



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 13, 2024 – 08:33 AM EDT

PDB ID : 1MPO
Title : MALTOPORIN MALTOHEXAOSE COMPLEX
Authors : Dutzler, R.; Schirmer, T.
Deposited on : 1996-01-11
Resolution : 2.80 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

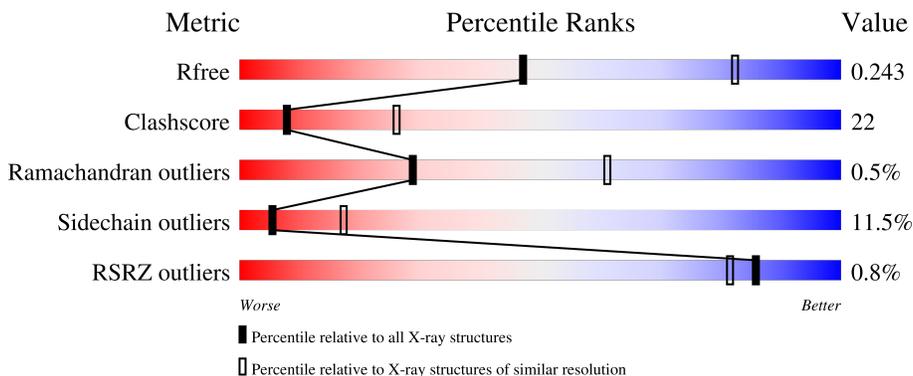
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	421	
1	B	421	
1	C	421	
2	D	5	
2	E	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	5	

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	GLC	D	1	-	-	X	-
2	GLC	E	1	-	-	X	-
2	GLC	E	5	-	-	-	X
2	GLC	F	1	-	-	X	-
2	GLC	F	5	-	-	-	X
3	MG	A	422	-	-	X	-
3	MG	B	422	-	-	X	-
3	MG	C	422	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10536 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 MALTOPORIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	421	3350	2110	571	655	14	101	0	0
1	B	421	3350	2110	571	655	14	101	0	0
1	C	421	3350	2110	571	655	14	101	0	0

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	D	5	56	30	26	0	0	0
2	E	5	56	30	26	0	0	0
2	F	5	56	30	26	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

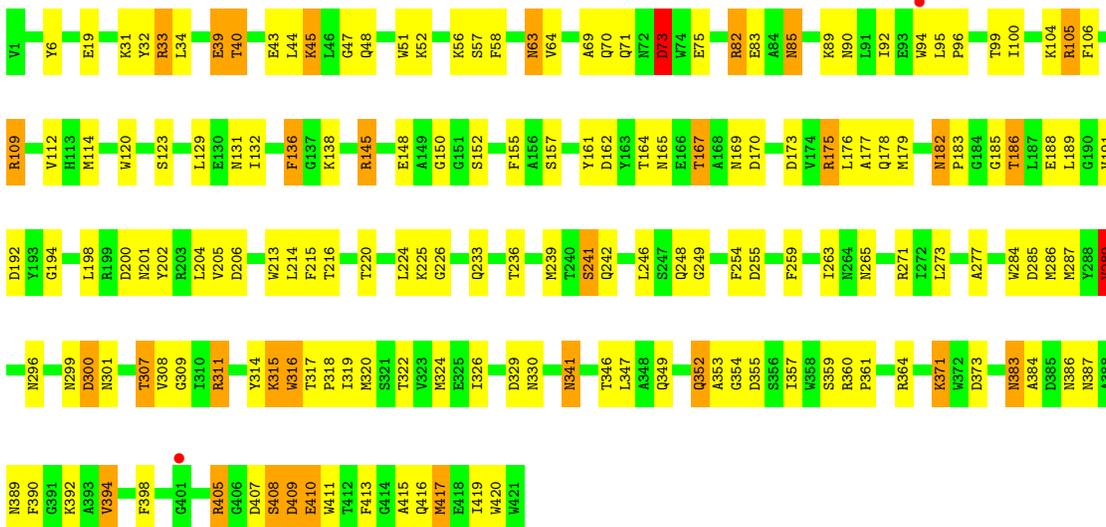
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total 106	O 106	0	0
4	B	106	Total 106	O 106	0	0
4	C	103	Total 103	O 103	0	0



- Molecule 1: MALTOPORIN

Chain C: 60% 32% 7%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D: 20% 60% 20%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E: 20% 60% 20%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F: 20% 60% 20%



4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	129.80Å 211.70Å 218.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 20.48 – 2.82	Depositor EDS
% Data completeness (in resolution range)	94.6 (8.00-2.80) 93.5 (20.48-2.82)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.43 (at 2.84Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.230 , 0.251 0.224 , 0.243	Depositor DCC
R_{free} test set	3384 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtrriage
Anisotropy	0.306	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 122.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.008 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.015 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10536	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: GLC, MG

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	0.95	3/3443 (0.1%)	1.05	9/4668 (0.2%)
1	B	0.95	3/3443 (0.1%)	1.05	9/4668 (0.2%)
1	C	0.95	3/3443 (0.1%)	1.05	9/4668 (0.2%)
All	All	0.95	9/10329 (0.1%)	1.05	27/14004 (0.2%)

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	2
1	B	0	2
1	C	0	2
All	All	0	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	316	TRP	CB-CG	-6.88	1.37	1.50
1	C	316	TRP	CB-CG	-6.87	1.37	1.50
1	B	316	TRP	CB-CG	-6.86	1.38	1.50
1	B	284	TRP	CB-CG	-5.98	1.39	1.50
1	C	284	TRP	CB-CG	-5.97	1.39	1.50

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	VAL	CB-CA-C	-7.55	97.05	111.40
1	C	289	VAL	CB-CA-C	-7.55	97.05	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	289	VAL	CB-CA-C	-7.54	97.08	111.40
1	C	73	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	73	ASP	CB-CG-OD1	5.96	123.66	118.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	32	TYR	Sidechain
1	A	6	TYR	Sidechain
1	B	32	TYR	Sidechain
1	B	6	TYR	Sidechain
1	C	6	TYR	Sidechain

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	3350	0	3070	136	0
1	B	3350	0	3070	135	0
1	C	3350	0	3070	135	0
2	D	56	0	48	10	0
2	E	56	0	48	10	0
2	F	56	0	48	10	0
3	A	1	0	0	2	0
3	B	1	0	0	2	0
3	C	1	0	0	2	0
4	A	106	0	0	6	0
4	B	106	0	0	6	0
4	C	103	0	0	6	0
All	All	10536	0	9354	407	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 22.

The worst 5 of 407 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:383:ASN:HB3	1:A:386:ASN:H	1.27	1.00
1:C:109:ARG:NH2	2:F:1:GLC:H62	1.77	0.99
1:A:109:ARG:NH2	2:D:1:GLC:H62	1.77	0.98
1:B:109:ARG:NH2	2:E:1:GLC:H62	1.77	0.97
1:B:383:ASN:HB3	1:B:386:ASN:H	1.27	0.96

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	419/421 (100%)	393 (94%)	24 (6%)	2 (0%)	29	61
1	B	419/421 (100%)	394 (94%)	23 (6%)	2 (0%)	29	61
1	C	419/421 (100%)	393 (94%)	24 (6%)	2 (0%)	29	61
All	All	1257/1263 (100%)	1180 (94%)	71 (6%)	6 (0%)	29	61

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	GLU
1	B	410	GLU
1	C	410	GLU
1	A	263	ILE
1	B	263	ILE

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	340/340 (100%)	301 (88%)	39 (12%)	5	17
1	B	340/340 (100%)	301 (88%)	39 (12%)	5	17
1	C	340/340 (100%)	301 (88%)	39 (12%)	5	17
All	All	1020/1020 (100%)	903 (88%)	117 (12%)	5	17

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	189	LEU
1	C	352	GLN
1	B	352	GLN
1	C	341	ASN
1	C	241	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	341	ASN
1	C	169	ASN
1	B	349	GLN
1	C	70	GLN
1	C	221	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](#)

15 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	GLC	D	1	2	12,12,12	0.32	0	17,17,17	0.65	0
2	GLC	D	2	2	11,11,12	0.42	0	15,15,17	0.94	1 (6%)
2	GLC	D	3	2	11,11,12	0.57	0	15,15,17	0.73	0
2	GLC	D	4	2	11,11,12	0.53	0	15,15,17	0.71	0
2	GLC	D	5	2	11,11,12	0.38	0	15,15,17	0.64	0
2	GLC	E	1	2	12,12,12	0.32	0	17,17,17	0.65	0
2	GLC	E	2	2	11,11,12	0.41	0	15,15,17	0.94	1 (6%)
2	GLC	E	3	2	11,11,12	0.58	0	15,15,17	0.73	0
2	GLC	E	4	2	11,11,12	0.54	0	15,15,17	0.71	0
2	GLC	E	5	2	11,11,12	0.38	0	15,15,17	0.62	0
2	GLC	F	1	2	12,12,12	0.32	0	17,17,17	0.65	0
2	GLC	F	2	2	11,11,12	0.43	0	15,15,17	0.93	1 (6%)
2	GLC	F	3	2	11,11,12	0.58	0	15,15,17	0.73	0
2	GLC	F	4	2	11,11,12	0.53	0	15,15,17	0.72	0
2	GLC	F	5	2	11,11,12	0.37	0	15,15,17	0.64	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
2	GLC	D	1	2	-	1/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	3	2	-	1/2/19/22	0/1/1/1
2	GLC	D	4	2	-	0/2/19/22	0/1/1/1
2	GLC	D	5	2	-	0/2/19/22	0/1/1/1
2	GLC	E	1	2	-	1/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	E	3	2	-	1/2/19/22	0/1/1/1
2	GLC	E	4	2	-	0/2/19/22	0/1/1/1
2	GLC	E	5	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	1/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	3	2	-	1/2/19/22	0/1/1/1
2	GLC	F	4	2	-	0/2/19/22	0/1/1/1
2	GLC	F	5	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	C1-O5-C5	2.58	115.68	112.19
2	F	2	GLC	C1-O5-C5	2.57	115.67	112.19
2	E	2	GLC	C1-O5-C5	2.54	115.64	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

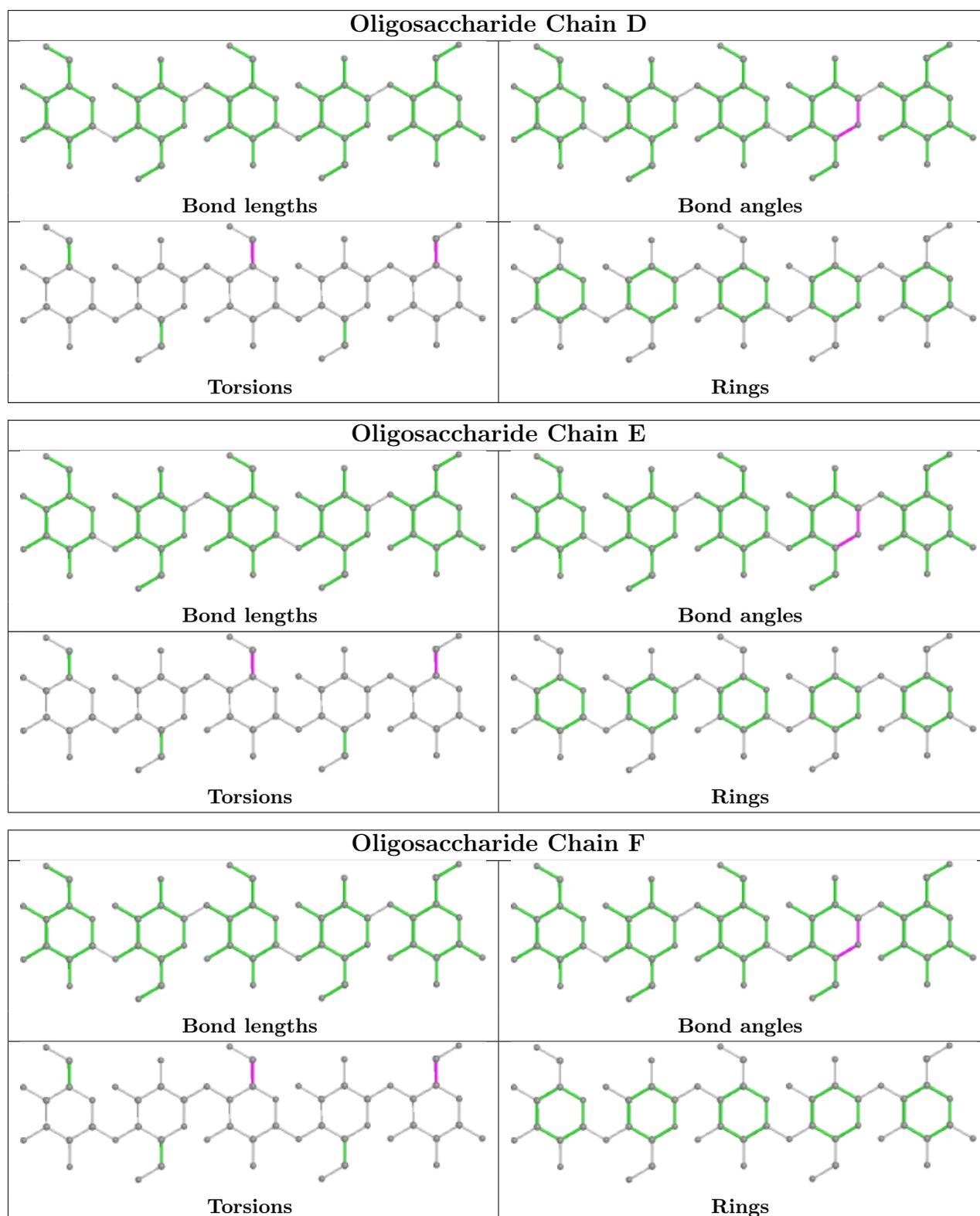
Mol	Chain	Res	Type	Atoms
2	E	3	GLC	O5-C5-C6-O6
2	F	3	GLC	O5-C5-C6-O6
2	D	3	GLC	O5-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	F	1	GLC	C4-C5-C6-O6

There are no ring outliers.

12 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	4	GLC	1	0
2	F	3	GLC	2	0
2	D	4	GLC	1	0
2	F	2	GLC	3	0
2	E	2	GLC	3	0
2	D	3	GLC	2	0
2	E	1	GLC	8	0
2	F	1	GLC	8	0
2	E	3	GLC	2	0
2	D	1	GLC	8	0
2	F	4	GLC	1	0
2	D	2	GLC	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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	421/421 (100%)	-0.53	4 (0%) 82 77	16, 40, 66, 83	35 (8%)
1	B	421/421 (100%)	-0.49	4 (0%) 82 77	16, 40, 66, 83	35 (8%)
1	C	421/421 (100%)	-0.60	2 (0%) 91 88	16, 40, 66, 83	35 (8%)
All	All	1263/1263 (100%)	-0.54	10 (0%) 86 81	16, 40, 66, 83	105 (8%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	94	TRP	3.3
1	A	184	GLY	2.4
1	B	185	GLY	2.2
1	A	155	PHE	2.2
1	A	94	TRP	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.

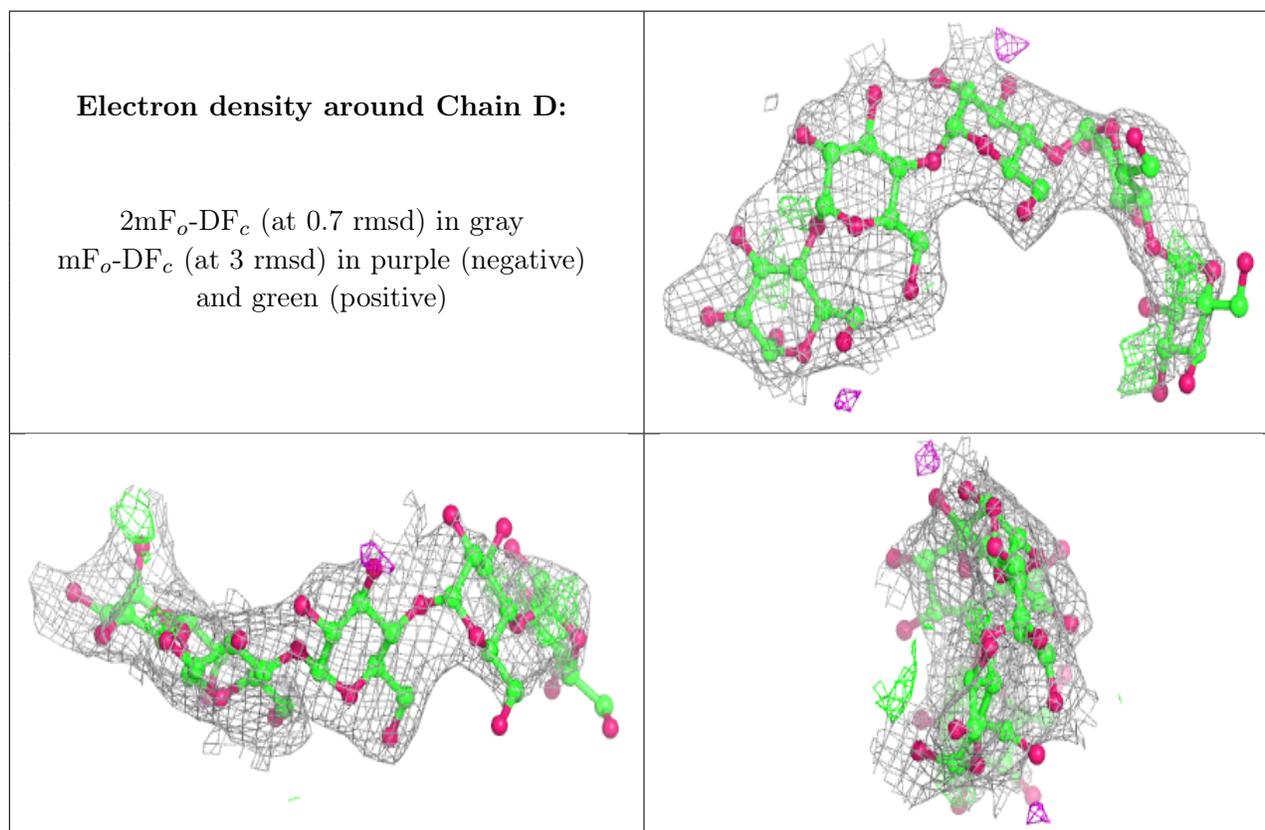
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	F	5	11/12	0.51	0.48	148,148,148,148	11
2	GLC	E	5	11/12	0.57	0.51	148,148,148,148	11
2	GLC	D	5	11/12	0.72	0.40	148,148,148,148	11

Continued on next page...

Continued from previous page...

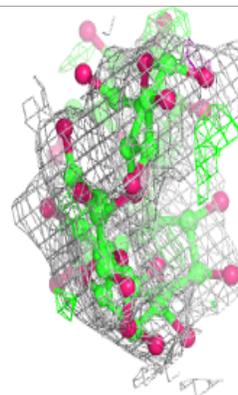
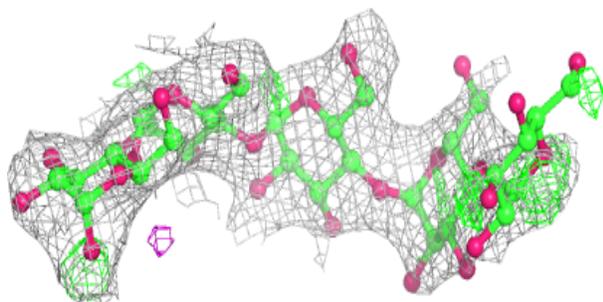
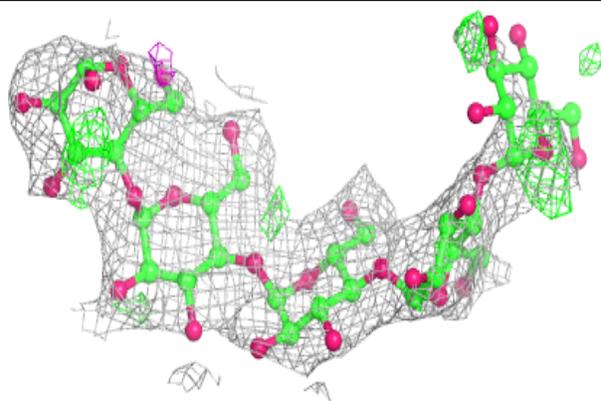
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	F	4	11/12	0.75	0.31	115,115,115,115	11
2	GLC	D	1	12/12	0.79	0.23	106,106,106,106	0
2	GLC	F	1	12/12	0.80	0.26	106,106,106,106	0
2	GLC	E	4	11/12	0.86	0.25	115,115,115,115	11
2	GLC	E	1	12/12	0.90	0.20	106,106,106,106	0
2	GLC	D	4	11/12	0.90	0.20	115,115,115,115	11
2	GLC	F	3	11/12	0.92	0.20	57,57,57,57	0
2	GLC	F	2	11/12	0.94	0.14	50,50,50,50	0
2	GLC	E	2	11/12	0.94	0.19	50,50,50,50	0
2	GLC	E	3	11/12	0.95	0.15	57,57,57,57	0
2	GLC	D	2	11/12	0.96	0.12	50,50,50,50	0
2	GLC	D	3	11/12	0.96	0.13	57,57,57,57	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.

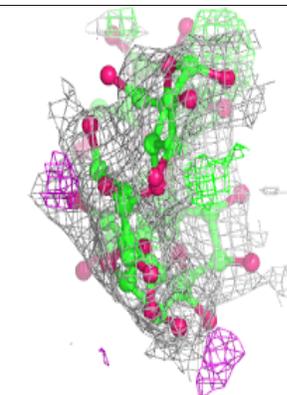
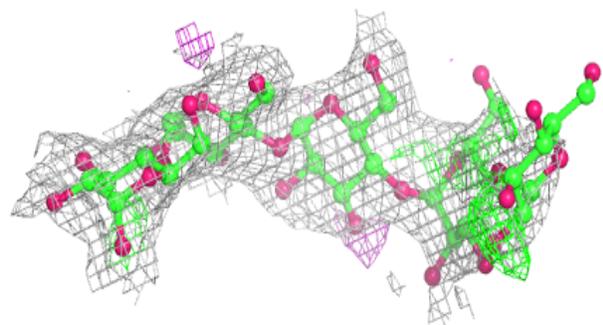
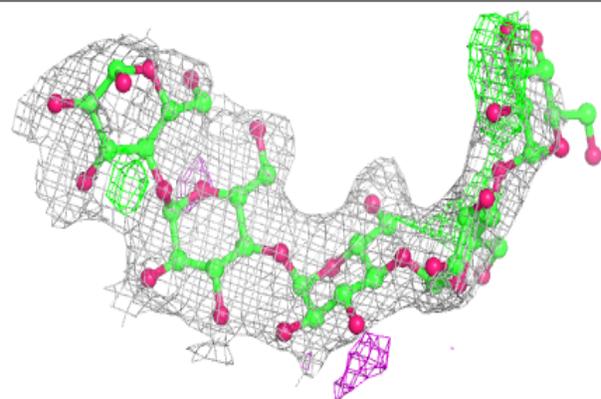


Electron density around Chain E:

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

**Electron density around Chain F:**

$2mF_o-DF_c$ (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
3	MG	A	422	1/1	0.98	0.11	11,11,11,11	1
3	MG	B	422	1/1	0.98	0.11	11,11,11,11	1
3	MG	C	422	1/1	0.99	0.09	11,11,11,11	1

6.5 Other polymers [i](#)

There are no such residues in this entry.