Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 06:45 AM EDT

PDB ID	:	6NAE
Title	:	Crystal Structure of Ebola zaire GP protein with bound ARN0074898
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2018-12-05
Resolution	:	2.75 Å(reported)

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	:	2.35.1
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 ⓘ

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

The reported resolution of this entry is 2.75 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.
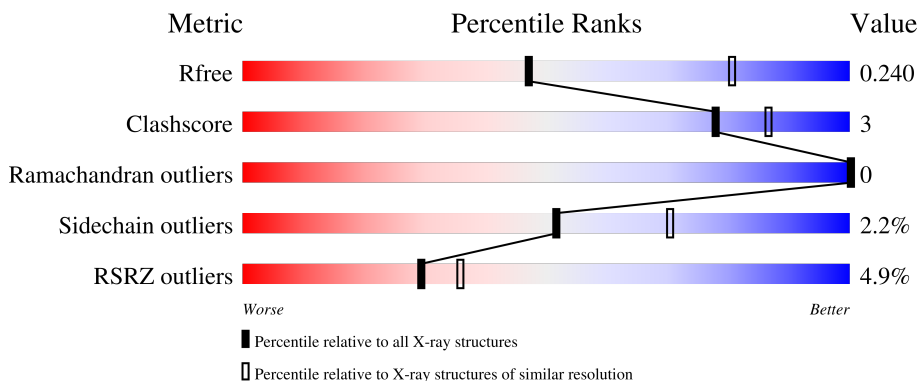
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	330	2% / 66% / 5% • / 28%
2	B	168	7% / 65% / 5% / 30%
3	C	5	40% / 60%

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
4	NAG	A	604	-	-	-	X

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 2972 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 Envelope glycoprotein,Envelope glycoprotein,Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total 1813	C 1160	N 310	O 338	S 5	0	3	0

There are 5 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

- Molecule 2 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	117	Total 897	C 569	N 158	O 164	S 6	0	1	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
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

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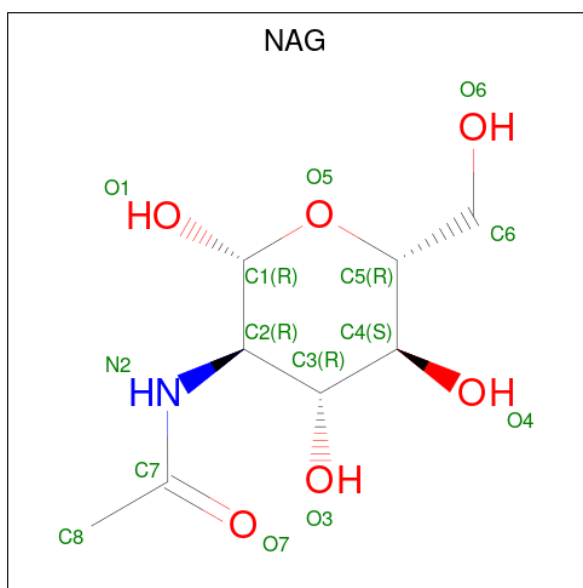| Chain	Residue	Modelled	Actual	Comment	Reference
B	642	ARG	-	expression tag	UNP Q05320
B	643	ASP	-	expression tag	UNP Q05320
B	644	GLY	-	expression tag	UNP Q05320
B	645	GLN	-	expression tag	UNP Q05320
B	646	ALA	-	expression tag	UNP Q05320
B	647	TYR	-	expression tag	UNP Q05320
B	648	VAL	-	expression 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.
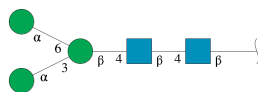
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	5	61	34	2	25	0	0	0

- 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
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
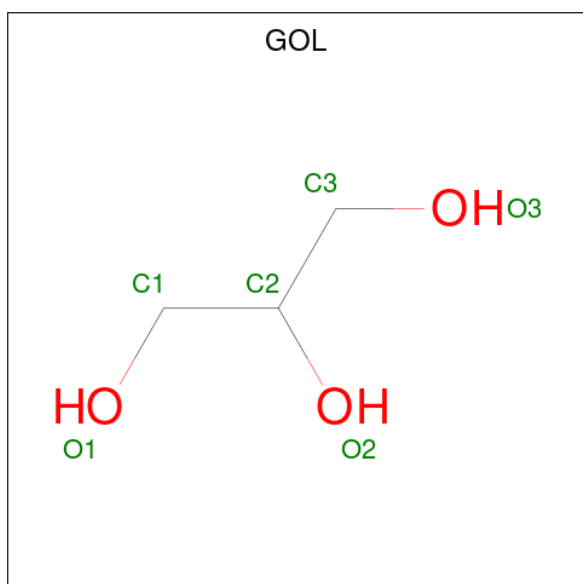
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total C O 6　3　3			0	0
5	A	1	Total C O 6　3　3			0	0
5	A	1	Total C O 6　3　3			0	0
5	A	1	Total C O 6　3　3			0	0
5	B	1	Total C O 6　3　3			0	0

- Molecule 6 is (1S,3R,5R,7S)-N-(trans-4-aminocyclohexyl)-3-methyl-5-phenyltricyclo[3.3.1.1 3,7]decane-1-carboxamide (three-letter code: KHG) (formula: $C_{24}H_{34}N_2O$).
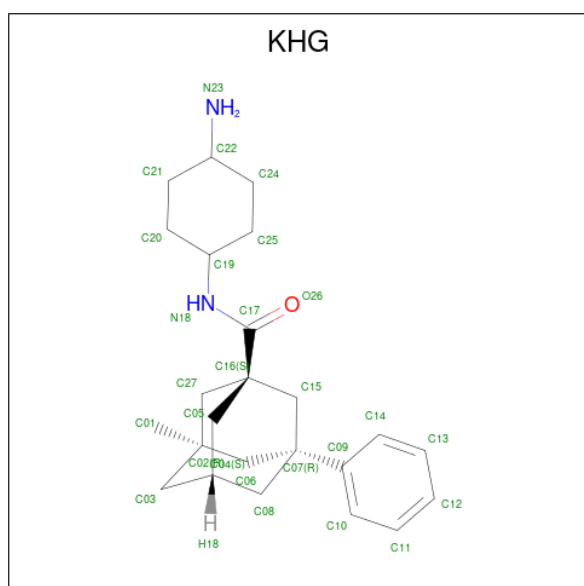
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total C N O 27　24　2　1				0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	57	Total O 57　57		0	0
7	B	31	Total O 31　31		0	0

3 Residue-property plots ⓘ

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.
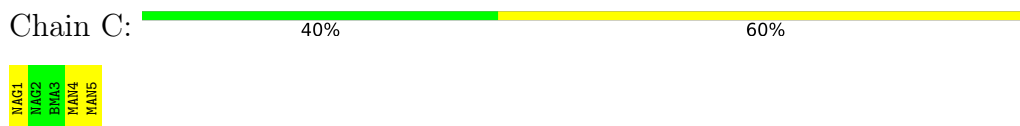
• Molecule 1: Envelope glycoprotein,Envelope glycoprotein,Envelope glycoprotein

Chain A:
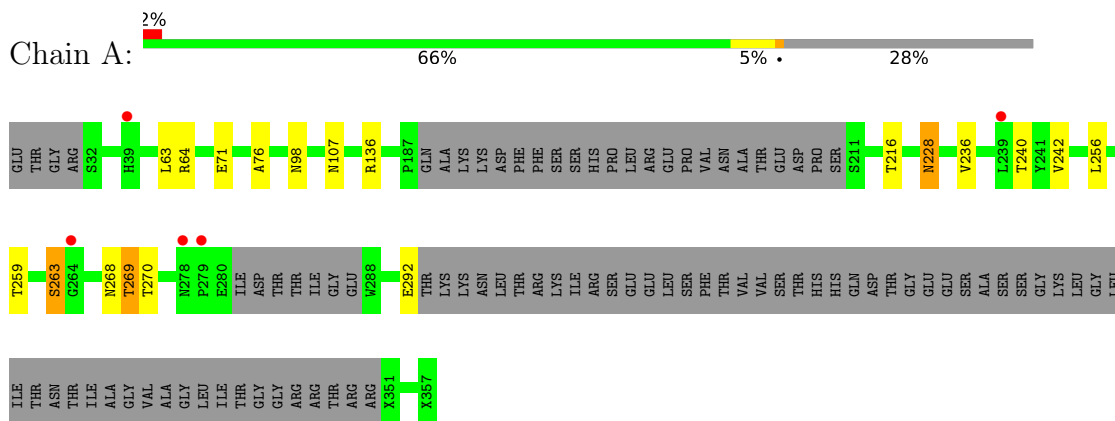
• Molecule 2: Envelope glycoprotein

Chain B:
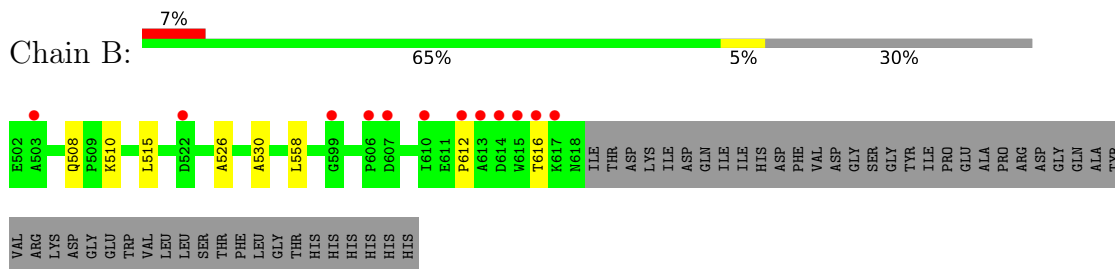
• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyrano se-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyra nose

Chain C:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	113.25Å　　113.25Å　　307.21Å 90.00°　　　90.00°　　　120.00°	Depositor
Resolution (Å)	49.55　–　2.75 49.55　–　2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.55-2.75) 100.0 (49.55-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.05 (at 2.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.193　,　0.240 0.193　,　0.240	Depositor DCC
R_{free} test set	2076 reflections (10.30%)	wwPDB-VP
Wilson B-factor (Å^2)	58.2	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 61.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2972	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: NAG, MAN, GOL, BMA, KHG

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	0.26	0/1832	0.46	0/2499
2	B	0.26	0/921	0.42	0/1256
All	All	0.26	0/2753	0.45	0/3755

There are no bond length outliers.

There are no bond angle outliers.

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	1813	0	1688	10	0
2	B	897	0	850	6	0
3	C	61	0	52	1	0
4	A	56	0	52	1	0
5	A	24	0	32	1	0
5	B	6	0	8	0	0
6	A	27	0	0	2	0
7	A	57	0	0	0	0
7	B	31	0	0	0	0
All	All	2972	0	2682	16	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 3.

All (16) 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)
2:B:526:ALA:HB1	2:B:530:ALA:HB3	1.65	0.76
1:A:228:ASN:OD1	1:A:228:ASN:N	2.19	0.70
1:A:136:ARG:HH22	1:A:216:THR:HG23	1.57	0.69
1:A:71:GLU:OE2	1:A:107:ASN:N	2.27	0.66
1:A:269:THR:OG1	1:A:270:THR:N	2.31	0.61
1:A:292:GLU:OE1	2:B:510:LYS:NZ	2.35	0.60
1:A:242:VAL:HG21	1:A:256:LEU:HD21	1.85	0.57
1:A:236:VAL:HG22	1:A:240:THR:HB	1.89	0.55
4:A:603:NAG:H83	4:A:603:NAG:H3	1.90	0.54
2:B:612:PRO:O	2:B:616:THR:N	2.42	0.51
6:A:608:KHG:C14	2:B:515:LEU:HD21	2.45	0.47
1:A:63:LEU:O	1:A:64[B]:ARG:HD2	2.16	0.45
2:B:508:GLN:OE1	3:C:1:NAG:O6	2.31	0.44
1:A:259:THR:O	1:A:263:SER:HB3	2.19	0.43
1:A:76:ALA:HA	5:A:606:GOL:H2	2.01	0.42
6:A:608:KHG:C13	2:B:515:LEU:HD21	2.51	0.41

There are no symmetry-related clashes.

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	228/330 (69%)	222 (97%)	6 (3%)	0	100	100
2	B	116/168 (69%)	106 (91%)	10 (9%)	0	100	100
All	All	344/498 (69%)	328 (95%)	16 (5%)	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	183/273 (67%)	178 (97%)	5 (3%)	44	65
2	B	89/139 (64%)	88 (99%)	1 (1%)	73	84
All	All	272/412 (66%)	266 (98%)	6 (2%)	52	70

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

Mol	Chain	Res	Type
1	A	98	ASN
1	A	228	ASN
1	A	263	SER
1	A	268	ASN
1	A	269	THR
2	B	558	LEU

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 ⓘ

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	3,2	14,14,15	0.21	0	17,19,21	0.63	0
3	NAG	C	2	3	14,14,15	0.24	0	17,19,21	0.55	0
3	BMA	C	3	3	11,11,12	0.91	0	15,15,17	0.78	0
3	MAN	C	4	3	11,11,12	0.78	0	15,15,17	0.94	1 (6%)
3	MAN	C	5	3	11,11,12	1.63	3 (27%)	15,15,17	2.16	4 (26%)

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	3,2	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	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	5	MAN	C1-C2	3.66	1.60	1.52
3	C	5	MAN	O5-C1	3.38	1.49	1.43
3	C	5	MAN	O5-C5	2.04	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	5	MAN	C1-O5-C5	6.88	121.52	112.19
3	C	5	MAN	C1-C2-C3	2.93	113.26	109.67
3	C	5	MAN	O5-C1-C2	2.40	114.47	110.77
3	C	5	MAN	O2-C2-C3	-2.23	105.66	110.14
3	C	4	MAN	O2-C2-C3	-2.17	105.78	110.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	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.

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings
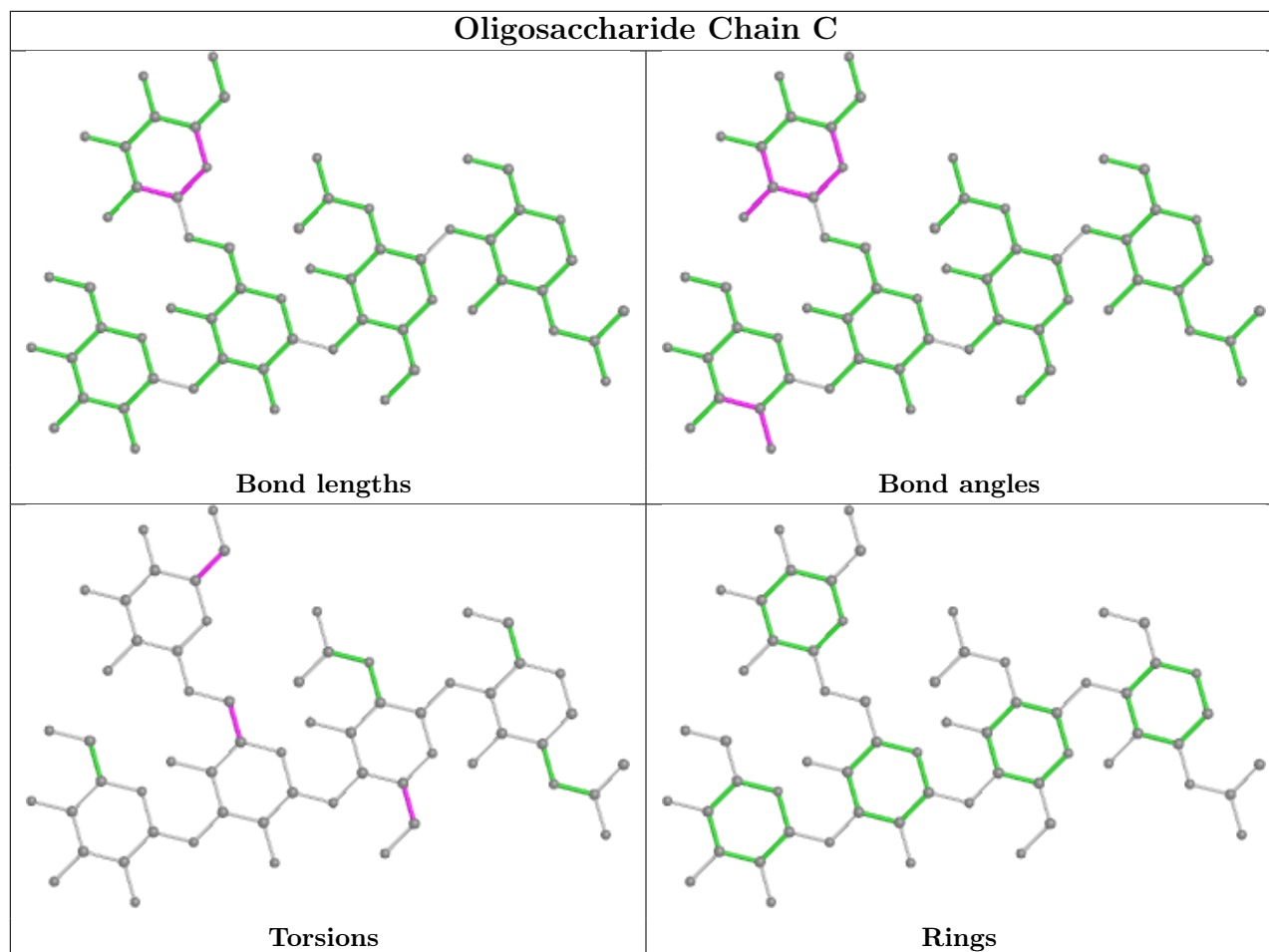
5.6 Ligand geometry ⓘ

10 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	602	1	14,14,15	0.21	0	17,19,21	0.47	0
5	GOL	B	706	-	5,5,5	0.96	0	5,5,5	1.00	0
4	NAG	A	601	1	14,14,15	0.28	0	17,19,21	0.60	0
5	GOL	A	605	-	5,5,5	0.91	0	5,5,5	1.00	0
4	NAG	A	604	1	14,14,15	0.17	0	17,19,21	0.35	0
5	GOL	A	607	-	5,5,5	0.90	0	5,5,5	1.00	0
5	GOL	A	606	-	5,5,5	0.95	0	5,5,5	0.97	0
4	NAG	A	603	1	14,14,15	0.43	0	17,19,21	1.32	2 (11%)
6	KHG	A	608	-	31,31,31	0.46	0	47,49,49	0.91	2 (4%)
5	GOL	A	609	-	5,5,5	0.92	0	5,5,5	0.98	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	602	1	-	2/6/23/26	0/1/1/1
5	GOL	B	706	-	-	0/4/4/4	-
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1
5	GOL	A	605	-	-	2/4/4/4	-
4	NAG	A	604	1	-	2/6/23/26	0/1/1/1
5	GOL	A	607	-	-	2/4/4/4	-
5	GOL	A	606	-	-	4/4/4/4	-
4	NAG	A	603	1	-	5/6/23/26	0/1/1/1
6	KHG	A	608	-	-	6/16/59/59	0/6/5/5
5	GOL	A	609	-	-	0/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	NAG	C2-N2-C7	4.35	129.09	122.90
6	A	608	KHG	C24-C25-C19	-2.13	109.12	111.48
4	A	603	NAG	C1-C2-N2	2.13	114.12	110.49
6	A	608	KHG	C08-C07-C09	-2.09	107.85	111.14

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	605	GOL	O1-C1-C2-C3
5	A	606	GOL	C1-C2-C3-O3
5	A	607	GOL	C1-C2-C3-O3
4	A	604	NAG	O5-C5-C6-O6
4	A	603	NAG	O5-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	A	602	NAG	O5-C5-C6-O6
4	A	604	NAG	C4-C5-C6-O6
4	A	601	NAG	O5-C5-C6-O6
4	A	603	NAG	C4-C5-C6-O6
4	A	603	NAG	C8-C7-N2-C2
4	A	603	NAG	O7-C7-N2-C2
4	A	602	NAG	C4-C5-C6-O6
5	A	605	GOL	O1-C1-C2-O2
5	A	606	GOL	O1-C1-C2-C3
5	A	606	GOL	O1-C1-C2-O2
5	A	607	GOL	O2-C2-C3-O3
5	A	606	GOL	O2-C2-C3-O3
6	A	608	KHG	C08-C07-C09-C10
6	A	608	KHG	C08-C07-C09-C14
6	A	608	KHG	C15-C07-C09-C10
6	A	608	KHG	C06-C07-C09-C10
6	A	608	KHG	C15-C07-C09-C14
6	A	608	KHG	C06-C07-C09-C14
4	A	603	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	606	GOL	1	0
4	A	603	NAG	1	0
6	A	608	KHG	2	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 KHG A 608

Bond lengths

Bond angles

Torsions

Rings
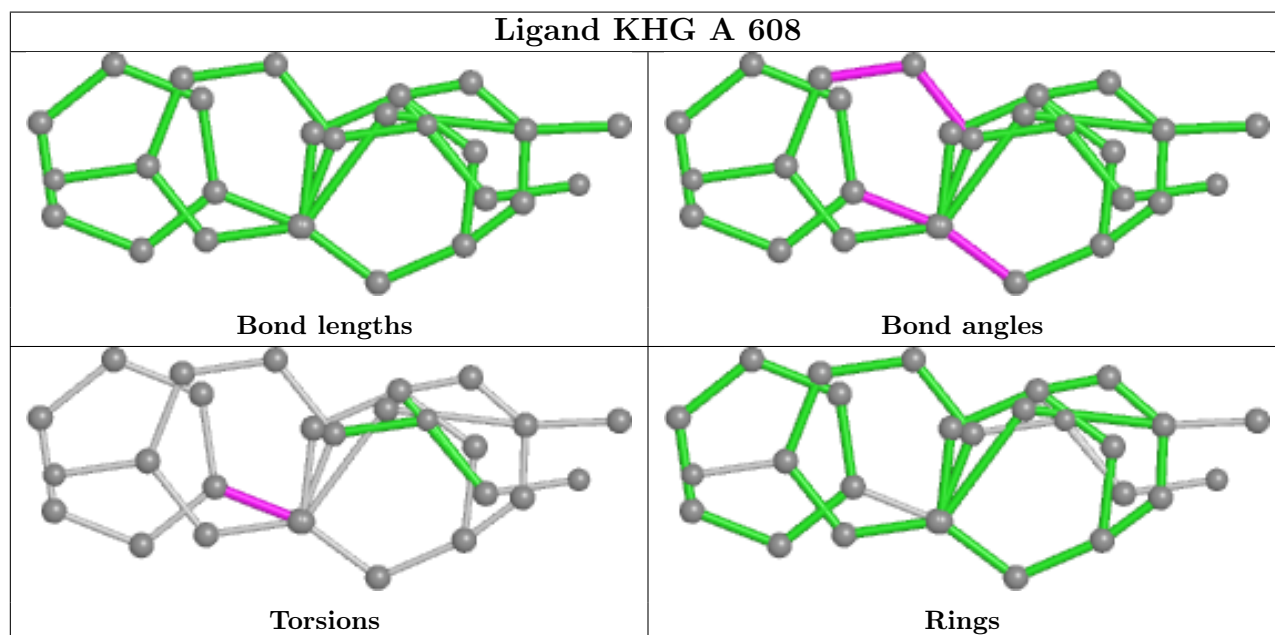
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	231/330 (70%)	0.35	5 (2%)	62	70	37, 56, 99, 132	0
2	B	117/168 (69%)	0.55	12 (10%)	6	7	39, 56, 118, 125	0
All	All	348/498 (69%)	0.42	17 (4%)	29	36	37, 56, 111, 132	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	613	ALA	5.9
2	B	610	ILE	4.0
2	B	614	ASP	3.8
2	B	616	THR	3.0
1	A	279	PRO	2.7
2	B	522	ASP	2.7
1	A	239	LEU	2.6
1	A	39	HIS	2.6
2	B	615	TRP	2.4
2	B	599	GLY	2.2
2	B	503	ALA	2.2
2	B	617	LYS	2.1
1	A	278	ASN	2.1
2	B	612	PRO	2.1
1	A	264	GLY	2.1
2	B	607	ASP	2.1
2	B	606	PRO	2.0

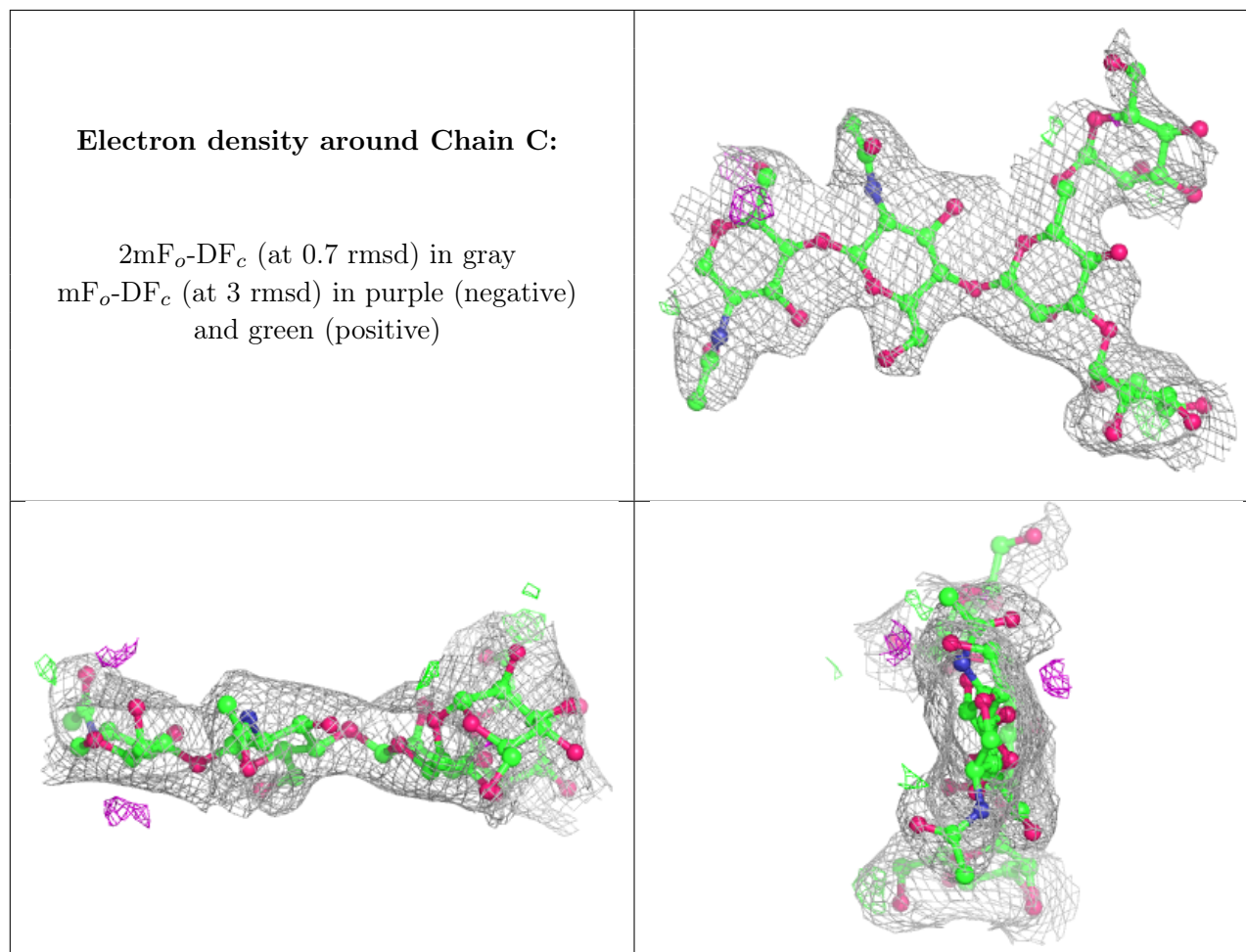## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 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
3	MAN	C	5	11/12	0.73	0.36	114,123,139,141	0
3	MAN	C	4	11/12	0.77	0.26	109,122,134,135	0
3	BMA	C	3	11/12	0.87	0.21	96,108,119,119	0
3	NAG	C	2	14/15	0.92	0.17	68,81,90,101	0
3	NAG	C	1	14/15	0.97	0.16	43,58,66,71	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.
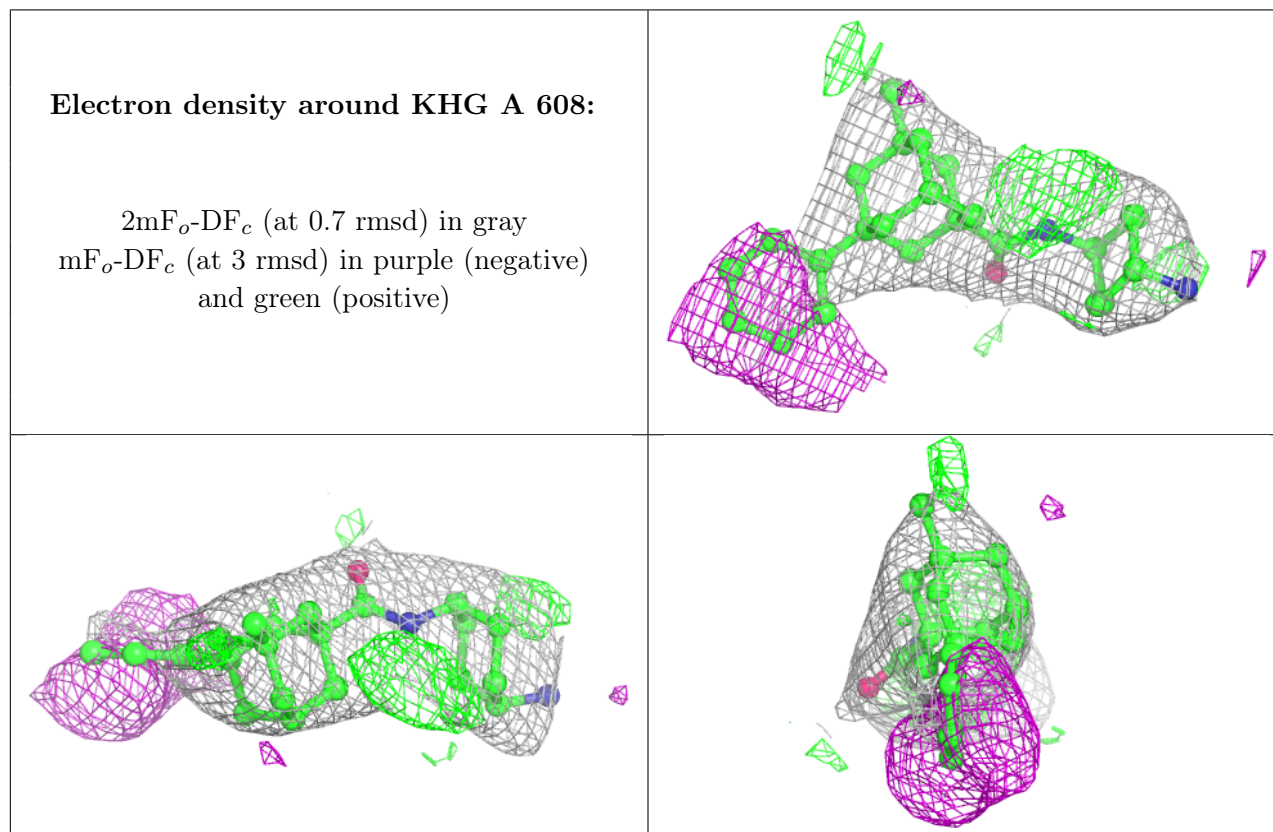

Electron density around Chain C:

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

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	GOL	A	609	6/6	0.50	0.24	78,97,105,112	0
5	GOL	A	606	6/6	0.69	0.34	69,79,93,94	0
4	NAG	A	604	14/15	0.73	0.42	130,151,168,168	0
4	NAG	A	603	14/15	0.82	0.48	118,127,140,144	0
5	GOL	B	706	6/6	0.84	0.45	64,66,76,78	0
5	GOL	A	607	6/6	0.85	0.27	90,90,101,112	0
5	GOL	A	605	6/6	0.86	0.25	80,82,90,98	0
6	KHG	A	608	27/27	0.86	0.29	53,73,87,96	0
4	NAG	A	602	14/15	0.92	0.28	93,109,118,119	0
4	NAG	A	601	14/15	0.95	0.22	57,76,84,84	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 KHG A 608:

$2mF_o-DF_c$ (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.