



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2024 – 02:29 pm GMT

PDB ID : 6Q3R
Title : ASPERGILLUS ACULEATUS GALACTANASE
Authors : Muderspach, S.J.; Torpenholt, S.; Lo Leggio, L.; Poulsen, J.C.N.
Deposited on : 2018-12-04
Resolution : 2.69 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

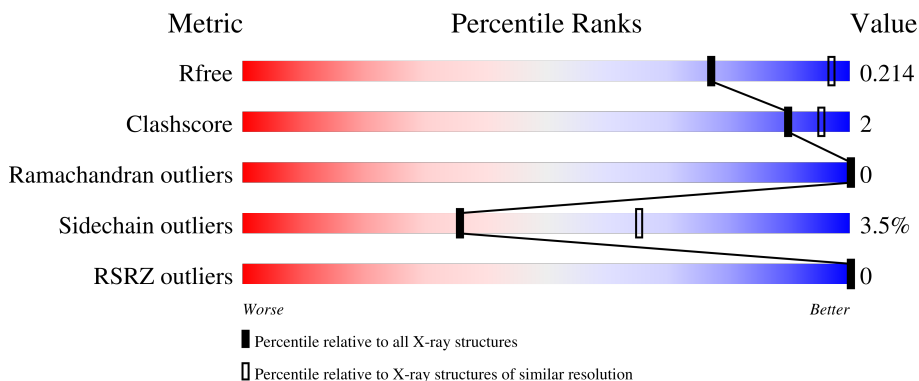
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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.



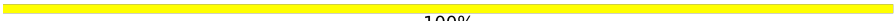
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	334	93% (green), 6% (orange), 1% (red)
1	B	334	92% (green), 7% (orange)
2	C	3	100% (yellow)
2	F	3	67% (yellow), 33% (orange)
3	D	2	50% (yellow), 50% (orange)

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	EDO	B	417	-	-	-	X

2 Entry composition [i](#)

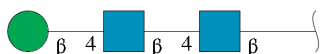
There are 11 unique types of molecules in this entry. The entry contains 5711 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Arabinogalactan endo-beta-1,4-galactanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	Total 2614	C 1671	N 403	O 534	S 6	0	3	0
1	B	334	Total 2598	C 1658	N 402	O 532	S 6	0	0	0

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	Total 39	C 22	N 2	O 15	0	0	0
2	F	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	D	2	Total 23	C 12	O 11	0	0	0
3	E	2	Total 23	C 12	O 11	0	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

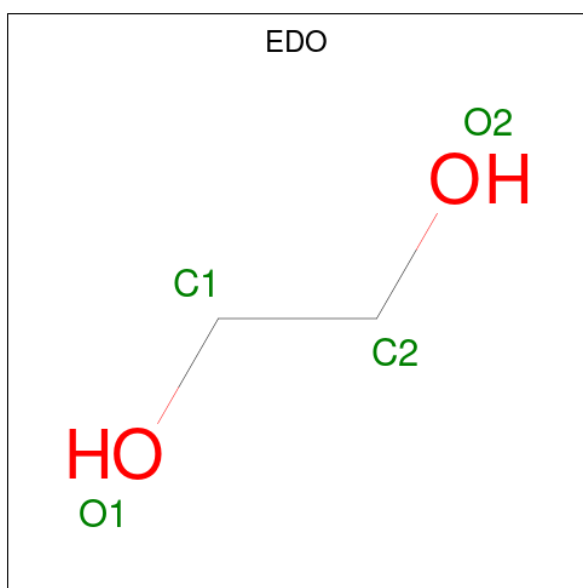
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total Ca 4 4	0	0
5	B	3	Total Ca 3 3	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



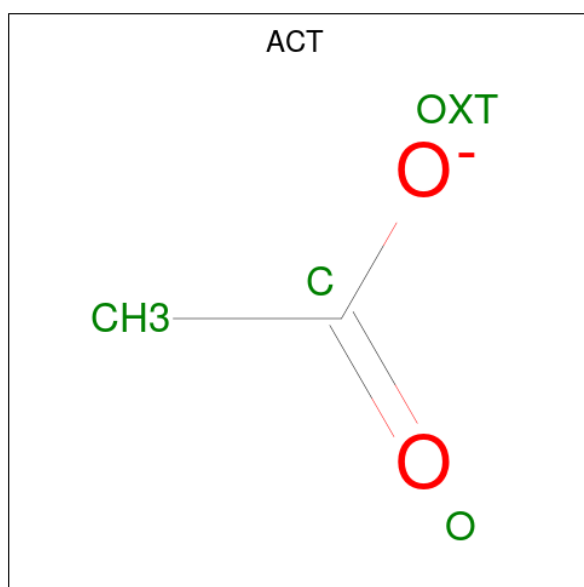
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

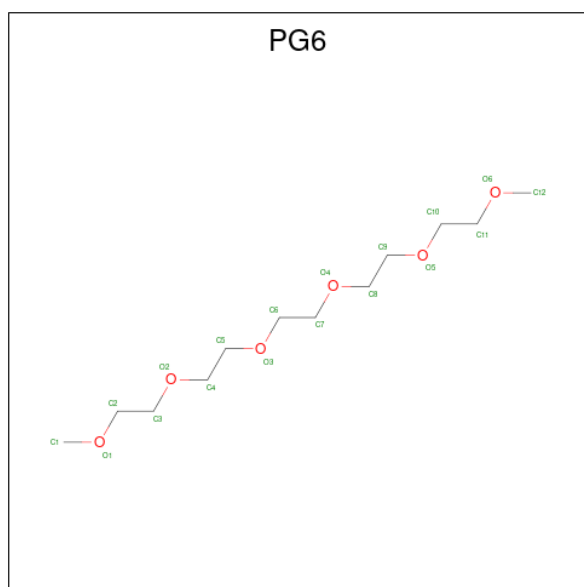
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



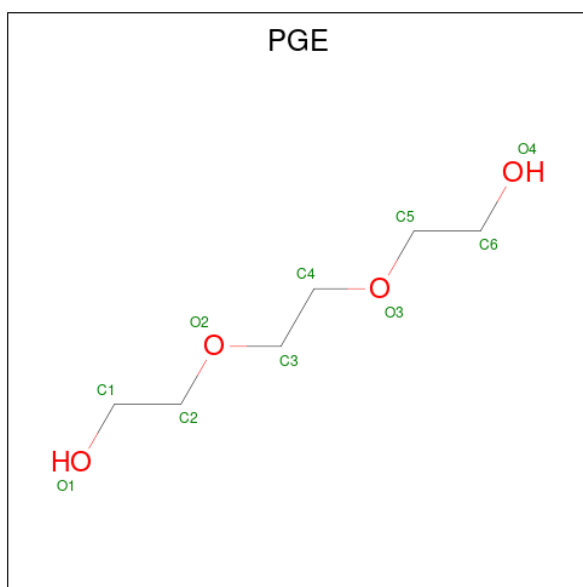
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANE (three-letter code: PG6) (formula: C₁₂H₂₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			18	12	6		

- Molecule 10 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	C O	0	0
			10	6 4		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	113	Total	O	0	0
			113	113		
11	B	109	Total	O	0	0
			109	109		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Arabinogalactan endo-beta-1,4-galactanase

Chain A:  93% 6%



- Molecule 1: Arabinogalactan endo-beta-1,4-galactanase

Chain B:  92% 7%




- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%



- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  67% 33%




- Molecule 3: beta-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain D:  50% 50%



- Molecule 3: beta-D-galactopyranose-(1-4)-beta-D-galactopyranose

Chain E:  100%

GAL1
GAL2

4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	200.20Å 200.20Å 106.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.17 – 2.69 47.13 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.17-2.69) 98.5 (47.13-2.69)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.145 , 0.211 0.154 , 0.214	Depositor DCC
R_{free} test set	1517 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtrriage
Anisotropy	0.569	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5711	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: PEG, BMA, ACT, PG6, NAG, EDO, PG4, GAL, PGE, CA

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	0.73	0/2689	0.88	3/3682 (0.1%)
1	B	0.71	0/2664	0.82	2/3649 (0.1%)
All	All	0.72	0/5353	0.85	5/7331 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	208	ASP	CB-CG-OD1	-5.65	113.21	118.30
1	A	58	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	45	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	138	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2614	0	2484	8	0
1	B	2598	0	2456	9	0
2	C	39	0	34	0	0
2	F	39	0	34	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	23	0	21	1	0
3	E	23	0	21	0	0
4	A	14	0	20	1	0
4	B	14	0	20	0	0
5	A	4	0	0	0	0
5	B	3	0	0	0	0
6	A	13	0	18	0	0
6	B	13	0	18	0	0
7	A	28	0	42	0	0
7	B	24	0	36	0	0
8	A	8	0	6	0	0
8	B	4	0	3	0	0
9	A	18	0	26	0	0
10	B	10	0	14	0	0
11	A	113	0	0	1	0
11	B	109	0	0	1	0
All	All	5711	0	5253	19	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 2.

All (19) 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:99:SER:H	1:A:109:GLN:HE22	1.38	0.71
1:A:106:LEU:HA	1:A:109:GLN:HE21	1.68	0.58
1:A:122:ALA:HB2	1:A:170:LEU:HD23	1.86	0.58
1:A:25:LEU:HD13	1:A:324:VAL:HG23	1.90	0.54
1:A:39:ALA:CB	1:A:328[A]:ILE:HG22	2.38	0.52
1:A:24:ASN:HB2	11:A:687:HOH:O	2.10	0.51
11:B:501:HOH:O	2:F:3:BMA:O2	2.19	0.50
1:B:122:ALA:HB2	1:B:170:LEU:HD23	1.96	0.47
1:B:235:GLN:HG3	1:B:289:THR:O	2.15	0.46
1:A:88:ASP:HB2	1:A:89:PRO:CD	2.47	0.45
1:B:42:ASN:C	1:B:42:ASN:HD22	2.20	0.44
1:B:25:LEU:HD13	1:B:324:VAL:HG23	2.00	0.43
1:A:42:ASN:HD22	1:A:42:ASN:C	2.22	0.42
1:B:46:GLN:HB3	1:B:62:ASN:OD1	2.20	0.41
1:B:4:TYR:HA	1:B:42:ASN:HD21	1.85	0.41
4:A:506:PEG:C2	3:D:2:GAL:O4	2.69	0.40
1:B:317:VAL:HG12	1:B:324:VAL:HG12	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ILE:HD12	1:B:207:PHE:CG	2.56	0.40
1:B:249:TRP:CD2	1:B:250:PRO:HD2	2.56	0.40

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	335/334 (100%)	322 (96%)	13 (4%)	0	100	100
1	B	332/334 (99%)	322 (97%)	10 (3%)	0	100	100
All	All	667/668 (100%)	644 (97%)	23 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	285/282 (101%)	275 (96%)	10 (4%)	36	65
1	B	282/282 (100%)	272 (96%)	10 (4%)	36	65
All	All	567/564 (100%)	547 (96%)	20 (4%)	36	65

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	25	LEU
1	A	42	ASN
1	A	77	TYR
1	A	125	ASP
1	A	127	ASP
1	A	149	SER
1	A	172	THR
1	A	217	PHE
1	A	280	LYS
1	B	15	LEU
1	B	26	ASN
1	B	42	ASN
1	B	77	TYR
1	B	91	ASP
1	B	123	GLU
1	B	160	SER
1	B	163	TRP
1	B	217	PHE
1	B	255	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	109	GLN
1	A	169	ASN
1	B	26	ASN
1	B	28	GLN
1	B	42	ASN
1	B	46	GLN
1	B	169	ASN

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

10 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	NAG	C	1	1,2	14,14,15	0.64	0	17,19,21	1.82	5 (29%)
2	NAG	C	2	2	14,14,15	0.76	0	17,19,21	0.96	1 (5%)
2	BMA	C	3	2	11,11,12	0.71	0	15,15,17	1.45	2 (13%)
3	GAL	D	1	3	12,12,12	0.78	0	17,17,17	1.61	4 (23%)
3	GAL	D	2	3	11,11,12	0.84	0	15,15,17	1.63	4 (26%)
3	GAL	E	1	3,5	12,12,12	0.69	0	17,17,17	1.73	5 (29%)
3	GAL	E	2	3	11,11,12	0.88	0	15,15,17	1.16	1 (6%)
2	NAG	F	1	1,2	14,14,15	0.59	0	17,19,21	1.47	3 (17%)
2	NAG	F	2	2	14,14,15	0.49	0	17,19,21	1.36	3 (17%)
2	BMA	F	3	2	11,11,12	0.77	0	15,15,17	1.78	4 (26%)

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	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
3	GAL	D	1	3	-	0/2/22/22	0/1/1/1
3	GAL	D	2	3	-	2/2/19/22	0/1/1/1
3	GAL	E	1	3,5	-	0/2/22/22	0/1/1/1
3	GAL	E	2	3	-	1/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	BMA	F	3	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	GAL	C1-C2-C3	4.48	115.18	109.67
2	F	3	BMA	O5-C5-C6	4.41	114.12	107.20
2	C	1	NAG	C1-O5-C5	4.22	117.91	112.19
2	C	3	BMA	C1-O5-C5	3.68	117.18	112.19
3	D	1	GAL	O2-C2-C1	3.61	117.54	109.16
2	C	1	NAG	C2-N2-C7	3.58	128.00	122.90
3	D	1	GAL	O1-C1-O5	-3.21	100.74	110.38
2	F	1	NAG	C2-N2-C7	3.09	127.30	122.90
3	E	1	GAL	O5-C1-C2	3.08	115.78	110.28
2	F	2	NAG	O5-C1-C2	-3.08	106.43	111.29
2	F	1	NAG	C1-O5-C5	2.91	116.13	112.19
3	D	1	GAL	C1-O5-C5	2.74	118.84	113.66
2	F	2	NAG	O5-C5-C6	2.69	111.42	107.20
3	E	1	GAL	O1-C1-O5	-2.67	102.35	110.38
2	C	1	NAG	O4-C4-C3	2.64	116.45	110.35
3	E	1	GAL	O3-C3-C4	2.58	116.31	110.35
2	C	3	BMA	O4-C4-C3	-2.58	104.39	110.35
2	C	2	NAG	C2-N2-C7	2.52	126.49	122.90
2	F	3	BMA	C3-C4-C5	2.52	114.73	110.24
2	F	3	BMA	C1-C2-C3	-2.38	106.75	109.67
2	C	1	NAG	C8-C7-N2	-2.28	112.24	116.10
3	E	1	GAL	O5-C5-C4	2.22	113.72	109.69
2	F	2	NAG	O4-C4-C3	-2.21	105.25	110.35
3	D	2	GAL	O5-C1-C2	-2.20	107.38	110.77
3	D	2	GAL	C1-O5-C5	2.17	115.13	112.19
3	E	2	GAL	C1-O5-C5	2.16	115.11	112.19
2	C	1	NAG	O7-C7-N2	2.15	125.91	121.95
2	F	1	NAG	C1-C2-N2	-2.08	106.93	110.49
3	D	2	GAL	O2-C2-C3	2.08	114.30	110.14
3	E	1	GAL	C1-C2-C3	2.08	114.62	110.31
2	F	3	BMA	O5-C5-C4	-2.06	105.80	110.83
3	D	1	GAL	O1-C1-C2	2.06	114.84	109.03

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2	GAL	O5-C5-C6-O6
2	F	3	BMA	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

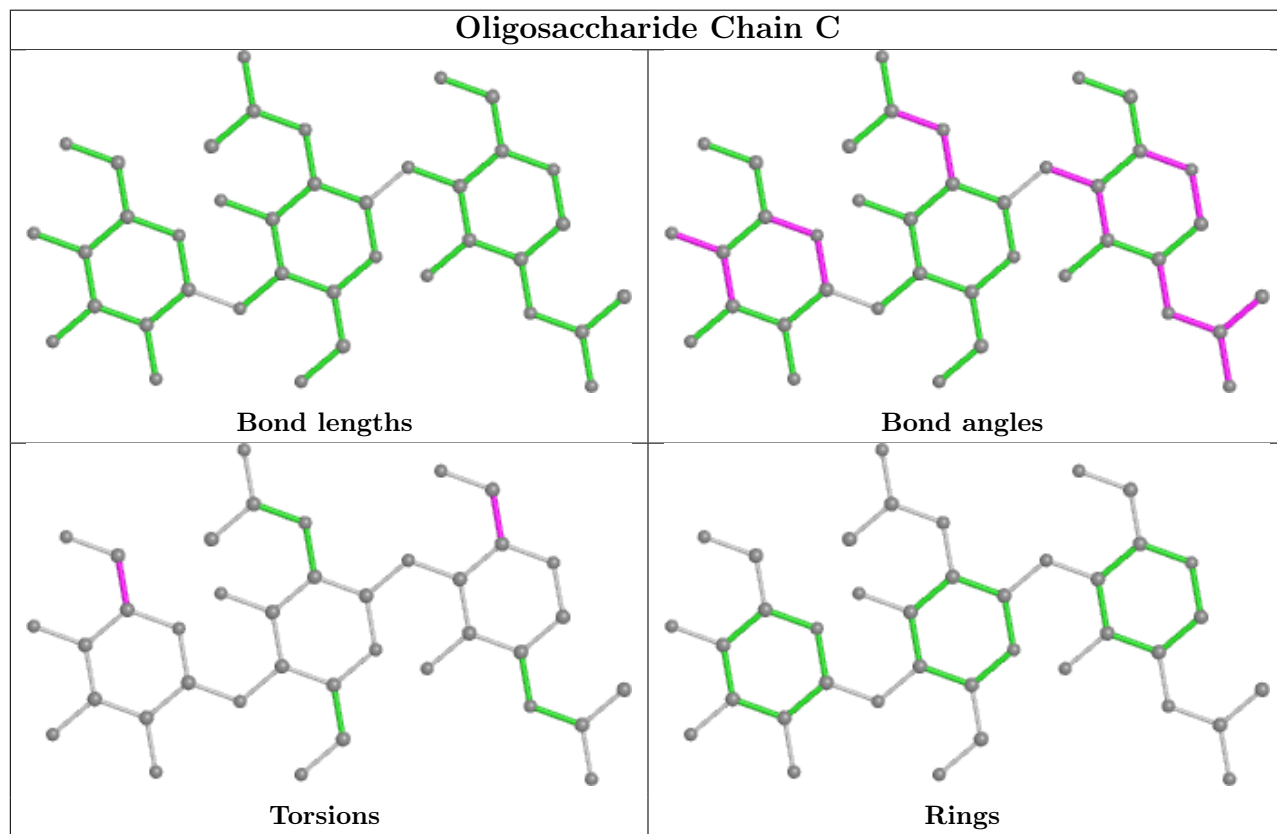
Mol	Chain	Res	Type	Atoms
2	F	3	BMA	C4-C5-C6-O6
3	D	2	GAL	C4-C5-C6-O6
3	E	2	GAL	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6

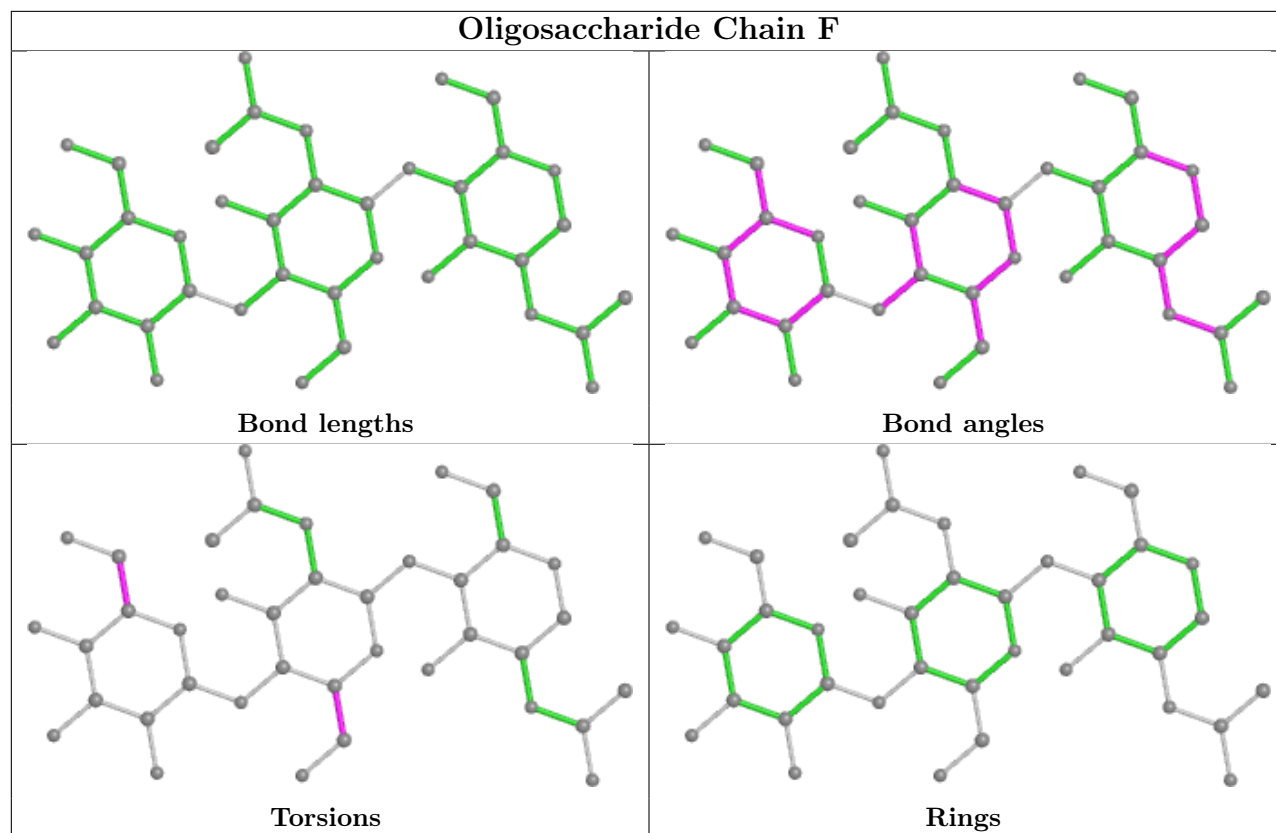
There are no ring outliers.

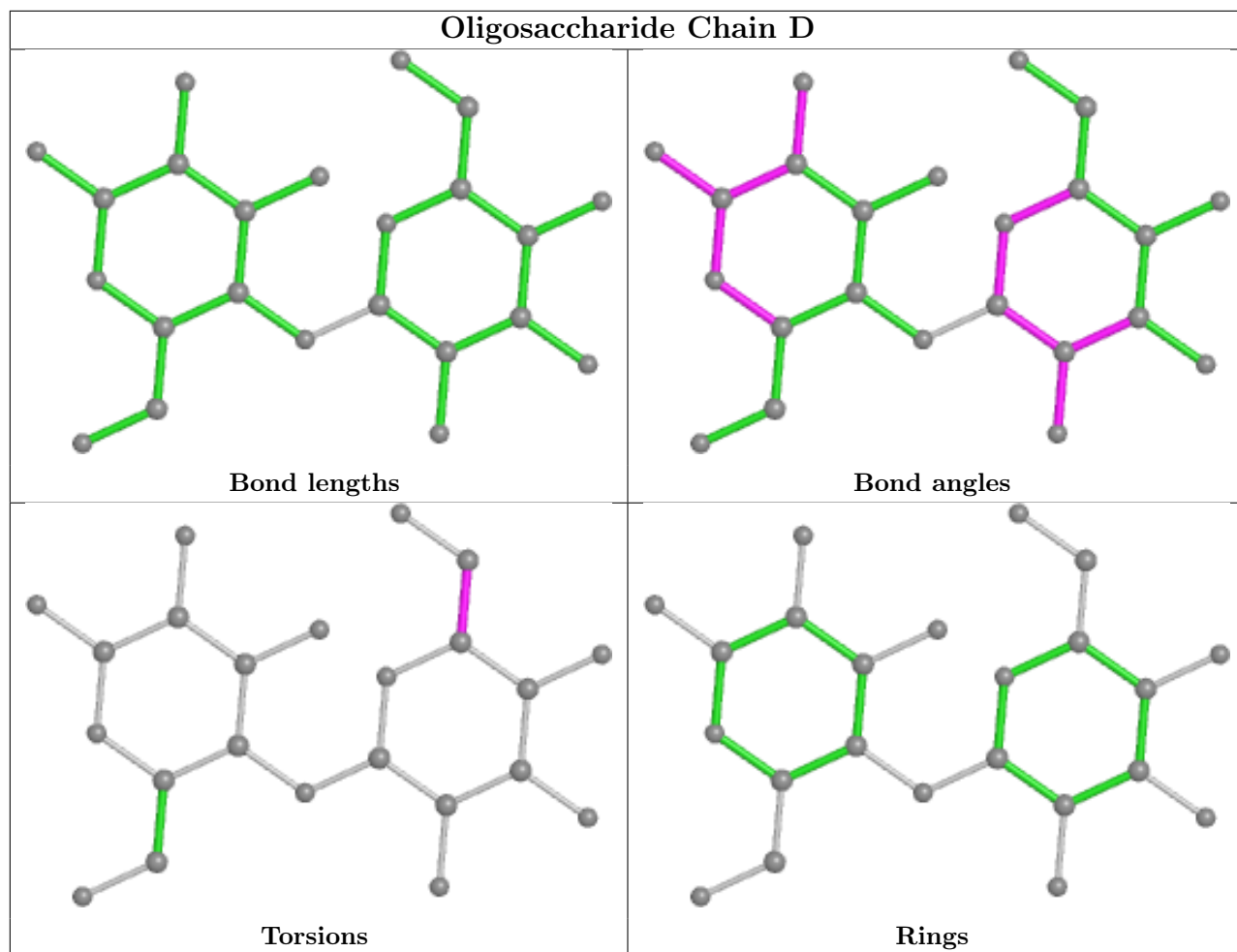
2 monomers are involved in 2 short contacts:

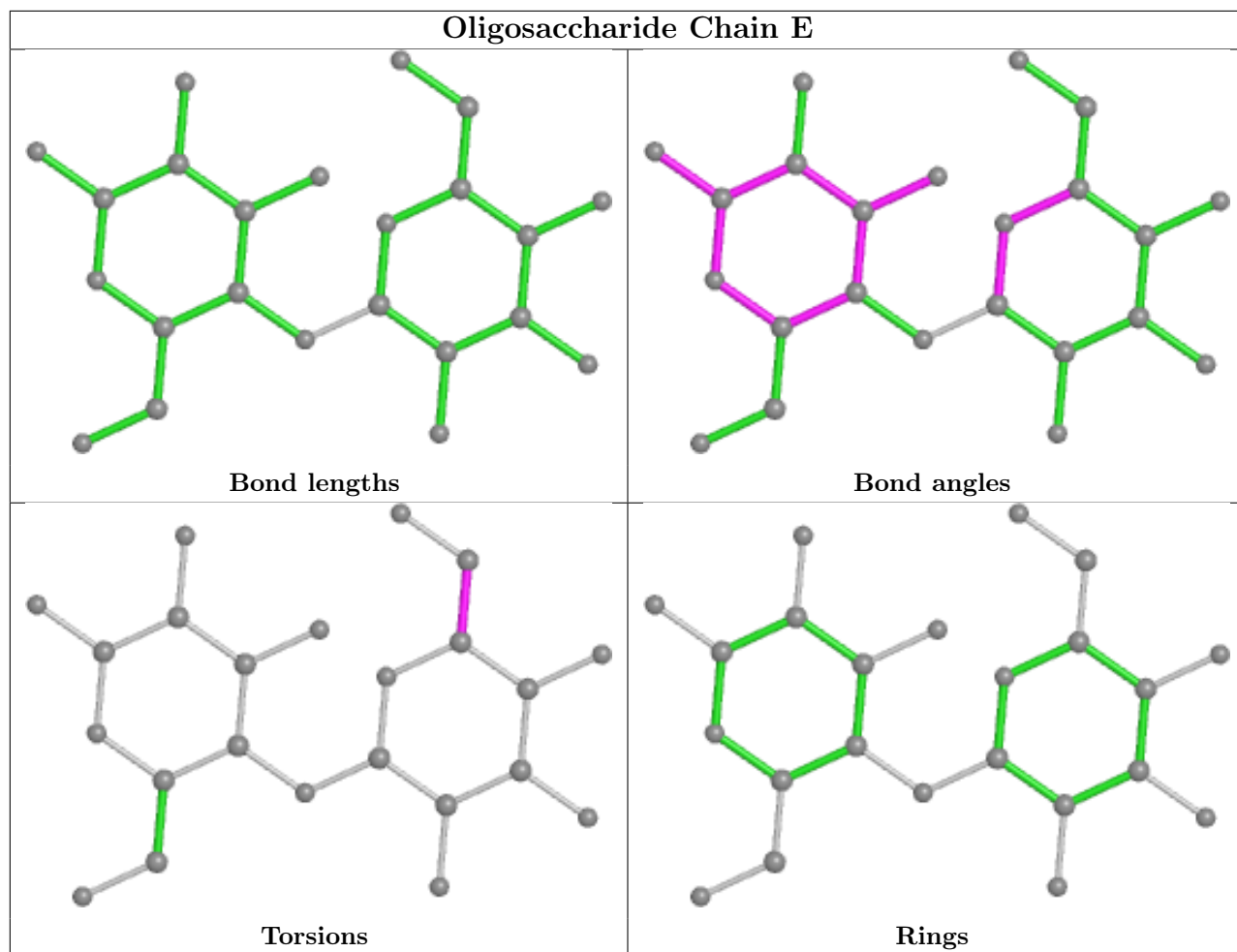
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3	BMA	1	0
3	D	2	GAL	1	0

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 31 ligands modelled in this entry, 7 are monoatomic - leaving 24 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	$\# Z > 2$
4	PEG	B	407	-	6,6,6	0.77	0	5,5,5	0.51	0
7	EDO	B	414	-	3,3,3	0.45	0	2,2,2	0.46	0
7	EDO	B	417	-	3,3,3	0.79	0	2,2,2	0.28	0
7	EDO	A	515	-	3,3,3	0.70	0	2,2,2	0.29	0
4	PEG	A	507	-	6,6,6	0.84	0	5,5,5	0.67	0
7	EDO	A	519	-	3,3,3	0.46	0	2,2,2	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	A	513	-	3,3,3	0.41	0	2,2,2	0.67	0
8	ACT	A	521	-	3,3,3	0.88	0	3,3,3	0.95	0
4	PEG	B	406	-	6,6,6	0.67	0	5,5,5	0.52	0
7	EDO	A	516	-	3,3,3	0.82	0	2,2,2	0.66	0
6	PG4	A	512	-	12,12,12	0.59	0	11,11,11	0.54	0
8	ACT	B	418	-	3,3,3	0.87	0	3,3,3	0.73	0
8	ACT	A	520	-	3,3,3	0.68	0	3,3,3	1.51	0
10	PGE	B	419	-	9,9,9	0.82	0	8,8,8	0.65	0
7	EDO	A	518	-	3,3,3	0.50	0	2,2,2	0.49	0
7	EDO	B	412	-	3,3,3	0.39	0	2,2,2	0.54	0
7	EDO	B	413	-	3,3,3	0.84	0	2,2,2	0.39	0
6	PG4	B	411	-	12,12,12	0.77	0	11,11,11	0.70	0
7	EDO	A	517	-	3,3,3	0.41	0	2,2,2	0.51	0
7	EDO	B	416	-	3,3,3	0.71	0	2,2,2	0.17	0
9	PG6	A	522	-	17,17,17	1.05	0	16,16,16	0.96	0
4	PEG	A	506	-	6,6,6	0.67	0	5,5,5	0.36	0
7	EDO	A	514	-	3,3,3	0.68	0	2,2,2	0.38	0
7	EDO	B	415	-	3,3,3	0.51	0	2,2,2	0.47	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
4	PEG	B	407	-	-	1/4/4/4	-
7	EDO	B	414	-	-	1/1/1/1	-
7	EDO	B	417	-	-	0/1/1/1	-
7	EDO	A	515	-	-	1/1/1/1	-
4	PEG	A	507	-	-	3/4/4/4	-
7	EDO	A	519	-	-	0/1/1/1	-
7	EDO	A	513	-	-	1/1/1/1	-
4	PEG	B	406	-	-	3/4/4/4	-
7	EDO	A	516	-	-	0/1/1/1	-
6	PG4	A	512	-	-	7/10/10/10	-
10	PGE	B	419	-	-	3/7/7/7	-
7	EDO	A	518	-	-	1/1/1/1	-
7	EDO	B	412	-	-	1/1/1/1	-
7	EDO	B	413	-	-	1/1/1/1	-
6	PG4	B	411	-	-	3/10/10/10	-
7	EDO	A	517	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	416	-	-	0/1/1/1	-
9	PG6	A	522	-	-	8/15/15/15	-
4	PEG	A	506	-	-	3/4/4/4	-
7	EDO	A	514	-	-	1/1/1/1	-
7	EDO	B	415	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	419	PGE	O2-C3-C4-O3
9	A	522	PG6	O5-C10-C11-O6
9	A	522	PG6	O1-C2-C3-O2
6	B	411	PG4	O2-C3-C4-O3
9	A	522	PG6	O2-C4-C5-O3
10	B	419	PGE	O3-C5-C6-O4
6	A	512	PG4	O2-C3-C4-O3
4	A	507	PEG	C1-C2-O2-C3
4	B	406	PEG	O1-C1-C2-O2
4	B	406	PEG	O2-C3-C4-O4
6	A	512	PG4	O3-C5-C6-O4
4	A	506	PEG	O1-C1-C2-O2
7	A	518	EDO	O1-C1-C2-O2
7	B	414	EDO	O1-C1-C2-O2
4	A	507	PEG	O2-C3-C4-O4
7	B	412	EDO	O1-C1-C2-O2
9	A	522	PG6	O4-C8-C9-O5
7	A	515	EDO	O1-C1-C2-O2
7	A	517	EDO	O1-C1-C2-O2
4	A	507	PEG	O1-C1-C2-O2
6	B	411	PG4	O1-C1-C2-O2
9	A	522	PG6	C4-C5-O3-C6
9	A	522	PG6	C2-C3-O2-C4
6	B	411	PG4	C1-C2-O2-C3
6	A	512	PG4	O4-C7-C8-O5
7	B	413	EDO	O1-C1-C2-O2
6	A	512	PG4	C1-C2-O2-C3
9	A	522	PG6	C6-C7-O4-C8

Continued on next page...

Continued from previous page...

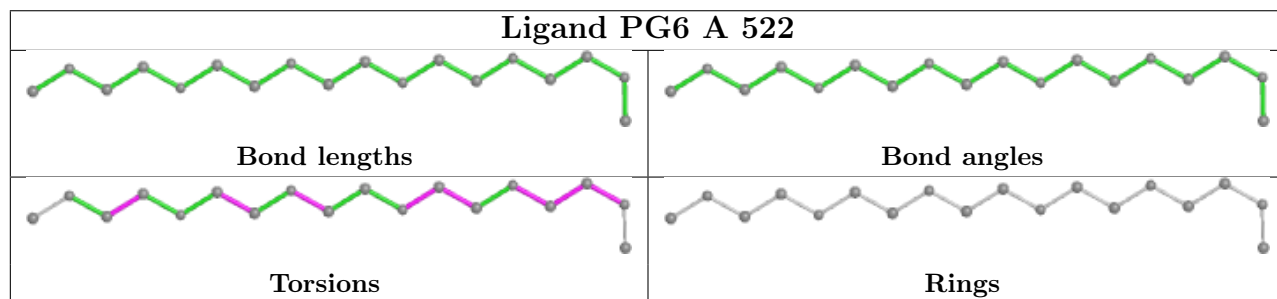
Mol	Chain	Res	Type	Atoms
4	A	506	PEG	C4-C3-O2-C2
10	B	419	PGE	C6-C5-O3-C4
6	A	512	PG4	C4-C3-O2-C2
6	A	512	PG4	O1-C1-C2-O2
4	A	506	PEG	C1-C2-O2-C3
9	A	522	PG6	C3-C2-O1-C1
6	A	512	PG4	C8-C7-O4-C6
4	B	406	PEG	C1-C2-O2-C3
7	A	513	EDO	O1-C1-C2-O2
7	A	514	EDO	O1-C1-C2-O2
7	B	415	EDO	O1-C1-C2-O2
4	B	407	PEG	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	506	PEG	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](#)

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	334/334 (100%)	-0.50	0 100 100	24, 37, 52, 77	0
1	B	334/334 (100%)	-0.55	0 100 100	28, 40, 54, 71	0
All	All	668/668 (100%)	-0.52	0 100 100	24, 38, 54, 77	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

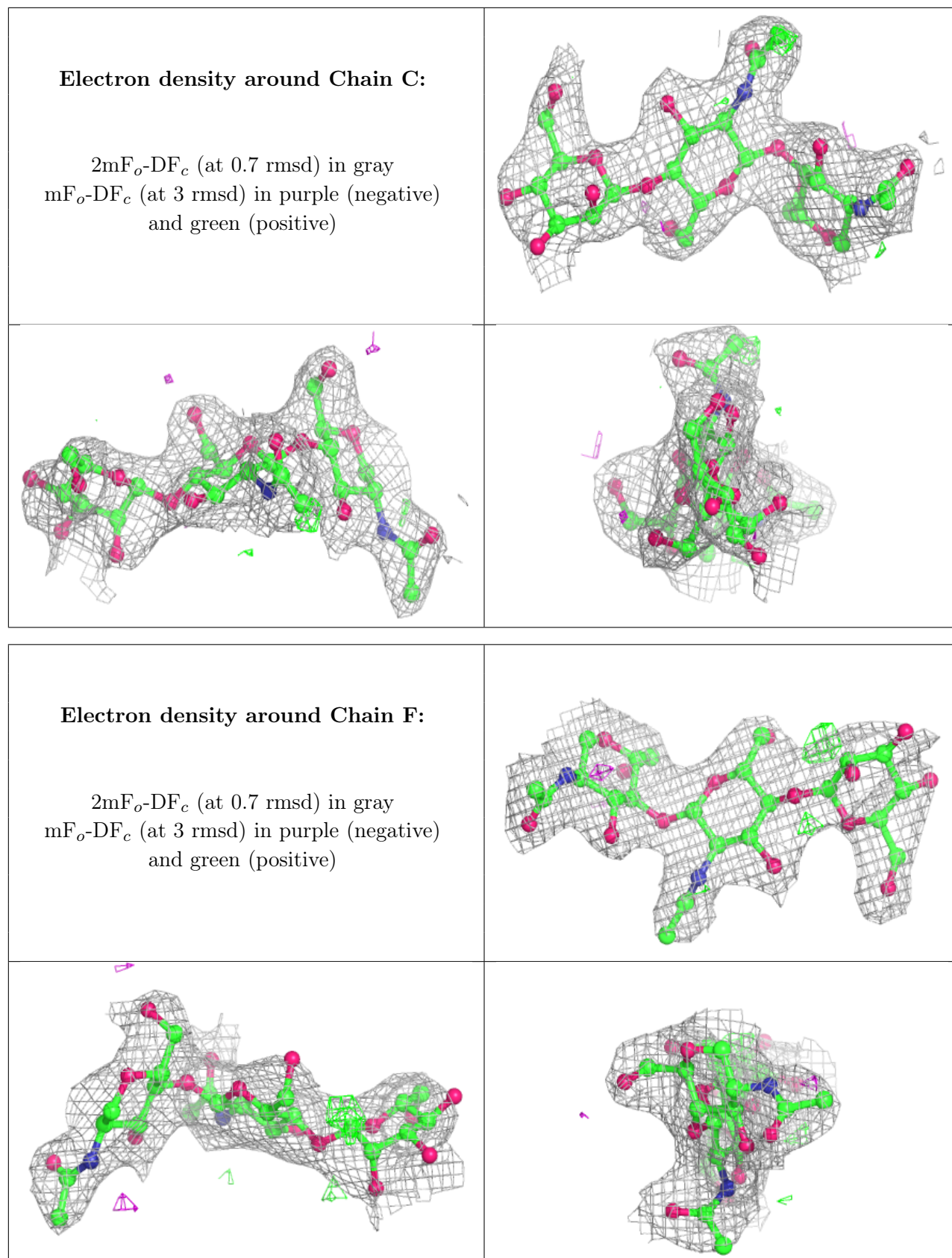
6.3 Carbohydrates [i](#)

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	BMA	C	3	11/12	0.90	0.19	67,77,83,83	0
2	BMA	F	3	11/12	0.91	0.23	68,84,90,91	0
2	NAG	C	2	14/15	0.96	0.11	45,49,56,60	0
3	GAL	D	2	11/12	0.96	0.17	35,41,45,47	0
3	GAL	E	2	11/12	0.96	0.12	37,39,43,43	0
3	GAL	D	1	12/12	0.97	0.12	35,46,52,57	0
2	NAG	F	2	14/15	0.97	0.14	45,51,60,67	0
3	GAL	E	1	12/12	0.97	0.14	37,44,50,57	0
2	NAG	C	1	14/15	0.97	0.11	35,39,48,49	0
2	NAG	F	1	14/15	0.98	0.14	31,34,37,42	0

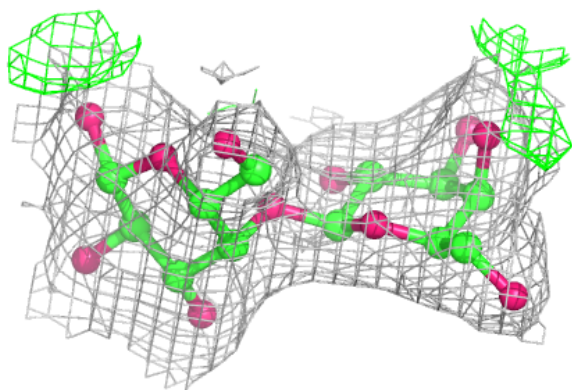
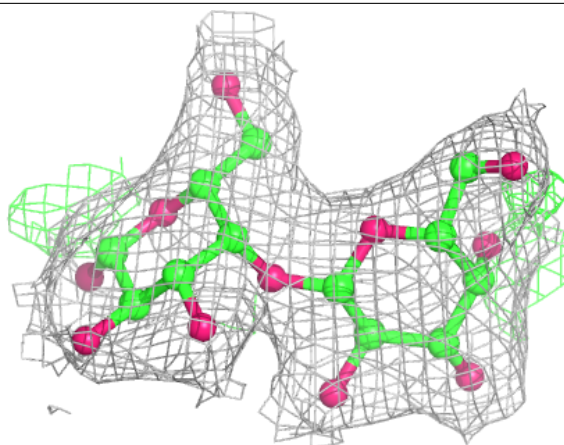
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

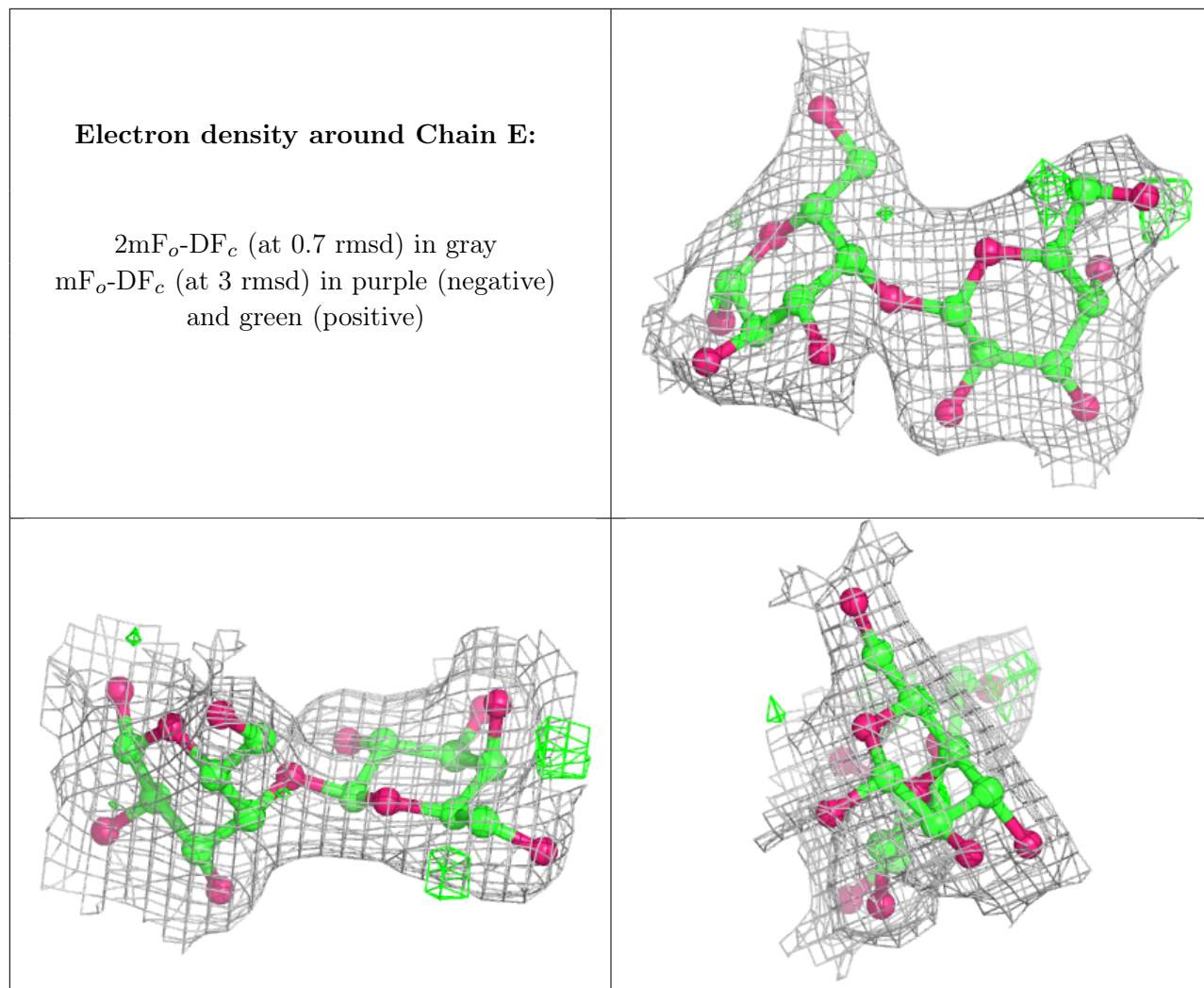
charide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain D:

$2mF_o-DF_c$ (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.

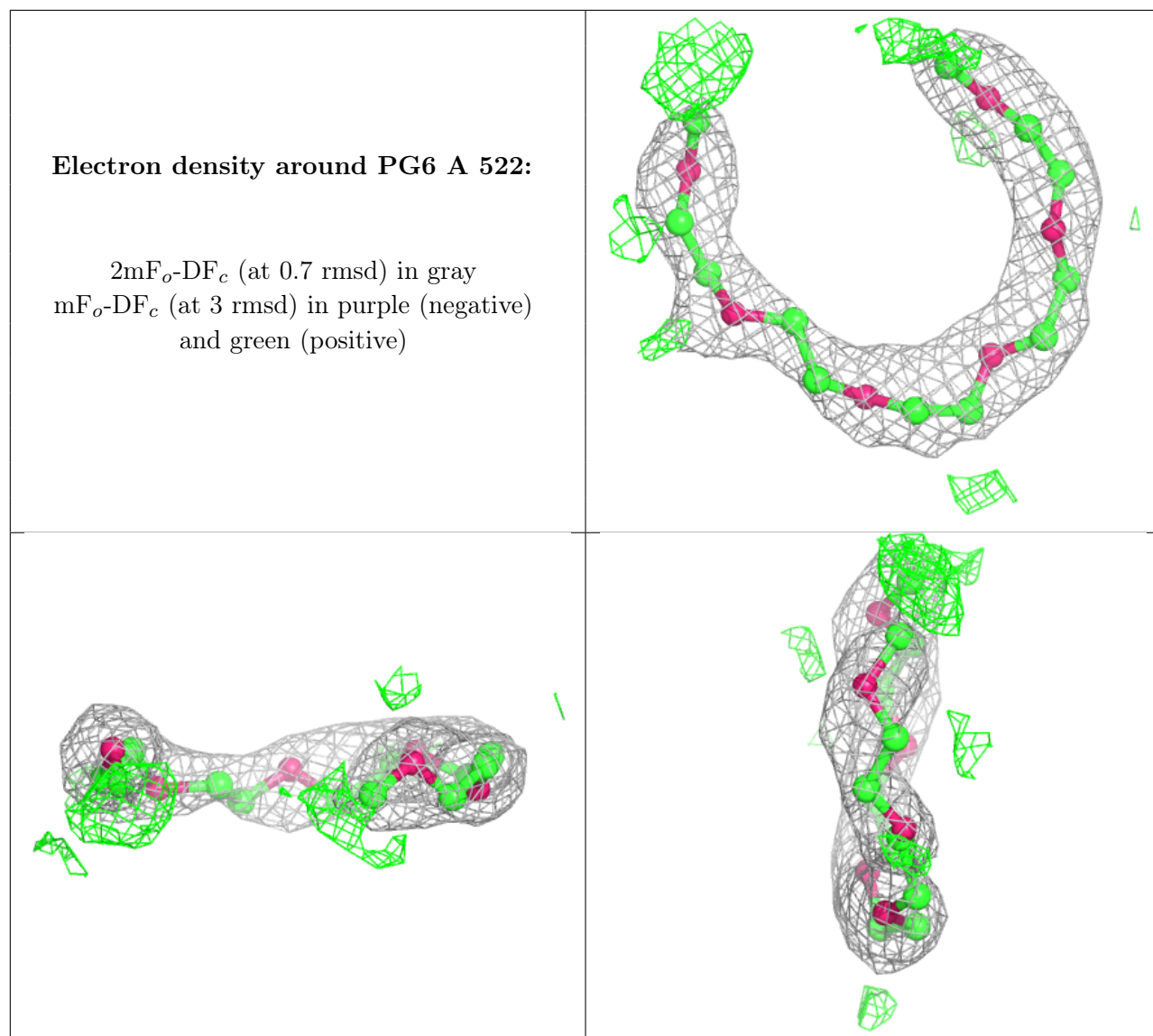
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	EDO	B	417	4/4	0.16	0.63	84,89,93,95	0
7	EDO	B	416	4/4	0.77	0.20	64,69,73,73	0
4	PEG	A	506	7/7	0.79	0.22	66,72,77,79	0
7	EDO	A	515	4/4	0.79	0.32	60,69,70,73	0
7	EDO	B	415	4/4	0.82	0.27	59,66,67,69	0
6	PG4	B	411	13/13	0.82	0.24	59,70,91,91	0
4	PEG	B	407	7/7	0.82	0.24	55,67,74,75	0
10	PGE	B	419	10/10	0.82	0.27	65,73,80,81	0
7	EDO	A	518	4/4	0.83	0.34	69,74,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	EDO	A	517	4/4	0.84	0.24	68,72,75,76	0
6	PG4	A	512	13/13	0.85	0.35	63,88,94,98	0
8	ACT	B	418	4/4	0.85	0.25	67,72,79,82	0
7	EDO	B	414	4/4	0.85	0.29	63,65,66,67	0
7	EDO	B	412	4/4	0.86	0.17	63,64,65,67	0
8	ACT	A	521	4/4	0.86	0.45	74,77,80,83	0
5	CA	A	511	1/1	0.87	0.07	72,72,72,72	0
4	PEG	B	406	7/7	0.87	0.17	53,61,69,70	0
7	EDO	A	514	4/4	0.88	0.24	57,60,62,66	0
7	EDO	A	516	4/4	0.88	0.16	45,47,49,50	0
7	EDO	B	413	4/4	0.90	0.22	46,51,53,57	0
5	CA	A	510	1/1	0.90	0.42	80,80,80,80	1
7	EDO	A	519	4/4	0.90	0.27	62,67,69,70	0
9	PG6	A	522	18/18	0.90	0.25	57,75,82,83	0
4	PEG	A	507	7/7	0.90	0.19	53,68,70,73	0
5	CA	B	409	1/1	0.94	0.19	64,64,64,64	1
7	EDO	A	513	4/4	0.94	0.20	55,58,58,58	0
5	CA	A	509	1/1	0.96	0.06	77,77,77,77	0
5	CA	B	408	1/1	0.97	0.07	70,70,70,70	0
8	ACT	A	520	4/4	0.97	0.16	39,40,43,43	0
5	CA	B	410	1/1	0.97	0.33	36,36,36,36	1
5	CA	A	508	1/1	0.98	0.15	51,51,51,51	0

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



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.