wwPDB X-ray Structure Validation Summary Report (i)

Jan 13, 2024 – 05:59 pm GMT

PDB ID	:	6YUT
Title	:	Structure of recombinant human beta-glucocerebrosidase in complex with N-acyl functionalised cyclophellitol aziridine
Authors	:	Rowland, R.J.; Davies, G.J.
Deposited on	:	2020-04-27
Resolution	:	1.76 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

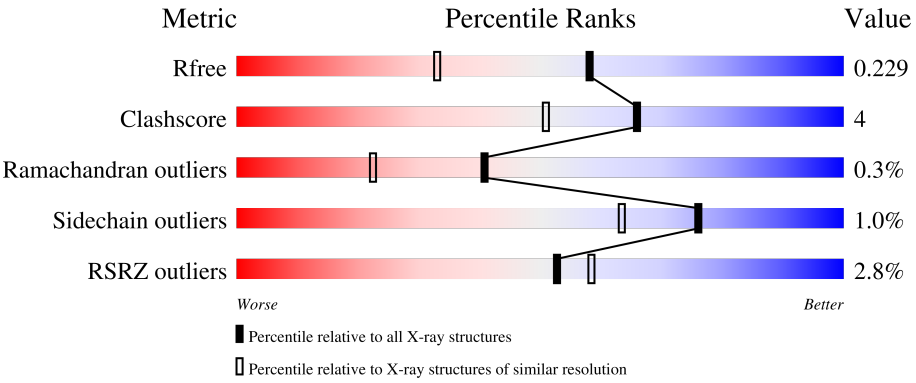
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	497	2% 95% 5%
1	BBB	497	3% 92% 7%
2	A	2	100%
2	B	2	50% 50%

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	NAG	BBB	503	-	-	-	X
3	NAG	BBB	504	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 16977 atoms, of which 8031 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	494	Total	C	H	N	O	S	212	7	0
			7819	2538	3871	677	717	16			
1	BBB	497	Total	C	H	N	O	S	211	4	0
			7815	2542	3866	673	717	17			

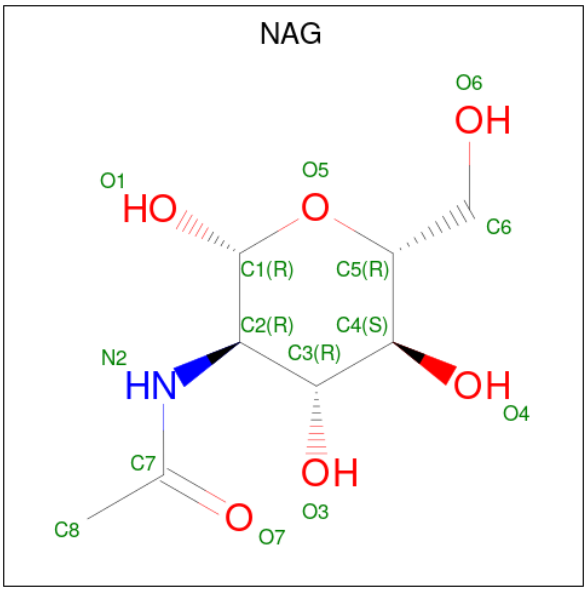
There are 2 discrepancies between the modelled and reference sequences:

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.

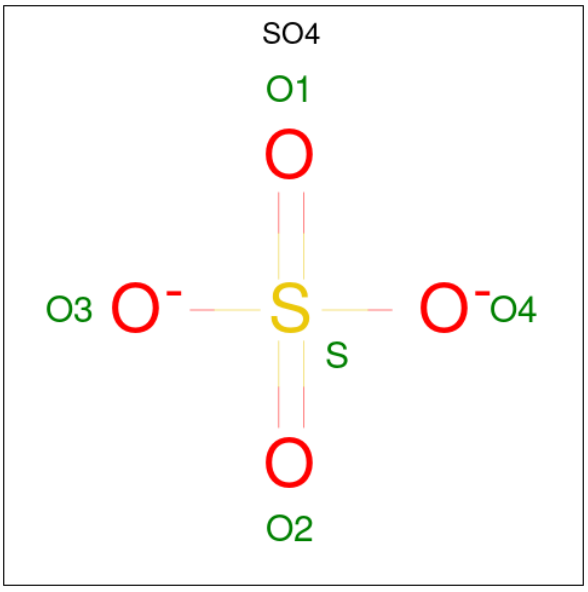
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	2	Total	C	H	N	O	5	0	0
			55	16	27	2	10			
2	B	2	Total	C	H	N	O	5	0	0
			55	16	27	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



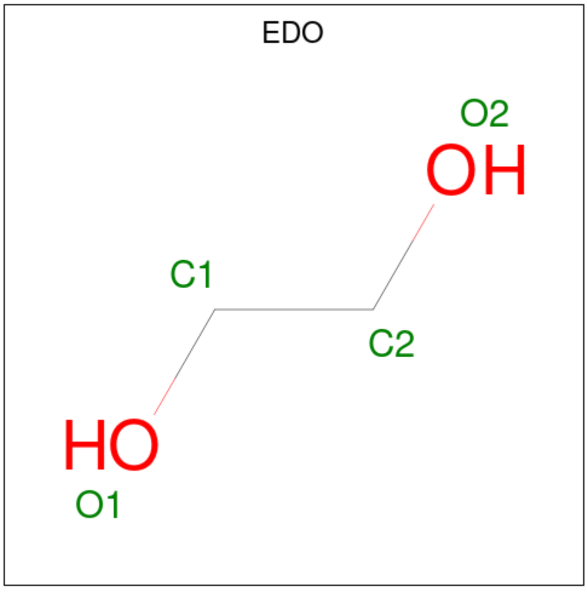
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
3	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
3	BBB	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
3	BBB	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- 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 10 2 6 2	1	0
5	AAA	1	Total C H O 10 2 6 2	1	0
5	AAA	1	Total C H O 10 2 6 2	1	0
5	AAA	1	Total C H O 10 2 6 2	1	0
5	AAA	1	Total C H O 10 2 6 2	1	0
5	AAA	1	Total C H O 10 2 6 2	1	0
5	AAA	1	Total C H O 10 2 6 2	1	0
5	AAA	1	Total C H O 10 2 6 2	1	0
5	AAA	1	Total C H O 10 2 6 2	1	0
5	BBB	1	Total C H O 10 2 6 2	1	0
5	BBB	1	Total C H O 10 2 6 2	1	0
5	BBB	1	Total C H O 10 2 6 2	1	0
5	BBB	1	Total C H O 10 2 6 2	1	0
5	BBB	1	Total C H O 10 2 6 2	1	0

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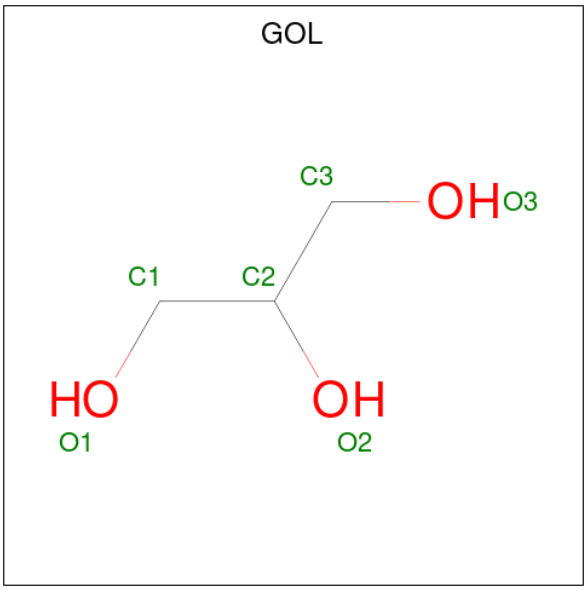
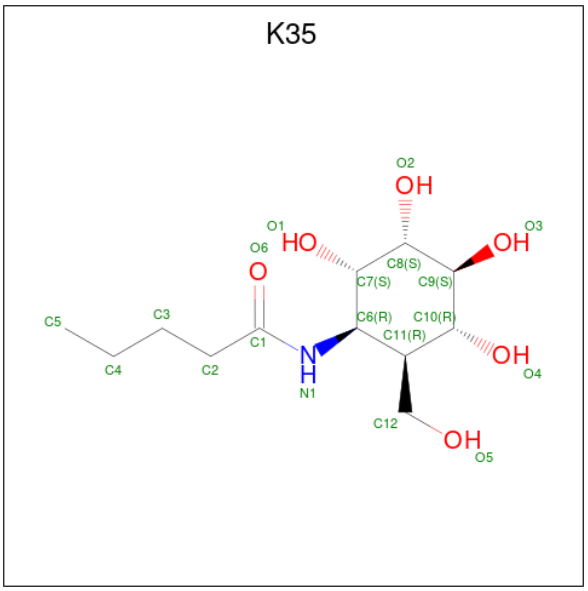
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
5	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
5	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
5	BBB	1	Total	C	H	O	1	0
			10	2	6	2		

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



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	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		

- Molecule 7 is {N}-[(1 {R},2 {R},3 {R},4 {S},5 {S},6 {S})-2-(hydroxymethyl)-3,4,5,6-tetrakis(oxidanyl)cyclohexyl]pentanamide (three-letter code: K35) (formula: $C_{12}H_{23}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	AAA	1	Total	C	H	N	O	4	0
			40	12	22	1	5		
7	BBB	1	Total	C	H	N	O	4	0
			40	12	22	1	5		

- Molecule 8 is water.

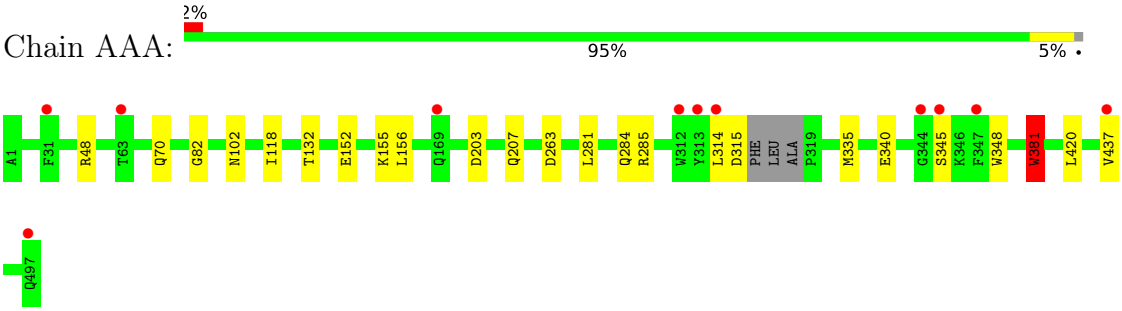
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	360	Total	O	0	0
			360	360		
8	BBB	375	Total	O	0	0
			375	375		

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.

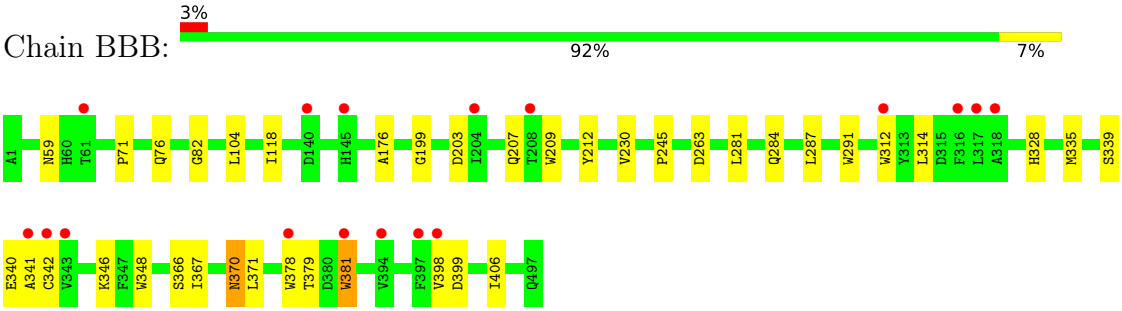
• Molecule 1: Glucosylceramidase

Chain AAA:



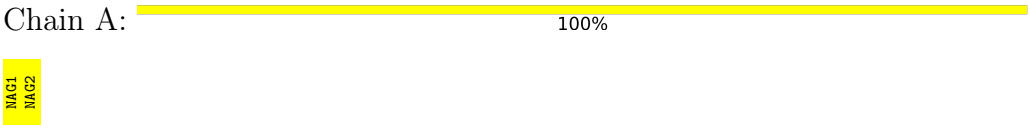
• Molecule 1: Glucosylceramidase

Chain BBB:



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

Chain A:



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

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	110.70Å 285.52Å 91.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.63 – 1.76 47.59 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.63-1.76) 99.8 (47.59-1.76)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.183 , 0.208 0.203 , 0.229	Depositor DCC
R_{free} test set	7160 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 39.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16977	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, K35, SO4, EDO

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	1/4067 (0.0%)	0.75	0/5545
1	BBB	0.69	1/4070 (0.0%)	0.77	0/5552
All	All	0.69	2/8137 (0.0%)	0.76	0/11097

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	340	GLU	CD-OE2	15.42	1.42	1.25
1	AAA	340	GLU	CD-OE2	14.70	1.41	1.25

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	AAA	3948	3871	3836	17	0
1	BBB	3949	3866	3836	42	0
2	A	28	27	25	0	0
2	B	28	27	25	0	0
3	AAA	28	28	26	1	0
3	BBB	28	28	26	1	0
4	AAA	30	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BBB	40	0	0	0	0
5	AAA	36	54	54	1	0
5	BBB	36	54	54	5	0
6	AAA	18	24	24	2	0
6	BBB	6	8	8	0	0
7	AAA	18	22	0	0	0
7	BBB	18	22	0	0	0
8	AAA	360	0	0	4	0
8	BBB	375	0	0	3	0
All	All	8946	8031	7914	64	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.

The worst 5 of 64 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:342[A]:CYS:SG	1:BBB:398:VAL:HG21	2.09	0.93
1:BBB:339:SER:HA	1:BBB:379:THR:HG22	1.64	0.79
1:AAA:102[A]:ASN:OD1	8:AAA:601:HOH:O	2.02	0.78
1:AAA:207:GLN:NE2	1:AAA:263:ASP:OD1	2.17	0.73
4:AAA:509:SO4:O3	8:AAA:602:HOH:O	2.07	0.72

There are no symmetry-related clashes.

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	497/497 (100%)	479 (96%)	16 (3%)	2 (0%)	34 17
1	BBB	499/497 (100%)	478 (96%)	20 (4%)	1 (0%)	47 29
All	All	996/994 (100%)	957 (96%)	36 (4%)	3 (0%)	41 22

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	425/424 (100%)	421 (99%)	4 (1%)	78	67
1	BBB	424/424 (100%)	420 (99%)	4 (1%)	78	67
All	All	849/848 (100%)	841 (99%)	8 (1%)	76	67

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

Mol	Chain	Res	Type
1	BBB	381	TRP
1	BBB	370	ASN
1	BBB	59	ASN
1	AAA	420	LEU
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 (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

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	$\#\|Z\| > 2$
2	NAG	A	1	2,1	14,14,15	0.47	0	17,19,21	1.18	2 (11%)
2	NAG	A	2	2	14,14,15	0.46	0	17,19,21	0.86	1 (5%)
2	NAG	B	1	2,1	14,14,15	0.57	0	17,19,21	0.85	0
2	NAG	B	2	2	14,14,15	0.57	0	17,19,21	1.30	4 (23%)

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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	2/6/23/26	0/1/1/1
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	NAG	O5-C1-C2	-2.82	106.84	111.29
2	A	1	NAG	O5-C5-C6	2.69	111.42	107.20
2	B	2	NAG	O5-C5-C6	2.54	111.18	107.20
2	B	2	NAG	O4-C4-C5	2.27	114.94	109.30
2	B	2	NAG	C3-C4-C5	-2.05	106.58	110.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

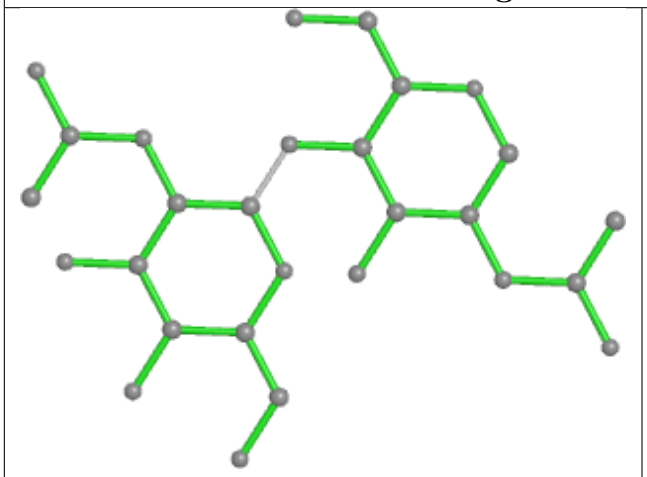
Mol	Chain	Res	Type	Atoms
2	A	2	NAG	O5-C5-C6-O6
2	A	2	NAG	C4-C5-C6-O6

There are no ring outliers.

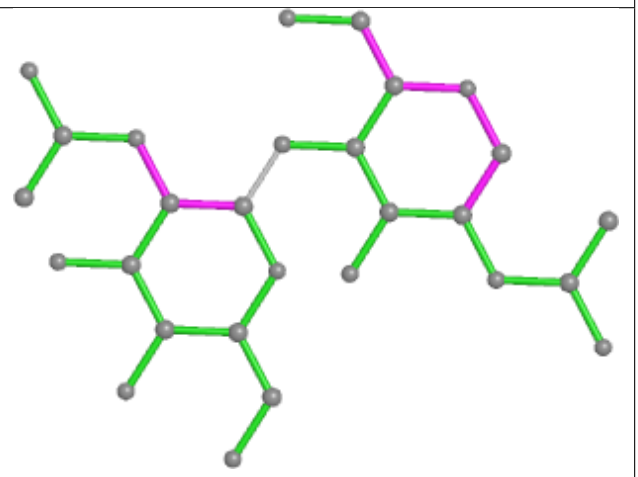
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

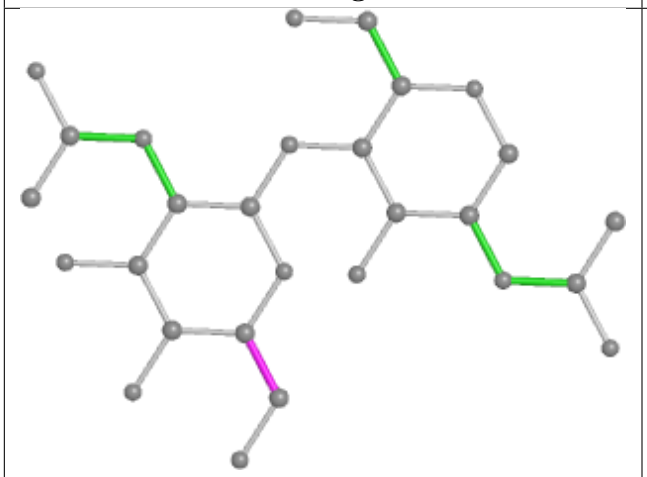
Oligosaccharide Chain A



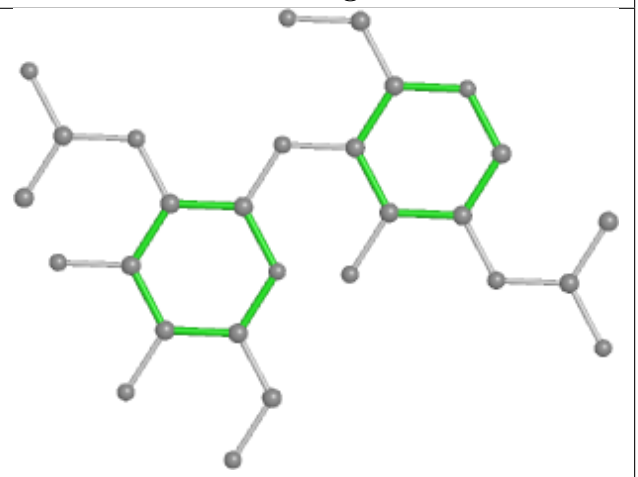
Bond lengths



Bond angles

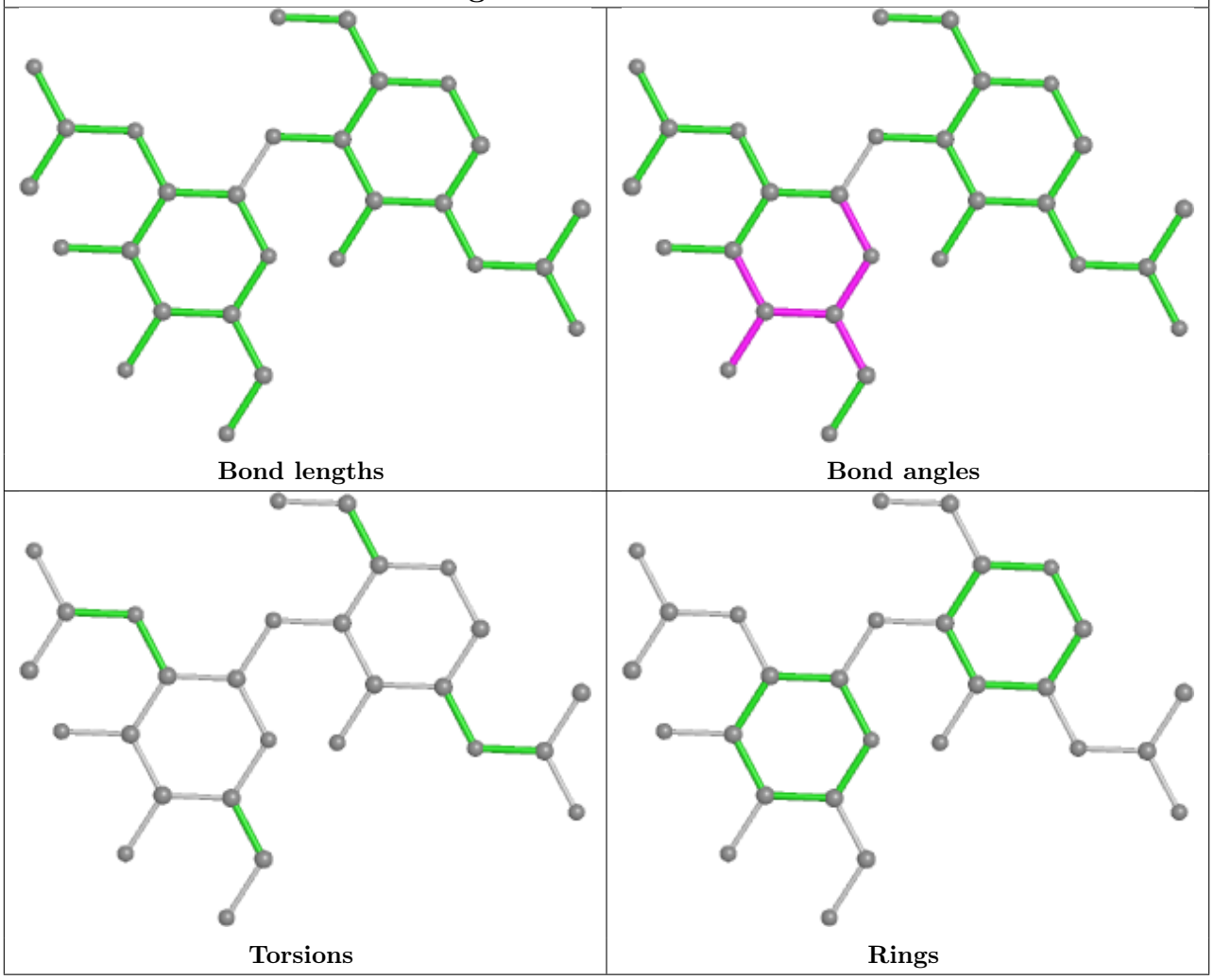


Torsions



Rings

Oligosaccharide Chain B



5.6 Ligand geometry (i)

42 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EDO	AAA	514	-	3,3,3	0.24	0	2,2,2	0.32	0
5	EDO	BBB	518	-	3,3,3	0.16	0	2,2,2	0.40	0
3	NAG	BBB	504	1	14,14,15	0.75	1 (7%)	17,19,21	1.74	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	K35	AAA	523	1	18,18,19	0.71	0	23,24,26	1.02	2 (8%)
4	SO4	AAA	507	-	4,4,4	0.38	0	6,6,6	0.08	0
7	K35	BBB	523	1	18,18,19	0.70	0	23,24,26	1.38	3 (13%)
5	EDO	AAA	518	-	3,3,3	0.11	0	2,2,2	0.39	0
4	SO4	AAA	509	-	4,4,4	0.35	0	6,6,6	0.09	0
5	EDO	BBB	513	-	3,3,3	0.15	0	2,2,2	0.21	0
5	EDO	AAA	517	-	3,3,3	0.22	0	2,2,2	0.42	0
4	SO4	BBB	511	-	4,4,4	0.35	0	6,6,6	0.11	0
5	EDO	AAA	512	-	3,3,3	0.13	0	2,2,2	0.22	0
5	EDO	BBB	516	-	3,3,3	0.07	0	2,2,2	0.34	0
3	NAG	AAA	503	1	14,14,15	0.73	0	17,19,21	0.94	0
5	EDO	AAA	519	-	3,3,3	0.08	0	2,2,2	0.14	0
5	EDO	BBB	514	-	3,3,3	0.10	0	2,2,2	0.18	0
4	SO4	AAA	505	-	4,4,4	0.47	0	6,6,6	0.19	0
4	SO4	BBB	507	-	4,4,4	0.39	0	6,6,6	0.12	0
5	EDO	AAA	516	-	3,3,3	0.08	0	2,2,2	0.07	0
4	SO4	AAA	508	-	4,4,4	0.40	0	6,6,6	0.12	0
4	SO4	BBB	508	-	4,4,4	0.37	0	6,6,6	0.14	0
4	SO4	BBB	505	-	4,4,4	0.40	0	6,6,6	0.15	0
5	EDO	BBB	517	-	3,3,3	0.22	0	2,2,2	0.45	0
5	EDO	AAA	515	-	3,3,3	0.05	0	2,2,2	0.11	0
4	SO4	BBB	512	-	4,4,4	0.37	0	6,6,6	0.11	0
6	GOL	BBB	522	-	5,5,5	0.15	0	5,5,5	0.41	0
4	SO4	AAA	506	-	4,4,4	0.33	0	6,6,6	0.22	0
5	EDO	BBB	519	-	3,3,3	0.14	0	2,2,2	0.11	0
6	GOL	AAA	522	-	5,5,5	0.11	0	5,5,5	0.30	0
5	EDO	BBB	521	-	3,3,3	0.07	0	2,2,2	0.23	0
3	NAG	BBB	503	1	14,14,15	0.49	0	17,19,21	1.31	2 (11%)
3	NAG	AAA	504	1	14,14,15	0.28	0	17,19,21	0.75	1 (5%)
5	EDO	BBB	520	-	3,3,3	0.05	0	2,2,2	0.50	0
5	EDO	BBB	515	-	3,3,3	0.10	0	2,2,2	0.41	0
5	EDO	AAA	513	-	3,3,3	0.09	0	2,2,2	0.27	0
4	SO4	BBB	506	-	4,4,4	0.40	0	6,6,6	0.13	0
6	GOL	AAA	520	-	5,5,5	0.14	0	5,5,5	0.48	0
4	SO4	BBB	510	-	4,4,4	0.36	0	6,6,6	0.10	0
4	SO4	BBB	509	-	4,4,4	0.37	0	6,6,6	0.05	0
4	SO4	AAA	510	-	4,4,4	0.37	0	6,6,6	0.10	0
6	GOL	AAA	521	-	5,5,5	0.21	0	5,5,5	0.57	0
5	EDO	AAA	511	-	3,3,3	0.05	0	2,2,2	0.11	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	AAA	514	-	-	1/1/1/1	-
5	EDO	BBB	518	-	-	1/1/1/1	-
3	NAG	BBB	504	1	-	2/6/23/26	0/1/1/1
7	K35	AAA	523	1	-	2/10/30/34	0/1/1/1
7	K35	BBB	523	1	-	3/10/30/34	0/1/1/1
5	EDO	AAA	518	-	-	1/1/1/1	-
5	EDO	BBB	513	-	-	0/1/1/1	-
5	EDO	AAA	517	-	-	1/1/1/1	-
5	EDO	AAA	512	-	-	0/1/1/1	-
5	EDO	BBB	516	-	-	1/1/1/1	-
3	NAG	AAA	503	1	-	2/6/23/26	0/1/1/1
5	EDO	AAA	519	-	-	0/1/1/1	-
5	EDO	BBB	514	-	-	1/1/1/1	-
5	EDO	AAA	516	-	-	1/1/1/1	-
5	EDO	BBB	517	-	-	1/1/1/1	-
5	EDO	AAA	515	-	-	0/1/1/1	-
6	GOL	BBB	522	-	-	0/4/4/4	-
5	EDO	BBB	519	-	-	1/1/1/1	-
6	GOL	AAA	522	-	-	2/4/4/4	-
5	EDO	BBB	521	-	-	0/1/1/1	-
3	NAG	BBB	503	1	-	2/6/23/26	0/1/1/1
3	NAG	AAA	504	1	-	0/6/23/26	0/1/1/1
5	EDO	BBB	520	-	-	0/1/1/1	-
5	EDO	BBB	515	-	-	1/1/1/1	-
5	EDO	AAA	513	-	-	1/1/1/1	-
6	GOL	AAA	520	-	-	2/4/4/4	-
6	GOL	AAA	521	-	-	0/4/4/4	-
5	EDO	AAA	511	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	504	NAG	C1-C2	2.18	1.55	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	BBB	504	NAG	C1-O5-C5	4.23	117.93	112.19
7	BBB	523	K35	C11-C6-N1	3.69	115.95	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	BBB	504	NAG	C2-N2-C7	3.59	128.01	122.90
3	BBB	503	NAG	C2-N2-C7	3.52	127.91	122.90
3	BBB	504	NAG	C8-C7-N2	3.21	121.54	116.10

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	AAA	520	GOL	C1-C2-C3-O3
6	AAA	522	GOL	C1-C2-C3-O3
6	AAA	522	GOL	O2-C2-C3-O3
7	BBB	523	K35	C1-C2-C3-C4
3	BBB	503	NAG	C1-C2-N2-C7

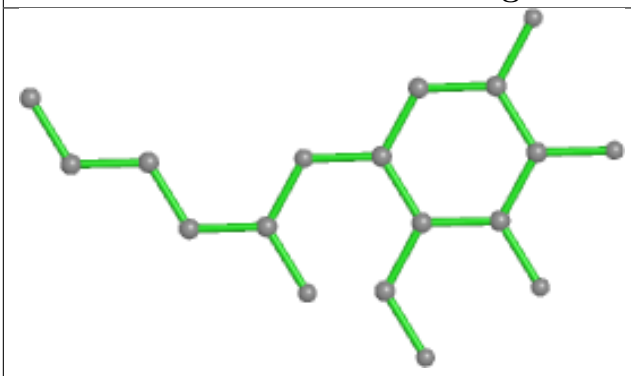
There are no ring outliers.

9 monomers are involved in 11 short contacts:

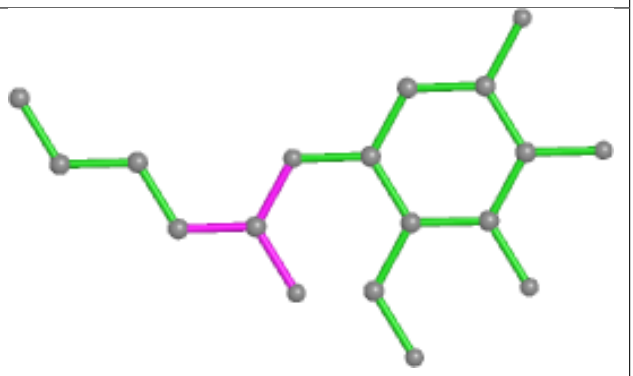
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AAA	514	EDO	1	0
3	BBB	504	NAG	1	0
4	AAA	509	SO4	1	0
3	AAA	503	NAG	1	0
5	BBB	519	EDO	1	0
5	BBB	521	EDO	3	0
5	BBB	520	EDO	1	0
6	AAA	520	GOL	1	0
6	AAA	521	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

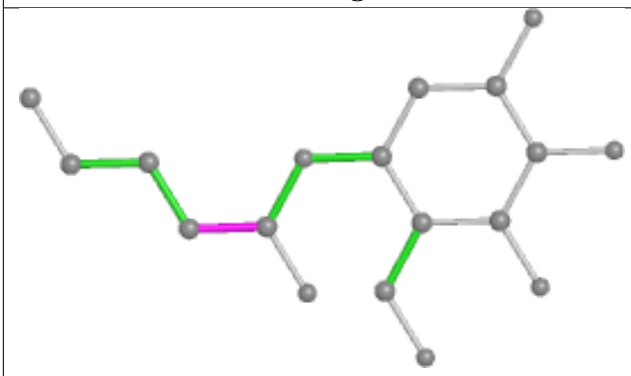
Ligand K35 AAA 523



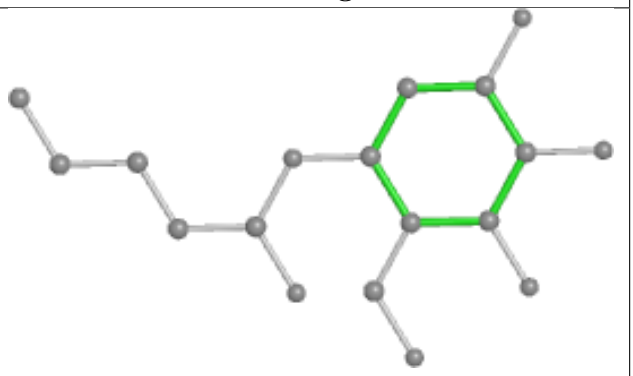
Bond lengths



Bond angles

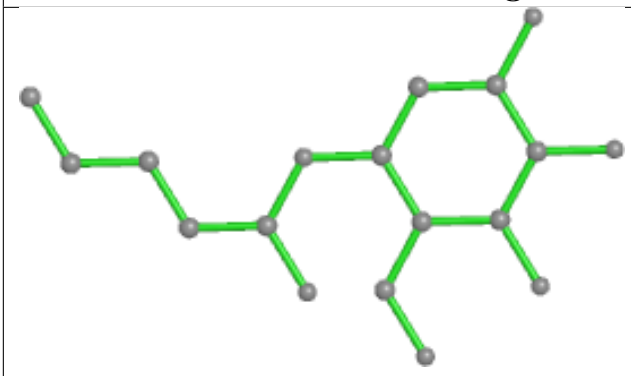


Torsions

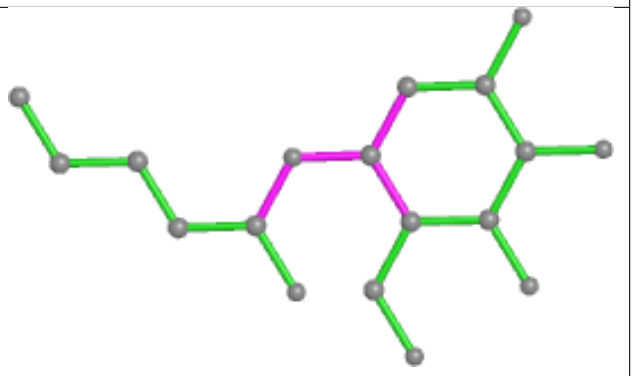


Rings

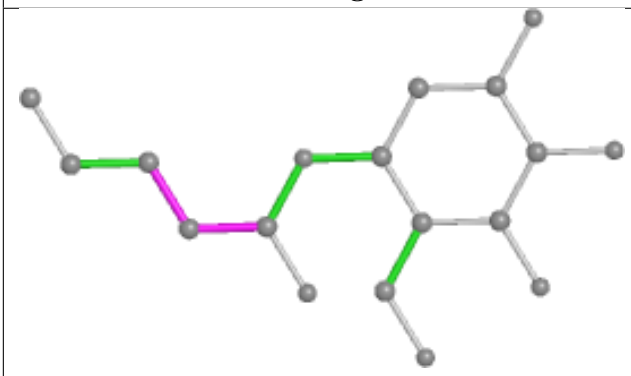
Ligand K35 BBB 523



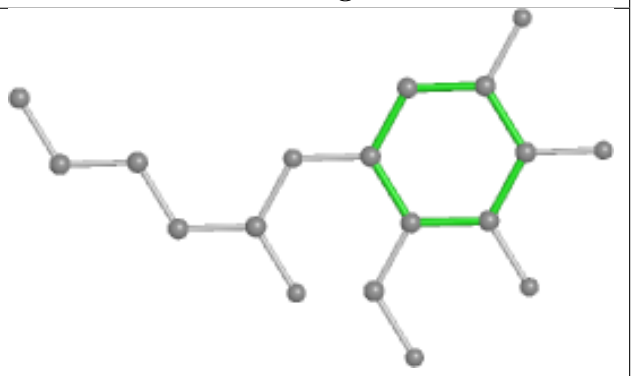
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	494/497 (99%)	-0.02	11 (2%)	62	69	21, 29, 50, 87	5 (1%)
1	BBB	497/497 (100%)	0.03	17 (3%)	45	51	20, 29, 49, 70	2 (0%)
All	All	991/994 (99%)	0.00	28 (2%)	53	58	20, 29, 50, 87	7 (0%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	345	SER	12.4
1	AAA	314	LEU	4.4
1	BBB	397	PHE	4.4
1	BBB	378	TRP	3.5
1	AAA	312	TRP	3.4

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

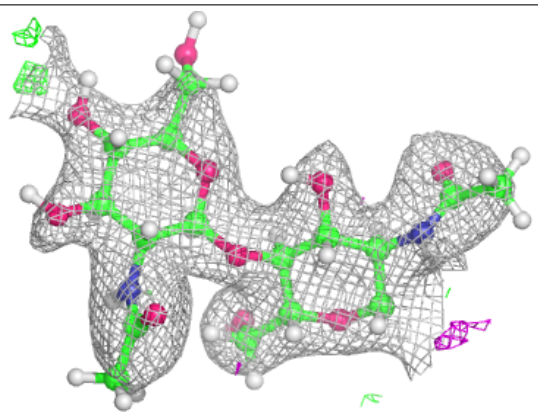
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

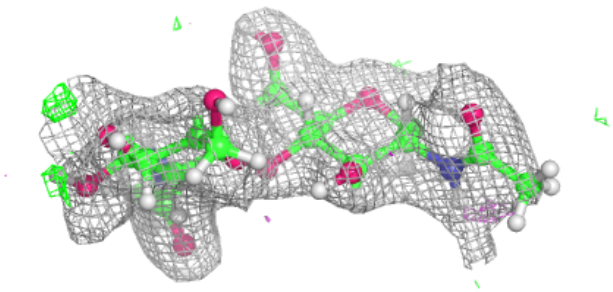
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	B	2	14/15	0.76	0.19	49,60,67,69	3
2	NAG	A	2	14/15	0.83	0.19	51,63,72,77	3
2	NAG	A	1	14/15	0.94	0.11	36,40,44,49	2
2	NAG	B	1	14/15	0.95	0.08	32,36,39,44	2

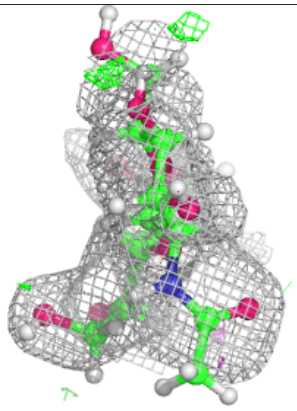
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

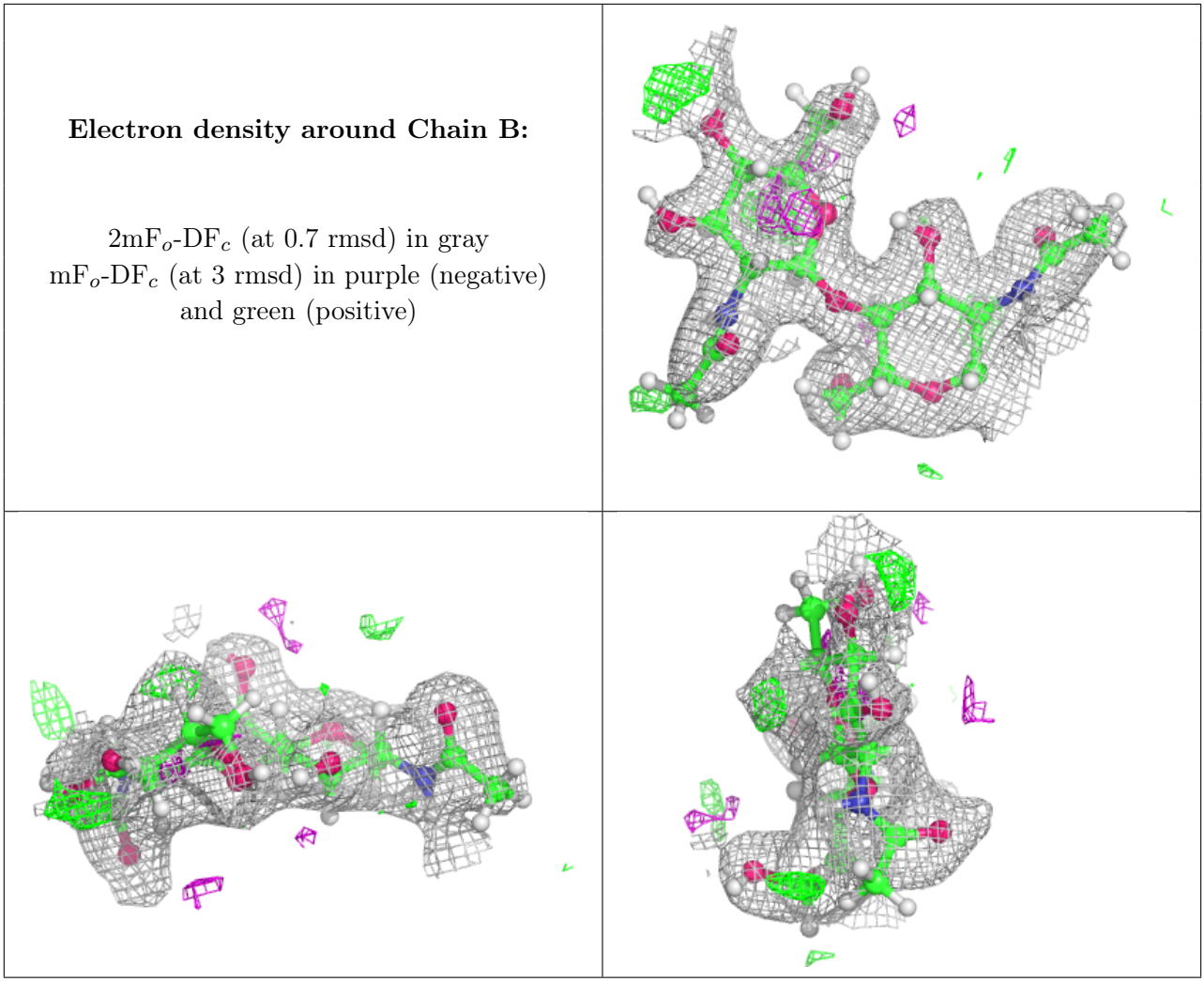






Electron density around Chain B:

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



6.4 Ligands

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	BBB	504	14/15	0.32	0.44	97,113,117,120	3
5	EDO	AAA	517	4/4	0.35	0.27	63,66,67,68	1
5	EDO	BBB	518	4/4	0.50	0.15	70,71,72,73	1
5	EDO	BBB	515	4/4	0.59	0.28	68,72,72,73	1
3	NAG	AAA	504	14/15	0.63	0.24	57,59,59,60	28
6	GOL	AAA	521	6/6	0.64	0.15	54,58,62,62	2
5	EDO	BBB	514	4/4	0.65	0.29	79,81,82,83	1
3	NAG	AAA	503	14/15	0.67	0.19	53,66,73,78	3
3	NAG	BBB	503	14/15	0.72	0.42	90,99,106,108	3

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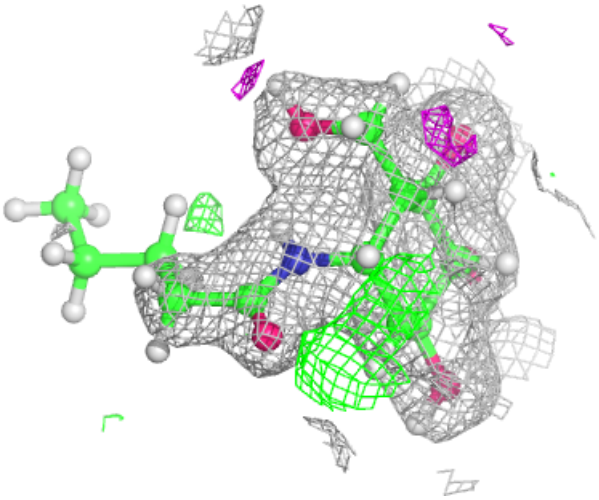
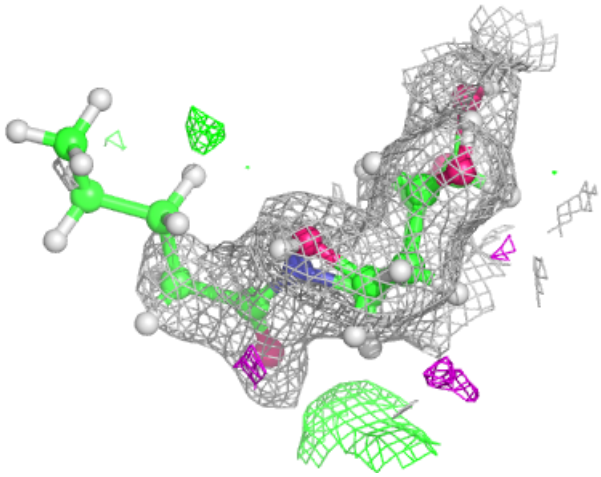
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	AAA	516	4/4	0.73	0.19	51,56,59,60	1
5	EDO	BBB	516	4/4	0.74	0.13	63,66,67,68	1
5	EDO	BBB	520	4/4	0.75	0.19	51,54,56,57	1
4	SO4	BBB	512	5/5	0.76	0.26	37,39,44,46	5
5	EDO	AAA	512	4/4	0.76	0.14	59,60,62,62	1
5	EDO	BBB	517	4/4	0.77	0.25	46,53,55,55	1
5	EDO	AAA	511	4/4	0.78	0.26	75,80,81,82	1
5	EDO	BBB	513	4/4	0.79	0.14	52,57,62,63	1
6	GOL	AAA	520	6/6	0.83	0.19	41,61,67,67	2
5	EDO	AAA	513	4/4	0.83	0.24	46,48,49,49	10
4	SO4	AAA	510	5/5	0.84	0.16	74,74,82,93	0
5	EDO	AAA	514	4/4	0.84	0.16	49,49,50,51	1
5	EDO	AAA	518	4/4	0.84	0.22	45,58,65,67	1
6	GOL	AAA	522	6/6	0.85	0.22	60,61,63,64	2
4	SO4	BBB	509	5/5	0.87	0.23	85,90,101,105	0
5	EDO	BBB	519	4/4	0.87	0.10	59,62,63,64	1
5	EDO	BBB	521	4/4	0.88	0.17	48,51,58,59	1
5	EDO	AAA	519	4/4	0.89	0.10	48,50,51,53	1
6	GOL	BBB	522	6/6	0.89	0.15	46,53,64,64	2
5	EDO	AAA	515	4/4	0.94	0.17	42,45,50,50	1
4	SO4	BBB	507	5/5	0.94	0.18	61,61,62,66	0
4	SO4	AAA	507	5/5	0.95	0.13	72,78,80,80	0
4	SO4	BBB	511	5/5	0.96	0.09	71,72,75,77	0
4	SO4	BBB	510	5/5	0.96	0.21	68,69,73,78	0
7	K35	AAA	523	18/19	0.96	0.10	22,28,65,66	4
7	K35	BBB	523	18/19	0.96	0.14	25,29,66,66	4
4	SO4	BBB	505	5/5	0.97	0.07	50,51,54,54	0
4	SO4	AAA	509	5/5	0.97	0.10	49,57,58,59	0
4	SO4	AAA	508	5/5	0.97	0.10	58,59,64,65	0
4	SO4	AAA	506	5/5	0.98	0.07	51,51,54,54	0
4	SO4	BBB	508	5/5	0.98	0.16	53,54,64,64	0
4	SO4	AAA	505	5/5	0.99	0.10	36,36,41,41	0
4	SO4	BBB	506	5/5	0.99	0.08	34,35,39,40	0

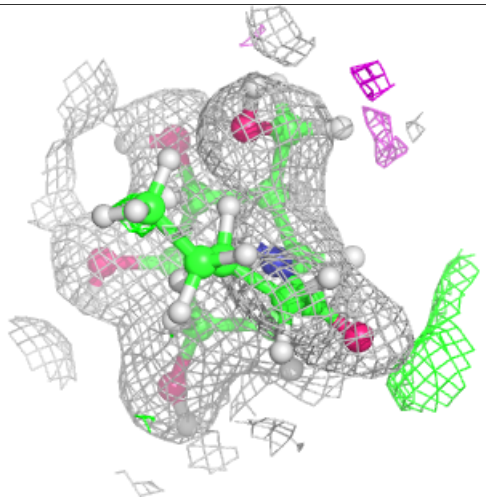
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around K35 AAA 523:

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

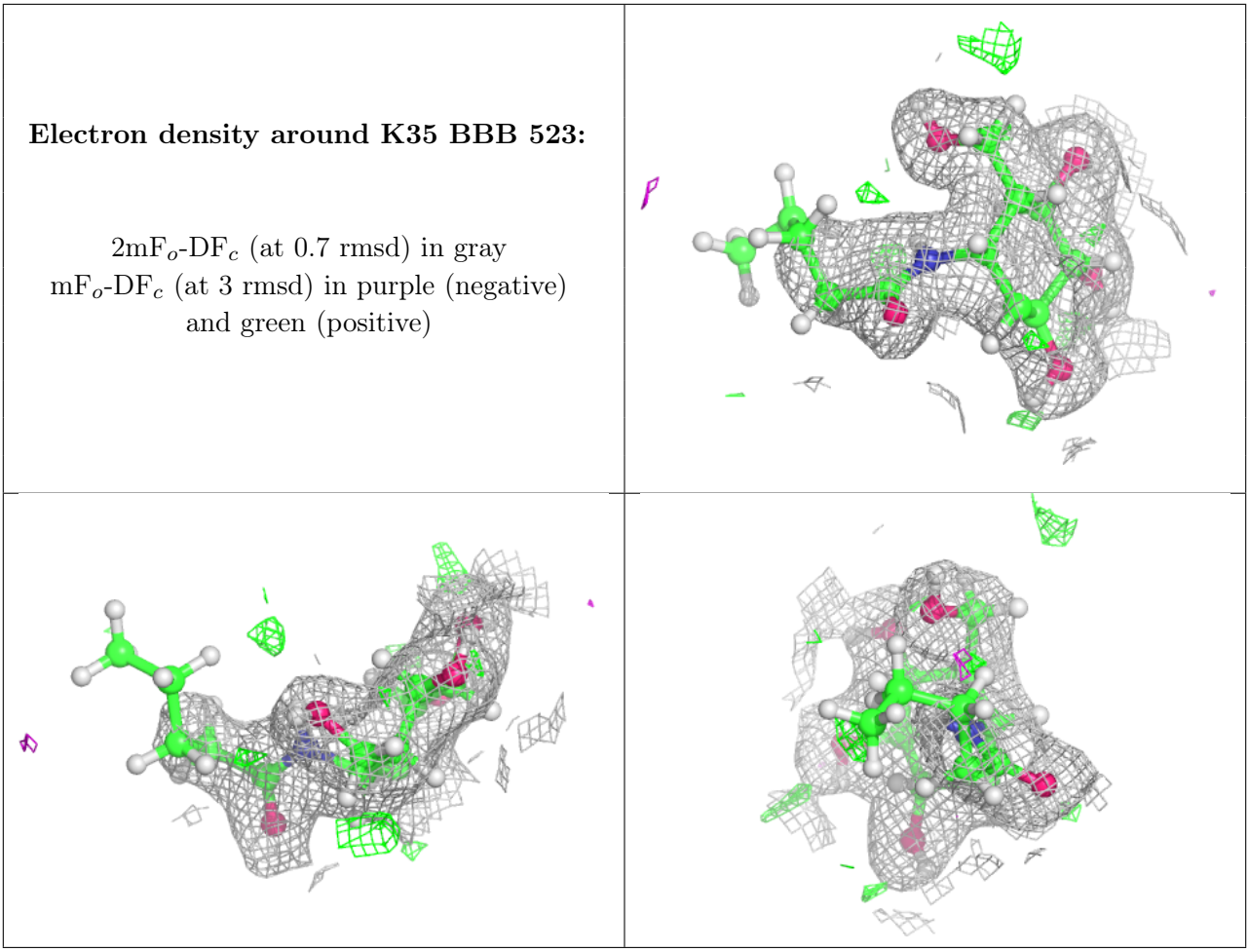






Electron density around K35 BBB 523:

$2mF_o$-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.