



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2020 – 08:03 PM EST

PDB ID : 6W5Y
Title : Inferred receptor binding domain of human endogenous retrovirus envelope EnvP(b)1
Authors : McCarthy, K.R.
Deposited on : 2020-03-14
Resolution : 2.50 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 ⓘ symbol.

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 : 2.14.6
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) : 2.14.6

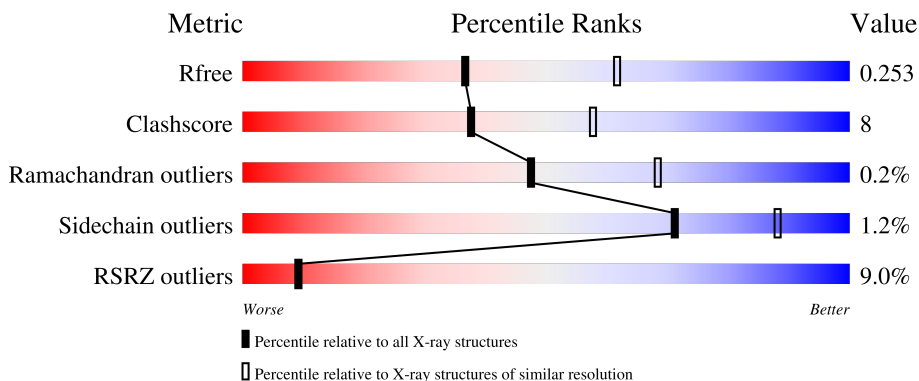
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	201	
1	B	201	
1	C	201	
2	D	3	
3	E	3	

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Mol	Chain	Length	Quality of chain
4	F	2	 100%

2 Entry composition [i](#)

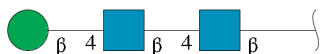
There are 6 unique types of molecules in this entry. The entry contains 4008 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EnvP(b)1 inferred receptor binding domain.

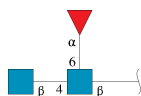
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	154	1215	780	202	226	7	0	0	0
1	B	163	1288	827	214	240	7	0	0	0
1	C	162	1280	823	213	237	7	0	0	0

- Molecule 2 is an oligosaccharide called 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			
2	D	3	39	22	2	15	0	0	0

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



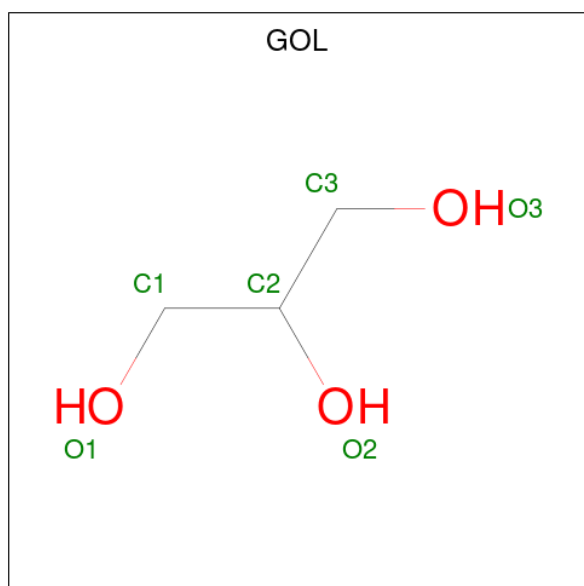
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	3	38	22	2	14	0	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	37	Total 37	O 37	0	0
6	B	35	Total 35	O 35	0	0
6	C	12	Total 12	O 12	0	0

MAG1
MAG2
BMA3

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

Chain E:  33% 67%

MAG1
MAG2
FUC3

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	243.31Å 37.35Å 66.99Å 90.00° 102.28° 90.00°	Depositor
Resolution (Å)	49.56 – 2.50 49.56 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.56-2.50) 99.9 (49.56-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.222 , 0.254 0.221 , 0.253	Depositor DCC
R_{free} test set	1012 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtrriage
Anisotropy	0.551	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4008	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% 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: GOL, BMA, NAG, FUC

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	0.29	0/1253	0.46	0/1717
1	B	0.32	0/1329	0.53	0/1821
1	C	0.31	0/1321	0.55	0/1810
All	All	0.31	0/3903	0.51	0/5348

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	171	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1215	0	1173	15	2
1	B	1288	0	1239	17	1
1	C	1280	0	1235	27	1
2	D	39	0	34	1	0
3	E	38	0	34	2	0
4	F	28	0	25	0	0
5	A	12	0	16	3	0
5	B	12	0	16	0	0
5	C	12	0	16	0	0
6	A	37	0	0	4	0
6	B	35	0	0	2	0
6	C	12	0	0	2	0
All	All	4008	0	3788	59	2

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 8.

The worst 5 of 59 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ARG:NH2	6:B:401:HOH:O	1.85	1.10
1:A:114:TYR:HH	1:B:53:HIS:N	1.65	0.93
1:B:175:ASN:ND2	6:B:402:HOH:O	2.04	0.90
1:A:186:GLY:O	6:A:401:HOH:O	2.08	0.71
1:C:100:ALA:HB2	1:C:177:PHE:CE2	2.29	0.68

All (2) 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:185:ARG:NH1	1:B:169:ASP:OD2[4_446]	1.42	0.78
1:A:202:SER:OG	1:C:188:ASP:OD2[2_556]	1.87	0.33

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	152/201 (76%)	144 (95%)	8 (5%)	0	100	100
1	B	161/201 (80%)	155 (96%)	5 (3%)	1 (1%)	25	43
1	C	160/201 (80%)	144 (90%)	16 (10%)	0	100	100
All	All	473/603 (78%)	443 (94%)	29 (6%)	1 (0%)	47	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	213	PRO

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	139/172 (81%)	137 (99%)	2 (1%)	67	86
1	B	146/172 (85%)	145 (99%)	1 (1%)	84	94
1	C	145/172 (84%)	143 (99%)	2 (1%)	67	86
All	All	430/516 (83%)	425 (99%)	5 (1%)	71	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	SER
1	A	97	GLU
1	B	214	TYR
1	C	63	SER
1	C	194	GLU

Some 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](#)

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	1	1,2	14,14,15	0.26	0	17,19,21	0.45	0
2	NAG	D	2	2	14,14,15	0.53	0	17,19,21	0.72	0
2	BMA	D	3	2	11,11,12	0.75	0	15,15,17	0.69	0
3	NAG	E	1	1,3	14,14,15	0.61	0	17,19,21	1.39	1 (5%)
3	NAG	E	2	3	14,14,15	0.62	1 (7%)	17,19,21	0.51	0
3	FUC	E	3	3	10,10,11	2.03	2 (20%)	14,14,16	1.86	3 (21%)
4	NAG	F	1	1,4	14,14,15	0.32	0	17,19,21	0.44	0
4	NAG	F	2	4	14,14,15	0.26	0	17,19,21	0.40	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
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	E	3	3	-	-	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3	FUC	C1-C2	5.26	1.64	1.52
3	E	3	FUC	O5-C1	3.15	1.48	1.43
3	E	2	NAG	C1-C2	2.24	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C1-O5-C5	4.57	118.39	112.19
3	E	3	FUC	C1-C2-C3	4.28	114.92	109.67
3	E	3	FUC	C1-O5-C5	3.90	121.62	112.78
3	E	3	FUC	O5-C5-C4	2.05	113.20	109.52

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

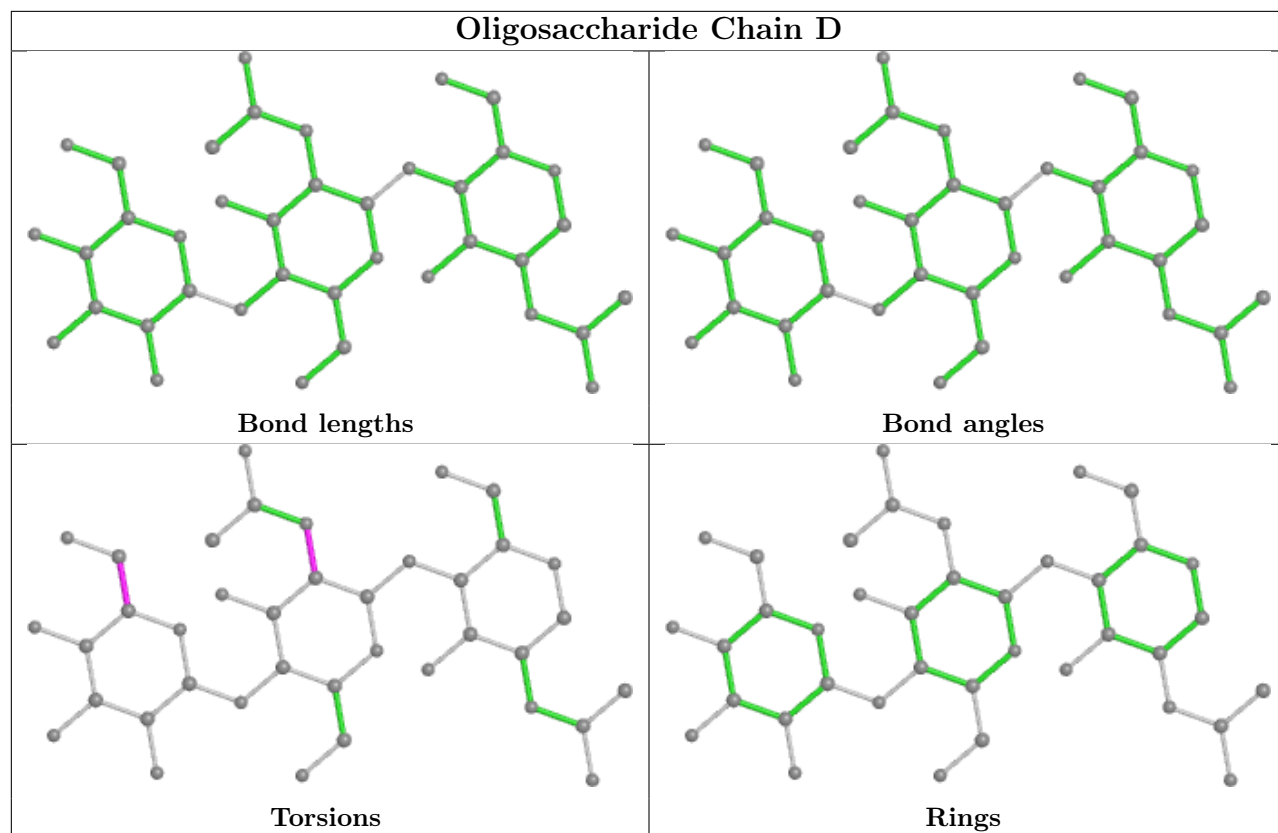
Mol	Chain	Res	Type	Atoms
2	D	3	BMA	O5-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
4	F	1	NAG	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6

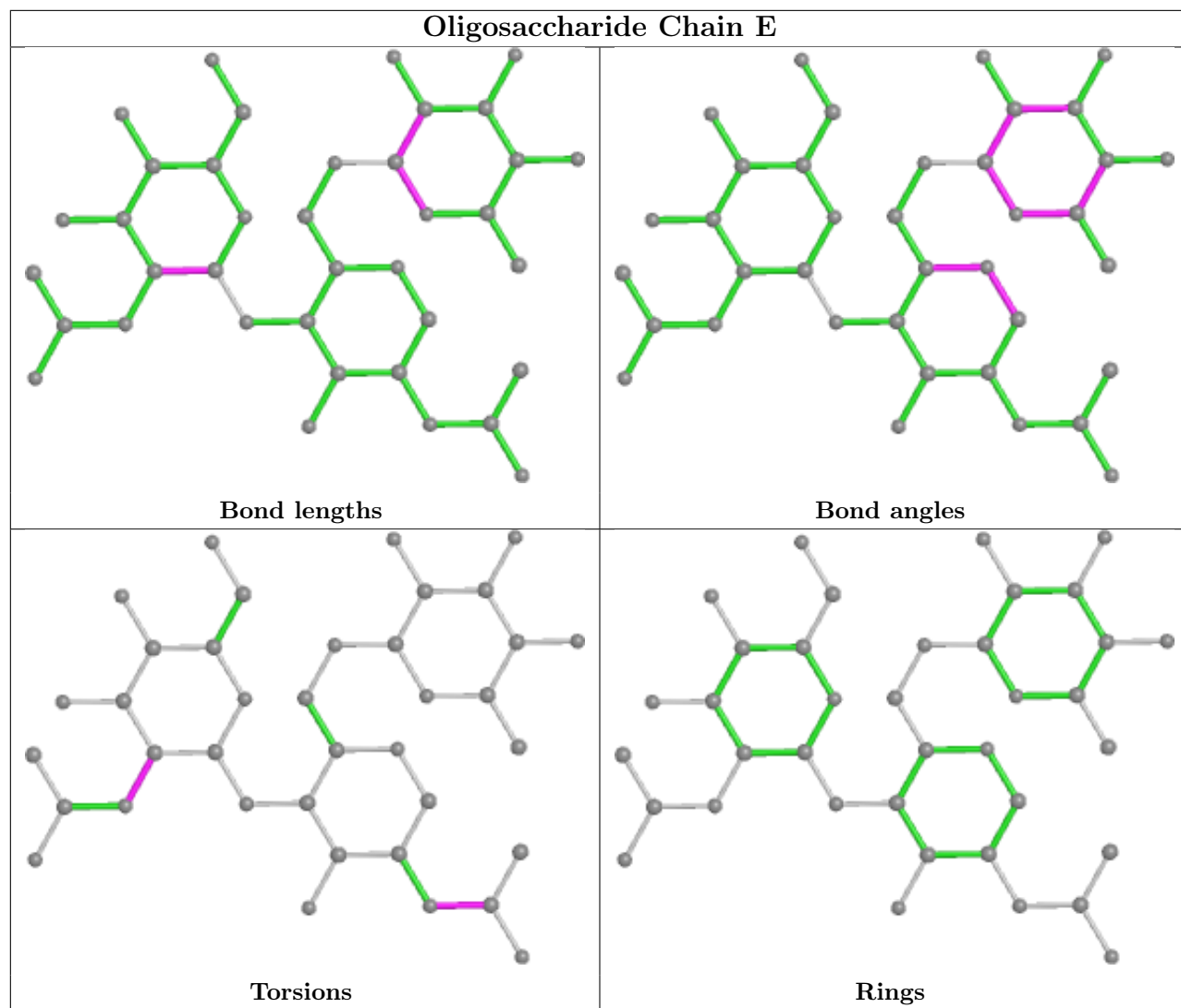
There are no ring outliers.

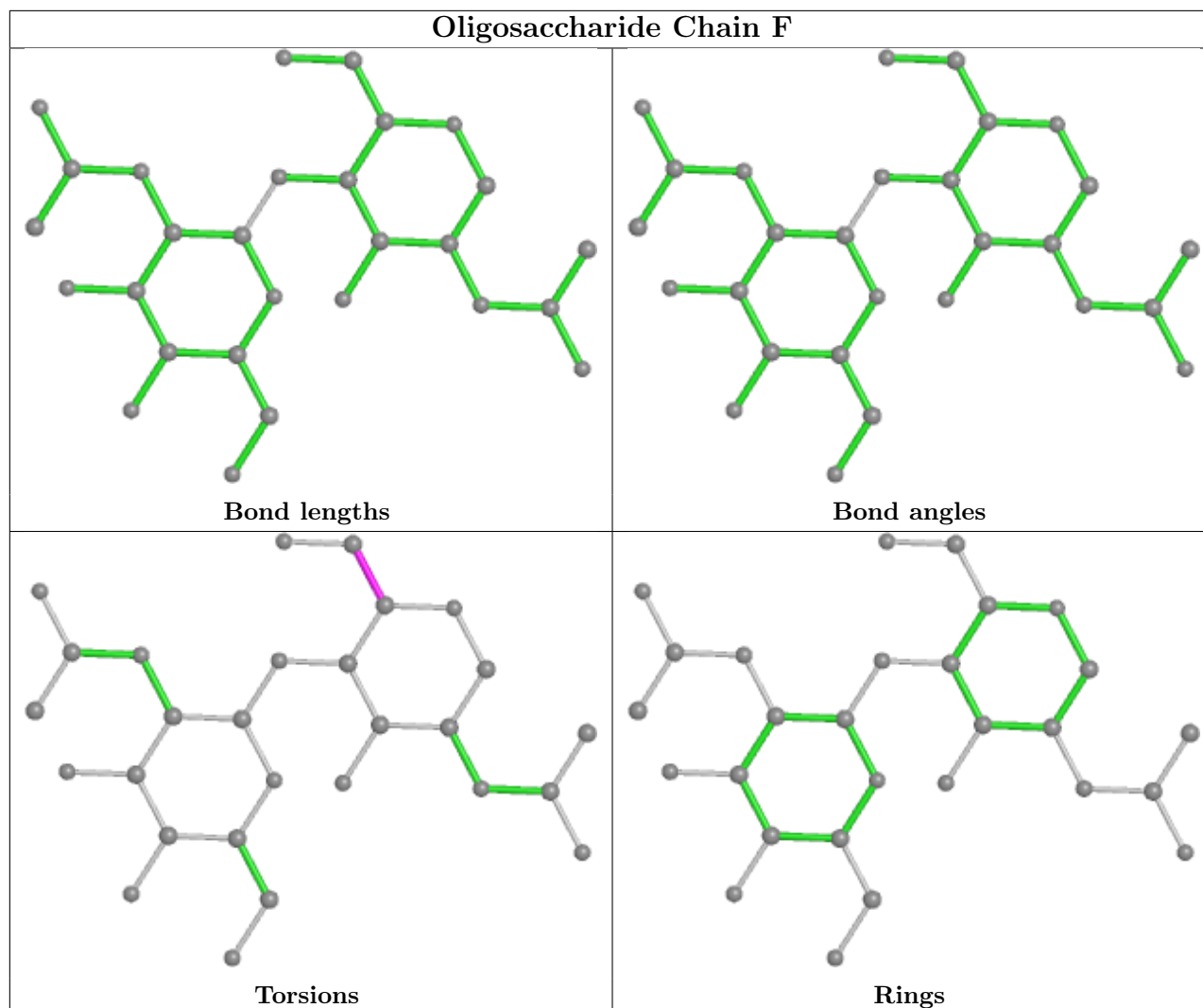
4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	2	0
2	D	3	BMA	1	0
3	E	1	NAG	2	0
2	D	2	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.







5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
5	GOL	A	302	-	5,5,5	0.93	0	5,5,5	1.01	0
5	GOL	C	302	-	5,5,5	0.89	0	5,5,5	1.01	0
5	GOL	B	302	-	5,5,5	0.95	0	5,5,5	0.93	0
5	GOL	B	301	-	5,5,5	0.91	0	5,5,5	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	C	301	-	5,5,5	0.90	0	5,5,5	0.92	0
5	GOL	A	301	-	5,5,5	0.87	0	5,5,5	1.09	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
5	GOL	A	302	-	-	2/4/4/4	-
5	GOL	C	302	-	-	2/4/4/4	-
5	GOL	B	302	-	-	0/4/4/4	-
5	GOL	B	301	-	-	2/4/4/4	-
5	GOL	C	301	-	-	2/4/4/4	-
5	GOL	A	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	301	GOL	C1-C2-C3-O3
5	A	301	GOL	O1-C1-C2-O2
5	A	302	GOL	C1-C2-C3-O3
5	C	302	GOL	O1-C1-C2-C3
5	B	301	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	302	GOL	1	0
5	A	301	GOL	2	0

5.7 Other polymers [i](#)

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 [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	A	154/201 (76%)	0.48	6 (3%) 39 42	27, 42, 66, 91	0
1	B	163/201 (81%)	0.56	9 (5%) 25 26	28, 43, 90, 129	0
1	C	162/201 (80%)	1.17	28 (17%) 1 1	42, 64, 115, 138	0
All	All	479/603 (79%)	0.74	43 (8%) 9 9	27, 49, 101, 138	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	106	PHE	8.3
1	B	212	TYR	6.0
1	C	104	PHE	5.9
1	C	212	TYR	5.9
1	C	148	PRO	5.2

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.

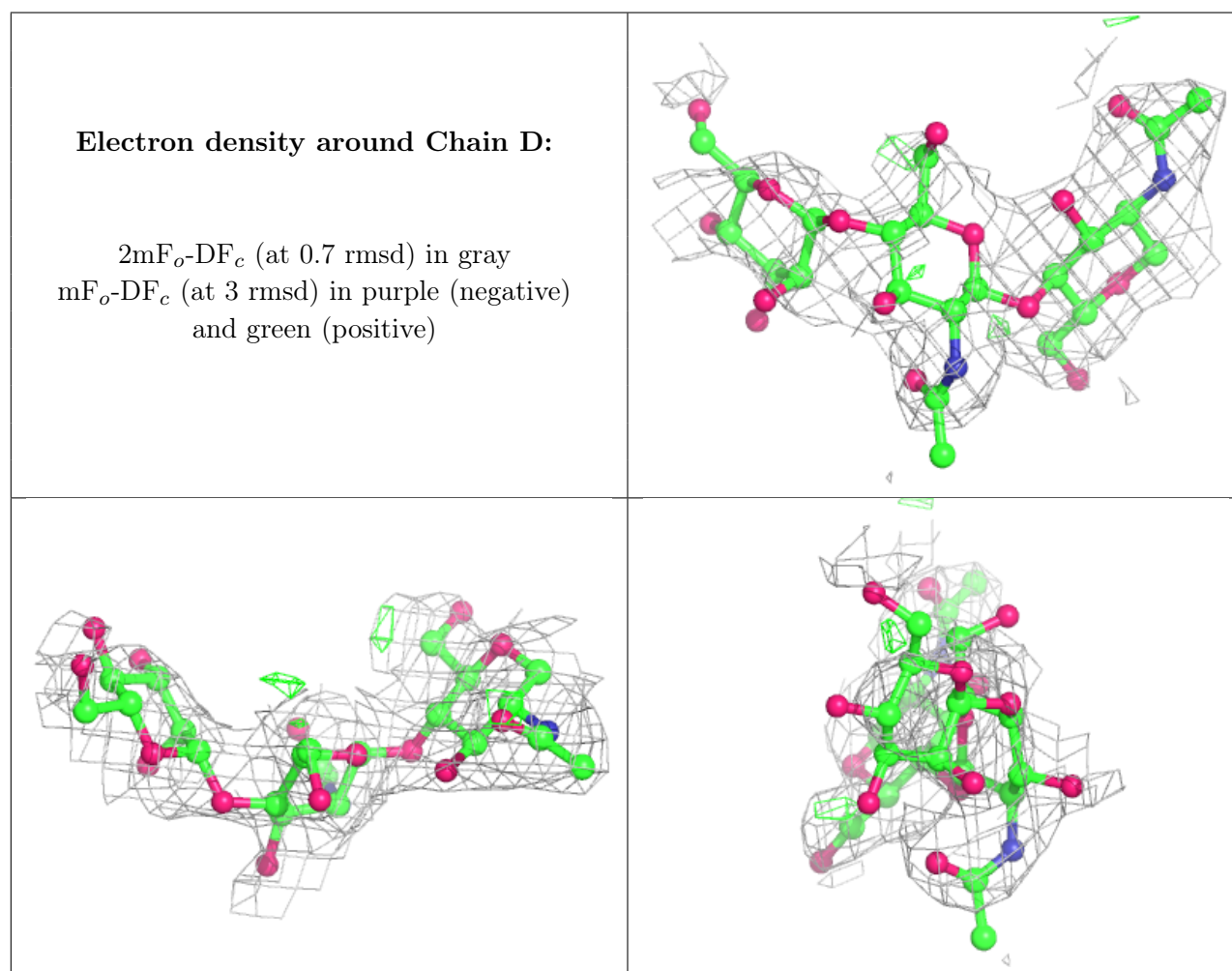
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	E	2	14/15	0.60	0.34	114,118,120,120	0
2	NAG	D	2	14/15	0.69	0.25	107,112,119,120	0
4	NAG	F	1	14/15	0.71	0.27	70,81,88,93	0

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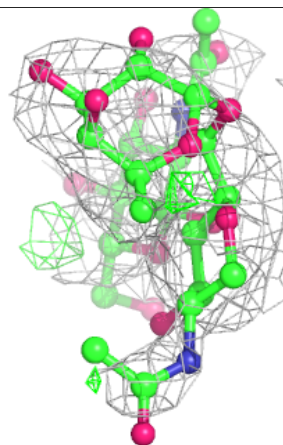
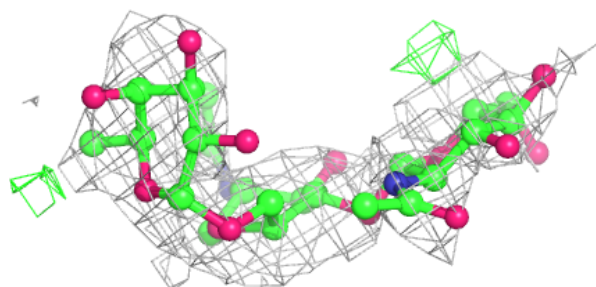
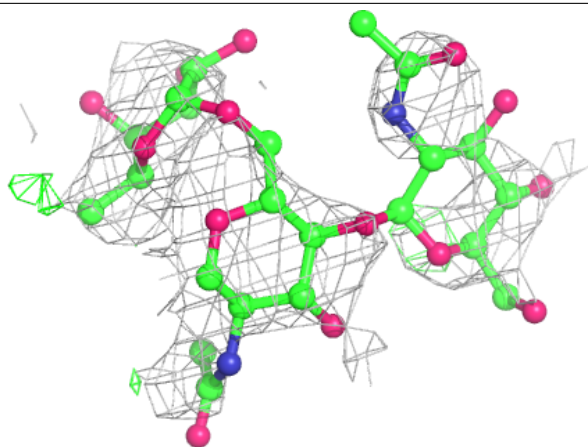
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FUC	E	3	10/11	0.72	0.26	111,114,115,115	0
2	BMA	D	3	11/12	0.73	0.35	119,121,122,122	0
3	NAG	E	1	14/15	0.76	0.32	79,95,107,107	0
2	NAG	D	1	14/15	0.79	0.23	60,70,84,99	0
4	NAG	F	2	14/15	0.84	0.27	100,104,106,106	0

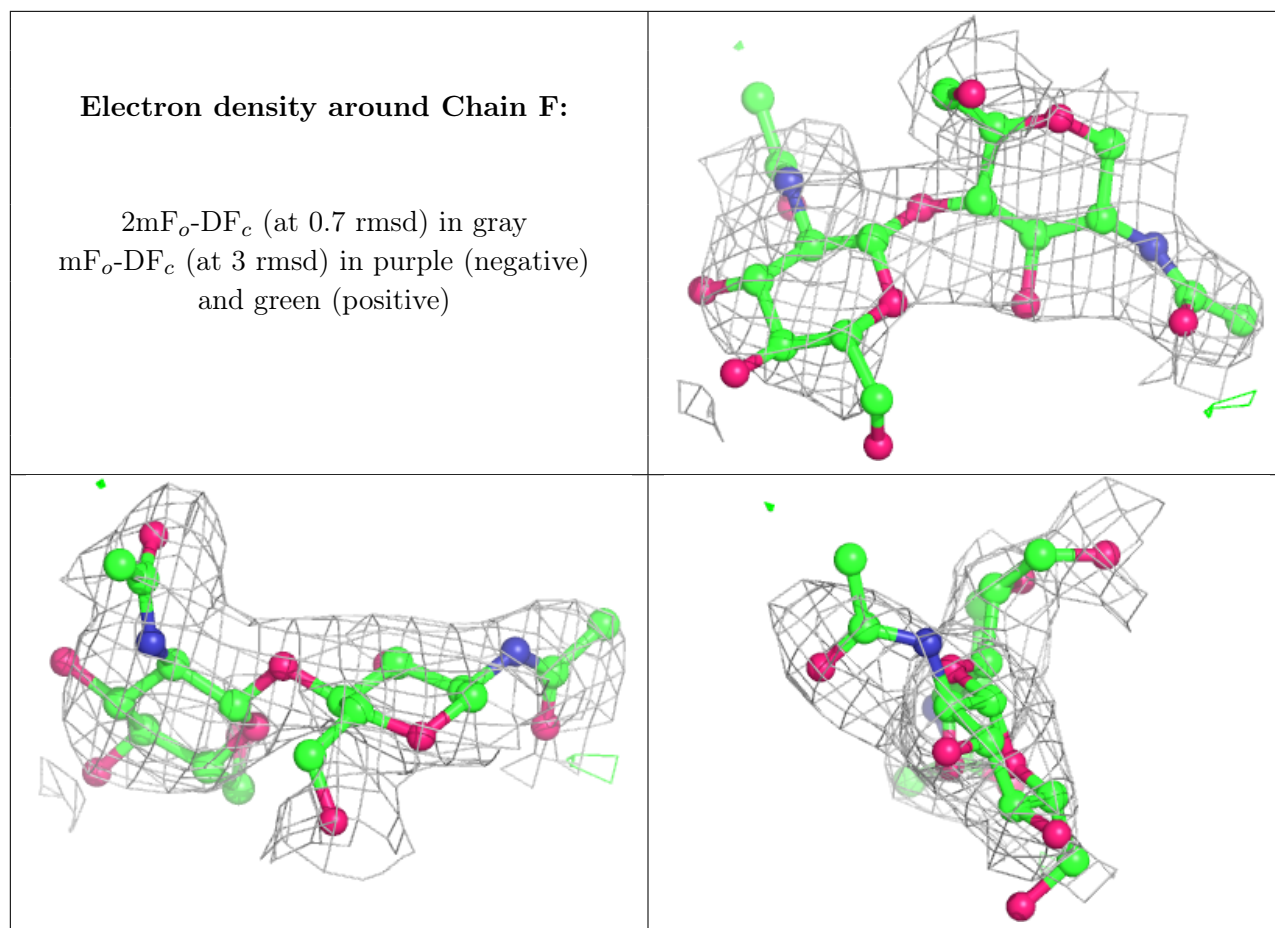
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain E:

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





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
5	GOL	C	302	6/6	0.64	0.28	84,85,86,87	0
5	GOL	C	301	6/6	0.74	0.28	75,78,79,80	0
5	GOL	B	302	6/6	0.76	0.23	70,71,72,72	0
5	GOL	B	301	6/6	0.86	0.24	78,79,81,82	0
5	GOL	A	301	6/6	0.88	0.19	58,59,59,60	0
5	GOL	A	302	6/6	0.91	0.15	42,47,48,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.