



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2024 – 01:12 PM JST

PDB ID : 8X8G
Title : Crystal structure of EndoSz mutant D234M, from Streptococcus equi subsp. Zooepidemicus Sz105, in complex with oligosaccharide G2S2-oxazoline
Authors : Guan, H.H.; Lin, C.C.; Hsieh, Y.C.; Chen, C.J.
Deposited on : 2023-11-27
Resolution : 2.27 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 : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

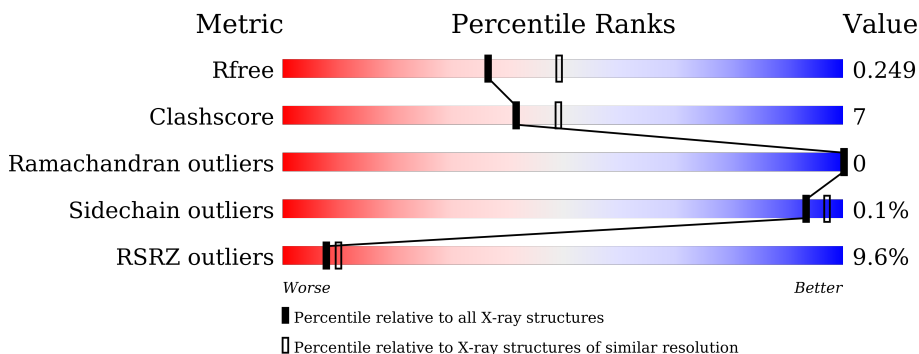
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 $\leq 5\%$. 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	961	
2	B	9	

2 Entry composition [i](#)

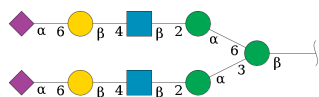
There are 5 unique types of molecules in this entry. The entry contains 7334 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 glycoside hydrolase.

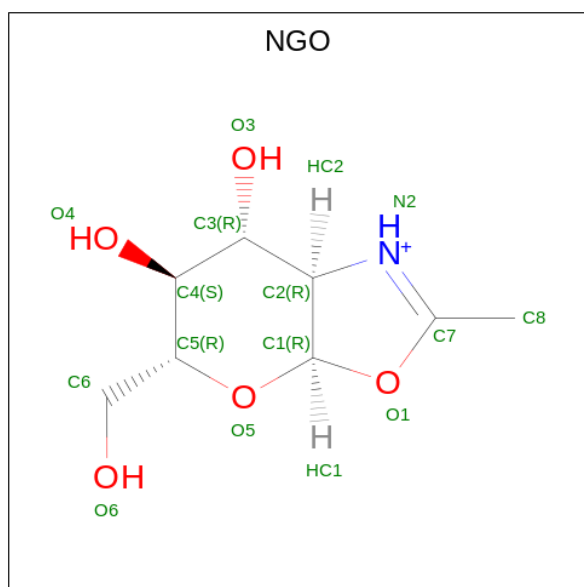
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	876	6902	4375	1152	1360	15	0	0	0

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	9	123	68	4	51	0	0	0

- Molecule 3 is 2-METHYL-4,5-DIHYDRO-(1,2-DIDEOXY-ALPHA-D-GLUCOPYRANOSO)[2,1-D]-1,3-OXAZOLE (three-letter code: NGO) (formula: C₈H₁₄NO₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	294	Total	O	0	0
			294	294		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.06Å 232.60Å 50.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.44 – 2.27 46.44 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.44-2.27) 99.6 (46.44-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.27Å)	Xtrriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.207 , 0.249 0.207 , 0.249	Depositor DCC
R_{free} test set	2846 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtrriage
Anisotropy	0.026	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7334	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: NAG, CA, GAL, SIA, MAN, NGO, BMA

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	0.31	0/7035	0.54	0/9501

There are no bond length outliers.

There are no bond angle outliers.

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	6902	0	6887	95	0
2	B	123	0	102	1	0
3	A	14	0	13	2	0
4	A	1	0	0	0	0
5	A	294	0	0	5	0
All	All	7334	0	7002	98	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 7.

All (98) 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)
3:A:10:NGO:HC2	5:A:1126:HOH:O	1.83	0.78
1:A:849:LYS:H	1:A:852:LEU:HD13	1.50	0.75
1:A:941:GLU:HA	1:A:944:VAL:HG12	1.73	0.71
1:A:302:LEU:HD22	1:A:343:MET:HB2	1.76	0.67
1:A:908:ARG:NH2	5:A:1109:HOH:O	2.27	0.66
1:A:848:VAL:O	1:A:849:LYS:HG2	1.96	0.64
1:A:919:MET:HE3	1:A:948:LYS:HB2	1.79	0.63
1:A:919:MET:HE1	1:A:948:LYS:HD3	1.80	0.63
3:A:10:NGO:C2	5:A:1126:HOH:O	2.44	0.63
1:A:602:GLU:OE1	1:A:602:GLU:N	2.29	0.62
1:A:713:THR:HG22	1:A:719:VAL:HG22	1.79	0.62
1:A:954:LYS:N	1:A:954:LYS:HD2	2.15	0.61
1:A:286:ASP:N	1:A:286:ASP:OD1	2.32	0.61
1:A:111:LYS:HD2	1:A:112:GLY:N	2.17	0.60
1:A:972:ILE:HG13	1:A:973:ASP:N	2.17	0.60
1:A:789:ASN:OD1	1:A:822:SER:HB2	2.03	0.58
1:A:745:LYS:HD2	1:A:746:PRO:HD2	1.86	0.58
1:A:234:MET:HA	1:A:280:ASP:OD1	2.04	0.57
1:A:302:LEU:HB3	1:A:399:PHE:CE1	2.41	0.55
1:A:111:LYS:HE3	1:A:469:ARG:HH21	1.71	0.54
1:A:810:PRO:HG3	1:A:881:LYS:HB3	1.87	0.54
1:A:450:GLN:H	1:A:450:GLN:CD	2.11	0.54
1:A:785:ASP:OD2	1:A:790:ASN:ND2	2.41	0.53
1:A:799:ASN:HB2	1:A:895:GLY:H	1.72	0.53
1:A:782:LYS:NZ	1:A:792:THR:O	2.34	0.53
1:A:852:LEU:H	1:A:852:LEU:HD12	1.75	0.52
1:A:833:ALA:HB3	1:A:864:TYR:HB3	1.92	0.52
1:A:845:SER:HB3	1:A:852:LEU:HD11	1.92	0.52
1:A:856:THR:HG22	1:A:857:GLU:N	2.25	0.52
1:A:925:LEU:HA	1:A:928:GLN:HE21	1.75	0.52
1:A:849:LYS:N	1:A:852:LEU:HD13	2.22	0.52
1:A:236:GLU:HG3	1:A:238:ASP:HB3	1.92	0.52
1:A:930:ASP:H	1:A:933:SER:CB	2.22	0.51
1:A:360:TYR:CE1	1:A:413:LYS:HG2	2.45	0.51
1:A:797:THR:OG1	1:A:798:SER:N	2.43	0.51
1:A:795:LEU:HA	1:A:898:SER:HA	1.93	0.50
1:A:961:ILE:O	1:A:965:PHE:N	2.40	0.50
1:A:773:GLY:H	1:A:854:LYS:HE2	1.74	0.50
1:A:845:SER:HB3	1:A:852:LEU:HD21	1.92	0.50
1:A:579:ALA:HB2	1:A:606:ILE:HG23	1.93	0.50
1:A:838:PHE:HE1	1:A:856:THR:HG21	1.76	0.49
1:A:742:ASN:ND2	5:A:1129:HOH:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:LEU:HB3	1:A:499:LEU:HD21	1.94	0.49
1:A:140:GLU:OE2	1:A:426:LYS:NZ	2.44	0.49
1:A:849:LYS:H	1:A:852:LEU:CD1	2.21	0.48
1:A:926:SER:HB2	1:A:940:LEU:HD23	1.95	0.48
1:A:165:LEU:HA	1:A:169:HIS:HB2	1.96	0.48
1:A:812:LEU:HD11	1:A:877:ASN:HB3	1.94	0.48
1:A:280:ASP:HB3	1:A:302:LEU:HB2	1.95	0.48
1:A:756:GLU:OE2	1:A:954:LYS:HG2	2.14	0.47
1:A:308:THR:OG1	1:A:312:LYS:HE3	2.15	0.47
1:A:604:ARG:CZ	1:A:686:ILE:HG12	2.44	0.47
1:A:636:TYR:OH	1:A:704:THR:O	2.25	0.47
1:A:819:PHE:CE2	1:A:870:GLU:HG3	2.49	0.47
1:A:104:LYS:HD3	1:A:105:ILE:H	1.80	0.46
1:A:972:ILE:HG13	1:A:973:ASP:H	1.80	0.46
1:A:445:TYR:O	1:A:469:ARG:NH1	2.47	0.46
1:A:838:PHE:HB3	1:A:882:TYR:HB2	1.97	0.46
1:A:797:THR:O	1:A:896:TYR:HA	2.16	0.46
1:A:856:THR:HG22	1:A:857:GLU:H	1.81	0.46
1:A:123:HIS:NE2	1:A:351:GLU:OE2	2.45	0.45
1:A:815:HIS:HB3	1:A:905:ILE:HB	1.98	0.45
1:A:487:ILE:HD12	1:A:507:LEU:HD21	1.99	0.45
1:A:706:LYS:NZ	5:A:1138:HOH:O	2.49	0.45
1:A:186:TRP:HB3	1:A:239:SER:O	2.17	0.44
1:A:330:TRP:CD1	1:A:389:PRO:HB3	2.53	0.44
1:A:775:ALA:HB1	1:A:796:SER:HB3	1.99	0.44
1:A:788:LEU:HD13	1:A:901:GLU:HG3	1.98	0.44
1:A:918:THR:HG21	1:A:965:PHE:HE1	1.82	0.44
1:A:654:ILE:HD12	1:A:659:LYS:HD2	1.99	0.44
1:A:793:THR:HG23	1:A:795:LEU:HD23	1.99	0.44
1:A:797:THR:HG22	1:A:801:ALA:HB2	2.00	0.43
2:B:9:SIA:H6	2:B:9:SIA:H92	1.45	0.43
1:A:488:LYS:HG2	1:A:509:GLN:OE1	2.19	0.43
1:A:104:LYS:HD3	1:A:104:LYS:HA	1.83	0.43
1:A:111:LYS:HD2	1:A:112:GLY:H	1.81	0.43
1:A:779:ASN:HA	1:A:782:LYS:HE2	2.00	0.43
1:A:660:LEU:HD11	1:A:752:ILE:HD11	2.00	0.43
1:A:943:LYS:HB3	1:A:968:VAL:HG22	2.00	0.43
1:A:602:GLU:O	1:A:606:ILE:HD12	2.19	0.42
1:A:111:LYS:CE	1:A:469:ARG:HH21	2.33	0.42
1:A:930:ASP:HA	1:A:933:SER:HB2	2.00	0.42
1:A:954:LYS:N	1:A:954:LYS:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:GLU:OE1	1:A:914:THR:HG23	2.20	0.42
1:A:183:THR:CG2	1:A:234:MET:HE3	2.50	0.42
1:A:812:LEU:O	1:A:906:GLY:HA3	2.20	0.41
1:A:852:LEU:HD12	1:A:852:LEU:N	2.36	0.41
1:A:797:THR:HG21	1:A:800:LYS:O	2.20	0.41
1:A:335:LYS:HE2	1:A:336:TYR:CE2	2.56	0.41
1:A:848:VAL:C	1:A:849:LYS:HZ2	2.23	0.41
1:A:361:ASP:OD1	1:A:380:ARG:HD2	2.20	0.41
1:A:112:GLY:HA2	1:A:113:PRO:C	2.41	0.41
1:A:615:THR:HA	1:A:620:VAL:HG21	2.02	0.41
1:A:234:MET:HE3	1:A:234:MET:HB2	1.91	0.40
1:A:268:PRO:HD2	1:A:297:TYR:O	2.22	0.40
1:A:466:VAL:HG22	1:A:476:PHE:CD2	2.56	0.40
1:A:496:LEU:HD22	1:A:499:LEU:HD13	2.03	0.40
1:A:969:LYS:O	1:A:972:ILE:HG12	2.21	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	874/961 (91%)	831 (95%)	43 (5%)	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	753/827 (91%)	752 (100%)	1 (0%)	93 97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	456	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	841	HIS
1	A	928	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](#)

9 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BMA	B	1	3,2	11,11,12	0.61	0	15,15,17	0.86	0
2	MAN	B	2	2	11,11,12	0.60	0	15,15,17	1.11	2 (13%)
2	NAG	B	3	2	14,14,15	0.30	0	17,19,21	0.62	0
2	GAL	B	4	2	11,11,12	0.82	1 (9%)	15,15,17	1.40	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	B	5	2	20,20,21	2.05	3 (15%)	24,28,31	1.68	3 (12%)
2	MAN	B	6	2	11,11,12	0.71	0	15,15,17	1.20	2 (13%)
2	NAG	B	7	2	14,14,15	0.42	0	17,19,21	0.57	0
2	GAL	B	8	2	11,11,12	0.61	0	15,15,17	1.15	2 (13%)
2	SIA	B	9	2	20,20,21	2.06	3 (15%)	24,28,31	1.75	9 (37%)

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	BMA	B	1	3,2	-	0/2/19/22	0/1/1/1
2	MAN	B	2	2	-	0/2/19/22	0/1/1/1
2	NAG	B	3	2	-	2/6/23/26	0/1/1/1
2	GAL	B	4	2	-	1/2/19/22	0/1/1/1
2	SIA	B	5	2	-	12/18/34/38	0/1/1/1
2	MAN	B	6	2	-	2/2/19/22	0/1/1/1
2	NAG	B	7	2	-	0/6/23/26	0/1/1/1
2	GAL	B	8	2	-	0/2/19/22	0/1/1/1
2	SIA	B	9	2	-	11/18/34/38	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	SIA	C2-C1	7.65	1.59	1.52
2	B	9	SIA	C2-C1	7.62	1.59	1.52
2	B	5	SIA	O6-C2	3.12	1.47	1.43
2	B	9	SIA	O6-C2	2.93	1.47	1.43
2	B	9	SIA	C7-C6	2.07	1.55	1.53
2	B	5	SIA	C7-C6	2.00	1.55	1.53
2	B	4	GAL	C1-C2	2.00	1.56	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9	SIA	C5-N5-C10	4.80	134.86	123.18
2	B	5	SIA	O1A-C1-C2	-4.46	112.03	122.57
2	B	5	SIA	C6-O6-C2	4.29	120.52	111.34
2	B	4	GAL	C1-O5-C5	3.49	116.92	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	MAN	O2-C2-C3	-2.96	104.22	110.14
2	B	2	MAN	C1-O5-C5	2.92	116.15	112.19
2	B	9	SIA	C4-C5-N5	2.61	115.54	110.38
2	B	6	MAN	C1-O5-C5	2.56	115.66	112.19
2	B	9	SIA	C4-C3-C2	2.45	114.20	109.81
2	B	8	GAL	C1-O5-C5	2.45	115.51	112.19
2	B	9	SIA	O1B-C1-O1A	2.36	129.46	124.09
2	B	5	SIA	O1B-C1-O1A	2.33	129.37	124.09
2	B	9	SIA	C11-C10-N5	2.31	120.00	116.10
2	B	9	SIA	C6-O6-C2	2.20	116.04	111.34
2	B	8	GAL	C1-C2-C3	2.17	112.33	109.67
2	B	9	SIA	O1A-C1-C2	-2.16	117.46	122.57
2	B	4	GAL	O2-C2-C3	-2.16	105.81	110.14
2	B	9	SIA	C3-C4-C5	-2.07	108.96	111.46
2	B	4	GAL	O2-C2-C1	2.01	113.27	109.15
2	B	9	SIA	O10-C10-C11	-2.01	118.33	122.06
2	B	2	MAN	O2-C2-C3	-2.00	106.13	110.14

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5	SIA	C5-C6-C7-C8
2	B	5	SIA	C5-C6-C7-O7
2	B	5	SIA	O6-C6-C7-C8
2	B	5	SIA	O6-C6-C7-O7
2	B	5	SIA	O8-C8-C9-O9
2	B	9	SIA	C6-C7-C8-C9
2	B	9	SIA	C6-C7-C8-O8
2	B	9	SIA	O7-C7-C8-O8
2	B	9	SIA	C7-C8-C9-O9
2	B	9	SIA	O8-C8-C9-O9
2	B	3	NAG	C4-C5-C6-O6
2	B	3	NAG	O5-C5-C6-O6
2	B	5	SIA	C7-C8-C9-O9
2	B	5	SIA	C11-C10-N5-C5
2	B	5	SIA	O10-C10-N5-C5
2	B	9	SIA	C11-C10-N5-C5
2	B	9	SIA	O10-C10-N5-C5
2	B	6	MAN	O5-C5-C6-O6
2	B	6	MAN	C4-C5-C6-O6
2	B	9	SIA	O7-C7-C8-C9

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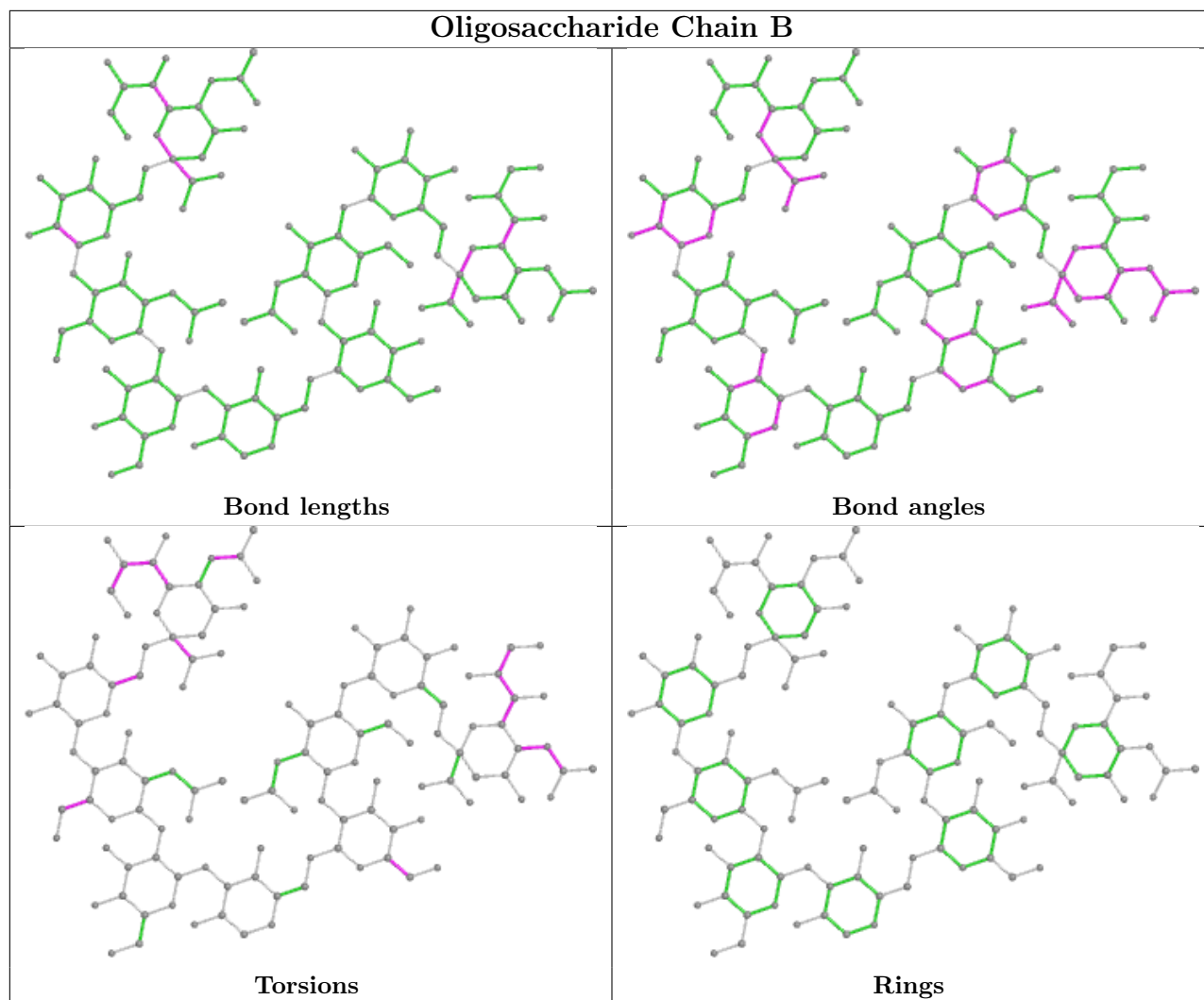
Mol	Chain	Res	Type	Atoms
2	B	5	SIA	C6-C7-C8-O8
2	B	4	GAL	O5-C5-C6-O6
2	B	5	SIA	C6-C7-C8-C9
2	B	9	SIA	C6-C5-N5-C10
2	B	9	SIA	O6-C6-C7-O7
2	B	5	SIA	O7-C7-C8-O8
2	B	5	SIA	O1A-C1-C2-O6
2	B	9	SIA	C4-C5-N5-C10

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	9	SIA	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
3	NGO	A	10	2	15,15,15	4.60	6 (40%)	15,22,22	3.57	7 (46%)

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	NGO	A	10	2	-	1/2/30/30	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	10	NGO	O1-C7	11.68	1.51	1.36
3	A	10	NGO	C1-C2	-8.43	1.36	1.52
3	A	10	NGO	O5-C1	7.81	1.61	1.41
3	A	10	NGO	C2-N2	4.39	1.52	1.47
3	A	10	NGO	C4-C5	-2.21	1.48	1.53
3	A	10	NGO	O5-C5	-2.15	1.39	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	10	NGO	O1-C7-C8	9.55	123.66	114.90
3	A	10	NGO	C1-O1-C7	-4.73	100.35	106.88
3	A	10	NGO	C1-O5-C5	-4.50	104.86	113.69
3	A	10	NGO	O5-C1-O1	4.37	117.01	109.24
3	A	10	NGO	C2-N2-C7	-4.01	103.75	106.46
3	A	10	NGO	O6-C6-C5	-3.34	99.82	111.29
3	A	10	NGO	C8-C7-N2	-2.16	123.81	127.04

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	10	NGO	O5-C5-C6-O6

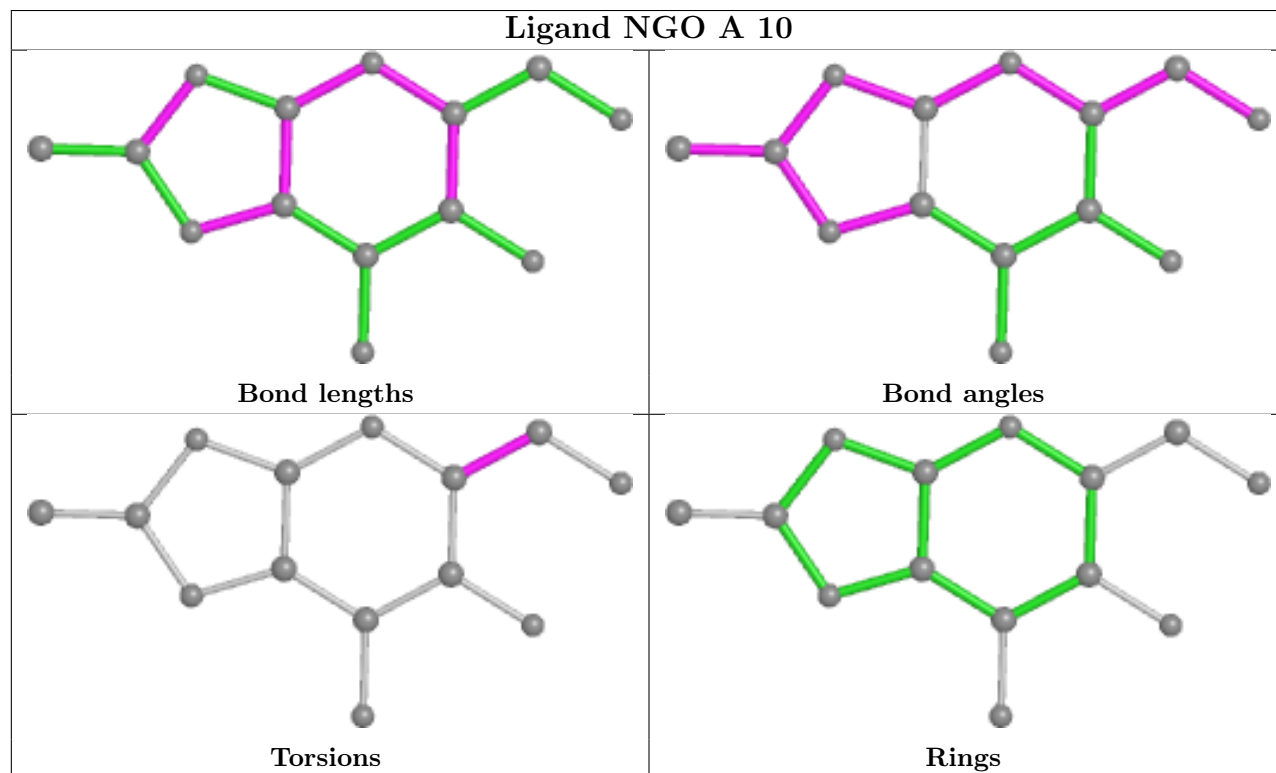
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	10	NGO	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 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

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(Å ²)	Q<0.9
1	A	876/961 (91%)	0.61	84 (9%) 8 10	28, 51, 108, 161	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	932	PHE	12.4
1	A	928	GLN	9.2
1	A	927	GLN	8.1
1	A	844	ASP	7.8
1	A	935	GLU	6.8
1	A	929	LYS	6.6
1	A	542	LYS	6.4
1	A	922	ALA	6.3
1	A	930	ASP	6.3
1	A	926	SER	5.9
1	A	933	SER	5.8
1	A	923	GLU	5.5
1	A	793	THR	5.4
1	A	847	LYS	5.3
1	A	541	ARG	5.2
1	A	841	HIS	5.1
1	A	788	LEU	5.0
1	A	414	ASN	4.9
1	A	845	SER	4.9
1	A	848	VAL	4.8
1	A	790	ASN	4.7
1	A	415	GLY	4.6
1	A	972	ILE	4.5
1	A	840	GLY	4.4
1	A	942	VAL	4.4
1	A	842	LEU	4.4
1	A	543	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	130	ALA	4.0
1	A	792	THR	3.9
1	A	791	ASP	3.8
1	A	158	TYR	3.8
1	A	789	ASN	3.6
1	A	910	PRO	3.5
1	A	843	GLU	3.4
1	A	934	GLN	3.4
1	A	824	ILE	3.4
1	A	846	SER	3.4
1	A	911	GLU	3.3
1	A	946	ALA	3.3
1	A	971	TYR	3.2
1	A	939	GLU	3.2
1	A	129	PRO	3.1
1	A	786	GLY	3.1
1	A	744	THR	3.1
1	A	921	ALA	3.1
1	A	823	LYS	3.0
1	A	931	LYS	2.9
1	A	540	ASP	2.9
1	A	937	LEU	2.9
1	A	132	LYS	2.9
1	A	915	VAL	2.9
1	A	925	LEU	2.9
1	A	537	LYS	2.8
1	A	798	SER	2.8
1	A	822	SER	2.8
1	A	973	ASP	2.7
1	A	851	SER	2.6
1	A	943	LYS	2.6
1	A	381	ALA	2.6
1	A	808	LYS	2.6
1	A	938	LYS	2.6
1	A	936	GLN	2.5
1	A	160	LEU	2.5
1	A	787	LEU	2.5
1	A	916	MET	2.4
1	A	945	ALA	2.4
1	A	438	VAL	2.4
1	A	924	GLU	2.4
1	A	850	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	912	ALA	2.3
1	A	416	PRO	2.3
1	A	968	VAL	2.2
1	A	385	ALA	2.2
1	A	858	TRP	2.1
1	A	743	SER	2.1
1	A	756	GLU	2.1
1	A	317	ASN	2.1
1	A	417	LYS	2.1
1	A	918	THR	2.1
1	A	852	LEU	2.0
1	A	545	ALA	2.0
1	A	131	GLU	2.0
1	A	379	THR	2.0
1	A	435	LEU	2.0

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

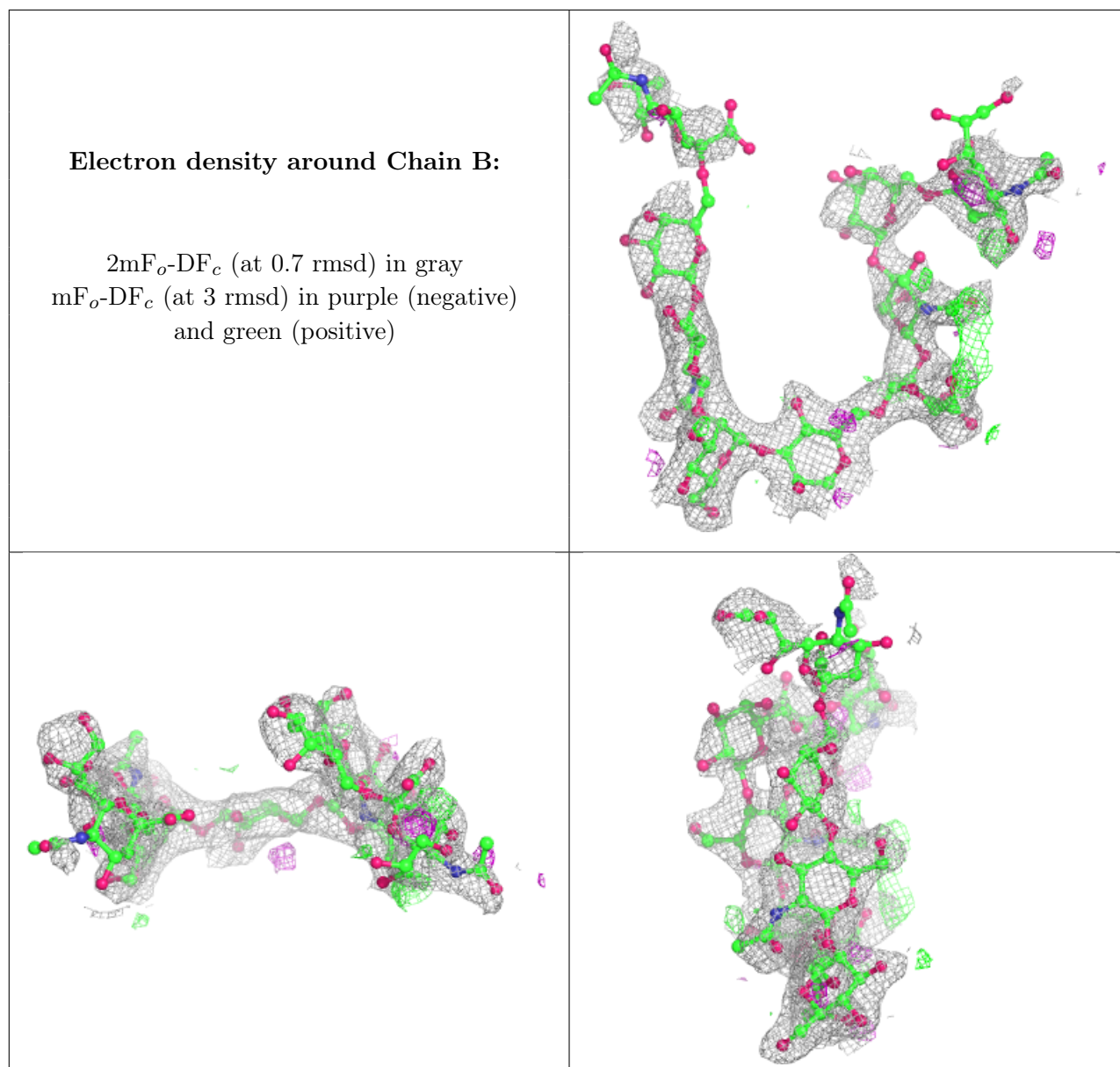
There are no non-standard protein/DNA/RNA residues in this entry.

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	SIA	B	9	20/21	0.53	0.32	92,106,118,118	0
2	SIA	B	5	20/21	0.61	0.39	88,129,138,138	0
2	NAG	B	7	14/15	0.74	0.24	72,89,102,111	0
2	GAL	B	8	11/12	0.76	0.21	109,114,118,119	0
2	GAL	B	4	11/12	0.84	0.28	80,99,119,131	0
2	MAN	B	6	11/12	0.87	0.15	55,63,67,71	0
2	NAG	B	3	14/15	0.91	0.14	48,62,69,80	0
2	MAN	B	2	11/12	0.95	0.12	36,39,48,51	0
2	BMA	B	1	11/12	0.95	0.11	31,40,53,55	0

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



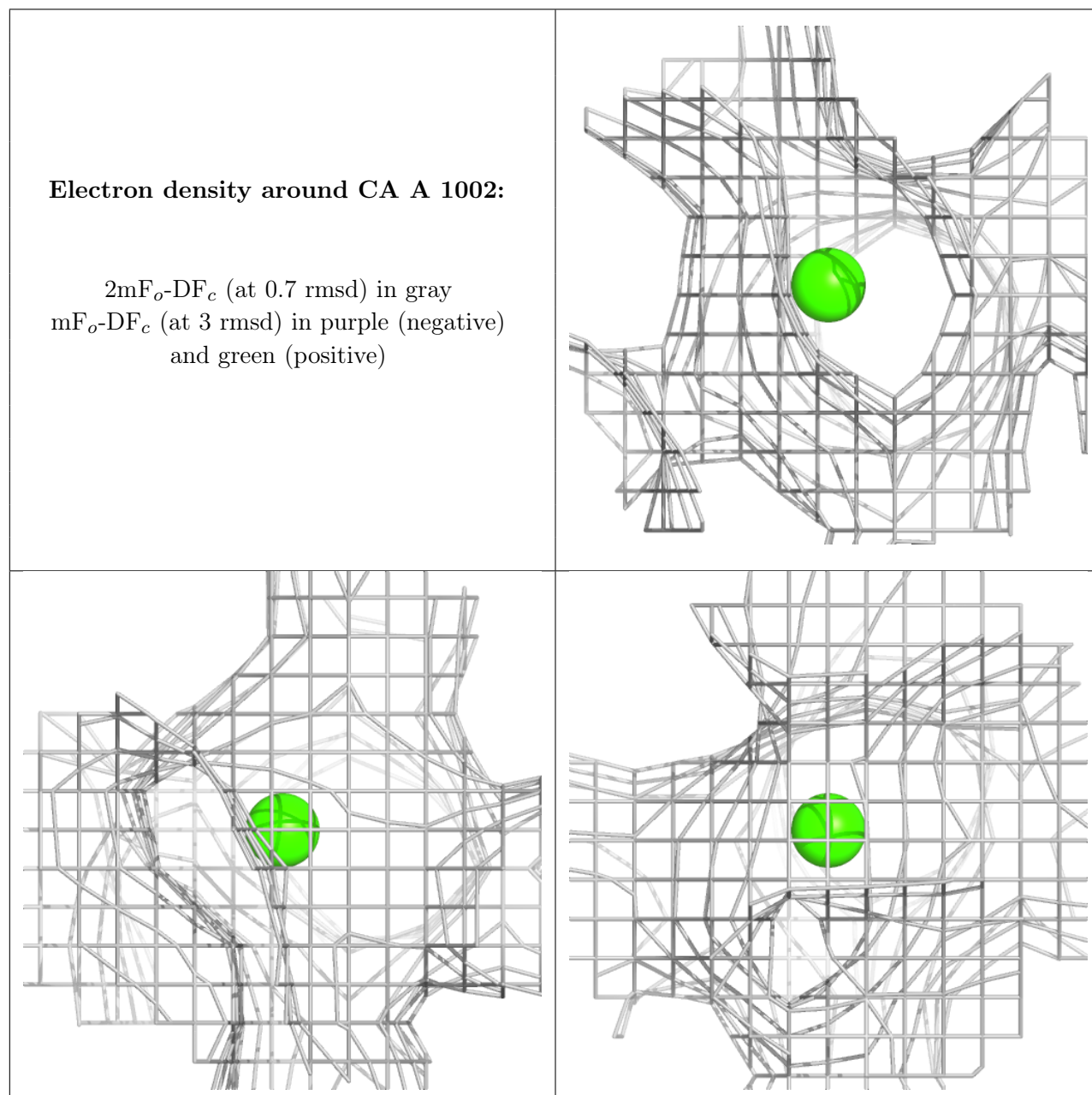
6.4 Ligands [i](#)

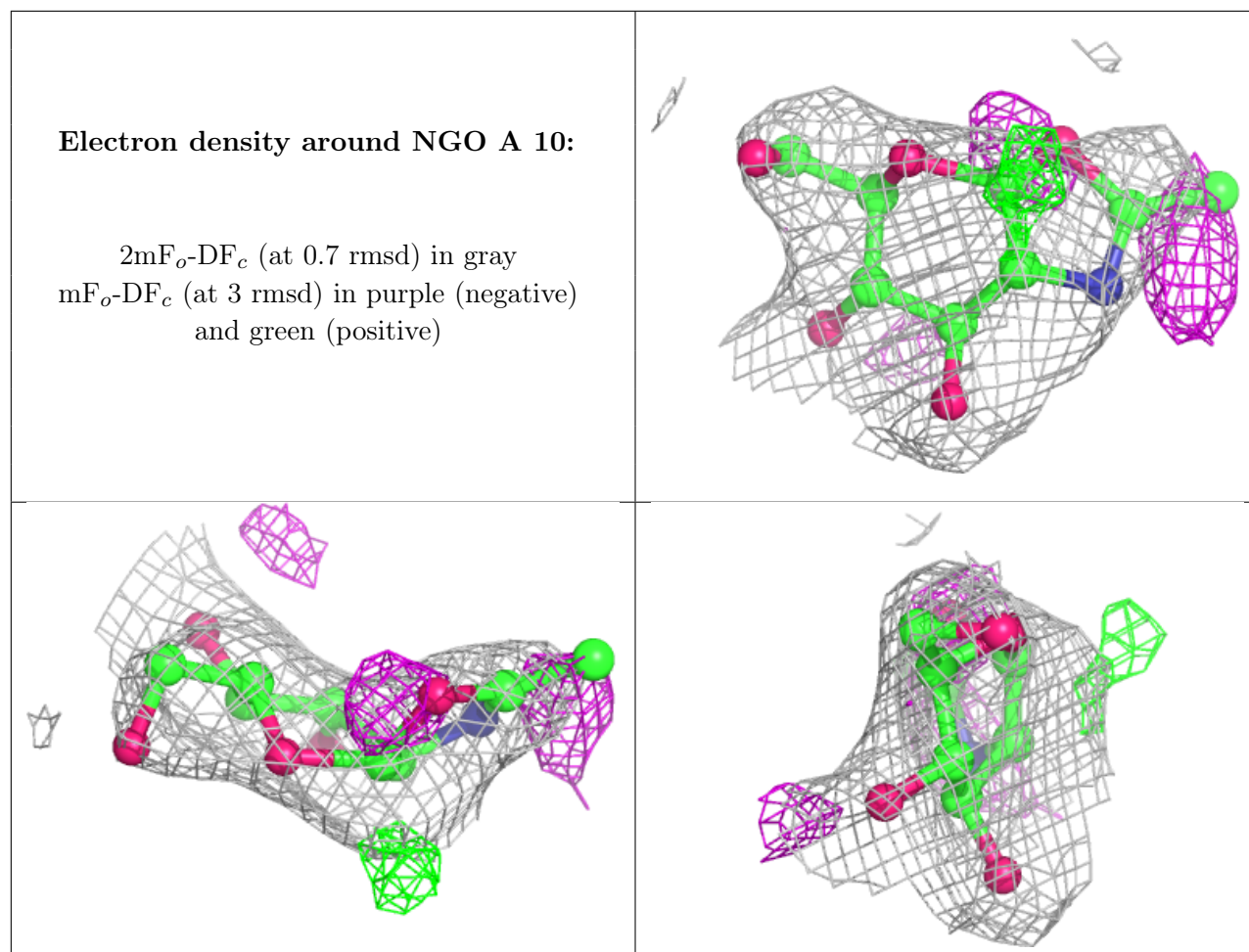
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
4	CA	A	1002	1/1	0.88	0.20	82,82,82,82	0
3	NGO	A	10	14/14	0.92	0.19	39,55,65,66	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.