



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 01:55 AM EDT

PDB ID : 7LYD
Title : Crystal Structure of Ebola zaire Envelope glycoprotein GP in complex with compound ARN0075146
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2021-03-06
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

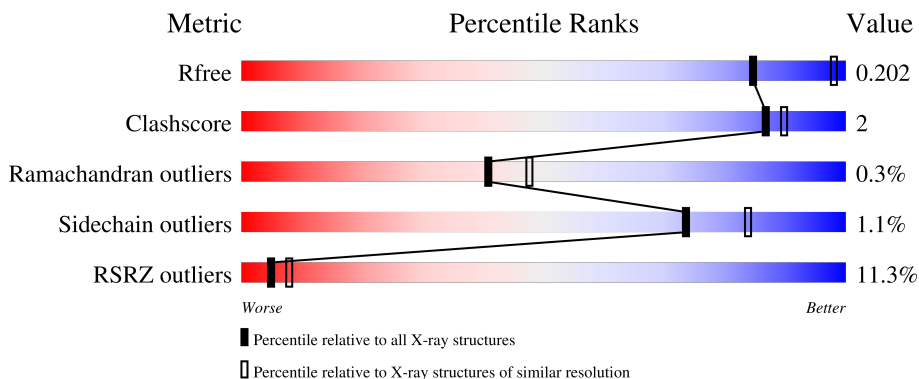
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	291	
2	B	168	
3	C	5	

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
3	MAN	C	4	-	-	-	X
3	MAN	C	5	-	-	-	X
4	NAG	A	604	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3123 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 GP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	240	1841	1179	311	346	5	0	3	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLU	-	expression tag	UNP Q05320
A	29	THR	-	expression tag	UNP Q05320
A	30	GLY	-	expression tag	UNP Q05320
A	31	ARG	-	expression tag	UNP Q05320
A	42	ALA	THR	engineered mutation	UNP Q05320
A	472	UNK	ASN	conflict	UNP Q05320
A	473	UNK	GLY	conflict	UNP Q05320
A	474	UNK	ALA	conflict	UNP Q05320
A	475	UNK	LYS	conflict	UNP Q05320
A	476	UNK	ASN	conflict	UNP Q05320
A	477	UNK	ILE	conflict	UNP Q05320

- Molecule 2 is a protein called GP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	128	944	596	168	174	6	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

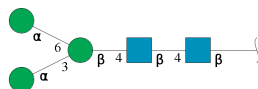
Chain	Residue	Modelled	Actual	Comment	Reference
B	613	ALA	HIS	engineered mutation	UNP Q05320
B	633	GLY	-	expression tag	UNP Q05320
B	634	SER	-	expression tag	UNP Q05320
B	635	GLY	-	expression tag	UNP Q05320
B	636	TYR	-	expression tag	UNP Q05320

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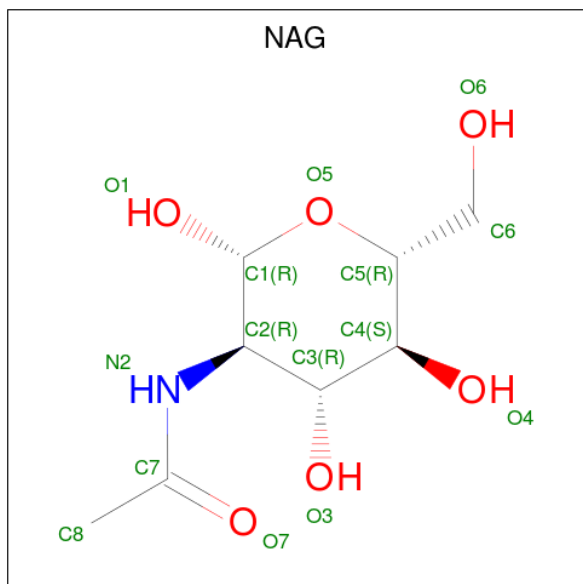
Chain	Residue	Modelled	Actual	Comment	Reference
B	637	ILE	-	expression tag	UNP Q05320
B	638	PRO	-	expression tag	UNP Q05320
B	639	GLU	-	expression tag	UNP Q05320
B	640	ALA	-	expression tag	UNP Q05320
B	641	PRO	-	expression tag	UNP Q05320
B	642	ARG	-	expression tag	UNP Q05320
B	643	ASP	-	expression tag	UNP Q05320
B	644	GLY	-	expression tag	UNP Q05320
B	645	GLN	-	expression tag	UNP Q05320
B	646	ALA	-	expression tag	UNP Q05320
B	647	TYR	-	expression tag	UNP Q05320
B	648	VAL	-	expression tag	UNP Q05320
B	649	ARG	-	expression tag	UNP Q05320
B	650	LYS	-	expression tag	UNP Q05320
B	651	ASP	-	expression tag	UNP Q05320
B	652	GLY	-	expression tag	UNP Q05320
B	653	GLU	-	expression tag	UNP Q05320
B	654	TRP	-	expression tag	UNP Q05320
B	655	VAL	-	expression tag	UNP Q05320
B	656	LEU	-	expression tag	UNP Q05320
B	657	LEU	-	expression tag	UNP Q05320
B	658	SER	-	expression tag	UNP Q05320
B	659	THR	-	expression tag	UNP Q05320
B	660	PHE	-	expression tag	UNP Q05320
B	661	LEU	-	expression tag	UNP Q05320
B	662	GLY	-	expression tag	UNP Q05320
B	663	THR	-	expression tag	UNP Q05320
B	664	HIS	-	expression tag	UNP Q05320
B	665	HIS	-	expression tag	UNP Q05320
B	666	HIS	-	expression tag	UNP Q05320
B	667	HIS	-	expression tag	UNP Q05320
B	668	HIS	-	expression tag	UNP Q05320
B	669	HIS	-	expression tag	UNP Q05320

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



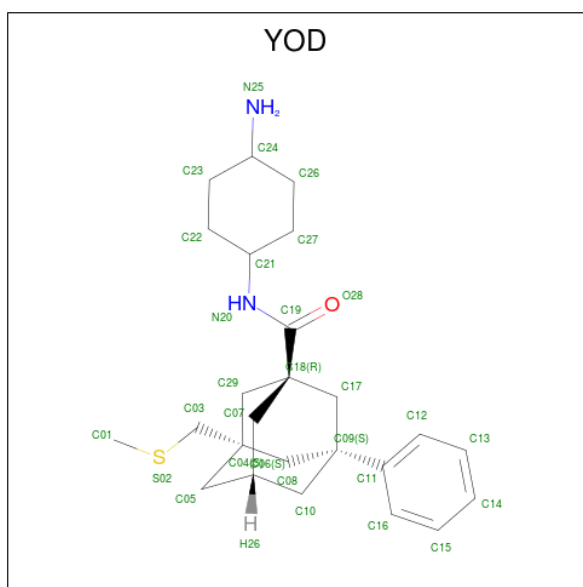
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	5	61	34	2	25	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



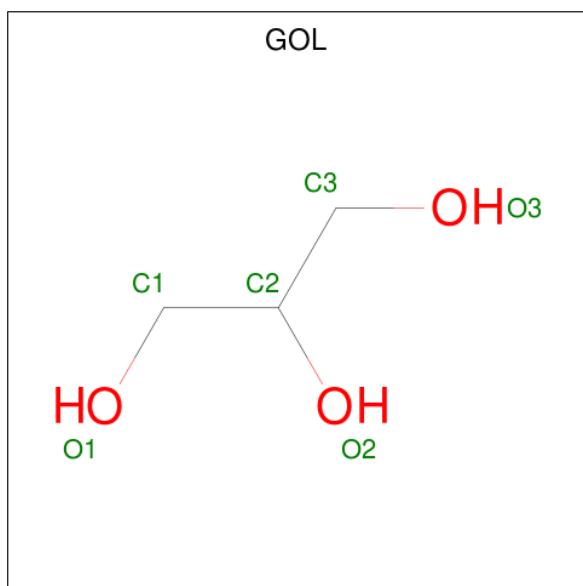
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0
4	A	1	14	8	1	5	0	0

- Molecule 5 is (1R,3S,5S,7S)-N-[(1r,4R)-4-aminocyclohexyl]-3-[(methylsulfanyl)methyl]-5-phenyladamantane-1-carboxamide (three-letter code: YOD) (formula: $C_{25}H_{36}N_2OS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	29	25	2	1	1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

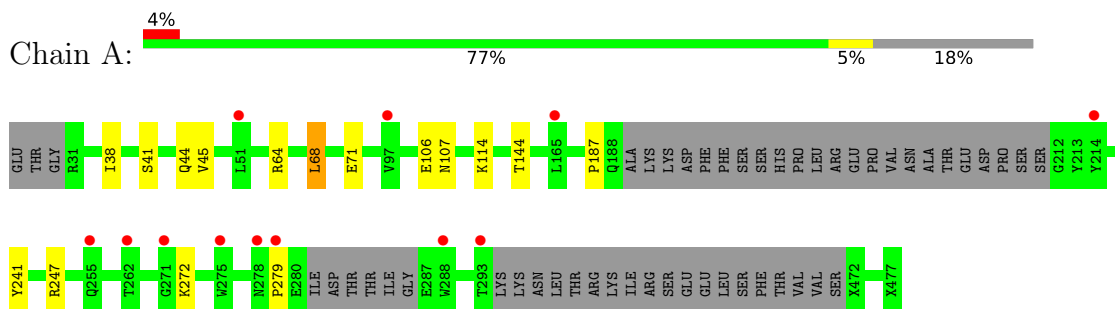
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	119	Total 119	O 119	0	0
7	B	61	Total 61	O 61	0	0

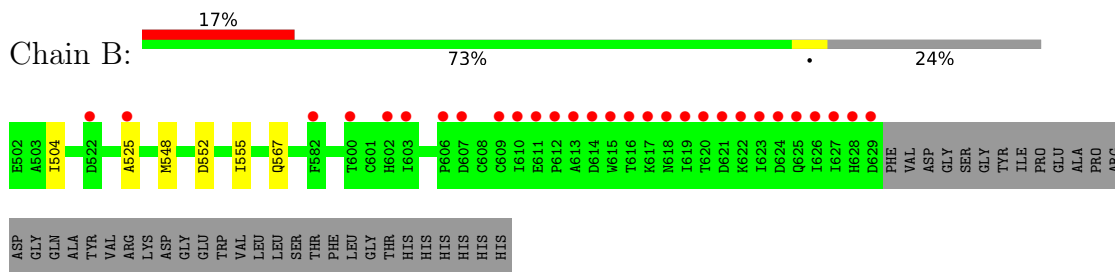
3 Residue-property plots [i](#)

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: GP1



- Molecule 2: GP2



- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	114.17Å 114.17Å 308.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.63 – 2.35 41.63 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.63-2.35) 99.9 (41.63-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.177 , 0.205 0.176 , 0.202	Depositor DCC
R_{free} test set	2035 reflections (6.23%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtrriage
Anisotropy	0.567	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3123	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, GOL, MAN, BMA, YOD

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	0.34	0/1866	0.57	1/2544 (0.0%)
2	B	0.31	0/965	0.49	0/1319
All	All	0.33	0/2831	0.54	1/3863 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	LEU	CA-CB-CG	-5.27	103.19	115.30

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	A	1841	0	1720	9	0
2	B	944	0	860	4	0
3	C	61	0	52	1	0
4	A	56	0	52	0	0
5	A	29	0	0	0	0
6	A	6	0	8	0	0
6	B	6	0	8	1	0
7	A	119	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	61	0	0	0	0
All	All	3123	0	2700	12	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 (12) 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:45:VAL:HG23	2:B:504:ILE:HD11	1.73	0.70
1:A:114:LYS:NZ	7:A:701:HOH:O	2.28	0.64
1:A:38:ILE:HD12	1:A:187:PRO:HG3	1.87	0.57
2:B:548:MET:HG2	2:B:555:ILE:HD11	1.87	0.56
1:A:114:LYS:O	1:A:144:THR:HA	2.11	0.51
1:A:247:ARG:NH1	1:A:279:PRO:O	2.46	0.45
2:B:567:GLN:HB2	6:B:701:GOL:H11	1.99	0.44
1:A:241:TYR:CD1	1:A:272:LYS:HE3	2.54	0.42
1:A:41:SER:O	2:B:552:ASP:HB3	2.19	0.42
1:A:71:GLU:OE2	1:A:106:GLU:HB3	2.19	0.42
3:C:3:BMA:H61	3:C:5:MAN:H2	1.72	0.41
1:A:71:GLU:OE2	1:A:107:ASN:N	2.54	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	231/291 (79%)	227 (98%)	4 (2%)	0	100	100
2	B	126/168 (75%)	122 (97%)	3 (2%)	1 (1%)	19	20
All	All	357/459 (78%)	349 (98%)	7 (2%)	1 (0%)	41	47

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	525	ALA

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	188/245 (77%)	185 (98%)	3 (2%)	62	75
2	B	88/139 (63%)	88 (100%)	0	100	100
All	All	276/384 (72%)	273 (99%)	3 (1%)	73	84

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

Mol	Chain	Res	Type
1	A	44	GLN
1	A	64	ARG
1	A	68	LEU

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](#)

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

5.5 Carbohydrates [i](#)

5 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	$\# Z > 2$
3	NAG	C	1	2,3	14,14,15	0.34	0	17,19,21	0.68	1 (5%)
3	NAG	C	2	3	14,14,15	0.37	0	17,19,21	0.52	0
3	BMA	C	3	3	11,11,12	1.21	2 (18%)	15,15,17	0.96	1 (6%)
3	MAN	C	4	3	11,11,12	1.19	1 (9%)	15,15,17	0.85	0
3	MAN	C	5	3	11,11,12	1.07	0	15,15,17	0.84	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	NAG	C	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
3	MAN	C	5	3	-	1/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	BMA	C2-C3	2.85	1.56	1.52
3	C	3	BMA	C1-C2	2.52	1.58	1.52
3	C	4	MAN	C2-C3	2.12	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C1-O5-C5	2.19	115.16	112.19
3	C	3	BMA	O3-C3-C2	2.11	114.03	109.99

There are no chirality outliers.

All (7) torsion outliers are listed below:

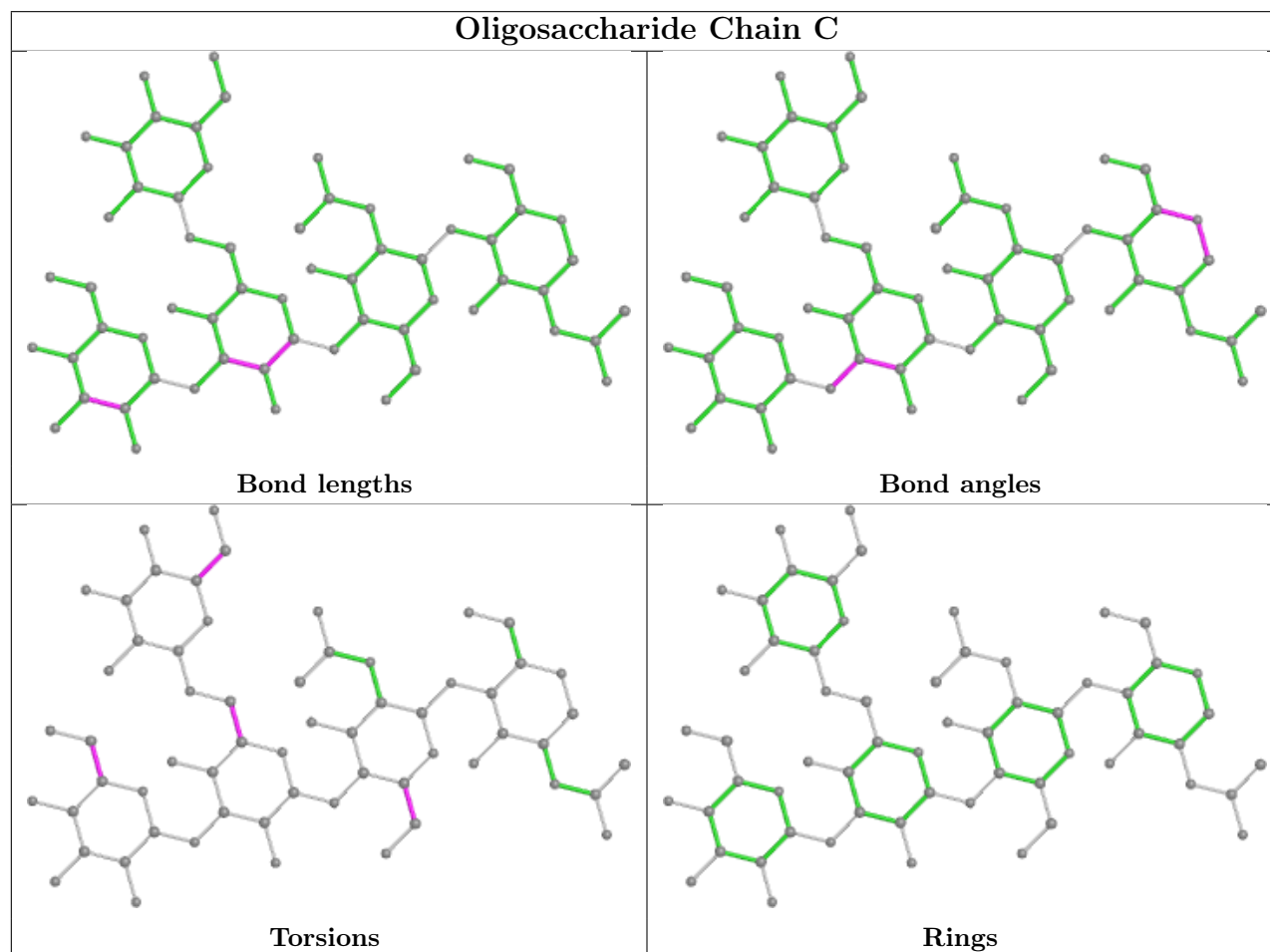
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6
3	C	5	MAN	C4-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3	BMA	1	0
3	C	5	MAN	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 oligosaccharide.



5.6 Ligand geometry

7 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
4	NAG	A	601	1	14,14,15	0.28	0	17,19,21	0.77	1 (5%)
4	NAG	A	604	1	14,14,15	0.58	0	17,19,21	0.59	0
5	YOD	A	605	-	33,33,33	0.99	1 (3%)	46,51,51	1.05	1 (2%)
4	NAG	A	602	1	14,14,15	0.32	0	17,19,21	0.46	0
4	NAG	A	603	1	14,14,15	0.20	0	17,19,21	0.57	0
6	GOL	A	606	-	5,5,5	1.03	0	5,5,5	0.94	0
6	GOL	B	701	-	5,5,5	0.78	0	5,5,5	1.01	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	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	NAG	A	604	1	-	2/6/23/26	0/1/1/1
5	YOD	A	605	-	-	0/20/63/63	0/6/5/5
4	NAG	A	602	1	-	2/6/23/26	0/1/1/1
4	NAG	A	603	1	-	4/6/23/26	0/1/1/1
6	GOL	A	606	-	-	0/4/4/4	-
6	GOL	B	701	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	605	YOD	C03-S02	4.27	1.90	1.80

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	605	YOD	C08-C09-C10	-2.89	106.61	108.23
4	A	601	NAG	C1-O5-C5	2.52	115.61	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

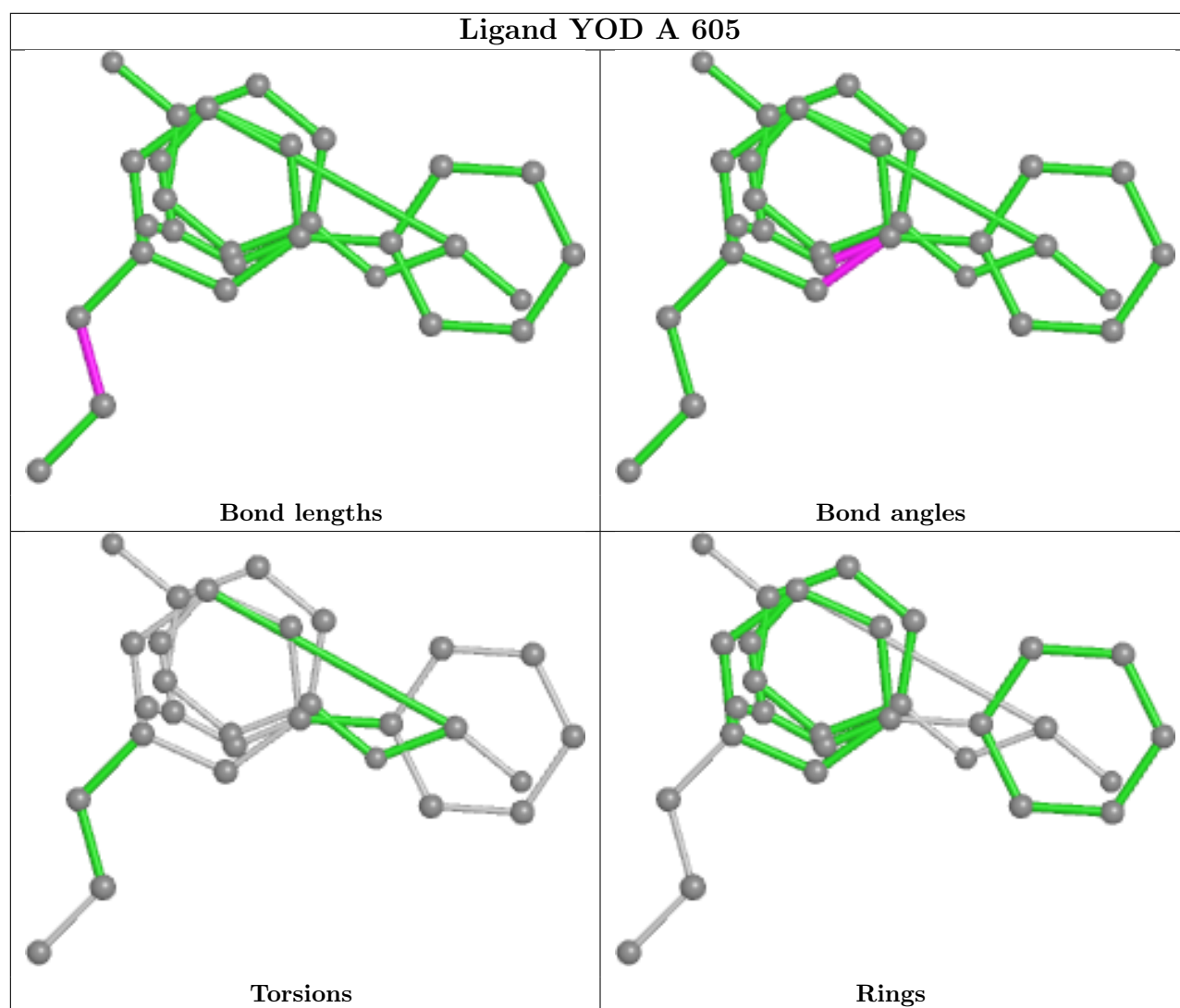
Mol	Chain	Res	Type	Atoms
4	A	602	NAG	O5-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	A	602	NAG	C4-C5-C6-O6
4	A	603	NAG	C8-C7-N2-C2
4	A	603	NAG	O7-C7-N2-C2
4	A	601	NAG	O5-C5-C6-O6
4	A	603	NAG	C4-C5-C6-O6
4	A	603	NAG	O5-C5-C6-O6
4	A	604	NAG	C3-C2-N2-C7
4	A	604	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	701	GOL	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 than 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	234/291 (80%)	0.27	12 (5%) 28 40	34, 54, 104, 138	0
2	B	128/168 (76%)	1.03	29 (22%) 0 1	36, 55, 181, 194	0
All	All	362/459 (78%)	0.54	41 (11%) 5 8	34, 55, 136, 194	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	620	THR	7.7
2	B	623	ILE	7.4
2	B	615	TRP	7.2
2	B	621	ASP	6.6
2	B	627	ILE	6.0
2	B	626	ILE	6.0
2	B	616	THR	5.9
1	A	278	ASN	5.2
2	B	613	ALA	4.8
2	B	617	LYS	4.5
2	B	618	ASN	4.5
2	B	622	LYS	4.3
2	B	610	ILE	4.2
2	B	625	GLN	4.1
2	B	619	ILE	4.1
2	B	628	HIS	4.1
1	A	279	PRO	3.9
2	B	624	ASP	3.8
2	B	612	PRO	3.7
2	B	629	ASP	3.7
2	B	522	ASP	3.4
2	B	614	ASP	3.4
1	A	214	TYR	3.4
2	B	603	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	525	ALA	2.9
1	A	51	LEU	2.9
2	B	600	THR	2.8
1	A	293	THR	2.7
2	B	609	CYS	2.6
1	A	255	GLN	2.6
2	B	607	ASP	2.5
2	B	602	HIS	2.4
2	B	582	PHE	2.4
1	A	275	TRP	2.3
2	B	606	PRO	2.3
1	A	97	VAL	2.1
1	A	288	TRP	2.1
1	A	271	GLY	2.0
1	A	165	LEU	2.0
2	B	611	GLU	2.0
1	A	262	THR	2.0

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

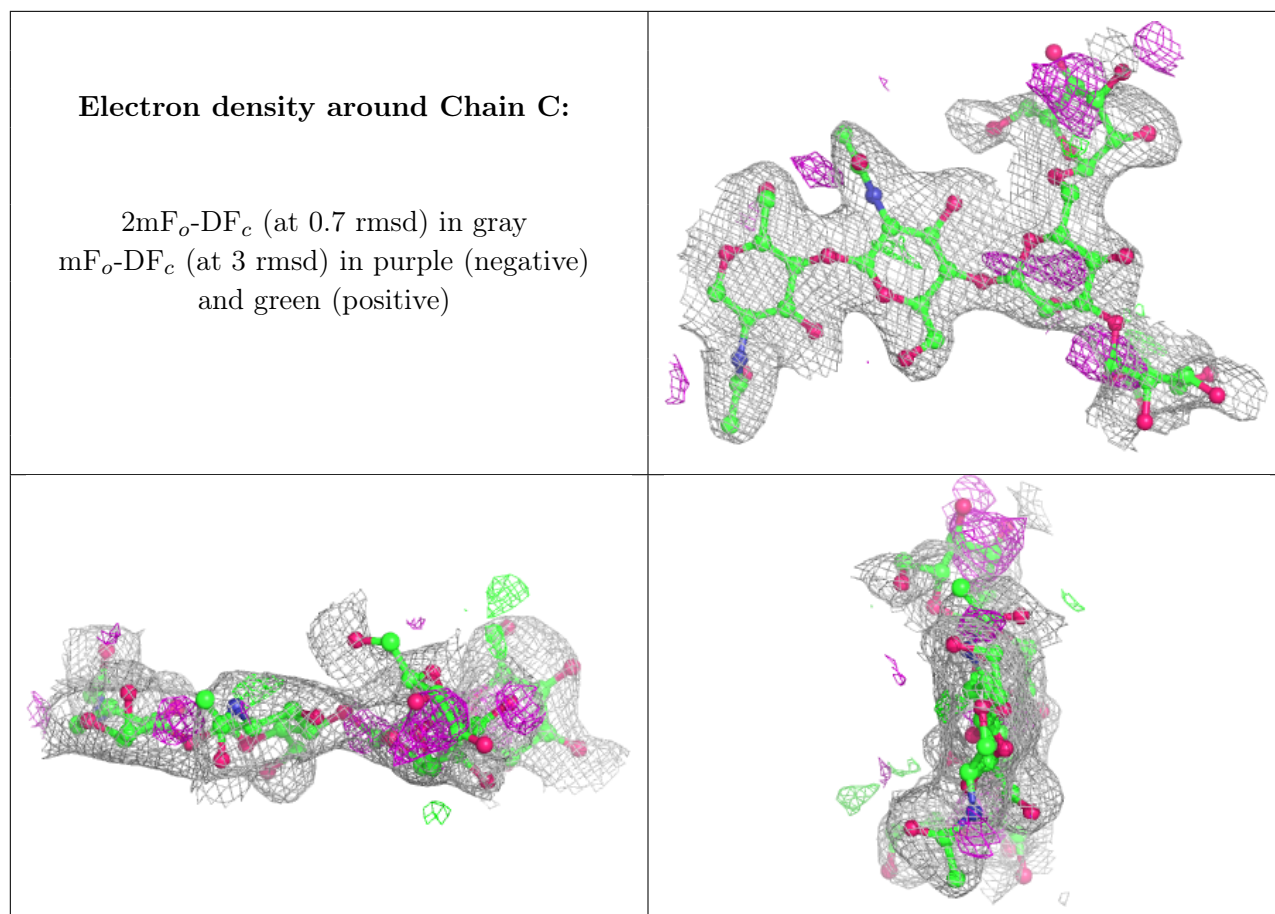
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	C	5	11/12	0.55	0.42	115,123,128,129	0
3	MAN	C	4	11/12	0.75	0.41	101,115,119,120	0
3	BMA	C	3	11/12	0.78	0.32	99,105,111,112	0
3	NAG	C	2	14/15	0.88	0.16	64,75,83,95	0
3	NAG	C	1	14/15	0.97	0.10	43,52,60,62	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.

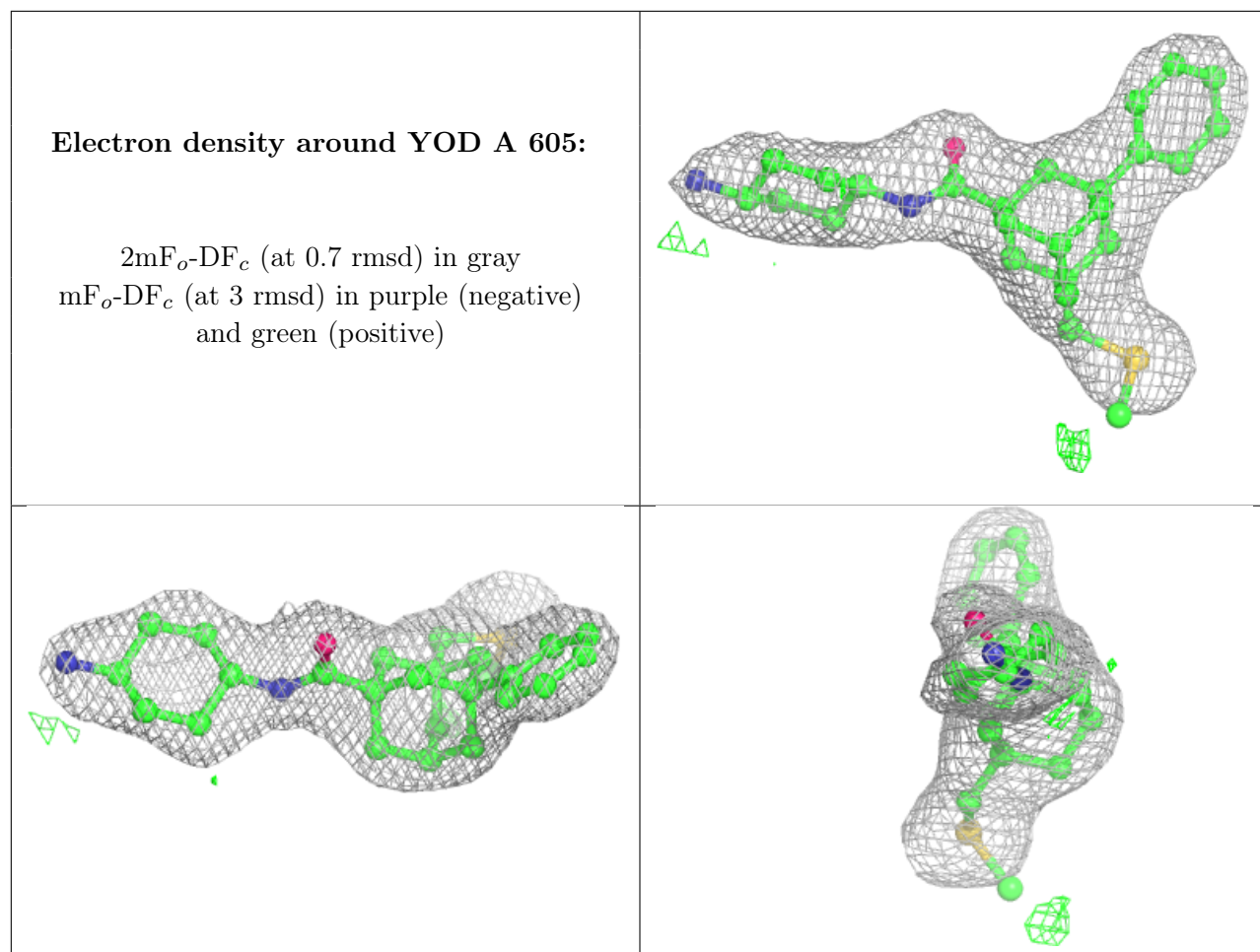


6.4 Ligands [i](#)

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
4	NAG	A	604	14/15	0.74	0.46	131,139,142,143	0
4	NAG	A	603	14/15	0.80	0.48	97,108,115,124	0
6	GOL	A	606	6/6	0.88	0.32	63,69,76,82	0
4	NAG	A	602	14/15	0.89	0.21	79,90,94,97	0
4	NAG	A	601	14/15	0.96	0.12	62,72,78,80	0
5	YOD	A	605	29/29	0.97	0.10	42,54,68,77	0
6	GOL	B	701	6/6	0.97	0.26	50,57,65,68	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.