wwPDB X-ray Structure Validation Summary Report (i)

Nov 9, 2024 – 02:31 PM EST

PDB ID	:	1MPO
Title	:	MALTOPORIN MALTOHEXAOSE COMPLEX
Authors	:	Dutzler, R.; Schirmer, T.
Deposited on	:	1996-01-11
Resolution	:	2.80 Å(reported)

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

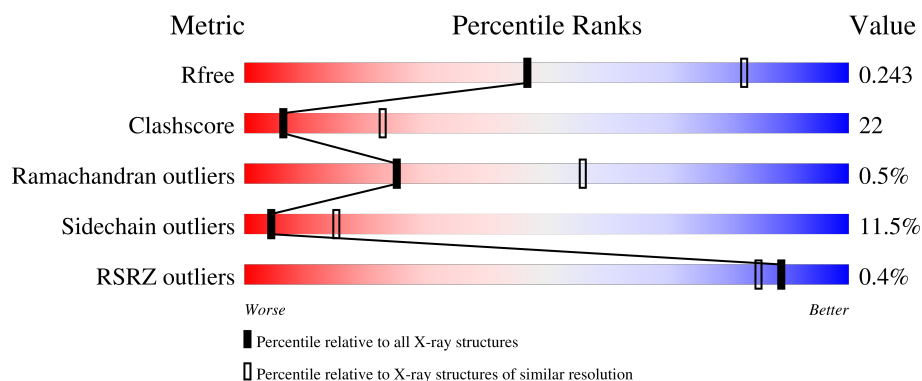|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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.
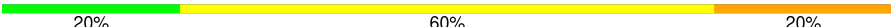
Metric	Percentile Ranks	Value
Rfree		0.243
Clashscore		22
Ramachandran outliers		0.5%
Sidechain outliers		11.5%
RSRZ outliers		0.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (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 <=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	60% 33% 7%
1	B	421	% 59% 33% 7%
1	C	421	60% 32% 7%
2	D	5	20% 60% 20%
2	E	5	20% 60% 20%

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	5	20% 60% 20%

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	F	1	-	-	X	-
3	MG	A	422	-	-	X	-
3	MG	B	422	-	-	X	-
3	MG	C	422	-	-	X	-

2 Entry composition ⓘ

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
1	A	421	Total 3350	C 2110	N 571	O 655	S 14	101	0	0
1	B	421	Total 3350	C 2110	N 571	O 655	S 14	101	0	0
1	C	421	Total 3350	C 2110	N 571	O 655	S 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-(1-4)-alpha-D-glucopyranose.
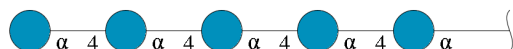
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	5	Total 56	C 30	O 26	0	0	0
2	E	5	Total 56	C 30	O 26	0	0	0
2	F	5	Total 56	C 30	O 26	0	0	0

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

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

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 c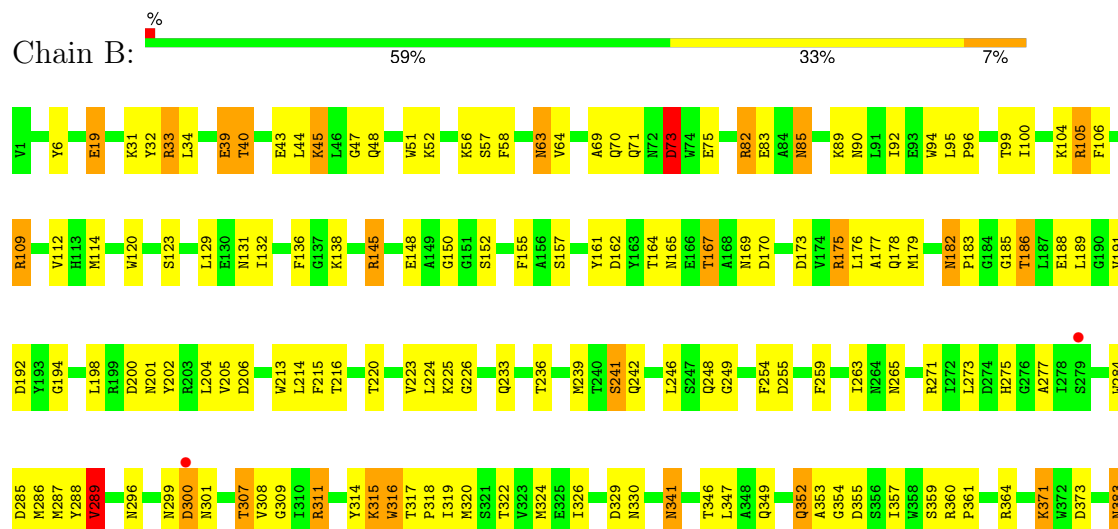olor-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: MALTOPORIN

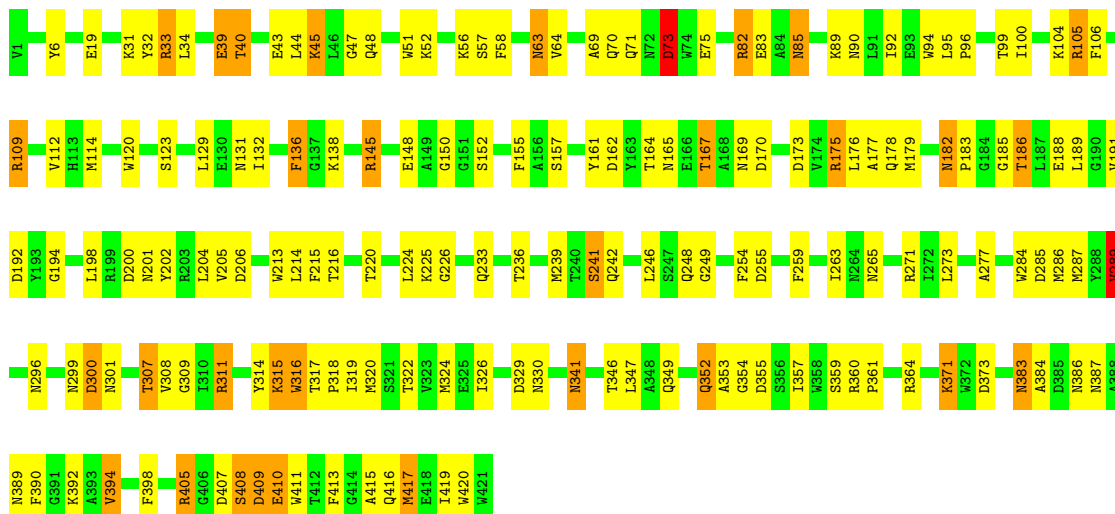Chain A:

- Molecule 1: MALTOPORIN

Chain B:

A384 D385 N386 A388 N389 F390 G391 K392 A393 V394 F398 N399 R405 G406 D407 S408 D409 E410 W411 T412 F413 G414 A415 Q416 M417 E418 I419 W420 W421

● Molecule 1: MALTOPORIN

Chain C:

V1 Y6 E19 K31 Y32 R33 L34 E39 T40 E43 L44 K45 L46 G47 Q48 W51 K52 K56 S57 F58 N63 V64 A69 Q70 Q71 N72 D73 W74 E75 R82 E83 A84 N85 K89 N90 L91 I92 E93 W94 L95 P96 T99 I100 K104 R105 F106

R109 V112 H113 M114 W120 S123 L129 E130 N131 I132 F136 G137 K138 R145 E148 A149 G150 G151 S152 F155 A156 S157 Y161 D162 Y163 T164 N165 E166 T167 A168 N169 D170 D173 V174 R175 L176 A177 Q178 M179 N182 P183 G184 G185 T186 L187 E188 L189 G190 V191

D192 Y193 G194 L198 R199 D200 N201 Y202 R203 L204 V205 D206 W213 L214 F215 T216 T220 L224 K225 G226 Q233 T236 M239 T240 S241 Q242 L246 S247 Q248 G249 F254 D255 F259 I263 N264 N265 R271 I272 L273 A277 W284 D285 M286 M287 Y288 V289

M296 N299 D300 N301 T307 V308 G309 I310 R311 Y314 K315 W316 T317 P318 I319 M320 S321 T322 V323 M324 E325 I326 D329 N330 N341 T346 L347 A348 Q349 Q352 A353 G354 D355 S356 I357 W358 S359 R360 P361 R364 K371 W372 D373 N383 A384 D385 N386 N387 A388

N389 F390 G391 K392 A393 V394 F398 R405 G406 D407 S408 D409 E410 W411 T412 F413 G414 A415 Q416 M417 E418 I419 W420 W421

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

Chain D:

GLC1 GLC2 GLC3 GLC4 GLC5

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

Chain E:

GLC1 GLC2 GLC3 GLC4 GLC5

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

Chain F:

GLC1 GLC2 GLC3 GLC4 GLC5

4 Data and refinement statistics ⓘ

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 8.00 – 2.82	Depositor EDS
% Data completeness (in resolution range)	94.6 (8.00-2.80) 89.8 (8.00-2.82)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.43 (at 2.84Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.230 , 0.251 0.224 , 0.243	Depositor DCC
R_{free} test set	3242 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 119.7	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
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	Xtriage
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

Xtriage'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.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 ⓘ

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 ⓘ

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	419/421 (100%)	393 (94%)	24 (6%)	2 (0%)	25	56
1	B	419/421 (100%)	394 (94%)	23 (6%)	2 (0%)	25	56
1	C	419/421 (100%)	393 (94%)	24 (6%)	2 (0%)	25	56
All	All	1257/1263 (100%)	1180 (94%)	71 (6%)	6 (0%)	25	56

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 ⓘ

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%)		4	15
1	B	340/340 (100%)	301 (88%)	39 (12%)		4	15
1	C	340/340 (100%)	301 (88%)	39 (12%)		4	15
All	All	1020/1020 (100%)	903 (88%)	117 (12%)		4	15

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 ⓘ

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 ⓘ

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	0.41	0	15,15,17	0.92	1 (6%)
2	GLC	D	3	2	11,11,12	0.55	0	15,15,17	0.70	0
2	GLC	D	4	2	11,11,12	0.53	0	15,15,17	0.64	0
2	GLC	D	5	2	11,11,12	0.38	0	15,15,17	0.63	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	0.40	0	15,15,17	0.91	1 (6%)
2	GLC	E	3	2	11,11,12	0.56	0	15,15,17	0.70	0
2	GLC	E	4	2	11,11,12	0.53	0	15,15,17	0.64	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	0.42	0	15,15,17	0.91	1 (6%)
2	GLC	F	3	2	11,11,12	0.56	0	15,15,17	0.70	0
2	GLC	F	4	2	11,11,12	0.53	0	15,15,17	0.65	0
2	GLC	F	5	2	11,11,12	0.37	0	15,15,17	0.63	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(^{o})	Ideal(^{o})
2	D	2	GLC	C1-O5-C5	2.61	115.68	112.19
2	F	2	GLC	C1-O5-C5	2.60	115.67	112.19
2	E	2	GLC	C1-O5-C5	2.57	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	F	2	GLC	3	0
2	F	3	GLC	2	0
2	E	2	GLC	3	0
2	D	2	GLC	3	0
2	E	4	GLC	1	0
2	F	1	GLC	8	0
2	D	1	GLC	8	0
2	D	3	GLC	2	0
2	E	1	GLC	8	0
2	E	3	GLC	2	0
2	F	4	GLC	1	0
2	D	4	GLC	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.

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings
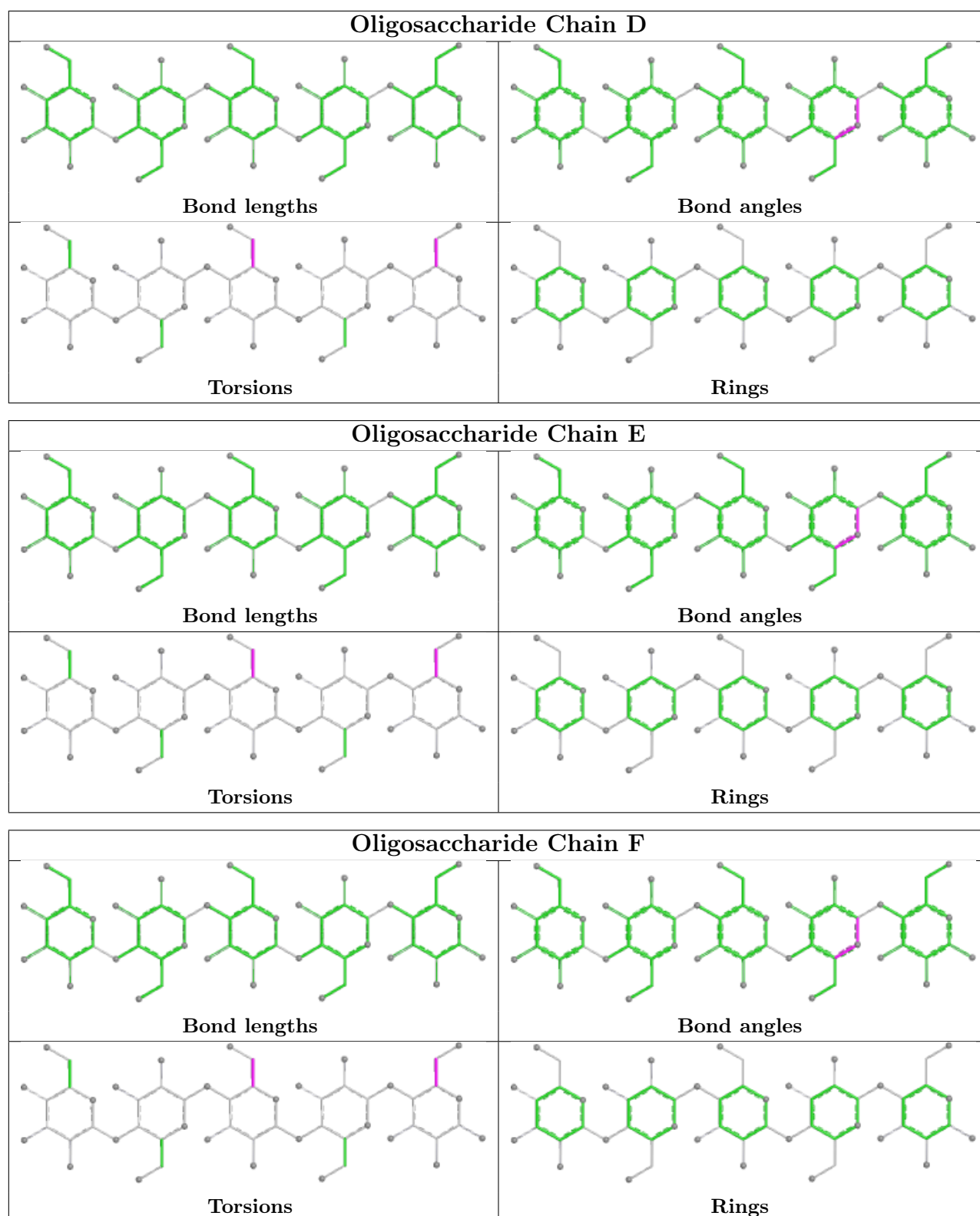
5.6   Ligand geometry   ⓘ

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 ⓘ

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(Å²)	Q<0.9
1	A	421/421 (100%)	-0.54	2 (0%)	87	83	16, 38, 63, 83	35 (8%)
1	B	421/421 (100%)	-0.53	3 (0%)	84	79	16, 38, 63, 83	35 (8%)
1	C	421/421 (100%)	-0.60	0	100	100	16, 38, 63, 83	35 (8%)
All	All	1263/1263 (100%)	-0.56	5 (0%)	89	85	16, 38, 63, 83	105 (8%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	SER	3.3
1	B	300	ASP	3.2
1	A	137	GLY	2.5
1	A	279	SER	2.4
1	B	399	ASN	2.4

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.
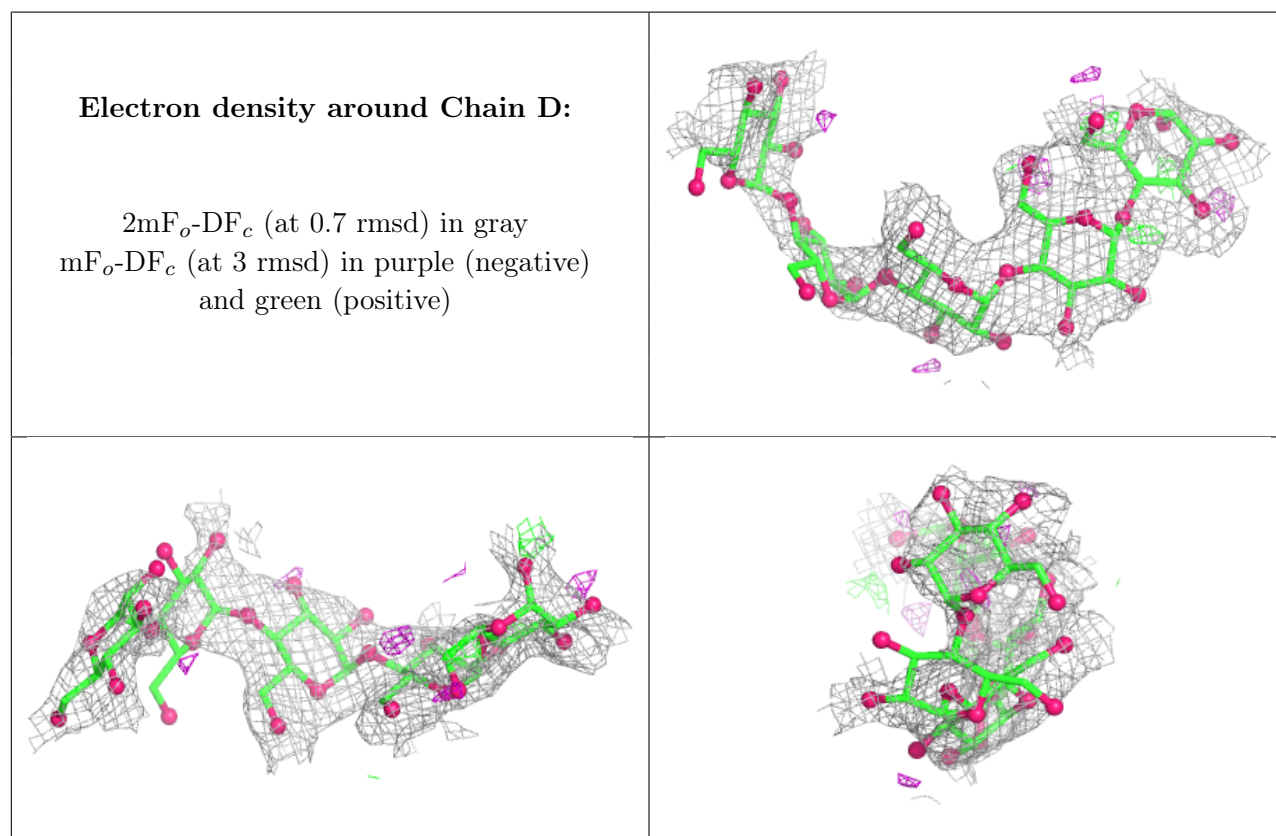
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	GLC	D	5	11/12	0.62	0.20	148,148,148,148	11
2	GLC	E	5	11/12	0.67	0.20	148,148,148,148	11
2	GLC	D	4	11/12	0.69	0.18	115,115,115,115	11

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	F	5	11/12	0.71	0.17	148,148,148,148	11
2	GLC	F	4	11/12	0.74	0.27	115,115,115,115	11
2	GLC	F	1	12/12	0.78	0.20	106,106,106,106	0
2	GLC	D	1	12/12	0.82	0.21	106,106,106,106	0
2	GLC	F	3	11/12	0.84	0.12	57,57,57,57	0
2	GLC	E	4	11/12	0.85	0.17	115,115,115,115	11
2	GLC	E	1	12/12	0.88	0.18	106,106,106,106	0
2	GLC	E	3	11/12	0.92	0.08	57,57,57,57	0
2	GLC	D	3	11/12	0.93	0.09	57,57,57,57	0
2	GLC	D	2	11/12	0.93	0.09	50,50,50,50	0
2	GLC	F	2	11/12	0.93	0.09	50,50,50,50	0
2	GLC	E	2	11/12	0.95	0.11	50,50,50,50	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.
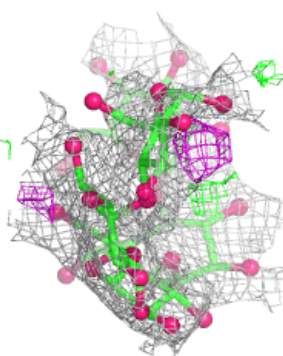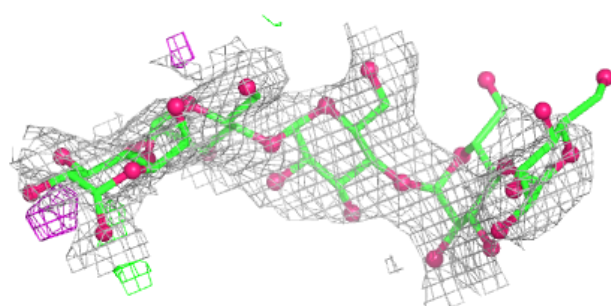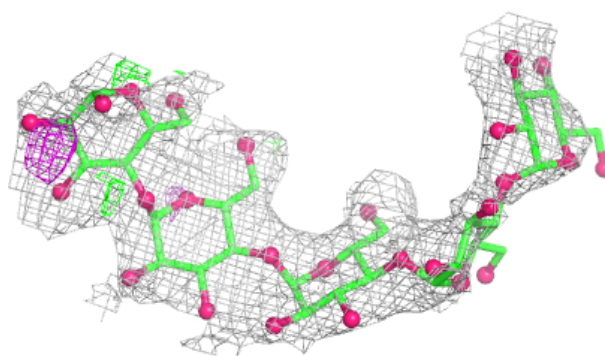

Electron density around Chain D:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
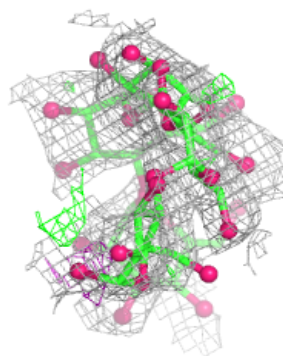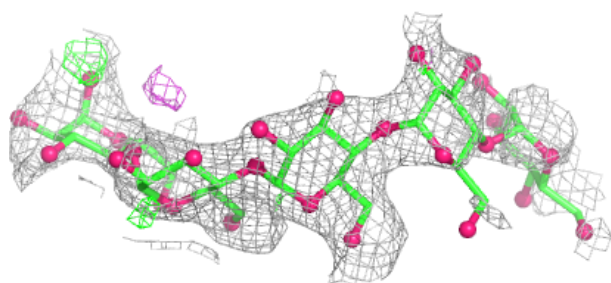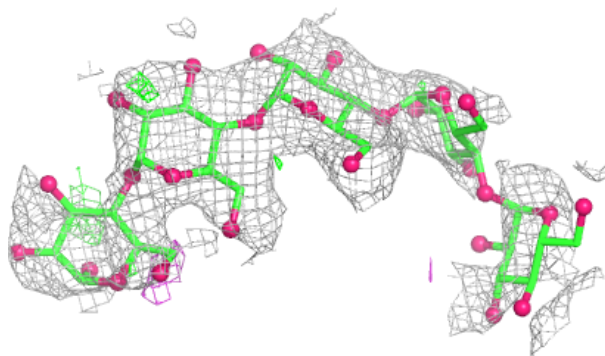
Electron density around Chain F:

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

6.4 Ligands ⓘ

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	0.95	0.08	11,11,11,11	1
3	MG	B	422	1/1	0.98	0.08	11,11,11,11	1
3	MG	C	422	1/1	1.00	0.06	11,11,11,11	1

6.5 Other polymers ⓘ

There are no such residues in this entry.