



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 07:36 PM BST

PDB ID : 6F6I
Title : CRYSTAL STRUCTURE OF EBOLAVIRUS GLYCOPROTEIN IN COMPLEX WITH PAROXETINE
Authors : Ren, J.; Zhao, Y.; Fry, E.E.; Stuart, D.I.
Deposited on : 2017-12-05
Resolution : 2.40 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 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)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

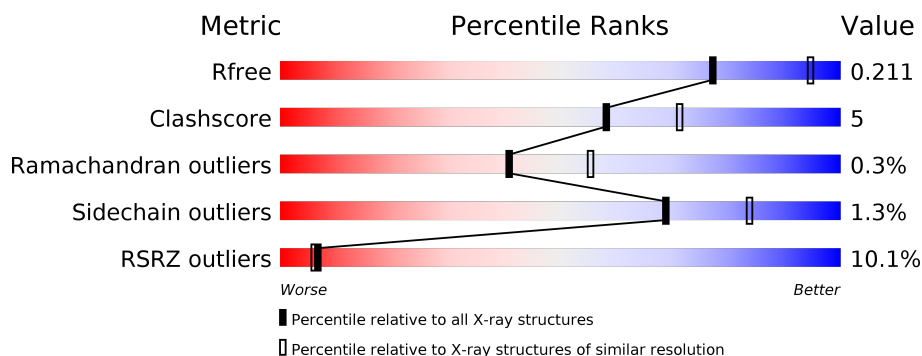
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	330	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>9%</div> <div>24%</div> </div> </div>
2	B	168	<div> <div>13%</div> <div> <div></div> <div>68%</div> <div>10%</div> <div>22%</div> </div> </div>
3	C	4	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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
4	NAG	A	502	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3320 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,GP,GP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	9	0
			2018	1289	342	382	5			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLU	-	expression tag	UNP A0A0E3NBB1
A	29	THR	-	expression tag	UNP A0A0E3NBB1
A	30	GLY	-	expression tag	UNP A0A0E3NBB1
A	31	ARG	-	expression tag	UNP A0A0E3NBB1
A	42	ALA	THR	engineered mutation	UNP A0A0E3NBB1

- Molecule 2 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	131	Total	C	N	O	S	0	0	0
			1035	660	177	192	6			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	613	ALA	HIS	engineered mutation	UNP A0A0U3BWW0
B	633	GLY	-	expression tag	UNP A0A0U3BWW0
B	634	SER	-	expression tag	UNP A0A0U3BWW0
B	635	GLY	-	expression tag	UNP A0A0U3BWW0
B	636	TYR	-	expression tag	UNP A0A0U3BWW0
B	637	ILE	-	expression tag	UNP A0A0U3BWW0
B	638	PRO	-	expression tag	UNP A0A0U3BWW0
B	639	GLU	-	expression tag	UNP A0A0U3BWW0
B	640	ALA	-	expression tag	UNP A0A0U3BWW0
B	641	PRO	-	expression tag	UNP A0A0U3BWW0
B	642	ARG	-	expression tag	UNP A0A0U3BWW0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	643	ASP	-	expression tag	UNP A0A0U3BWW0
B	644	GLY	-	expression tag	UNP A0A0U3BWW0
B	645	GLN	-	expression tag	UNP A0A0U3BWW0
B	646	ALA	-	expression tag	UNP A0A0U3BWW0
B	647	TYR	-	expression tag	UNP A0A0U3BWW0
B	648	VAL	-	expression tag	UNP A0A0U3BWW0
B	649	ARG	-	expression tag	UNP A0A0U3BWW0
B	650	LYS	-	expression tag	UNP A0A0U3BWW0
B	651	ASP	-	expression tag	UNP A0A0U3BWW0
B	652	GLY	-	expression tag	UNP A0A0U3BWW0
B	653	GLU	-	expression tag	UNP A0A0U3BWW0
B	654	TRP	-	expression tag	UNP A0A0U3BWW0
B	655	VAL	-	expression tag	UNP A0A0U3BWW0
B	656	LEU	-	expression tag	UNP A0A0U3BWW0
B	657	LEU	-	expression tag	UNP A0A0U3BWW0
B	658	SER	-	expression tag	UNP A0A0U3BWW0
B	659	THR	-	expression tag	UNP A0A0U3BWW0
B	660	PHE	-	expression tag	UNP A0A0U3BWW0
B	661	LEU	-	expression tag	UNP A0A0U3BWW0
B	662	GLY	-	expression tag	UNP A0A0U3BWW0
B	663	THR	-	expression tag	UNP A0A0U3BWW0
B	664	HIS	-	expression tag	UNP A0A0U3BWW0
B	665	HIS	-	expression tag	UNP A0A0U3BWW0
B	666	HIS	-	expression tag	UNP A0A0U3BWW0
B	667	HIS	-	expression tag	UNP A0A0U3BWW0
B	668	HIS	-	expression tag	UNP A0A0U3BWW0
B	669	HIS	-	expression tag	UNP A0A0U3BWW0

- Molecule 3 is an oligosaccharide called 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.



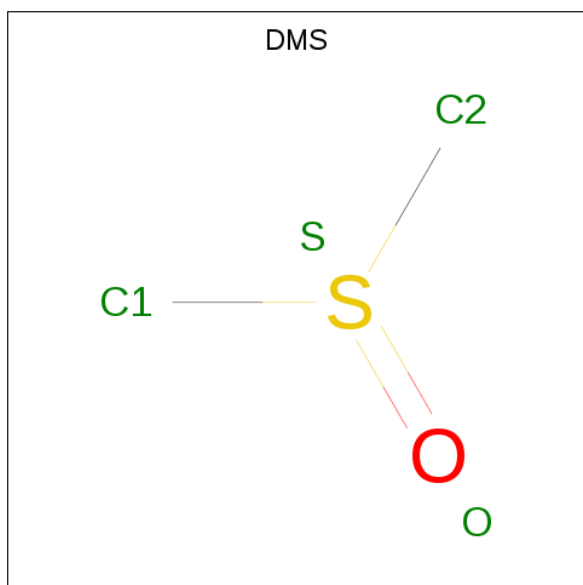
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



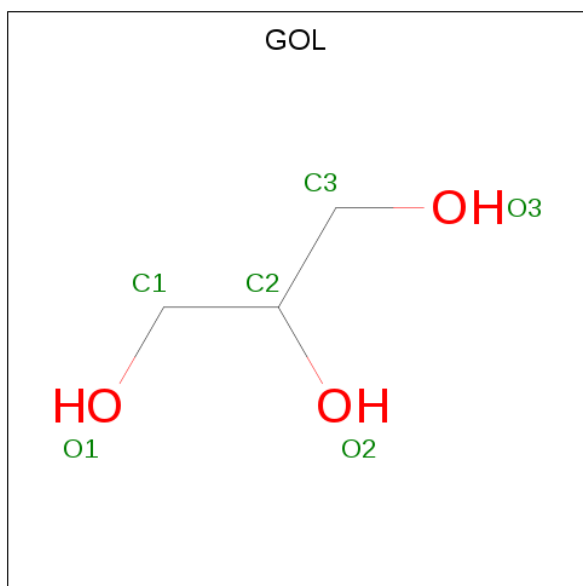
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



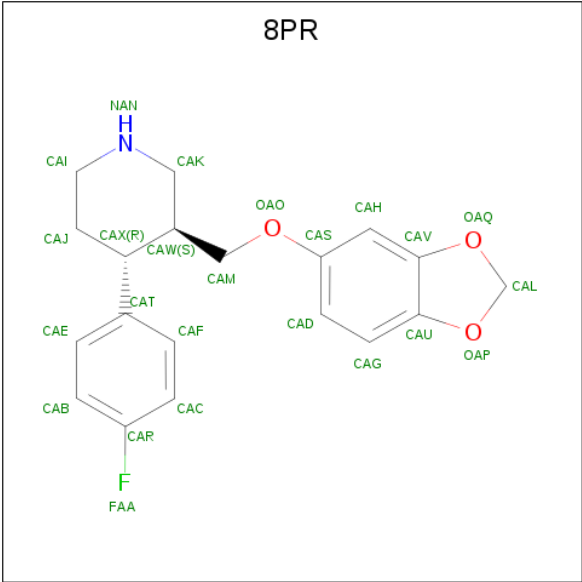
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		

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



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

- Molecule 7 is Paroxetine (three-letter code: 8PR) (formula: $C_{19}H_{20}FNO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	F	N	O	0	0
			24	19	1	1	3		

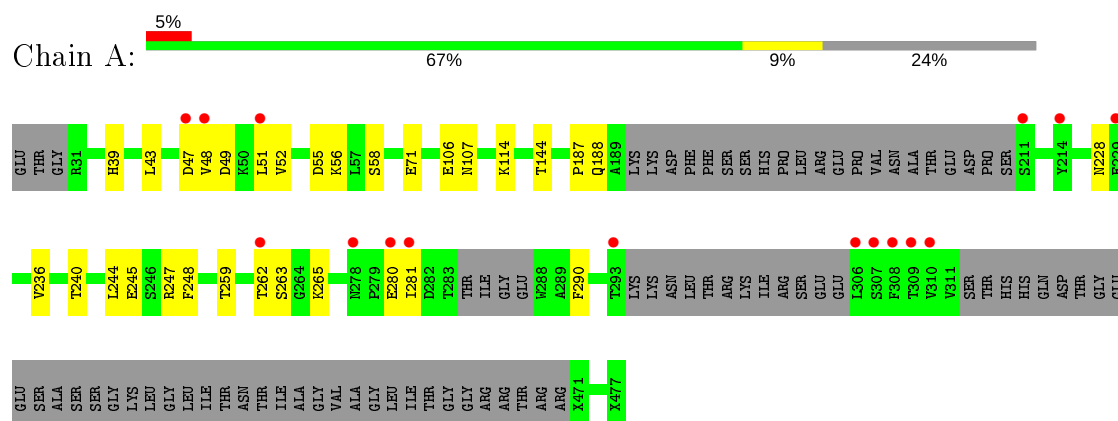
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	68	Total	O	0	0
			68	68		
8	B	35	Total	O	0	0
			35	35		

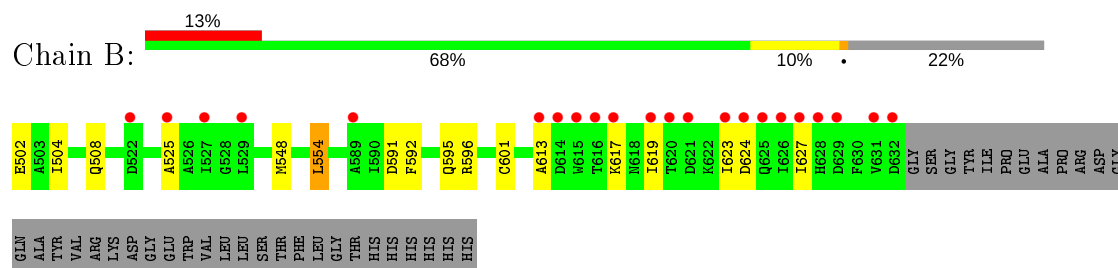
3 Residue-property plots [i](#)

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: Envelope glycoprotein,GP,GP1



- Molecule 2: Envelope glycoprotein



- Molecule 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	113.68Å 113.68Å 306.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.01 – 2.40 52.01 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (52.01-2.40) 99.8 (52.01-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.39Å)	Xtriage
Refinement program	PHENIX (dev_2940: ???)	Depositor
R, R_{free}	0.192 , 0.212 0.192 , 0.211	Depositor DCC
R_{free} test set	1521 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3320	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, DMS, 8PR, MAN

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	0.25	0/2036	0.45	0/2766
2	B	0.27	0/1060	0.44	0/1445
All	All	0.25	0/3096	0.45	0/4211

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	2018	0	1938	22	0
2	B	1035	0	1001	14	0
3	C	50	0	43	1	0
4	A	56	0	52	0	0
5	A	4	0	6	0	0
6	A	18	0	24	1	0
6	B	12	0	16	0	0
7	A	24	0	20	0	0
8	A	68	0	0	0	0
8	B	35	0	0	0	0
All	All	3320	0	3100	30	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 5.

All (30) 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:52[B]:VAL:O	2:B:596:ARG:NH2	2.35	0.59
1:A:187:PRO:HA	6:A:508:GOL:H32	1.84	0.59
1:A:56:LYS:HZ3	1:A:58:SER:HB3	1.68	0.58
1:A:106:GLU:HG3	1:A:290:PHE:CD1	2.39	0.58
1:A:56:LYS:NZ	1:A:58:SER:HB3	2.23	0.54
1:A:71:GLU:OE2	1:A:107:ASN:N	2.36	0.54
2:B:623:ILE:HD12	2:B:627:ILE:HG12	1.90	0.53
1:A:247:ARG:NH1	1:A:281:ILE:O	2.40	0.53
1:A:52[A]:VAL:O	2:B:596:ARG:NH2	2.41	0.53
1:A:228:ASN:OD1	1:A:228:ASN:N	2.41	0.52
1:A:48[B]:VAL:HG21	2:B:591:ASP:HB3	1.91	0.52
2:B:613:ALA:O	2:B:617:LYS:HG2	2.15	0.46
2:B:624:ASP:HA	2:B:627:ILE:HG13	1.99	0.44
1:A:236:VAL:HB	1:A:240:THR:HB	1.98	0.44
2:B:548:MET:HE3	2:B:548:MET:HB2	1.80	0.44
2:B:504:ILE:H	2:B:504:ILE:HG13	1.65	0.44
2:B:619:ILE:O	2:B:623:ILE:HG23	2.18	0.44
1:A:48[B]:VAL:HB	2:B:592:PHE:HA	2.00	0.43
1:A:47[A]:ASP:OD1	2:B:502:GLU:N	2.50	0.43
1:A:56:LYS:O	1:A:188:GLN:NE2	2.52	0.43
1:A:49[B]:ASP:HA	2:B:595:GLN:HG2	2.01	0.43
1:A:39[A]:HIS:HE2	1:A:55:ASP:CG	2.22	0.43
1:A:244:LEU:HD12	1:A:248:PHE:HD2	1.85	0.42
2:B:554:LEU:HD12	2:B:554:LEU:HA	1.89	0.42
2:B:508:GLN:NE2	3:C:1:NAG:O6	2.53	0.41
1:A:259:THR:HA	1:A:262:THR:HG22	2.03	0.41
1:A:263:SER:HB3	1:A:265:LYS:NZ	2.35	0.41
1:A:245:GLU:OE2	1:A:247:ARG:NH2	2.55	0.40
1:A:114:LYS:O	1:A:144:THR:HA	2.21	0.40
1:A:280:GLU:HG2	1:A:281:ILE:HG13	2.03	0.40

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	245/330 (74%)	237 (97%)	8 (3%)	0	100	100
2	B	129/168 (77%)	119 (92%)	9 (7%)	1 (1%)	19	29
All	All	374/498 (75%)	356 (95%)	17 (4%)	1 (0%)	41	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	525	ALA

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	216/273 (79%)	213 (99%)	3 (1%)	67	82
2	B	109/139 (78%)	107 (98%)	2 (2%)	59	76
All	All	325/412 (79%)	320 (98%)	5 (2%)	69	80

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

Mol	Chain	Res	Type
1	A	43	LEU
1	A	51[A]	LEU
1	A	51[B]	LEU
2	B	554	LEU
2	B	601	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	139	HIS
1	A	243	GLN
2	B	508	GLN
2	B	514	ASN
2	B	595	GLN

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 ⓘ

4 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	0.54	0
3	NAG	C	2	3	14,14,15	0.20	0	17,19,21	0.48	0
3	BMA	C	3	3	11,11,12	0.53	0	15,15,17	0.77	0
3	MAN	C	4	3	11,11,12	1.60	2 (18%)	15,15,17	2.13	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	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	MAN	C1-C2	4.31	1.62	1.52
3	C	4	MAN	O5-C1	2.66	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	4	MAN	C1-O5-C5	5.77	120.01	112.19
3	C	4	MAN	C1-C2-C3	3.98	114.56	109.67
3	C	4	MAN	O5-C1-C2	2.94	115.31	110.77
3	C	4	MAN	O2-C2-C3	-2.29	105.54	110.14

There are no chirality outliers.

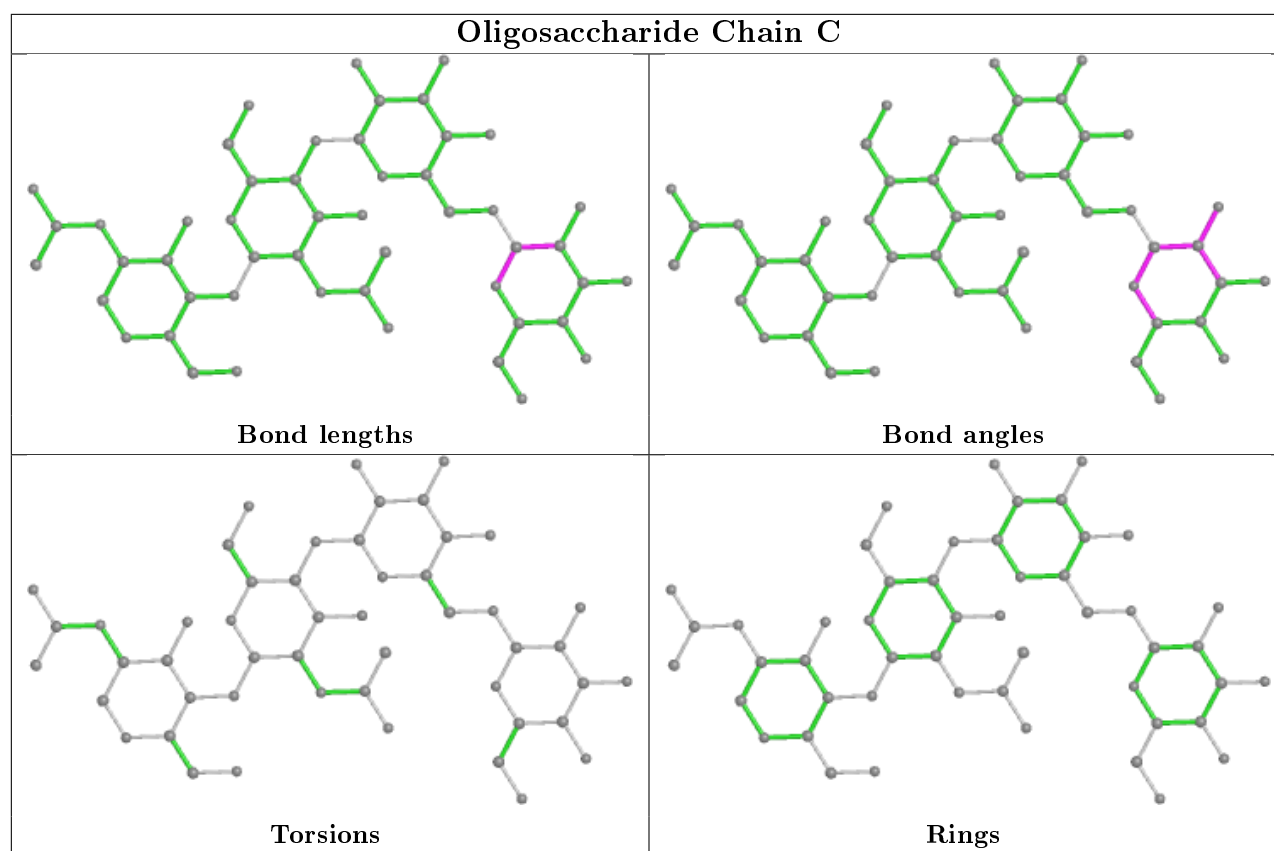
There are no torsion outliers.

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.



5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
6	GOL	A	506	-	5,5,5	0.90	0	5,5,5	1.00	0
4	NAG	A	503	1	14,14,15	0.29	0	17,19,21	0.45	0
7	8PR	A	509	-	26,27,27	1.44	5 (19%)	33,37,37	2.15	15 (45%)
4	NAG	A	504	1	14,14,15	0.69	1 (7%)	17,19,21	0.94	1 (5%)
6	GOL	A	507	-	5,5,5	0.89	0	5,5,5	1.00	0
6	GOL	A	508	-	5,5,5	0.91	0	5,5,5	0.98	0
6	GOL	B	706	-	5,5,5	0.91	0	5,5,5	0.98	0
4	NAG	A	502	1	14,14,15	0.19	0	17,19,21	0.50	0
6	GOL	B	705	-	5,5,5	0.92	0	5,5,5	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	505	-	3,3,3	0.65	0	3,3,3	0.49	0
4	NAG	A	501	1	14,14,15	0.23	0	17,19,21	0.47	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
6	GOL	A	506	-	-	2/4/4/4	-
4	NAG	A	503	1	-	0/6/23/26	0/1/1/1
7	8PR	A	509	-	-	3/9/26/26	0/4/4/4
4	NAG	A	504	1	-	0/6/23/26	0/1/1/1
6	GOL	A	507	-	-	2/4/4/4	-
6	GOL	A	508	-	-	4/4/4/4	-
6	GOL	B	706	-	-	2/4/4/4	-
4	NAG	A	502	1	-	1/6/23/26	0/1/1/1
6	GOL	B	705	-	-	2/4/4/4	-
4	NAG	A	501	1	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	509	8PR	CAT-CAX	4.09	1.58	1.51
7	A	509	8PR	OAQ-CAV	2.60	1.42	1.38
7	A	509	8PR	OAP-CAU	2.53	1.41	1.38
4	A	504	NAG	C1-C2	2.45	1.56	1.52
7	A	509	8PR	CAK-NAN	2.30	1.50	1.46
7	A	509	8PR	CAJ-CAX	-2.16	1.51	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	509	8PR	CAE-CAT-CAX	-4.81	111.98	121.08
7	A	509	8PR	CAJ-CAX-CAW	3.69	113.90	109.62
7	A	509	8PR	CAF-CAT-CAX	3.69	128.06	121.08
4	A	504	NAG	C1-O5-C5	3.23	116.56	112.19
7	A	509	8PR	OAQ-CAV-CAH	3.00	131.87	127.85
7	A	509	8PR	OAQ-CAS-CAH	-2.98	105.58	119.86
7	A	509	8PR	CAK-CAW-CAX	2.83	114.42	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	509	8PR	OAO-CAS-CAD	2.83	133.86	119.94
7	A	509	8PR	CAT-CAX-CAW	-2.64	108.55	113.69
7	A	509	8PR	CAJ-CAX-CAT	-2.58	107.83	112.57
7	A	509	8PR	CAL-OAP-CAU	2.33	108.37	105.34
7	A	509	8PR	OAP-CAU-CAG	2.29	131.98	127.81
7	A	509	8PR	CAM-CAW-CAX	-2.18	108.13	112.05
7	A	509	8PR	FAA-CAR-CAB	2.16	122.21	118.54
7	A	509	8PR	CAL-OAQ-CAV	2.13	108.11	105.34
7	A	509	8PR	CAC-CAR-CAB	-2.06	120.09	122.83

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	506	GOL	O1-C1-C2-C3
6	A	508	GOL	C1-C2-C3-O3
6	A	508	GOL	O2-C2-C3-O3
6	A	508	GOL	O1-C1-C2-C3
6	B	706	GOL	O1-C1-C2-C3
6	A	508	GOL	O1-C1-C2-O2
6	B	706	GOL	O1-C1-C2-O2
4	A	502	NAG	O5-C5-C6-O6
4	A	501	NAG	C4-C5-C6-O6
6	A	506	GOL	O1-C1-C2-O2
6	A	507	GOL	O2-C2-C3-O3
6	B	705	GOL	O1-C1-C2-O2
6	A	507	GOL	C1-C2-C3-O3
4	A	501	NAG	O5-C5-C6-O6
6	B	705	GOL	O1-C1-C2-C3
7	A	509	8PR	OAO-CAM-CAW-CAK
7	A	509	8PR	CAH-CAS-OAO-CAM
7	A	509	8PR	CAD-CAS-OAO-CAM

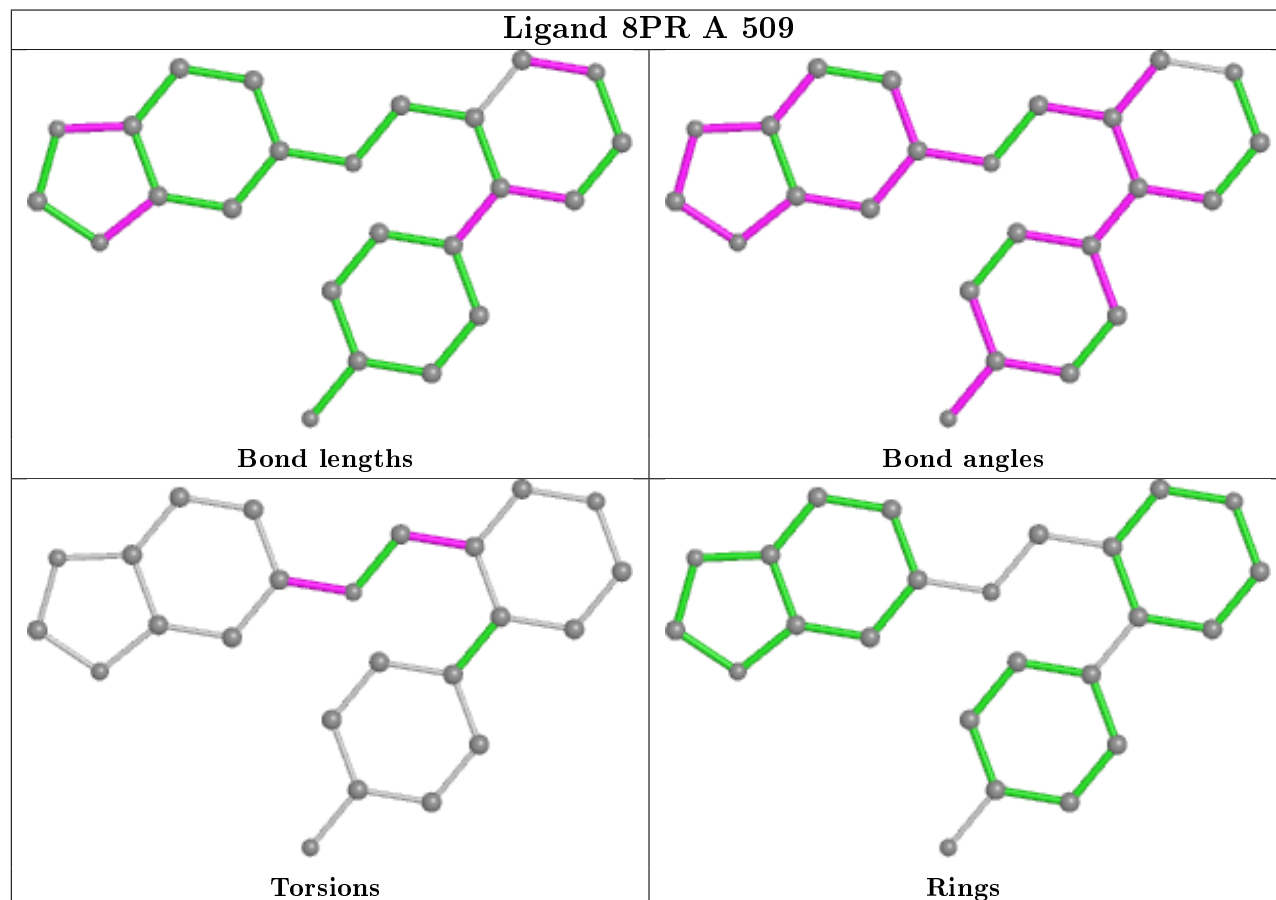
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	508	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	244/330 (73%)	0.44	16 (6%) 18 17	43, 70, 143, 197	0
2	B	131/168 (77%)	0.92	22 (16%) 1 1	48, 67, 198, 210	0
All	All	375/498 (75%)	0.61	38 (10%) 7 6	43, 69, 175, 210	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	620	THR	9.1
2	B	522	ASP	7.3
1	A	308	PHE	7.0
1	A	293	THR	6.9
2	B	615	TRP	6.7
2	B	619	ILE	6.5
2	B	625	GLN	5.7
2	B	629	ASP	5.4
2	B	623	ILE	5.2
2	B	616	THR	5.2
1	A	309	THR	4.9
2	B	613	ALA	4.8
2	B	621	ASP	4.7
2	B	626	ILE	4.6
1	A	307	SER	4.5
1	A	211	SER	4.0
2	B	628	HIS	3.9
1	A	310	VAL	3.8
1	A	229	GLU	3.8
1	A	306	LEU	3.8
2	B	617	LYS	3.5
2	B	627	ILE	3.5
2	B	631	VAL	3.3
2	B	632	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	278	ASN	3.0
1	A	262	THR	3.0
1	A	280	GLU	2.8
1	A	48[A]	VAL	2.8
2	B	527	ILE	2.8
1	A	214	TYR	2.7
2	B	614	ASP	2.7
1	A	281	ILE	2.7
2	B	589	ALA	2.6
2	B	525	ALA	2.5
2	B	624	ASP	2.3
1	A	47[A]	ASP	2.1
2	B	529	LEU	2.1
1	A	51[A]	LEU	2.0

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

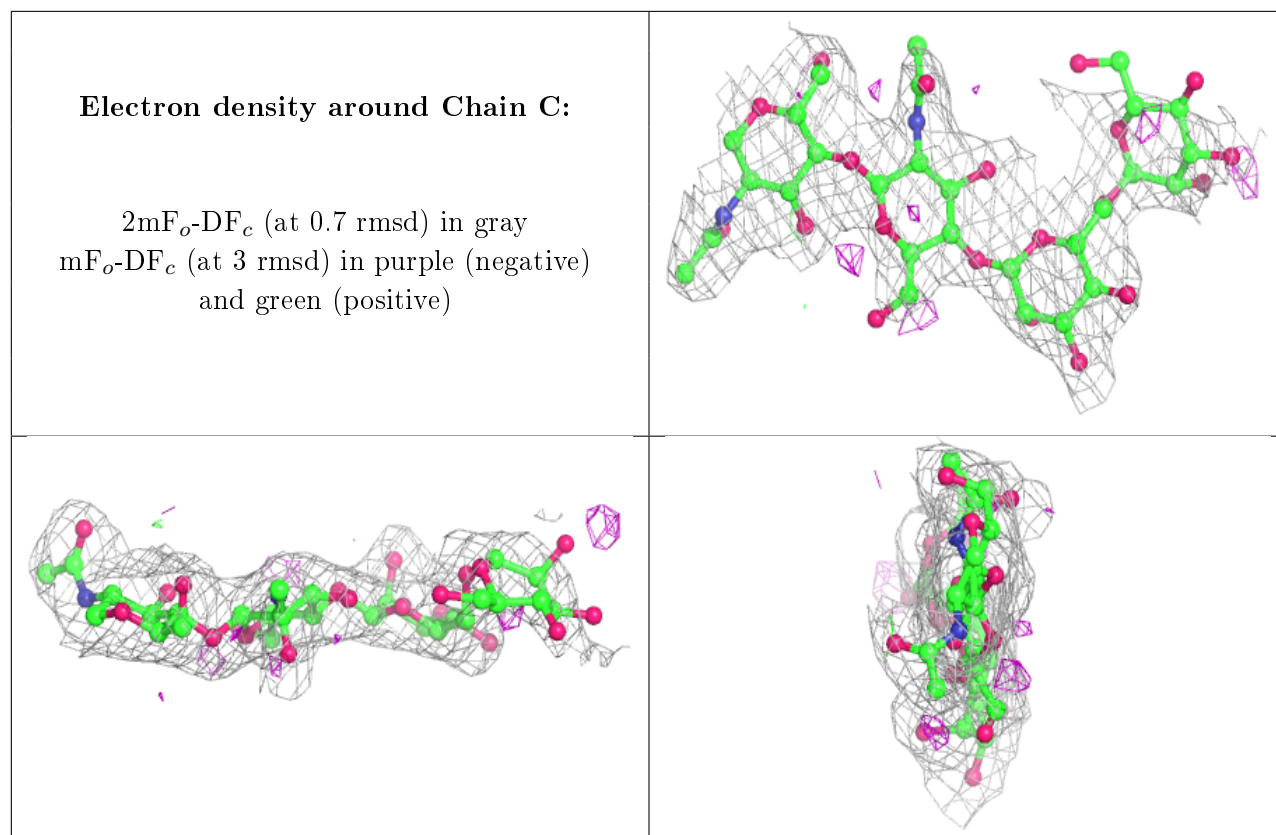
There are no non-standard protein/DNA/RNA residues in this entry.

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	4	11/12	0.73	0.50	164,169,174,174	0
3	BMA	C	3	11/12	0.80	0.35	129,134,148,158	0
3	NAG	C	2	14/15	0.88	0.28	98,107,119,125	0
3	NAG	C	1	14/15	0.97	0.12	49,64,75,79	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 ⓘ

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.

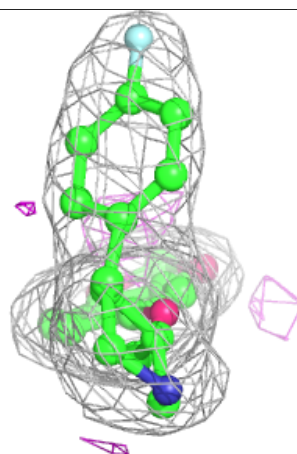
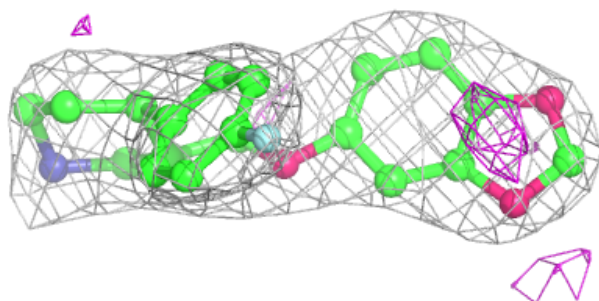
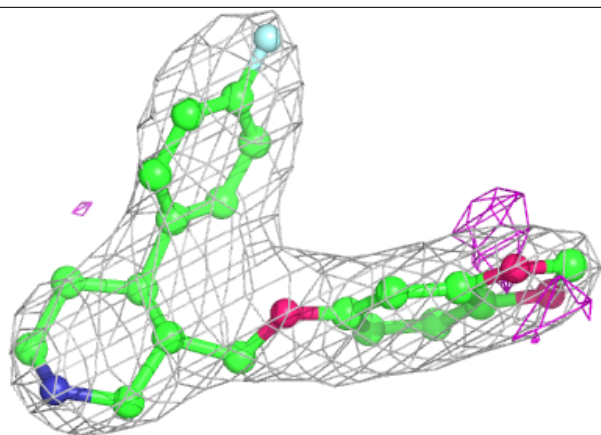
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	502	14/15	0.59	0.58	137,162,167,167	0
6	GOL	A	506	6/6	0.77	0.33	95,110,113,118	0
6	GOL	B	706	6/6	0.78	0.34	98,107,110,112	0
6	GOL	A	507	6/6	0.80	0.19	92,101,105,113	0
4	NAG	A	504	14/15	0.81	0.63	128,142,149,153	0
4	NAG	A	503	14/15	0.86	0.17	117,122,136,139	0
6	GOL	A	508	6/6	0.86	0.17	99,102,106,107	0
6	GOL	B	705	6/6	0.91	0.34	78,88,92,99	0
7	8PR	A	509	24/24	0.92	0.18	66,85,96,98	0
5	DMS	A	505	4/4	0.92	0.15	94,94,102,106	0
4	NAG	A	501	14/15	0.94	0.17	66,82,90,91	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 8PR A 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 ⓘ

There are no such residues in this entry.