



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:01 AM UTC

PDB ID : 7BM6 / pdb_00007bm6
Title : Structure-function analysis of a new PL17 oligoalginate lyase from the marine bacterium *Zobellia galactanivorans* DsijT
Authors : Czjzek, M.; Roret, T.; Jouanneau, D.; Le Duff, N.; Jeudy, A.
Deposited on : 2021-01-19
Resolution : 2.16 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

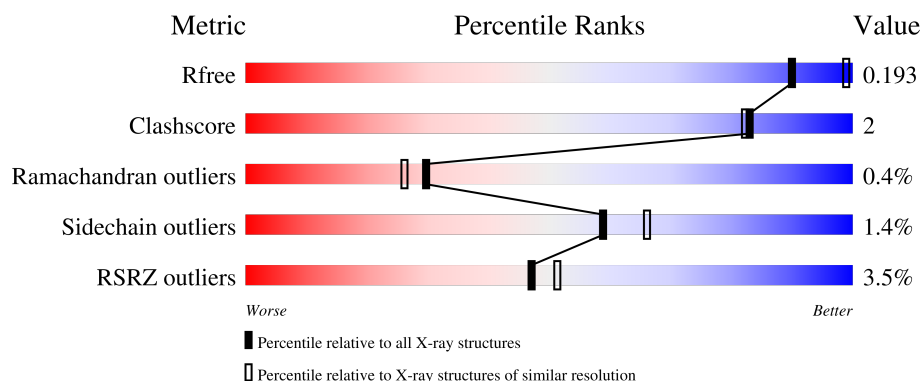
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	751	3% 90% 6% ••
1	B	751	4% 90% 6% •
2	C	2	100%
2	D	2	100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12658 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.

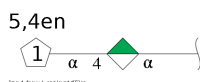
- Molecule 1 is a protein called Alginate lyase, family PL17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	7	0
			5840	3721	985	1120	14			
1	B	727	Total	C	N	O	S	0	8	0
			5846	3724	985	1124	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	ALA	TYR	engineered mutation	UNP G0LCA3
B	274	ALA	TYR	engineered mutation	UNP G0LCA3

- Molecule 2 is an oligosaccharide called 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-alpha-D-mannopyranuronic acid.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			24	12	12			
2	D	2	Total	C	O	0	0	0
			24	12	12			

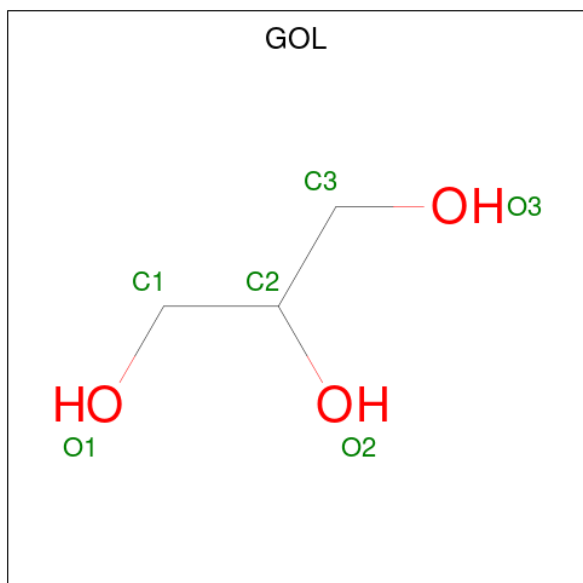
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

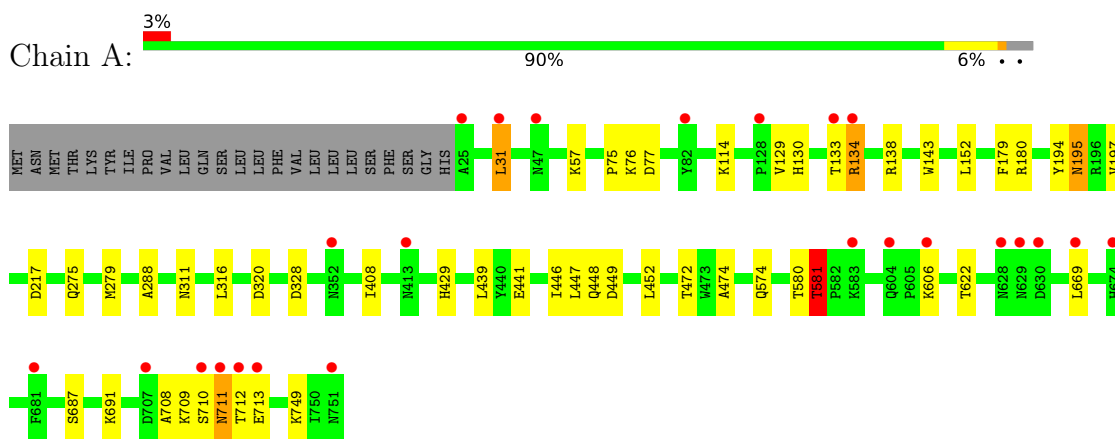
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	475	Total	O	0	0
			475	475		
6	B	437	Total	O	0	0
			437	437		

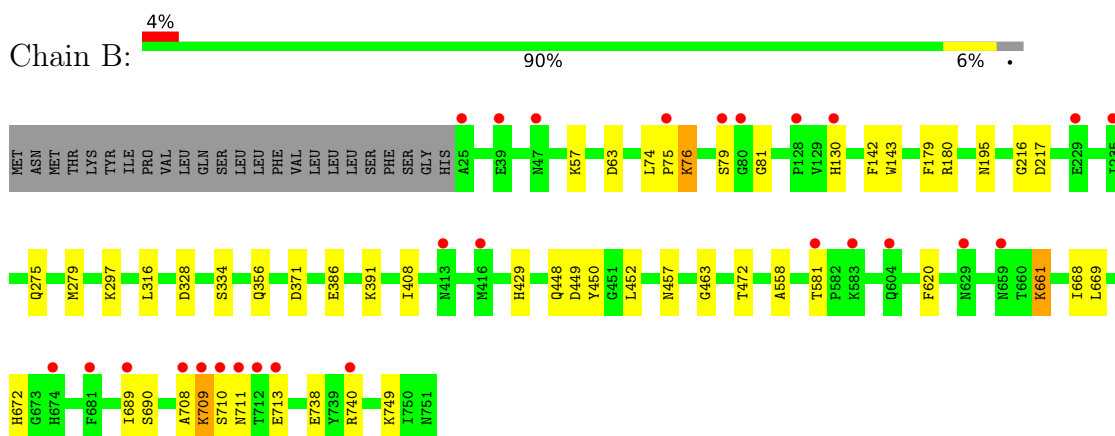
3 Residue-property plots [i](#)

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: Alginate lyase, family PL17



- Molecule 1: Alginate lyase, family PL17



- Molecule 2: 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-alpha-D-mannopyranuronic acid



- Molecule 2: 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-alpha-D-mannopyranuronic acid

Chain D:

100%

HA1
HA2

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	164.13Å 164.13Å 168.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.00 – 2.16 45.00 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.00-2.16) 99.8 (45.00-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.153 , 0.182 0.166 , 0.193	Depositor DCC
R_{free} test set	6752 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12658	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL, MAV, MAW, 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	1.08	1/5995 (0.0%)	1.01	11/8111 (0.1%)
1	B	1.08	3/6010 (0.0%)	1.01	10/8132 (0.1%)
All	All	1.08	4/12005 (0.0%)	1.01	21/16243 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	581	THR	C-O	-5.44	1.20	1.25
1	B	216	GLY	C-O	-5.31	1.18	1.24
1	B	63	ASP	C-O	-5.27	1.18	1.24
1	B	450	TYR	C-O	-5.11	1.18	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	449	ASP	N-CA-C	-9.16	94.32	109.07
1	B	195	ASN	N-CA-C	8.41	121.88	112.97
1	A	448	GLN	N-CA-C	7.33	121.37	110.52
1	A	197	VAL	N-CA-C	-7.26	96.54	106.85
1	A	474	ALA	N-CA-C	7.02	119.53	111.11
1	B	581	THR	CB-CA-C	-6.45	101.96	110.34
1	A	179	PHE	N-CA-C	6.25	117.75	111.07
1	B	448	GLN	N-CA-C	6.23	120.07	110.42
1	A	152	LEU	N-CA-C	5.83	117.64	111.28
1	B	334	SER	N-CA-C	5.75	116.68	108.74
1	B	581	THR	CA-C-N	-5.71	114.08	119.85
1	B	581	THR	C-N-CA	-5.71	114.08	119.85
1	A	580	THR	CB-CA-C	-5.67	99.81	109.51
1	B	450	TYR	N-CA-C	5.63	118.14	111.33
1	A	194	TYR	N-CA-C	5.36	118.98	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	449	ASP	N-CA-C	-5.32	99.84	108.52
1	A	472	THR	N-CA-C	5.28	117.94	111.82
1	B	179	PHE	N-CA-C	5.24	116.80	111.14
1	B	472	THR	N-CA-C	5.17	118.85	112.54
1	A	77	ASP	N-CA-C	5.12	118.36	110.42
1	A	195	ASN	N-CA-C	5.11	119.00	112.26

There are no chirality outliers.

There are no planarity outliers.

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	5840	0	5673	33	0
1	B	5846	0	5679	22	0
2	C	24	0	13	0	0
2	D	24	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	B	6	0	8	0	0
6	A	475	0	0	4	0
6	B	437	0	0	0	0
All	All	12658	0	11386	55	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 (55) 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:439:LEU:CD2	1:A:669:LEU:HD23	1.84	1.07
1:A:311[B]:ASN:ND2	6:A:901:HOH:O	1.94	0.98
1:A:439:LEU:CD2	1:A:669:LEU:CD2	2.43	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:LEU:HD23	1:A:669:LEU:CD2	2.08	0.82
1:A:439:LEU:HD22	1:A:669:LEU:HD23	1.62	0.81
1:B:79:SER:OG	1:B:463:GLY:O	2.07	0.73
1:A:31:LEU:HD23	1:A:288:ALA:HB1	1.75	0.68
1:A:439:LEU:HD23	1:A:669:LEU:HD21	1.76	0.67
1:B:713:GLU:OE1	1:B:749:LYS:NZ	2.29	0.66
1:A:581:THR:OG1	6:A:902:HOH:O	2.14	0.65
1:A:709:LYS:C	1:A:711:ASN:H	2.05	0.64
1:A:31:LEU:HD23	1:A:288:ALA:CB	2.27	0.64
1:A:709:LYS:O	1:A:711:ASN:N	2.33	0.61
1:A:439:LEU:HD21	1:A:669:LEU:HD23	1.79	0.60
1:A:320:ASP:OD2	6:A:903:HOH:O	2.16	0.60
1:A:709:LYS:C	1:A:711:ASN:N	2.58	0.59
1:B:275:GLN:O	1:B:279:MET:HG2	2.03	0.58
1:A:275:GLN:O	1:A:279:MET:HG2	2.03	0.57
1:B:708:ALA:C	1:B:710:SER:H	2.13	0.57
1:B:130:HIS:CD2	1:B:142:PHE:C	2.83	0.57
1:A:711:ASN:C	1:A:713:GLU:H	2.13	0.56
1:A:574:GLN:NE2	6:A:909:HOH:O	2.40	0.54
1:A:31:LEU:CD2	1:A:288:ALA:HB1	2.37	0.54
1:A:180:ARG:NH1	1:A:217:ASP:OD2	2.24	0.53
1:A:279:MET:HE2	1:A:279:MET:HA	1.90	0.52
1:B:180:ARG:NH1	1:B:217:ASP:OD2	2.30	0.52
1:A:711:ASN:O	1:A:713:GLU:N	2.43	0.52
1:B:316:LEU:HD23	1:B:408:ILE:HD11	1.91	0.51
1:B:279:MET:HA	1:B:279:MET:HE2	1.91	0.51
1:B:690:SER:CA	1:B:709:LYS:HG3	2.41	0.51
1:B:328:ASP:HB2	1:B:429:HIS:HB3	1.94	0.49
1:A:134:ARG:O	1:A:143:TRP:HZ3	1.96	0.49
1:B:668:ILE:HG21	1:B:689:ILE:HD11	1.93	0.49
1:A:328:ASP:HB2	1:A:429:HIS:HB3	1.93	0.49
1:A:133:THR:HG22	1:A:138:ARG:CZ	2.43	0.49
1:A:316:LEU:HD23	1:A:408:ILE:HD11	1.95	0.48
1:A:129:VAL:O	1:A:130:HIS:C	2.59	0.46
1:B:690:SER:HB2	1:B:709:LYS:HG3	1.98	0.46
1:B:74:LEU:HD12	1:B:75:PRO:HD2	1.97	0.46
1:A:447:LEU:HD12	1:A:669:LEU:HD22	1.99	0.45
1:B:79:SER:C	1:B:81:GLY:H	2.25	0.45
1:B:79:SER:HB2	1:B:457:ASN:HA	1.99	0.45
1:B:738:GLU:OE2	1:B:740:ARG:NH2	2.49	0.45
1:A:711:ASN:C	1:A:713:GLU:N	2.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:LYS:HB3	1:A:691:LYS:HE3	1.86	0.43
1:B:558:ALA:C	1:B:661:LYS:HG2	2.44	0.43
1:B:708:ALA:C	1:B:710:SER:N	2.73	0.42
1:B:130:HIS:CG	1:B:143:TRP:HA	2.55	0.42
1:A:622:THR:HG21	1:A:687:SER:HB2	2.01	0.41
1:B:74:LEU:O	1:B:75:PRO:C	2.64	0.41
1:B:620:PHE:HB2	1:B:672:HIS:O	2.21	0.41
1:A:441:GLU:CB	1:A:446[B]:ILE:HD11	2.51	0.41
1:A:708:ALA:HB3	1:A:713:GLU:HB2	2.03	0.41
1:B:356:GLN:HA	1:B:386:GLU:O	2.21	0.40
1:A:75:PRO:O	1:A:76[B]:LYS:HD3	2.22	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	731/751 (97%)	695 (95%)	33 (4%)	3 (0%)	30	26
1	B	734/751 (98%)	701 (96%)	30 (4%)	3 (0%)	30	26
All	All	1465/1502 (98%)	1396 (95%)	63 (4%)	6 (0%)	30	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	712	THR
1	A	710	SER
1	A	711	ASN
1	B	76	LYS
1	B	711	ASN
1	B	709	LYS

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	624/642 (97%)	615 (99%)	9 (1%)	59	66
1	B	626/642 (98%)	618 (99%)	8 (1%)	61	68
All	All	1250/1284 (97%)	1233 (99%)	17 (1%)	59	66

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	57	LYS
1	A	114	LYS
1	A	134	ARG
1	A	195	ASN
1	A	452	LEU
1	A	581	THR
1	A	606	LYS
1	A	749	LYS
1	B	57	LYS
1	B	76	LYS
1	B	297	LYS
1	B	371	ASP
1	B	391	LYS
1	B	452	LEU
1	B	661	LYS
1	B	669	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	144	GLN
1	A	177	ASN
1	A	205	ASN
1	A	561	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	571	GLN
1	A	617	ASN
1	A	646	ASN
1	A	674	HIS
1	A	686	ASN
1	B	144	GLN
1	B	147	ASN
1	B	205	ASN
1	B	275	GLN
1	B	485	GLN
1	B	571	GLN
1	B	574	GLN
1	B	617	ASN
1	B	686	ASN

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 ⓘ

4 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	MAV	C	1	2	13,13,13	0.63	0	18,19,19	1.25	2 (11%)
2	MAW	C	2	2	10,11,12	2.29	3 (30%)	12,15,17	1.72	3 (25%)
2	MAV	D	1	2	13,13,13	0.73	0	18,19,19	1.45	3 (16%)
2	MAW	D	2	2	10,11,12	2.28	2 (20%)	12,15,17	2.22	3 (25%)

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	MAV	C	1	2	-	0/4/24/24	0/1/1/1
2	MAW	C	2	2	-	0/4/17/20	0/1/1/1
2	MAV	D	1	2	-	0/4/24/24	0/1/1/1
2	MAW	D	2	2	-	0/4/17/20	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	MAW	O5-C5	6.48	1.46	1.37
2	C	2	MAW	O5-C5	6.05	1.45	1.37
2	C	2	MAW	C3-C4	2.51	1.53	1.50
2	C	2	MAW	O6B-C6	-2.39	1.24	1.30
2	D	2	MAW	C3-C4	2.22	1.53	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	MAW	O5-C5-C4	-5.64	119.76	124.94
2	D	2	MAW	O5-C5-C6	3.28	117.87	111.85
2	C	2	MAW	O5-C5-C4	-3.27	121.93	124.94
2	D	1	MAV	C1-O5-C5	3.15	116.85	112.22
2	C	1	MAV	C1-O5-C5	2.99	116.62	112.22
2	D	2	MAW	O6B-C6-C5	2.85	120.52	114.06
2	C	2	MAW	C1-C2-C3	2.83	113.76	109.64
2	D	1	MAV	C3-C4-C5	2.48	113.56	109.30
2	C	2	MAW	O5-C5-C6	2.32	116.11	111.85
2	D	1	MAV	O6B-C6-C5	2.26	121.81	113.64
2	C	1	MAV	O6B-C6-O6A	-2.22	119.05	124.08

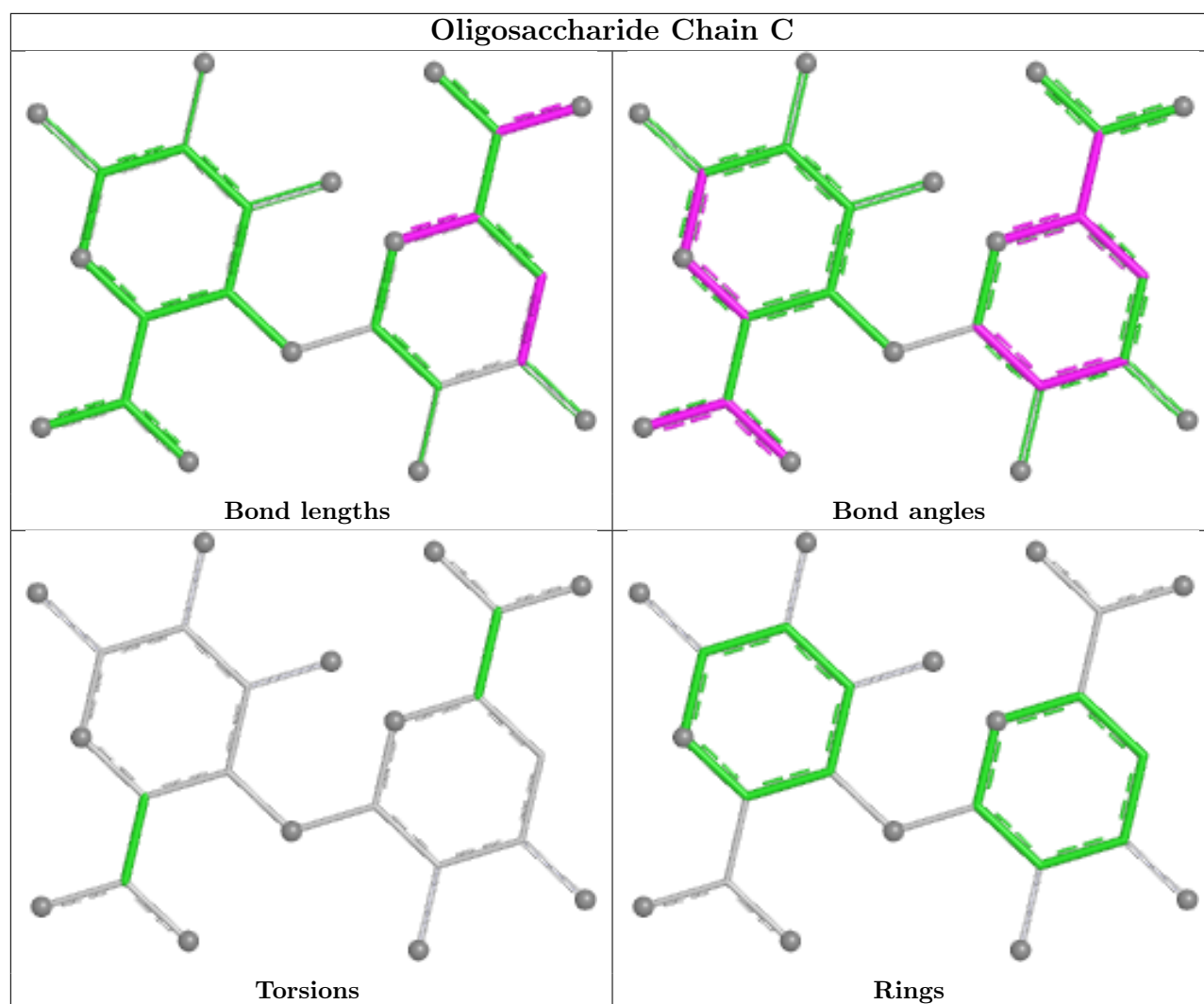
There are no chirality outliers.

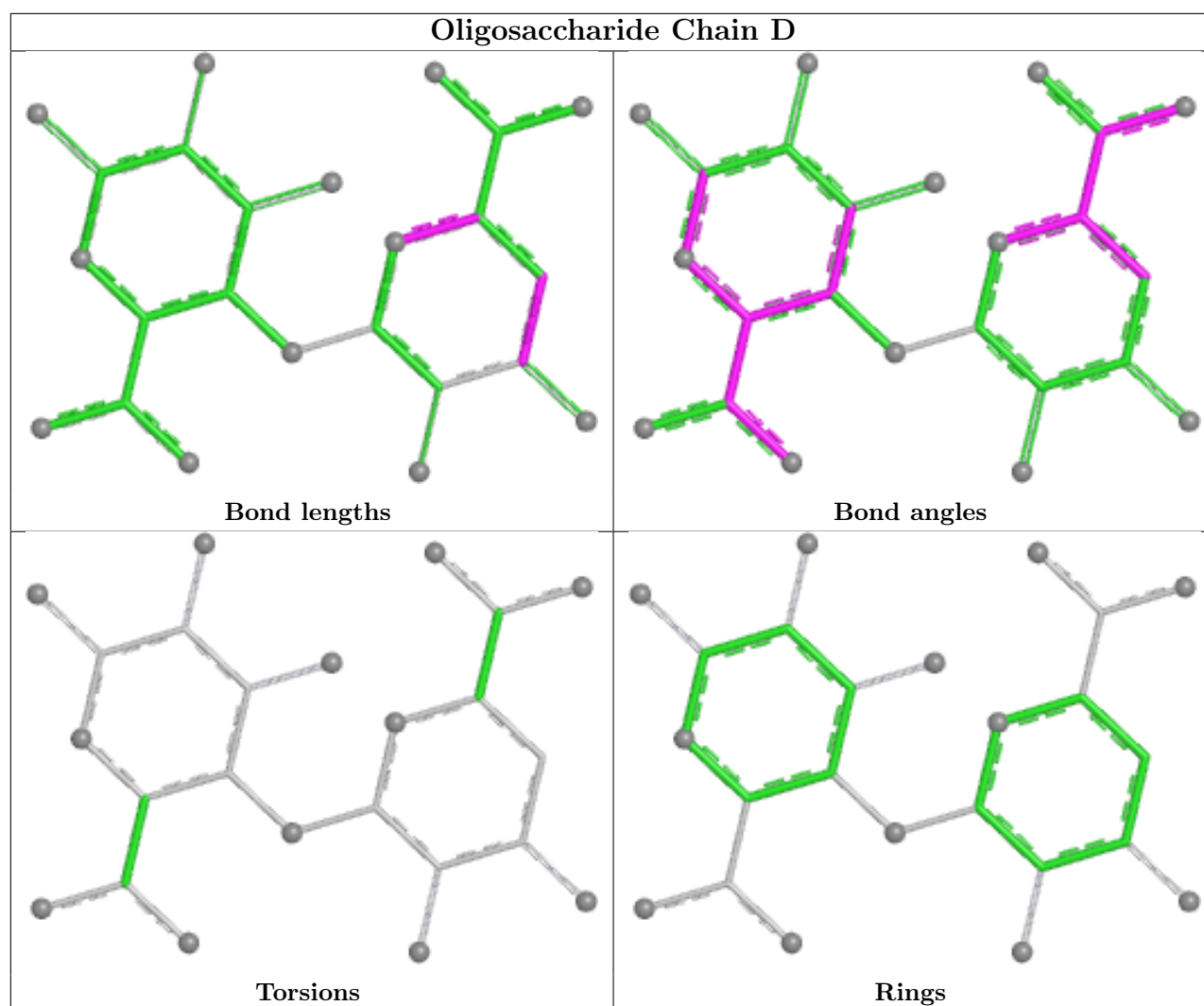
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 7 ligands modelled in this entry, 6 are 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	$\# Z > 2$
5	GOL	B	804	-	5,5,5	0.51	0	5,5,5	0.56	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
5	GOL	B	804	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	804	GOL	C1-C2-C3-O3
5	B	804	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	727/751 (96%)	0.00	24 (3%)	49	53	16, 30, 47, 91	6 (0%)
1	B	727/751 (96%)	0.12	27 (3%)	45	49	13, 31, 48, 104	8 (1%)
All	All	1454/1502 (96%)	0.06	51 (3%)	47	51	13, 31, 47, 104	14 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	712	THR	7.8
1	B	710	SER	7.5
1	B	711	ASN	7.2
1	A	712	THR	6.7
1	B	25	ALA	6.3
1	B	709	LYS	6.2
1	A	25	ALA	5.4
1	A	134	ARG	5.1
1	B	75	PRO	4.9
1	A	133	THR	4.4
1	A	711	ASN	4.4
1	B	713	GLU	4.3
1	B	128	PRO	4.1
1	B	79	SER	4.1
1	A	128	PRO	3.8
1	B	604	GLN	3.6
1	A	674	HIS	3.5
1	A	707	ASP	3.2
1	B	674	HIS	3.1
1	A	710	SER	3.1
1	A	751[A]	ASN	3.0
1	A	413	ASN	2.8
1	A	31	LEU	2.8
1	A	604	GLN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	583	LYS	2.7
1	B	629	ASN	2.6
1	B	413	ASN	2.6
1	B	416	MET	2.6
1	A	629	ASN	2.5
1	A	606	LYS	2.4
1	A	681	PHE	2.4
1	B	47	ASN	2.4
1	A	352	ASN	2.4
1	B	689	ILE	2.4
1	B	39	GLU	2.3
1	B	659	ASN	2.3
1	A	713	GLU	2.3
1	B	130	HIS	2.2
1	B	581	THR	2.2
1	A	669	LEU	2.2
1	B	229	GLU	2.1
1	B	681	PHE	2.1
1	A	47	ASN	2.1
1	B	583	LYS	2.1
1	A	628	ASN	2.0
1	B	740	ARG	2.0
1	A	82	TYR	2.0
1	B	235	ILE	2.0
1	B	708	ALA	2.0
1	A	630	ASP	2.0
1	B	80	GLY	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($\text{\AA}^2$)	Q<0.9
2	MAV	C	1	13/13	0.91	0.13	30,42,59,65	0

Continued on next page...

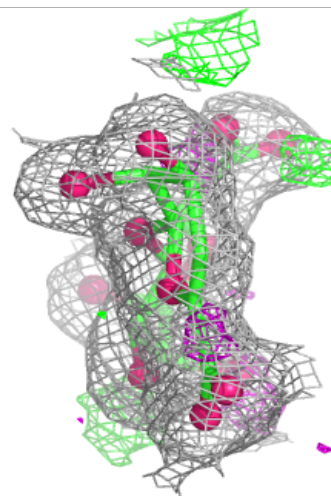
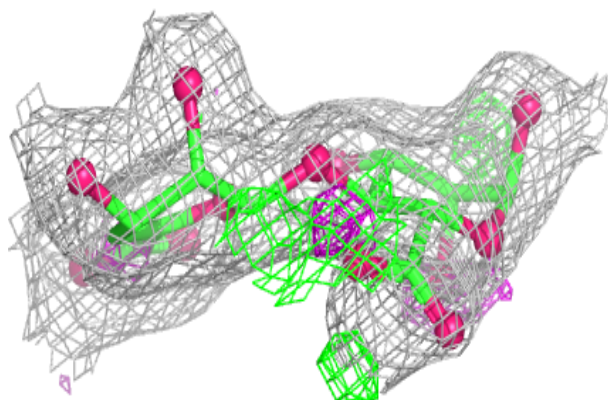
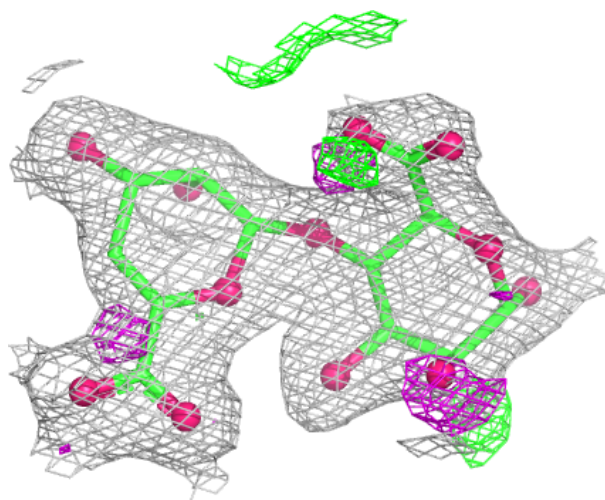
Continued from previous page...

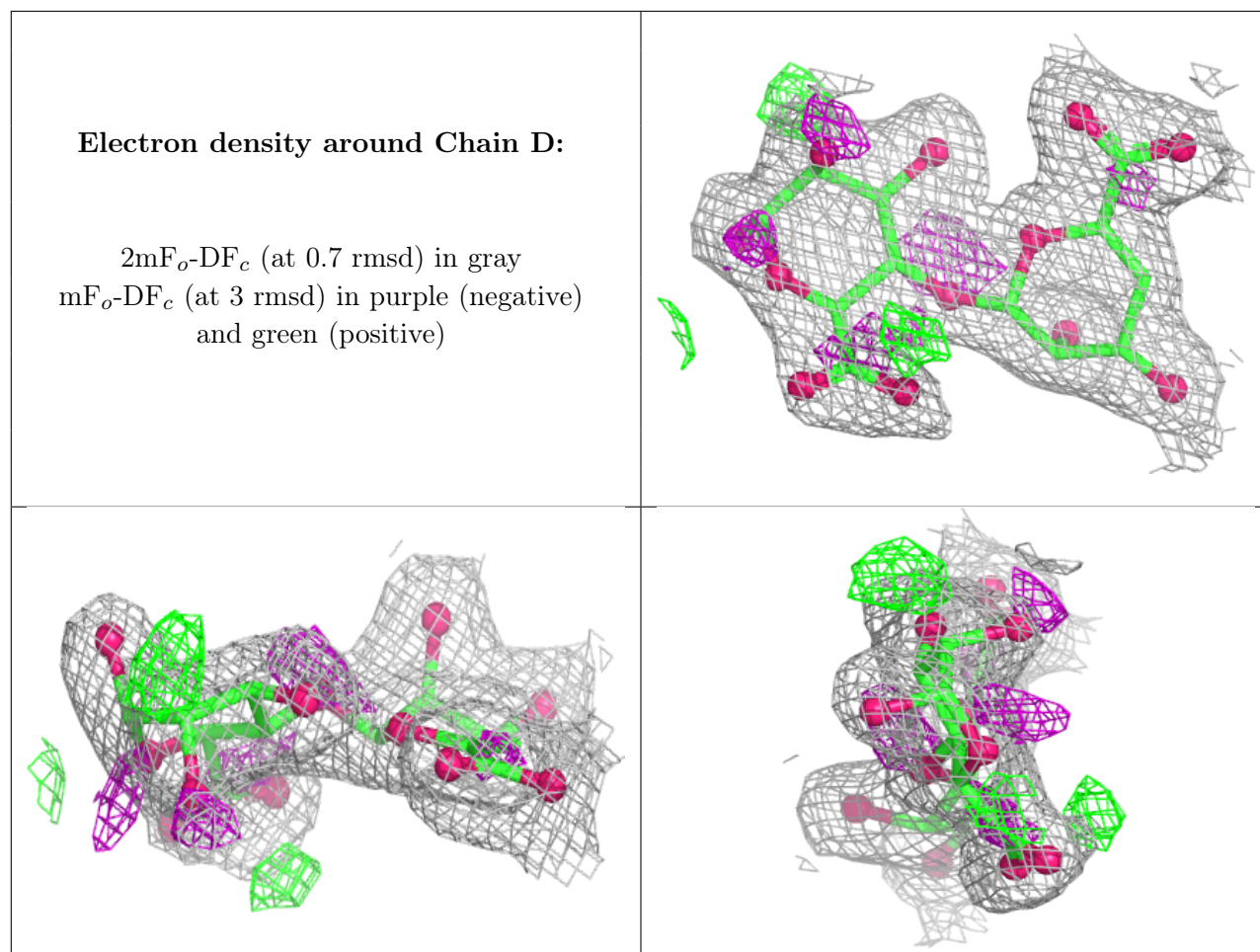
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAV	D	1	13/13	0.92	0.11	27,36,50,52	0
2	MAW	C	2	11/12	0.97	0.07	26,30,33,35	0
2	MAW	D	2	11/12	0.97	0.07	24,29,36,38	0

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 C:

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.

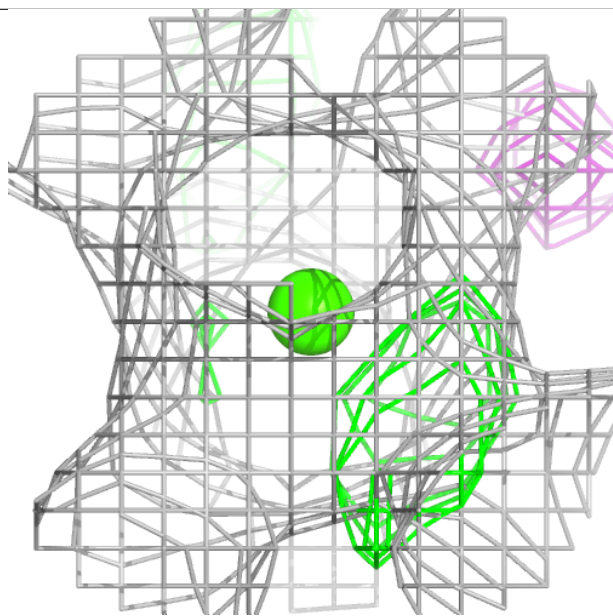
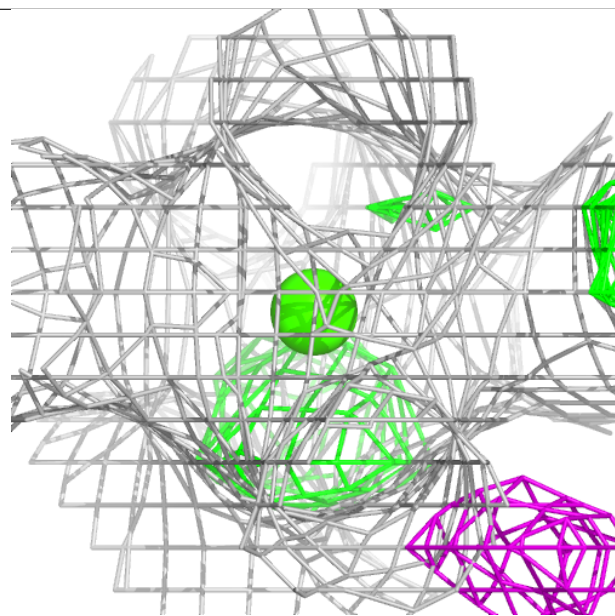
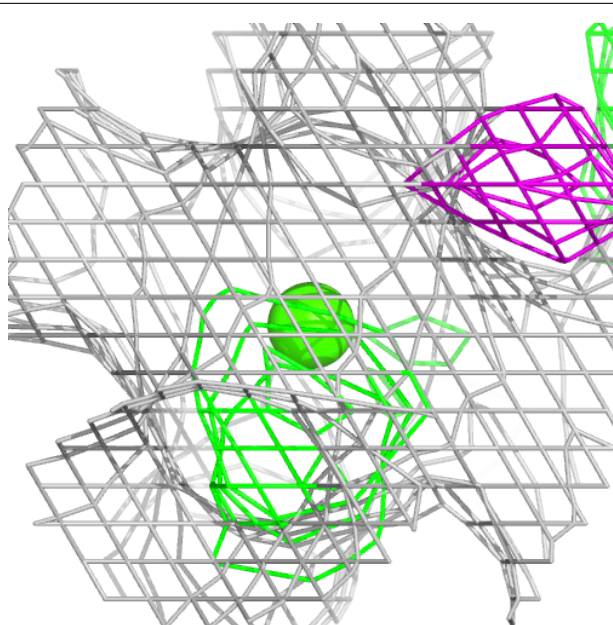
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	803	1/1	0.94	0.08	45,45,45,45	0
4	MG	B	801	1/1	0.96	0.10	42,42,42,42	0
4	MG	B	803	1/1	0.96	0.08	28,28,28,28	0
5	GOL	B	804	6/6	0.96	0.10	34,39,39,42	0
3	CA	A	801	1/1	0.99	0.03	17,17,17,17	0
4	MG	A	802	1/1	0.99	0.13	37,37,37,37	0
3	CA	B	802	1/1	1.00	0.02	17,17,17,17	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.

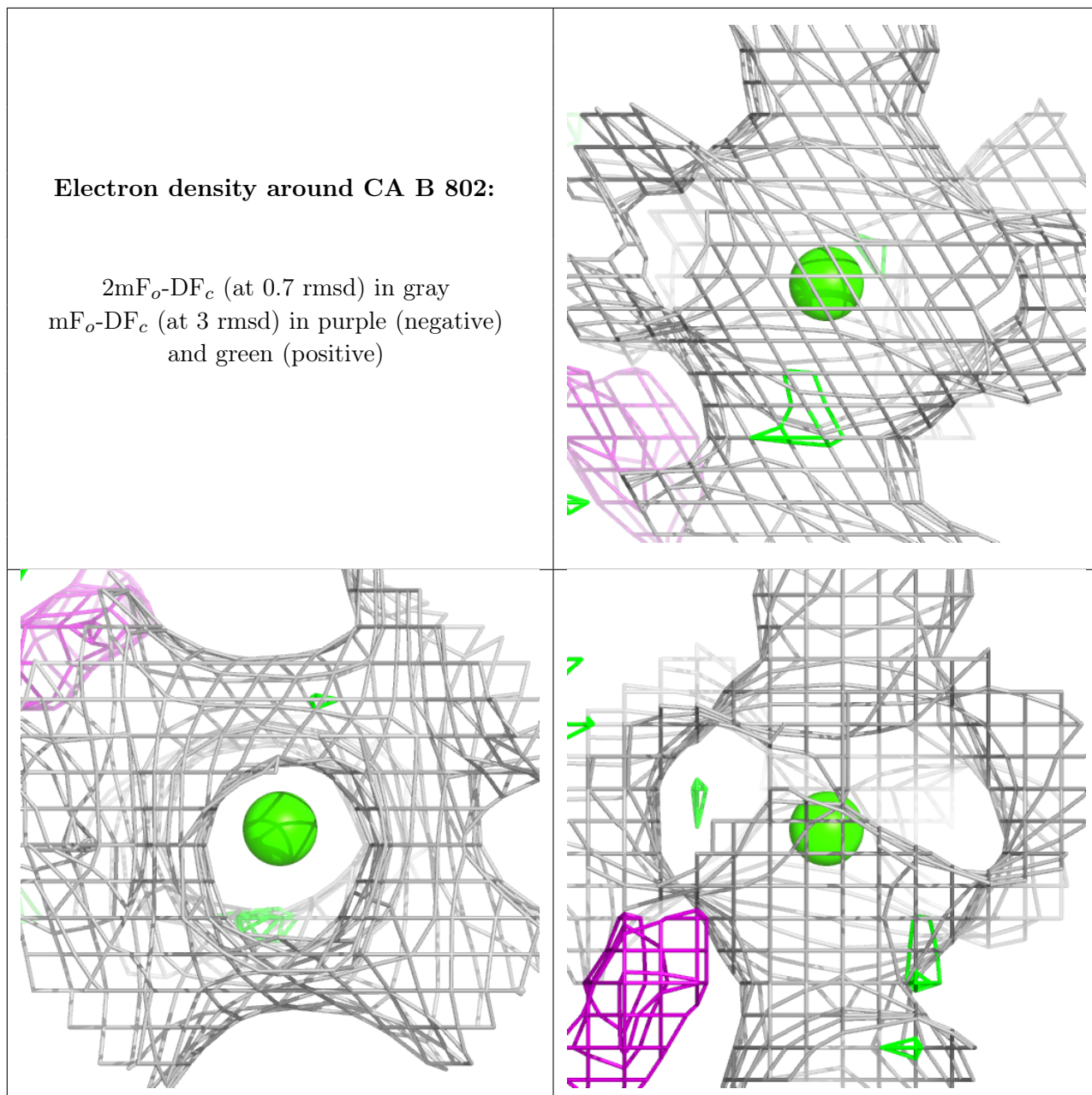
Electron density around CA A 801:

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



Electron density around CA B 802:

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

**6.5 Other polymers** ⓘ

There are no such residues in this entry.