



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2021 – 05:16 am GMT

PDB ID : 6YTP
Title : Structure of recombinant human beta-glucocerebrosidase in complex with
azide tagged cyclophellitol epoxide inhibitor
Authors : Rowland, R.J.; Davies, G.J.
Deposited on : 2020-04-24
Resolution : 1.70 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 : 1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

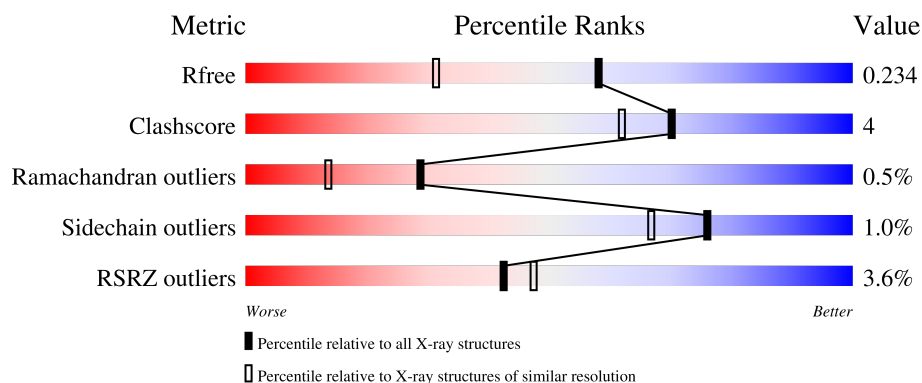
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	AAA	497	
1	BBB	497	
2	A	2	
2	B	2	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 16941 atoms, of which 8042 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.

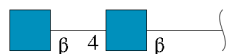
- Molecule 1 is a protein called Glucosylceramidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	497	Total	C	H	N	O	S	214	9	0
			7895	2566	3907	682	724	16			
1	BBB	497	Total	C	H	N	O	S	207	8	0
			7871	2560	3898	675	721	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	495	HIS	ARG	conflict	UNP P04062
BBB	495	HIS	ARG	conflict	UNP P04062

- Molecule 2 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
2	A	2	Total	C	H	N	O		5	0	0
			55	16	27	2	10				
2	B	2	Total	C	H	N	O		5	0	0
			56	16	28	2	10				

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



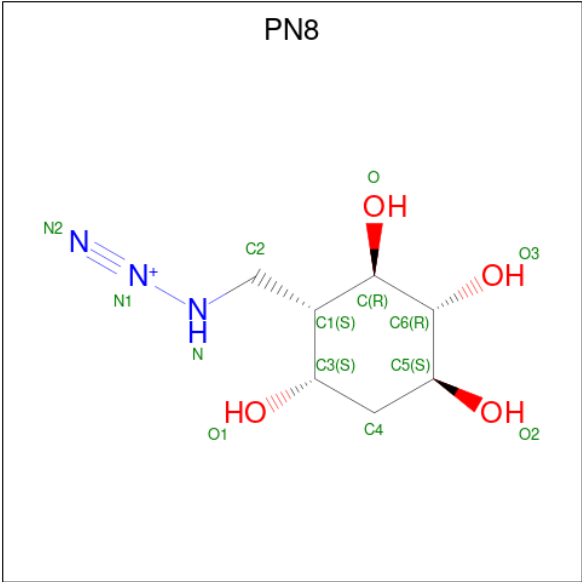
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
5	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
5	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
5	BBB	1	Total	C	H	O	1	0
			10	2	6	2		

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



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

- Molecule 7 is (1 {S},2 {R},3 {R},4 {S},5 {S})-4-[[(\$l^{5}\$-azanylidyne-\$l^{5}\$-azanyl)amino]methyl]cyclohexane-1,2,3,5-tetrol (three-letter code: PN8) (formula: C₇H₁₄N₃O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	AAA	1	Total	C	H	N	O	4	0
			27	7	13	3	4		
7	BBB	1	Total	C	H	N	O	4	0
			27	7	13	3	4		

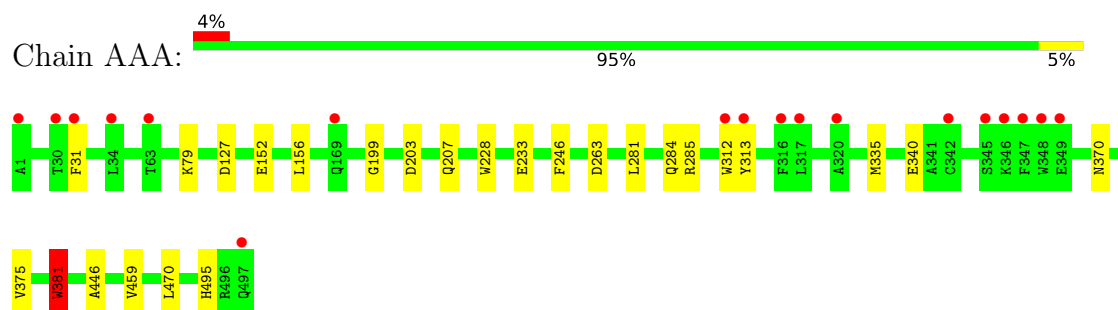
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	338	Total	O	0	0
			338	338		
8	BBB	323	Total	O	0	0
			323	323		

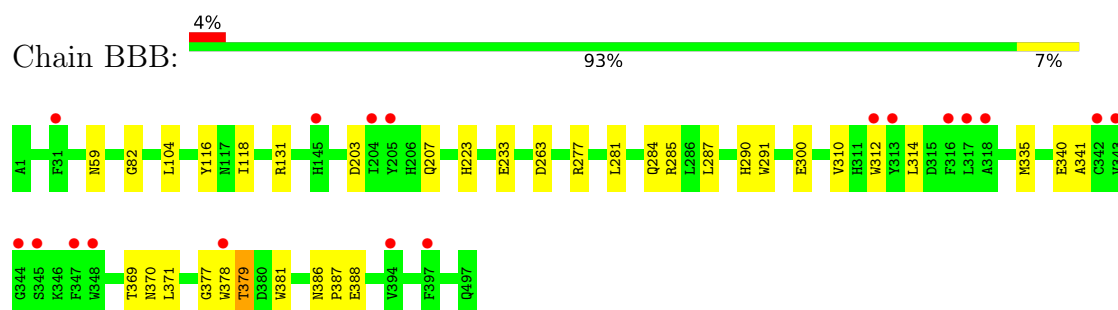
3 Residue-property plots [i](#)

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.

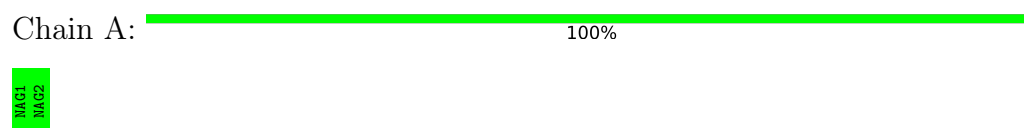
- Molecule 1: Glucosylceramidase



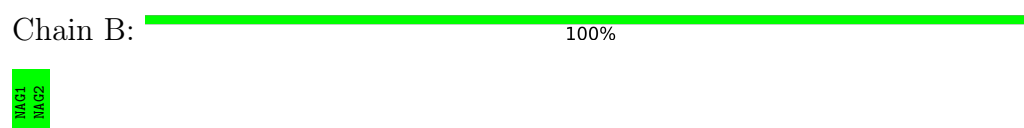
- Molecule 1: Glucosylceramidase



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



- Molecule 2: 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	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.89Å 285.77Å 91.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.20 – 1.70 68.11 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (68.20-1.70) 99.9 (68.11-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.186 , 0.212 0.208 , 0.234	Depositor DCC
R_{free} test set	7842 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16941	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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, PN8, EDO, SO4, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AAA	0.68	1/4110 (0.0%)	0.76	0/5607
1	BBB	0.70	1/4094 (0.0%)	0.77	1/5584 (0.0%)
All	All	0.69	2/8204 (0.0%)	0.76	1/11191 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	340	GLU	CD-OE2	16.61	1.44	1.25
1	AAA	340	GLU	CD-OE2	15.07	1.42	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	379	THR	CA-CB-OG1	-5.75	96.91	109.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	3988	3907	3867	23	0
1	BBB	3973	3898	3863	32	0
2	A	28	27	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	28	28	25	0	0
3	AAA	14	14	13	0	0
3	BBB	14	14	13	0	0
4	AAA	35	0	0	1	0
4	BBB	40	0	0	0	0
5	AAA	32	48	48	0	0
5	BBB	16	24	24	1	0
6	AAA	12	16	16	1	0
6	BBB	30	40	40	6	0
7	AAA	14	13	0	1	0
7	BBB	14	13	0	0	0
8	AAA	338	0	0	2	0
8	BBB	323	0	0	4	0
All	All	8899	8042	7934	59	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 4.

All (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:BBB:370:ASN:CB	1:BBB:378:TRP:HE1	1.89	0.86
1:AAA:285:ARG:CZ	1:AAA:312:TRP:HZ3	1.91	0.82
1:BBB:370:ASN:HB3	1:BBB:378:TRP:HE1	1.45	0.81
1:BBB:207:GLN:NE2	1:BBB:263:ASP:OD1	2.17	0.78
1:AAA:207:GLN:NE2	1:AAA:263:ASP:OD1	2.18	0.73
1:AAA:285:ARG:CZ	1:AAA:312:TRP:CZ3	2.74	0.69
1:AAA:370:ASN:HD22	1:AAA:375:VAL:HG11	1.59	0.67
1:BBB:388:GLU:OE1	8:BBB:601:HOH:O	2.14	0.66
1:BBB:310[B]:VAL:HG12	8:BBB:676:HOH:O	1.95	0.65
1:BBB:312:TRP:HE1	1:BBB:370:ASN:HD21	1.46	0.63
1:AAA:152:GLU:HA	1:AAA:156[A]:LEU:HD12	1.82	0.61
1:AAA:285:ARG:NE	1:AAA:312:TRP:HZ3	1.97	0.61
1:BBB:312:TRP:CE3	1:BBB:341:ALA:HB1	2.36	0.61
6:AAA:519:GOL:O2	8:AAA:601:HOH:O	2.12	0.60
1:BBB:82:GLY:HA3	1:BBB:118:ILE:O	2.04	0.56
1:BBB:131:ARG:HH22	6:BBB:517:GOL:H11	1.71	0.56
1:BBB:131:ARG:HH22	6:BBB:517:GOL:C1	2.19	0.56
7:AAA:521:PN8:O1	7:AAA:521:PN8:N1	2.41	0.53
1:AAA:285:ARG:NE	1:AAA:312:TRP:CZ3	2.75	0.53
1:BBB:312:TRP:CE3	1:BBB:341:ALA:CB	2.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:207:GLN:HE22	1:AAA:263:ASP:HA	1.74	0.52
1:AAA:285:ARG:HD3	1:AAA:312:TRP:CH2	2.45	0.52
1:AAA:284:GLN:OE1	1:AAA:313:TYR:CE1	2.63	0.52
1:BBB:312:TRP:HE1	1:BBB:370:ASN:ND2	2.09	0.50
1:BBB:207:GLN:HE22	1:BBB:263:ASP:HA	1.76	0.50
1:BBB:223:HIS:HE1	8:BBB:873:HOH:O	1.93	0.50
1:AAA:284:GLN:NE2	1:AAA:313:TYR:CD1	2.81	0.49
1:BBB:203:ASP:OD1	1:BBB:203:ASP:C	2.51	0.48
1:BBB:370:ASN:HB2	1:BBB:378:TRP:HE1	1.74	0.46
1:BBB:277:ARG:HH11	6:BBB:520:GOL:H32	1.79	0.46
1:AAA:381:TRP:HA	1:AAA:381:TRP:CE3	2.51	0.46
1:AAA:127:ASP:HB3	1:AAA:246:PHE:CG	2.51	0.46
1:AAA:312:TRP:HE1	1:AAA:370:ASN:HD21	1.62	0.46
1:AAA:284:GLN:NE2	1:AAA:313:TYR:CE1	2.84	0.46
1:BBB:377:GLY:C	1:BBB:378:TRP:CE3	2.89	0.46
1:BBB:277:ARG:HH11	6:BBB:520:GOL:C3	2.29	0.45
1:AAA:31:PHE:CB	1:AAA:495:HIS:CE1	2.99	0.45
1:AAA:79:LYS:HE2	1:AAA:228:TRP:CE2	2.52	0.44
1:AAA:284:GLN:NE2	1:AAA:284:GLN:HA	2.32	0.44
1:BBB:285:ARG:HB3	1:BBB:310[B]:VAL:HG11	2.00	0.44
1:BBB:371:LEU:HD21	1:BBB:378:TRP:CH2	2.51	0.44
1:BBB:371:LEU:CD2	1:BBB:378:TRP:CH2	3.01	0.44
1:AAA:446:ALA:HA	1:AAA:459:VAL:O	2.18	0.43
1:AAA:199:GLY:HA3	1:AAA:203:ASP:OD2	2.19	0.43
6:BBB:520:GOL:H11	8:BBB:800:HOH:O	2.18	0.43
1:BBB:378:TRP:CE3	1:BBB:378:TRP:N	2.88	0.42
1:BBB:82:GLY:HA2	1:BBB:116:TYR:CD2	2.53	0.42
1:BBB:287:LEU:HB3	1:BBB:291:TRP:CD1	2.55	0.42
1:BBB:290:HIS:ND1	6:BBB:519:GOL:H11	2.34	0.42
1:AAA:381:TRP:HA	1:AAA:381:TRP:HE3	1.85	0.42
1:AAA:152:GLU:O	1:AAA:156[B]:LEU:HB2	2.20	0.41
4:AAA:508:SO4:O3	8:AAA:603:HOH:O	2.18	0.41
1:BBB:285:ARG:HB3	1:BBB:310[B]:VAL:CG1	2.50	0.41
1:BBB:284:GLN:HG3	1:BBB:314:LEU:HD12	2.01	0.41
1:BBB:369:THR:HG21	5:BBB:514:EDO:C1	2.50	0.41
1:BBB:386:ASN:HB2	1:BBB:387:PRO:CD	2.50	0.41
1:BBB:377:GLY:C	1:BBB:378:TRP:CD2	2.94	0.41
1:AAA:207:GLN:NE2	1:AAA:263:ASP:HA	2.34	0.41
1:BBB:104:LEU:C	1:BBB:104:LEU:HD23	2.42	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	AAA	504/497 (101%)	488 (97%)	13 (3%)	3 (1%)	25	11
1	BBB	503/497 (101%)	482 (96%)	19 (4%)	2 (0%)	34	18
All	All	1007/994 (101%)	970 (96%)	32 (3%)	5 (0%)	29	13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	233	GLU
1	AAA	381	TRP
1	BBB	233	GLU
1	BBB	281	LEU
1	AAA	281	LEU

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	AAA	427/424 (101%)	424 (99%)	3 (1%)	84	77
1	BBB	428/424 (101%)	422 (99%)	6 (1%)	67	53
All	All	855/848 (101%)	846 (99%)	9 (1%)	76	63

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	335	MET

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Mol	Chain	Res	Type
1	AAA	381	TRP
1	AAA	470	LEU
1	BBB	59	ASN
1	BBB	300[A]	GLU
1	BBB	300[B]	GLU
1	BBB	335	MET
1	BBB	379	THR
1	BBB	381	TRP

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 ⓘ

4 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

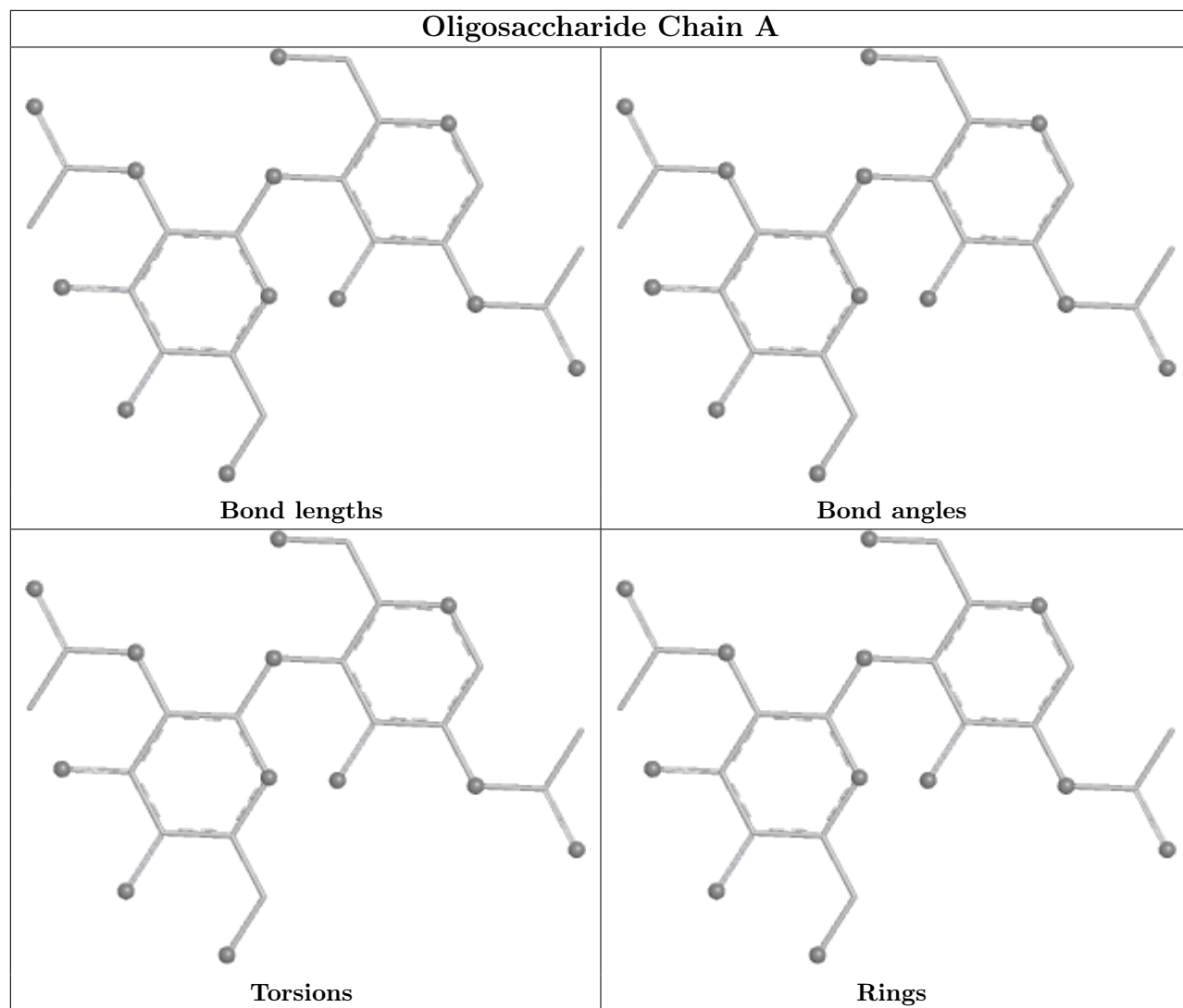
There are no chirality outliers.

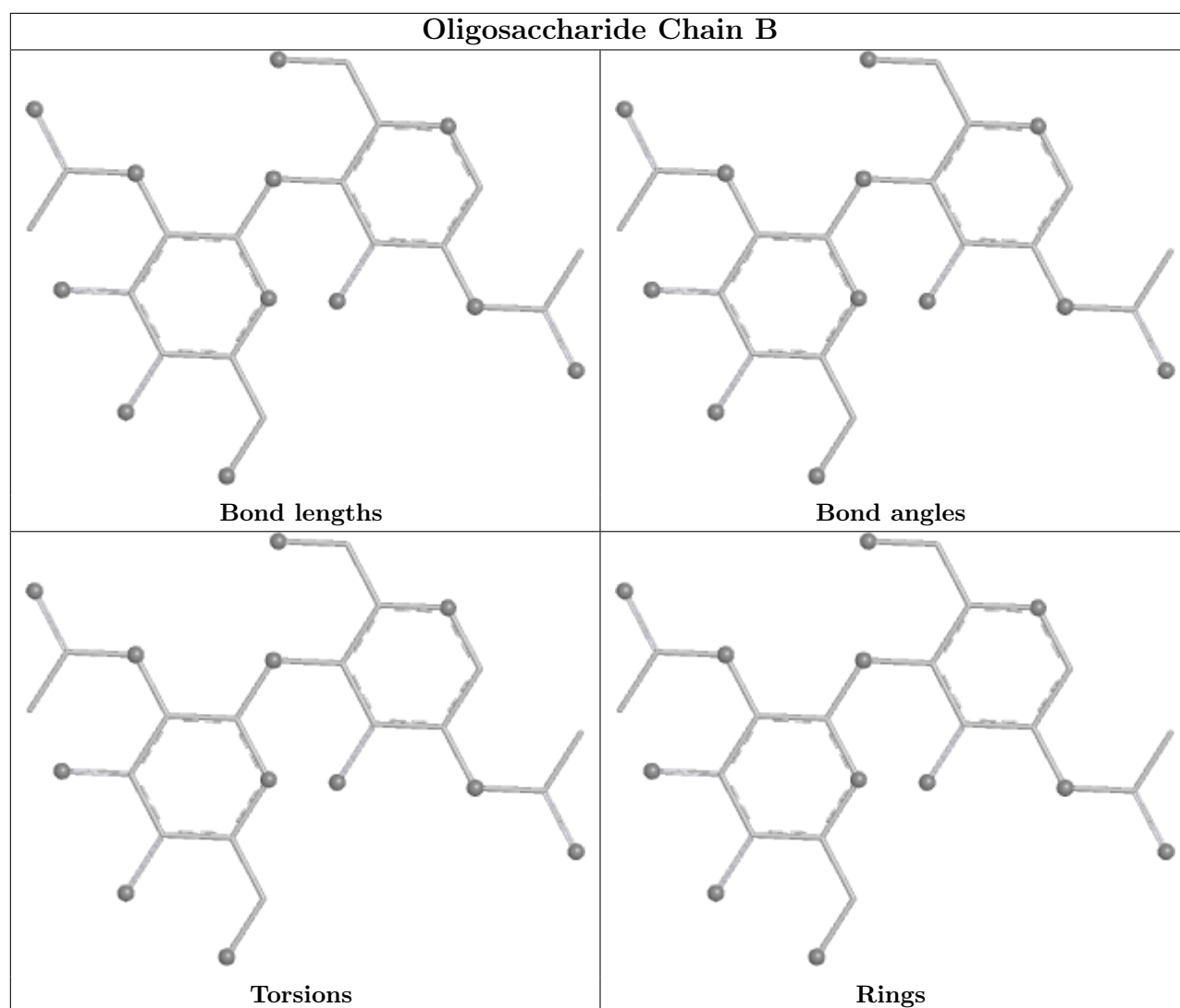
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

38 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

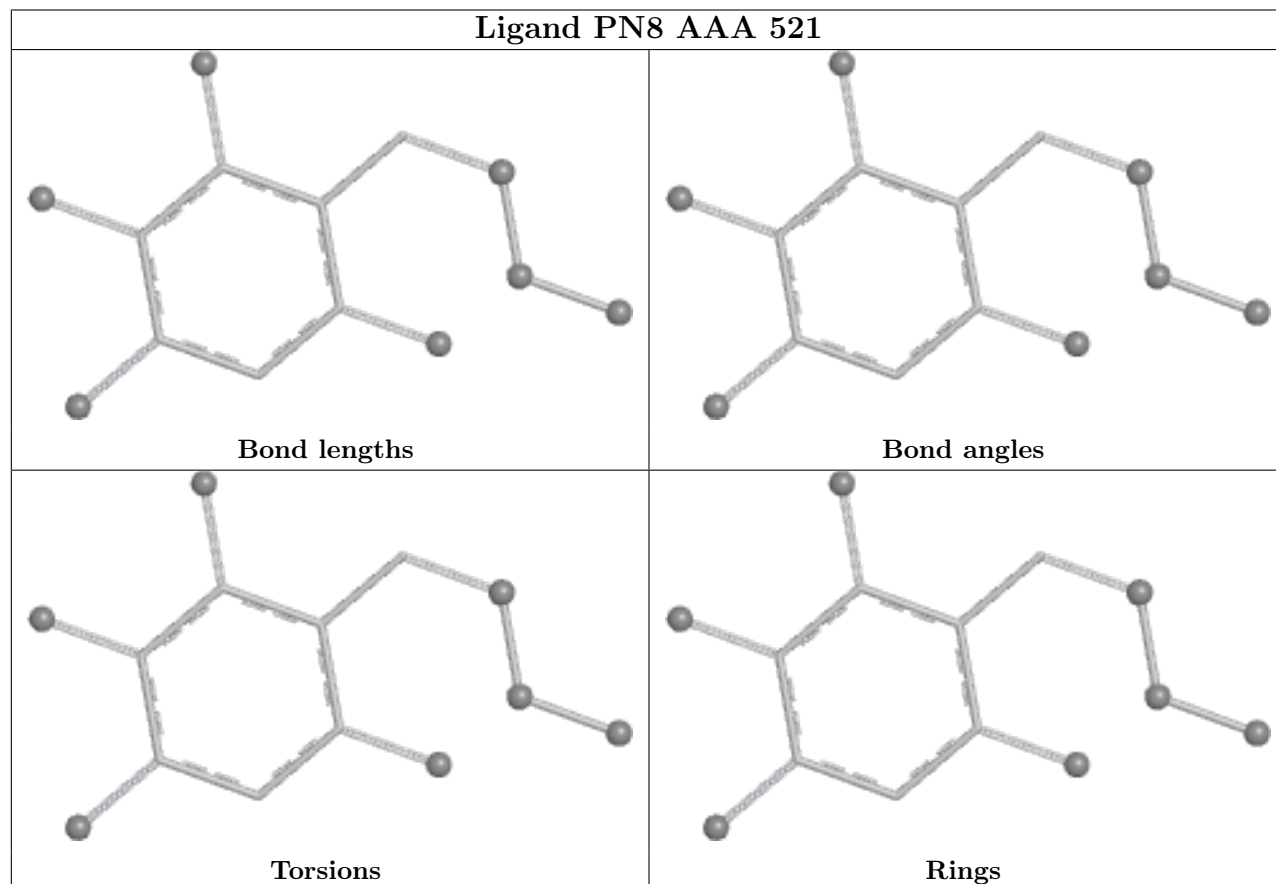
There are no torsion outliers.

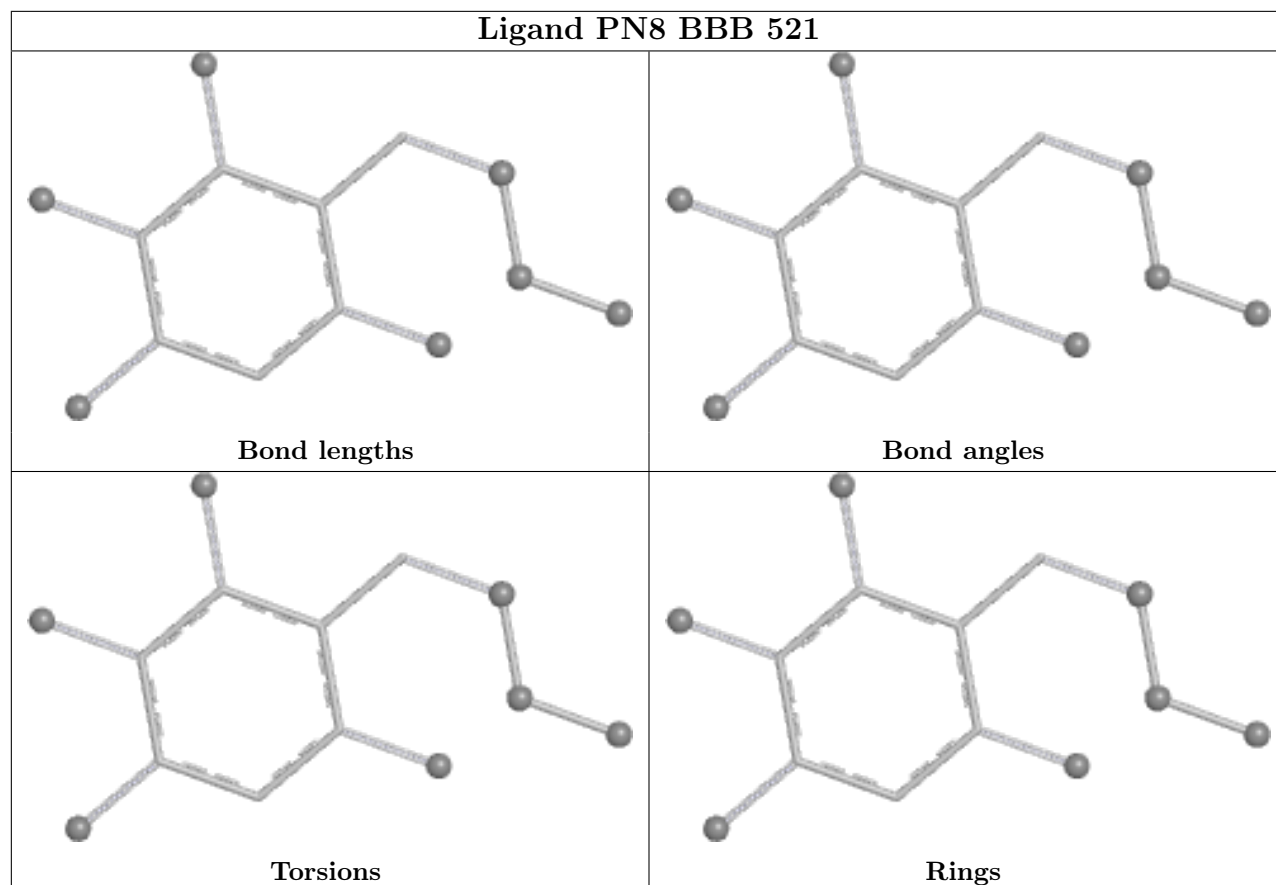
There are no ring outliers.

No monomer is involved in short contacts.

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	AAA	497/497 (100%)	0.11	18 (3%)	42	47	21, 30, 51, 91	9 (1%)
1	BBB	497/497 (100%)	0.00	18 (3%)	42	47	21, 31, 51, 83	8 (1%)
All	All	994/994 (100%)	0.05	36 (3%)	42	47	21, 30, 51, 91	17 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	347	PHE	21.2
1	BBB	316[A]	PHE	15.2
1	AAA	312	TRP	5.3
1	BBB	347	PHE	4.7
1	BBB	378	TRP	4.5
1	AAA	316	PHE	4.2
1	BBB	313	TYR	3.7
1	AAA	348	TRP	3.7
1	BBB	394[A]	VAL	3.5
1	AAA	349[A]	GLU	3.4
1	AAA	317	LEU	3.4
1	AAA	497	GLN	3.3
1	AAA	169	GLN	3.2
1	BBB	312	TRP	3.2
1	BBB	345	SER	3.1
1	BBB	397	PHE	2.9
1	BBB	317	LEU	2.8
1	AAA	346	LYS	2.8
1	AAA	31	PHE	2.8
1	BBB	348	TRP	2.5
1	AAA	345	SER	2.5
1	BBB	31	PHE	2.4
1	BBB	342	CYS	2.4
1	BBB	343	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	34	LEU	2.4
1	AAA	313	TYR	2.4
1	BBB	344	GLY	2.4
1	AAA	30[A]	THR	2.4
1	AAA	63	THR	2.3
1	AAA	342	CYS	2.3
1	AAA	320	ALA	2.3
1	BBB	204	ILE	2.2
1	BBB	145	HIS	2.2
1	AAA	1	ALA	2.2
1	BBB	205	TYR	2.0
1	BBB	318	ALA	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 ⓘ

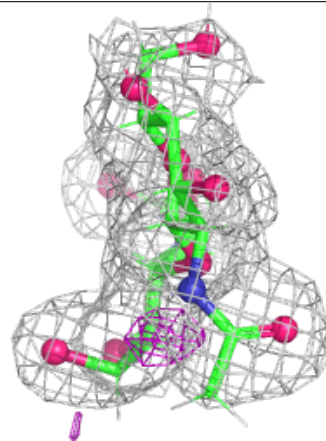
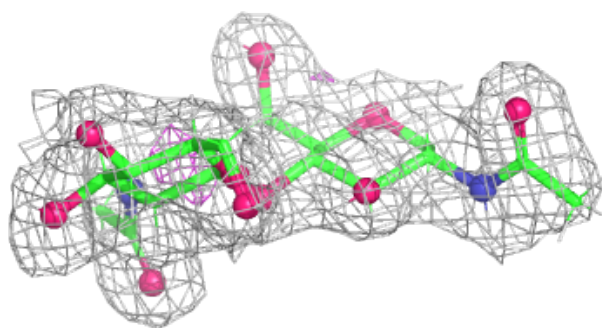
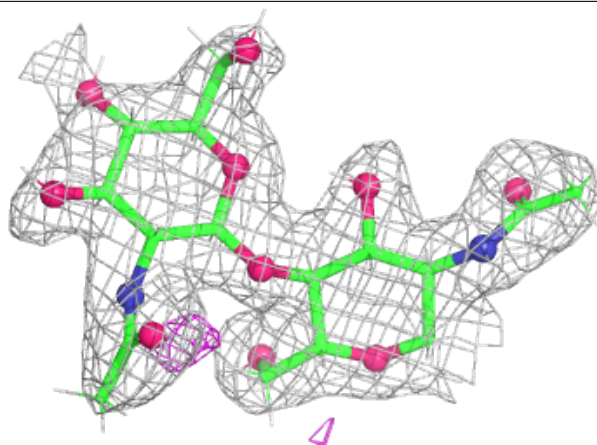
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

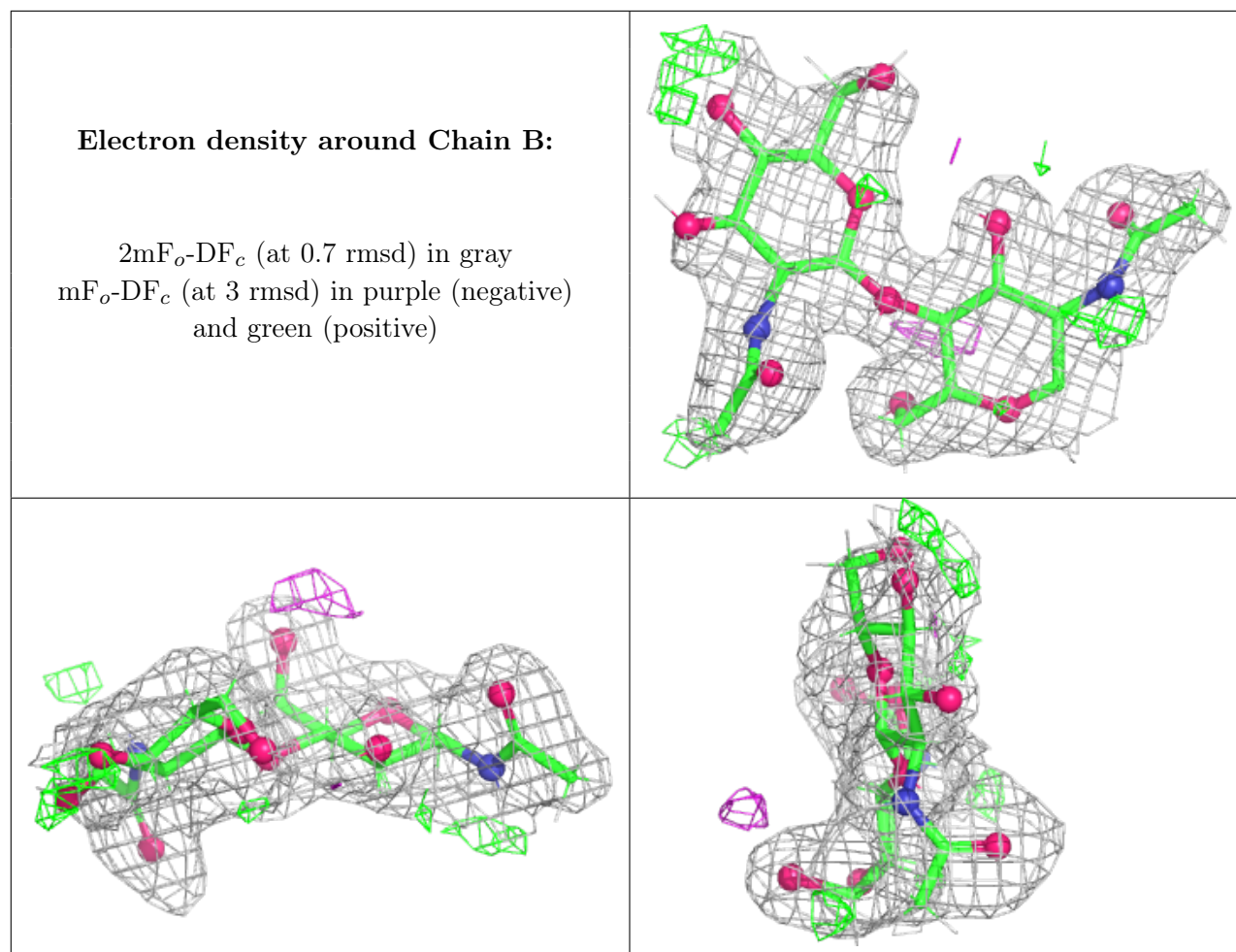
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	2	14/15	0.81	0.18	51,72,76,81	3
2	NAG	A	2	14/15	0.87	0.16	42,55,66,67	3
2	NAG	A	1	14/15	0.93	0.10	33,40,44,47	2
2	NAG	B	1	14/15	0.94	0.09	34,41,43,48	2

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 A:

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
6	GOL	BBB	520	6/6	0.47	0.27	74,78,84,85	2
5	EDO	BBB	515	4/4	0.57	0.28	61,64,66,68	1
5	EDO	AAA	512	4/4	0.58	0.17	55,58,58,60	1
3	NAG	BBB	503	14/15	0.60	0.40	90,110,122,122	3
6	GOL	BBB	518	6/6	0.63	0.17	70,72,73,74	2
4	SO4	AAA	510	5/5	0.70	0.26	98,100,107,114	0
6	GOL	BBB	517	6/6	0.72	0.16	49,57,64,64	2
3	NAG	AAA	503	14/15	0.74	0.17	56,62,69,69	3
5	EDO	AAA	513	4/4	0.76	0.18	59,63,64,65	1
5	EDO	BBB	514	4/4	0.77	0.17	65,66,67,67	1
4	SO4	BBB	508	5/5	0.83	0.16	89,92,95,104	0

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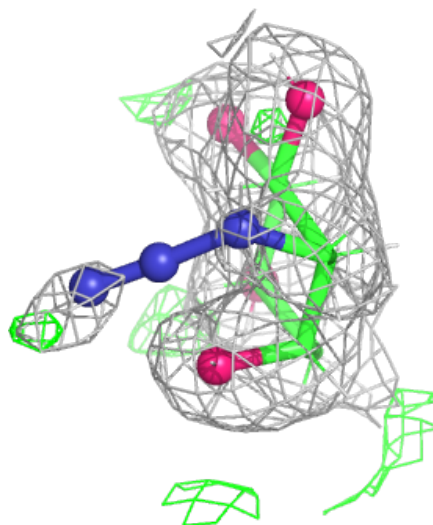
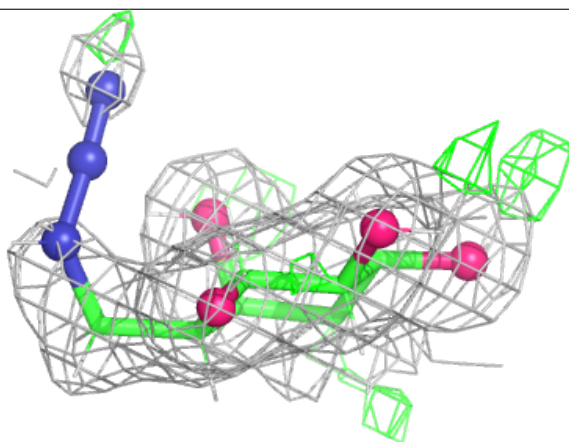
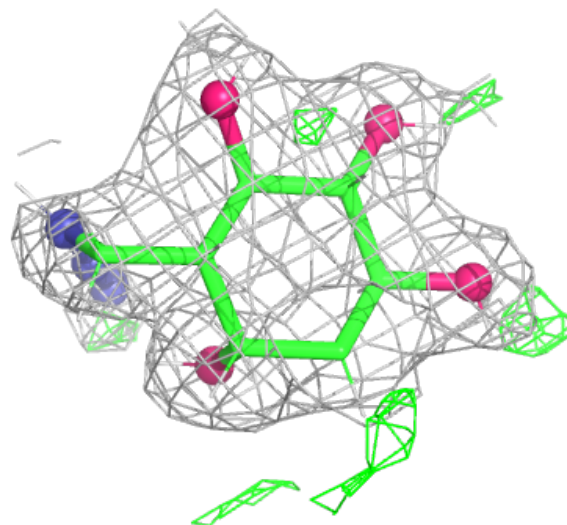
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	AAA	518	4/4	0.84	0.15	62,65,66,67	1
5	EDO	AAA	517	4/4	0.84	0.20	51,61,64,64	1
5	EDO	AAA	516	4/4	0.85	0.22	64,68,70,71	1
5	EDO	AAA	515	4/4	0.86	0.22	54,61,66,67	1
6	GOL	AAA	519	6/6	0.87	0.14	36,51,59,60	2
4	SO4	BBB	509	5/5	0.87	0.14	60,62,66,72	5
6	GOL	BBB	519	6/6	0.88	0.17	62,65,69,69	2
4	SO4	AAA	509	5/5	0.88	0.14	81,84,90,96	0
5	EDO	BBB	512	4/4	0.89	0.18	69,74,78,78	1
5	EDO	AAA	511	4/4	0.90	0.13	58,63,64,65	1
5	EDO	AAA	514	4/4	0.91	0.27	61,62,62,63	1
6	GOL	BBB	516	6/6	0.91	0.11	46,54,62,62	2
5	EDO	BBB	513	4/4	0.91	0.20	55,60,64,65	1
6	GOL	AAA	520	6/6	0.93	0.10	41,51,59,62	2
4	SO4	BBB	506	5/5	0.93	0.14	73,75,81,83	0
4	SO4	AAA	506	5/5	0.93	0.10	74,79,80,82	0
4	SO4	BBB	511	5/5	0.94	0.11	76,76,86,88	0
4	SO4	BBB	510	5/5	0.94	0.17	66,67,79,80	0
7	PN8	BBB	521	14/14	0.94	0.13	30,33,37,39	8
7	PN8	AAA	521	14/14	0.95	0.12	25,28,37,42	8
4	SO4	AAA	507	5/5	0.96	0.08	63,64,66,72	0
4	SO4	AAA	508	5/5	0.96	0.09	62,67,70,74	0
4	SO4	BBB	507	5/5	0.97	0.13	60,61,67,68	0
4	SO4	BBB	504	5/5	0.97	0.08	51,55,58,60	0
4	SO4	AAA	505	5/5	0.98	0.06	47,50,52,53	0
4	SO4	BBB	505	5/5	0.99	0.10	35,36,39,42	0
4	SO4	AAA	504	5/5	0.99	0.12	36,38,38,46	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.

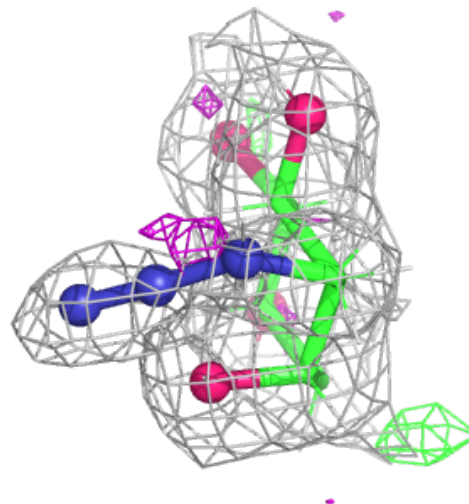
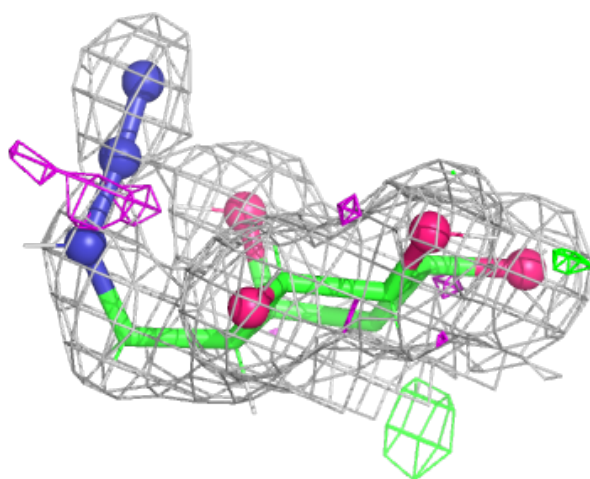
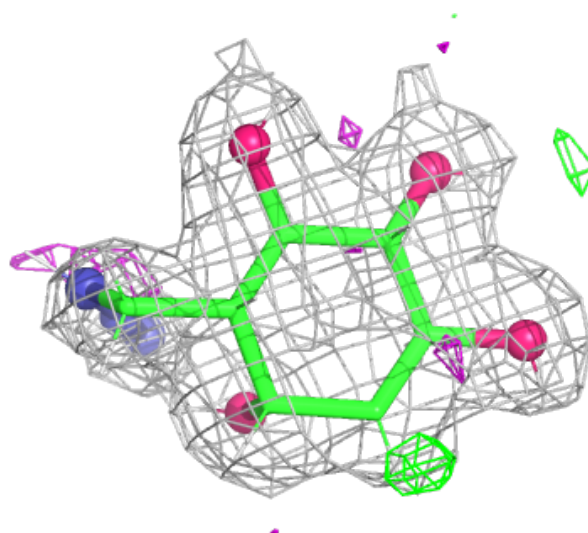
Electron density around PN8 BBB 521:

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



Electron density around PN8 AAA 521:

$2mF_o-DF_c$ (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.