:H	1.36	0.73
2:B:170:GLN:HE22	2:B:449:LYS:H	1.37	0.72
2:B:266:HIS:HD2	2:B:268:GLY:H	1.40	0.68
2:B:381:GLN:HE22	2:B:487:VAL:H	1.48	0.61
2:B:266:HIS:HE1	7:B:3011:FPP:O2B	1.86	0.59
1:A:148:TRP:O	1:A:152:HIS:HD2	1.87	0.57
2:B:440:ASP:H	2:B:518:GLN:NE2	2.00	0.57
1:A:226:HIS:H	2:B:20:ASN:HD21	1.53	0.56
5:B:522:3FX:HAJA	9:B:1900:HOH:O	2.08	0.54
2:B:381:GLN:NE2	2:B:487:VAL:H	2.06	0.53
2:B:139:HIS:CE1	2:B:188:VAL:HB	2.45	0.52
2:B:305:GLN:NE2	2:B:376:ASN:H	2.06	0.49
2:B:328:TRP:CZ2	2:B:502:ASN:HB2	2.47	0.49
2:B:298:LEU:HD11	2:B:374:ILE:HG12	1.96	0.48
2:B:268:GLY:HA3	7:B:3011:FPP:C8	2.45	0.47
2:B:323:ASP:HB3	2:B:326:TYR:CD2	2.50	0.46
2:B:464:GLN:HE22	2:B:467:ARG:NH1	2.01	0.45
2:B:139:HIS:HB3	2:B:142:PRO:CG	2.47	0.45
2:B:62:ARG:H	2:B:389:GLN:NE2	2.07	0.44
2:B:305:GLN:HE22	2:B:376:ASN:N	2.06	0.44
2:B:86:ALA:HA	2:B:136:GLN:HE22	1.82	0.44
1:A:226:HIS:H	2:B:20:ASN:ND2	2.14	0.44
1:A:156:SER:O	1:A:160:THR:HG23	2.18	0.43
2:B:271:SER:HB2	2:B:329:TRP:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:CYS:HB3	2:B:410:HIS:CD2	2.54	0.43
1:A:254:PRO:HG2	1:A:275:PRO:HG2	2.00	0.42
2:B:262[B]:MET:HA	2:B:262[B]:MET:CE	2.49	0.42
2:B:66:HIS:HD1	2:B:397:GLY:N	2.09	0.42
2:B:170:GLN:NE2	2:B:449:LYS:H	2.12	0.42
2:B:398:LEU:HB2	2:B:411:THR:HA	2.02	0.42
2:B:491:ASP:OD2	5:B:522:3FX:NAL	2.51	0.41
1:A:60:LEU:HA	1:A:83:LEU:HD13	2.01	0.41
7:B:3011:FPP:H102	8:B:3012:778:C29	2.50	0.41
2:B:277:HIS:O	2:B:281:THR:HG23	2.19	0.41
2:B:404:LYS:HA	2:B:404:LYS:HD2	1.96	0.41
2:B:170:GLN:HE22	2:B:449:LYS:N	2.12	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	309/349 (88%)	301 (97%)	8 (3%)	0	100	100
2	B	480/520 (92%)	470 (98%)	10 (2%)	0	100	100
All	All	789/869 (91%)	771 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	285/316 (90%)	285 (100%)	0	100	100
2	B	404/436 (93%)	403 (100%)	1 (0%)	93	95
All	All	689/752 (92%)	688 (100%)	1 (0%)	93	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	404	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	110	GLN
1	A	152	HIS
1	A	187	ASN
1	A	211	GLN
2	B	20	ASN
2	B	108	GLN
2	B	136	GLN
2	B	170	GLN
2	B	219	ASN
2	B	228	GLN
2	B	266	HIS
2	B	304	GLN
2	B	305	GLN
2	B	319	ASN
2	B	381	GLN
2	B	389	GLN
2	B	414	ASN
2	B	464	GLN
2	B	495	ASN
2	B	518	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$
3	GLC	C	1	3	11,11,12	0.94	0	15,15,17	0.73	0
3	FRU	C	2	3	11,12,12	1.21	1 (9%)	10,18,18	1.01	1 (10%)
3	GLC	D	1	3	11,11,12	0.86	0	15,15,17	0.67	0
3	FRU	D	2	3	11,12,12	1.21	2 (18%)	10,18,18	0.75	0
3	GLC	E	1	3	11,11,12	0.84	0	15,15,17	0.76	0
3	FRU	E	2	3	11,12,12	1.19	1 (9%)	10,18,18	0.95	1 (10%)

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
3	GLC	C	1	3	-	0/2/19/22	0/1/1/1
3	FRU	C	2	3	-	2/5/24/24	0/1/1/1
3	GLC	D	1	3	-	2/2/19/22	0/1/1/1
3	FRU	D	2	3	-	0/5/24/24	0/1/1/1
3	GLC	E	1	3	-	0/2/19/22	0/1/1/1
3	FRU	E	2	3	-	0/5/24/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	FRU	O2-C2	3.18	1.46	1.40
3	E	2	FRU	O2-C2	2.63	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	FRU	O2-C2	2.60	1.45	1.40
3	D	2	FRU	O5-C2	2.21	1.46	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	FRU	C6-C5-C4	-2.49	109.09	115.09
3	E	2	FRU	C6-C5-C4	-2.45	109.18	115.09

There are no chirality outliers.

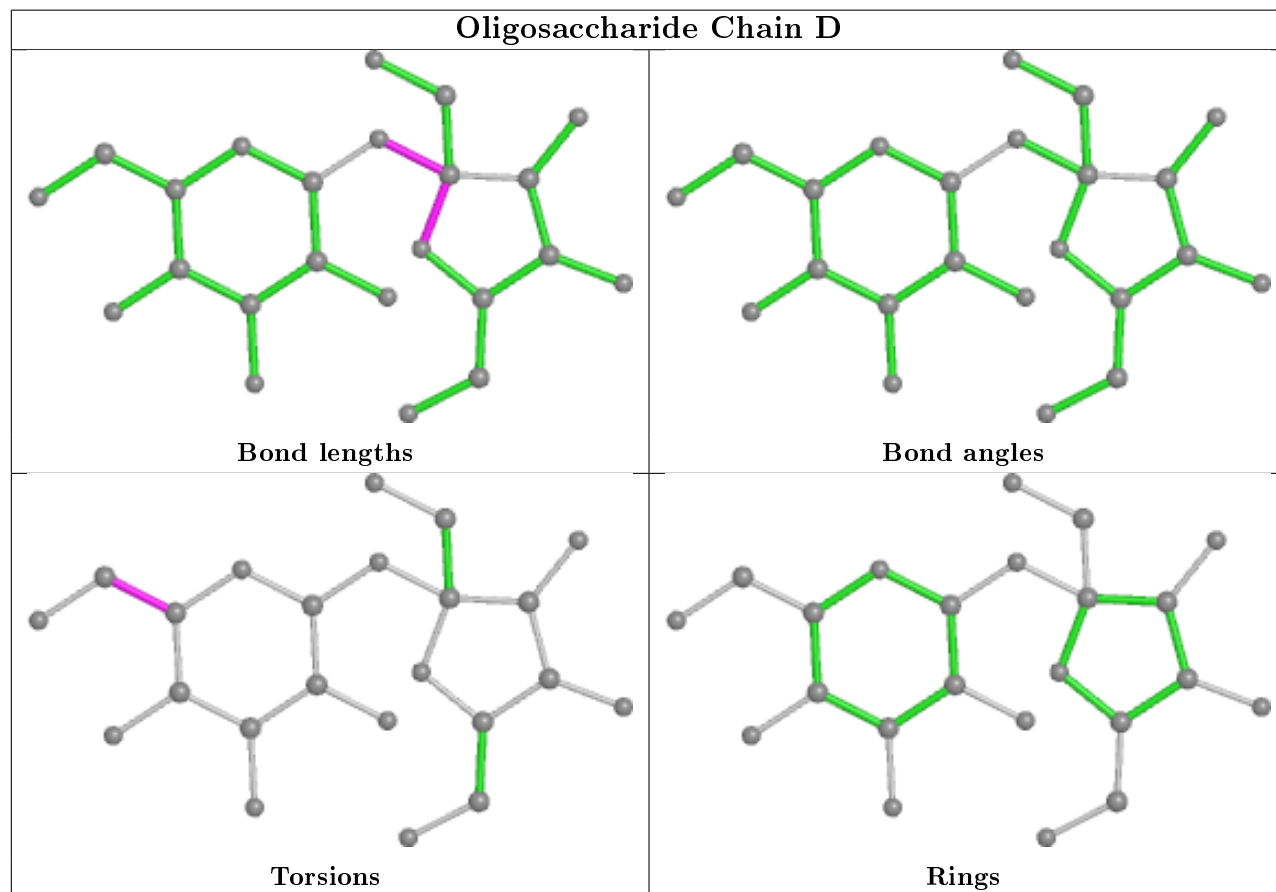
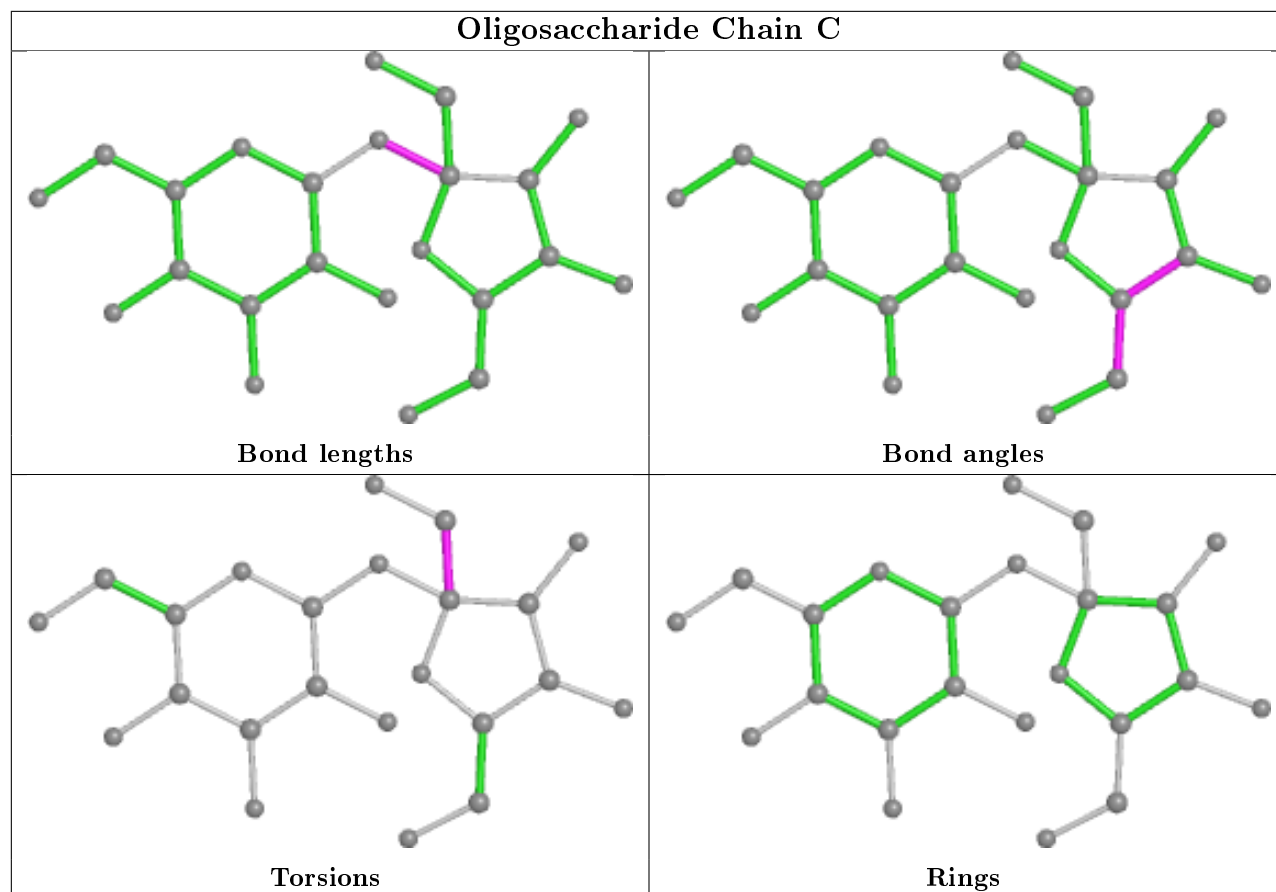
All (4) torsion outliers are listed below:

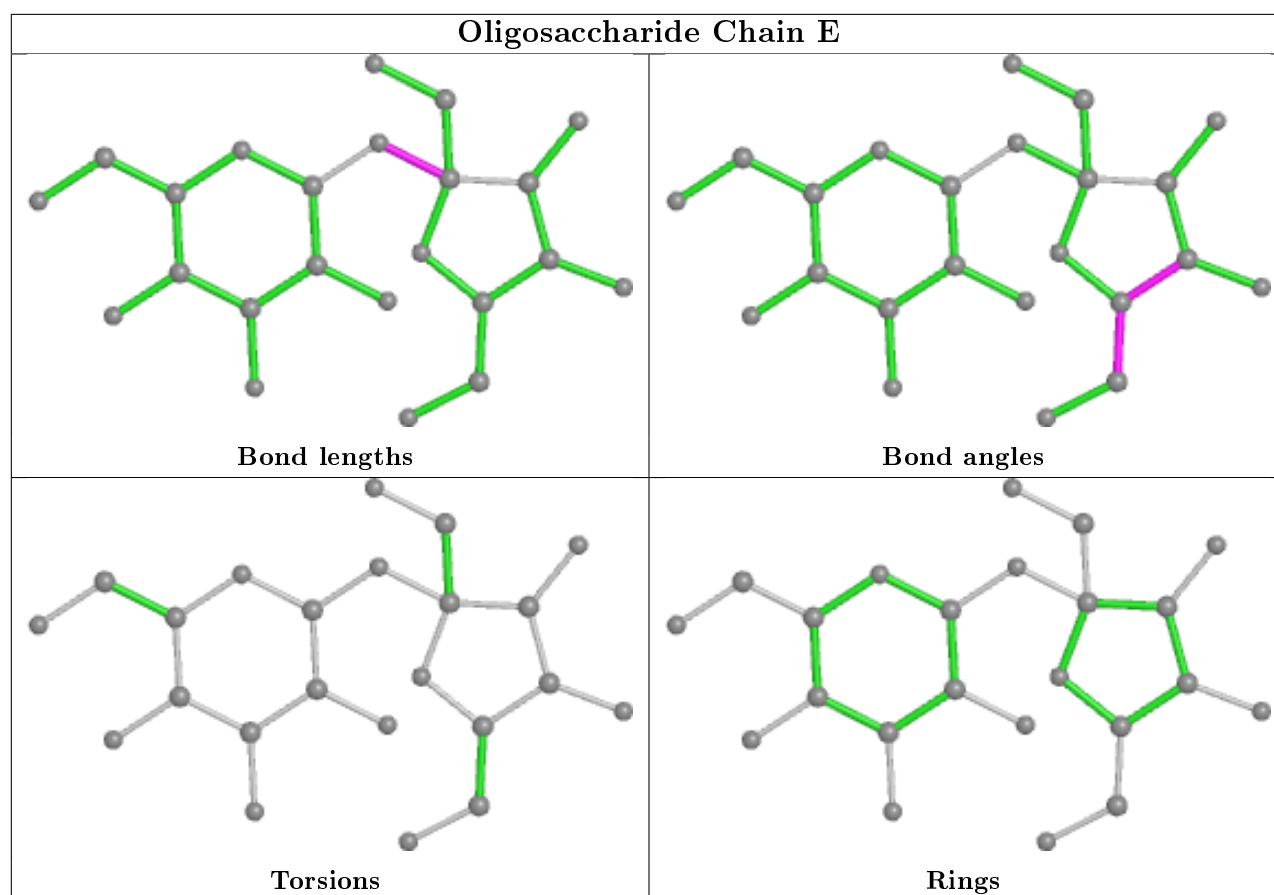
Mol	Chain	Res	Type	Atoms
3	C	2	FRU	O1-C1-C2-O2
3	D	1	GLC	C4-C5-C6-O6
3	C	2	FRU	O1-C1-C2-O5
3	D	1	GLC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	3FX	B	524	-	15,15,15	0.89	0	16,20,20	1.10	2 (12%)
5	3FX	B	523	-	15,15,15	0.94	0	16,20,20	1.25	2 (12%)
5	3FX	B	522	-	15,15,15	1.02	0	16,20,20	1.15	2 (12%)
8	778	B	3012	4	29,32,32	1.08	2 (6%)	39,44,44	1.20	4 (10%)
7	FPP	B	3011	-	21,23,23	1.87	6 (28%)	27,31,31	0.99	2 (7%)
6	SO4	B	525	-	4,4,4	0.17	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	3FX	B	522	-	-	2/10/18/18	0/1/1/1
5	3FX	B	524	-	-	4/10/18/18	0/1/1/1
8	778	B	3012	4	-	2/14/27/27	0/4/4/4
7	FPP	B	3011	-	-	6/25/25/25	-
5	3FX	B	523	-	-	4/10/18/18	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	3012	778	C8-N9	3.76	1.42	1.36
7	B	3011	FPP	C11-C12	-3.18	1.40	1.50
7	B	3011	FPP	C2-C3	3.09	1.40	1.33
7	B	3011	FPP	C7-C8	3.09	1.40	1.33
7	B	3011	FPP	C6-C7	-3.09	1.40	1.50
7	B	3011	FPP	C1-C2	-2.93	1.40	1.49
7	B	3011	FPP	C12-C13	2.56	1.39	1.32
8	B	3012	778	C3-C7	2.21	1.54	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	3012	778	N18-C17-N11	-3.70	106.76	112.26
5	B	522	3FX	OAD-SAO-CAK	3.46	111.06	106.94
5	B	523	3FX	OAB-SAO-CAK	3.20	110.84	105.74
5	B	524	3FX	OAD-SAO-CAK	2.84	110.31	106.94
5	B	523	3FX	OAA-SAO-CAK	2.72	110.18	106.94
8	B	3012	778	C3-C7-C12	-2.49	126.13	129.46
8	B	3012	778	C7-C3-N1	-2.32	107.56	113.12
7	B	3011	FPP	PA-O3A-PB	-2.18	125.35	132.83
5	B	524	3FX	OAB-SAO-CAK	2.16	109.18	105.74
7	B	3011	FPP	C15-C13-C14	2.10	119.25	114.60
5	B	522	3FX	OAB-SAO-CAK	2.06	109.02	105.74
8	B	3012	778	C3-N1-C4	2.06	113.24	110.53

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	524	3FX	SAO-CAK-CAM-OAC
5	B	524	3FX	SAO-CAK-CAM-CAJ
5	B	523	3FX	NAL-CAJ-CAM-OAC
5	B	524	3FX	CAI-CAN-NAL-CAJ
5	B	523	3FX	CAI-CAN-NAL-CAJ
5	B	523	3FX	NAL-CAJ-CAM-CAK
7	B	3011	FPP	C4-C3-C5-C6
7	B	3011	FPP	C2-C3-C5-C6
5	B	522	3FX	SAO-CAK-CAM-OAC
7	B	3011	FPP	PB-O3A-PA-O1A
7	B	3011	FPP	C10-C8-C9-C11
8	B	3012	778	N11-C16-C25-C28
8	B	3012	778	N11-C16-C25-C29
5	B	524	3FX	CAH-CAN-NAL-CAJ
5	B	523	3FX	CAH-CAN-NAL-CAJ
5	B	522	3FX	SAO-CAK-CAM-CAJ
7	B	3011	FPP	C7-C8-C9-C11
7	B	3011	FPP	PB-O3A-PA-O2A

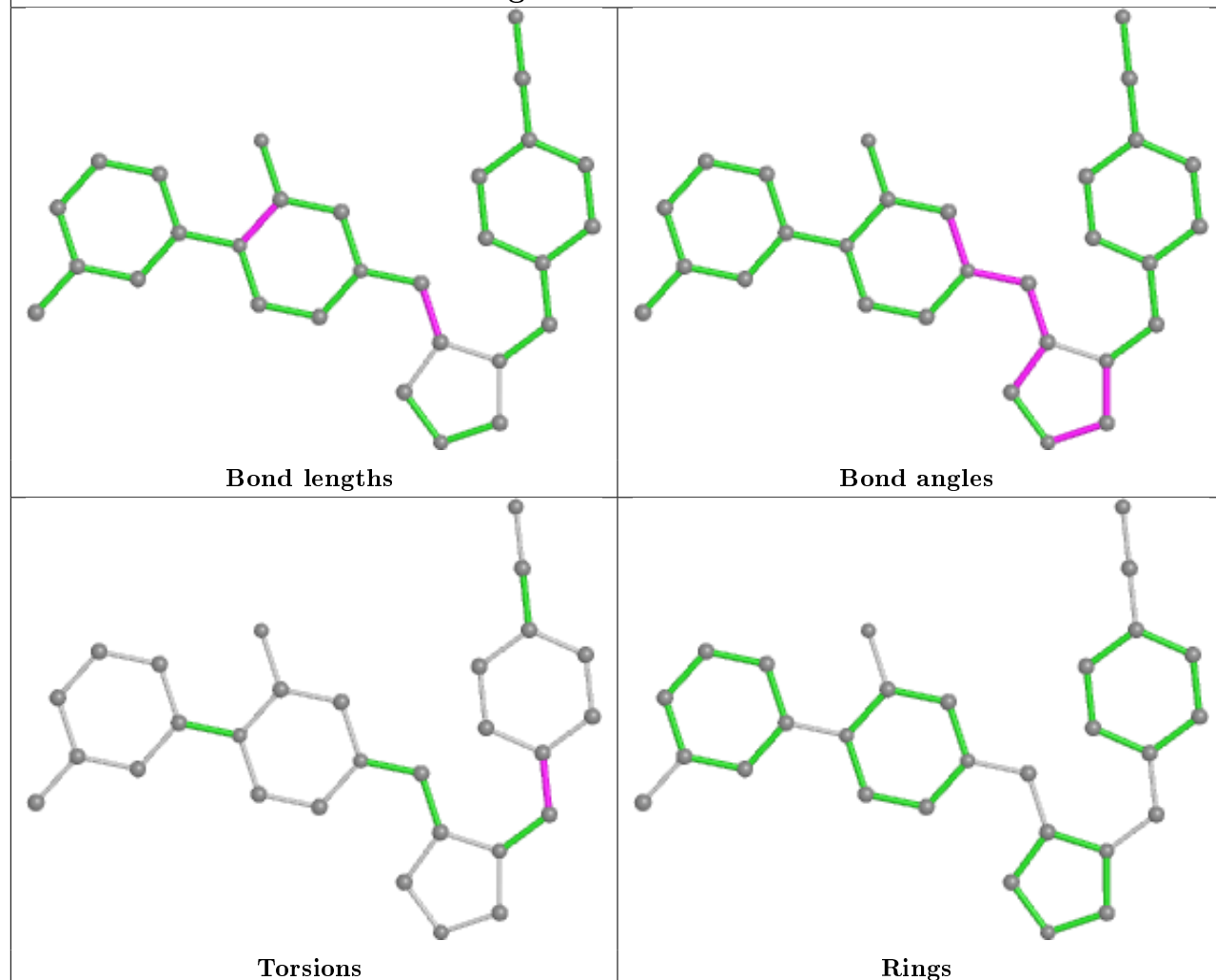
There are no ring outliers.

3 monomers are involved in 5 short contacts:

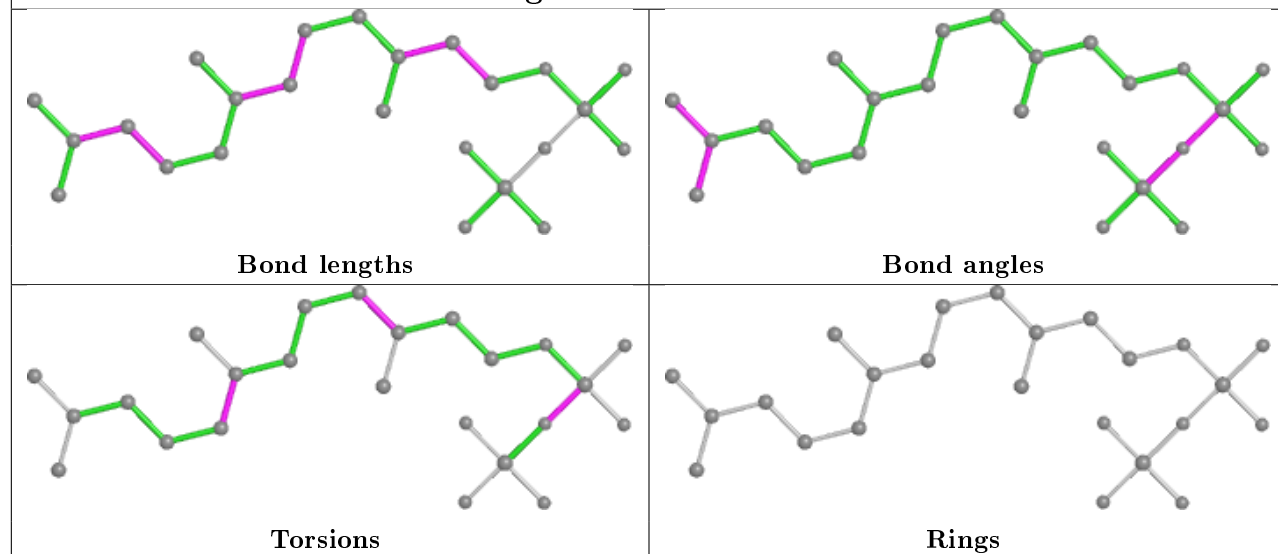
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	522	3FX	2	0
8	B	3012	778	1	0
7	B	3011	FPP	3	0

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.

Ligand 778 B 3012



Ligand FPP B 3011



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	315/349 (90%)	0.03	18 (5%) 23 23	17, 29, 48, 55	0
2	B	485/520 (93%)	0.15	19 (3%) 39 38	14, 22, 37, 57	0
All	All	800/869 (92%)	0.10	37 (4%) 32 31	14, 25, 45, 57	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	349	VAL	6.5
1	A	5	THR	5.8
2	B	347	ARG	4.7
2	B	371	ILE	4.6
1	A	334	ALA	4.5
2	B	481	GLU	4.4
1	A	208	ARG	4.3
2	B	255	GLU	4.2
2	B	51	VAL	4.1
1	A	13	ARG	3.9
2	B	50	LEU	3.9
2	B	348	LYS	3.7
1	A	207	SER	3.6
1	A	272	PHE	3.6
1	A	205	THR	3.5
2	B	257	SER	3.5
2	B	52	SER	3.2
2	B	2	ALA	3.1
1	A	7	ILE	3.1
1	A	139	LEU	3.1
2	B	453	PRO	2.8
2	B	53	GLU	2.7
1	A	302	ASN	2.6
1	A	304	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	6	TYR	2.5
2	B	346	SER	2.4
1	A	105	ASN	2.3
1	A	257	ALA	2.3
1	A	11	GLN	2.3
2	B	452	ALA	2.2
1	A	278	PRO	2.2
1	A	211	GLN	2.2
1	A	274	MET	2.1
2	B	372	PRO	2.0
2	B	233	GLY	2.0
2	B	268	GLY	2.0
2	B	330	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

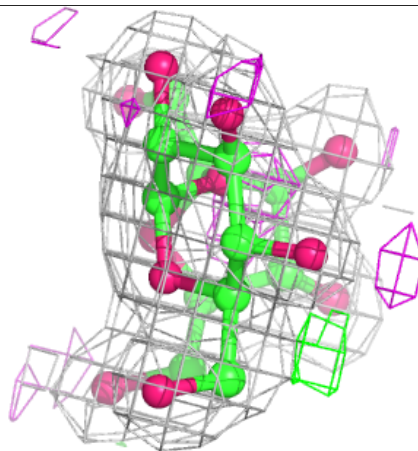
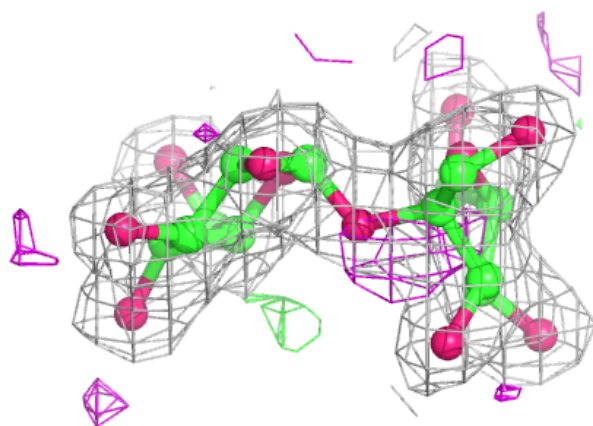
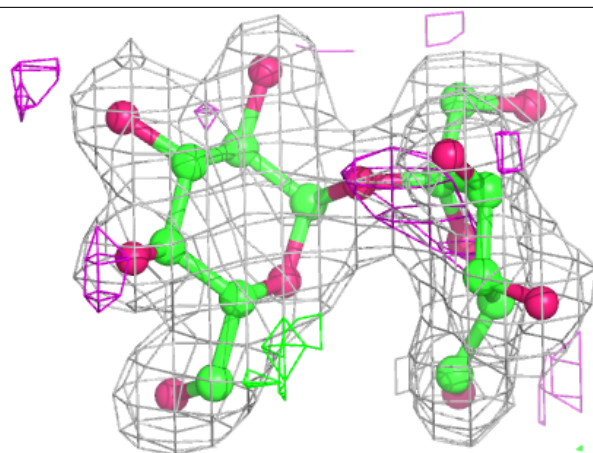
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GLC	E	1	11/12	0.86	0.15	43,43,43,44	0
3	FRU	E	2	12/12	0.88	0.18	44,44,45,45	0
3	FRU	D	2	12/12	0.90	0.12	30,31,31,32	0
3	FRU	C	2	12/12	0.93	0.22	36,36,37,37	0
3	GLC	C	1	11/12	0.95	0.13	35,36,36,36	0
3	GLC	D	1	11/12	0.95	0.11	29,31,31,32	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.

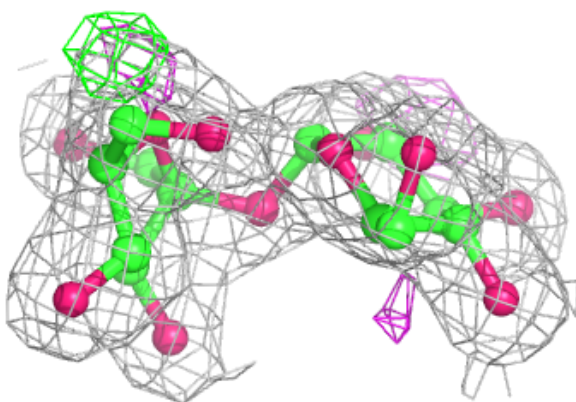
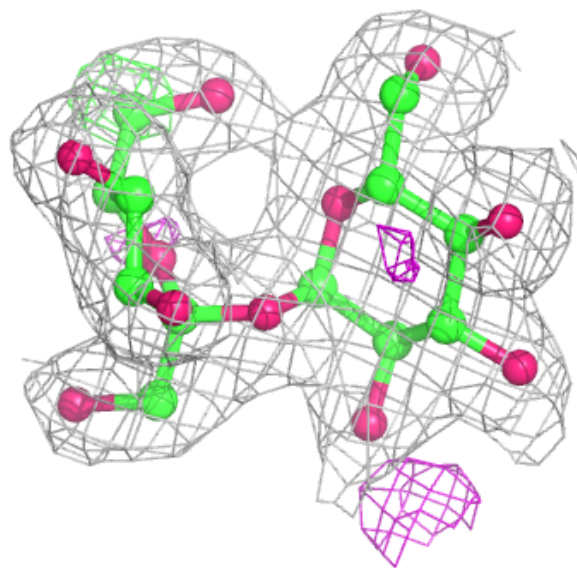
Electron density around Chain C:

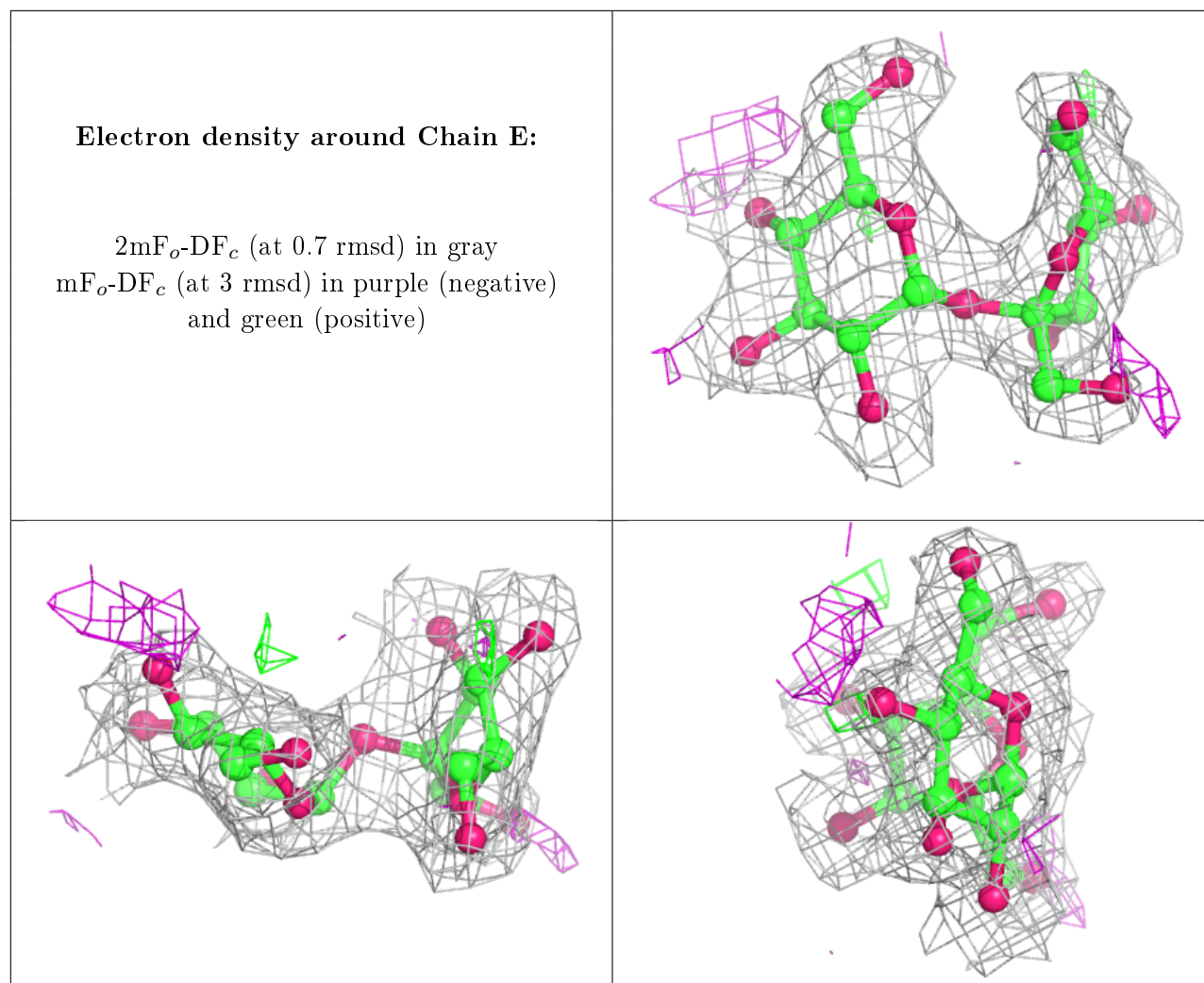
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

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.

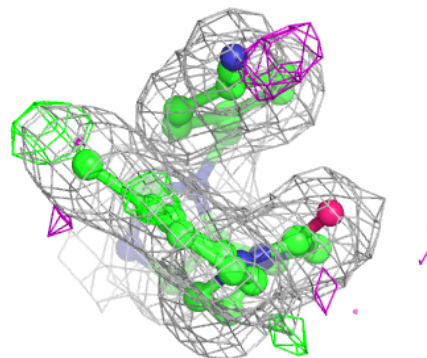
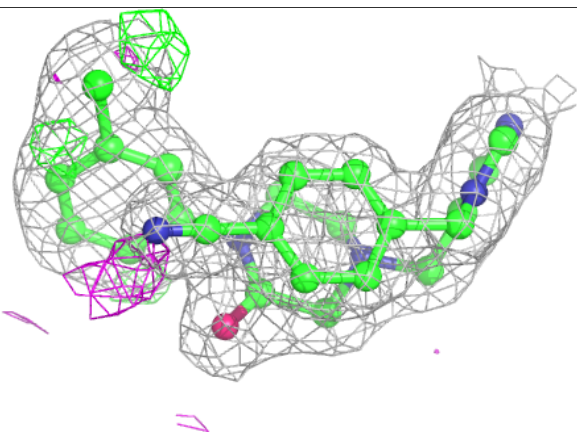
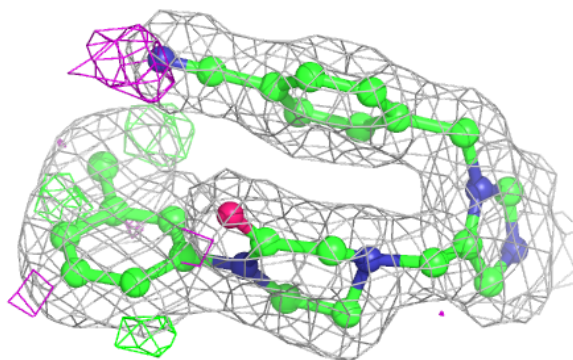
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	3FX	B	524	15/15	0.82	0.19	46,48,53,54	0
6	SO4	B	525	5/5	0.91	0.18	38,39,39,39	0
8	778	B	3012	29/29	0.96	0.15	17,19,26,30	0
5	3FX	B	523	15/15	0.96	0.14	37,39,39,40	0
7	FPP	B	3011	24/24	0.97	0.18	17,19,19,20	0
5	3FX	B	522	15/15	0.97	0.13	20,21,22,22	0
4	ZN	B	521	1/1	1.00	0.10	17,17,17,17	0

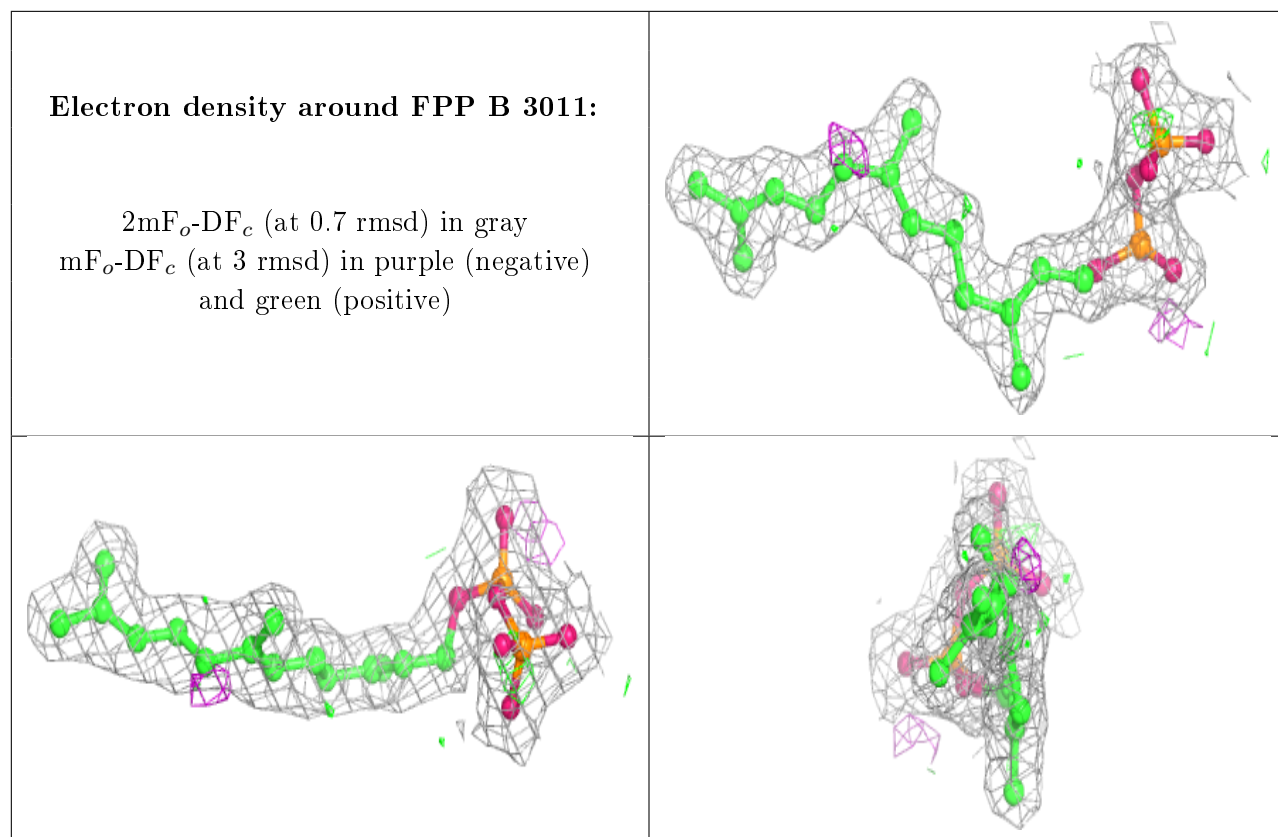
The following is a graphical depiction of the model fit to experimental electron density of all

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 778 B 3012:

$2mF_o-DF_c$ (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.