Full wwPDB X-ray Structure Validation Report ⓘ

Nov 18, 2024 – 04:58 PM EST

PDB ID	:	9E92
Title	:	Acanthamoeba Polyphaga Mimivirus R699
Deposited on	:	2024-11-07
Resolution	:	1.50 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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:

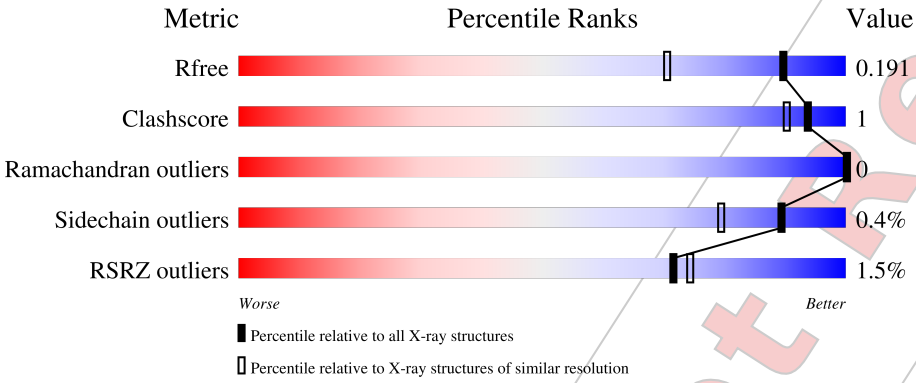
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 1.50 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}	164625	3717 (1.50-1.50)
Clashscore	180529	4048 (1.50-1.50)
Ramachandran outliers	177936	3970 (1.50-1.50)
Sidechain outliers	177891	3967 (1.50-1.50)
RSRZ outliers	164620	3718 (1.50-1.50)

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	458	94%
1	B	458	3% 92%
2	C	2	100%

Validation Pipeline (wwPDB-VP) : 2.39

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16070 atoms, of which 7543 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.

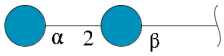
- Molecule 1 is a protein called R699.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	448	7465	2419	3711	615	698	22	103	11	0
			Total	C	H	N	O	S			
1	B	439	7458	2414	3715	620	688	21	105	16	0

There are 8 discrepancies between the modelled and reference sequences:

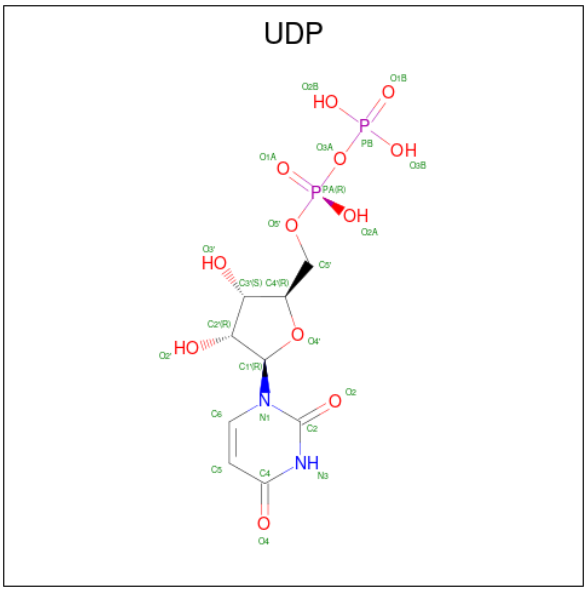
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q5UNV6
A	-1	PRO	-	expression tag	UNP Q5UNV6
A	0	GLY	-	expression tag	UNP Q5UNV6
A	1	SER	-	expression tag	UNP Q5UNV6
B	-2	GLY	-	expression tag	UNP Q5UNV6
B	-1	PRO	-	expression tag	UNP Q5UNV6
B	0	GLY	-	expression tag	UNP Q5UNV6
B	1	SER	-	expression tag	UNP Q5UNV6

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	H	O			
2	C	2	46	12	23	11	4	0	0

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).

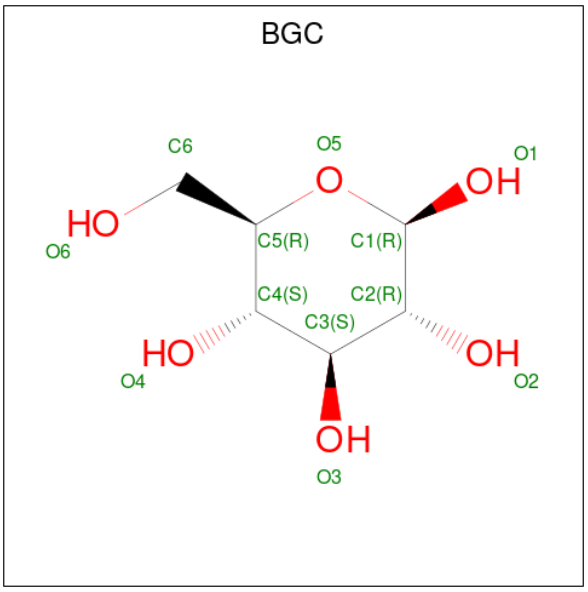


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	2	0
			36	9	11	2	12	2		
3	B	1	Total	C	H	N	O	P	2	0
			36	9	11	2	12	2		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

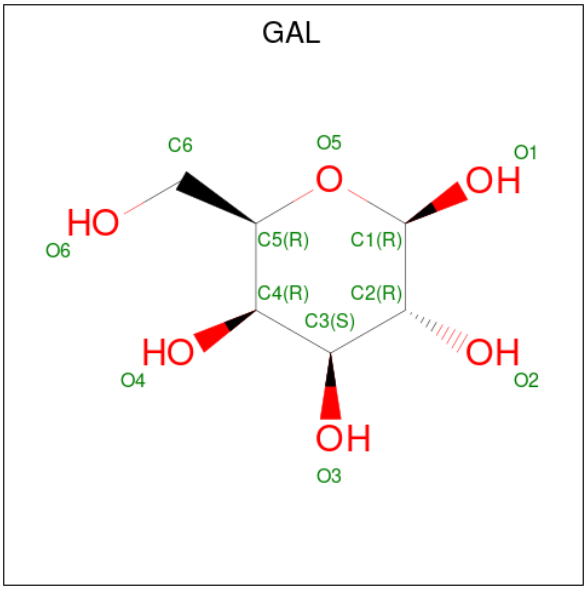
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	B	1	Total	Mn	0	0
			1	1		

- Molecule 5 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 24 6 12 6	4	0
5	A	1	Total C H O 24 6 12 6	4	0
5	B	1	Total C H O 24 6 12 6	4	0
5	B	1	Total C H O 24 6 12 6	4	0

- Molecule 6 is beta-D-galactopyranose (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	4	0
			24	6	12	6		
6	B	1	Total	C	H	O	4	0
			24	6	12	6		

- Molecule 7 is water.

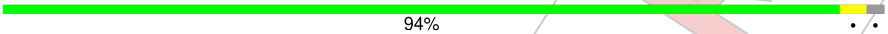
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	482	Total	O	0	0
			482	482		
7	B	401	Total	O	0	0
			401	401		

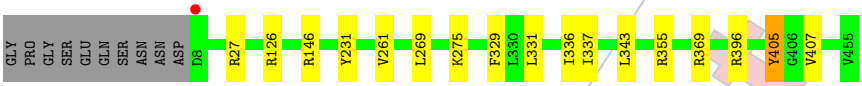
3 Residue-property plots (i)

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: R699

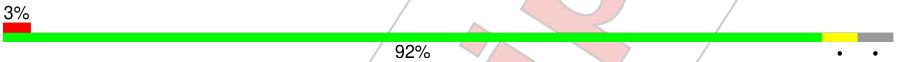
Chain A:

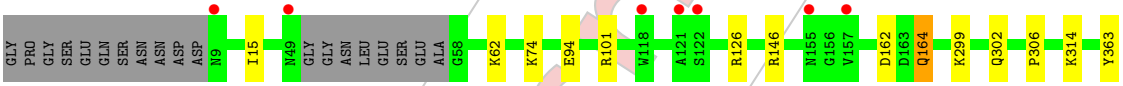


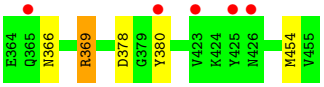


- Molecule 1: R699

Chain B:

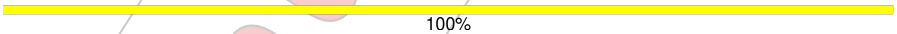






- Molecule 2: alpha-D-glucopyranose-(1-2)-beta-D-glucopyranose

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.15Å 125.00Å 72.76Å 90.00° 118.30° 90.00°	Depositor
Resolution (Å)	60.97 – 1.50 60.97 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (60.97-1.50) 98.7 (60.97-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.166 , 0.189 0.167 , 0.191	Depositor DCC
R_{free} test set	8738 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	17.2	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 37.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	16070	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, GLC, UDP, MN, GAL

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	0.58	0/3859	0.91	6/5209 (0.1%)
1	B	0.59	0/3848	0.90	11/5189 (0.2%)
All	All	0.58	0/7707	0.91	17/10398 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	396	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	231	TYR	CB-CG-CD1	6.09	124.65	121.00
1	A	126	ARG	CD-NE-CZ	6.06	132.09	123.60
1	A	355	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	A	27	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	396	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B	94[A]	GLU	CG-CD-OE1	-5.54	107.22	118.30
1	B	94[B]	GLU	CG-CD-OE1	-5.54	107.22	118.30
1	B	94[A]	GLU	CG-CD-OE2	5.28	128.85	118.30
1	B	94[B]	GLU	CG-CD-OE2	5.28	128.85	118.30
1	B	101[A]	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	101[B]	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	454	MET	CG-SD-CE	-5.22	91.85	100.20
1	B	126	ARG	NE-CZ-NH2	-5.20	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	164	GLN	N-CA-CB	-5.20	101.24	110.60
1	B	369[A]	ARG	NE-CZ-NH1	-5.01	117.79	120.30
1	B	369[B]	ARG	NE-CZ-NH1	-5.01	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	369	ARG	Sidechain
1	A	405	TYR	Peptide

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	3754	3711	3701	7	0
1	B	3743	3715	3699	12	0
2	C	23	23	21	0	0
3	A	25	11	11	0	0
3	B	25	11	11	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	24	24	24	0	0
5	B	24	24	24	0	0
6	A	12	12	12	1	0
6	B	12	12	12	0	0
7	A	482	0	0	0	0
7	B	401	0	0	0	0
All	All	8527	7543	7515	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 1.

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:B:162:ASP:OD1	1:B:164:GLN:HB3	1.96	0.66
1:B:314:LYS:HE2	1:B:314:LYS:HA	1.86	0.57
1:B:15:ILE:HG21	1:B:62:LYS:HG2	1.90	0.54
1:B:74:LYS:HA	1:B:74:LYS:HE3	1.91	0.53
1:A:331[B]:LEU:CD1	1:A:407:VAL:HG22	2.39	0.52
1:B:363:TYR:CE1	1:B:369[A]:ARG:CZ	2.94	0.51
1:B:302:GLN:HG2	1:B:306:PRO:HA	1.93	0.50
1:B:363:TYR:CE2	1:B:369[A]:ARG:NH2	2.80	0.50
1:B:366:ASN:OD1	1:B:369[B]:ARG:NH2	2.45	0.49
1:A:331[B]:LEU:HD12	1:A:407:VAL:HG22	1.95	0.49
1:B:378:ASP:O	1:B:380[A]:TYR:CD2	2.66	0.49
1:B:378:ASP:O	1:B:380[A]:TYR:CE2	2.68	0.46
1:B:363:TYR:CZ	1:B:369[A]:ARG:NH2	2.84	0.45
1:A:337:ILE:HD11	1:A:407:VAL:HG21	2.00	0.43
1:A:261:VAL:HB	1:A:269:LEU:HD13	2.00	0.43
1:A:329:PHE:CD2	1:A:343[A]:LEU:HD21	2.54	0.42
1:A:275:LYS:HG3	1:A:336:ILE:HG23	2.01	0.42
1:B:363:TYR:CE1	1:B:369[A]:ARG:NH1	2.89	0.40
1:A:405:TYR:CE1	6:A:505:GAL:H62	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	457/458 (100%)	451 (99%)	6 (1%)	0	100	100
1	B	451/458 (98%)	444 (98%)	7 (2%)	0	100	100
All	All	908/916 (99%)	895 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	418/415 (101%)	417 (100%)	1 (0%)	92 83
1	B	417/415 (100%)	415 (100%)	2 (0%)	86 75
All	All	835/830 (101%)	832 (100%)	3 (0%)	89 79

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ARG
1	B	146	ARG
1	B	299	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

2 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	BGC	C	1	2	12,12,12	0.80	0	17,17,17	1.14	1 (5%)
2	GLC	C	2	2	11,11,12	0.49	0	15,15,17	1.38	2 (13%)

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	BGC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	BGC	O5-C1-C2	-3.37	104.37	110.30
2	C	2	GLC	C1-C2-C3	3.34	114.50	109.64
2	C	2	GLC	C1-O5-C5	2.46	115.48	112.19

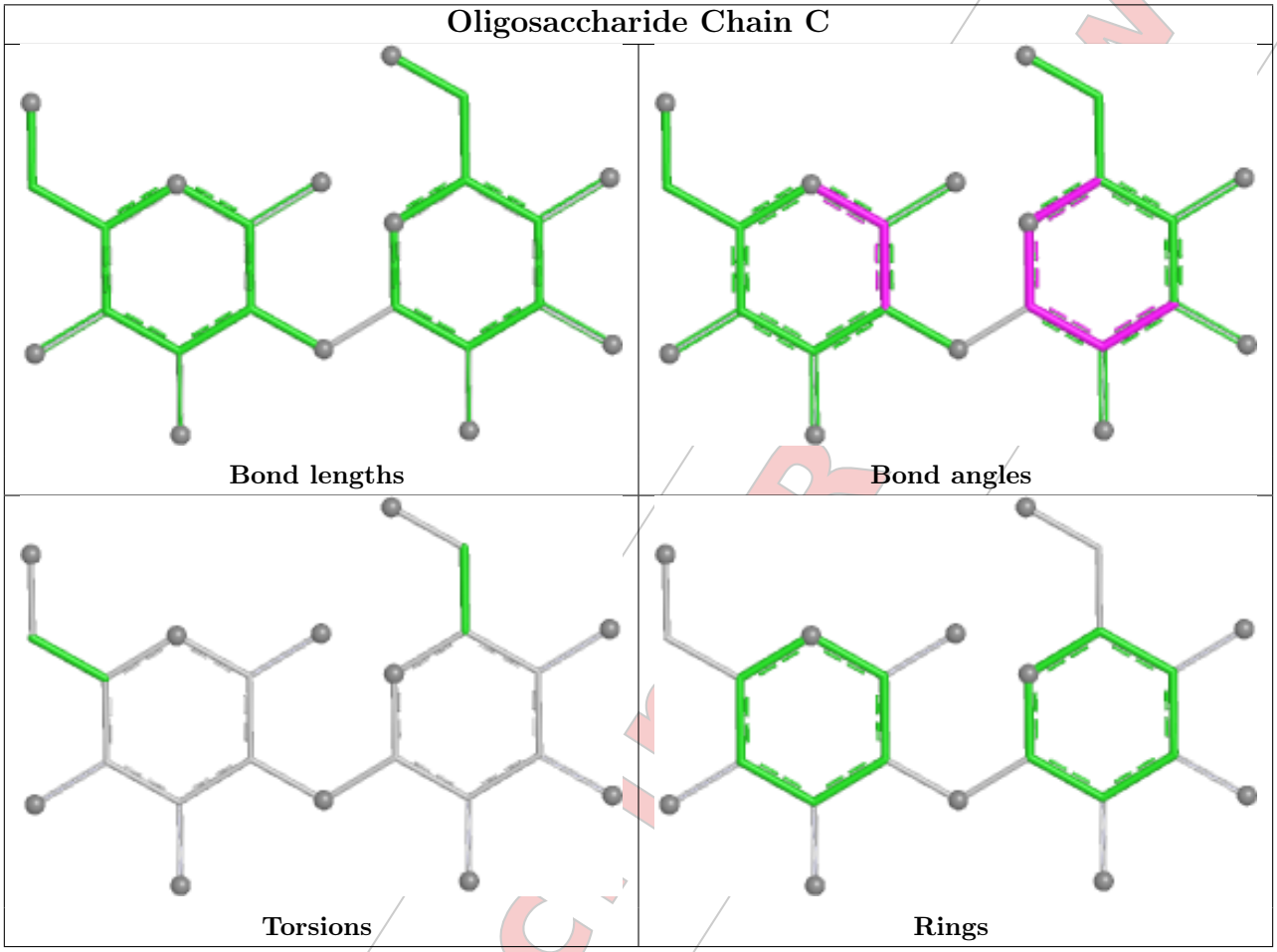
There are no chirality outliers.

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

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	BGC	A	503	-	12,12,12	0.73	0	17,17,17	0.76	0
3	UDP	B	501	4	25,26,26	0.48	0	38,40,40	1.51	6 (15%)
6	GAL	B	505	-	12,12,12	0.33	0	17,17,17	0.55	0
3	UDP	A	501	4	25,26,26	0.98	2 (8%)	38,40,40	1.24	2 (5%)
6	GAL	A	505	-	12,12,12	0.56	0	17,17,17	0.99	0
5	BGC	A	504	-	12,12,12	0.67	0	17,17,17	0.91	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BGC	B	504	-	12,12,12	0.54	0	17,17,17	0.87	0
5	BGC	B	503	-	12,12,12	0.57	0	17,17,17	0.92	1 (5%)

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	BGC	A	503	-	-	0/2/22/22	0/1/1/1
3	UDP	B	501	4	-	1/16/32/32	0/2/2/2
6	GAL	B	505	-	-	0/2/22/22	0/1/1/1
3	UDP	A	501	4	-	7/16/32/32	0/2/2/2
6	GAL	A	505	-	-	0/2/22/22	0/1/1/1
5	BGC	A	504	-	-	0/2/22/22	0/1/1/1
5	BGC	B	504	-	-	0/2/22/22	0/1/1/1
5	BGC	B	503	-	-	0/2/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	UDP	PA-O3A	-3.27	1.56	1.59
3	A	501	UDP	PB-O1B	-2.10	1.43	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	UDP	O3'-C3'-C2'	-3.97	99.07	111.82
3	A	501	UDP	O3B-PB-O3A	-3.89	91.59	104.64
3	B	501	UDP	O3'-C3'-C4'	2.97	119.61	111.08
3	B	501	UDP	O2A-PA-O1A	2.42	123.72	112.44
3	A	501	UDP	O2B-PB-O1B	2.37	120.08	110.83
3	B	501	UDP	C1'-N1-C2	-2.34	113.39	117.59
5	A	504	BGC	O1-C1-C2	2.31	115.68	108.98
5	A	504	BGC	O1-C1-O5	-2.21	103.84	110.41
3	B	501	UDP	O2-C2-N1	-2.18	119.97	122.80
5	B	503	BGC	O1-C1-C2	2.14	115.20	108.98
3	B	501	UDP	O2A-PA-O3A	2.05	112.80	107.27

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	UDP	PA-O3A-PB-O2B
3	A	501	UDP	C5'-O5'-PA-O2A
3	A	501	UDP	C4'-C5'-O5'-PA
3	B	501	UDP	C4'-C5'-O5'-PA
3	A	501	UDP	PB-O3A-PA-O1A
3	A	501	UDP	PB-O3A-PA-O2A
3	A	501	UDP	PA-O3A-PB-O1B
3	A	501	UDP	PA-O3A-PB-O3B

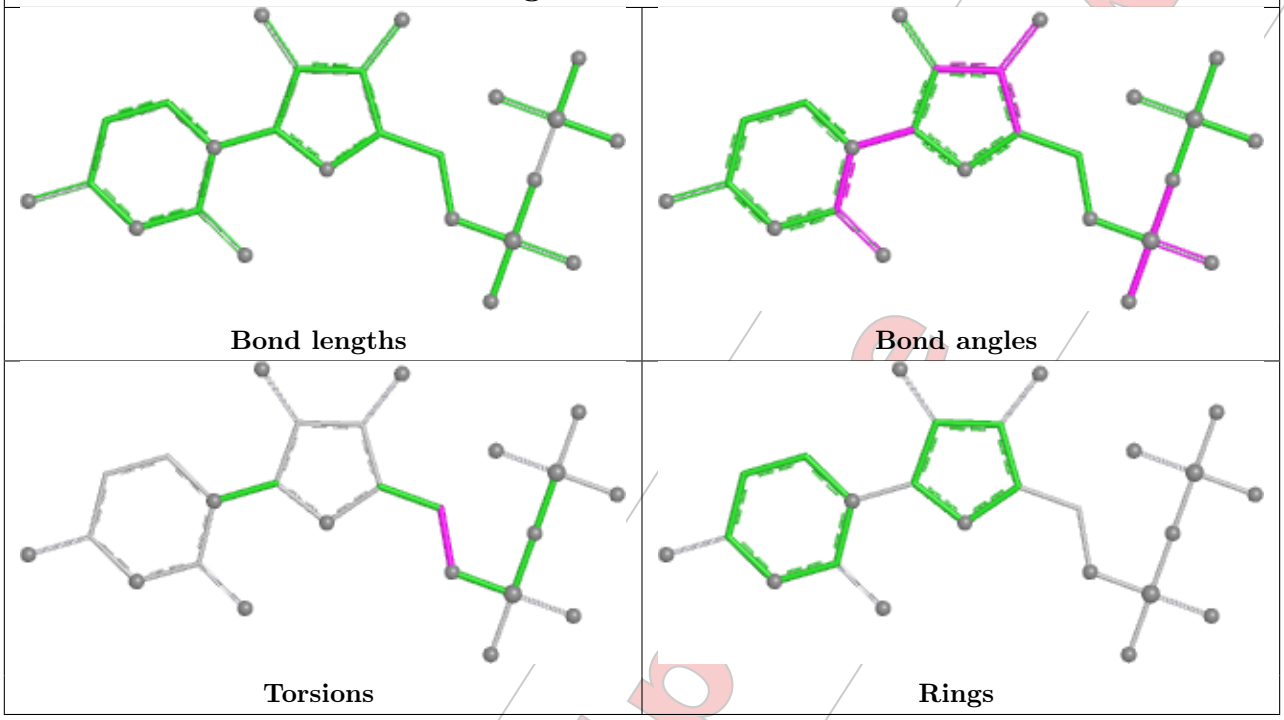
There are no ring outliers.

1 monomer is involved in 1 short contact:

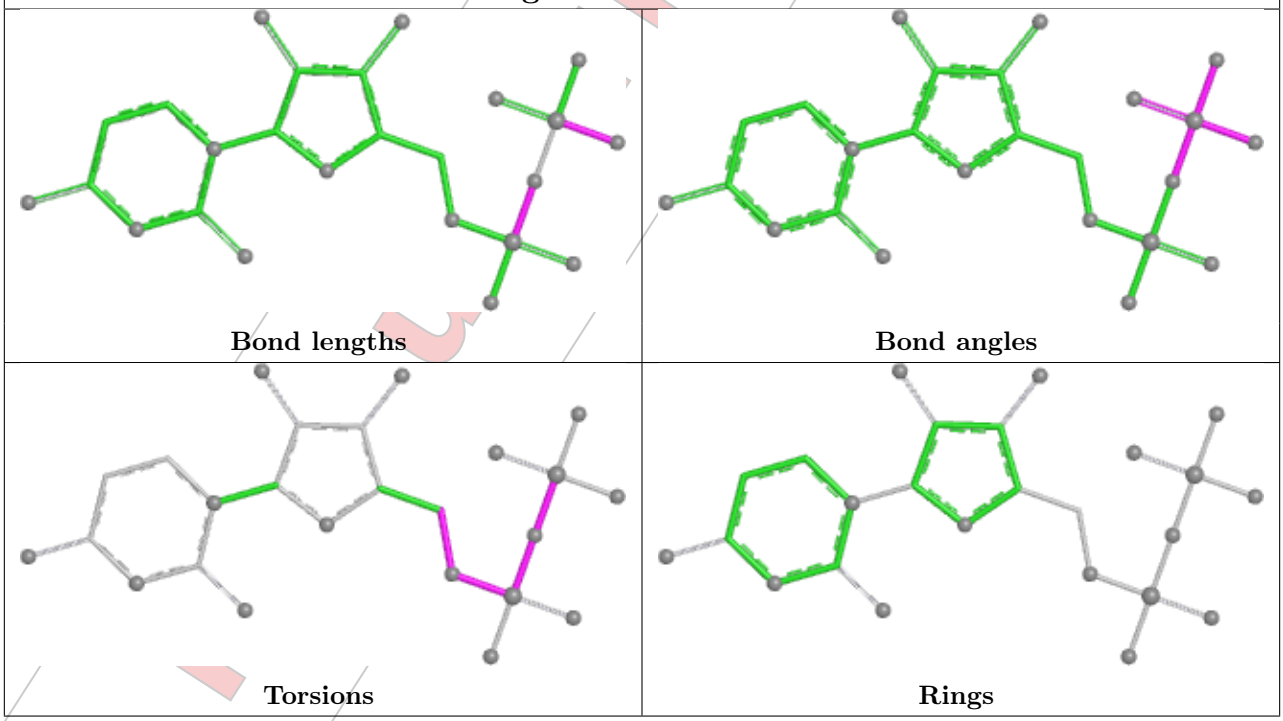
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	505	GAL	1	0

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

Ligand UDP B 501



Ligand UDP A 501



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, 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	448/458 (97%)	-0.27	1 (0%)	92	92	7, 18, 33, 52	13 (2%)
1	B	439/458 (95%)	-0.16	12 (2%)	56	59	5, 17, 38, 63	16 (3%)
All	All	887/916 (96%)	-0.22	13 (1%)	71	74	5, 17, 36, 63	29 (3%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	423	VAL	4.6
1	B	380[A]	TYR	4.0
1	B	121	ALA	3.6
1	B	49	ASN	3.4
1	B	118	TRP	3.3
1	A	8	ASP	3.0
1	B	365	GLN	3.0
1	B	157	VAL	2.7
1	B	9	ASN	2.4
1	B	426	ASN	2.3
1	B	155	ASN	2.2
1	B	122	SER	2.2
1	B	425	TYR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

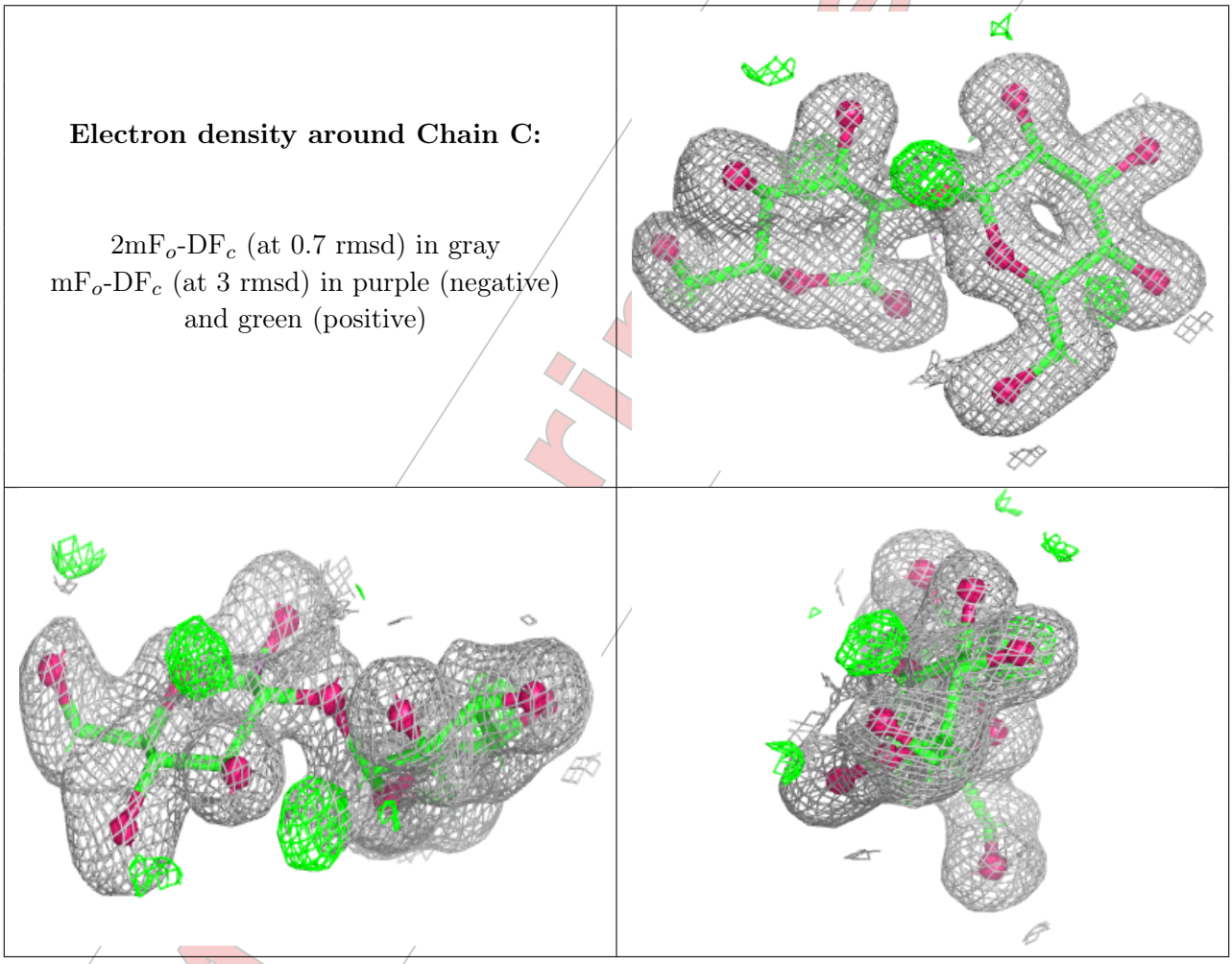
6.3 Carbohydrates

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	BGC	C	1	12/12	0.91	0.10	24,27,34,37	4
2	GLC	C	2	11/12	0.97	0.05	12,14,15,16	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

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
3	UDP	B	501	25/25	0.83	0.18	8,18,21,23	36

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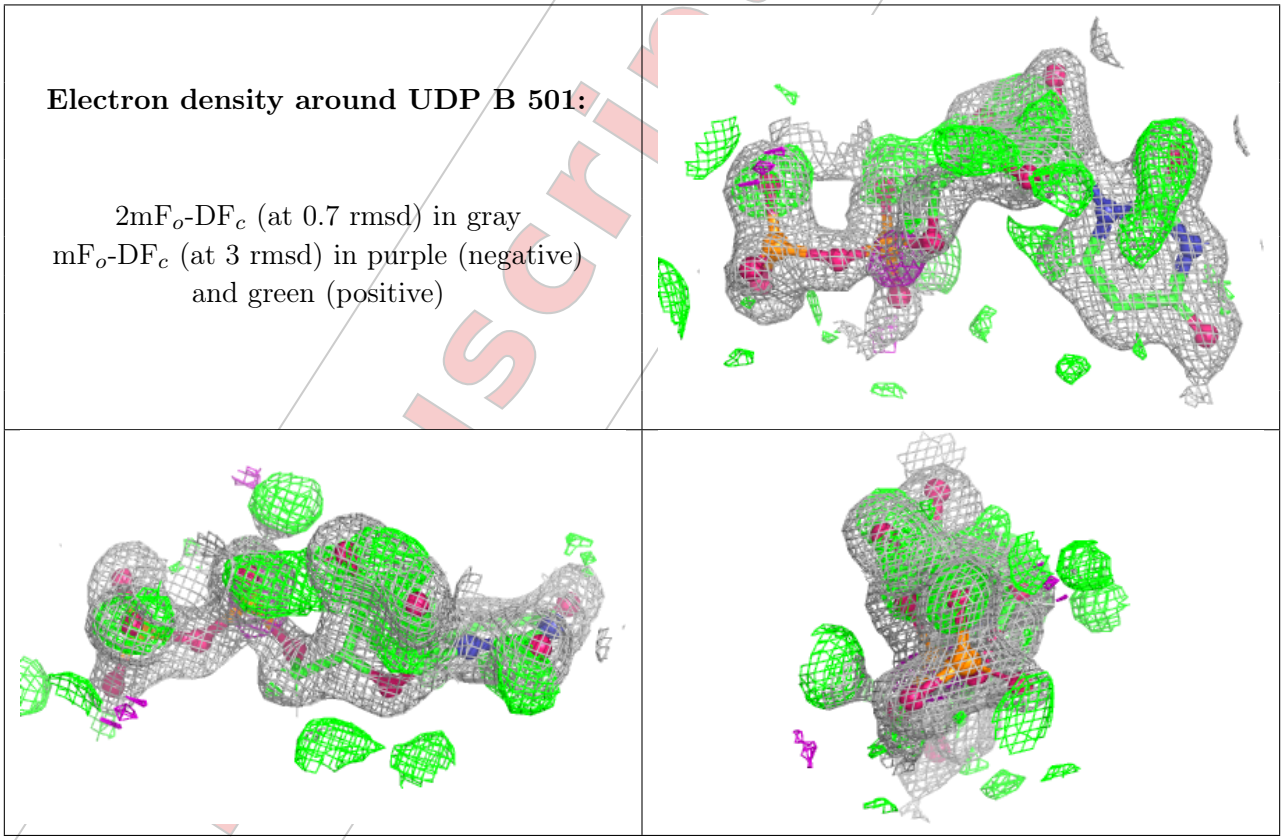
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GAL	A	505	12/12	0.88	0.12	22,28,33,37	24
5	BGC	B	503	12/12	0.93	0.10	15,19,27,28	24
5	BGC	A	503	12/12	0.95	0.07	18,21,26,30	4
6	GAL	B	505	12/12	0.95	0.07	21,23,24,27	4
5	BGC	B	504	12/12	0.97	0.06	19,21,23,28	4
3	UDP	A	501	25/25	0.98	0.06	14,15,24,28	2
5	BGC	A	504	12/12	0.98	0.05	18,19,22,22	4
4	MN	A	502	1/1	1.00	0.02	13,13,13,13	0
4	MN	B	502	1/1	1.00	0.01	12,12,12,12	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.

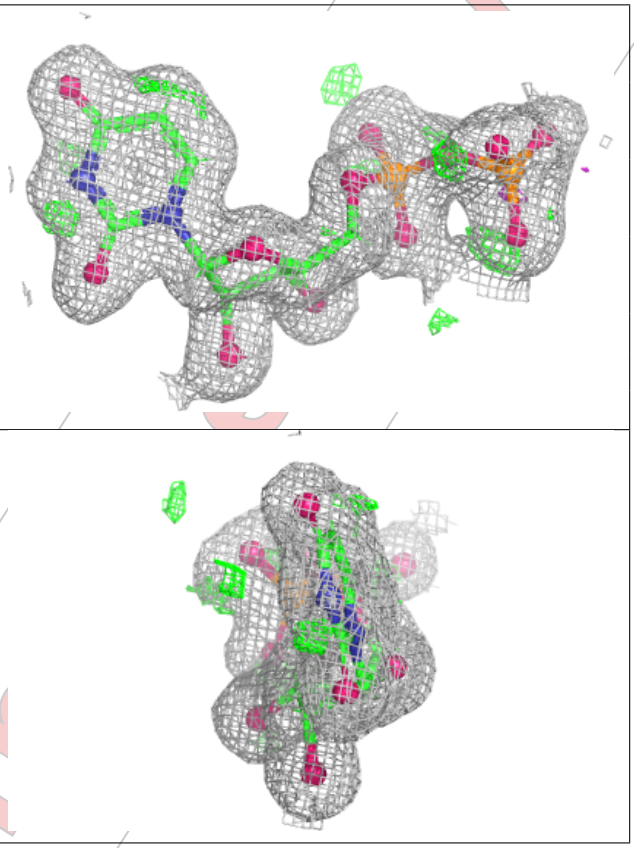
Electron density around UDP B 501:

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



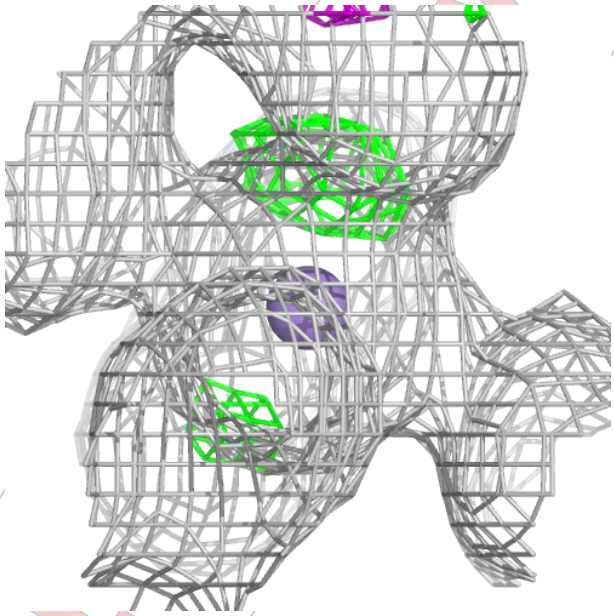
Electron density around UDP A 501:

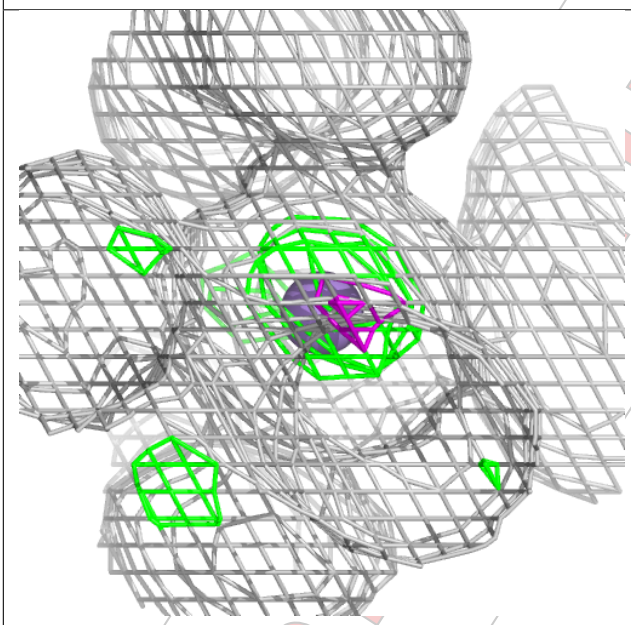
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

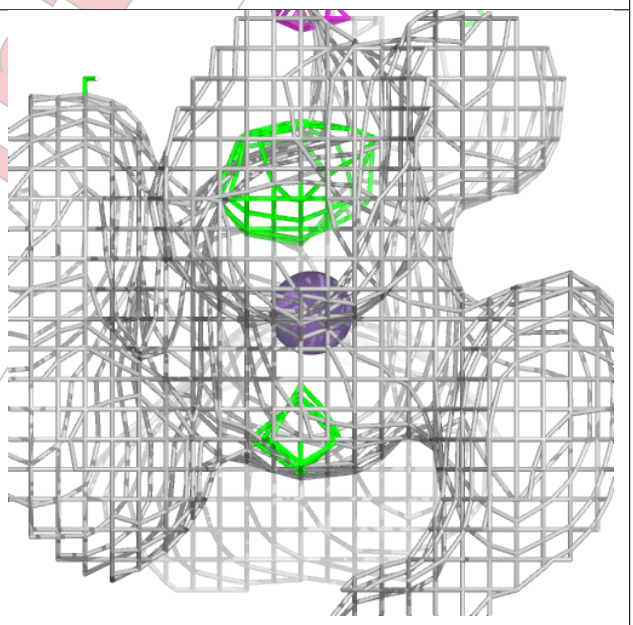


Electron density around MN A 502:

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







Electron density around MN B 502:

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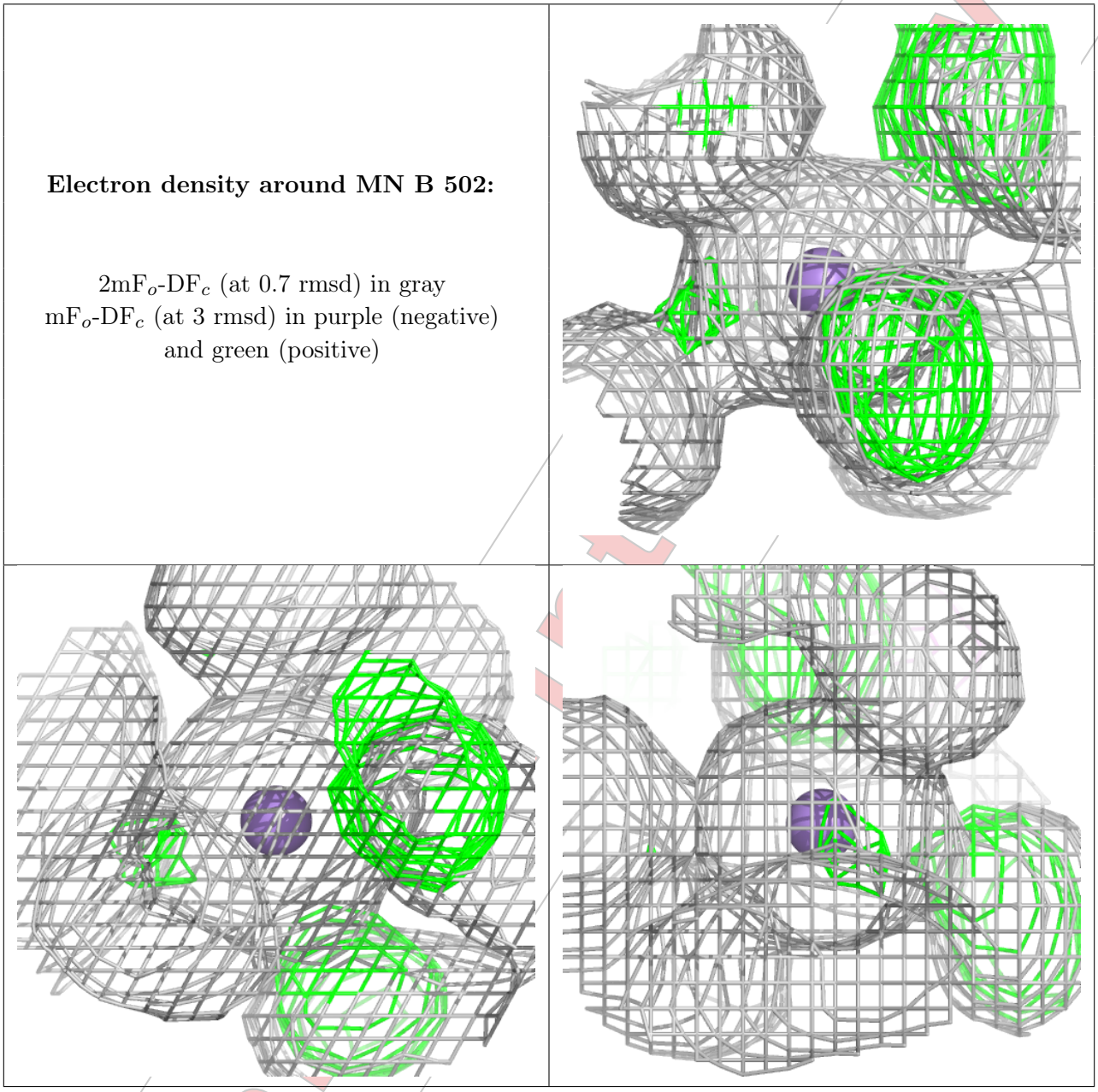
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.