Full wwPDB X-ray Structure Validation Report (i)

Jun 3, 2020 – 12:42 PM BST

PDB ID	:	6Z8L
Title	:	Alpha-Amylase in complex with probe fragments
Deposited on	:	2020-06-02
Resolution	:	1.40 Å(reported)

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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

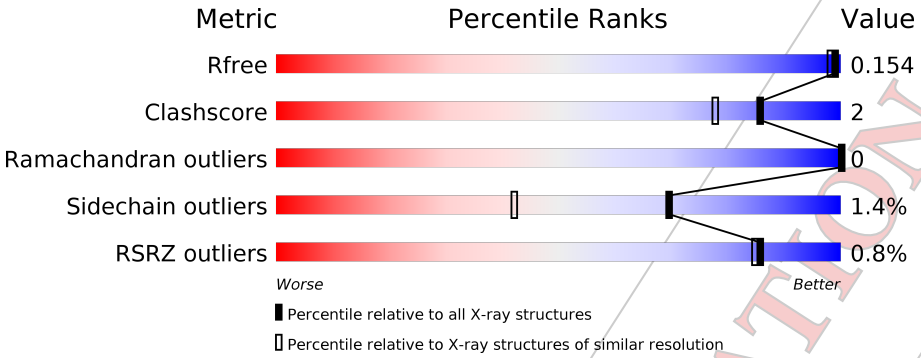
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

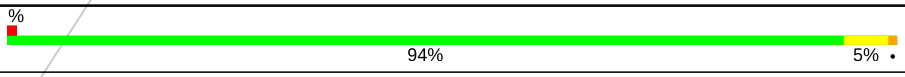
The reported resolution of this entry is 1.40 Å.

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}	111664	1450 (1.40-1.40)
Clashscore	122126	1541 (1.40-1.40)
Ramachandran outliers	120053	1500 (1.40-1.40)
Sidechain outliers	120020	1499 (1.40-1.40)
RSRZ outliers	108989	1412 (1.40-1.40)

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 on 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	496	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	A	901	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8274 atoms, of which 3838 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.

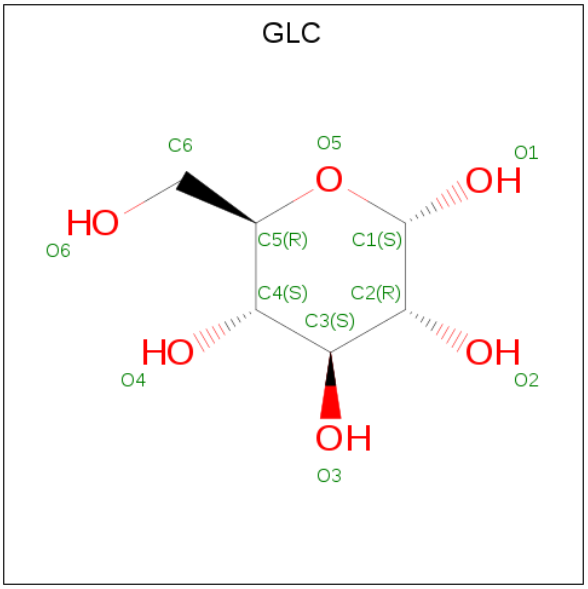
- Molecule 1 is a protein called Pancreatic alpha-amylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	496	7702	2510	3738	698	735	21	0	4	0

There is a discrepancy between the modelled and reference sequences:

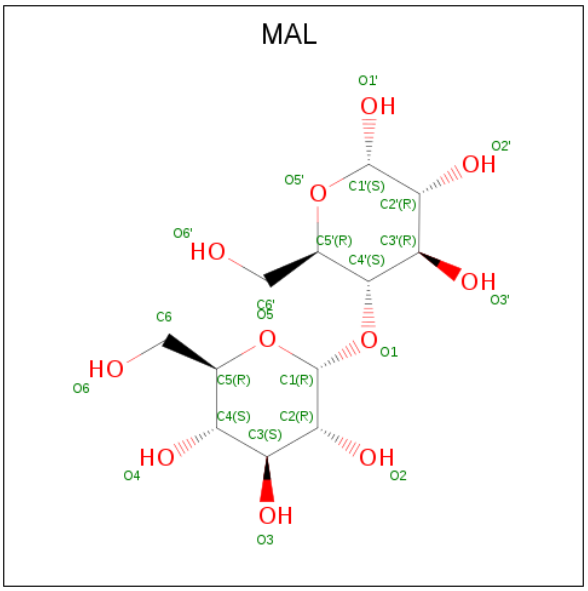
Chain	Residue	Modelled	Actual	Comment	Reference
A	287	MET	VAL	conflict	UNP P04746

- Molecule 2 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



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

- Molecule 3 is MALTOSE (three-letter code: MAL) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 45 12 22 11	0	0
3	A	1	Total C H O 45 12 22 11	0	0
3	A	1	Total C H O 45 12 22 11	0	0
3	A	1	Total C H O 45 12 22 11	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

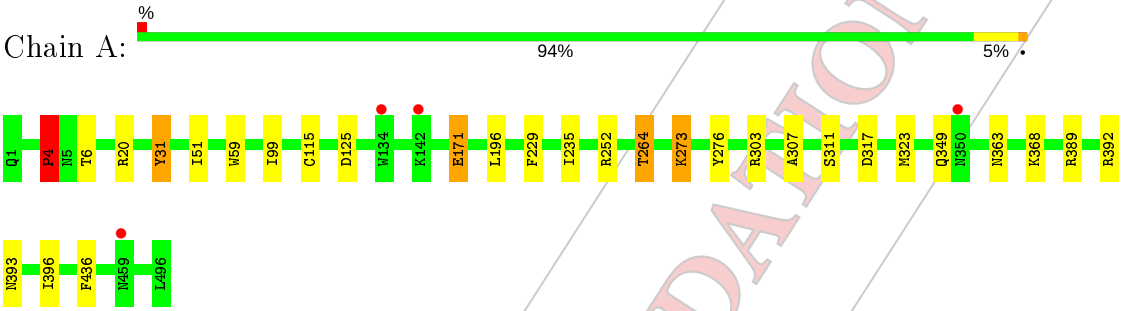
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	366	Total O 366 366	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Pancreatic alpha-amylase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.87Å 73.73Å 135.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.43 – 1.40 48.43 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.43-1.40) 99.7 (48.43-1.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 1.40Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.142 , 0.154 0.142 , 0.154	Depositor DCC
R_{free} test set	5308 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	8274	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: CA, GLC, PCA, MAL, CL

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	0.56	3/4083 (0.1%)	0.78	7/5544 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	PRO	CG-CD	9.24	1.81	1.50
1	A	31	TYR	CD2-CE2	-6.18	1.30	1.39
1	A	31	TYR	CE2-CZ	-5.45	1.31	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	252	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	323	MET	CG-SD-CE	-5.71	91.07	100.20
1	A	389	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	4	PRO	CA-N-CD	-5.21	104.20	111.50
1	A	303	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	317	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	A	20	ARG	NE-CZ-NH1	5.02	122.81	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	3964	3738	3741	19	1
2	A	12	12	11	1	0
3	A	92	88	83	0	1
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	366	0	0	3	2
All	All	4436	3838	3835	19	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:PRO:CD	1:A:4:PRO:CG	1.81	1.43
1:A:4:PRO:HG2	1:A:6:THR:H	1.50	0.77
1:A:363:ASN:ND2	6:A:1002:HOH:O	2.25	0.69
1:A:99:ILE:HD11	1:A:196[B]:LEU:HD11	1.84	0.58
1:A:99:ILE:CG1	1:A:196[B]:LEU:HD11	2.35	0.56
1:A:31:TYR:OH	1:A:392:ARG:HG3	2.07	0.55
1:A:99:ILE:HG12	1:A:196[B]:LEU:HD11	1.90	0.54
1:A:125:ASP:OD1	6:A:1001:HOH:O	2.18	0.54
1:A:264:THR:HG22	1:A:311:SER:CB	2.39	0.52
1:A:235:ILE:HG21	1:A:307:ALA:HB2	1.92	0.52
1:A:99:ILE:CD1	1:A:196[B]:LEU:HD11	2.38	0.52
1:A:273:LYS:HE2	1:A:276:TYR:OH	2.11	0.51
1:A:349:GLN:NE2	6:A:1010:HOH:O	2.45	0.49
1:A:393:ASN:HA	1:A:396:ILE:HG22	1.96	0.47
1:A:363:ASN:OD1	1:A:368[B]:LYS:HE3	2.13	0.47
1:A:4:PRO:HA	1:A:229:PHE:CG	2.50	0.46
1:A:51:ILE:HD13	1:A:59:TRP:HZ3	1.83	0.44
1:A:393:ASN:O	1:A:396:ILE:HG22	2.21	0.41
1:A:171:GLU:HB3	2:A:901:GLC:O4	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASN:OD1	3:A:904:MAL:O6'[1_655]	1.83	0.37
6:A:1007:HOH:O	6:A:1128:HOH:O[4_555]	1.92	0.28
6:A:1074:HOH:O	6:A:1190:HOH:O[3_544]	2.06	0.14

5.3 Torsion angles

5.3.1 Protein backbone

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	498/496 (100%)	488 (98%)	10 (2%)	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	422/418 (101%)	416 (99%)	6 (1%)	69 42

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	A	115	CYS
1	A	171	GLU
1	A	264	THR
1	A	273	LYS
1	A	436	PHE

Some 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 (i)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\|>2$
1	PCA	A	1	1	7,8,9	1.66	1 (14%)	9,10,12	1.97	2 (22%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CD-N	3.78	1.44	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	PCA	CA-N-CD	-2.94	103.53	113.58
1	A	1	PCA	CG-CD-N	2.66	115.28	108.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	MAL	A	902	-	24,24,24	1.47	4 (16%)	35,35,35	0.74	0
3	MAL	A	904	-	24,24,24	1.36	2 (8%)	35,35,35	1.40	5 (14%)
2	GLC	A	901	-	12,12,12	0.58	0	17,17,17	2.03	5 (29%)
3	MAL	A	903	-	24,24,24	1.58	4 (16%)	35,35,35	1.40	6 (17%)
3	MAL	A	905	-	24,24,24	1.48	4 (16%)	35,35,35	0.79	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
3	MAL	A	902	-	-	0/8/48/48	0/2/2/2
3	MAL	A	904	-	-	2/8/48/48	0/2/2/2
2	GLC	A	901	-	1/1/5/5	0/2/22/22	0/1/1/1
3	MAL	A	903	-	-	5/8/48/48	0/2/2/2
3	MAL	A	905	-	-	1/8/48/48	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	MAL	O5'-C1'	3.80	1.52	1.42
3	A	903	MAL	O2'-C2'	3.68	1.51	1.43
3	A	904	MAL	O2'-C2'	3.56	1.51	1.43
3	A	902	MAL	O2'-C2'	3.52	1.51	1.43
3	A	905	MAL	O2'-C2'	3.51	1.51	1.43
3	A	905	MAL	O5'-C1'	3.04	1.50	1.42
3	A	902	MAL	O5'-C1'	2.87	1.50	1.42
3	A	902	MAL	O5-C1	2.81	1.49	1.41
3	A	905	MAL	O5-C1	2.69	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	MAL	O5-C1	2.53	1.48	1.41
3	A	904	MAL	C3'-C2'	-2.24	1.46	1.52
3	A	905	MAL	C3'-C2'	-2.02	1.47	1.52
3	A	902	MAL	O5-C5	2.02	1.49	1.44
3	A	903	MAL	C4-C3	-2.02	1.47	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	GLC	O1-C1-C2	5.33	124.03	109.03
3	A	903	MAL	C3'-C4'-C5'	-3.37	103.21	110.93
2	A	901	GLC	O5-C1-C2	3.26	116.10	110.28
2	A	901	GLC	O1-C1-O5	3.09	119.67	110.38
3	A	904	MAL	O5'-C1'-C2'	3.06	115.75	110.28
3	A	903	MAL	O1-C1-C2	2.97	115.79	108.10
3	A	903	MAL	O1-C4'-C5'	2.83	117.21	109.45
3	A	904	MAL	O1-C4'-C3'	2.79	114.70	107.28
3	A	904	MAL	O3'-C3'-C2'	-2.78	103.92	110.35
2	A	901	GLC	O2-C2-C1	2.57	115.11	109.16
3	A	903	MAL	O2-C2-C3	-2.37	104.86	110.35
2	A	901	GLC	C1-C2-C3	-2.34	105.46	110.31
3	A	903	MAL	O2-C2-C1	2.33	115.69	110.05
3	A	904	MAL	O5'-C5'-C4'	2.30	114.59	109.75
3	A	903	MAL	O5'-C1'-C2'	2.26	114.31	110.28
3	A	904	MAL	C1-O5-C5	-2.25	109.27	113.69

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	901	GLC	C1

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	904	MAL	C3'-C4'-O1-C1
3	A	903	MAL	O5'-C5'-C6'-O6'
3	A	903	MAL	C4'-C5'-C6'-O6'
3	A	903	MAL	C2-C1-O1-C4'
3	A	903	MAL	O5-C1-O1-C4'
3	A	904	MAL	C5'-C4'-O1-C1
3	A	903	MAL	O5-C5-C6-O6
3	A	905	MAL	C5'-C4'-O1-C1

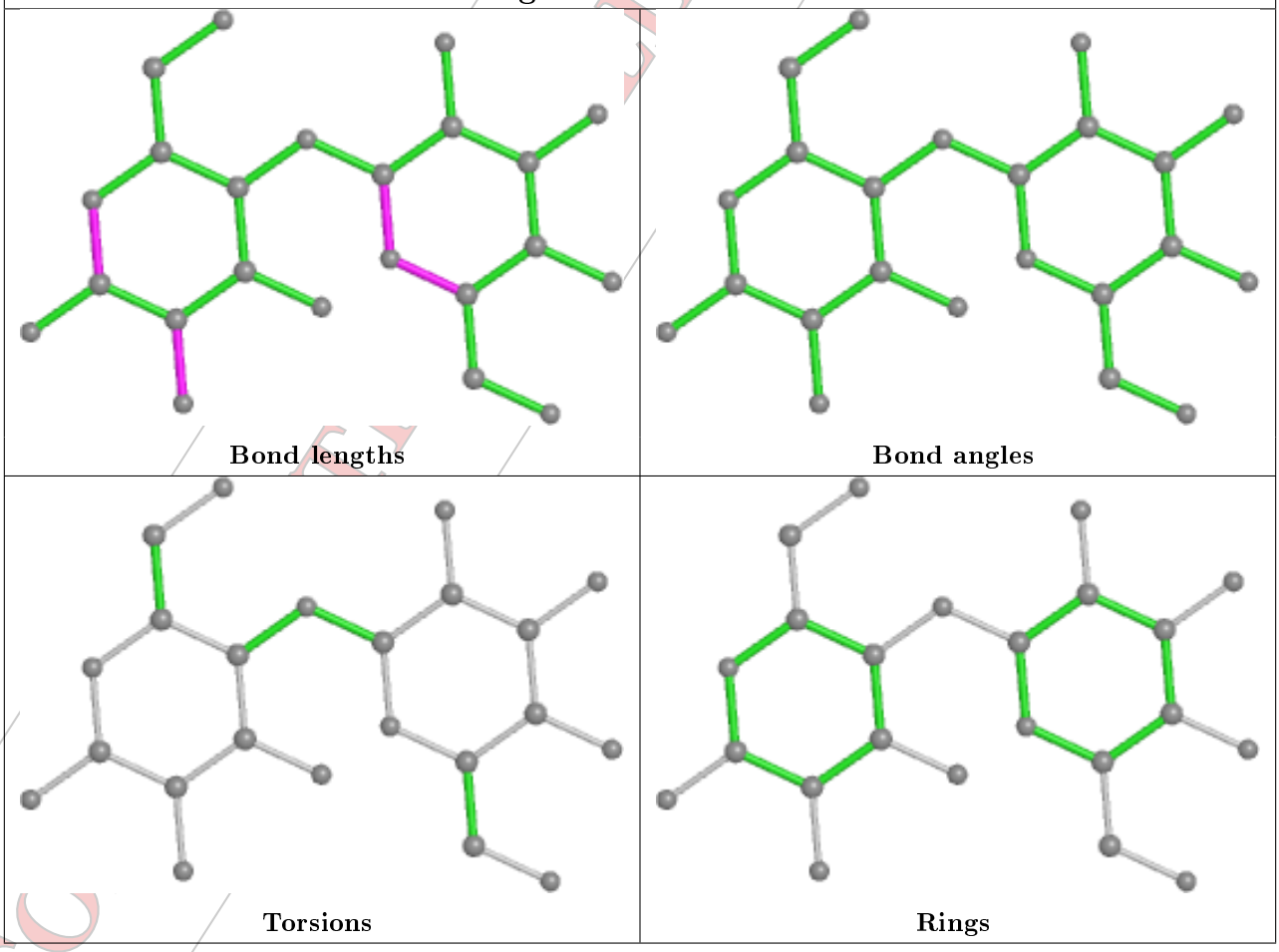
There are no ring outliers.

2 monomers are involved in 2 short contacts:

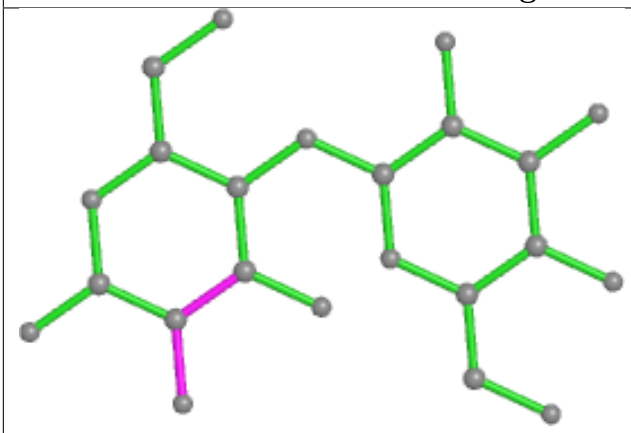
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	904	MAL	0	1
2	A	901	GLC	1	0

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.

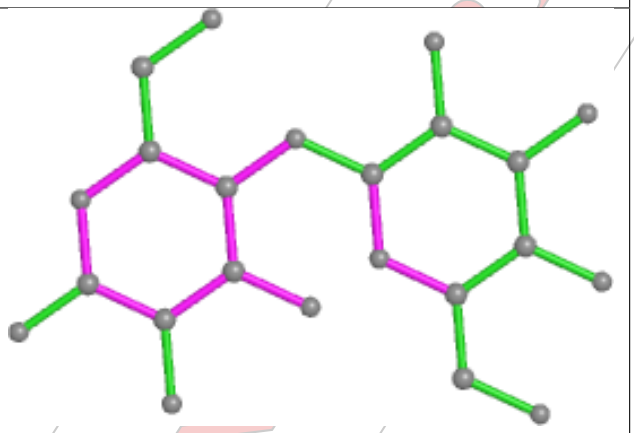
Ligand MAL A 902



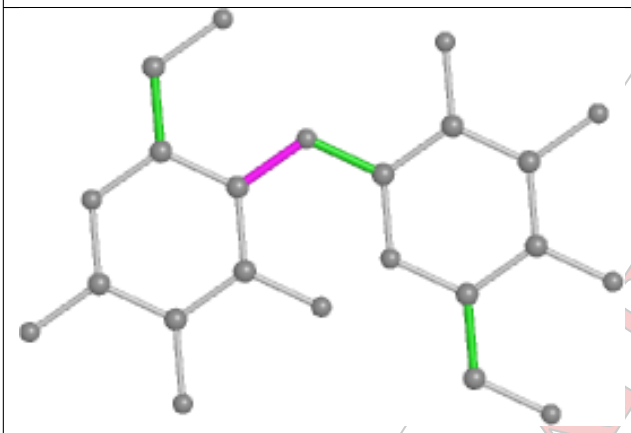
Ligand MAL A 904



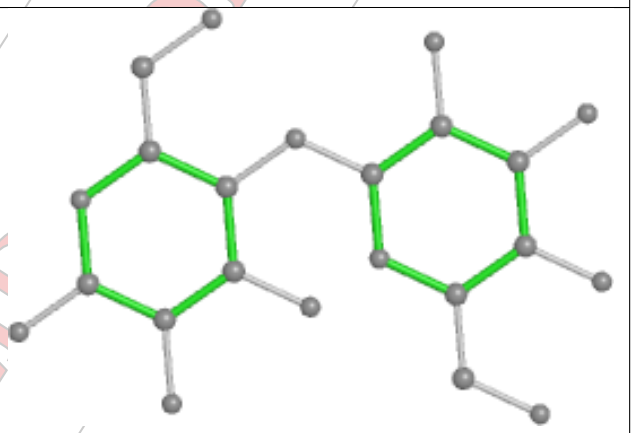
Bond lengths



Bond angles

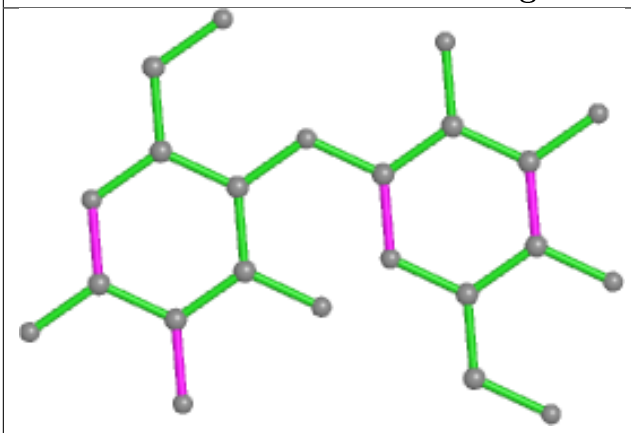


Torsions

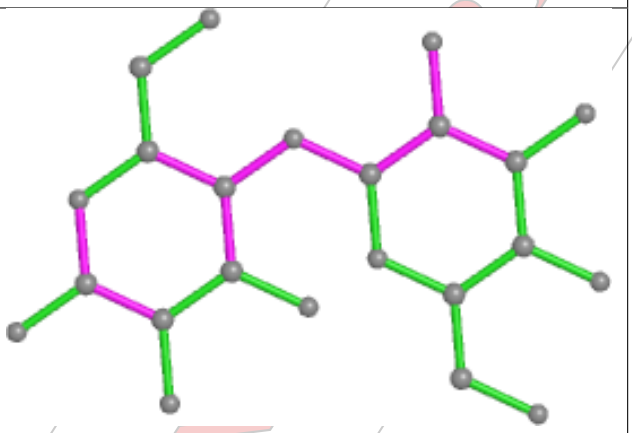


Rings

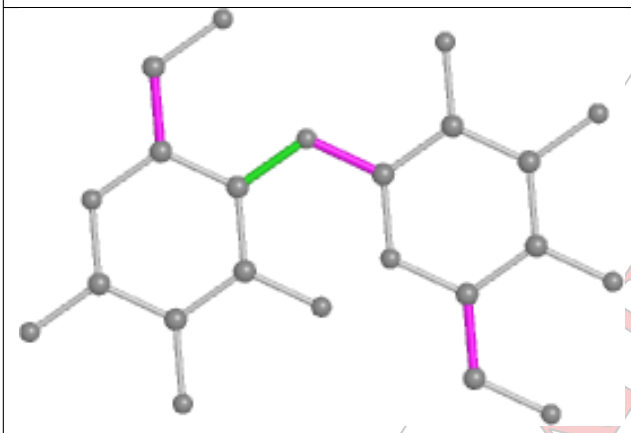
Ligand MAL A 903



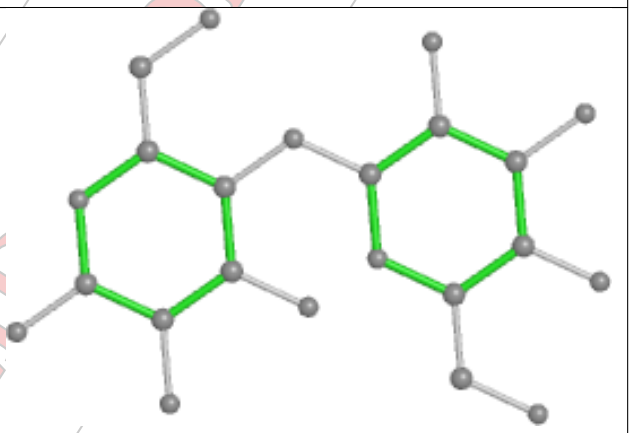
Bond lengths



Bond angles

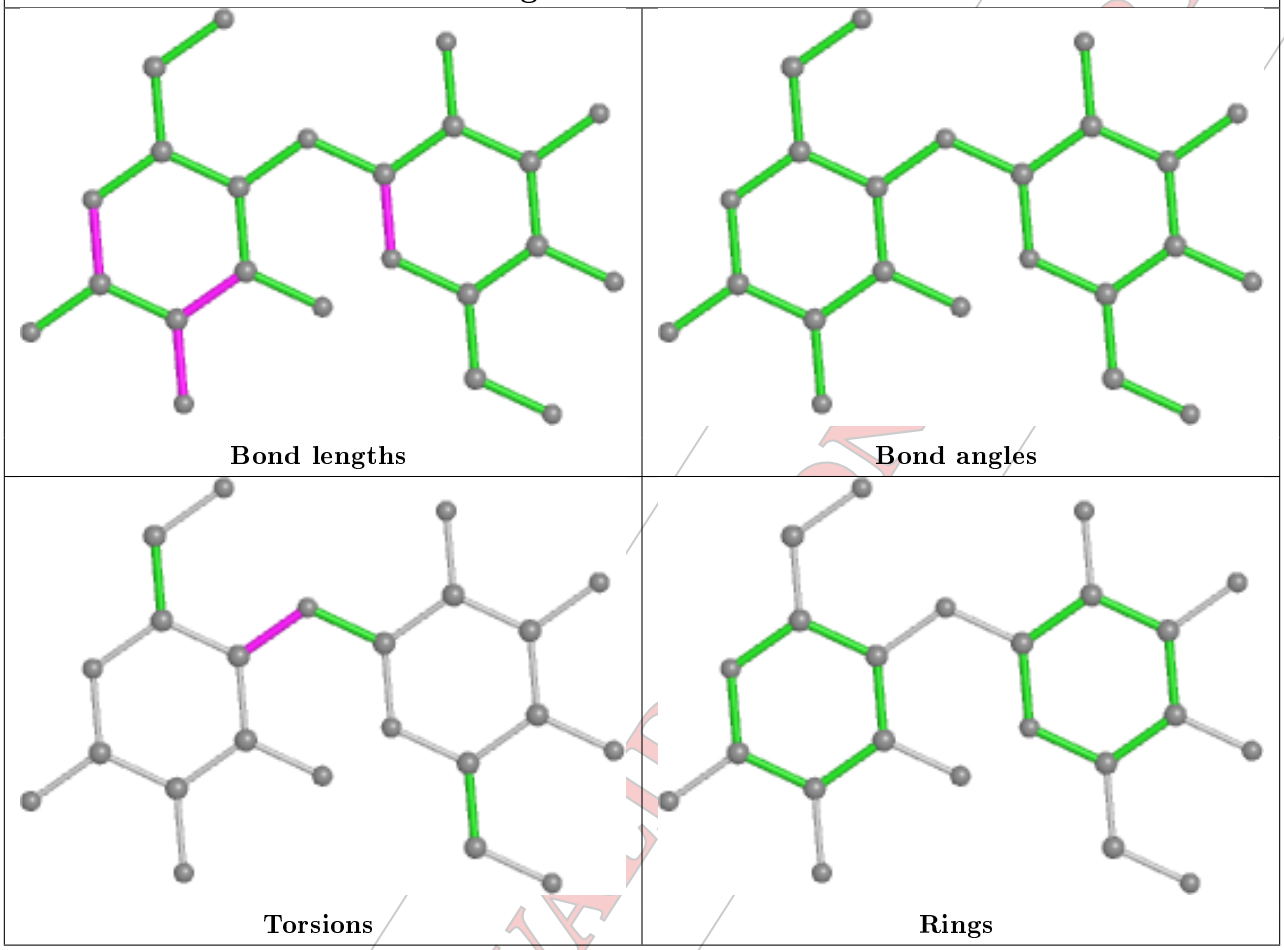


Torsions



Rings

Ligand MAL A 905



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	495/496 (99%)	-0.68	4 (0%)	86 85	13, 20, 36, 73	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	TRP	4.2
1	A	350	ASN	3.7
1	A	459	ASN	2.6
1	A	142	LYS	2.2

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

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
1	PCA	A	1	8/9	0.98	0.05	16,19,22,23	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

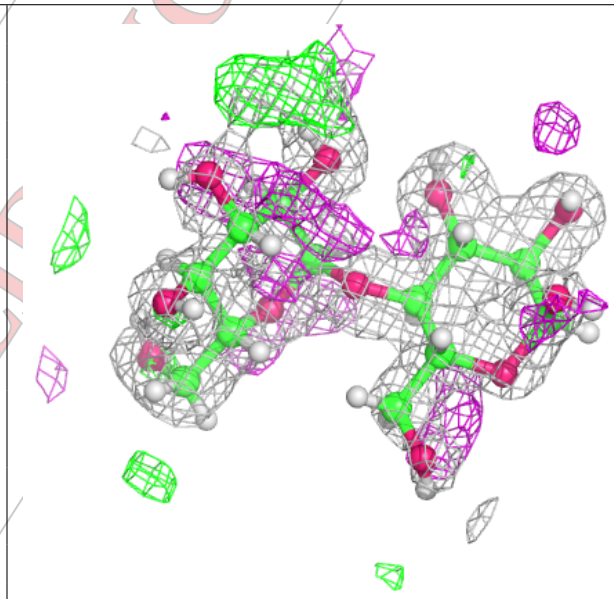
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

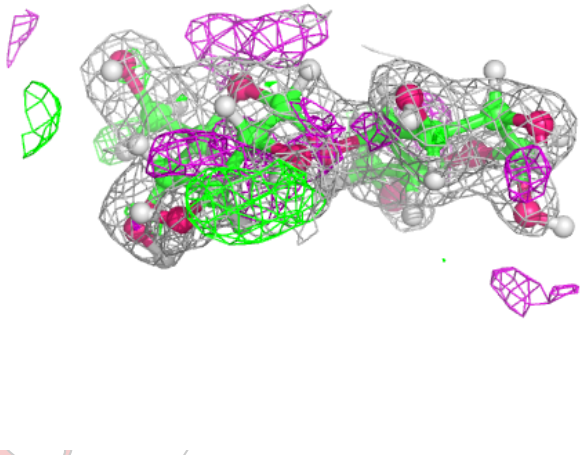
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAL	A	905	23/23	0.78	0.16	31,58,74,88	0
3	MAL	A	902	23/23	0.81	0.18	27,62,77,79	0
3	MAL	A	903	23/23	0.81	0.19	33,74,98,113	0
3	MAL	A	904	23/23	0.89	0.09	22,35,65,78	0
2	GLC	A	901	12/12	0.92	0.13	28,39,57,65	0
4	CA	A	906	1/1	0.99	0.05	18,18,18,18	0
5	CL	A	907	1/1	1.00	0.04	16,16,16,16	0

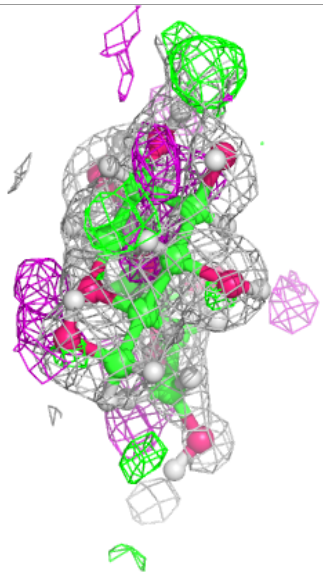
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MAL A 905:

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

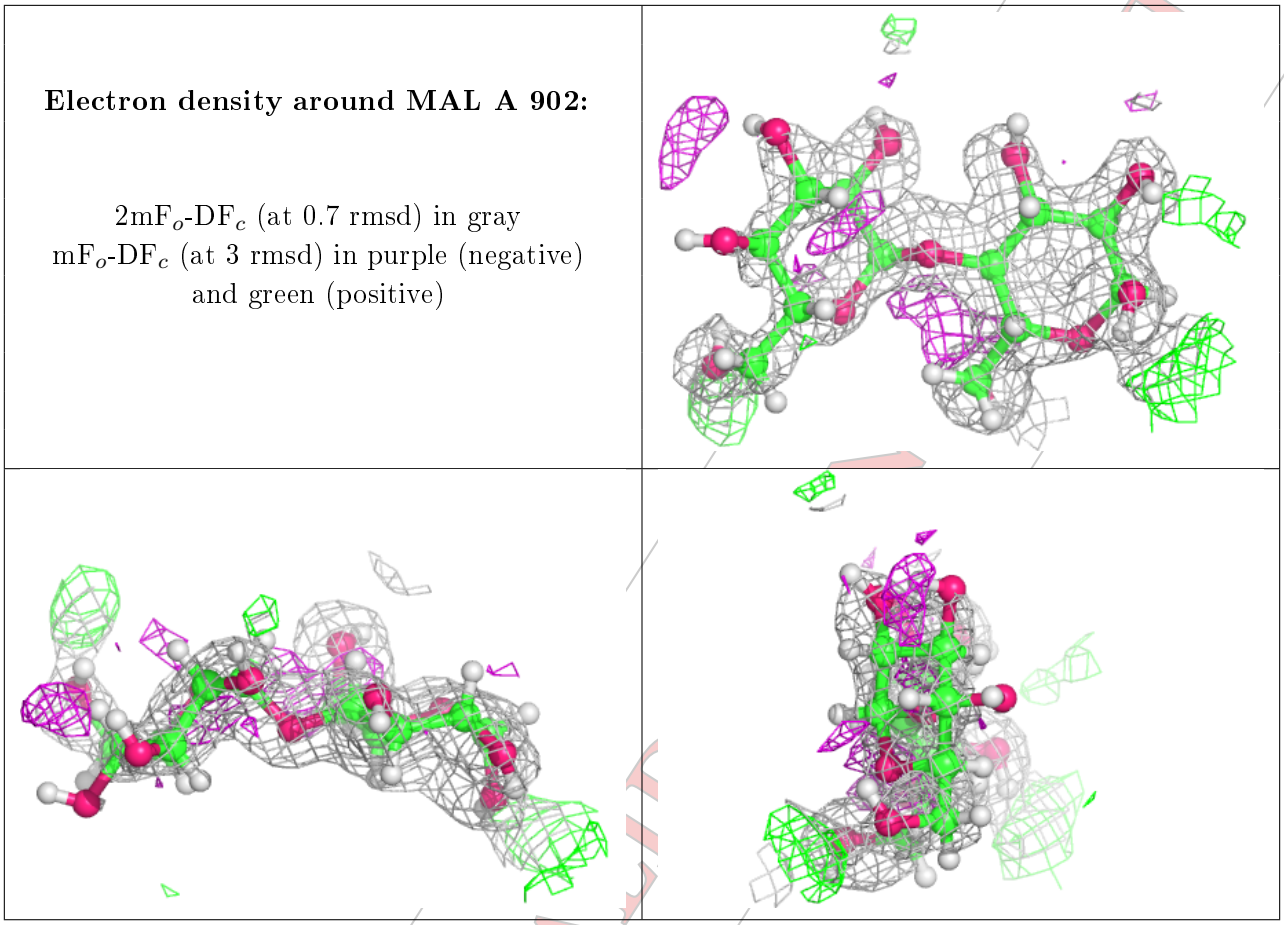






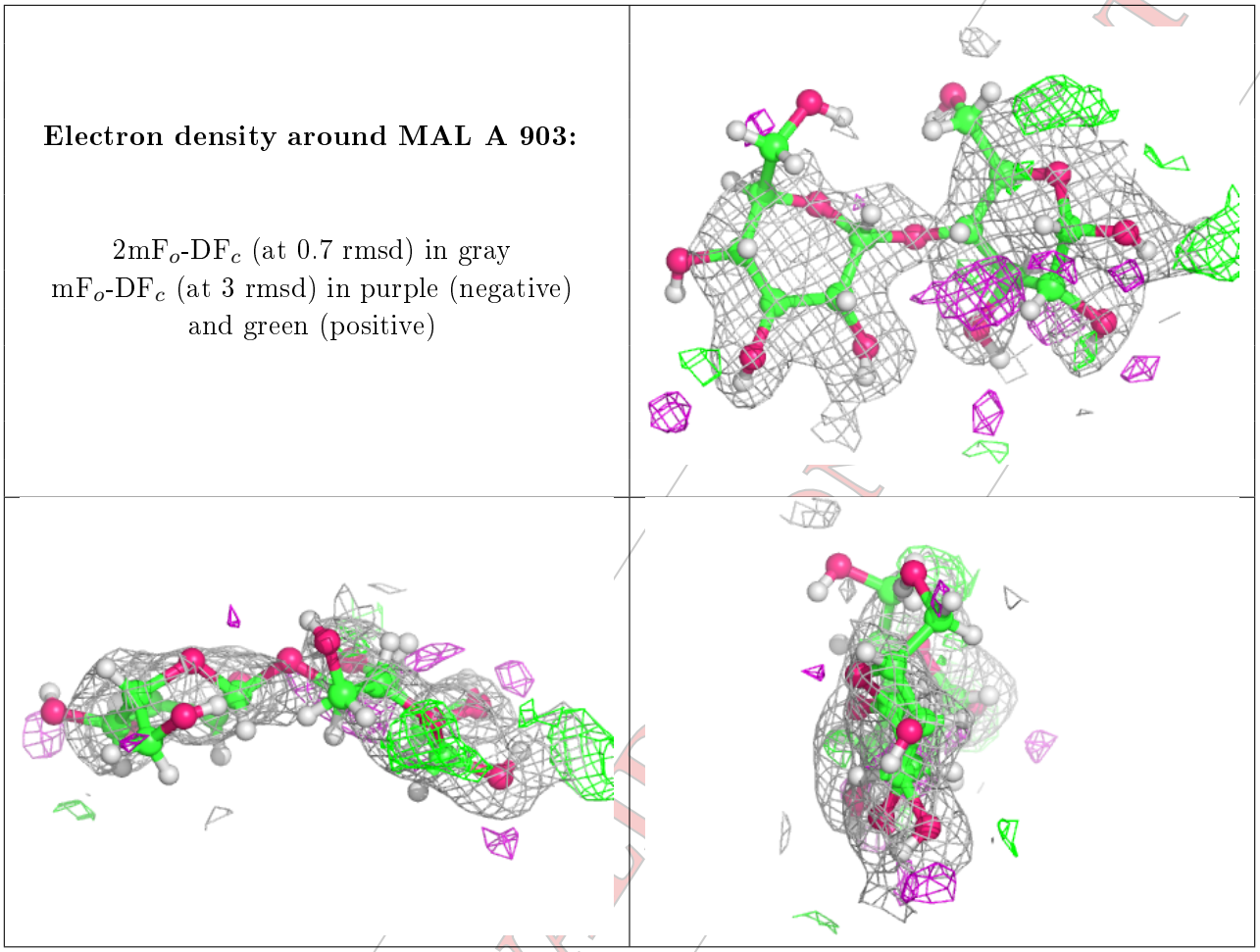
Electron density around MAL A 902:

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



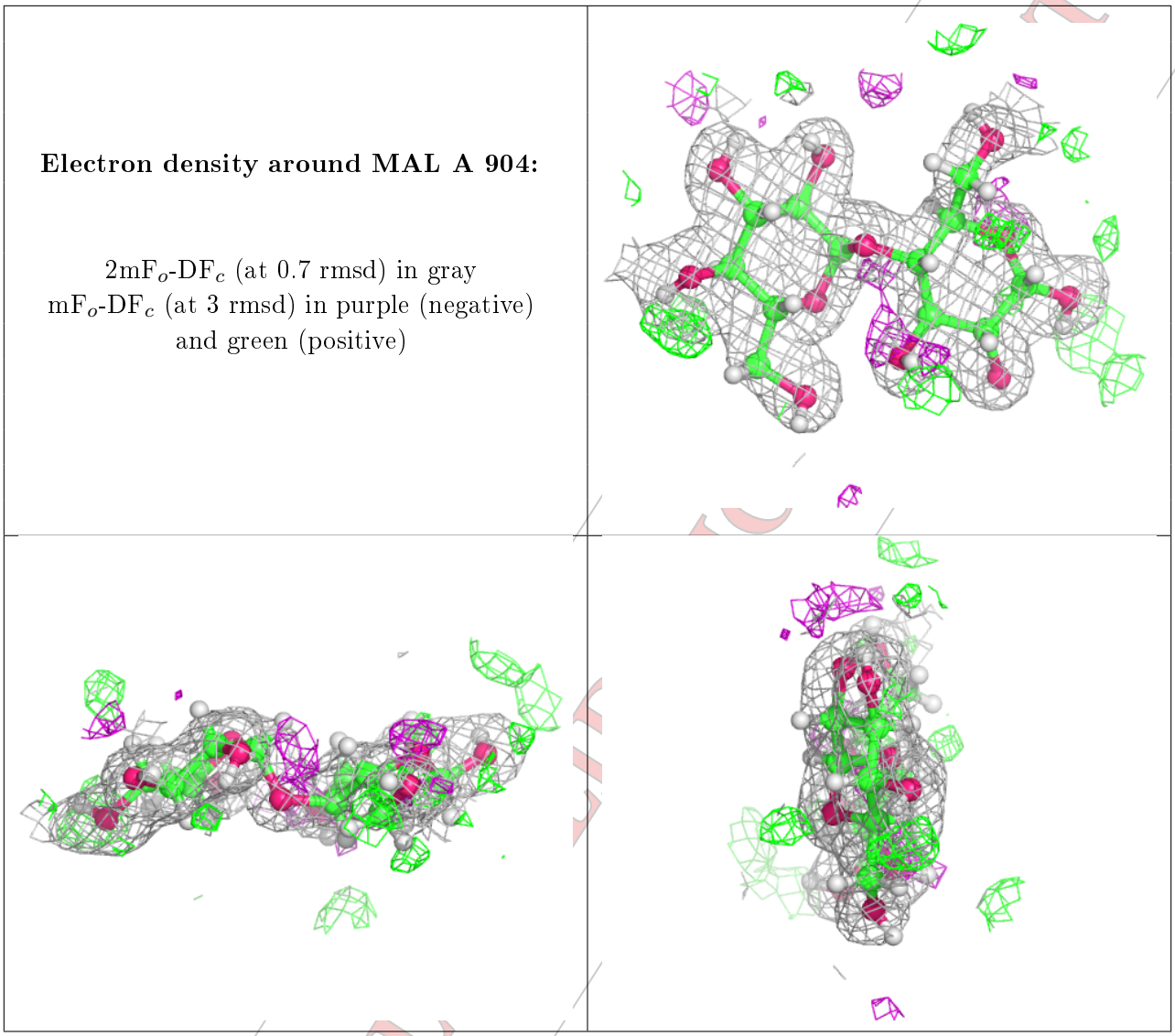
Electron density around MAL A 903:

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



Electron density around MAL A 904:

$2mF_o$-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.