



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 11, 2022 – 01:09 pm BST

PDB ID : 6TJK
Title : Crystal Structure of Recombinant GBA in Complex with Bis-Tris Propane
Authors : Rowland, R.J.; Davies, G.J.
Deposited on : 2019-11-26
Resolution : 1.56 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
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) : 2.27

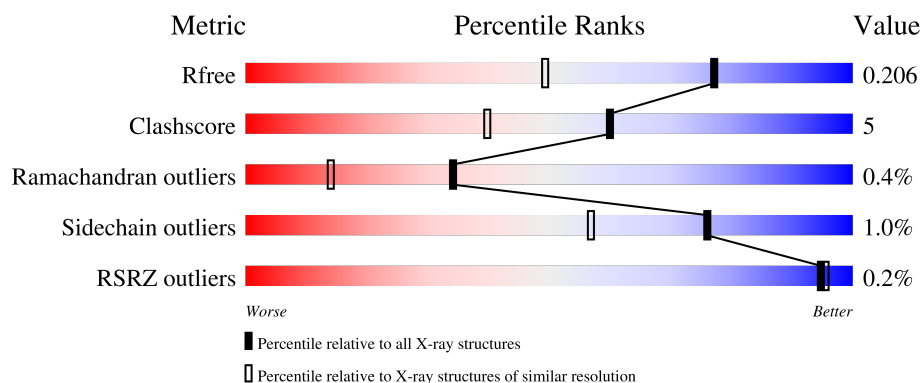
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	<div> <div style="width: 89%;"></div> <div style="width: 11%;"></div> </div> <div>89% 11%</div>
1	BBB	497	<div> <div style="width: 92%;"></div> <div style="width: 8%;"></div> </div> <div>92% 8%</div>
2	A	4	<div> <div style="width: 100%;"></div> </div> <div>100%</div>
2	B	4	<div> <div style="width: 25%;"></div> <div style="width: 50%;"></div> <div style="width: 25%;"></div> </div> <div>25% 50% 25%</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
5	EDO	AAA	517	-	-	X	-
5	EDO	BBB	1915	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17633 atoms, of which 8321 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 Lysosomal acid glucosylceramidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	497	Total	C	H	N	O	S	203	4	0
			7839	2548	3883	676	716	16			
1	BBB	497	Total	C	H	N	O	S	217	13	0
			7993	2591	3962	692	732	16			

- Molecule 2 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
2	A	4	Total	C	H	N	O	12	0	0
			100	28	50	2	20			
2	B	4	Total	C	H	N	O	11	0	0
			100	28	50	2	20			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



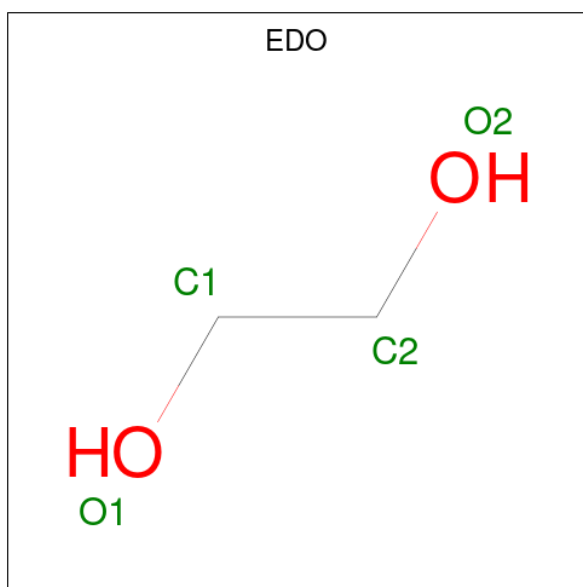
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	AAA	1	Total	O	S	0	0
			5	4	1		
3	BBB	1	Total	O	S	0	0
			5	4	1		
3	BBB	1	Total	O	S	0	0
			5	4	1		
3	BBB	1	Total	O	S	0	0
			5	4	1		
3	BBB	1	Total	O	S	0	0
			5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

- 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	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
4	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
4	BBB	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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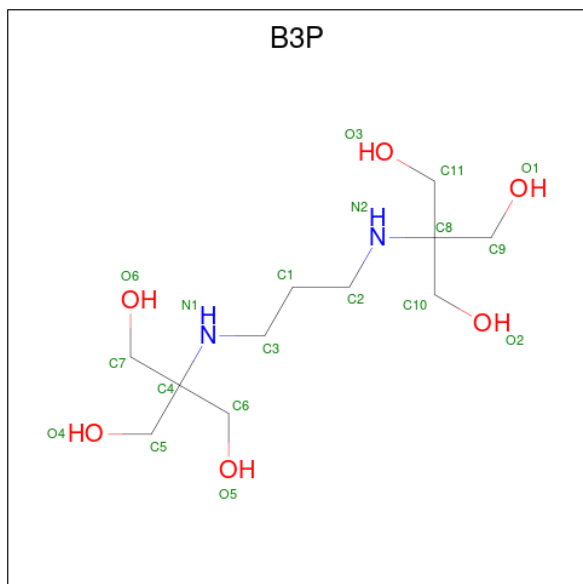
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	2	1
			20	4	12	4		
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	2	1
			20	4	12	4		
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	2	1
			20	4	12	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		
5	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
5	BBB	1	Total	C	H	O	2	1
			20	4	12	4		
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		
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		
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		
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 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	AAA	1	Total	C	H	N	O	5	0
			45	11	26	2	6		
6	BBB	1	Total	C	H	N	O	5	0
			45	11	26	2	6		

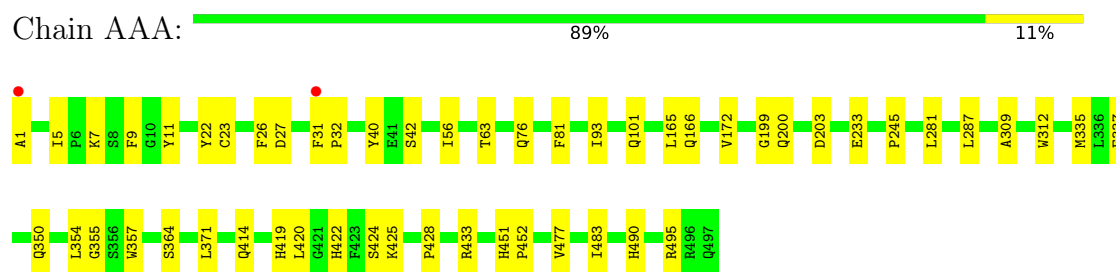
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	402	Total	O	0	5
			407	407		
7	BBB	493	Total	O	0	7
			500	500		

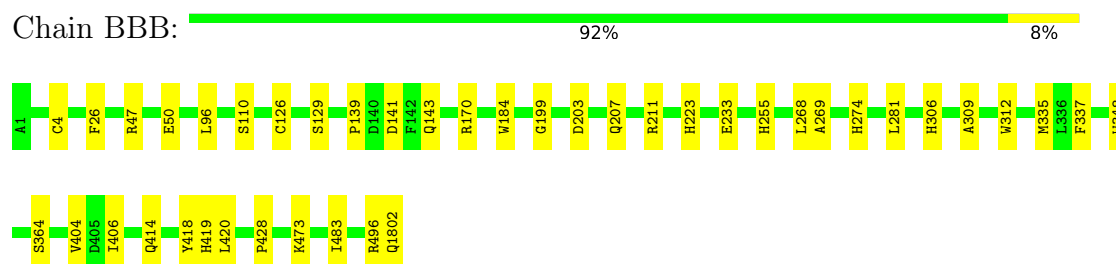
3 Residue-property plots [i](#)

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.

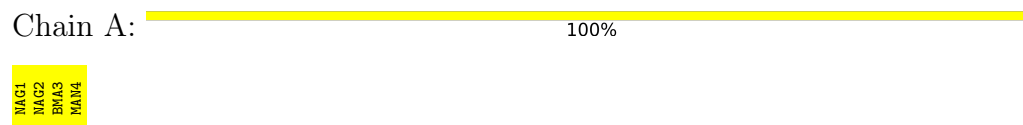
- Molecule 1: Lysosomal acid glucosylceramidase



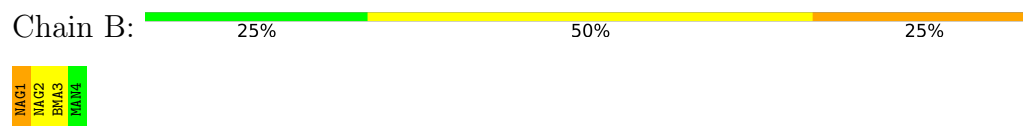
- Molecule 1: Lysosomal acid glucosylceramidase



- Molecule 2: 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



- Molecule 2: 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	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.74Å 156.22Å 68.26Å 90.00° 102.47° 90.00°	Depositor
Resolution (Å)	66.74 – 1.56 66.65 – 1.56	Depositor EDS
% Data completeness (in resolution range)	96.7 (66.74-1.56) 96.8 (66.65-1.56)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.56Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.165 , 0.199 0.176 , 0.206	Depositor DCC
R_{free} test set	7465 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17633	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% 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: EDO, NAG, SO4, B3P, MAN, BMA

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	0/4076	0.80	0/5560
1	BBB	0.72	1/4151 (0.0%)	0.81	1/5661 (0.0%)
All	All	0.70	1/8227 (0.0%)	0.81	1/11221 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	496	ARG	C-N	8.96	1.54	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	1802	GLN	CA-C-O	-5.45	108.66	120.10

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	3956	3883	3855	31	1
1	BBB	4031	3962	3926	39	1
2	A	50	50	43	0	0
2	B	50	50	43	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AAA	25	0	0	0	0
3	BBB	25	0	0	0	0
4	AAA	28	28	26	0	0
4	BBB	14	14	13	0	0
5	AAA	84	126	126	8	0
5	BBB	104	156	156	17	0
6	AAA	19	26	26	1	0
6	BBB	19	26	26	0	0
7	AAA	407	0	0	4	0
7	BBB	500	0	0	14	0
All	All	9312	8321	8240	77	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 5.

The worst 5 of 77 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:AAA:433[A]:ARG:NH1	7:AAA:601[A]:HOH:O	1.93	0.99
1:BBB:110[A]:SER:OG	7:BBB:2001:HOH:O	2.05	0.75
1:BBB:143[C]:GLN:O	1:BBB:211:ARG:NH1	2.25	0.69
1:BBB:406[B]:ILE:HD13	1:BBB:406[B]:ILE:O	1.96	0.66
5:BBB:1905:EDO:H12	7:BBB:2333:HOH:O	1.94	0.66

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:BBB:473:LYS:HZ3	2:B:1:NAG:HO3[1_655]	1.14	0.46
1:AAA:63:THR:H	1:AAA:200:GLN:HE21[1_556]	1.21	0.39

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	AAA	499/497 (100%)	479 (96%)	18 (4%)	2 (0%)	34	14
1	BBB	508/497 (102%)	490 (96%)	16 (3%)	2 (0%)	34	14
All	All	1007/994 (101%)	969 (96%)	34 (3%)	4 (0%)	34	14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	233	GLU
1	AAA	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	425/424 (100%)	421 (99%)	4 (1%)	78	61
1	BBB	434/424 (102%)	430 (99%)	4 (1%)	78	61
All	All	859/848 (101%)	851 (99%)	8 (1%)	76	61

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	483	ILE
1	BBB	420	LEU
1	BBB	312	TRP
1	AAA	483	ILE
1	BBB	335	MET

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 ⓘ

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	A	1	1,2	14,14,15	0.70	0	17,19,21	1.27	1 (5%)
2	NAG	A	2	2	14,14,15	0.57	0	17,19,21	1.45	2 (11%)
2	BMA	A	3	2	11,11,12	0.44	0	15,15,17	1.33	3 (20%)
2	MAN	A	4	2	11,11,12	0.41	0	15,15,17	1.38	1 (6%)
2	NAG	B	1	1,2	14,14,15	0.94	0	17,19,21	1.10	1 (5%)
2	NAG	B	2	2	14,14,15	0.67	0	17,19,21	1.78	5 (29%)
2	BMA	B	3	2	11,11,12	0.51	0	15,15,17	1.53	3 (20%)
2	MAN	B	4	2	11,11,12	0.35	0	15,15,17	0.91	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	A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1
2	BMA	A	3	2	-	1/2/19/22	0/1/1/1
2	MAN	A	4	2	-	0/2/19/22	0/1/1/1
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	1/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	NAG	O5-C1-C2	-4.03	104.92	111.29
2	B	2	NAG	C1-O5-C5	3.67	117.16	112.19
2	B	2	NAG	C8-C7-N2	-3.45	110.25	116.10
2	A	4	MAN	C1-C2-C3	3.14	113.53	109.67
2	B	3	BMA	C1-O5-C5	2.74	115.90	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

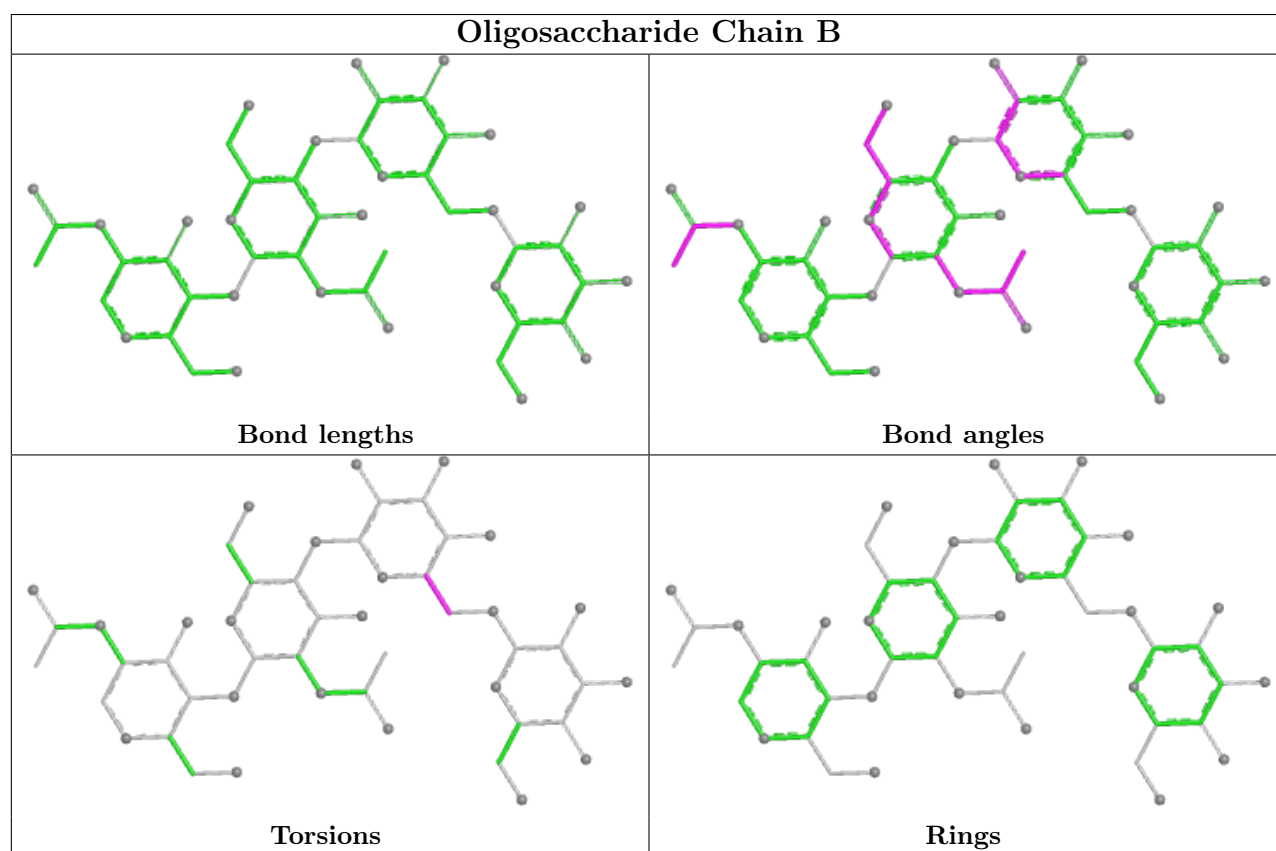
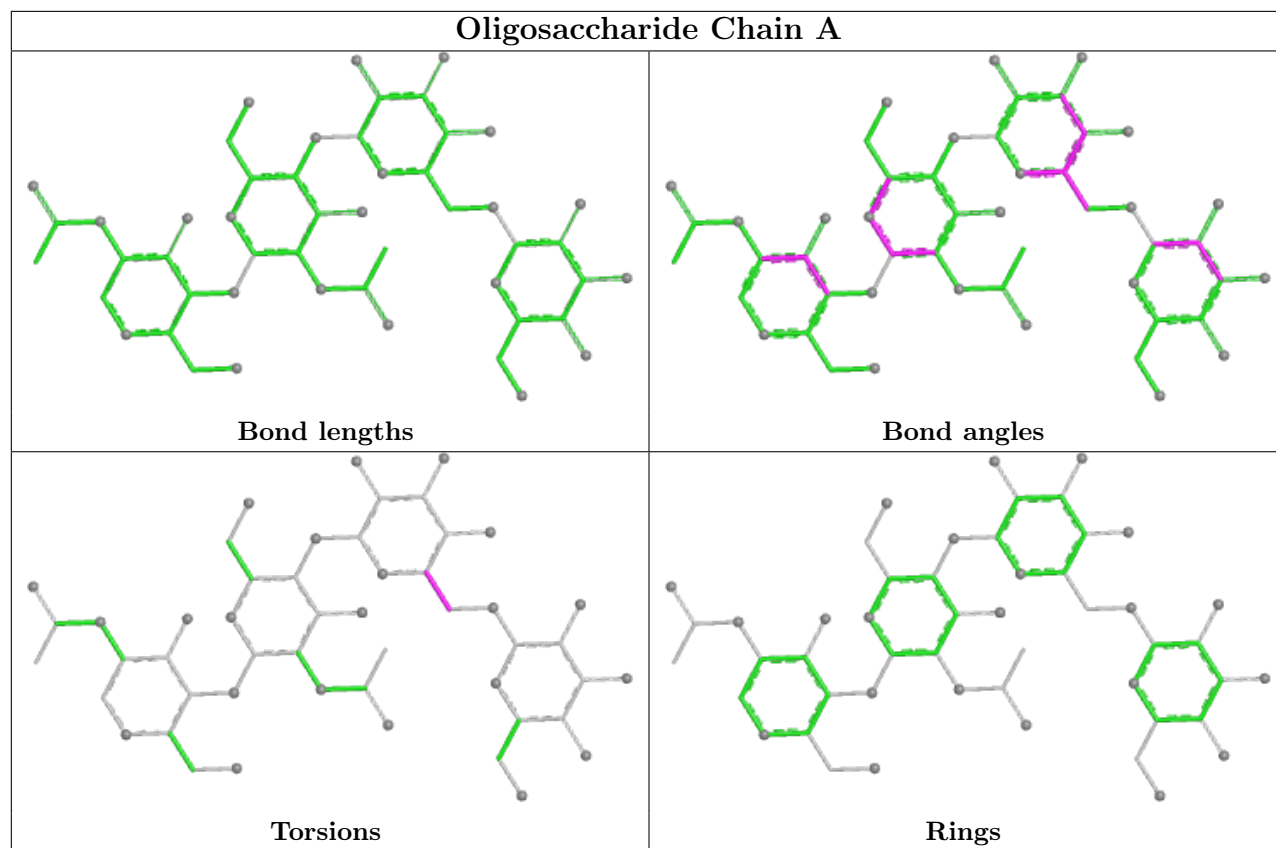
Mol	Chain	Res	Type	Atoms
2	A	3	BMA	C4-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	0	1

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

62 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	AAA	503	1	14,14,15	1.01	0	17,19,21	2.01	5 (29%)
3	SO4	AAA	505	-	4,4,4	0.43	0	6,6,6	0.15	0
3	SO4	BBB	1904	-	4,4,4	0.38	0	6,6,6	0.31	0
4	NAG	BBB	1903	1	14,14,15	0.96	0	17,19,21	1.55	3 (17%)
5	EDO	BBB	1910	-	3,3,3	0.38	0	2,2,2	0.55	0
6	B3P	AAA	524	-	18,18,18	0.33	0	21,23,23	1.06	1 (4%)
3	SO4	AAA	502	-	4,4,4	0.45	0	6,6,6	0.22	0
5	EDO	BBB	1919	-	3,3,3	0.22	0	2,2,2	0.69	0
5	EDO	BBB	1909	-	3,3,3	0.14	0	2,2,2	0.40	0
5	EDO	AAA	513	-	3,3,3	0.09	0	2,2,2	0.21	0
3	SO4	BBB	1902	-	4,4,4	0.45	0	6,6,6	0.37	0
5	EDO	BBB	1917	-	3,3,3	0.09	0	2,2,2	0.31	0
5	EDO	BBB	1908	-	3,3,3	0.75	0	2,2,2	1.20	0
6	B3P	BBB	1927	-	18,18,18	0.53	0	21,23,23	1.03	1 (4%)
3	SO4	BBB	1926	-	4,4,4	0.50	0	6,6,6	0.14	0
4	NAG	AAA	523	1	14,14,15	0.48	0	17,19,21	1.37	2 (11%)
5	EDO	AAA	510	-	3,3,3	0.52	0	2,2,2	0.57	0
3	SO4	AAA	518	-	4,4,4	0.54	0	6,6,6	0.14	0
5	EDO	BBB	1914	-	3,3,3	0.06	0	2,2,2	0.67	0
5	EDO	BBB	1911	-	3,3,3	0.06	0	2,2,2	0.10	0
5	EDO	AAA	516	-	3,3,3	0.14	0	2,2,2	0.39	0
5	EDO	AAA	511	-	3,3,3	0.12	0	2,2,2	0.13	0
5	EDO	AAA	517	-	3,3,3	0.20	0	2,2,2	0.19	0
5	EDO	BBB	1901	-	3,3,3	0.11	0	2,2,2	0.28	0
5	EDO	AAA	515[A]	-	3,3,3	0.16	0	2,2,2	0.26	0
5	EDO	BBB	1923	-	3,3,3	0.17	0	2,2,2	0.09	0
5	EDO	AAA	508	-	3,3,3	0.08	0	2,2,2	0.09	0
3	SO4	BBB	1924	-	4,4,4	0.43	0	6,6,6	0.18	0
5	EDO	AAA	515[B]	-	3,3,3	0.22	0	2,2,2	0.27	0
5	EDO	BBB	1915	-	3,3,3	0.73	0	2,2,2	0.65	0
5	EDO	BBB	1916	-	3,3,3	0.24	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	BBB	1921	-	3,3,3	0.20	0	2,2,2	0.25	0
5	EDO	AAA	512	-	3,3,3	0.02	0	2,2,2	0.19	0
5	EDO	BBB	1918	-	3,3,3	0.29	0	2,2,2	0.66	0
5	EDO	AAA	526	-	3,3,3	0.20	0	2,2,2	0.07	0
5	EDO	AAA	521	-	3,3,3	0.20	0	2,2,2	0.28	0
5	EDO	AAA	527	-	3,3,3	0.13	0	2,2,2	0.23	0
5	EDO	AAA	522	-	3,3,3	0.15	0	2,2,2	0.28	0
5	EDO	BBB	1928	-	3,3,3	0.10	0	2,2,2	0.08	0
5	EDO	AAA	509	-	3,3,3	0.20	0	2,2,2	0.19	0
5	EDO	BBB	1931	-	3,3,3	0.26	0	2,2,2	0.55	0
5	EDO	AAA	525[A]	-	3,3,3	0.08	0	2,2,2	0.17	0
5	EDO	BBB	1906[A]	-	3,3,3	0.29	0	2,2,2	0.51	0
3	SO4	AAA	519	-	4,4,4	0.41	0	6,6,6	0.12	0
5	EDO	BBB	1906[B]	-	3,3,3	0.28	0	2,2,2	0.21	0
5	EDO	AAA	520	-	3,3,3	0.45	0	2,2,2	0.47	0
5	EDO	AAA	525[B]	-	3,3,3	0.11	0	2,2,2	0.14	0
5	EDO	BBB	1930	-	3,3,3	0.07	0	2,2,2	0.20	0
5	EDO	BBB	1913[B]	-	3,3,3	0.13	0	2,2,2	0.23	0
5	EDO	AAA	506	-	3,3,3	0.11	0	2,2,2	0.25	0
5	EDO	BBB	1905	-	3,3,3	0.67	0	2,2,2	0.28	0
5	EDO	BBB	1912	-	3,3,3	0.23	0	2,2,2	0.43	0
5	EDO	BBB	1907	-	3,3,3	0.14	0	2,2,2	0.18	0
5	EDO	BBB	1913[A]	-	3,3,3	0.11	0	2,2,2	0.25	0
5	EDO	BBB	1920	-	3,3,3	0.30	0	2,2,2	0.15	0
3	SO4	AAA	501	-	4,4,4	0.44	0	6,6,6	0.32	0
5	EDO	BBB	1922	-	3,3,3	0.15	0	2,2,2	0.10	0
5	EDO	BBB	1929	-	3,3,3	0.35	0	2,2,2	0.33	0
5	EDO	AAA	514	-	3,3,3	0.24	0	2,2,2	0.21	0
5	EDO	AAA	504	-	3,3,3	0.19	0	2,2,2	0.34	0
3	SO4	BBB	1925	-	4,4,4	0.42	0	6,6,6	0.08	0
5	EDO	AAA	507	-	3,3,3	0.22	0	2,2,2	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
4	NAG	AAA	503	1	-	2/6/23/26	0/1/1/1
5	EDO	BBB	1910	-	-	0/1/1/1	-
4	NAG	BBB	1903	1	-	2/6/23/26	0/1/1/1
6	B3P	AAA	524	-	-	6/28/28/28	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	BBB	1919	-	-	0/1/1/1	-
5	EDO	BBB	1909	-	-	0/1/1/1	-
5	EDO	AAA	513	-	-	1/1/1/1	-
5	EDO	BBB	1917	-	-	0/1/1/1	-
5	EDO	BBB	1908	-	-	0/1/1/1	-
6	B3P	BBB	1927	-	-	3/28/28/28	-
4	NAG	AAA	523	1	-	2/6/23/26	0/1/1/1
5	EDO	AAA	510	-	-	1/1/1/1	-
5	EDO	BBB	1914	-	-	1/1/1/1	-
5	EDO	BBB	1911	-	-	0/1/1/1	-
5	EDO	AAA	516	-	-	0/1/1/1	-
5	EDO	AAA	511	-	-	0/1/1/1	-
5	EDO	AAA	517	-	-	1/1/1/1	-
5	EDO	BBB	1901	-	-	0/1/1/1	-
5	EDO	AAA	515[A]	-	-	0/1/1/1	-
5	EDO	BBB	1923	-	-	1/1/1/1	-
5	EDO	AAA	508	-	-	0/1/1/1	-
5	EDO	AAA	515[B]	-	-	0/1/1/1	-
5	EDO	BBB	1915	-	-	0/1/1/1	-
5	EDO	BBB	1916	-	-	1/1/1/1	-
5	EDO	BBB	1921	-	-	0/1/1/1	-
5	EDO	AAA	512	-	-	1/1/1/1	-
5	EDO	BBB	1918	-	-	1/1/1/1	-
5	EDO	AAA	526	-	-	1/1/1/1	-
5	EDO	AAA	521	-	-	1/1/1/1	-
5	EDO	AAA	527	-	-	1/1/1/1	-
5	EDO	AAA	522	-	-	0/1/1/1	-
5	EDO	BBB	1928	-	-	1/1/1/1	-
5	EDO	AAA	509	-	-	1/1/1/1	-
5	EDO	BBB	1931	-	-	1/1/1/1	-
5	EDO	AAA	525[A]	-	-	0/1/1/1	-
5	EDO	BBB	1906[A]	-	-	1/1/1/1	-
5	EDO	BBB	1906[B]	-	-	0/1/1/1	-
5	EDO	AAA	520	-	-	0/1/1/1	-
5	EDO	AAA	525[B]	-	-	1/1/1/1	-
5	EDO	BBB	1930	-	-	1/1/1/1	-
5	EDO	BBB	1913[B]	-	-	0/1/1/1	-
5	EDO	AAA	506	-	-	0/1/1/1	-
5	EDO	BBB	1905	-	-	0/1/1/1	-
5	EDO	BBB	1912	-	-	0/1/1/1	-
5	EDO	BBB	1907	-	-	0/1/1/1	-
5	EDO	BBB	1913[A]	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	BBB	1920	-	-	1/1/1/1	-
5	EDO	BBB	1929	-	-	1/1/1/1	-
5	EDO	BBB	1922	-	-	0/1/1/1	-
5	EDO	AAA	514	-	-	1/1/1/1	-
5	EDO	AAA	504	-	-	1/1/1/1	-
5	EDO	AAA	507	-	-	1/1/1/1	-

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AAA	503	NAG	C1-O5-C5	5.03	119.00	112.19
4	BBB	1903	NAG	O5-C5-C6	3.72	113.04	107.20
4	AAA	523	NAG	C4-C3-C2	-3.68	105.62	111.02
4	AAA	503	NAG	O5-C5-C6	3.55	112.77	107.20
4	BBB	1903	NAG	C1-O5-C5	3.20	116.53	112.19

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	AAA	524	B3P	N1-C4-C5-O4
6	AAA	524	B3P	C6-C4-C5-O4
6	AAA	524	B3P	O2-C10-C8-C11
6	BBB	1927	B3P	O2-C10-C8-N2
6	BBB	1927	B3P	O2-C10-C8-C11

There are no ring outliers.

15 monomers are involved in 25 short contacts:

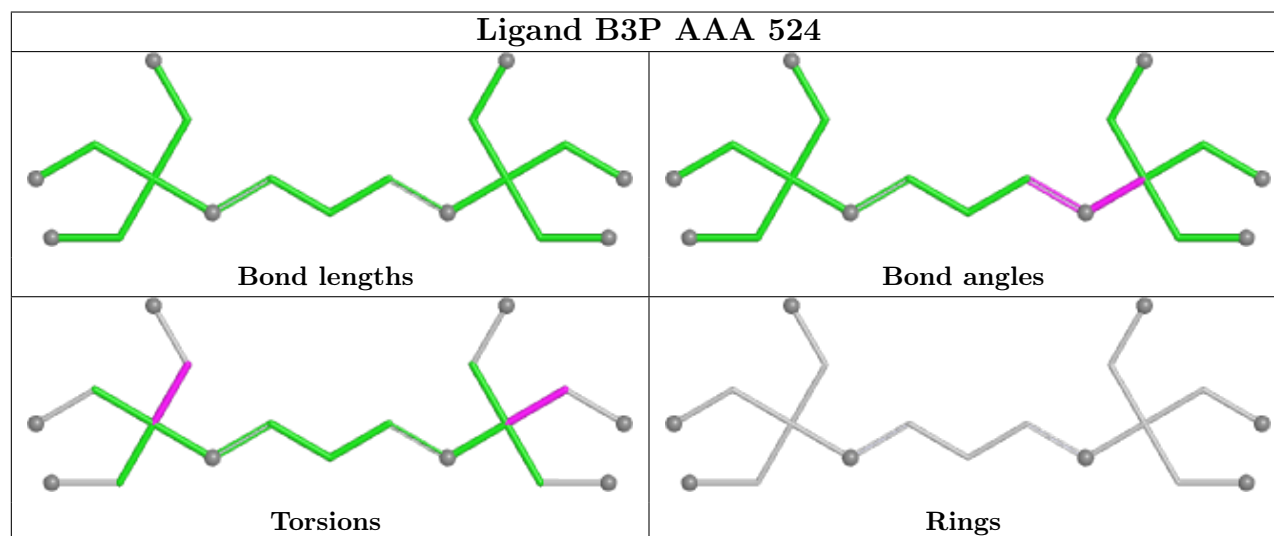
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	AAA	524	B3P	1	0
5	BBB	1919	EDO	3	0
5	BBB	1909	EDO	2	0
5	BBB	1917	EDO	1	0
5	AAA	517	EDO	4	0
5	AAA	515[B]	EDO	1	0
5	BBB	1915	EDO	4	0
5	BBB	1918	EDO	1	0
5	BBB	1906[A]	EDO	1	0
5	BBB	1906[B]	EDO	3	0

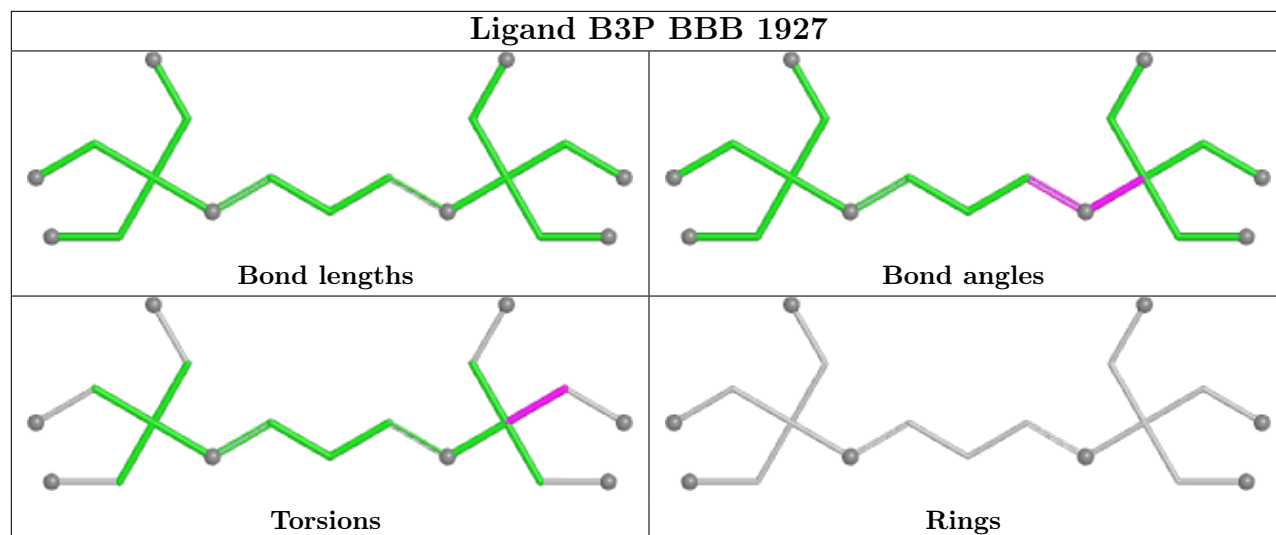
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AAA	520	EDO	1	0
5	AAA	525[B]	EDO	1	0
5	BBB	1930	EDO	1	0
5	BBB	1905	EDO	1	0
5	AAA	507	EDO	1	0

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 [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	AAA	497/497 (100%)	-0.43	2 (0%) 92 94	16, 24, 38, 59	3 (0%)
1	BBB	497/497 (100%)	-0.52	0 100 100	13, 19, 30, 40	5 (1%)
All	All	994/994 (100%)	-0.47	2 (0%) 95 95	13, 22, 34, 59	8 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	1	ALA	6.6
1	AAA	31	PHE	3.5

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

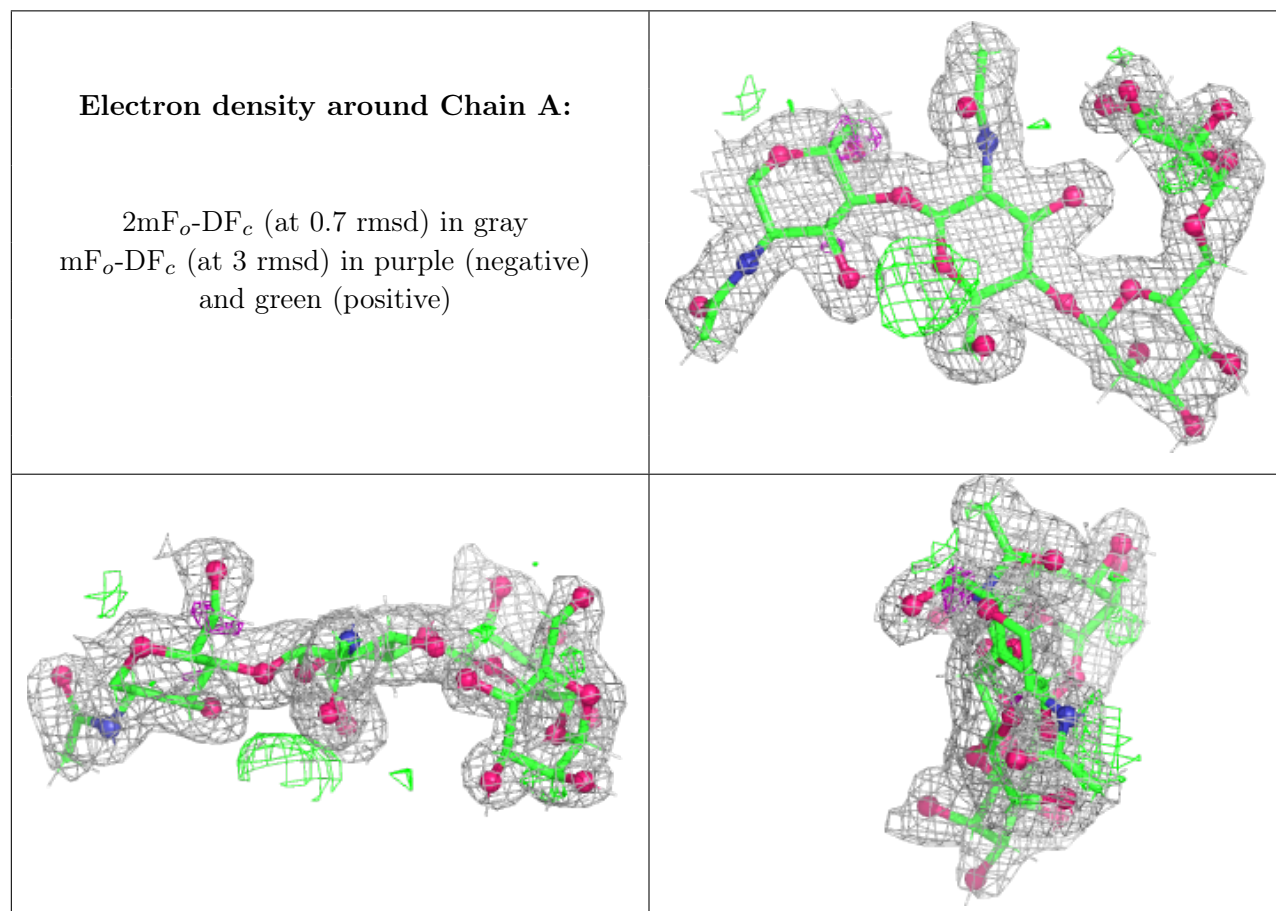
There are no non-standard protein/DNA/RNA residues in this entry.

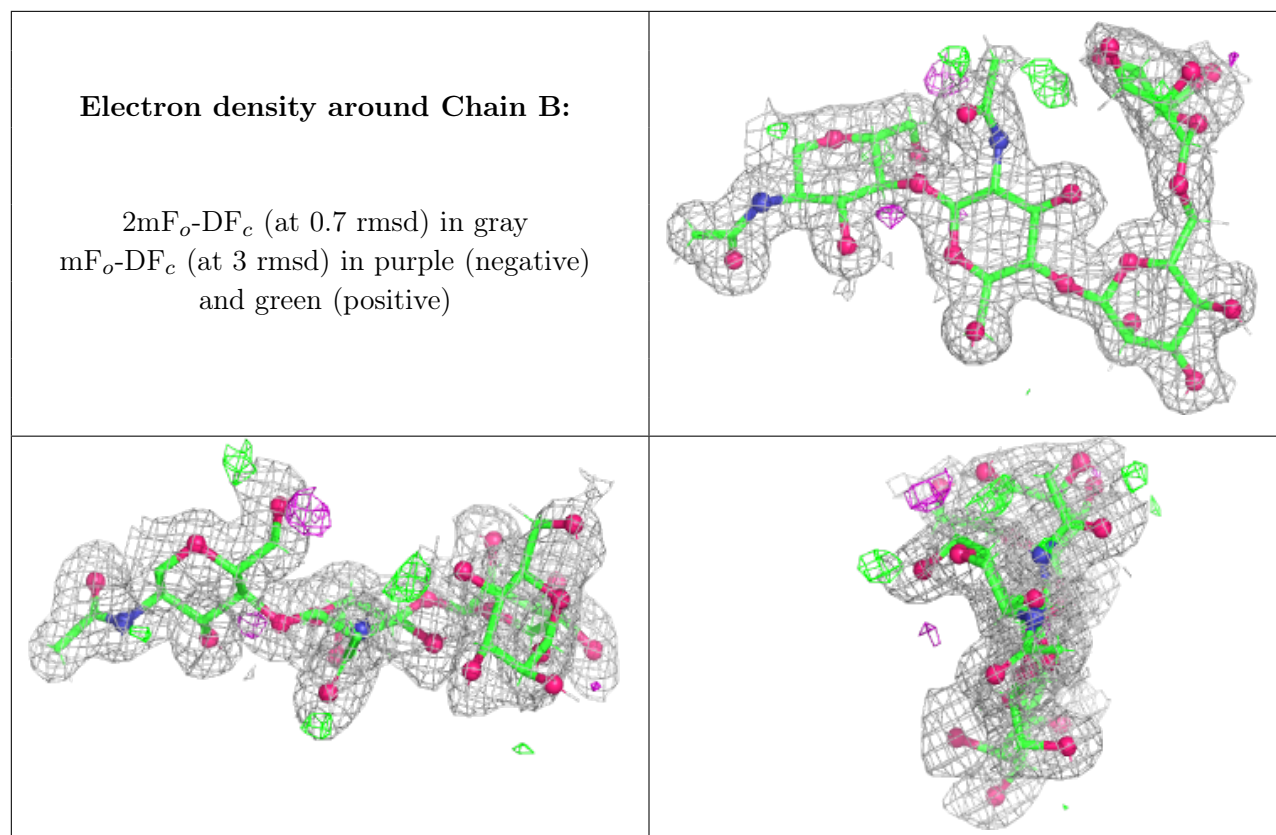
6.3 Carbohydrates [i](#)

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
2	BMA	B	3	11/12	0.75	0.14	47,54,59,60	3
2	MAN	B	4	11/12	0.79	0.16	64,72,76,77	4
2	MAN	A	4	11/12	0.86	0.12	25,33,36,36	22
2	BMA	A	3	11/12	0.88	0.18	44,52,56,60	4
2	NAG	B	1	14/15	0.93	0.08	20,24,28,28	2
2	NAG	B	2	14/15	0.94	0.08	22,30,35,38	2
2	NAG	A	1	14/15	0.95	0.12	25,28,37,43	2
2	NAG	A	2	14/15	0.95	0.07	27,30,34,39	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.





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	AAA	523	14/15	0.55	0.30	48,50,52,54	28
5	EDO	BBB	1928	4/4	0.70	0.27	35,37,39,40	10
4	NAG	BBB	1903	14/15	0.72	0.14	43,52,58,64	3
5	EDO	BBB	1912	4/4	0.73	0.13	48,53,53,55	1
5	EDO	BBB	1917	4/4	0.76	0.18	47,52,52,53	1
4	NAG	AAA	503	14/15	0.76	0.17	52,58,68,69	3
5	EDO	AAA	527	4/4	0.77	0.24	21,25,28,29	10
5	EDO	AAA	514	4/4	0.77	0.17	49,52,56,56	1
5	EDO	BBB	1914	4/4	0.79	0.13	40,41,43,45	1
5	EDO	AAA	517	4/4	0.82	0.15	22,23,26,26	10
5	EDO	BBB	1929	4/4	0.83	0.27	39,43,59,63	1
5	EDO	AAA	504	4/4	0.84	0.16	42,46,57,60	1
5	EDO	AAA	511	4/4	0.84	0.12	40,43,45,45	1
5	EDO	AAA	521	4/4	0.84	0.15	38,40,45,47	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	BBB	1906[B]	4/4	0.85	0.15	23,24,25,25	10
5	EDO	BBB	1901	4/4	0.85	0.11	55,59,62,64	1
5	EDO	BBB	1906[A]	4/4	0.85	0.15	22,23,23,24	10
5	EDO	BBB	1930	4/4	0.85	0.14	49,51,57,59	1
5	EDO	BBB	1908	4/4	0.86	0.12	25,32,36,36	1
5	EDO	AAA	510	4/4	0.86	0.15	39,42,43,44	1
5	EDO	BBB	1918	4/4	0.86	0.14	42,43,46,46	1
5	EDO	AAA	513	4/4	0.88	0.21	32,32,33,33	10
5	EDO	BBB	1916	4/4	0.88	0.10	39,42,43,45	1
5	EDO	BBB	1919	4/4	0.88	0.20	37,39,41,41	1
5	EDO	AAA	522	4/4	0.89	0.10	54,57,59,60	1
5	EDO	BBB	1907	4/4	0.89	0.22	38,43,48,49	1
5	EDO	BBB	1921	4/4	0.90	0.09	33,41,42,42	1
3	SO4	AAA	518	5/5	0.90	0.16	30,35,38,40	5
5	EDO	AAA	526	4/4	0.91	0.09	58,59,59,60	1
5	EDO	BBB	1910	4/4	0.91	0.08	32,38,39,40	1
3	SO4	BBB	1925	5/5	0.91	0.16	42,43,45,47	5
5	EDO	AAA	512	4/4	0.92	0.11	59,61,62,62	1
5	EDO	BBB	1922	4/4	0.92	0.11	39,43,45,46	1
5	EDO	AAA	509	4/4	0.92	0.15	30,35,43,43	1
3	SO4	AAA	505	5/5	0.92	0.12	34,35,37,41	5
3	SO4	BBB	1926	5/5	0.92	0.14	34,46,51,53	5
5	EDO	BBB	1915	4/4	0.93	0.13	28,32,37,37	1
3	SO4	BBB	1924	5/5	0.93	0.18	34,38,39,39	5
5	EDO	AAA	508	4/4	0.93	0.10	37,47,48,48	1
5	EDO	AAA	515[A]	4/4	0.93	0.15	24,26,28,29	10
5	EDO	AAA	515[B]	4/4	0.93	0.15	30,30,32,32	10
5	EDO	BBB	1911	4/4	0.93	0.11	53,53,53,54	1
3	SO4	AAA	519	5/5	0.93	0.15	37,41,41,47	5
5	EDO	BBB	1913[A]	4/4	0.93	0.13	25,26,29,30	10
5	EDO	BBB	1913[B]	4/4	0.93	0.13	36,37,38,38	10
5	EDO	AAA	520	4/4	0.93	0.10	18,19,21,21	10
5	EDO	AAA	525[A]	4/4	0.94	0.13	34,35,36,36	10
5	EDO	AAA	525[B]	4/4	0.94	0.13	31,34,34,35	10
5	EDO	AAA	507	4/4	0.94	0.09	28,34,38,38	1
5	EDO	BBB	1909	4/4	0.94	0.08	31,38,44,45	1
5	EDO	AAA	506	4/4	0.95	0.12	41,44,44,45	1
5	EDO	AAA	516	4/4	0.95	0.12	37,39,39,40	1
5	EDO	BBB	1931	4/4	0.95	0.12	20,30,40,40	1
5	EDO	BBB	1923	4/4	0.96	0.20	39,41,41,42	1
6	B3P	AAA	524	19/19	0.96	0.08	18,21,31,47	5
5	EDO	BBB	1905	4/4	0.97	0.07	19,20,21,21	1

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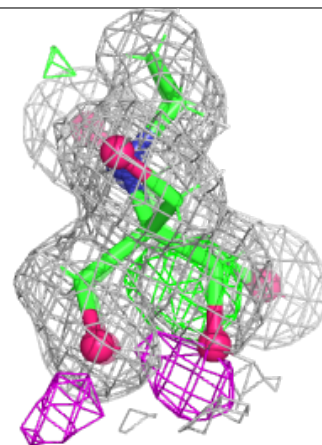
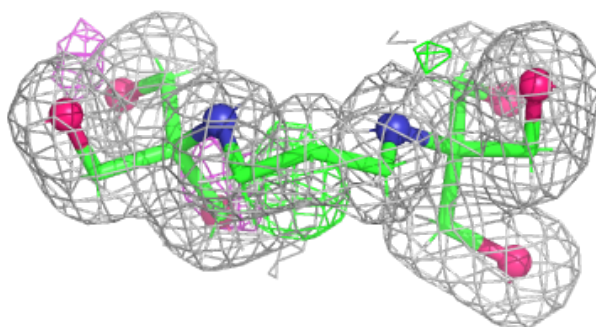
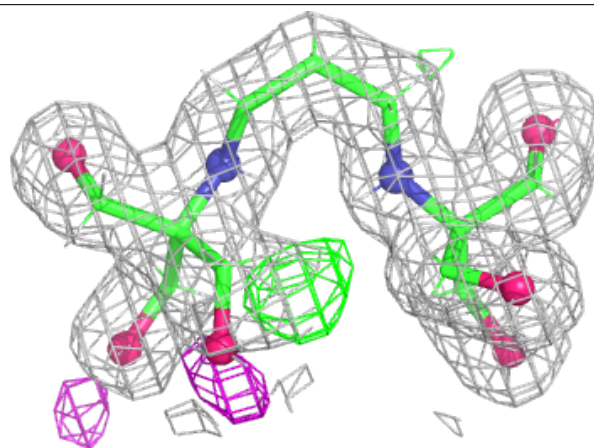
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	BBB	1920	4/4	0.97	0.07	28,30,33,35	1
6	B3P	BBB	1927	19/19	0.97	0.07	14,19,30,30	5
3	SO4	BBB	1904	5/5	0.99	0.05	31,31,32,33	0
3	SO4	AAA	502	5/5	0.99	0.06	36,38,40,40	0
3	SO4	AAA	501	5/5	0.99	0.07	24,29,33,37	0
3	SO4	BBB	1902	5/5	0.99	0.07	24,25,29,34	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.

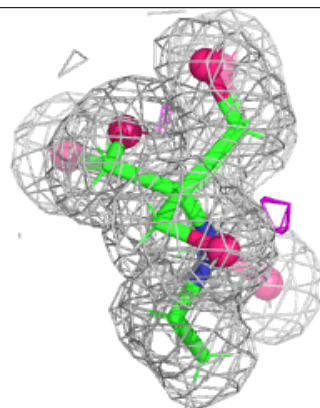
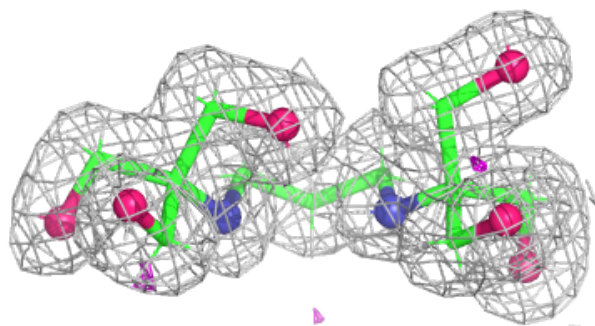
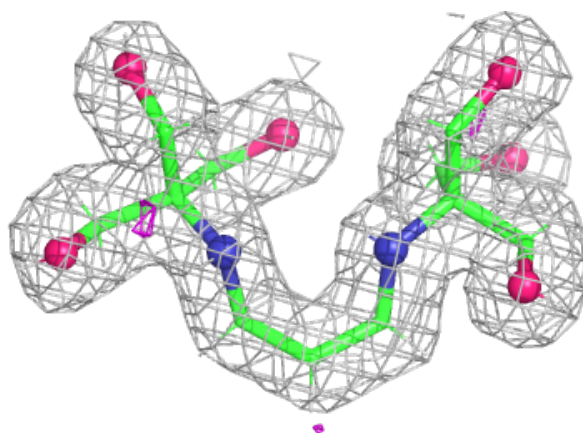
Electron density around B3P AAA 524:

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 B3P BBB 1927:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.