



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 10:26 AM BST

PDB ID : 4CU4
Title : FhuA from E. coli in complex with the lasso peptide microcin J25 (MccJ25)
Authors : Mathavan, I.; Rebuffat, S.; Beis, K.
Deposited on : 2014-03-17
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

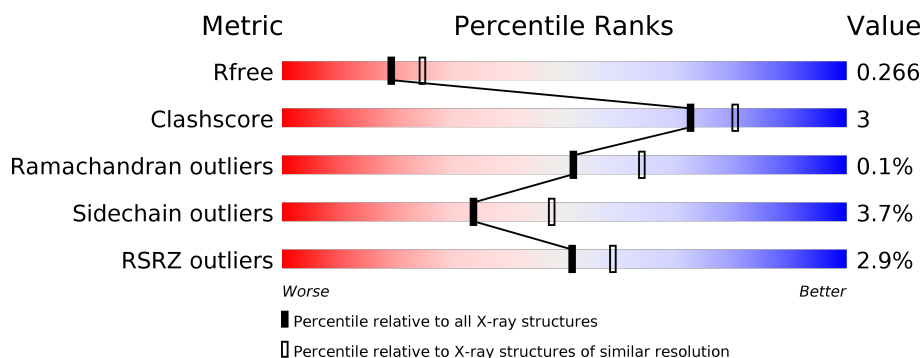
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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 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	706	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>..</div> </div> </div>
2	B	21	<div> <div>10%</div> <div> <div></div> <div>86%</div> <div>14%</div> </div> </div>
3	C	6	<div> <div></div> <div>100%</div> </div>

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
7	LDA	A	1738	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 6260 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 FERRICHRONE-IRON RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	693	5430	3423	920	1072	15	0	3	0

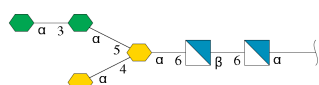
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	SER	-	expression tag	UNP P06971
A	407	SER	-	expression tag	UNP P06971
A	408	HIS	-	expression tag	UNP P06971
A	409	HIS	-	expression tag	UNP P06971
A	410	HIS	-	expression tag	UNP P06971
A	411	HIS	-	expression tag	UNP P06971
A	412	HIS	-	expression tag	UNP P06971
A	413	HIS	-	expression tag	UNP P06971
A	414	GLY	-	expression tag	UNP P06971
A	415	SER	-	expression tag	UNP P06971
A	416	SER	-	expression tag	UNP P06971

- Molecule 2 is a protein called MICROCIN J25.

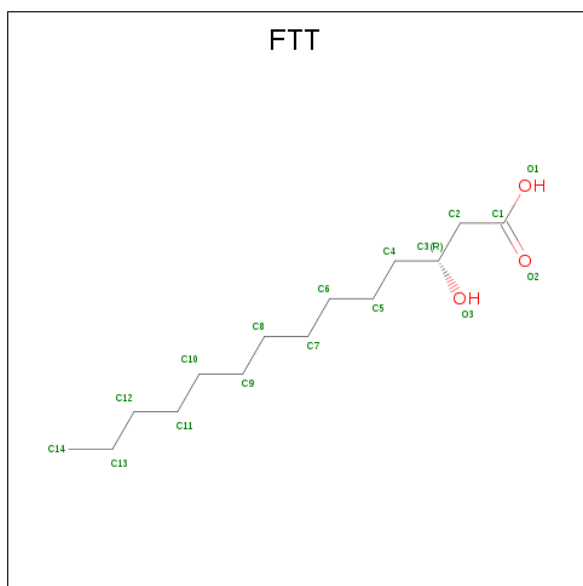
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	21	150	101	23	26	0	0	0

- Molecule 3 is an oligosaccharide called L-glycero-alpha-D-manno-heptopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose.



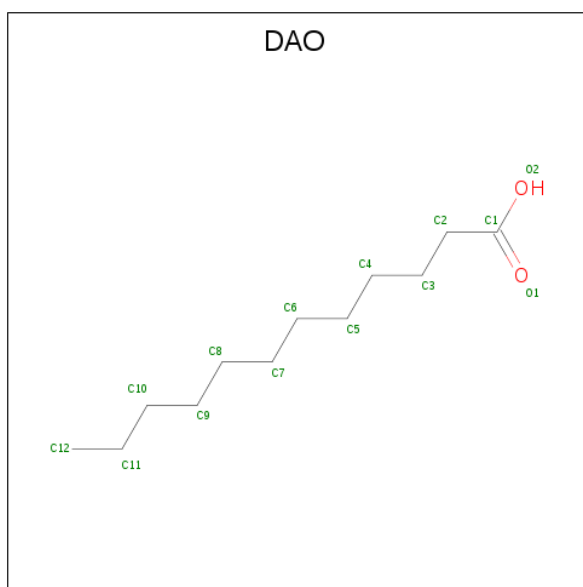
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	0	0	0
			78	42	2	34			

- Molecule 4 is 3-HYDROXY-TETRADECANOIC ACID (three-letter code: FTT) (formula: $C_{14}H_{28}O_3$).



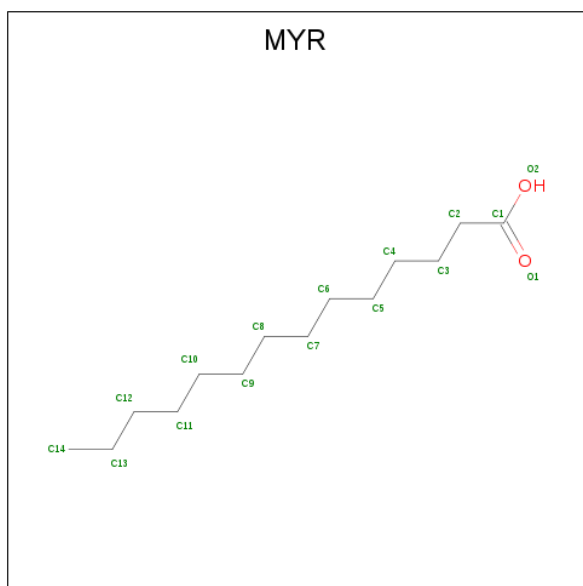
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	14	2		
4	A	1	Total	C	O	0	0
			16	14	2		
4	A	1	Total	C	O	0	0
			16	14	2		
4	A	1	Total	C	O	0	0
			16	14	2		

- Molecule 5 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).



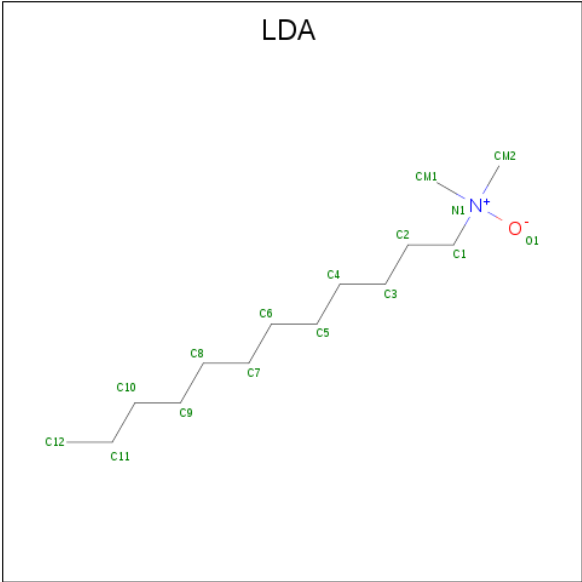
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	12	1		

- Molecule 6 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			15	14	1		

- Molecule 7 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



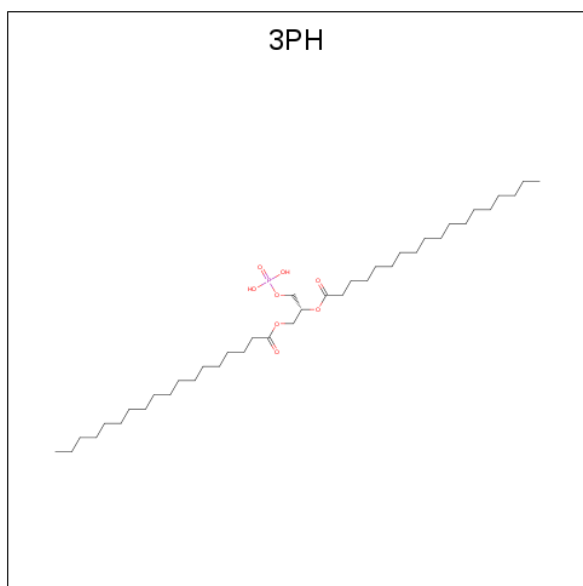
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			16	14	1	1		
7	A	1	Total	C	N	O	0	0
			16	14	1	1		
7	A	1	Total	C	N	O	0	0
			16	14	1	1		
7	A	1	Total	C	N	O	0	0
			16	14	1	1		
7	A	1	Total	C	N	O	0	0
			16	14	1	1		
7	A	1	Total	C	N	O	0	0
			16	14	1	1		
7	A	1	Total	C	N	O	0	0
			12	10	1	1		
7	A	1	Total	C	N	O	0	0
			16	14	1	1		
7	A	1	Total	C	N	O	0	0
			13	11	1	1		
7	A	1	Total	C	N	O	0	0
			14	12	1	1		
7	A	1	Total	C			0	0
			9	9				
7	A	1	Total	C			0	0
			10	10				
7	A	1	Total	C	N	O	0	0
			11	9	1	1		

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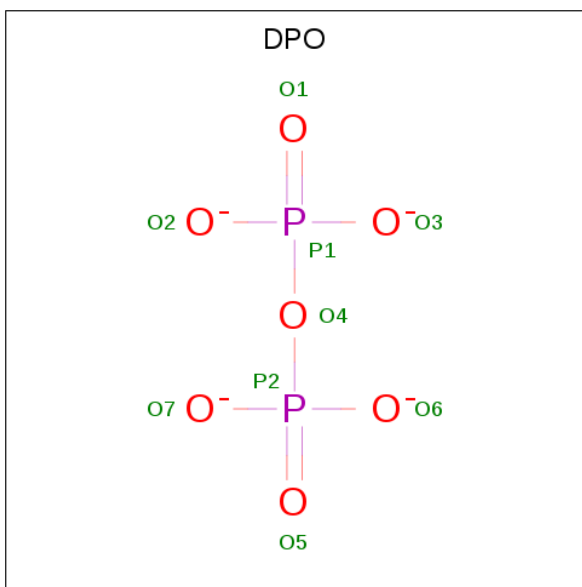
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			11	9	1	1		
7	A	1	Total	C	N	O	0	0
			16	14	1	1		
7	A	1	Total	C	N	O	0	0
			14	12	1	1		
7	A	1	Total	C	N	O	0	0
			12	10	1	1		
7	A	1	Total	C	N	O	0	0
			16	14	1	1		
7	A	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 8 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



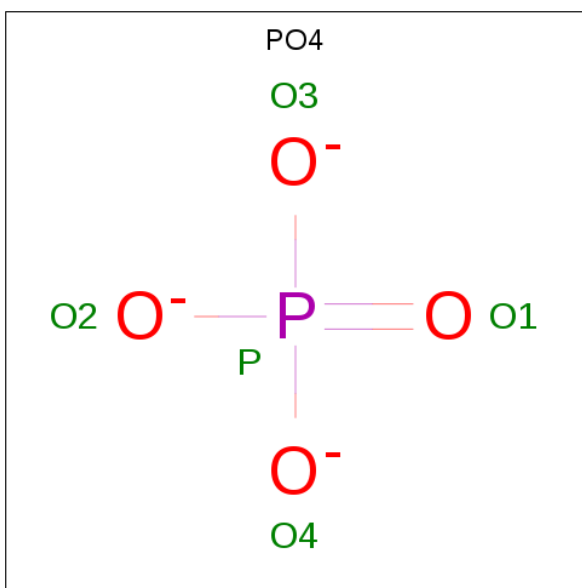
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	O	P	0	0
			35	26	8	1		

- Molecule 9 is DIPHOSPHATE (three-letter code: DPO) (formula: O_7P_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	P	0	0
			9	7	2		
9	A	1	Total	O	P	0	0
			8	6	2		

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	P	0	0
			4	3	1		
10	A	1	Total	O	P	0	0
			4	3	1		

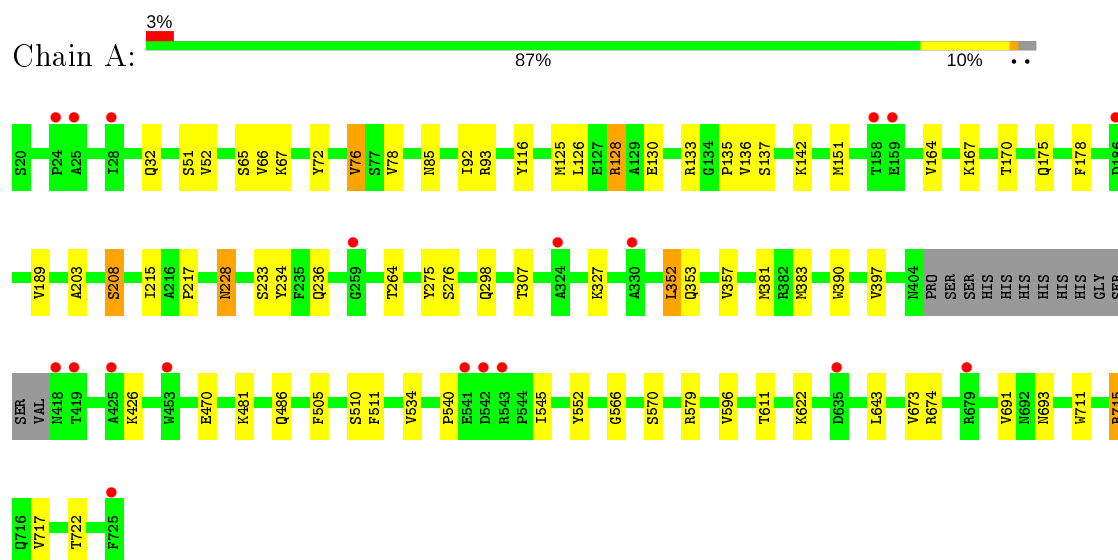
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	167	Total 167	O 167	0	0
11	B	1	Total 1	O 1	0	0

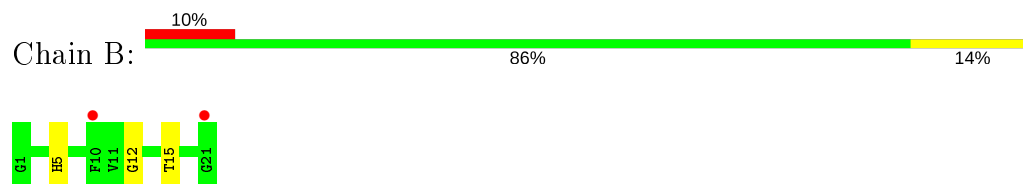
3 Residue-property plots [i](#)

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.

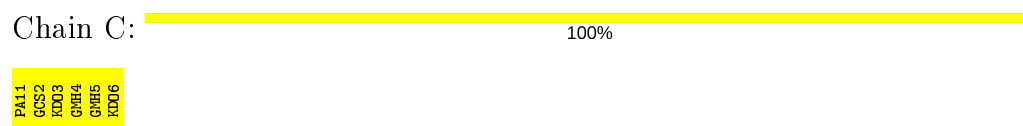
• Molecule 1: FERRICHRONE-IRON RECEPTOR



• Molecule 2: MICROCIN J25



• Molecule 3: L-glycero-alpha-D-manno-heptopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	95.98Å 277.05Å 106.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.46 – 2.30 30.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.46-2.30) 98.5 (30.46-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.31Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.212 , 0.255 0.219 , 0.266	Depositor DCC
R_{free} test set	3172 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.853	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6260	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: PA1, LDA, GMH, FTT, PO4, MYR, DAO, 3PH, GCS, KDO, DPO

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	0.53	0/5572	0.71	1/7569 (0.0%)
2	B	0.62	0/156	0.62	0/211
All	All	0.53	0/5728	0.71	1/7780 (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	A	352	LEU	CA-CB-CG	6.30	129.78	115.30

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	5430	0	5157	36	0
2	B	150	0	137	2	0
3	C	78	0	56	0	0
4	A	64	0	106	2	0
5	A	13	0	23	1	0
6	A	15	0	27	0	0
7	A	282	0	517	4	0
8	A	35	0	43	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	17	0	0	0	0
10	A	8	0	0	0	0
11	A	167	0	0	2	0
11	B	1	0	0	0	0
All	All	6260	0	6066	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.

The worst 5 of 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)
1:A:228:ASN:C	1:A:228:ASN:HD22	1.90	0.74
1:A:203:ALA:HB3	1:A:208:SER:HB3	1.76	0.68
1:A:66:VAL:HG23	11:A:3015:HOH:O	1.97	0.64
7:A:1732:LDA:H52	8:A:1744:3PH:H222	1.82	0.62
1:A:51:SER:OG	1:A:133:ARG:NH2	2.32	0.62

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	692/706 (98%)	667 (96%)	24 (4%)	1 (0%)	51	64
2	B	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
All	All	711/727 (98%)	685 (96%)	25 (4%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	566	GLY

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	577/586 (98%)	555 (96%)	22 (4%)	33	47
2	B	14/14 (100%)	14 (100%)	0	100	100
All	All	591/600 (98%)	569 (96%)	22 (4%)	34	48

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	TYR
1	A	353	GLN
1	A	715	ARG
1	A	327	LYS
1	A	352	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	GLN
1	A	716	GLN
1	A	309	GLN
1	A	228	ASN
1	A	299	ASN

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	PA1	C	1	9,3,4	11,11,12	0.77	1 (9%)	12,15,17	1.50	2 (16%)
3	GCS	C	2	10,3,4	11,11,12	1.10	1 (9%)	12,15,17	1.30	2 (16%)
3	KDO	C	3	3	12,15,16	0.41	0	16,21,24	1.18	2 (12%)
3	GMH	C	4	9,3	13,13,14	0.39	0	17,18,20	1.14	1 (5%)
3	GMH	C	5	10,3	13,13,14	0.43	0	17,18,20	1.13	1 (5%)
3	KDO	C	6	3	12,15,16	0.34	0	16,21,24	1.38	2 (12%)

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	PA1	C	1	9,3,4	-	0/2/19/22	0/1/1/1
3	GCS	C	2	10,3,4	-	1/2/19/22	0/1/1/1
3	KDO	C	3	3	-	2/6/26/30	0/1/1/1
3	GMH	C	4	9,3	-	0/6/23/26	0/1/1/1
3	GMH	C	5	10,3	-	2/6/23/26	0/1/1/1
3	KDO	C	6	3	-	2/6/26/30	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	GCS	C1-C2	3.27	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	PA1	C1-C2	2.48	1.55	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	GMH	C1-O5-C5	4.12	118.23	111.48
3	C	4	GMH	C1-O5-C5	3.88	117.84	111.48
3	C	6	KDO	C7-C6-C5	3.82	120.36	114.03
3	C	2	GCS	O3-C3-C2	3.35	115.96	109.81
3	C	1	PA1	O3-C3-C2	-3.33	103.70	109.81

There are no chirality outliers.

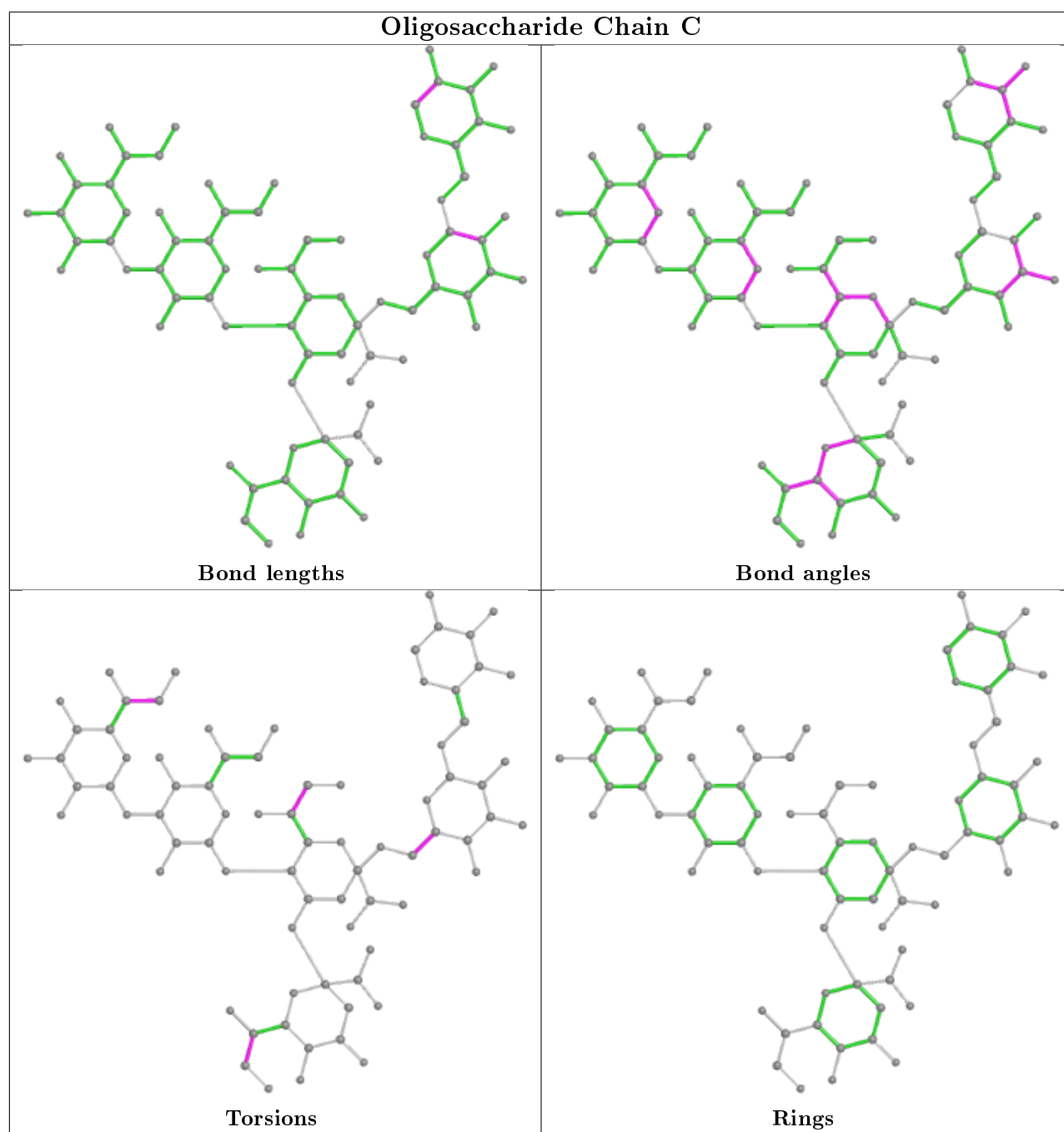
5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	5	GMH	O6-C6-C7-O7
3	C	6	KDO	O7-C7-C8-O8
3	C	3	KDO	C6-C7-C8-O8
3	C	3	KDO	O7-C7-C8-O8
3	C	5	GMH	C5-C6-C7-O7

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](#)

31 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
7	LDA	A	1738	-	9,9,15	0.20	0	8,8,17	0.10	0
7	LDA	A	1727	-	12,15,15	0.34	0	14,17,17	0.50	0
6	MYR	A	1014	4	14,14,15	0.61	1 (7%)	13,13,15	0.58	1 (7%)
5	DAO	A	1012	4	12,12,13	0.63	1 (8%)	11,11,13	0.58	0
7	LDA	A	1731	-	12,15,15	0.34	0	14,17,17	0.22	0
10	PO4	A	2001	3	0,3,4	0.00	-	0,3,6	0.00	-
7	LDA	A	1742	-	10,13,15	0.41	0	12,15,17	0.59	0
10	PO4	A	2005	3	0,3,4	0.00	-	0,3,6	0.00	-
8	3PH	A	1744	-	34,34,47	0.48	0	38,39,52	0.63	1 (2%)
9	DPO	A	2004	3	3,7,8	0.69	0	6,10,13	0.91	0
7	LDA	A	1737	-	8,8,15	0.21	0	7,7,17	0.09	0
7	LDA	A	1745	-	12,15,15	0.32	0	14,17,17	0.44	0
4	FTT	A	1011	3,5	15,15,16	0.29	0	15,15,17	0.66	1 (6%)
7	LDA	A	1730	-	12,15,15	0.35	0	14,17,17	0.25	0
7	LDA	A	1736	-	10,13,15	0.46	0	12,15,17	0.26	0
4	FTT	A	1013	3,6	15,15,16	0.19	0	15,15,17	0.31	0
7	LDA	A	1740	-	7,10,15	0.45	0	9,12,17	0.87	0
7	LDA	A	1729	-	12,15,15	0.39	0	14,17,17	0.39	0
7	LDA	A	1732	-	12,15,15	0.34	0	14,17,17	1.64	2 (14%)
4	FTT	A	1009	3	15,15,16	0.28	0	15,15,17	0.57	0
7	LDA	A	1741	-	12,15,15	0.35	0	14,17,17	0.59	0
7	LDA	A	1726	-	12,15,15	0.38	0	14,17,17	0.68	0
4	FTT	A	1010	3	15,15,16	0.24	0	15,15,17	0.94	1 (6%)
7	LDA	A	1735	-	9,12,15	0.40	0	11,14,17	0.58	0
7	LDA	A	1746	-	12,15,15	0.33	0	14,17,17	0.68	0
7	LDA	A	1743	-	8,11,15	0.44	0	10,13,17	0.62	0
7	LDA	A	1734	-	12,15,15	0.41	0	14,17,17	0.33	0
7	LDA	A	1728	-	12,15,15	0.34	0	14,17,17	0.25	0
7	LDA	A	1733	-	8,11,15	0.43	0	10,13,17	0.66	0
9	DPO	A	2000	3	6,8,8	1.05	0	13,13,13	3.87	5 (38%)
7	LDA	A	1739	-	7,10,15	0.43	0	9,12,17	0.41	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
7	LDA	A	1738	-	-	6/7/7/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FTT	A	1010	3	-	8/14/14/15	-
6	MYR	A	1014	4	-	7/11/12/13	-
5	DAO	A	1012	4	-	3/9/10/11	-
7	LDA	A	1731	-	-	4/13/13/13	-
7	LDA	A	1742	-	-	4/11/11/13	-
8	3PH	A	1744	-	-	19/36/36/49	-
9	DPO	A	2004	3	-	0/2/5/6	-
7	LDA	A	1737	-	-	3/6/6/13	-
7	LDA	A	1745	-	-	9/13/13/13	-
4	FTT	A	1011	3,5	-	8/14/14/15	-
7	LDA	A	1730	-	-	6/13/13/13	-
7	LDA	A	1736	-	-	4/11/11/13	-
4	FTT	A	1013	3,6	-	10/14/14/15	-
7	LDA	A	1740	-	-	2/8/8/13	-
7	LDA	A	1729	-	-	8/13/13/13	-
7	LDA	A	1732	-	-	5/13/13/13	-
4	FTT	A	1009	3	-	9/14/14/15	-
7	LDA	A	1741	-	-	7/13/13/13	-
7	LDA	A	1726	-	-	7/13/13/13	-
7	LDA	A	1727	-	-	8/13/13/13	-
7	LDA	A	1735	-	-	3/10/10/13	-
7	LDA	A	1746	-	-	6/13/13/13	-
7	LDA	A	1743	-	-	2/9/9/13	-
7	LDA	A	1734	-	-	9/13/13/13	-
7	LDA	A	1728	-	-	11/13/13/13	-
7	LDA	A	1733	-	-	4/9/9/13	-
9	DPO	A	2000	3	-	3/6/6/6	-
7	LDA	A	1739	-	-	3/8/8/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1014	MYR	O1-C1	2.11	1.31	1.19
5	A	1012	DAO	O1-C1	2.06	1.31	1.19

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2000	DPO	P2-O4-P1	11.49	172.26	132.83
9	A	2000	DPO	O2-P1-O1	-5.68	88.43	110.68
7	A	1732	LDA	CM2-N1-C1	4.30	119.27	110.23
7	A	1732	LDA	CM1-N1-C1	-4.09	101.63	110.23
9	A	2000	DPO	O3-P1-O1	3.41	124.02	110.68

There are no chirality outliers.

5 of 178 torsion outliers are listed below:

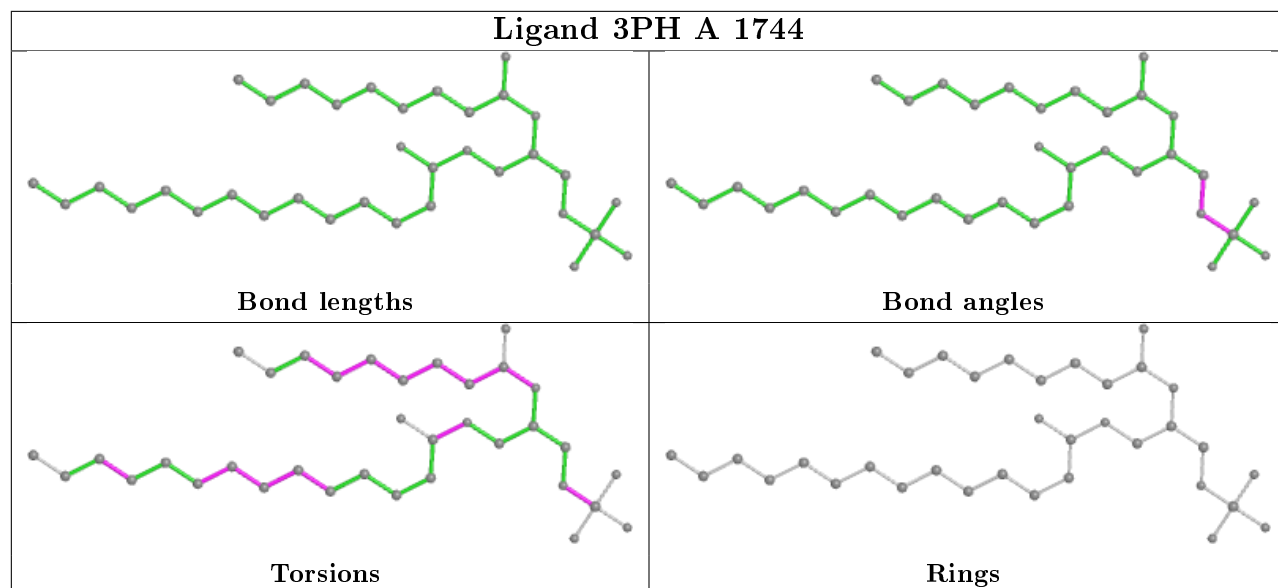
Mol	Chain	Res	Type	Atoms
7	A	1727	LDA	C2-C1-N1-CM1
8	A	1744	3PH	C1-O11-P-O13
8	A	1744	3PH	C1-O11-P-O14
8	A	1744	3PH	O22-C21-O21-C2
7	A	1745	LDA	C2-C1-N1-CM1

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1012	DAO	1	0
8	A	1744	3PH	3	0
7	A	1732	LDA	1	0
4	A	1009	FTT	2	0
7	A	1741	LDA	1	0
7	A	1726	LDA	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	693/706 (98%)	-0.18	19 (2%) 54 62	36, 53, 75, 104	0
2	B	21/21 (100%)	0.45	2 (9%) 8 11	56, 70, 80, 95	0
All	All	714/727 (98%)	-0.16	21 (2%) 51 58	36, 53, 76, 104	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	158	THR	3.8
1	A	725	PHE	3.7
1	A	28	ILE	3.4
1	A	418	ASN	3.0
1	A	635	ASP	2.8

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.

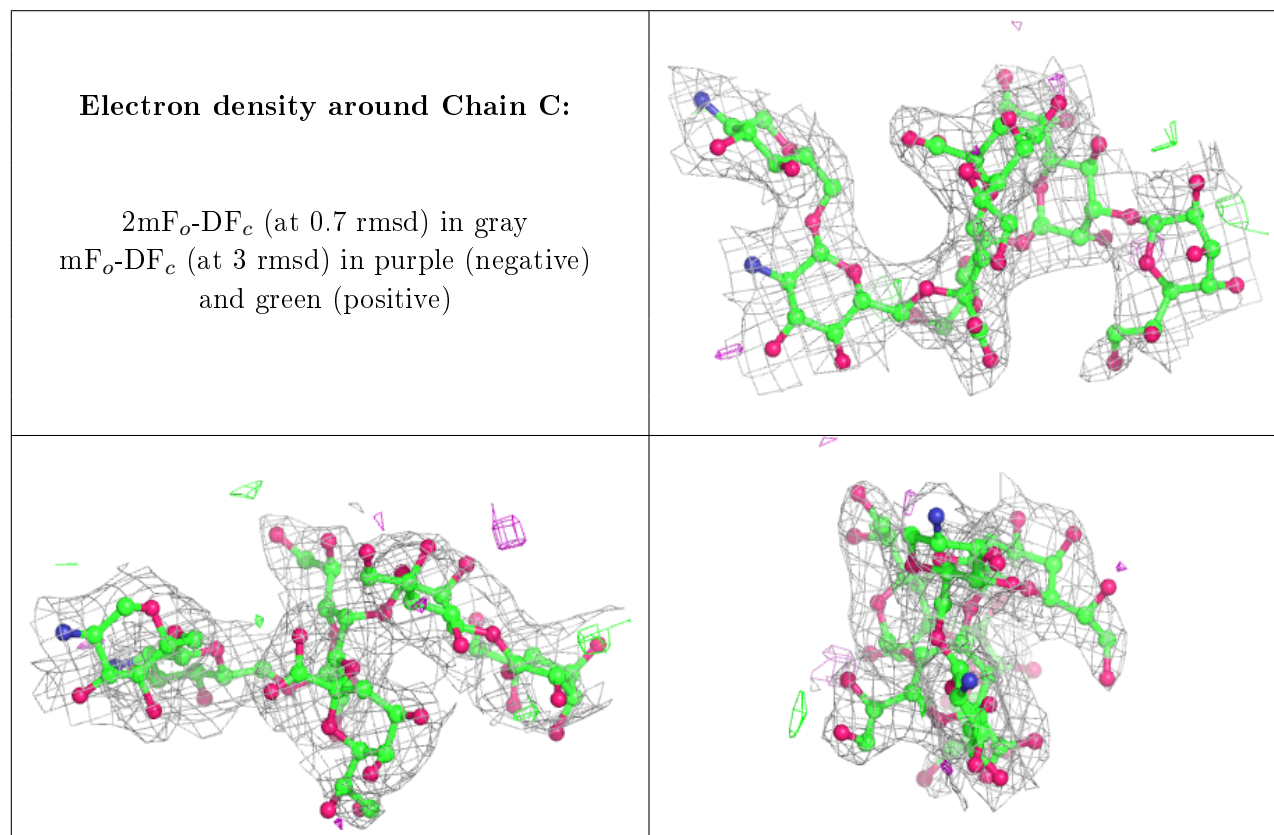
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GMH	C	5	13/14	0.85	0.28	109,117,120,127	0
3	KDO	C	6	15/16	0.90	0.21	69,81,89,90	0
3	GMH	C	4	13/14	0.94	0.15	74,81,92,100	0
3	KDO	C	3	15/16	0.95	0.12	66,73,77,79	0
3	GCS	C	2	11/12	0.95	0.08	50,54,67,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PA1	C	1	11/12	0.97	0.07	47,47,51,51	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.



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.

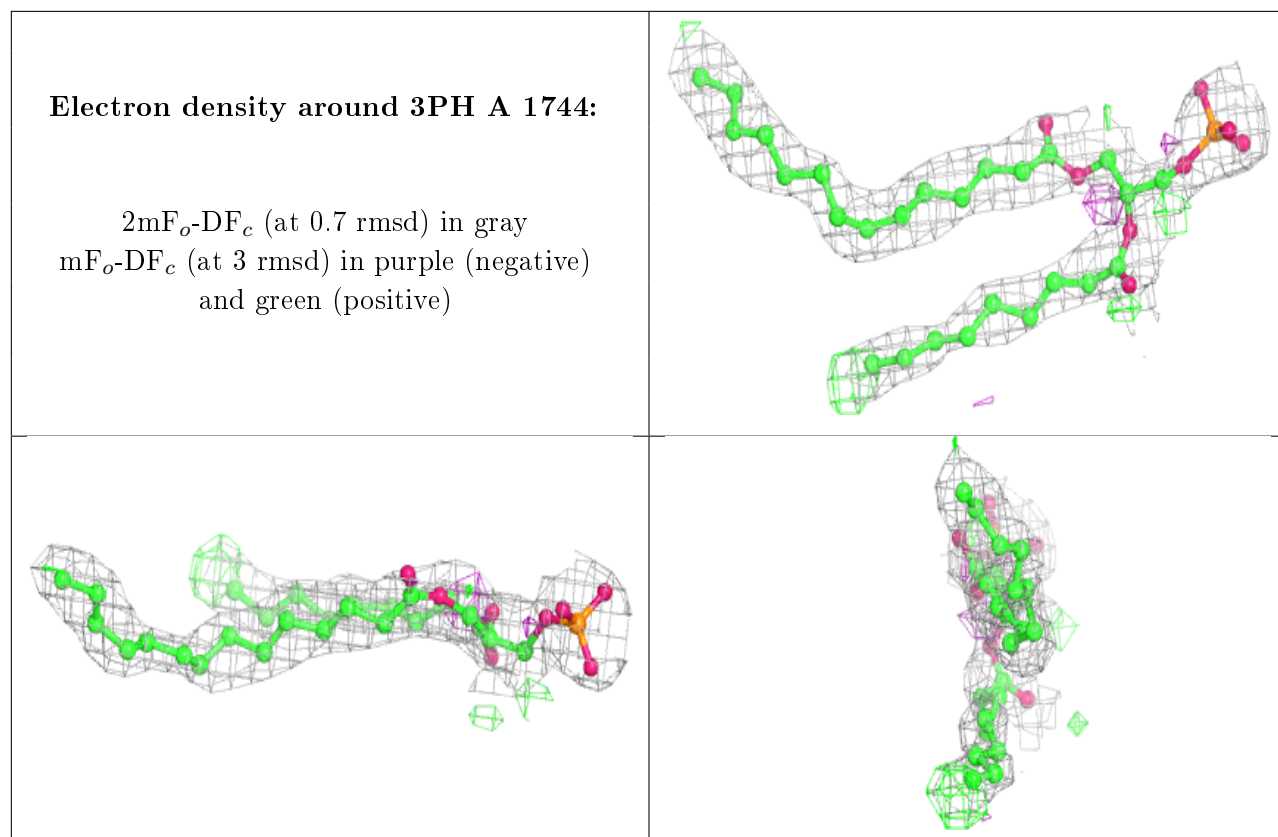
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	LDA	A	1729	16/16	0.55	0.27	70,74,97,99	0
7	LDA	A	1746	16/16	0.59	0.34	76,79,99,101	0
7	LDA	A	1742	14/16	0.62	0.30	78,88,103,104	0
7	LDA	A	1736	14/16	0.62	0.30	63,77,91,92	0
7	LDA	A	1733	12/16	0.64	0.28	91,99,106,106	0
7	LDA	A	1745	16/16	0.69	0.27	83,85,104,106	0
8	3PH	A	1744	35/48	0.71	0.25	55,85,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	LDA	A	1728	16/16	0.73	0.21	46,60,89,89	0
7	LDA	A	1735	13/16	0.73	0.29	53,65,91,92	0
7	LDA	A	1739	11/16	0.73	0.31	55,67,85,86	0
7	LDA	A	1732	16/16	0.74	0.27	64,77,91,91	0
7	LDA	A	1740	11/16	0.74	0.33	80,84,95,95	0
6	MYR	A	1014	15/16	0.76	0.39	81,86,92,92	0
7	LDA	A	1743	12/16	0.78	0.22	68,74,90,91	0
7	LDA	A	1738	10/16	0.78	0.41	87,92,94,94	0
7	LDA	A	1737	9/16	0.80	0.32	79,81,83,84	0
7	LDA	A	1734	16/16	0.81	0.23	64,77,96,96	0
7	LDA	A	1730	16/16	0.82	0.26	71,75,89,90	0
7	LDA	A	1731	16/16	0.82	0.32	81,83,91,92	0
10	PO4	A	2005	4/5	0.85	0.29	133,134,134,134	0
7	LDA	A	1726	16/16	0.86	0.25	67,72,76,78	0
9	DPO	A	2000	9/9	0.88	0.19	47,56,71,74	0
7	LDA	A	1741	16/16	0.90	0.14	64,68,79,82	0
9	DPO	A	2004	8/9	0.90	0.14	88,98,105,107	0
4	FTT	A	1013	16/17	0.91	0.15	59,68,73,79	0
7	LDA	A	1727	16/16	0.93	0.17	51,58,69,71	0
4	FTT	A	1010	16/17	0.94	0.13	52,60,74,74	0
4	FTT	A	1009	16/17	0.95	0.15	46,63,73,73	0
5	DAO	A	1012	13/14	0.95	0.13	45,61,69,69	0
4	FTT	A	1011	16/17	0.97	0.11	50,53,57,58	0
10	PO4	A	2001	4/5	0.98	0.05	60,66,66,71	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.