Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2021 – 05:08 am GMT

PDB ID	:	7BM6
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 following versions of software and data (see references ⓘ) were used in the production of this report:

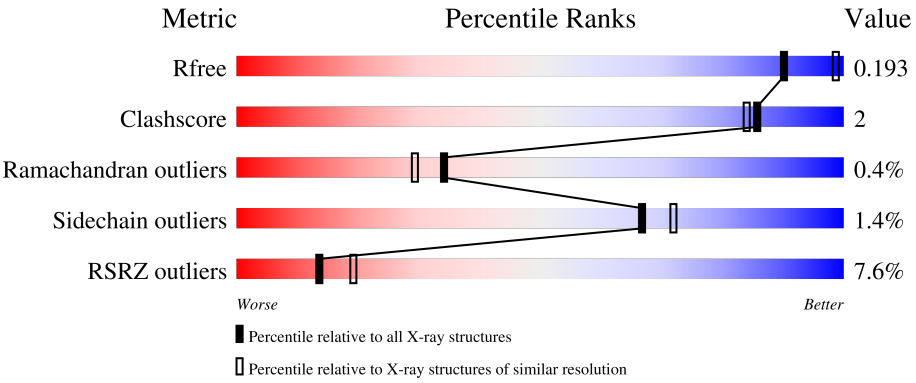
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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 <=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	6% 91% 6%
1	B	751	9% 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.

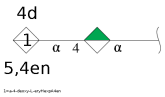
- Molecule 1 is a protein called Alginate lyase, family PL17.

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				

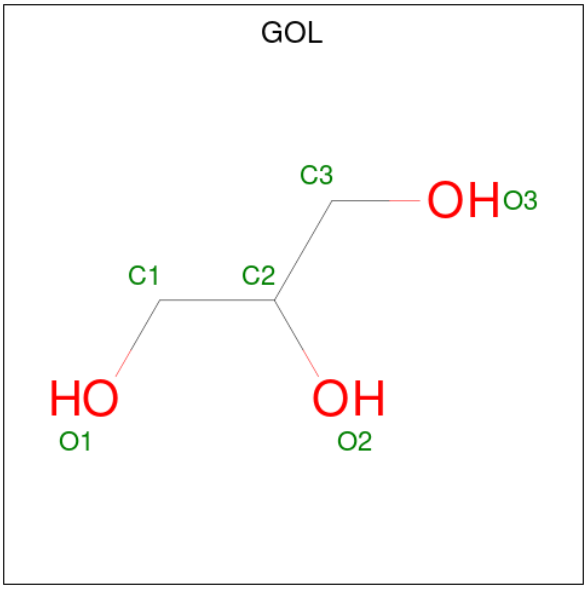
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

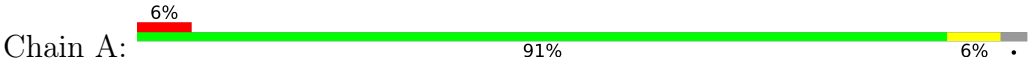
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	475	Total O 475 475	0	0
6	B	437	Total O 437 437	0	0

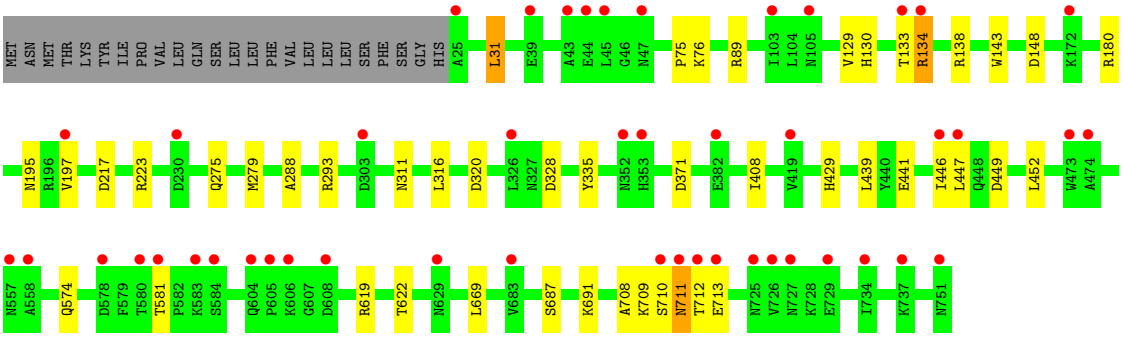
3 Residue-property plots (i)

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

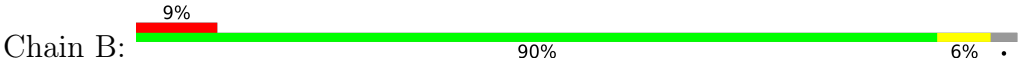
Chain A:

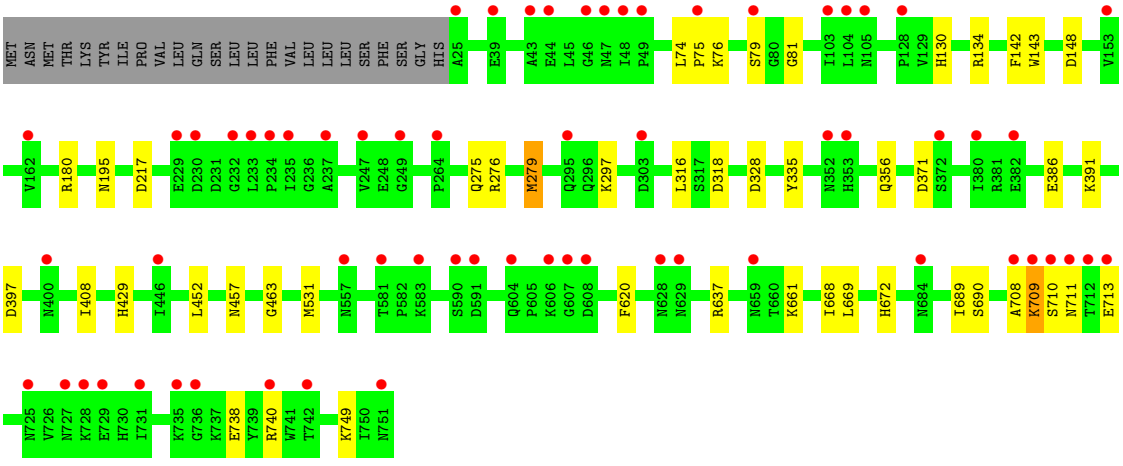




• Molecule 1: Alginate lyase, family PL17

Chain B:



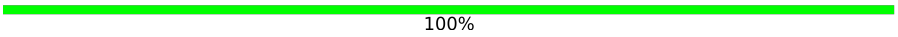


• Molecule 2: 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-alpha-D-mannopyranuronic acid

Chain C:

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

Chain D:



4 Data and refinement statistics (i)

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 47.38 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.00-2.16) 99.8 (47.38-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [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 (4.93%)	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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MAV, MG, 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	0.83	0/5995	0.85	6/8111 (0.1%)
1	B	0.84	0/6010	0.85	7/8132 (0.1%)
All	All	0.84	0/12005	0.85	13/16243 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	637	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	619	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	A	449	ASP	N-CA-C	-6.18	94.32	111.00
1	B	397	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	B	318	ASP	CB-CG-OD1	5.98	123.68	118.30
1	B	279	MET	CG-SD-CE	5.91	109.66	100.20
1	A	223	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	397	ASP	CB-CG-OD1	5.76	123.49	118.30
1	B	531	MET	CG-SD-CE	5.58	109.12	100.20
1	A	293	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	197	VAL	N-CA-C	-5.36	96.54	111.00
1	A	89	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	B	134	ARG	NE-CZ-NH1	5.19	122.90	120.30

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	31	0
1	B	5846	0	5679	19	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	50	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 (50) 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
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: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:709:LYS:C	1:A:711:ASN:H	2.05	0.60
1:A:320:ASP:OD2	6:A:903:HOH:O	2.16	0.60
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:A:709:LYS:C	1:A:711:ASN:N	2.58	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ARG:NH1	1:A:217:ASP:OD2	2.24	0.53
1:B:708:ALA:C	1:B:710:SER:H	2.13	0.53
1:B:130:HIS:CD2	1:B:142:PHE:C	2.83	0.52
1:B:180:ARG:NH1	1:B:217:ASP:OD2	2.30	0.52
1:A:711:ASN:C	1:A:713:GLU:H	2.13	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: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: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: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:691:LYS:HB3	1:A:691:LYS:HE3	1.86	0.43
1:B:130:HIS:CG	1:B:143:TRP:HA	2.55	0.42
1:A:129:VAL:O	1:A:130:HIS:C	2.59	0.42
1:A:622:THR:HG21	1:A:687:SER:HB2	2.01	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
1:B:79:SER:C	1:B:81:GLY:H	2.25	0.40
1:B:708:ALA:C	1:B:710:SER:N	2.73	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%)	34	29
1	B	734/751 (98%)	701 (96%)	30 (4%)	3 (0%)	34	29
All	All	1465/1502 (98%)	1396 (95%)	63 (4%)	6 (0%)	34	29

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 (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	624/642 (97%)	617 (99%)	7 (1%)	73	78
1	B	626/642 (98%)	616 (98%)	10 (2%)	62	67
All	All	1250/1284 (97%)	1233 (99%)	17 (1%)	67	72

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

Mol	Chain	Res	Type
1	A	31	LEU
1	A	134	ARG
1	A	148	ASP
1	A	195	ASN
1	A	335	TYR
1	A	371	ASP
1	A	452	LEU

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Mol	Chain	Res	Type
1	B	148	ASP
1	B	195	ASN
1	B	276	ARG
1	B	297	LYS
1	B	335	TYR
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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	686	ASN
1	B	275	GLN
1	B	574	GLN
1	B	634	HIS
1	B	686	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)

4 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

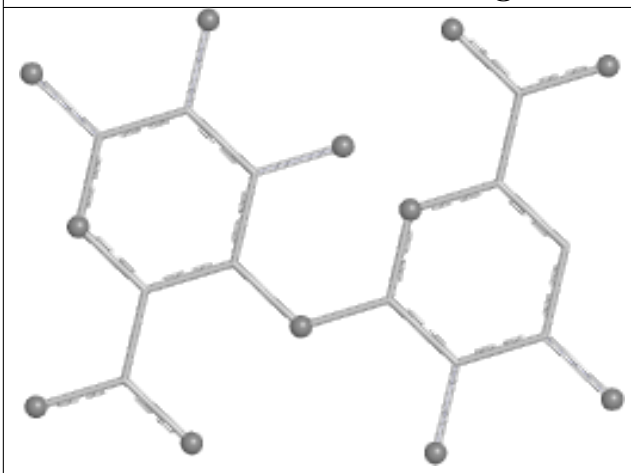
There are no torsion outliers.

There are no ring outliers.

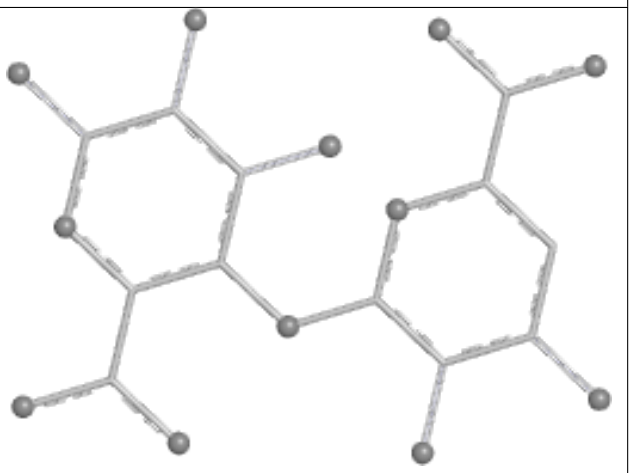
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

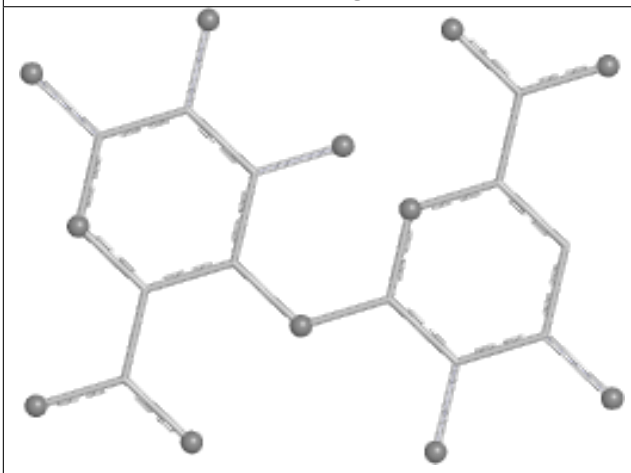
Oligosaccharide Chain C



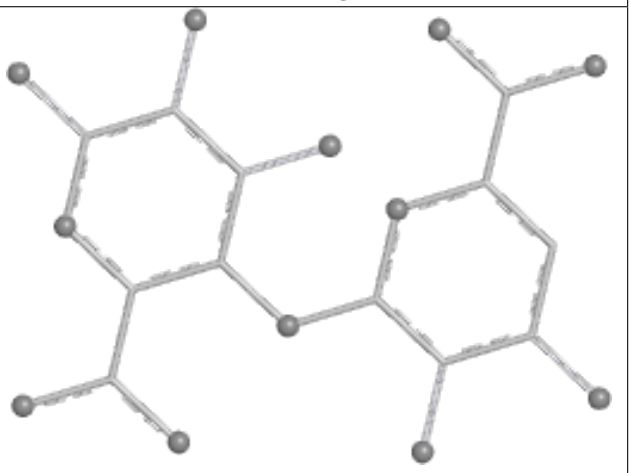
Bond lengths



Bond angles

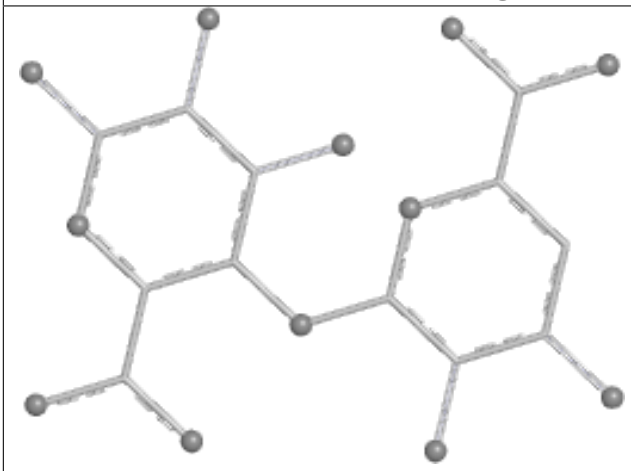


Torsions

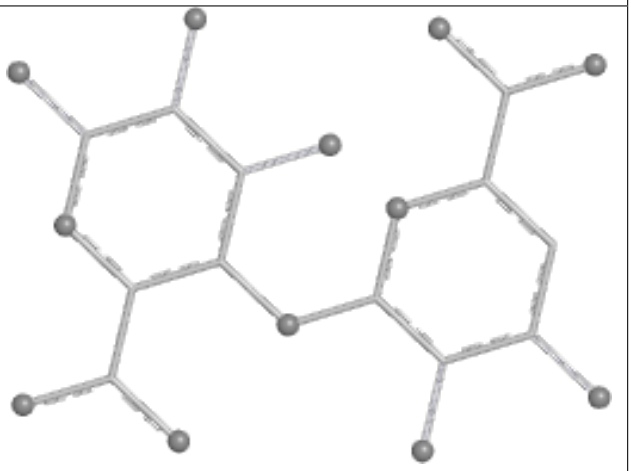


Rings

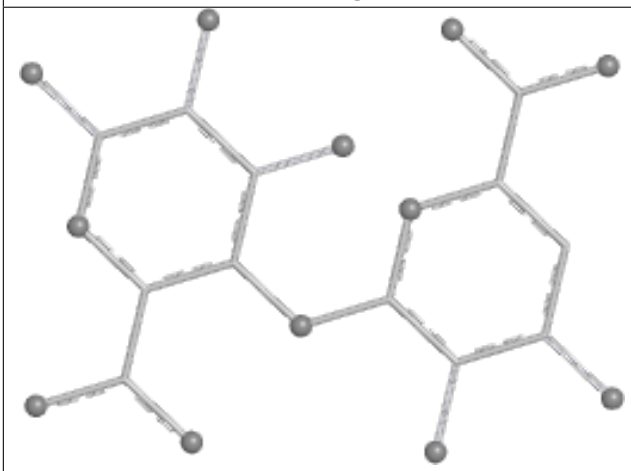
Oligosaccharide Chain D



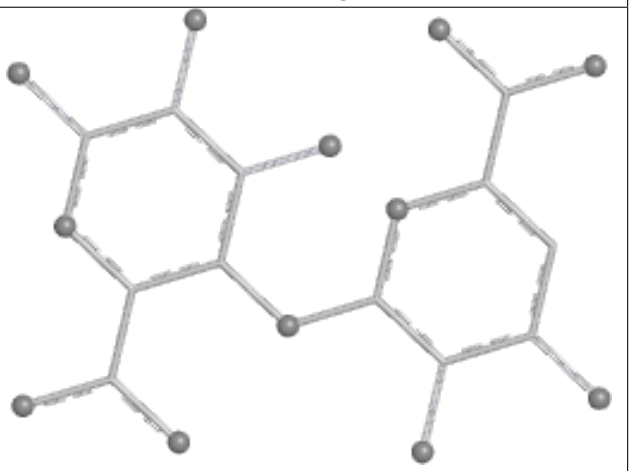
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (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, 95^{th} 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%)	0.76	47 (6%)	18	25	22, 30, 47, 91	0
1	B	727/751 (96%)	0.80	64 (8%)	10	14	23, 31, 48, 104	0
All	All	1454/1502 (96%)	0.78	111 (7%)	13	19	22, 31, 47, 104	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	711	ASN	9.9
1	A	711	ASN	9.1
1	B	712	THR	8.0
1	A	583	LYS	6.5
1	A	710	SER	5.9
1	B	230	ASP	5.8
1	B	710	SER	5.5
1	A	25	ALA	5.0
1	B	25	ALA	4.8
1	B	606	LYS	4.8
1	B	352	ASN	4.6
1	A	712	THR	4.5
1	A	751[A]	ASN	4.3
1	A	604	GLN	4.2
1	A	134	ARG	3.9
1	A	303	ASP	3.6
1	B	709	LYS	3.5
1	A	133	THR	3.4
1	B	382	GLU	3.4
1	B	629	ASN	3.4
1	B	736	GLY	3.4
1	A	606	LYS	3.3
1	B	229	GLU	3.3
1	A	629	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	48	ILE	3.3
1	B	725	ASN	3.2
1	B	75	PRO	3.2
1	B	247	VAL	3.2
1	A	725	ASN	3.1
1	B	372	SER	3.1
1	B	303	ASP	3.1
1	A	446[A]	ILE	3.0
1	A	447	LEU	3.0
1	A	578	ASP	3.0
1	B	47	ASN	3.0
1	B	234	PRO	3.0
1	B	583	LYS	2.9
1	B	43	ALA	2.9
1	B	105	ASN	2.8
1	A	726	VAL	2.8
1	B	128	PRO	2.8
1	B	104	LEU	2.8
1	A	557	ASN	2.8
1	B	740	ARG	2.8
1	B	590	SER	2.8
1	B	604	GLN	2.7
1	B	727	ASN	2.7
1	A	581	THR	2.6
1	A	729	GLU	2.6
1	B	235	ILE	2.6
1	B	742[A]	THR	2.6
1	A	197	VAL	2.5
1	B	79	SER	2.5
1	B	735	LYS	2.5
1	A	47	ASN	2.5
1	B	232	GLY	2.5
1	B	233	LEU	2.5
1	B	607	GLY	2.5
1	A	608	ASP	2.5
1	B	731	ILE	2.5
1	B	557	ASN	2.5
1	A	382	GLU	2.5
1	B	400	ASN	2.4
1	B	49	PRO	2.4
1	A	352	ASN	2.4
1	B	103	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	591	ASP	2.3
1	A	727	ASN	2.3
1	B	608	ASP	2.3
1	A	44	GLU	2.3
1	A	230	ASP	2.3
1	A	105	ASN	2.3
1	A	473	TRP	2.3
1	A	734	ILE	2.3
1	A	419	VAL	2.2
1	B	264	PRO	2.2
1	B	380	ILE	2.2
1	A	474	ALA	2.2
1	B	581	THR	2.2
1	B	713	GLU	2.2
1	B	729	GLU	2.2
1	B	751	ASN	2.2
1	A	45	LEU	2.2
1	B	162	VAL	2.2
1	A	43	ALA	2.2
1	A	39	GLU	2.2
1	B	628	ASN	2.2
1	A	683	VAL	2.1
1	B	153	VAL	2.1
1	B	237	ALA	2.1
1	B	249	GLY	2.1
1	A	584	SER	2.1
1	A	353	HIS	2.1
1	B	44	GLU	2.1
1	B	708	ALA	2.1
1	A	713	GLU	2.1
1	A	737	LYS	2.1
1	A	558	ALA	2.1
1	A	580	THR	2.1
1	B	684[A]	ASN	2.1
1	B	353	HIS	2.1
1	B	728	LYS	2.1
1	B	46	GLY	2.1
1	A	326	LEU	2.0
1	A	605	PRO	2.0
1	B	39	GLU	2.0
1	A	103	ILE	2.0
1	B	659	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	446	ILE	2.0
1	A	172	LYS	2.0
1	B	295	GLN	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)

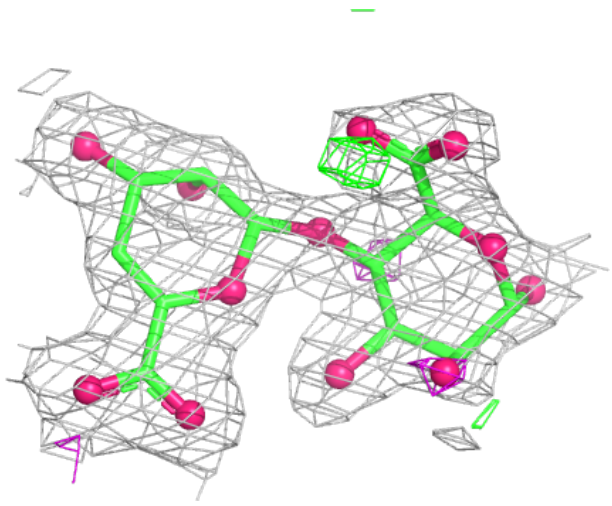
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

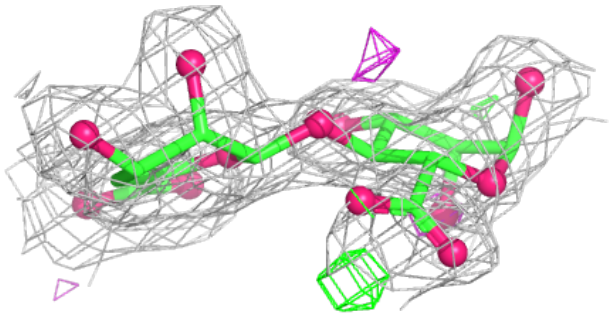
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAV	C	1	13/13	0.77	0.28	30,42,59,65	0
2	MAV	D	1	13/13	0.79	0.27	27,36,50,52	0
2	MAW	D	2	11/12	0.81	0.18	24,29,36,38	0
2	MAW	C	2	11/12	0.83	0.17	26,30,33,35	0

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:

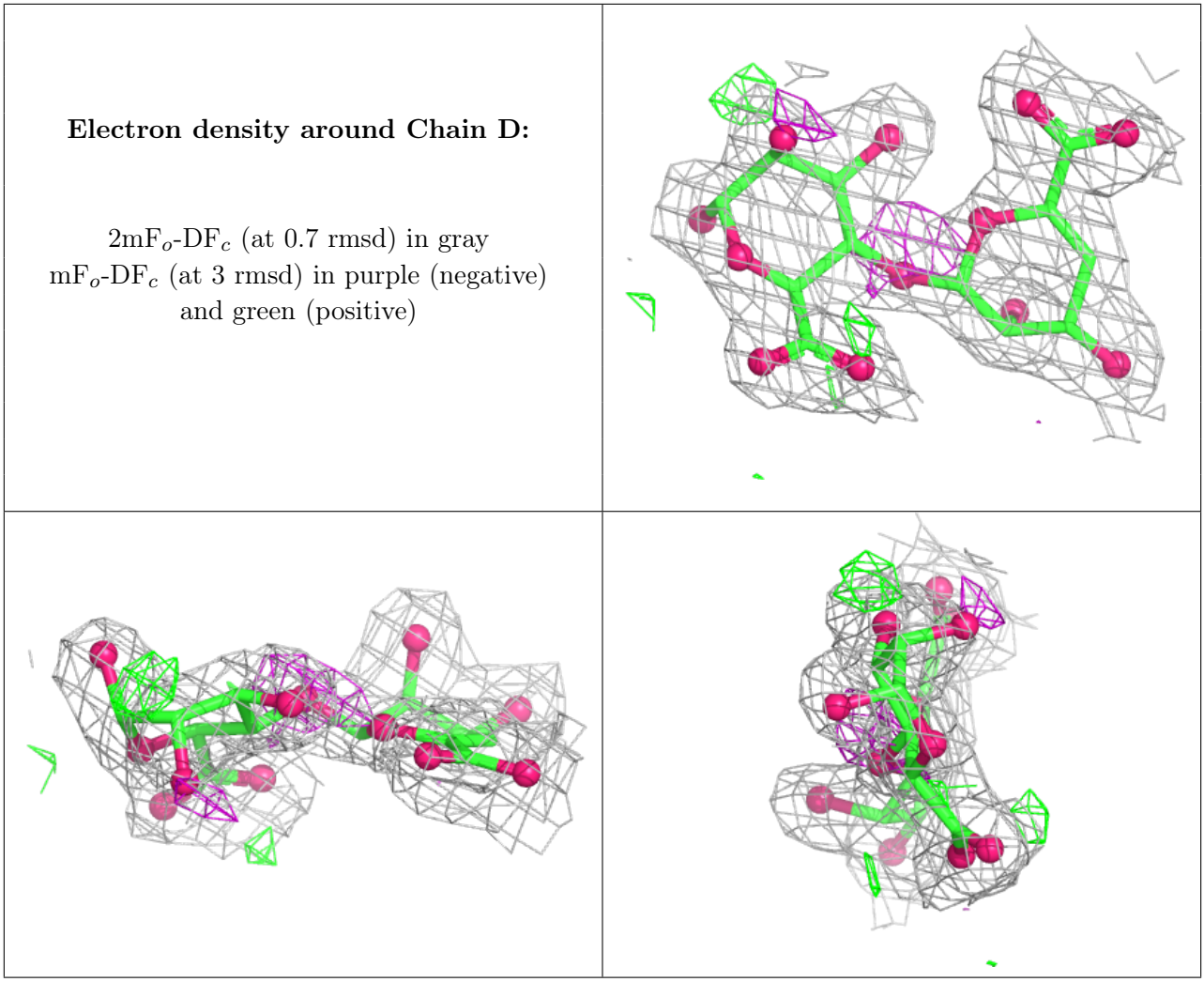
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





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

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, 95^{th} 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.

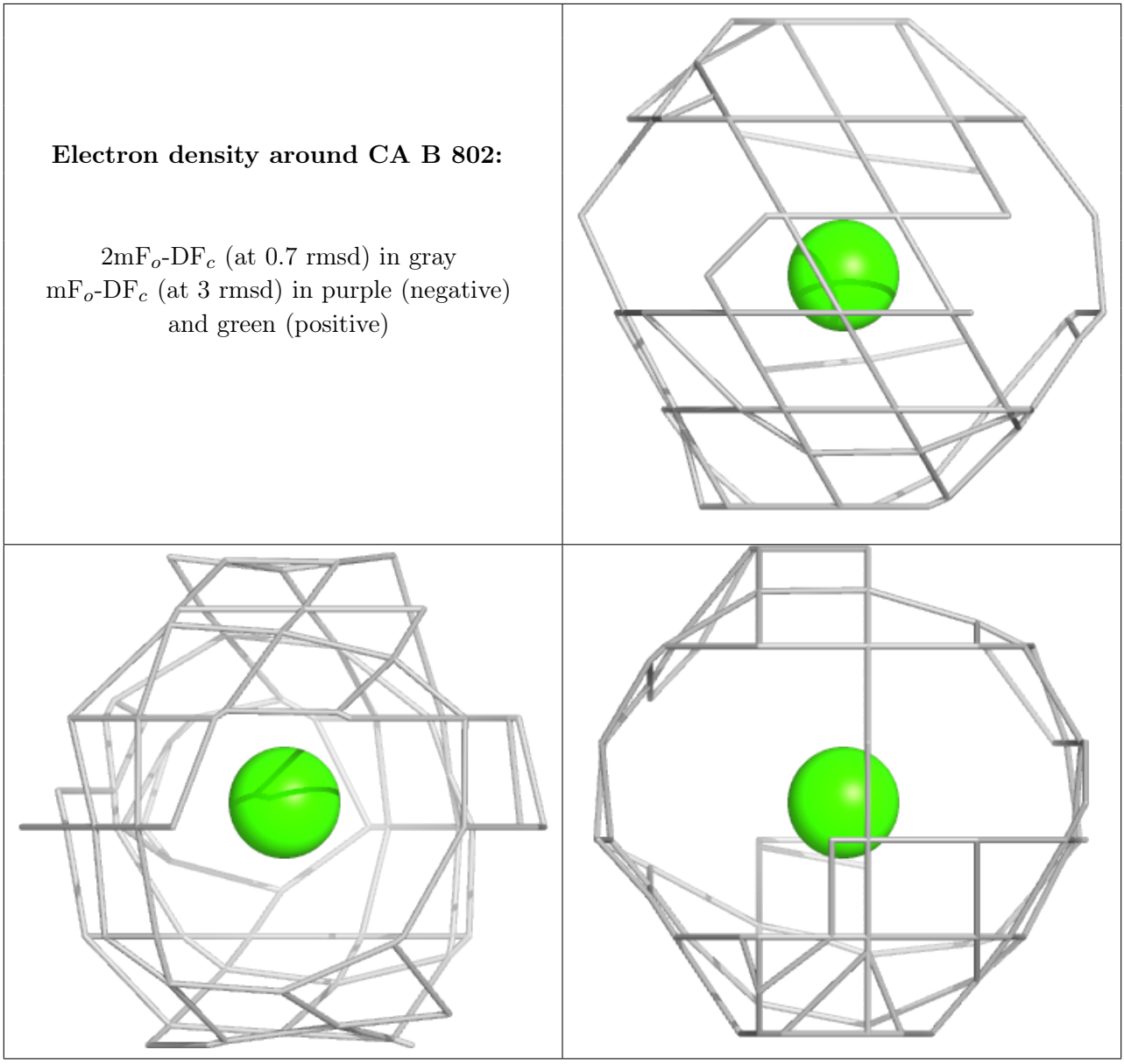
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	803	1/1	0.73	0.13	45,45,45,45	0
5	GOL	B	804	6/6	0.84	0.19	34,39,39,42	0
4	MG	B	801	1/1	0.94	0.18	42,42,42,42	0
4	MG	B	803	1/1	0.96	0.31	28,28,28,28	0
4	MG	A	802	1/1	0.96	0.15	37,37,37,37	0
3	CA	B	802	1/1	1.00	0.12	17,17,17,17	0
3	CA	A	801	1/1	1.00	0.15	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.

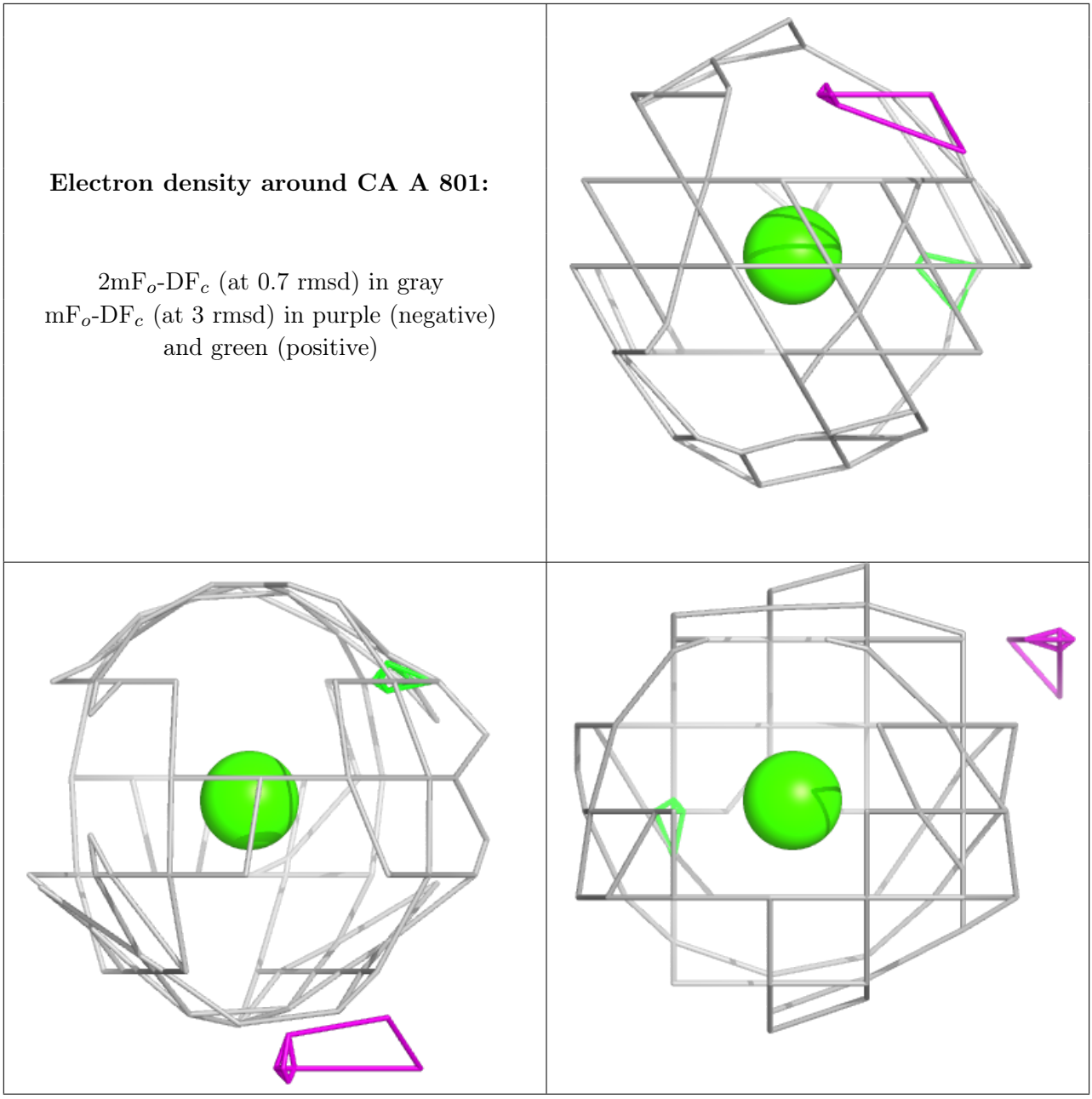
Electron density around CA B 802:

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



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)



6.5 Other polymers (i)

There are no such residues in this entry.