



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 27, 2024 – 10:09 PM EDT

PDB ID : 1QFG
Title : E. COLI FERRIC HYDROXAMATE RECEPTOR (FHUA)
Authors : Ferguson, A.D.; Welte, W.; Hofmann, E.; Lindner, B.; Holst, O.; Coulton, J.W.; Diederichs, K.
Deposited on : 1999-04-10
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

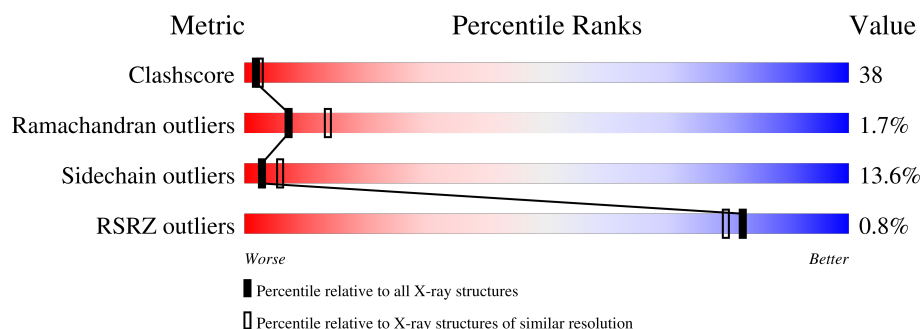
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	725	<div> <div></div> <div>46%</div> <div>40%</div> <div>9%</div> <div>..</div> </div>
2	B	9	<div> <div>11%</div> <div>56%</div> <div>33%</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
10	GOL	A	1103	-	X	-	-
10	GOL	A	1104	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	GOL	A	1105	-	-	X	-
10	GOL	A	1106	-	X	-	-
10	GOL	A	1107	-	X	X	-
10	GOL	A	1108	-	X	-	-
5	FTT	A	1013	-	-	X	-
7	MYR	A	1014	-	-	X	-
9	DPO	A	2000	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 6077 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.

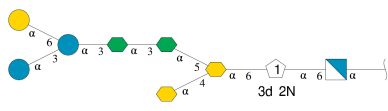
- Molecule 1 is a protein called PROTEIN (FERRIC HYDROXAMATE UPTAKE RECEPTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	707	5524	3475	944	1091	14	0	0	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 an oligosaccharide called alpha-D-glucopyranose-(1-3)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-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-2,3-dideoxy-alpha-D-glucopyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose.

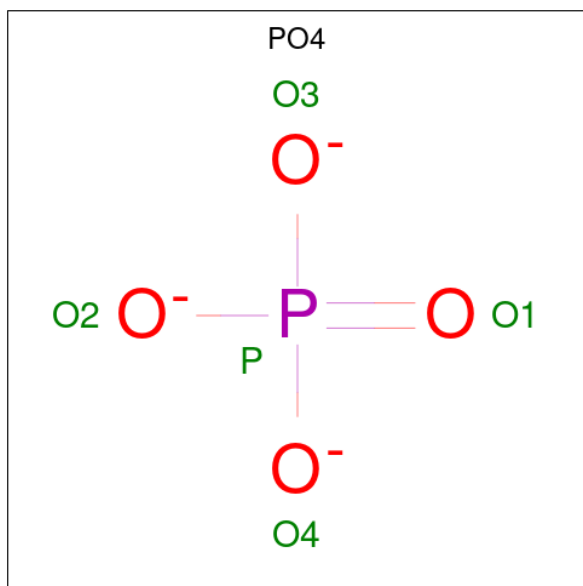


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	9	110	60	2	48	0	0	0

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

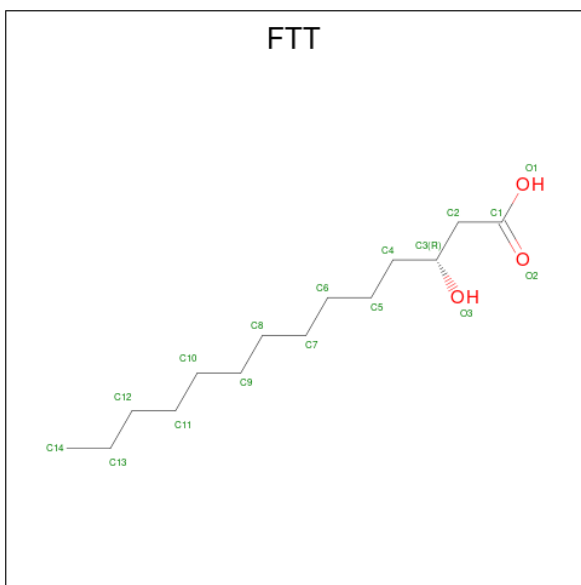
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



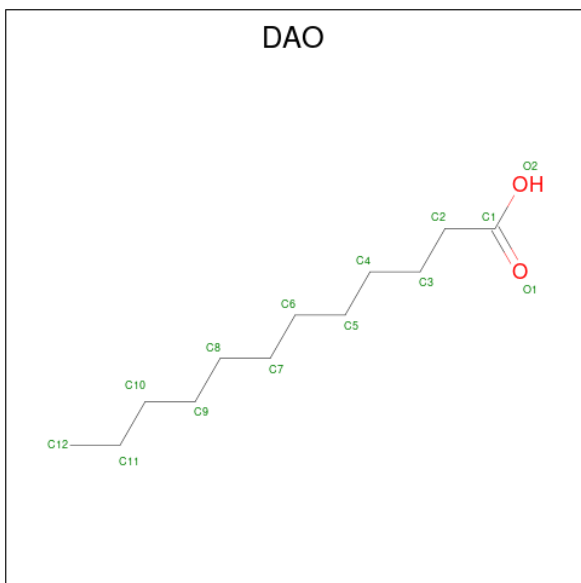
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 4 3 1	0	0
4	A	1	Total O P 4 3 1	0	0

- Molecule 5 is 3-HYDROXY-TETRADECANOIC ACID (three-letter code: FTT) (formula: C₁₄H₂₈O₃).



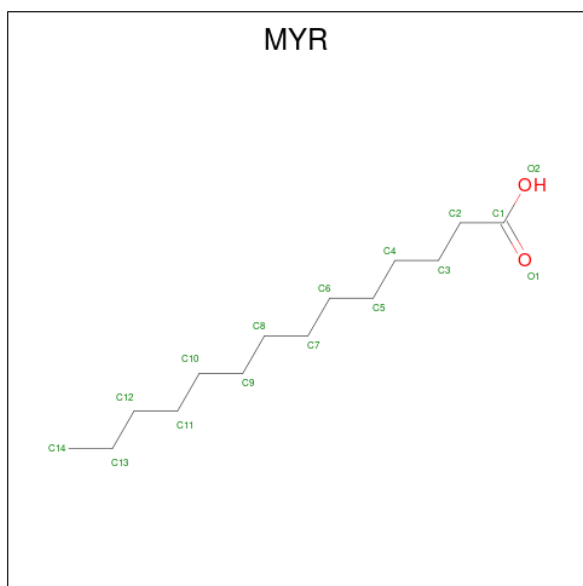
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	14	2		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			16	14	2		
5	A	1	Total	C	O	0	0
			17	14	3		

- Molecule 6 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).



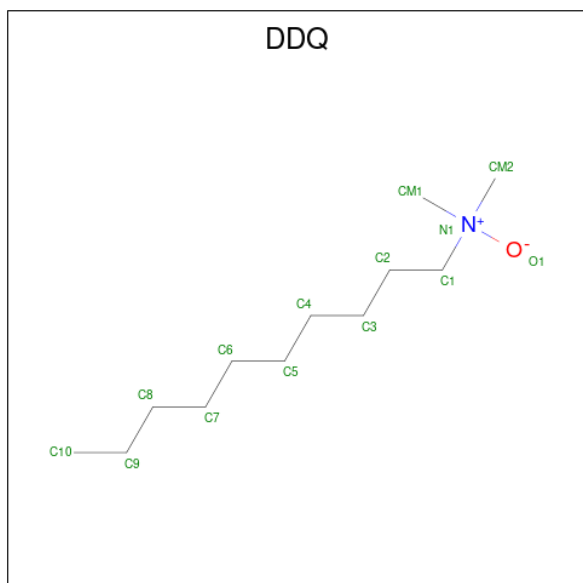
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	12	1		

- Molecule 7 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



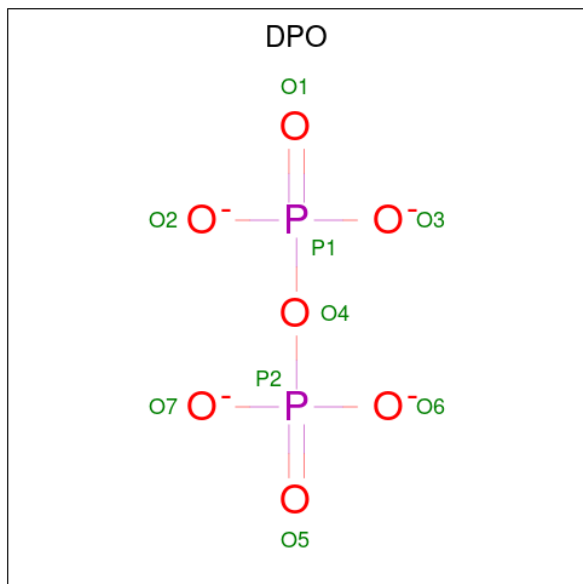
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			15	14	1		

- Molecule 8 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula: $C_{12}H_{27}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	12	1	1		
8	A	1	Total	C	N	O	0	0
			14	12	1	1		
8	A	1	Total	C	N	O	0	0
			14	12	1	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
			8	6	2		
9	A	1	Total	O	P	0	0
			8	6	2		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

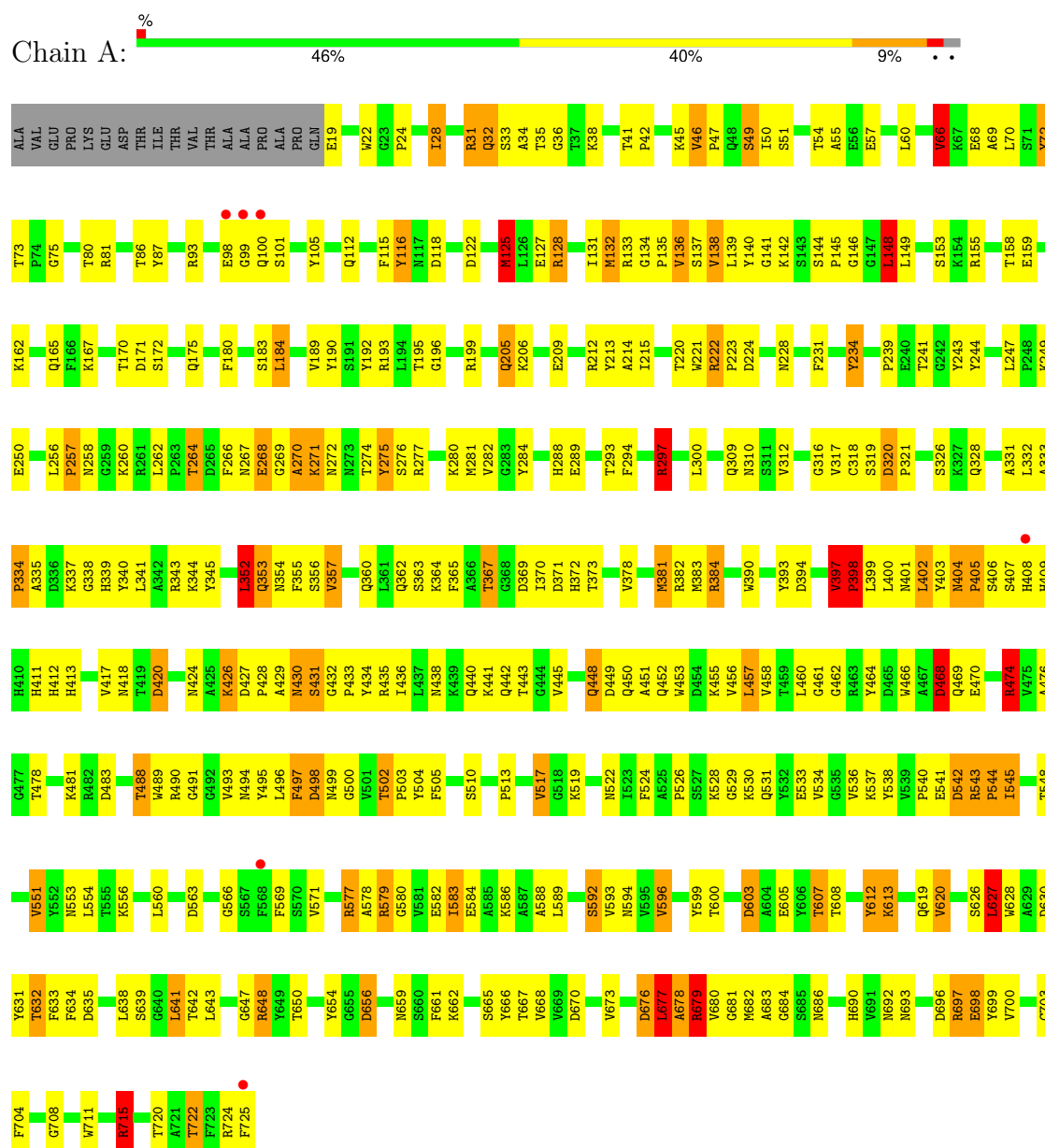
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	244	Total	O	0	0
			244	244		

3 Residue-property plots

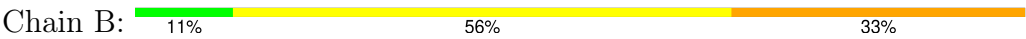
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PROTEIN (FERRIC HYDROXAMATE UPTAKE RECEPTOR)



• Molecule 2: alpha-D-glucopyranose-(1-3)-[alpha-D-galactopyranose-(1-6)]alpha-D-glucopyranose-(1-3)-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-ulop
yranosonic acid-(2-6)-2-amino-2,3-dideoxy-alpha-D-glucopyranose-(1-6)-2-amino-2-deoxy-alpha-D-
glucopyranose



PA11	GM2	KD03	GMH4	GMH5	GLC6	GLC7	GLA8	KD09
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4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	171.55Å 171.55Å 87.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.30 – 2.50 42.30 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.30-2.50) 99.4 (42.30-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.45Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.271 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6077	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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, FTT, GLA, DAO, KDO, MYR, GOL, GLC, NI, DDQ, DPO, GMH, GCN, PO4

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	1.21	9/5664 (0.2%)	1.28	31/7696 (0.4%)

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	7

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	698	GLU	CG-CD	9.99	1.67	1.51
1	A	66	VAL	CB-CG2	-9.46	1.32	1.52
1	A	277	ARG	CZ-NH1	6.67	1.41	1.33
1	A	397	VAL	CA-CB	6.63	1.68	1.54
1	A	275	TYR	CE2-CZ	-6.09	1.30	1.38

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	648	ARG	NE-CZ-NH1	-11.18	114.71	120.30
1	A	352	LEU	CA-CB-CG	9.23	136.52	115.30
1	A	125	MET	CG-SD-CE	-9.06	85.71	100.20
1	A	577	ARG	NE-CZ-NH1	-8.49	116.05	120.30
1	A	474	ARG	NE-CZ-NH1	8.10	124.35	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	TYR	Sidechain
1	A	213	TYR	Sidechain
1	A	234	TYR	Sidechain
1	A	599	TYR	Sidechain
1	A	72	TYR	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	5524	0	5223	404	0
2	B	110	0	84	3	0
3	A	1	0	0	0	0
4	A	8	0	0	0	0
5	A	56	0	83	18	0
6	A	13	0	23	3	0
7	A	15	0	27	9	0
8	A	42	0	81	5	0
9	A	16	0	0	5	0
10	A	48	0	39	18	0
11	A	244	0	0	40	0
All	All	6077	0	5560	437	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 38.

The worst 5 of 437 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)
10:A:1109:GOL:O1	10:A:1109:GOL:C1	1.64	1.44
10:A:1103:GOL:C1	10:A:1103:GOL:O1	1.65	1.44
10:A:1105:GOL:C1	10:A:1105:GOL:O1	1.66	1.43
10:A:1104:GOL:O1	10:A:1104:GOL:C1	1.65	1.42
10:A:1107:GOL:O1	10:A:1107:GOL:C1	1.65	1.41

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	705/725 (97%)	639 (91%)	54 (8%)	12 (2%)	7 14

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	ALA
1	A	420	ASP
1	A	677	LEU
1	A	679	ARG
1	A	682	MET

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	587/601 (98%)	507 (86%)	80 (14%)	3 6

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	534	VAL
1	A	620	VAL
1	A	543	ARG
1	A	583	ILE
1	A	641	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	430	ASN
1	A	522	ASN
1	A	690	HIS
1	A	619	GLN
1	A	310	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 ⓘ

9 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PA1	B	1	5,2,9	11,11,12	0.90	0	15,15,17	1.83	4 (26%)
2	GCN	B	2	5,2	10,10,11	1.50	3 (30%)	13,13,15	3.57	5 (38%)
2	KDO	B	3	2	15,15,16	1.37	1 (6%)	17,21,24	1.42	2 (11%)
2	GMH	B	4	2	13,13,14	1.42	1 (7%)	16,18,20	1.16	1 (6%)
2	GMH	B	5	2	13,13,14	2.67	7 (53%)	16,18,20	1.56	3 (18%)
2	GLC	B	6	2	11,11,12	0.68	0	15,15,17	1.35	3 (20%)
2	GLC	B	7	2	11,11,12	1.42	2 (18%)	15,15,17	0.95	1 (6%)
2	GLA	B	8	2	11,11,12	0.84	0	15,15,17	0.63	0
2	KDO	B	9	2	15,15,16	1.22	3 (20%)	17,21,24	1.56	5 (29%)

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	PA1	B	1	5,2,9	-	2/2/18/22	0/1/1/1
2	GCN	B	2	5,2	-	0/2/15/18	0/1/1/1
2	KDO	B	3	2	-	0/10/26/30	0/1/1/1
2	GMH	B	4	2	-	0/6/23/26	0/1/1/1
2	GMH	B	5	2	-	0/6/23/26	1/1/1/1
2	GLC	B	6	2	-	2/2/19/22	0/1/1/1
2	GLC	B	7	2	-	2/2/19/22	0/1/1/1
2	GLA	B	8	2	-	0/2/19/22	0/1/1/1
2	KDO	B	9	2	-	2/10/26/30	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	GMH	C2-C3	4.86	1.59	1.52
2	B	5	GMH	O5-C5	3.99	1.48	1.43
2	B	4	GMH	C2-C3	3.91	1.58	1.52
2	B	5	GMH	O4-C4	3.75	1.52	1.43
2	B	5	GMH	C7-C6	3.30	1.60	1.52

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	GCN	C1-O5-C5	8.23	123.21	112.19
2	B	2	GCN	C3-C2-C1	6.87	115.42	109.87
2	B	1	PA1	C4-C3-C2	-4.95	102.52	112.65
2	B	2	GCN	C3-C4-C5	-4.47	105.06	110.76
2	B	3	KDO	C3-C4-C5	-3.99	104.92	110.67

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	9	KDO	C6-C7-C8-O8
2	B	9	KDO	O7-C7-C8-O8
2	B	7	GLC	O5-C5-C6-O6
2	B	1	PA1	C4-C5-C6-O6
2	B	7	GLC	C4-C5-C6-O6

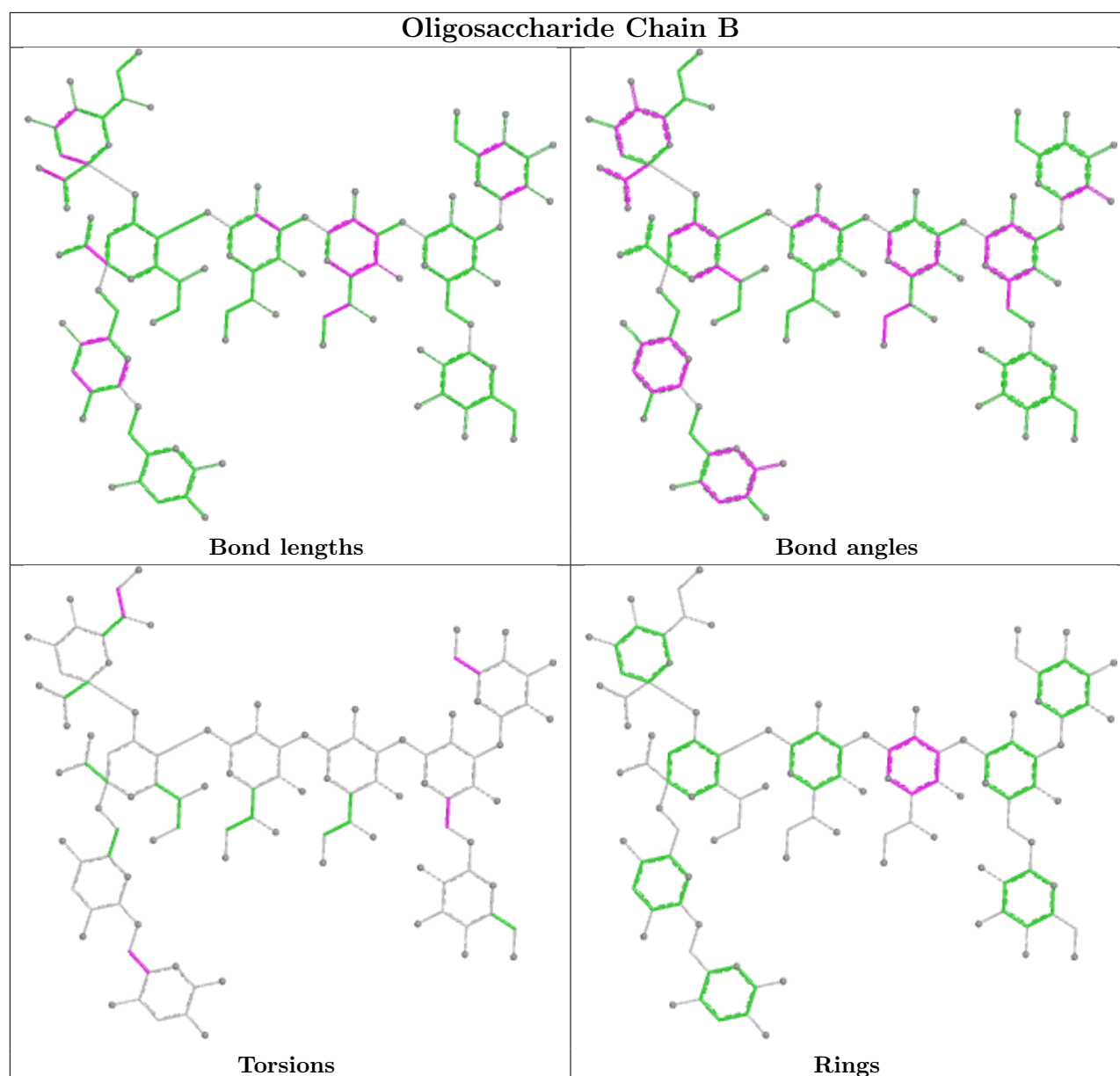
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5	GMH	C1-C2-C3-C4-C5-O5

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	KDO	1	0
2	B	1	PA1	2	0
2	B	4	GMH	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 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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
10	GOL	A	1103	-	5,5,5	4.64	5 (100%)	5,5,5	0.31	0
10	GOL	A	1104	-	5,5,5	4.61	5 (100%)	5,5,5	0.23	0
4	PO4	A	2001	-	0,3,4	-	-	0,3,6	-	-
10	GOL	A	1109	-	5,5,5	4.89	5 (100%)	5,5,5	0.31	0
9	DPO	A	2000	2	3,7,8	1.70	1 (33%)	6,10,13	0.93	0
5	FTT	A	1010	2	6,6,16	1.56	1 (16%)	6,7,17	1.07	1 (16%)
8	DDQ	A	1102	-	11,13,13	1.01	1 (9%)	12,15,15	1.20	1 (8%)
7	MYR	A	1014	5	14,14,15	1.04	1 (7%)	13,13,15	0.79	1 (7%)
8	DDQ	A	1101	-	11,13,13	0.84	0	12,15,15	0.90	0
5	FTT	A	1011	6,2	14,15,16	0.68	0	15,15,17	1.31	3 (20%)
10	GOL	A	1105	-	5,5,5	4.43	3 (60%)	5,5,5	0.58	0
10	GOL	A	1108	-	5,5,5	4.46	5 (100%)	5,5,5	0.54	0
8	DDQ	A	1100	-	11,13,13	0.99	1 (9%)	12,15,15	0.57	0
5	FTT	A	1013	7,2	16,16,16	1.15	2 (12%)	16,17,17	1.94	4 (25%)
9	DPO	A	2004	-	4,7,8	3.70	3 (75%)	5,10,13	2.35	3 (60%)
10	GOL	A	1106	-	5,5,5	4.74	5 (100%)	5,5,5	0.38	0
6	DAO	A	1012	5	12,12,13	1.27	1 (8%)	11,11,13	0.81	0
4	PO4	A	2005	3	0,3,4	-	-	0,3,6	-	-
5	FTT	A	1009	2	14,15,16	0.49	0	15,15,17	1.13	1 (6%)
10	GOL	A	1107	-	5,5,5	4.35	4 (80%)	5,5,5	0.75	0
10	GOL	A	1110	-	5,5,5	4.48	3 (60%)	5,5,5	0.77	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
10	GOL	A	1103	-	-	2/4/4/4	-
10	GOL	A	1104	-	-	3/4/4/4	-
10	GOL	A	1109	-	-	0/4/4/4	-
9	DPO	A	2000	2	-	1/2/5/6	-
5	FTT	A	1010	2	-	2/4/4/15	-
8	DDQ	A	1102	-	-	4/11/11/11	-
7	MYR	A	1014	5	-	5/12/12/13	-
8	DDQ	A	1101	-	-	0/11/11/11	-
5	FTT	A	1011	6,2	-	1/14/14/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	A	1105	-	-	2/4/4/4	-
10	GOL	A	1108	-	-	4/4/4/4	-
8	DDQ	A	1100	-	-	4/11/11/11	-
5	FTT	A	1013	7,2	-	4/15/15/15	-
9	DPO	A	2004	-	-	0/2/5/6	-
10	GOL	A	1106	-	-	2/4/4/4	-
6	DAO	A	1012	5	-	2/10/10/11	-
5	FTT	A	1009	2	-	3/14/14/15	-
10	GOL	A	1107	-	-	4/4/4/4	-
10	GOL	A	1110	-	-	2/4/4/4	-

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1106	GOL	C3-C2	-7.88	1.21	1.51
10	A	1109	GOL	C3-C2	-7.58	1.22	1.51
10	A	1104	GOL	C3-C2	-7.34	1.23	1.51
10	A	1103	GOL	C3-C2	-7.26	1.24	1.51
10	A	1105	GOL	C3-C2	-6.96	1.25	1.51

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1013	FTT	O3-C3-C4	5.10	122.95	109.35
5	A	1013	FTT	C5-C4-C3	3.87	125.36	114.68
9	A	2004	DPO	O6-P2-O4	3.82	117.40	104.64
8	A	1102	DDQ	CM2-N1-C1	3.20	116.97	110.23
5	A	1011	FTT	O2-C1-C2	-3.09	116.37	125.38

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1009	FTT	C1-C2-C3-O3
5	A	1010	FTT	C1-C2-C3-C4
5	A	1010	FTT	C1-C2-C3-O3
5	A	1013	FTT	C1-C2-C3-C4
5	A	1013	FTT	C1-C2-C3-O3

There are no ring outliers.

15 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1103	GOL	2	0
10	A	1104	GOL	2	0
10	A	1109	GOL	2	0
9	A	2000	DPO	4	0
7	A	1014	MYR	9	0
5	A	1011	FTT	1	0
10	A	1105	GOL	4	0
10	A	1108	GOL	1	0
8	A	1100	DDQ	5	0
5	A	1013	FTT	11	0
9	A	2004	DPO	1	0
6	A	1012	DAO	3	0
5	A	1009	FTT	6	0
10	A	1107	GOL	4	0
10	A	1110	GOL	3	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	707/725 (97%)	0.15	6 (0%) 82 79	34, 63, 94, 119	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	GLN	3.9
1	A	99	GLY	3.2
1	A	568	PHE	3.1
1	A	98	GLU	2.6
1	A	725	PHE	2.2

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.

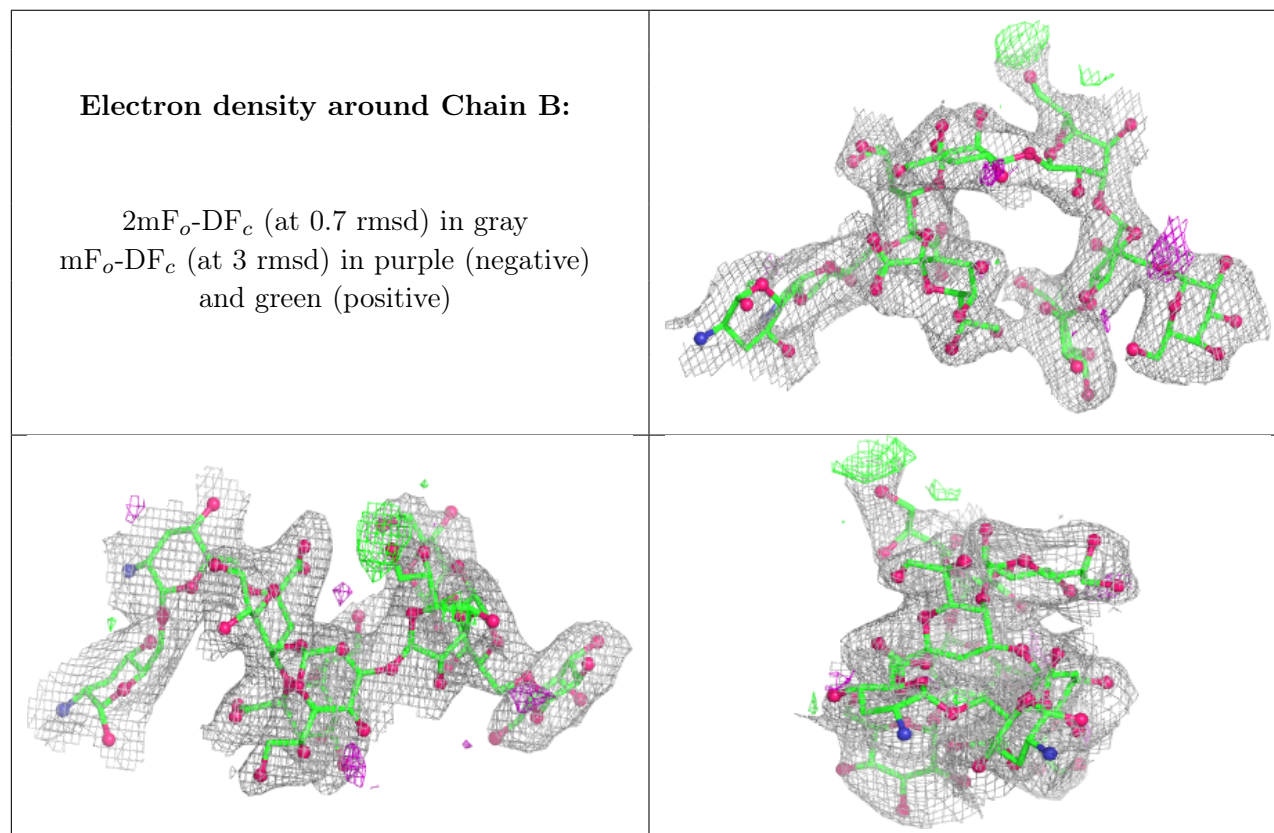
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	B	7	11/12	0.67	0.13	93,104,107,109	0
2	GLA	B	8	11/12	0.80	0.10	92,97,102,103	0
2	GMH	B	5	13/14	0.84	0.14	51,70,96,97	0
2	KDO	B	9	15/16	0.89	0.10	64,73,81,83	0
2	GLC	B	6	11/12	0.90	0.12	76,86,96,98	0
2	KDO	B	3	15/16	0.95	0.08	49,58,64,71	0
2	PA1	B	1	11/12	0.95	0.07	48,57,65,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GMH	B	4	13/14	0.96	0.08	52,56,68,75	0
2	GCN	B	2	10/11	0.97	0.06	35,45,53,54	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
8	DDQ	A	1102	14/14	0.75	0.23	53,86,138,138	0
4	PO4	A	2005	4/5	0.76	0.14	68,69,83,88	0
10	GOL	A	1105	6/6	0.79	0.15	91,100,103,104	0
10	GOL	A	1110	6/6	0.79	0.35	74,100,107,111	0
8	DDQ	A	1101	14/14	0.82	0.20	62,82,104,108	0
5	FTT	A	1010	7/17	0.84	0.15	67,78,91,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	FTT	A	1009	16/17	0.86	0.13	61,67,82,88	0
8	DDQ	A	1100	14/14	0.86	0.19	76,84,94,97	0
5	FTT	A	1013	17/17	0.87	0.15	59,75,84,85	0
7	MYR	A	1014	15/16	0.88	0.15	70,75,81,82	0
10	GOL	A	1107	6/6	0.88	0.24	74,79,82,88	0
10	GOL	A	1103	6/6	0.88	0.13	81,83,83,83	0
10	GOL	A	1106	6/6	0.90	0.16	86,100,102,104	0
6	DAO	A	1012	13/14	0.92	0.10	57,60,69,75	0
10	GOL	A	1104	6/6	0.92	0.11	78,81,86,97	0
10	GOL	A	1108	6/6	0.92	0.17	46,77,91,99	0
10	GOL	A	1109	6/6	0.92	0.25	88,94,95,98	0
9	DPO	A	2004	8/9	0.92	0.09	64,82,91,92	0
9	DPO	A	2000	8/9	0.94	0.09	56,69,75,82	4
5	FTT	A	1011	16/17	0.95	0.08	41,55,60,62	0
3	NI	A	1030	1/1	0.96	0.05	95,95,95,95	0
4	PO4	A	2001	4/5	0.97	0.09	54,68,68,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.