



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 29, 2022 – 12:11 am GMT

PDB ID : 5NUR
Title : Structural basis for maintenance of bacterial outer membrane lipid asymmetry
Authors : Abellon-Ruiz, J.; Kaptan, S.S.; Basle, A.; Claudi, B.; Bumann, D.;
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Deposited on : 2017-05-01
Resolution : 3.29 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.3
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

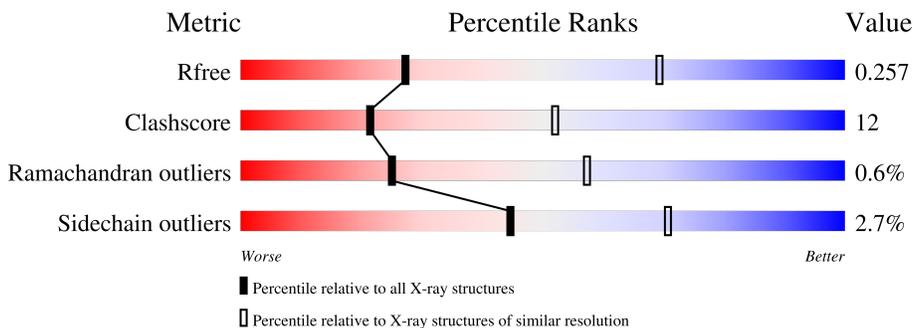
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	340	
1	C	340	
1	E	340	
2	B	236	
2	D	236	
2	F	236	
3	G	4	

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Mol	Chain	Length	Quality of chain
4	H	4	 75% 25%
5	I	3	 67% 33%

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
3	GP1	G	1	X	-	-	-
4	GP1	H	1	X	-	-	-
5	GP1	I	1	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12920 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 Outer membrane protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	340	Total 2627	C 1654	N 438	O 532	S 3	0	0	0
1	A	340	Total 2627	C 1654	N 438	O 532	S 3	0	0	0
1	E	340	Total 2627	C 1654	N 438	O 532	S 3	0	0	0

- Molecule 2 is a protein called ABC transporter permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	199	Total 1597	C 1031	N 271	O 287	S 8	0	0	0
2	B	198	Total 1586	C 1025	N 267	O 286	S 8	0	0	0
2	F	198	Total 1586	C 1025	N 267	O 286	S 8	0	0	0

- Molecule 3 is an oligosaccharide called 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-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	G	4	Total 61	C 28	N 2	O 29	P 2	0	0	0

- Molecule 4 is an oligosaccharide called 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(3-4)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	H	4	Total 61	C 28	N 2	O 29	P 2	0	0	0

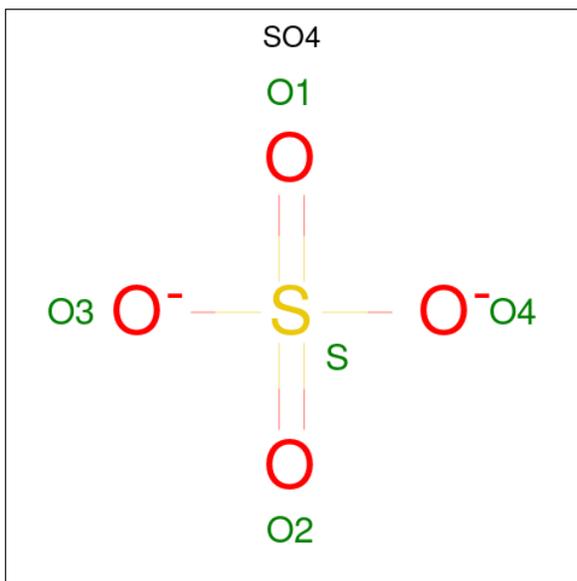
- Molecule 5 is an oligosaccharide called 3-deoxy- α -D-manno-oct-2-ulopyranosonic acid-(3-6)-2-amino-2-deoxy-4-O-phospho-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phospho- α -D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	N	O				P
5	I	3	46	20	2	22	2	0	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	C	1	1	1	0	0
6	A	1	1	1	0	0
6	E	1	1	1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



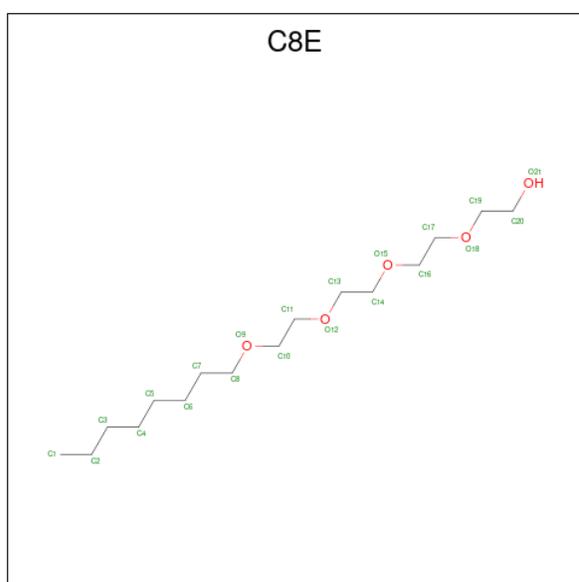
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
7	C	1	5	4	1	0	0
7	C	1	5	4	1	0	0
7	C	1	5	4	1	0	0
7	A	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).

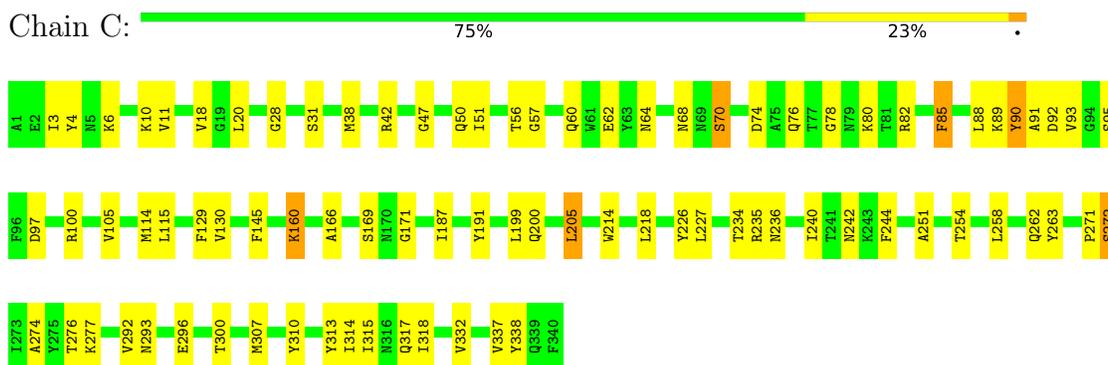


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			17	14	3		
8	A	1	Total	C	O	0	0
			21	16	5		
8	E	1	Total	C	O	0	0
			21	16	5		

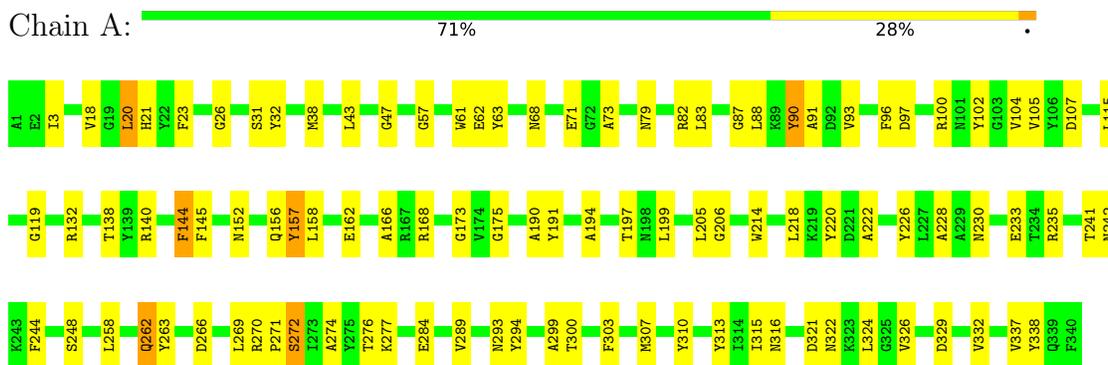
3 Residue-property plots [i](#)

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. 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. 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: Outer membrane protein F



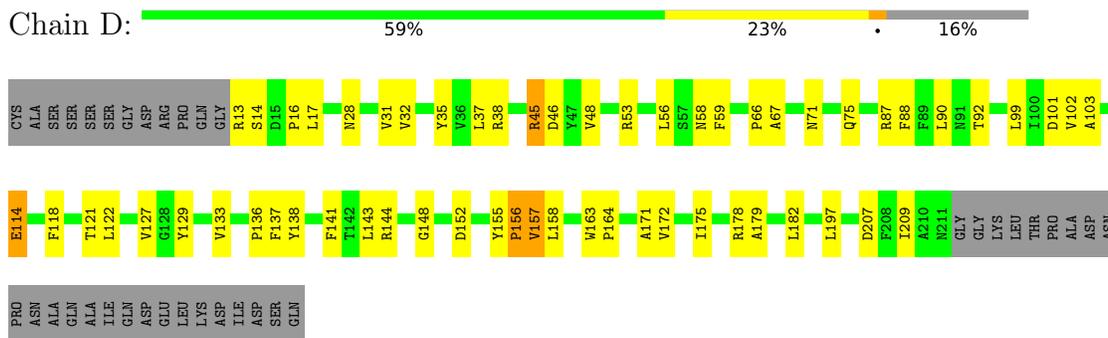
- Molecule 1: Outer membrane protein F



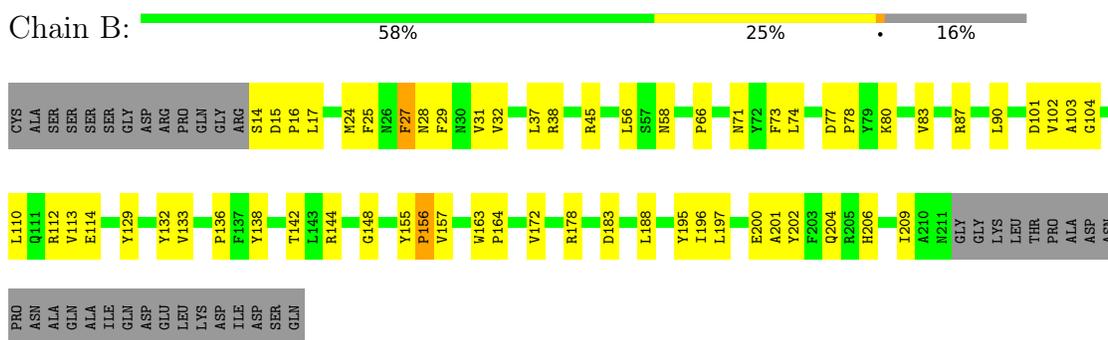
- Molecule 1: Outer membrane protein F



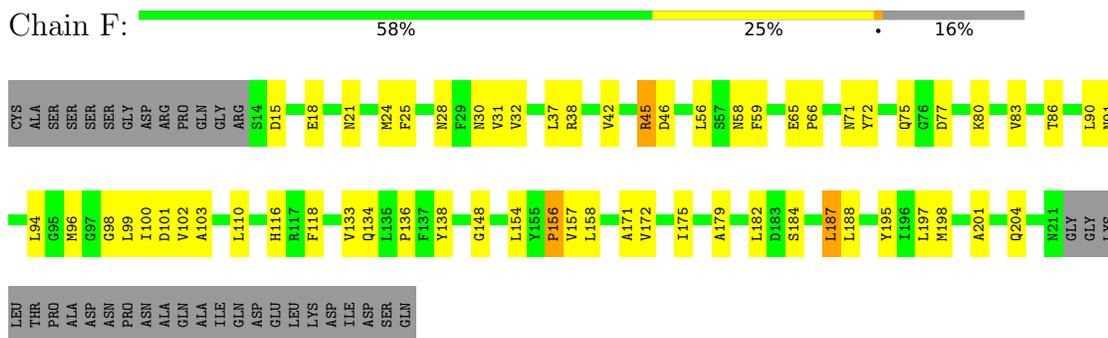
- Molecule 2: ABC transporter permease



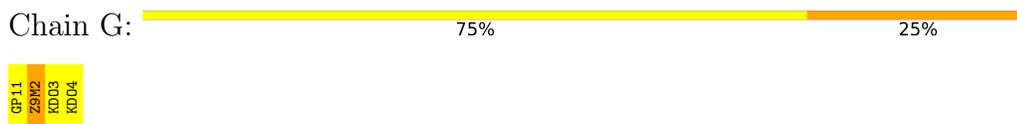
- Molecule 2: ABC transporter permease



- Molecule 2: ABC transporter permease



- Molecule 3: 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-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose



- Molecule 4: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(3-4)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

Chain H:  75% 25%

GP11
Z9M2
KD03
KD04

- Molecule 5: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(3-6)-2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose

Chain I:  67% 33%

GP11
Z9M2
KD03

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	190.55Å 179.66Å 133.39Å 90.00° 116.55° 90.00°	Depositor
Resolution (Å)	47.40 – 3.29 54.27 – 3.29	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.40-3.29) 99.4 (54.27-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.26Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.219 , 0.259 0.220 , 0.257	Depositor DCC
R_{free} test set	2950 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	95.8	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12920	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: GP1, SO4, CA, Z9M, C8E, KDO

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	0.59	0/2683	0.76	1/3628 (0.0%)
1	C	0.54	0/2683	0.74	1/3628 (0.0%)
1	E	0.53	0/2683	0.73	0/3628
2	B	0.46	0/1636	0.68	0/2227
2	D	0.50	0/1647	0.72	0/2241
2	F	0.40	0/1636	0.62	1/2227 (0.0%)
All	All	0.52	0/12968	0.72	3/17579 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	154	LEU	CA-CB-CG	6.30	129.80	115.30
1	C	205	LEU	CB-CG-CD2	-5.24	102.10	111.00
1	A	43	LEU	CB-CG-CD1	-5.14	102.26	111.00

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	2627	0	2444	83	0
1	C	2627	0	2444	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2627	0	2444	57	0
2	B	1586	0	1512	33	0
2	D	1597	0	1525	40	0
2	F	1586	0	1512	41	0
3	G	61	0	27	1	0
4	H	61	0	27	1	0
5	I	46	0	16	2	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
7	A	10	0	0	0	0
7	C	15	0	0	0	0
7	E	15	0	0	2	0
8	A	38	0	61	7	0
8	E	21	0	34	4	0
All	All	12920	0	12046	300	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 12.

The worst 5 of 300 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:289:VAL:HG11	1:A:324:LEU:HD11	1.45	0.97
1:E:262:GLN:HG2	1:E:272:SER:HB2	1.58	0.84
2:F:30:ASN:O	2:F:32:VAL:N	2.10	0.83
2:B:66:PRO:HG2	2:B:157:VAL:HG21	1.60	0.83
1:A:289:VAL:HG21	1:A:324:LEU:HD12	1.62	0.81

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	338/340 (99%)	315 (93%)	22 (6%)	1 (0%)	41 71
1	C	338/340 (99%)	316 (94%)	21 (6%)	1 (0%)	41 71
1	E	338/340 (99%)	317 (94%)	20 (6%)	1 (0%)	41 71
2	B	196/236 (83%)	175 (89%)	19 (10%)	2 (1%)	15 46
2	D	197/236 (84%)	173 (88%)	22 (11%)	2 (1%)	15 46
2	F	196/236 (83%)	175 (89%)	19 (10%)	2 (1%)	15 46
All	All	1603/1728 (93%)	1471 (92%)	123 (8%)	9 (1%)	25 57

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	91	ALA
1	A	91	ALA
1	E	91	ALA
2	F	31	VAL
2	D	156	PRO

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	263/263 (100%)	254 (97%)	9 (3%)	37 65
1	C	263/263 (100%)	257 (98%)	6 (2%)	50 73
1	E	263/263 (100%)	258 (98%)	5 (2%)	57 77
2	B	167/197 (85%)	162 (97%)	5 (3%)	41 68
2	D	168/197 (85%)	164 (98%)	4 (2%)	49 73
2	F	167/197 (85%)	161 (96%)	6 (4%)	35 63
All	All	1291/1380 (94%)	1256 (97%)	35 (3%)	44 71

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	272	SER

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Mol	Chain	Res	Type
2	F	37	LEU
2	F	116	HIS
1	A	100	ARG
1	A	90	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	64	ASN
1	C	66	GLN
2	F	75	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](#)

11 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	GP1	G	1	3	15,16,16	1.83	5 (33%)	23,24,24	3.65	4 (17%)
3	Z9M	G	2	3	15,15,16	2.31	3 (20%)	18,22,24	1.32	2 (11%)
3	KDO	G	3	3	15,15,16	2.35	2 (13%)	19,21,24	1.33	3 (15%)
3	KDO	G	4	6,3	15,15,16	2.18	4 (26%)	19,21,24	1.91	6 (31%)
4	GP1	H	1	4	15,16,16	2.09	5 (33%)	23,24,24	3.31	8 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	Z9M	H	2	4	15,15,16	2.29	4 (26%)	18,22,24	1.03	1 (5%)
4	KDO	H	3	4	15,15,16	2.19	6 (40%)	19,21,24	1.68	3 (15%)
4	KDO	H	4	4,6	15,15,16	2.10	3 (20%)	19,21,24	1.78	3 (15%)
5	GP1	I	1	5	15,16,16	1.96	6 (40%)	23,24,24	3.79	8 (34%)
5	Z9M	I	2	5	15,15,16	2.11	3 (20%)	18,22,24	1.23	2 (11%)
5	KDO	I	3	5,6	15,15,16	2.15	4 (26%)	19,21,24	3.26	7 (36%)

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	GP1	G	1	3	1/1/6/6	1/6/27/27	0/1/1/1
3	Z9M	G	2	3	-	4/7/24/27	0/1/1/1
3	KDO	G	3	3	-	2/10/26/30	0/1/1/1
3	KDO	G	4	6,3	-	8/10/26/30	0/1/1/1
4	GP1	H	1	4	1/1/6/6	3/6/27/27	0/1/1/1
4	Z9M	H	2	4	-	4/7/24/27	0/1/1/1
4	KDO	H	3	4	-	6/10/26/30	0/1/1/1
4	KDO	H	4	4,6	-	5/10/26/30	0/1/1/1
5	GP1	I	1	5	1/1/6/6	4/6/27/27	0/1/1/1
5	Z9M	I	2	5	-	1/7/24/27	0/1/1/1
5	KDO	I	3	5,6	-	4/10/26/30	0/1/1/1

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3	KDO	O6-C2	7.14	1.53	1.43
3	G	4	KDO	O6-C2	6.34	1.52	1.43
4	H	3	KDO	O6-C2	6.28	1.52	1.43
5	I	3	KDO	O6-C2	6.10	1.51	1.43
3	G	2	Z9M	P1-O4	5.83	1.70	1.59

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	GP1	O6-C6-C5	15.78	165.42	111.29
5	I	1	GP1	O6-C6-C5	15.21	163.48	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	GP1	O6-C6-C5	11.35	150.23	111.29
5	I	3	KDO	O6-C6-C5	7.50	118.41	107.87
5	I	3	KDO	O6-C2-C3	6.38	119.24	110.46

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	1	GP1	C3
4	H	1	GP1	C3
5	I	1	GP1	C3

5 of 42 torsion outliers are listed below:

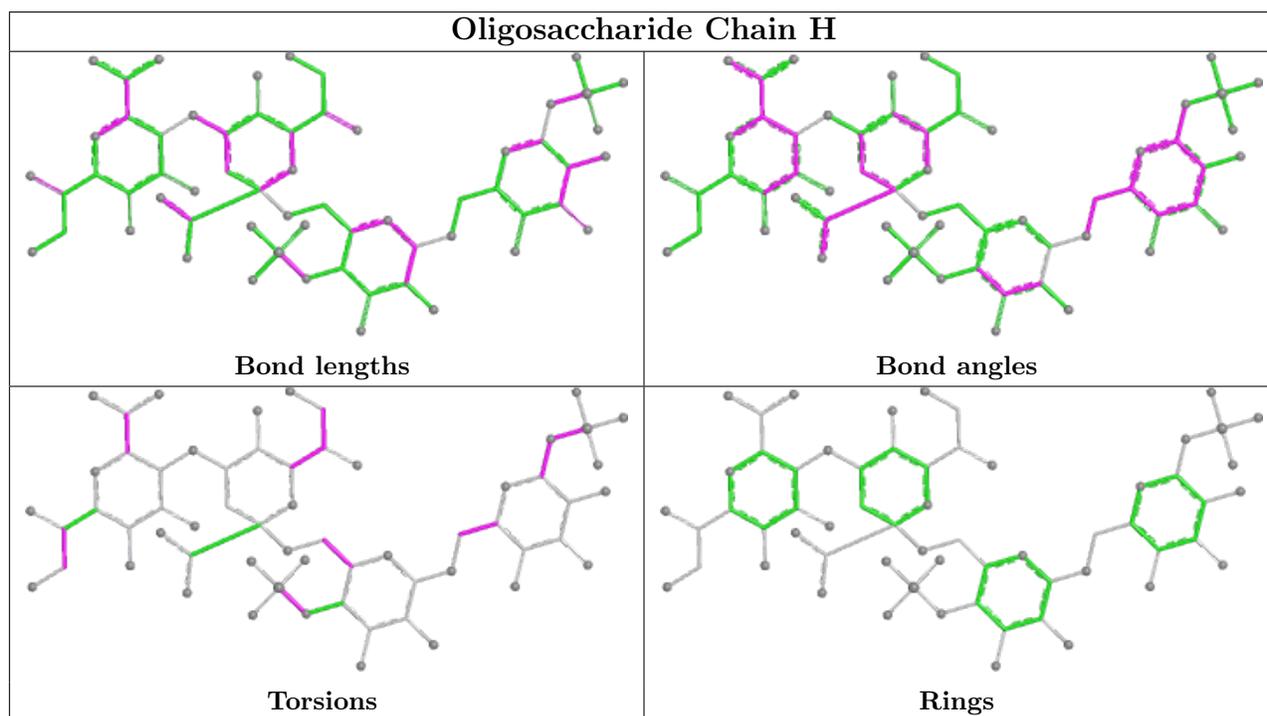
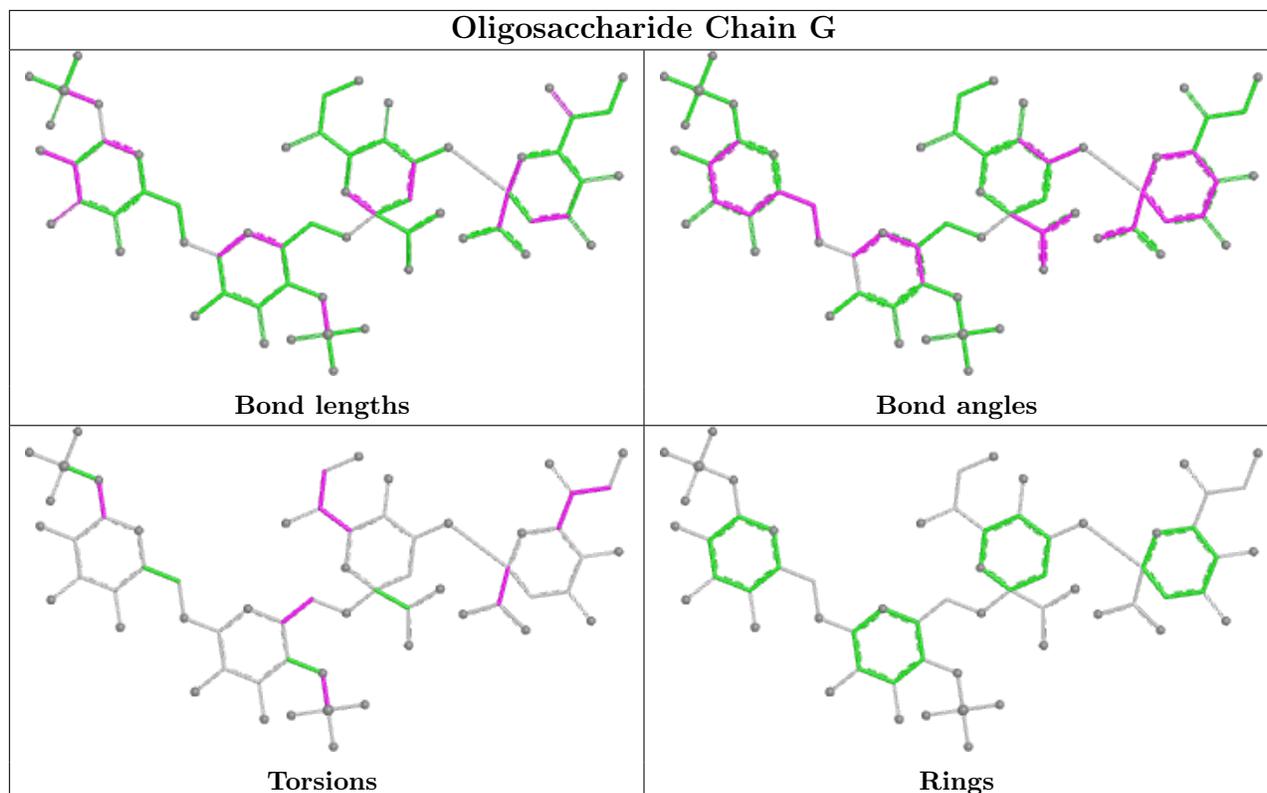
Mol	Chain	Res	Type	Atoms
3	G	3	KDO	O6-C6-C7-O7
3	G	4	KDO	O1A-C1-C2-O6
3	G	4	KDO	C5-C6-C7-O7
3	G	4	KDO	C5-C6-C7-C8
3	G	4	KDO	O6-C6-C7-O7

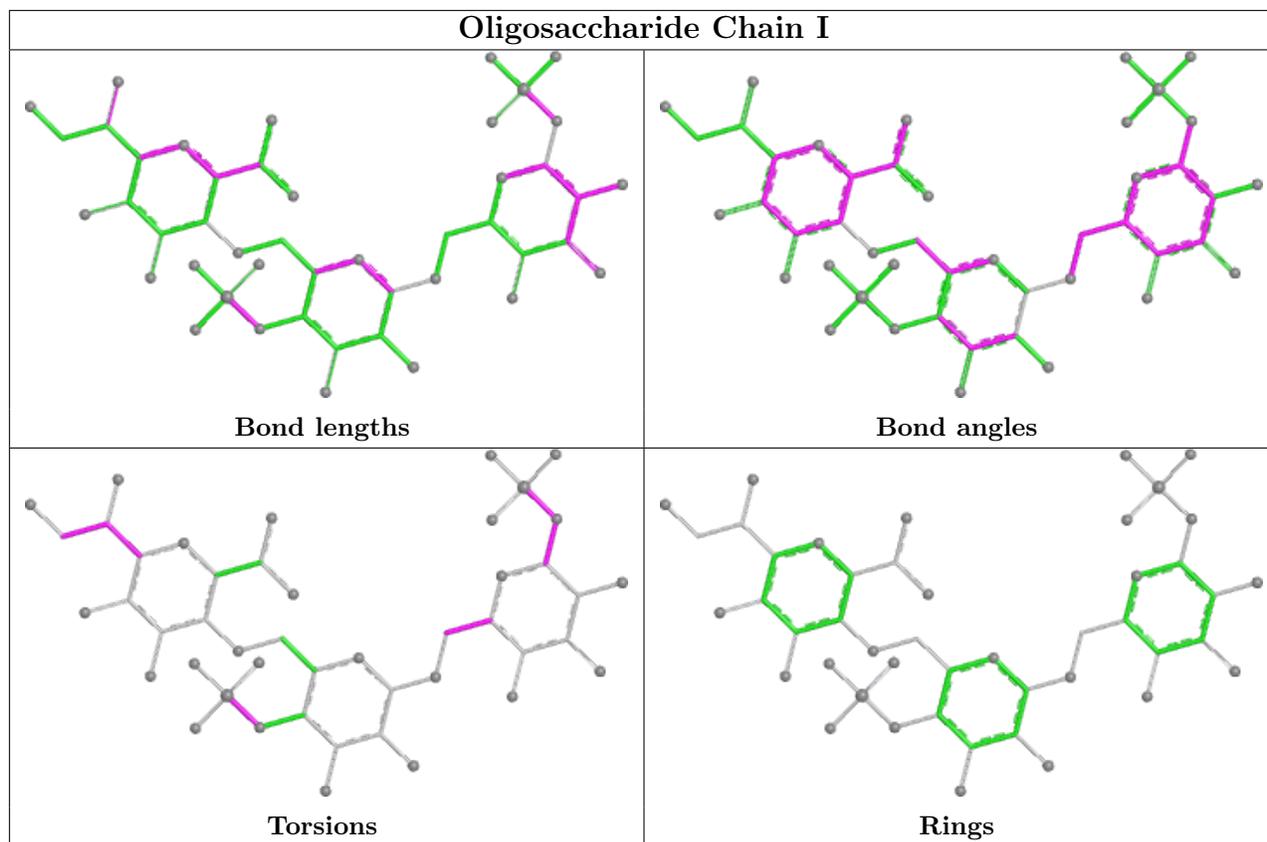
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	Z9M	1	0
4	H	4	KDO	1	0
5	I	2	Z9M	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 oligosaccharide.





5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	$\# Z > 2$
7	SO4	C	404	-	4,4,4	0.18	0	6,6,6	0.74	0
7	SO4	E	405	-	4,4,4	0.08	0	6,6,6	0.30	0
7	SO4	C	402	-	4,4,4	0.16	0	6,6,6	0.29	0
8	C8E	A	402	-	20,20,20	0.48	0	19,19,19	0.58	0
8	C8E	E	401	-	20,20,20	0.47	0	19,19,19	0.41	0
7	SO4	E	403	-	4,4,4	0.15	0	6,6,6	0.20	0
7	SO4	A	405	-	4,4,4	0.22	0	6,6,6	0.71	0
7	SO4	C	403	-	4,4,4	0.16	0	6,6,6	0.29	0
7	SO4	E	404	-	4,4,4	0.21	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	A	404	-	4,4,4	0.15	0	6,6,6	0.23	0
8	C8E	A	401	-	16,16,20	0.66	0	15,15,19	0.84	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
8	C8E	E	401	-	-	11/18/18/18	-
8	C8E	A	402	-	-	12/18/18/18	-
8	C8E	A	401	-	-	10/14/14/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	401	C8E	O9-C10-C11-O12
8	E	401	C8E	O9-C10-C11-O12
8	A	402	C8E	O18-C19-C20-O21
8	A	402	C8E	O9-C10-C11-O12
8	A	402	C8E	C3-C4-C5-C6

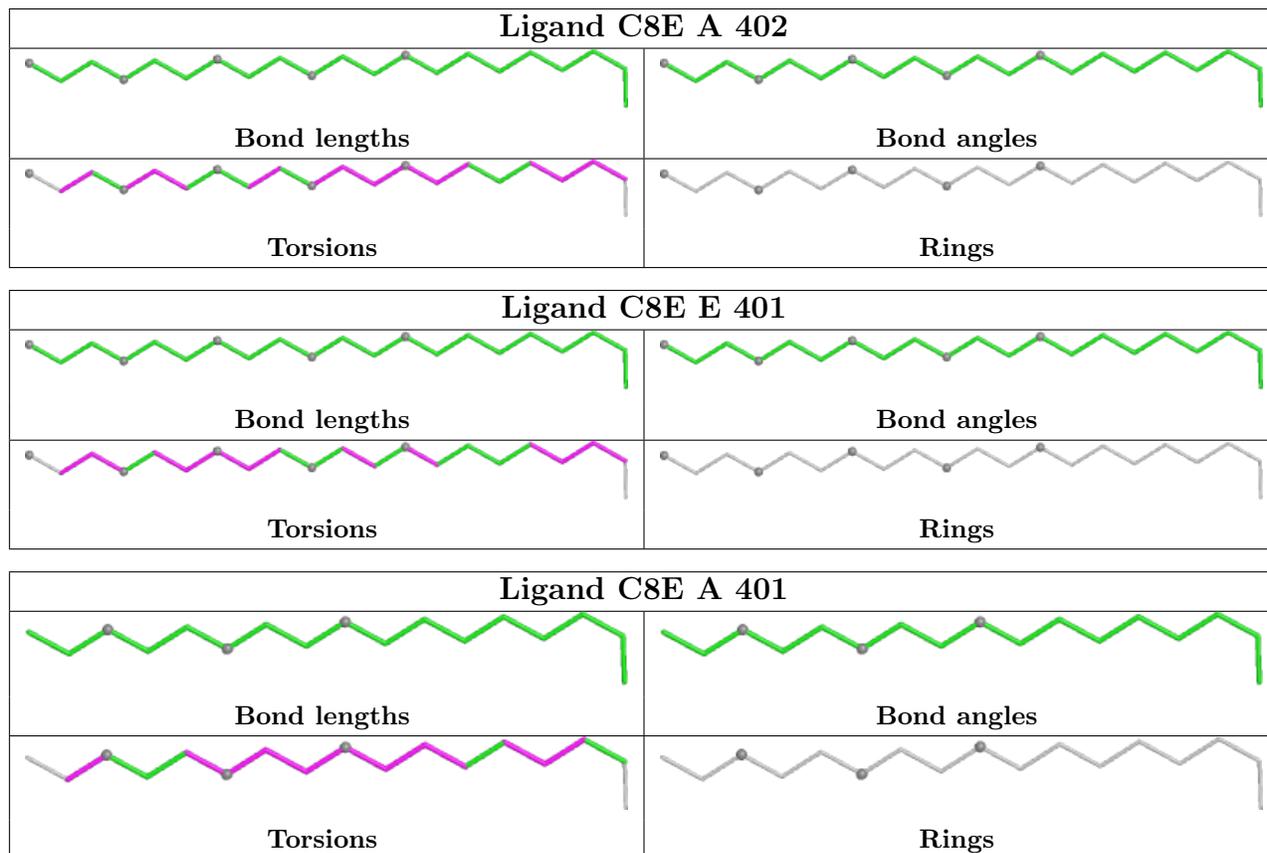
There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	405	SO4	1	0
8	A	402	C8E	6	0
8	E	401	C8E	4	0
7	E	404	SO4	1	0
8	A	401	C8E	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 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](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.

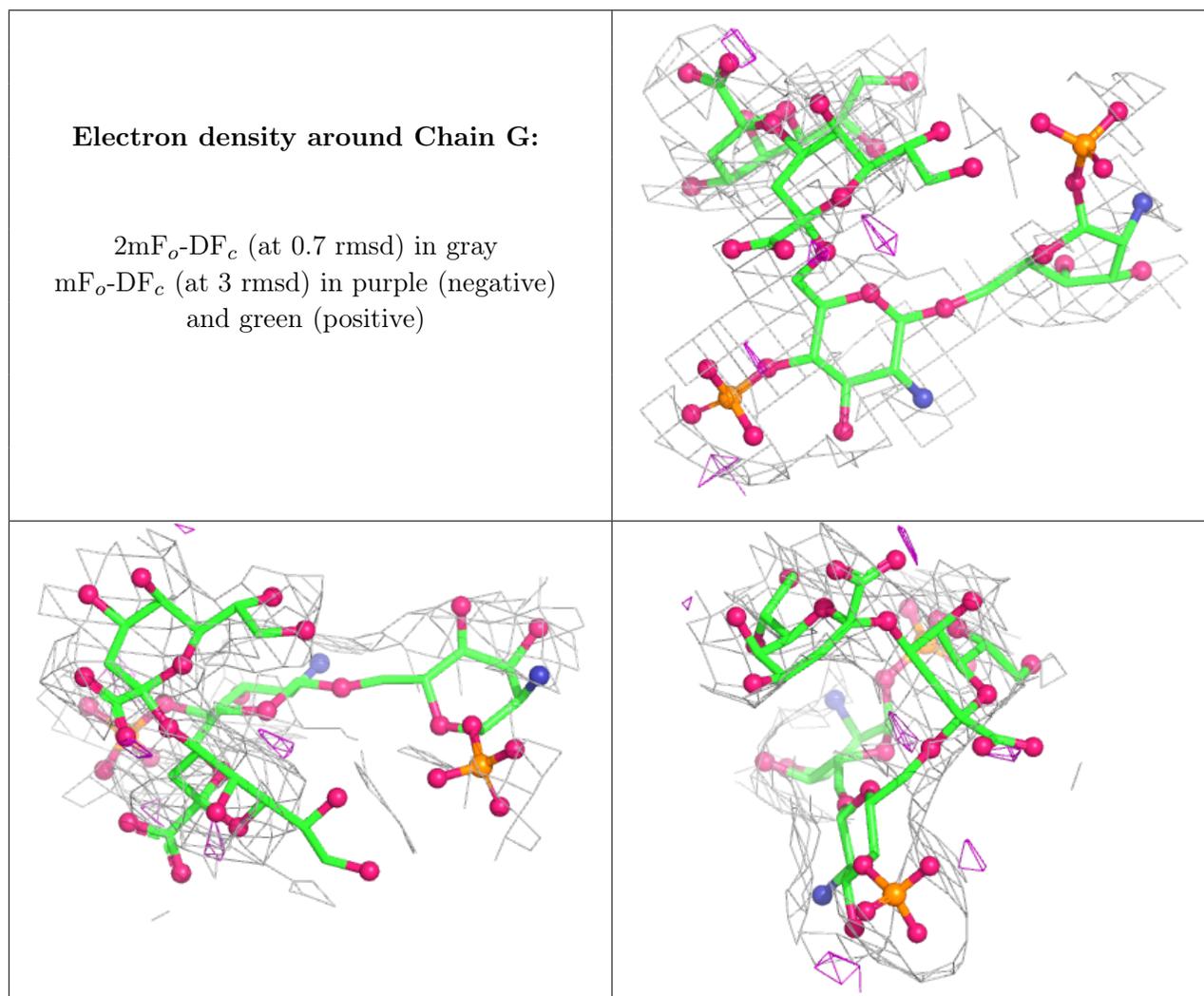
6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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6.3 Carbohydrates [i](#)

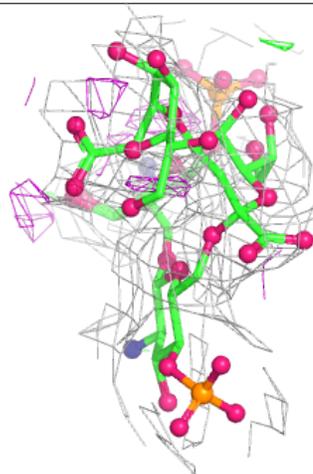
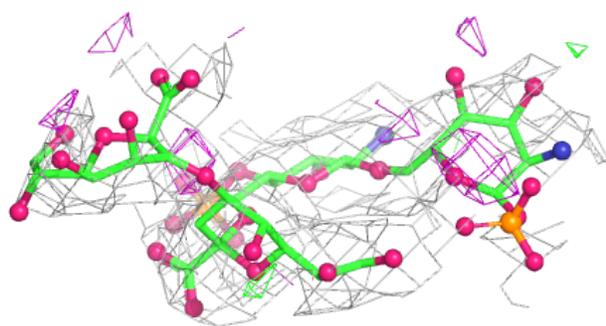
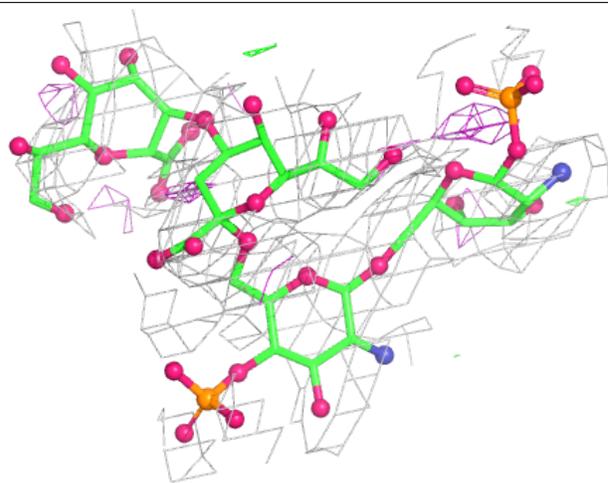
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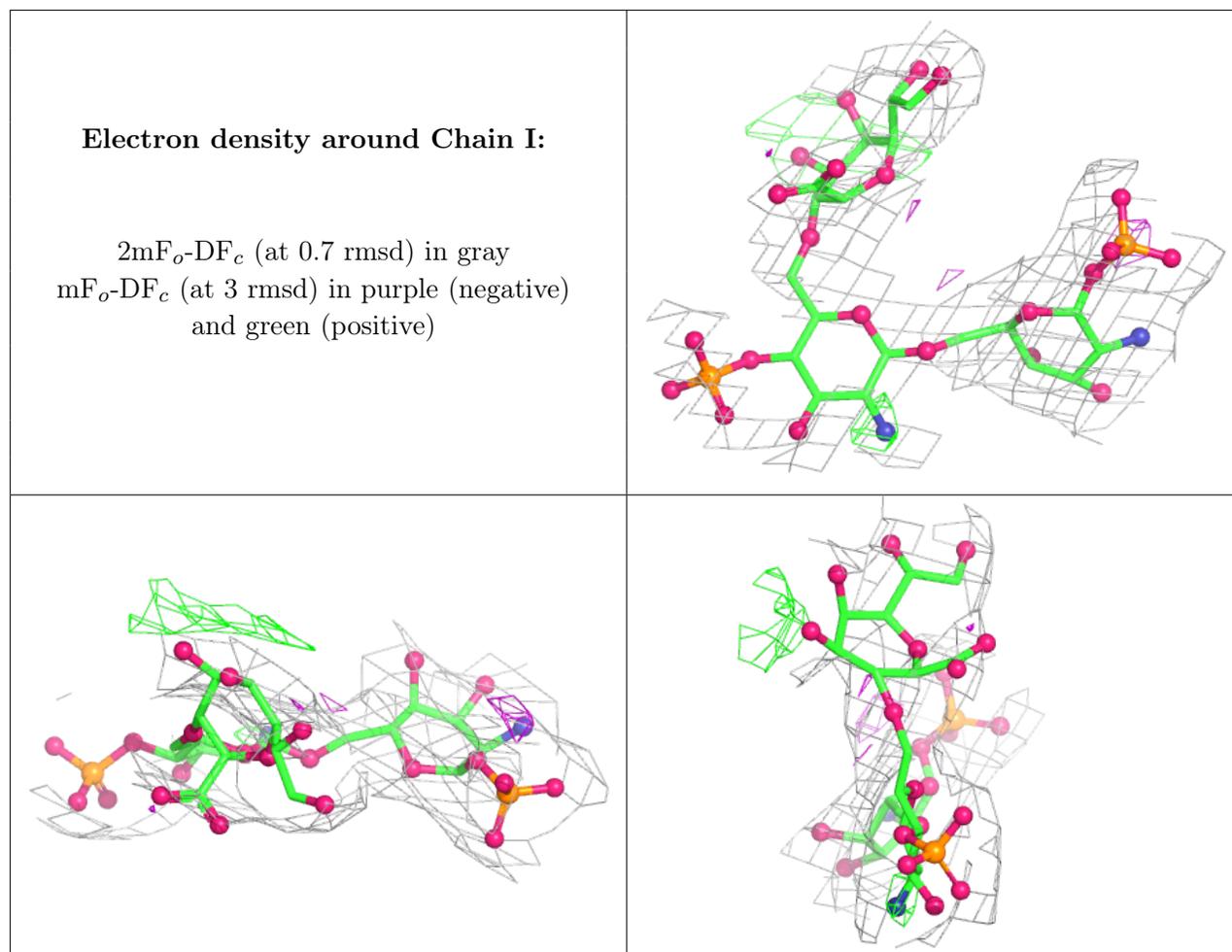
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain H:

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





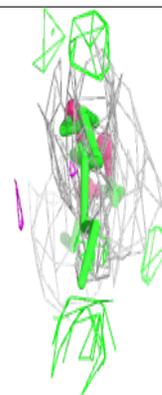
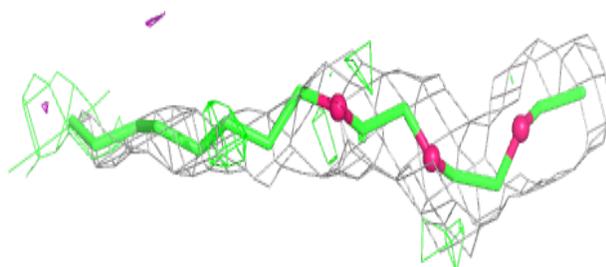
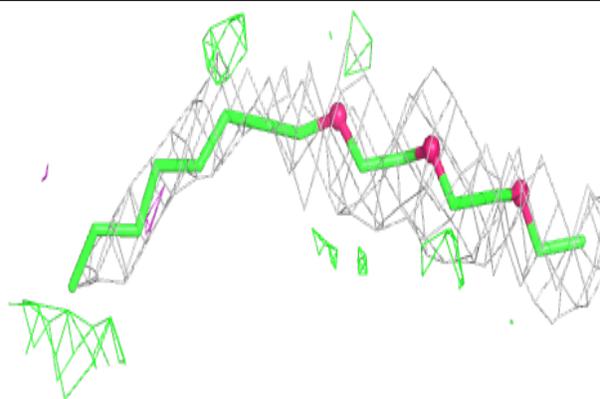
6.4 Ligands [\(i\)](#)

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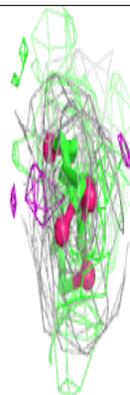
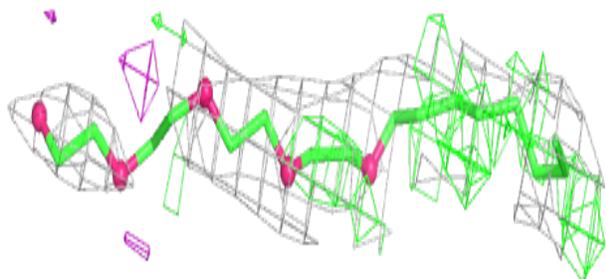
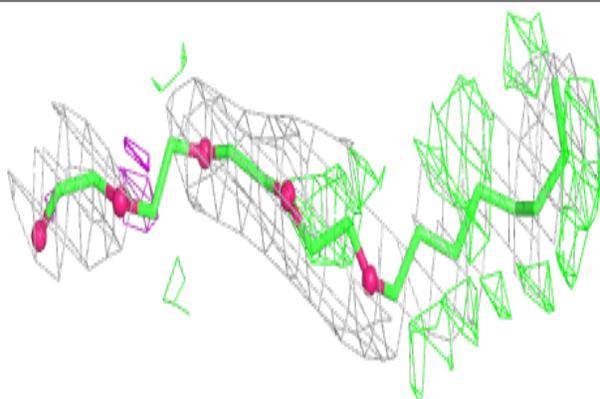
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

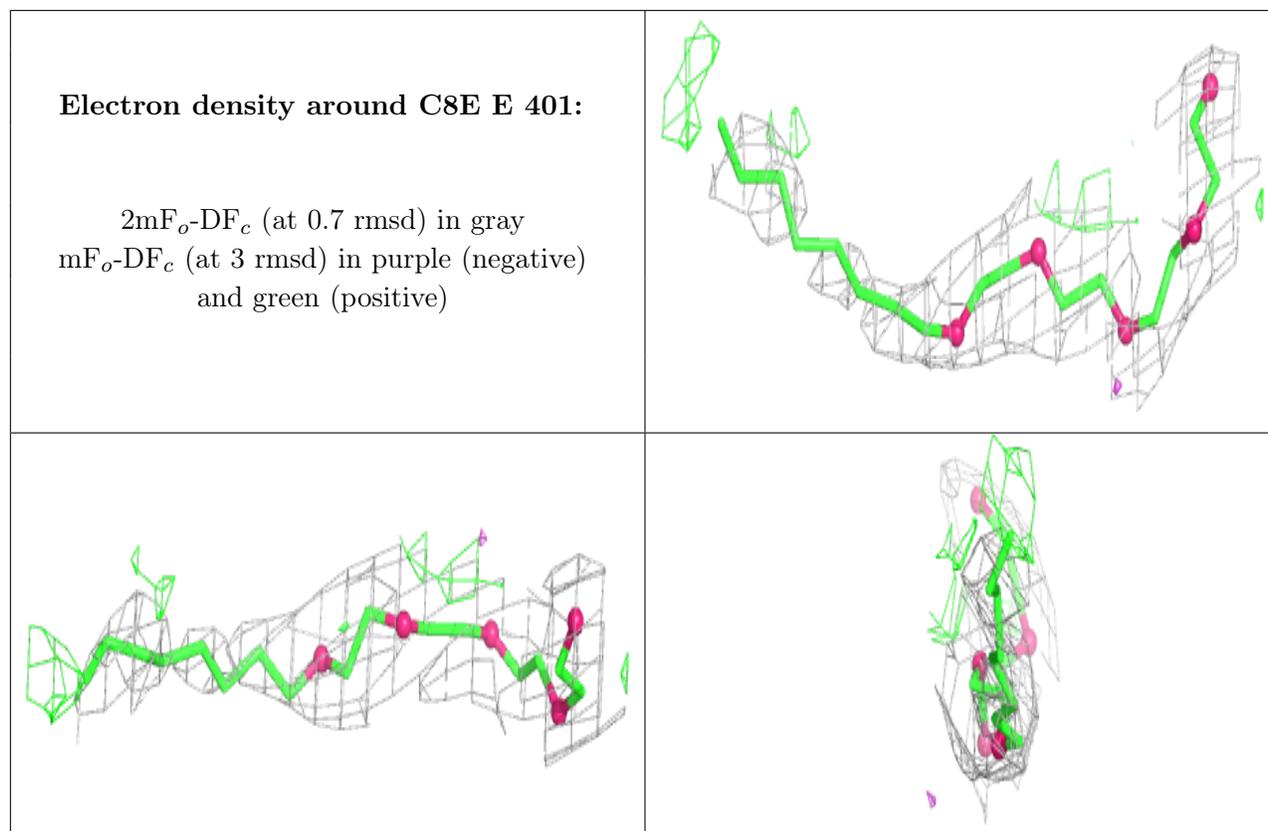
Electron density around C8E A 401:

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

**Electron density around C8E A 402:**

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





6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.