wwPDB X-ray Structure Validation Summary Report (i)

Jan 15, 2024 – 02:08 pm GMT

PDB ID	:	6YOZ
Title	:	HiCel7B labelled with b-1,4-glucosyl cyclophellitol
Authors	:	McGregor, N.G.S.; Davies, G.J.
Deposited on	:	2020-04-15
Resolution	:	1.88 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

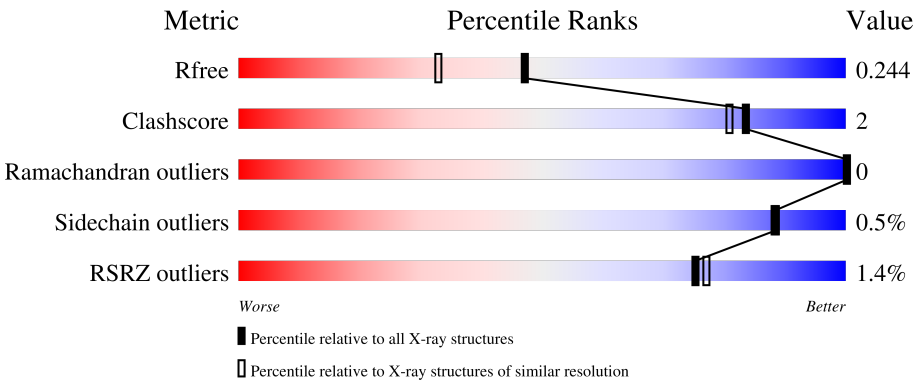
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	AAA	400	2% 96%
1	BBB	400	% 96%

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
7	ACM	AAA	511	-	-	X	-

2 Entry composition (i)

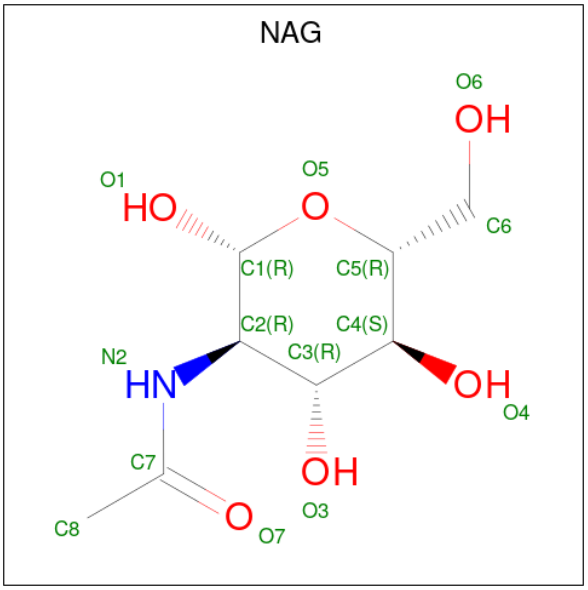
There are 8 unique types of molecules in this entry. The entry contains 12702 atoms, of which 5891 are hydrogens and 0 are deuteriums.

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 Endoglucanase 1.

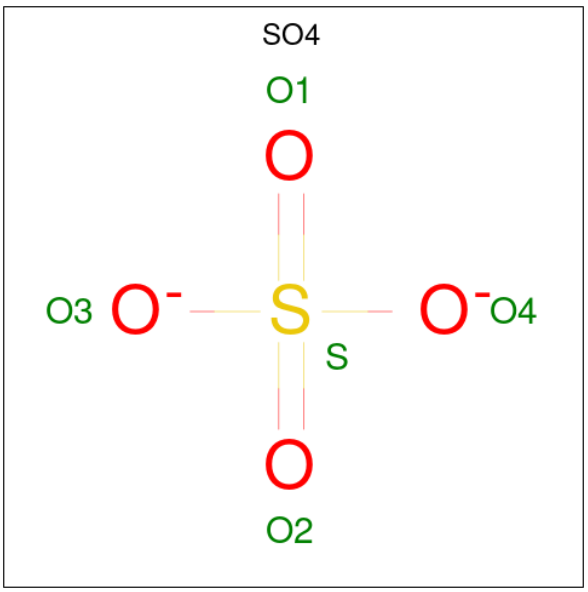
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	400	5955	1926	2896	521	582	30	155	1	0
1	BBB	398	5911	1915	2862	519	586	29	156	1	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



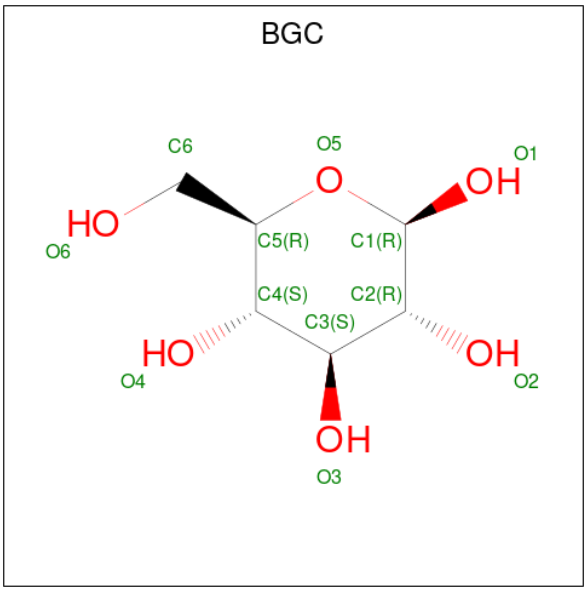
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	AAA	1	28	8	14	1	5	3	0
2	AAA	1	28	8	14	1	5	3	0
2	BBB	1	28	8	14	1	5	3	0
2	BBB	1	28	8	14	1	5	3	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



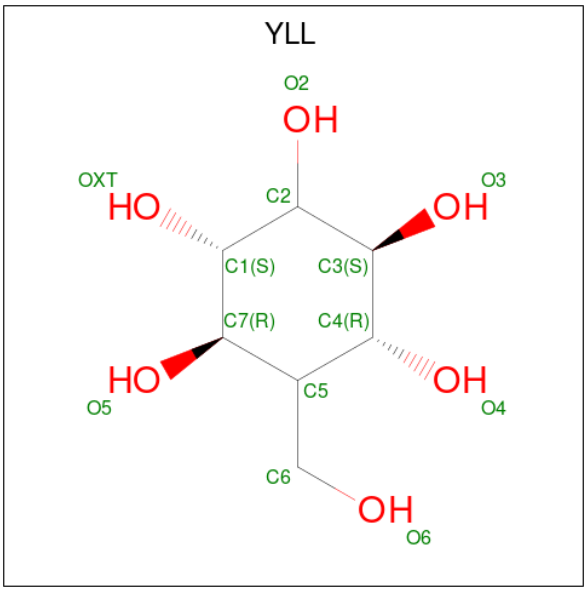
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	AAA	1	5	4	1		0	0
			Total	O	S			
3	AAA	1	5	4	1		0	0
			Total	O	S			
3	AAA	1	5	4	1		0	0
			Total	O	S			
3	AAA	1	5	4	1		0	0
			Total	O	S			
3	AAA	1	5	4	1		0	0
			Total	O	S			
3	BBB	1	5	4	1		0	0
			Total	O	S			
3	BBB	1	5	4	1		0	0
			Total	O	S			
3	BBB	1	5	4	1		0	0
			Total	O	S			
3	BBB	1	5	4	1		0	0
			Total	O	S			
3	BBB	1	5	4	1		0	0
			Total	O	S			
3	BBB	1	5	4	1		0	0
			Total	O	S			
3	BBB	1	5	4	1		0	0

- Molecule 4 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	AAA	1	22	6	11	5	4	0
			Total	C	H	O		
4	BBB	1	22	6	11	5	4	0

- Molecule 5 is (1R,2S,3S,4S,5R,6R)-6-(HYDROXYMETHYL)CYCLOHEXANE-1,2,3,4,5-PENTOL (three-letter code: YLL) (formula: $C_7H_{14}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	AAA	1	25	7	13	5	5	0

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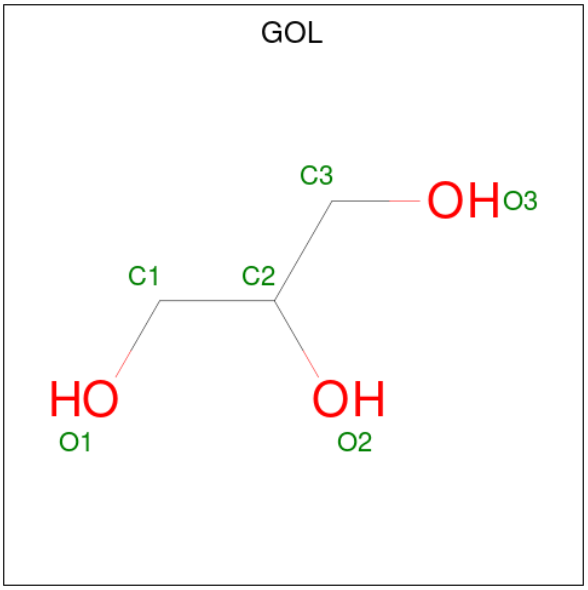
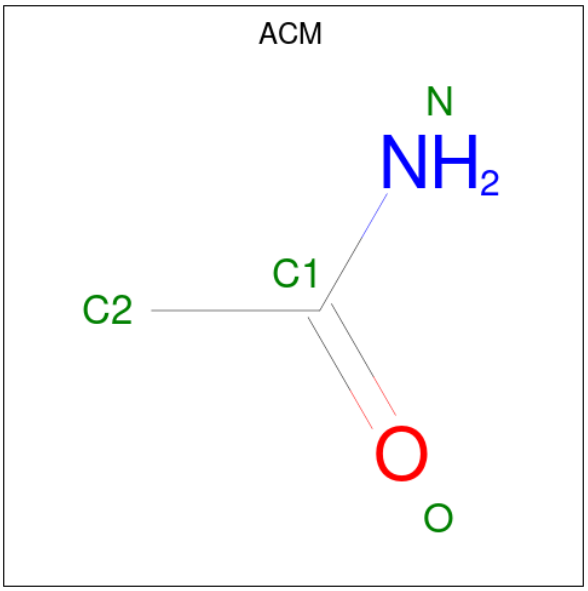
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	BBB	1	25	7	13	5	4	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	AAA	1	14	3	8	3	2	0
			Total	C	H	O		
6	AAA	1	14	3	8	3	2	0
			Total	C	H	O		
6	BBB	1	14	3	8	3	2	0

- Molecule 7 is ACETAMIDE (three-letter code: ACM) (formula: C_2H_5NO).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
7	AAA	1	9	2	5	1	1	2	0

- Molecule 8 is water.

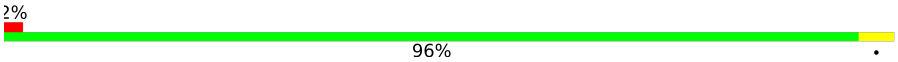
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	AAA	270	270	270	0	0
			Total	O		
8	BBB	249	249	249	0	0

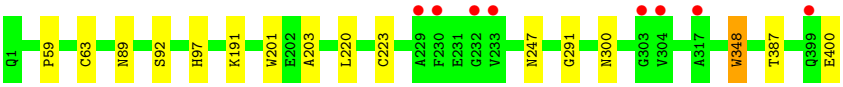
3 Residue-property plots (i)

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: Endoglucanase 1

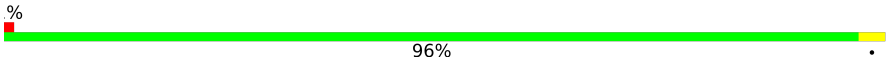
Chain AAA:

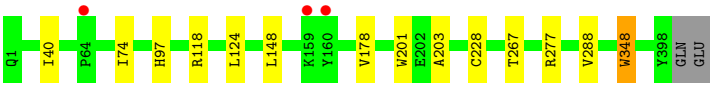




- Molecule 1: Endoglucanase 1

Chain BBB:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	102.00Å 102.00Å 278.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.62 – 1.88 57.55 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.9 (57.62-1.88) 100.0 (57.55-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.202 , 0.236 0.210 , 0.244	Depositor DCC
R_{free} test set	5995 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	35.7	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 62.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12702	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: SO4, YLL, PCA, GOL, ACM, NAG, BGC

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	AAA	0.79	0/3136	0.88	0/4257
1	BBB	0.78	0/3126	0.93	1/4248 (0.0%)
All	All	0.78	0/6262	0.91	1/8505 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	277	ARG	NE-CZ-NH2	-5.27	117.67	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	3059	2896	2866	14	0
1	BBB	3049	2862	2830	11	0
2	AAA	28	28	26	6	0
2	BBB	28	28	26	0	0
3	AAA	25	0	0	1	0
3	BBB	35	0	0	1	0
4	AAA	11	11	10	0	0
4	BBB	11	11	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AAA	12	13	11	0	0
5	BBB	12	13	11	0	0
6	AAA	12	16	16	0	0
6	BBB	6	8	8	2	0
7	AAA	4	5	5	2	5
8	AAA	270	0	0	1	0
8	BBB	249	0	0	0	0
All	All	6811	5891	5819	26	5

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.

The worst 5 of 26 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:AAA:247:ASN:ND2	2:AAA:501:NAG:C2	2.44	0.79
3:AAA:510:SO4:O4	8:AAA:601:HOH:O	1.99	0.78
1:AAA:247:ASN:CG	2:AAA:501:NAG:C1	2.54	0.74
1:AAA:89:ASN:ND2	2:AAA:502:NAG:C2	2.58	0.59
1:AAA:300:ASN:HD21	2:AAA:501:NAG:H61	1.67	0.59

All (5) 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)
7:AAA:511:ACM:C1	7:AAA:511:ACM:N[6_565]	1.43	0.77
7:AAA:511:ACM:HN1	7:AAA:511:ACM:H23[6_565]	0.94	0.66
7:AAA:511:ACM:N	7:AAA:511:ACM:N[6_565]	1.54	0.66
7:AAA:511:ACM:C2	7:AAA:511:ACM:HN1[6_565]	1.32	0.28
7:AAA:511:ACM:N	7:AAA:511:ACM:C2[6_565]	1.93	0.27

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	AAA	399/400 (100%)	393 (98%)	6 (2%)	0	100	100
1	BBB	397/400 (99%)	386 (97%)	11 (3%)	0	100	100
All	All	796/800 (100%)	779 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	321/332 (97%)	319 (99%)	2 (1%)	86	86
1	BBB	319/332 (96%)	318 (100%)	1 (0%)	92	92
All	All	640/664 (96%)	637 (100%)	3 (0%)	88	88

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

Mol	Chain	Res	Type
1	AAA	92	SER
1	AAA	348	TRP
1	BBB	348	TRP

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	PCA	BBB	1	1	7,8,9	0.51	0	9,10,12	0.93	0
1	PCA	AAA	1	1	7,8,9	0.24	0	9,10,12	1.08	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
1	PCA	BBB	1	1	-	0/0/11/13	0/1/1/1
1	PCA	AAA	1	1	-	0/0/11/13	0/1/1/1

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.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

24 ligands 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	$\#\|Z\| > 2$
3	SO4	BBB	510	-	4,4,4	0.39	0	6,6,6	0.15	0
5	YLL	BBB	509	1,4	12,12,13	0.78	0	14,17,19	1.35	2 (14%)
6	GOL	BBB	511	-	5,5,5	0.20	0	5,5,5	0.79	0
3	SO4	BBB	512	-	4,4,4	0.38	0	6,6,6	0.11	0
3	SO4	AAA	504	-	4,4,4	0.31	0	6,6,6	0.30	0
3	SO4	AAA	510	-	4,4,4	0.26	0	6,6,6	0.35	0
3	SO4	BBB	505	-	4,4,4	0.19	0	6,6,6	0.30	0
4	BGC	AAA	506	5	11,11,12	0.96	0	15,15,17	1.44	2 (13%)
5	YLL	AAA	507	1,4	12,12,13	0.67	1 (8%)	14,17,19	1.09	2 (14%)
6	GOL	AAA	508	-	5,5,5	0.70	0	5,5,5	1.31	0
3	SO4	BBB	503	-	4,4,4	0.55	0	6,6,6	0.24	0
2	NAG	BBB	501	1	14,14,15	0.87	0	17,19,21	2.43	9 (52%)
3	SO4	BBB	502	-	4,4,4	0.58	0	6,6,6	0.23	0
7	ACM	AAA	511	-	3,3,3	2.12	1 (33%)	3,3,3	1.59	1 (33%)
4	BGC	BBB	508	5	11,11,12	0.95	0	15,15,17	1.29	1 (6%)
3	SO4	BBB	504	-	4,4,4	0.44	0	6,6,6	0.18	0
3	SO4	AAA	512	-	4,4,4	0.39	0	6,6,6	0.19	0
2	NAG	BBB	507	1	14,14,15	1.32	2 (14%)	17,19,21	2.01	5 (29%)
2	NAG	AAA	501	1	14,14,15	0.93	1 (7%)	17,19,21	2.14	6 (35%)
3	SO4	AAA	505	-	4,4,4	0.38	0	6,6,6	0.22	0
3	SO4	AAA	503	-	4,4,4	0.44	0	6,6,6	0.21	0
3	SO4	BBB	506	-	4,4,4	0.49	0	6,6,6	0.09	0
2	NAG	AAA	502	1	14,14,15	1.11	2 (14%)	17,19,21	1.53	1 (5%)
6	GOL	AAA	509	-	5,5,5	0.08	0	5,5,5	0.22	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
4	BGC	BBB	508	5	-	0/2/19/22	0/1/1/1
5	YLL	BBB	509	1,4	-	0/2/22/26	0/1/1/1
6	GOL	BBB	511	-	-	2/4/4/4	-
5	YLL	AAA	507	1,4	-	0/2/22/26	0/1/1/1
2	NAG	AAA	501	1	-	2/6/23/26	0/1/1/1
6	GOL	AAA	508	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGC	AAA	506	5	-	0/2/19/22	0/1/1/1
2	NAG	BBB	501	1	-	0/6/23/26	0/1/1/1
2	NAG	BBB	507	1	-	2/6/23/26	0/1/1/1
2	NAG	AAA	502	1	-	2/6/23/26	0/1/1/1
6	GOL	AAA	509	-	-	0/4/4/4	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	AAA	511	ACM	O-C1	3.66	1.32	1.24
2	BBB	507	NAG	C1-C2	2.89	1.56	1.52
2	AAA	502	NAG	C1-C2	-2.87	1.48	1.52
2	AAA	502	NAG	O5-C1	-2.65	1.39	1.43
2	BBB	507	NAG	O5-C1	2.55	1.47	1.43

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	501	NAG	O5-C1-C2	5.79	120.43	111.29
2	AAA	501	NAG	O5-C1-C2	5.12	119.38	111.29
2	BBB	507	NAG	O5-C5-C6	4.75	114.65	107.20
2	AAA	502	NAG	O6-C6-C5	-4.49	95.89	111.29
2	BBB	501	NAG	C6-C5-C4	-4.41	102.67	113.00

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	AAA	508	GOL	O1-C1-C2-C3
6	BBB	511	GOL	C1-C2-C3-O3
2	AAA	501	NAG	C4-C5-C6-O6
2	AAA	502	NAG	C4-C5-C6-O6
2	BBB	507	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	BBB	511	GOL	2	0
3	AAA	510	SO4	1	0

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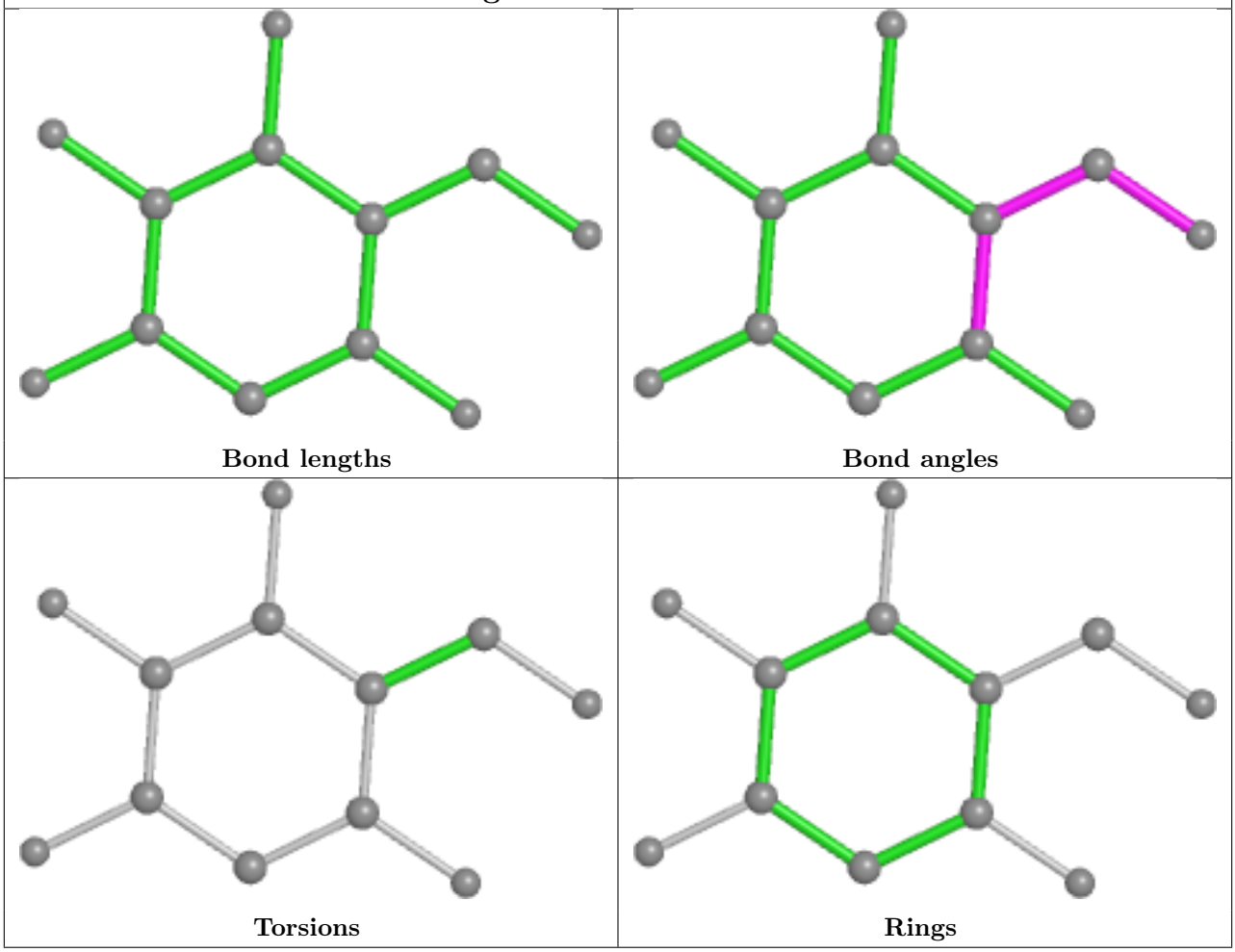
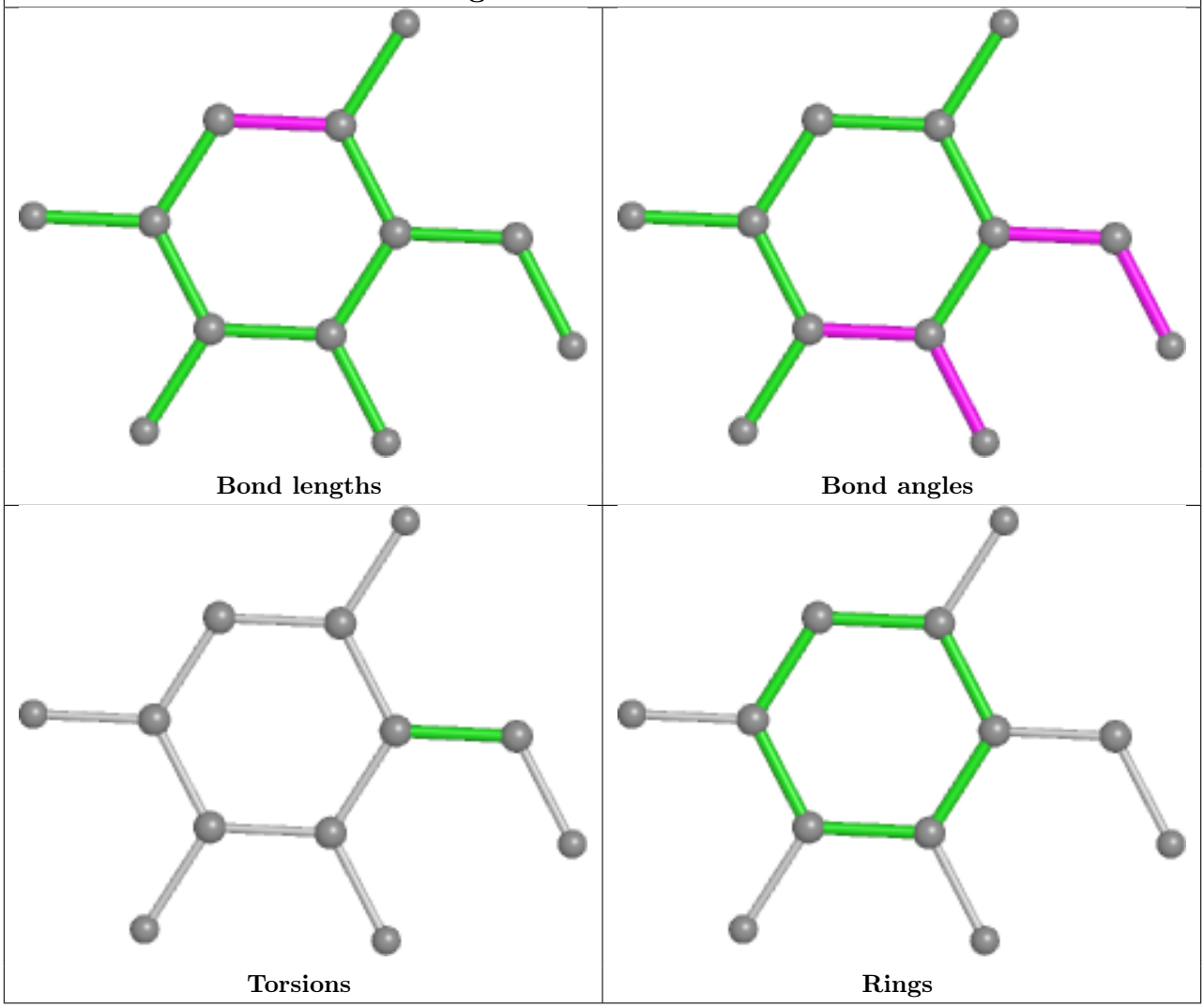
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	AAA	511	ACM	2	5
3	BBB	504	SO4	1	0
2	AAA	501	NAG	3	0
2	AAA	502	NAG	3	0

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 YLL BBB 509



Ligand YLL AAA 507



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	AAA	399/400 (99%)	0.40	8 (2%)	65	67	24, 35, 51, 71	0
1	BBB	397/400 (99%)	0.18	3 (0%)	86	87	23, 34, 50, 68	0
All	All	796/800 (99%)	0.29	11 (1%)	75	77	23, 34, 51, 71	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	160	TYR	3.7
1	AAA	229	ALA	3.1
1	AAA	233	VAL	2.8
1	AAA	399	GLN	2.8
1	AAA	232	GLY	2.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PCA	AAA	1	8/9	0.96	0.09	28,30,31,32	0
1	PCA	BBB	1	8/9	0.96	0.12	36,41,44,45	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

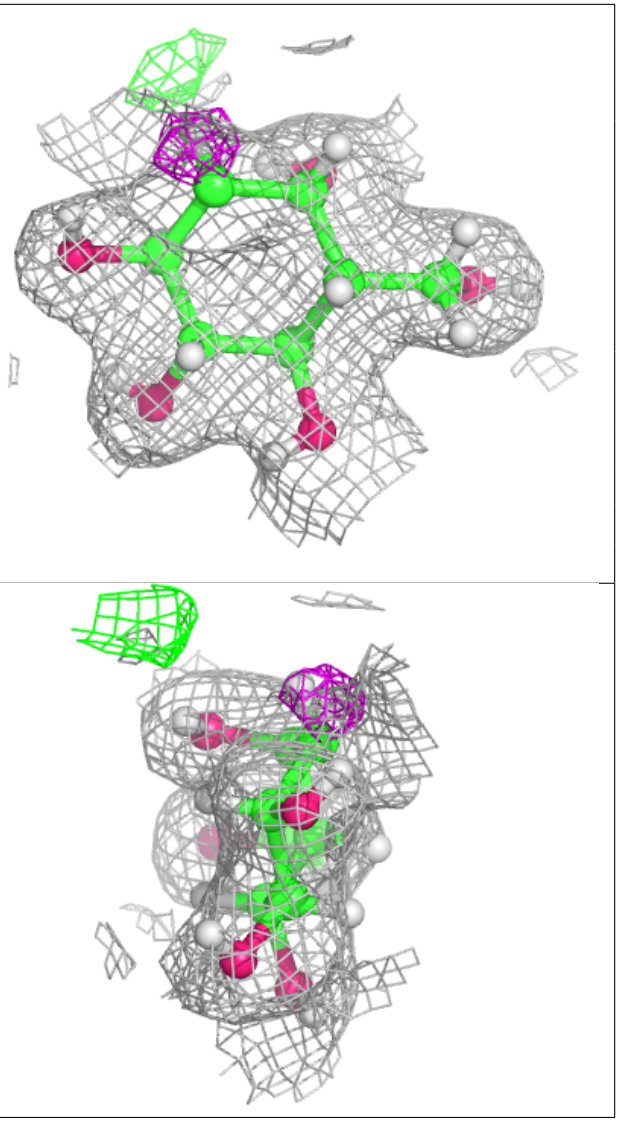
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	AAA	508	6/6	0.66	0.20	38,45,49,49	2
2	NAG	BBB	507	14/15	0.78	0.15	49,58,63,63	3
7	ACM	AAA	511	4/4	0.81	0.23	30,49,62,62	4
3	SO4	AAA	512	5/5	0.83	0.36	80,92,100,111	0
6	GOL	BBB	511	6/6	0.84	0.24	42,46,55,55	2
5	YLL	AAA	507	12/13	0.90	0.12	0,29,31,32	5
3	SO4	BBB	510	5/5	0.90	0.14	61,73,80,84	0
3	SO4	AAA	504	5/5	0.91	0.20	60,70,82,90	0
6	GOL	AAA	509	6/6	0.91	0.27	58,65,78,78	2
2	NAG	AAA	502	14/15	0.92	0.14	39,48,57,63	3
3	SO4	BBB	512	5/5	0.93	0.25	42,42,47,47	5
2	NAG	AAA	501	14/15	0.93	0.21	42,53,61,66	3
2	NAG	BBB	501	14/15	0.94	0.12	37,43,58,61	3
3	SO4	AAA	510	5/5	0.94	0.22	50,62,85,87	0
3	SO4	AAA	503	5/5	0.94	0.16	54,66,74,79	0
5	YLL	BBB	509	12/13	0.94	0.12	22,24,26,29	4
3	SO4	AAA	505	5/5	0.95	0.11	65,65,79,82	0
4	BGC	BBB	508	11/12	0.95	0.14	0,23,24,24	4
3	SO4	BBB	506	5/5	0.96	0.14	60,64,67,80	0
4	BGC	AAA	506	11/12	0.96	0.11	0,29,32,34	4
3	SO4	BBB	504	5/5	0.96	0.11	57,60,62,75	0
3	SO4	BBB	505	5/5	0.97	0.11	46,46,52,66	0
3	SO4	BBB	503	5/5	0.97	0.12	52,52,61,63	0
3	SO4	BBB	502	5/5	0.98	0.10	39,48,58,65	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.

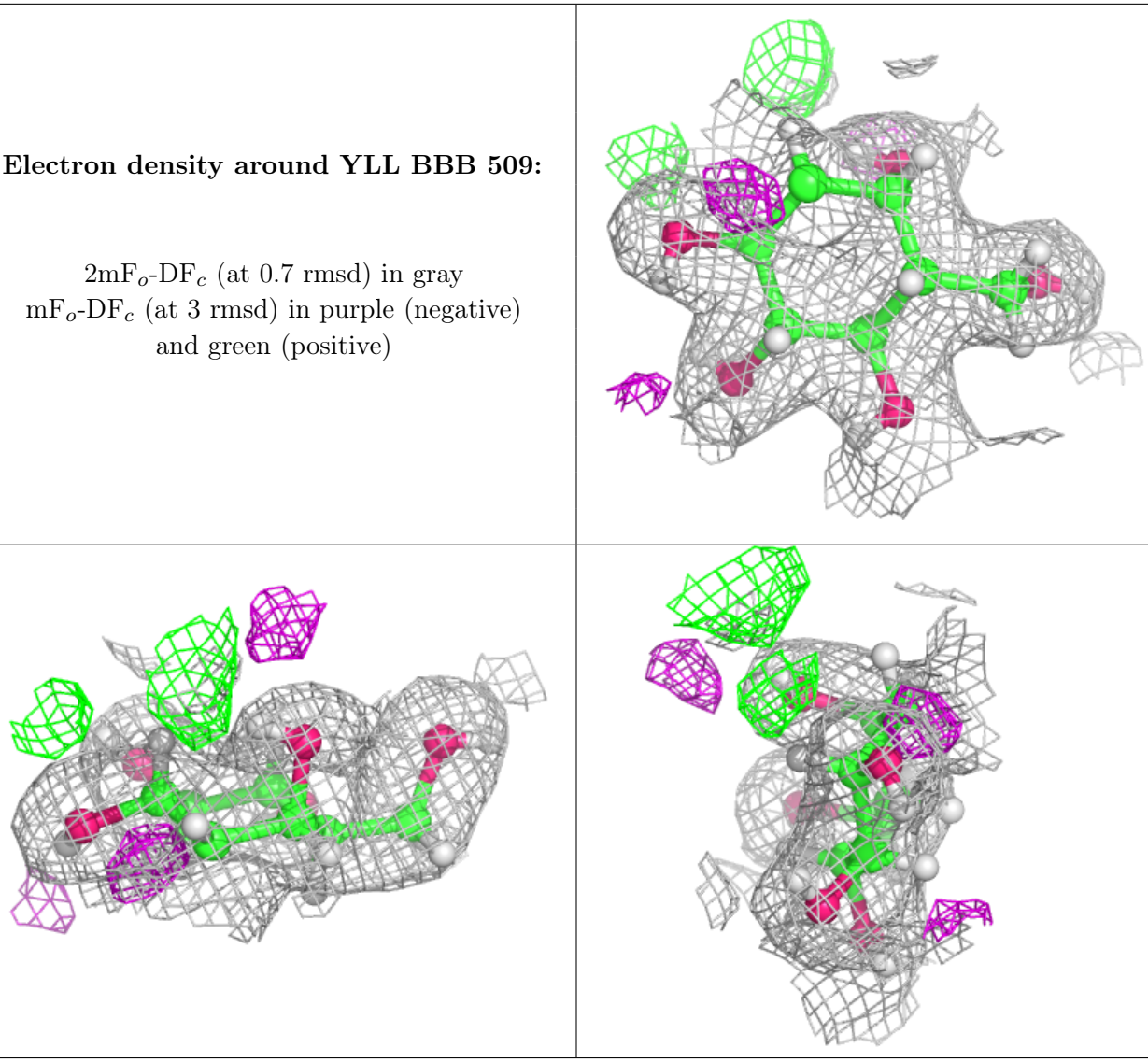
Electron density around YLL AAA 507:

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



Electron density around YLL BBB 509:

$2mF_o$-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.