



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:52 PM UTC

PDB ID : 6Z39 / pdb_00006z39
Title : Structure of recombinant human beta-glucocerebrosidase in complex with BODIPY functionalised epoxide activity based probe
Authors : Rowland, R.J.; Davies, G.J.
Deposited on : 2020-05-19
Resolution : 1.70 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

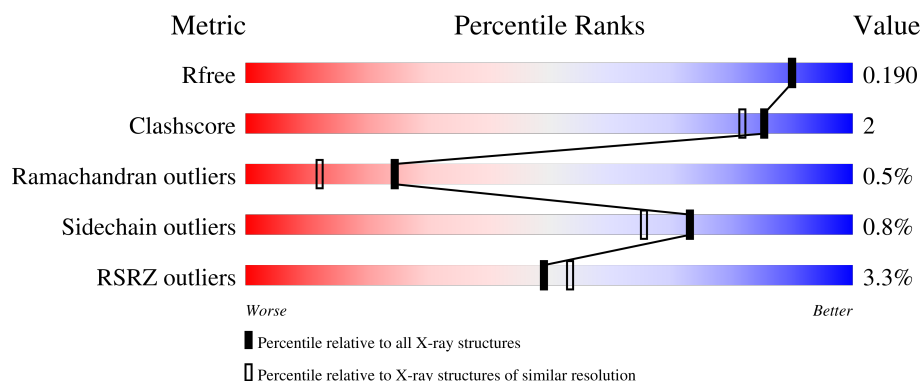
1 Overall quality at a glance

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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	4% 95% 5%
1	BBB	497	2% 95% ..
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
4	Q65	AAA	504	X	-	-	-
7	EDO	BBB	515	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17226 atoms, of which 8077 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	206	8	0
			7884	2562	3903	680	723	16			
1	BBB	497	Total	C	H	N	O	S	202	1	0
			7794	2535	3861	670	711	17			

There are 2 discrepancies between the modelled and reference sequences:

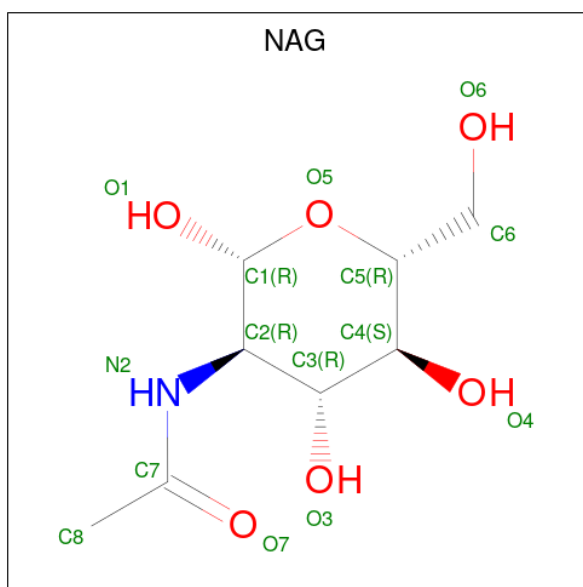
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	495	HIS	ARG	conflict	UNP P04062
BBB	495	HIS	ARG	conflict	UNP P04062

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



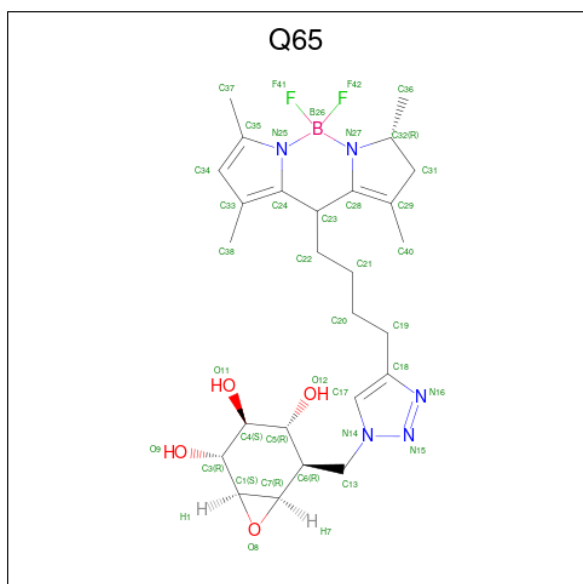
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	2	Total	C	H	N	O	5	0	0
			55	16	27	2	10			
2	B	2	Total	C	H	N	O	5	0	0
			55	16	27	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



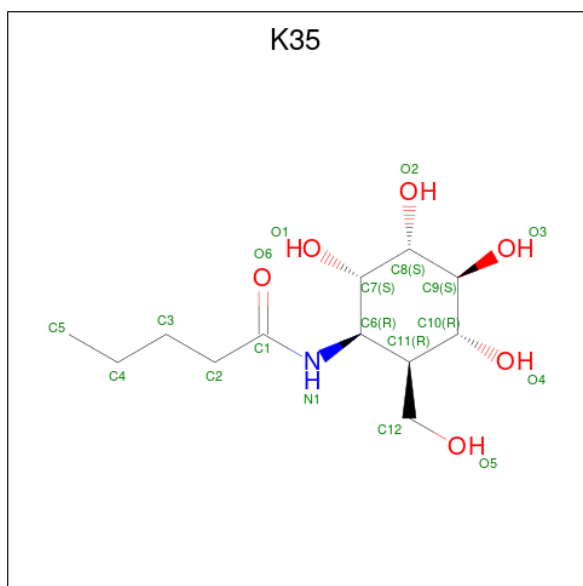
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	H	N	O	3	0
			28	8	14	1	5		
3	BBB	1	Total	C	H	N	O	3	0
			28	8	14	1	5		

- Molecule 4 is (1 {S},2 {R},3 {S},4 {R},5 {R},6 {R})-5-[[4-[4-[(12 {R})-2,2-bis(fluoranyl)-4,6,10,12-tetramethyl-1,3-diaza-2 λ^4 -boratricyclo[7.3.0.0 3,7]dodeca-4,6,9-trien-8-yl]butyl]-1,2,3-triazol-1-yl]methyl]-7-oxabicyclo[4.1.0]heptane-2,3,4-triol (CCD ID: Q65) (formula: C₂₆H₃₇BF₂N₅O₄) (labeled as "Ligand of Interest" by depositor).



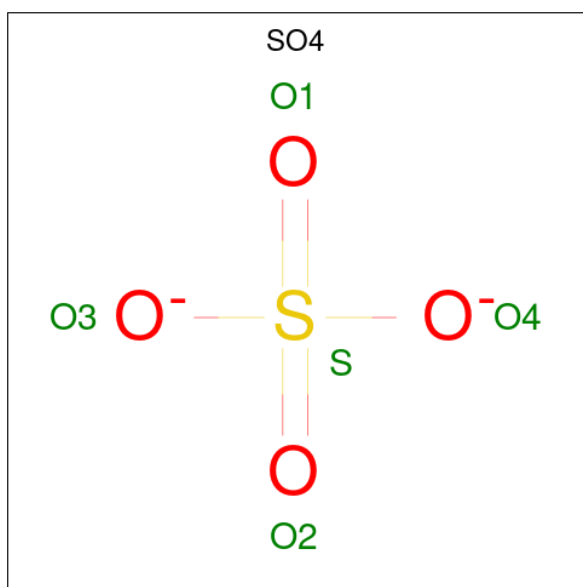
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	AAA	1	Total	B	C	F	H	N	O	3	0
			73	1	26	2	35	5	4		

- Molecule 5 is {N}-[(1 {R},2 {R},3 {R},4 {S},5 {S},6 {S})-2-(hydroxymethyl)-3,4,5,6-tetra kis(oxidanyl)cyclohexyl]pentanamide (CCD ID: K35) (formula: C₁₂H₂₃NO₆).



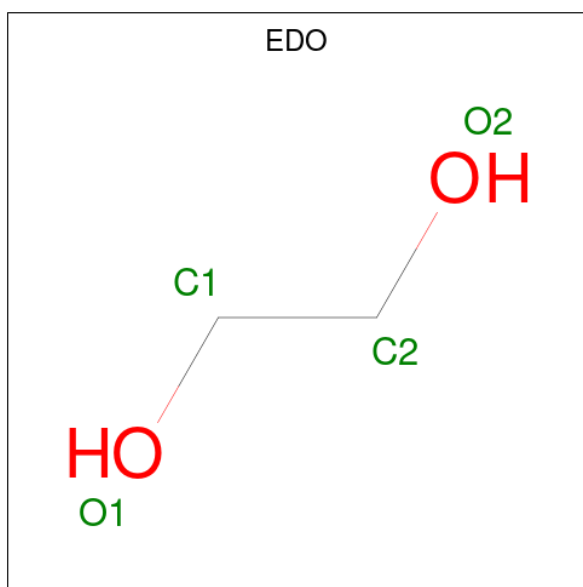
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	AAA	1	Total	C	H	N	O	4	0
			40	12	22	1	5		
5	BBB	1	Total	C	H	N	O	4	0
			40	12	22	1	5		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



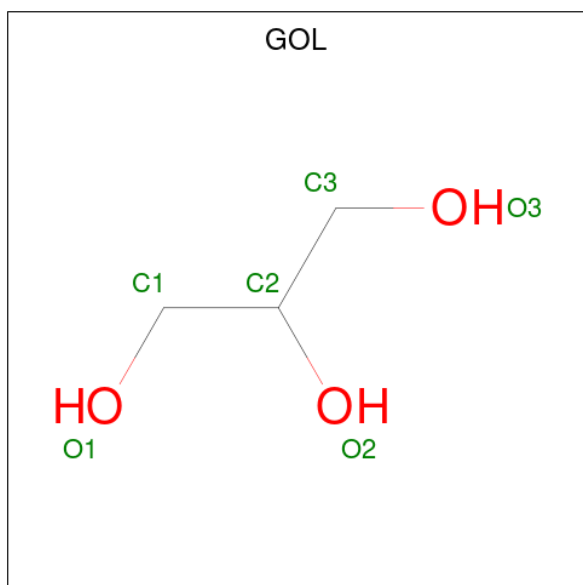
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
7	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
7	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
7	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
7	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
7	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
7	AAA	1	Total	C	H	O	1	0
			10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

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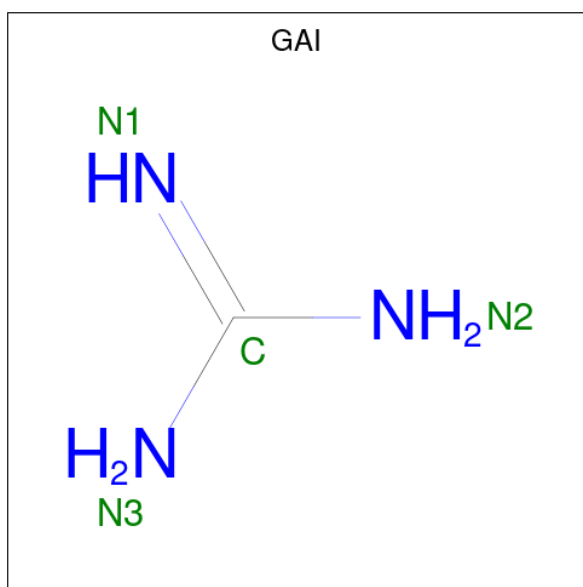
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
7	BBB	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



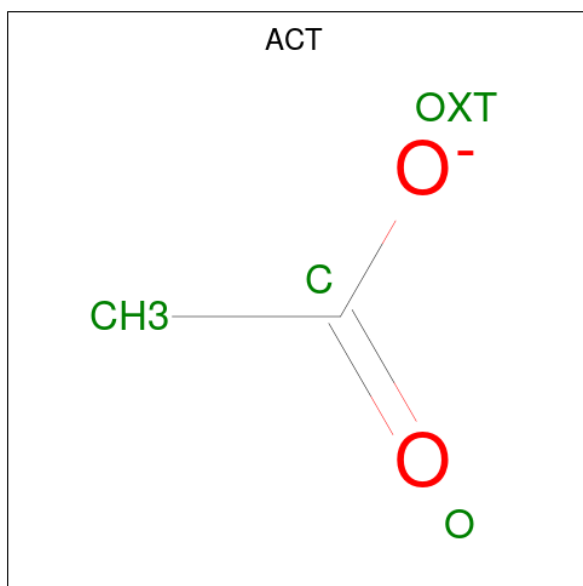
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
8	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
8	BBB	1	Total	C	H	O	2	0
			14	3	8	3		
8	BBB	1	Total	C	H	O	2	0
			14	3	8	3		
8	BBB	1	Total	C	H	O	2	0
			14	3	8	3		
8	BBB	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 9 is GUANIDINE (CCD ID: GAI) (formula: CH_5N_3).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	AAA	1	Total	C	H	N	4	0
			9	1	5	3		

- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	BBB	1	Total	C	H	O	0	0
			7	2	3	2		

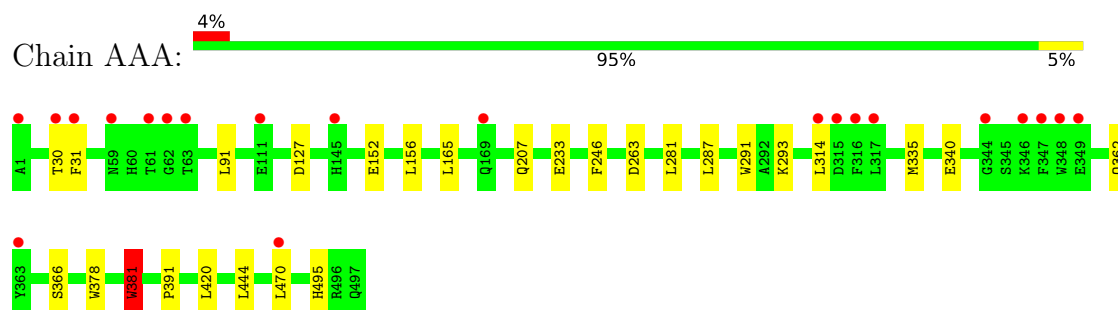
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	AAA	446	Total 446	O 446	0	0
11	BBB	458	Total 458	O 458	0	0

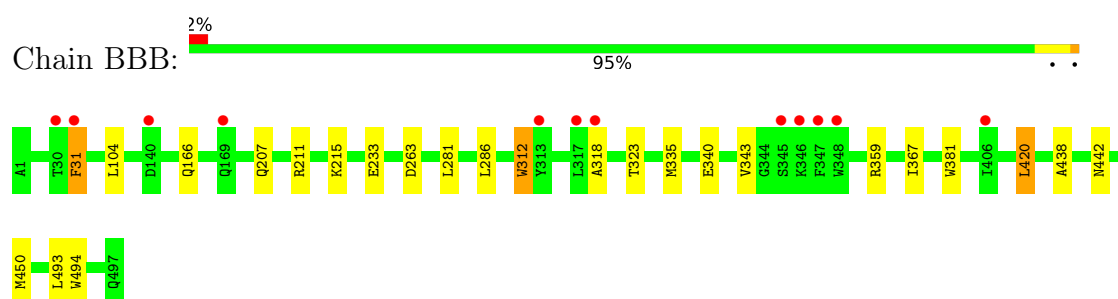
3 Residue-property plots [i](#)

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.

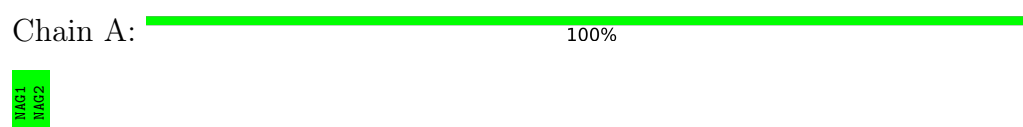
- Molecule 1: Glucosylceramidase



- 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	111.17Å 285.62Å 91.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	103.82 – 1.70 103.82 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (103.82-1.70) 99.9 (103.82-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.163 , 0.180 0.172 , 0.190	Depositor DCC
R_{free} test set	7997 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 38.3	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	0.97	EDS
Total number of atoms	17226	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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, SO4, Q65, EDO, GOL, GAI, K35, ACT

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	0.95	1/4102 (0.0%)	1.15	0/5593
1	BBB	0.96	1/4054 (0.0%)	1.17	1/5527 (0.0%)
All	All	0.95	2/8156 (0.0%)	1.16	1/11120 (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	9.20	1.42	1.25
1	AAA	340	GLU	CD-OE2	8.64	1.41	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	31	PHE	CB-CA-C	6.92	117.63	109.47

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	3981	3903	3870	17	0
1	BBB	3933	3861	3839	18	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	27	25	0	0
3	AAA	14	14	13	0	0
3	BBB	14	14	13	0	0
4	AAA	38	35	0	0	0
5	AAA	18	22	0	0	0
5	BBB	18	22	0	0	0
6	AAA	30	0	0	0	0
6	BBB	35	0	0	0	0
7	AAA	40	60	60	2	0
7	BBB	24	36	36	7	0
8	AAA	12	16	16	0	0
8	BBB	24	32	32	0	0
9	AAA	4	5	4	0	0
10	BBB	4	3	3	0	0
11	AAA	446	0	0	2	0
11	BBB	458	0	0	3	0
All	All	9149	8077	7936	35	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 2.

The worst 5 of 35 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:442:ASN:HD21	7:BBB:518:EDO:H12	1.50	0.77
1:BBB:31:PHE:HB3	7:BBB:515:EDO:H21	1.72	0.72
1:AAA:366[A]:SER:OG	1:AAA:378:TRP:CH2	2.45	0.70
1:AAA:207:GLN:NE2	1:AAA:263:ASP:OD1	2.23	0.66
1:BBB:215:LYS:NZ	11:BBB:602:HOH:O	2.29	0.65

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	503/497 (101%)	488 (97%)	12 (2%)	3 (1%)	21	9
1	BBB	496/497 (100%)	482 (97%)	12 (2%)	2 (0%)	30	16
All	All	999/994 (100%)	970 (97%)	24 (2%)	5 (0%)	24	12

All (5) Ramachandran outliers are listed below:

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

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%)	76	69
1	BBB	423/424 (100%)	419 (99%)	4 (1%)	70	62
All	All	850/848 (100%)	843 (99%)	7 (1%)	73	65

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	312	TRP
1	BBB	335	MET
1	BBB	420	LEU
1	BBB	381	TRP
1	AAA	420	LEU

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.

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	0.43	0	17,19,21	0.63	0
2	NAG	A	2	2	14,14,15	0.45	0	17,19,21	0.73	0
2	NAG	B	1	2,1	14,14,15	0.45	0	17,19,21	0.77	0
2	NAG	B	2	2	14,14,15	0.53	0	17,19,21	1.53	6 (35%)

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	-	0/6/23/26	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 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	3.10	116.35	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-C2-N2	2.56	114.46	110.43
2	B	2	NAG	O5-C1-C2	-2.30	107.73	111.29
2	B	2	NAG	C6-C5-C4	-2.17	107.68	113.02
2	B	2	NAG	O5-C5-C6	2.15	111.85	107.66

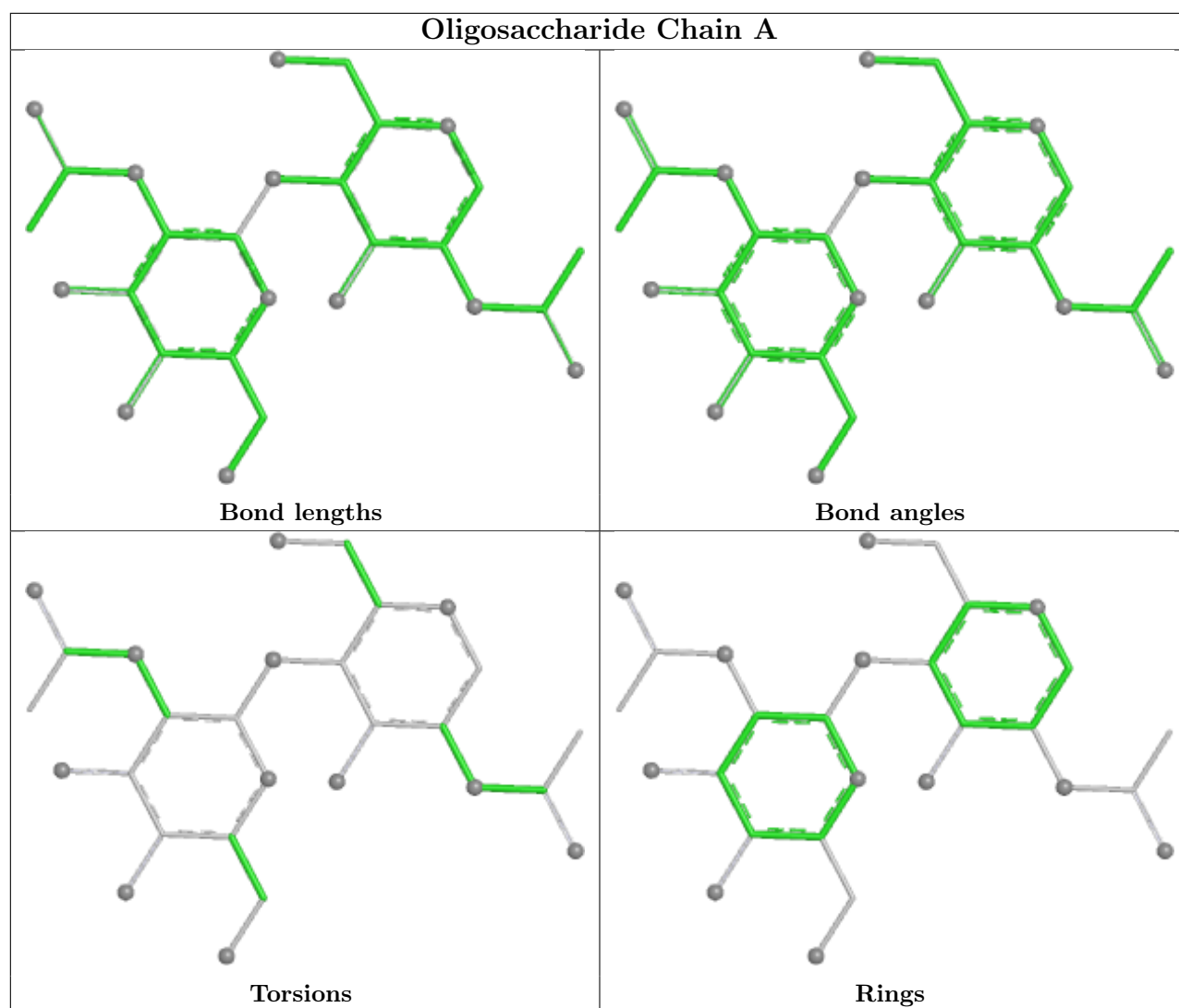
There are no chirality outliers.

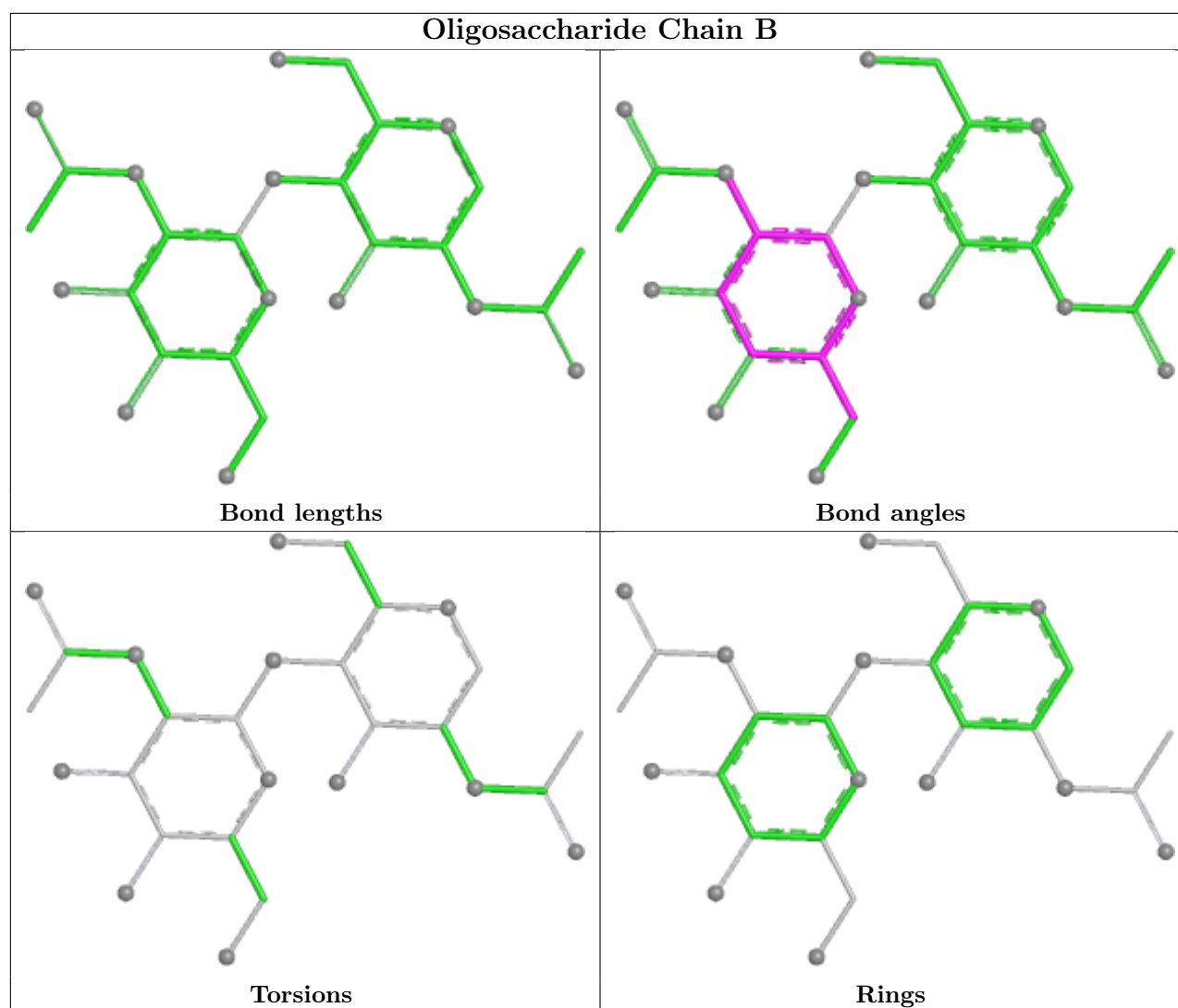
There are no torsion outliers.

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](#)

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	$\# Z > 2$
6	SO4	BBB	510	-	4,4,4	0.32	0	6,6,6	0.09	0
5	K35	AAA	505	1	18,18,19	0.54	0	23,24,26	1.35	4 (17%)
8	GOL	AAA	523	-	5,5,5	0.15	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	BBB	512	-	4,4,4	0.34	0	6,6,6	0.07	0
6	SO4	AAA	509	-	4,4,4	0.33	0	6,6,6	0.07	0
7	EDO	BBB	517	-	3,3,3	0.06	0	2,2,2	0.12	0
7	EDO	BBB	515	-	3,3,3	0.11	0	2,2,2	0.39	0
9	GAI	AAA	524	-	3,3,3	0.47	0	3,3,3	0.57	0
6	SO4	AAA	508	-	4,4,4	0.32	0	6,6,6	0.06	0
6	SO4	BBB	507	-	4,4,4	0.34	0	6,6,6	0.16	0
6	SO4	BBB	511	-	4,4,4	0.31	0	6,6,6	0.09	0
7	EDO	AAA	518	-	3,3,3	0.08	0	2,2,2	0.14	0
7	EDO	AAA	512	-	3,3,3	0.06	0	2,2,2	0.07	0
7	EDO	BBB	514	-	3,3,3	0.08	0	2,2,2	0.13	0
6	SO4	AAA	506	-	4,4,4	0.44	0	6,6,6	0.15	0
5	K35	BBB	505	1	18,18,19	0.39	0	23,24,26	1.79	2 (8%)
4	Q65	AAA	504	-	42,43,43	4.55	9 (21%)	51,68,68	3.35	22 (43%)
6	SO4	AAA	510	-	4,4,4	0.31	0	6,6,6	0.10	0
7	EDO	AAA	521	-	3,3,3	0.08	0	2,2,2	0.21	0
7	EDO	AAA	514	-	3,3,3	0.12	0	2,2,2	0.15	0
6	SO4	BBB	509	-	4,4,4	0.35	0	6,6,6	0.05	0
8	GOL	BBB	520	-	5,5,5	0.13	0	5,5,5	0.34	0
3	NAG	AAA	503	1	14,14,15	0.38	0	17,19,21	1.23	1 (5%)
8	GOL	AAA	522	-	5,5,5	0.15	0	5,5,5	0.50	0
8	GOL	BBB	521	-	5,5,5	0.16	0	5,5,5	0.49	0
7	EDO	AAA	513	-	3,3,3	0.04	0	2,2,2	0.10	0
7	EDO	AAA	515	-	3,3,3	0.09	0	2,2,2	0.05	0
8	GOL	BBB	519	-	5,5,5	0.09	0	5,5,5	0.23	0
7	EDO	BBB	518	-	3,3,3	0.05	0	2,2,2	0.21	0
10	ACT	BBB	504	-	3,3,3	1.07	0	3,3,3	0.78	0
7	EDO	AAA	516	-	3,3,3	0.08	0	2,2,2	0.07	0
6	SO4	BBB	506	-	4,4,4	0.35	0	6,6,6	0.20	0
6	SO4	BBB	508	-	4,4,4	0.34	0	6,6,6	0.06	0
6	SO4	AAA	511	-	4,4,4	0.32	0	6,6,6	0.08	0
7	EDO	BBB	516	-	3,3,3	0.07	0	2,2,2	0.16	0
7	EDO	AAA	519	-	3,3,3	0.07	0	2,2,2	0.11	0
8	GOL	BBB	522	-	5,5,5	0.12	0	5,5,5	0.30	0
7	EDO	AAA	517	-	3,3,3	0.14	0	2,2,2	0.24	0
7	EDO	AAA	520	-	3,3,3	0.06	0	2,2,2	0.16	0
7	EDO	BBB	513	-	3,3,3	0.11	0	2,2,2	0.08	0
6	SO4	AAA	507	-	4,4,4	0.36	0	6,6,6	0.22	0
3	NAG	BBB	503	1	14,14,15	0.41	0	17,19,21	1.05	2 (11%)

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	K35	AAA	505	1	-	2/10/30/34	0/1/1/1
8	GOL	AAA	523	-	-	4/4/4/4	-
7	EDO	BBB	517	-	-	1/1/1/1	-
7	EDO	BBB	515	-	-	1/1/1/1	-
7	EDO	AAA	518	-	-	1/1/1/1	-
7	EDO	AAA	512	-	-	0/1/1/1	-
7	EDO	BBB	514	-	-	1/1/1/1	-
5	K35	BBB	505	1	-	2/10/30/34	0/1/1/1
4	Q65	AAA	504	-	1/1/12/12	2/11/72/72	0/6/6/6
7	EDO	AAA	521	-	-	1/1/1/1	-
7	EDO	AAA	514	-	-	1/1/1/1	-
8	GOL	BBB	520	-	-	2/4/4/4	-
3	NAG	AAA	503	1	-	2/6/23/26	0/1/1/1
8	GOL	AAA	522	-	-	2/4/4/4	-
8	GOL	BBB	521	-	-	4/4/4/4	-
7	EDO	AAA	513	-	-	1/1/1/1	-
7	EDO	AAA	515	-	-	0/1/1/1	-
8	GOL	BBB	519	-	-	0/4/4/4	-
7	EDO	BBB	518	-	-	1/1/1/1	-
7	EDO	AAA	516	-	-	1/1/1/1	-
7	EDO	BBB	516	-	-	1/1/1/1	-
7	EDO	AAA	519	-	-	1/1/1/1	-
8	GOL	BBB	522	-	-	2/4/4/4	-
7	EDO	AAA	517	-	-	1/1/1/1	-
7	EDO	AAA	520	-	-	0/1/1/1	-
7	EDO	BBB	513	-	-	0/1/1/1	-
3	NAG	BBB	503	1	-	0/6/23/26	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	504	Q65	C29-C28	23.29	1.49	1.33
4	AAA	504	Q65	C31-C29	-13.23	1.39	1.51
4	AAA	504	Q65	C24-C33	8.00	1.47	1.37
4	AAA	504	Q65	N16-N15	5.32	1.40	1.32
4	AAA	504	Q65	N14-N15	3.64	1.40	1.34

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AAA	504	Q65	C33-C24-N25	-11.86	103.60	109.83
4	AAA	504	Q65	C22-C23-C24	8.70	121.20	111.86
4	AAA	504	Q65	C22-C23-C28	8.24	120.71	111.86
4	AAA	504	Q65	C37-C35-C34	-7.59	117.20	129.90
5	BBB	505	K35	C11-C6-N1	6.66	119.21	111.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	AAA	504	Q65	C23

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	AAA	522	GOL	C1-C2-C3-O3
8	AAA	523	GOL	O1-C1-C2-O2
8	AAA	523	GOL	O1-C1-C2-C3
8	AAA	523	GOL	C1-C2-C3-O3
8	BBB	520	GOL	O1-C1-C2-O2

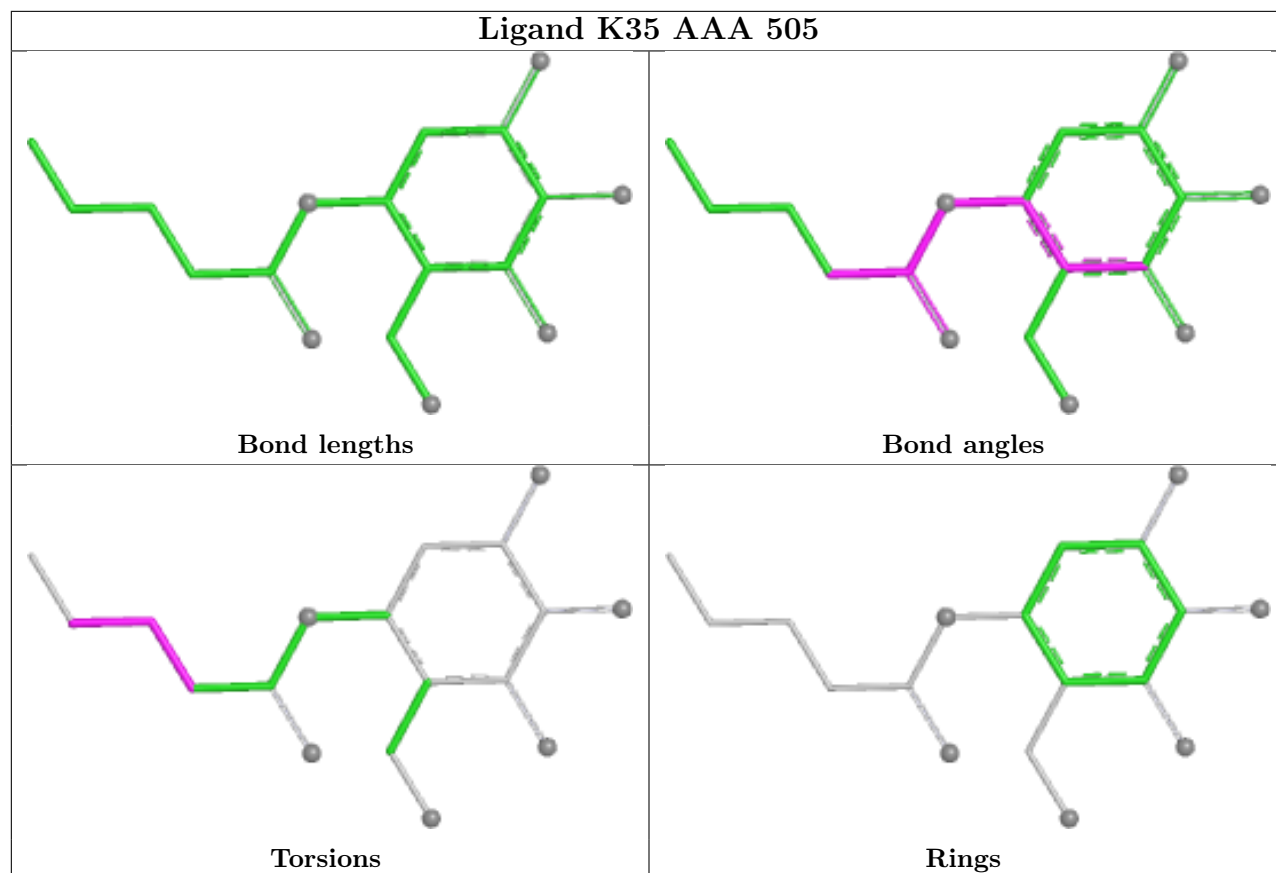
There are no ring outliers.

4 monomers are involved in 9 short contacts:

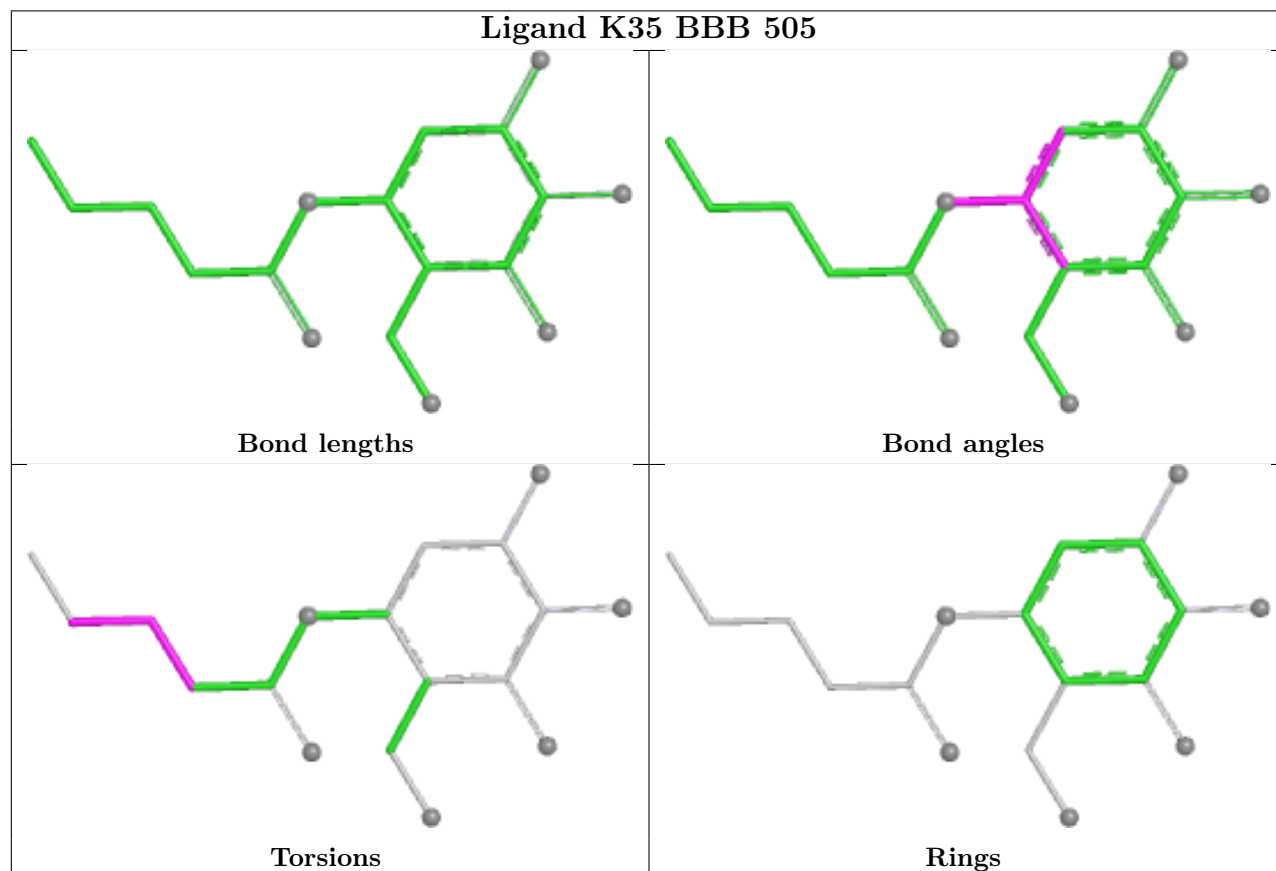
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	BBB	515	EDO	5	0
7	AAA	521	EDO	1	0
7	BBB	518	EDO	2	0
7	AAA	517	EDO	1	0

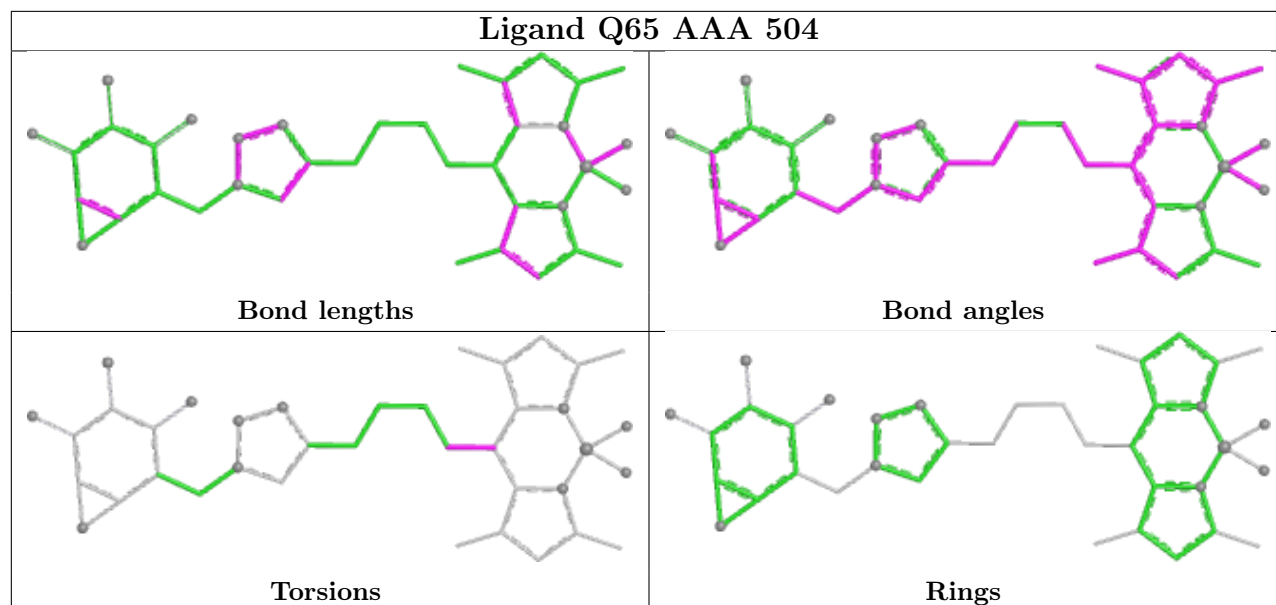
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand K35 AAA 505



Ligand K35 BBB 505





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%)	-0.16	21 (4%) 40 45	9, 21, 36, 58	13 (2%)
1	BBB	497/497 (100%)	-0.28	12 (2%) 59 64	10, 21, 35, 46	4 (0%)
All	All	994/994 (100%)	-0.22	33 (3%) 49 53	9, 21, 35, 58	17 (1%)

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	347	PHE	15.9
1	BBB	169	GLN	5.0
1	AAA	316	PHE	4.5
1	AAA	348	TRP	4.2
1	AAA	31	PHE	4.0

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

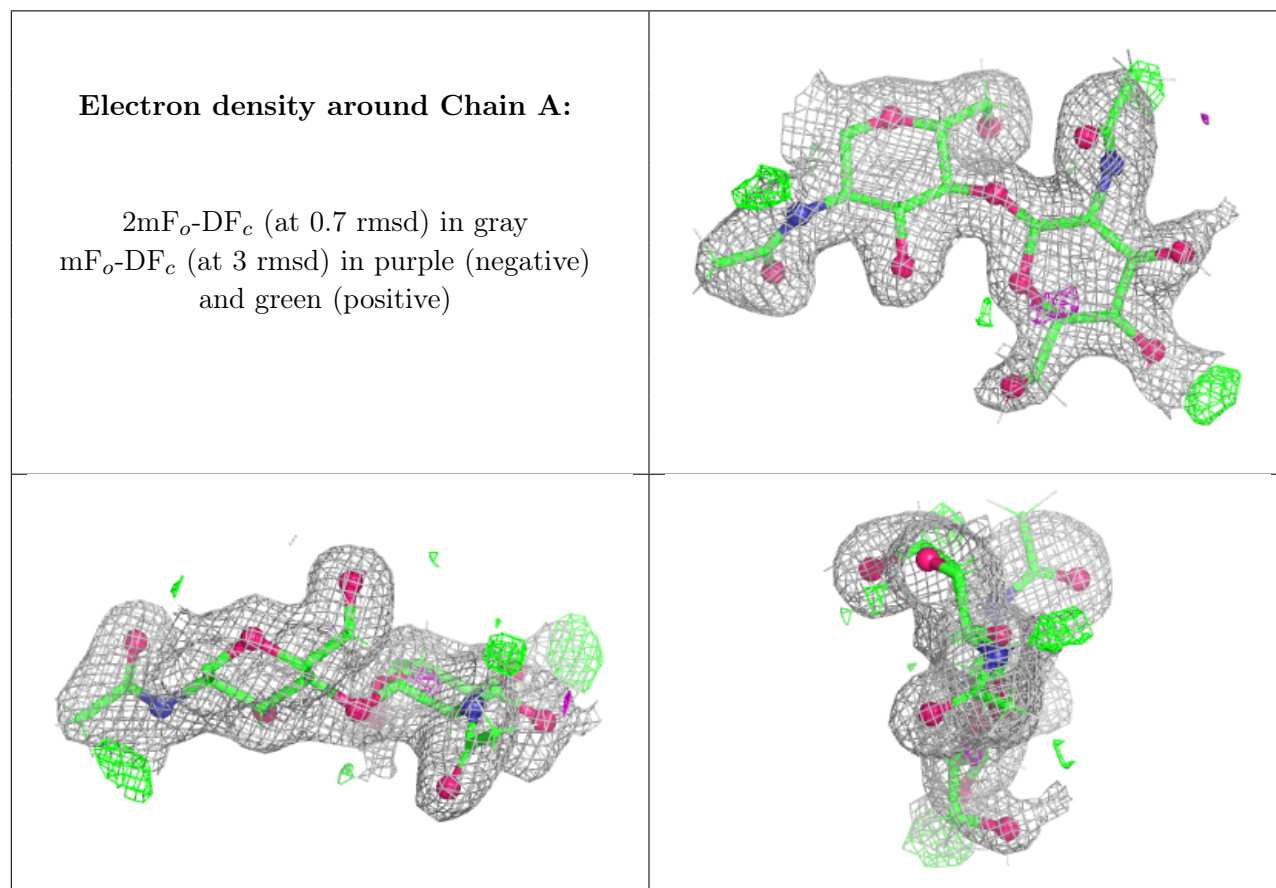
There are no non-standard protein/DNA/RNA residues in this entry.

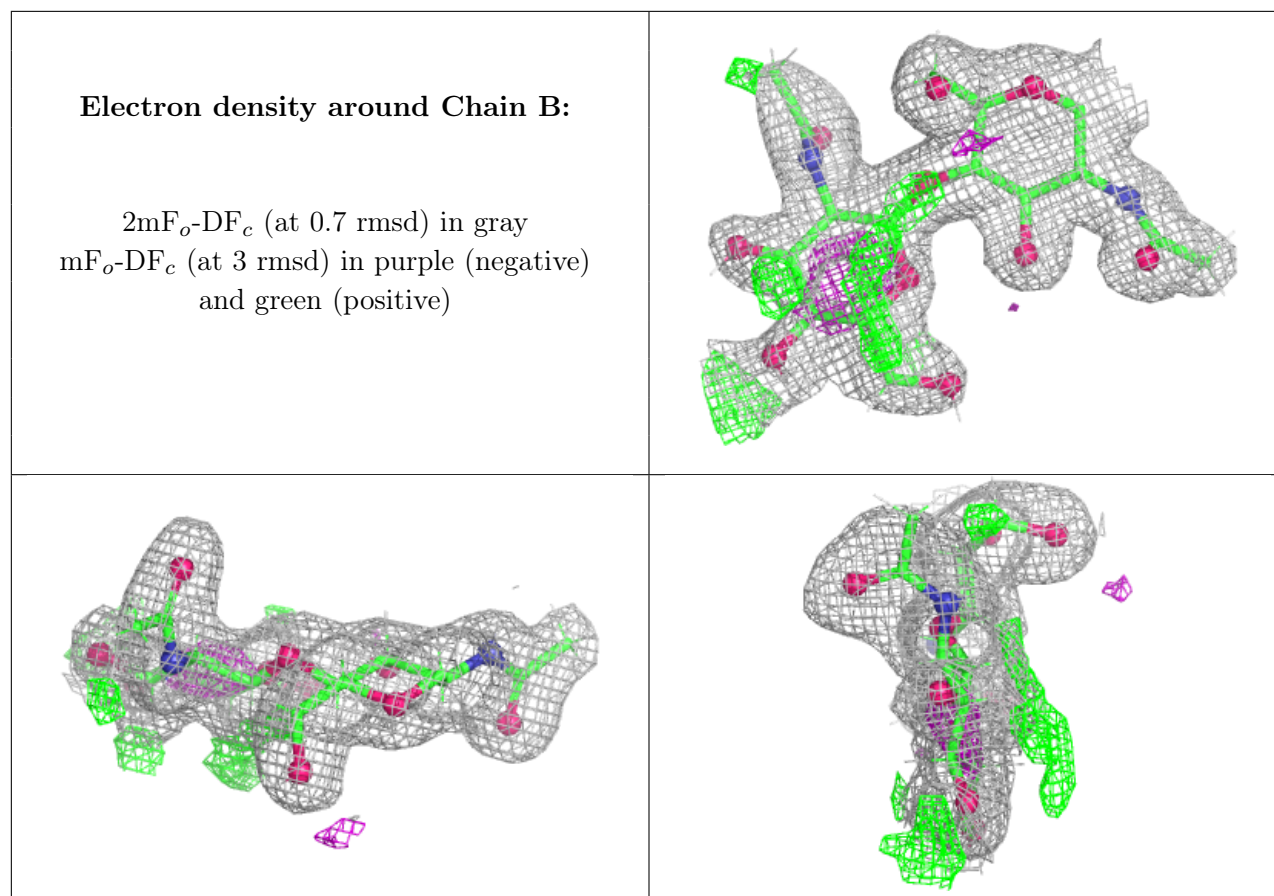
6.3 Carbohydrates [i](#)

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	NAG	A	1	14/15	-	-	26,30,34,37	2
2	NAG	A	2	14/15	-	-	42,49,53,57	3
2	NAG	B	1	14/15	-	-	25,28,30,36	2
2	NAG	B	2	14/15	-	-	43,50,56,58	3

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 [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($\text{\AA}^2$)	Q<0.9
6	SO4	BBB	512	5/5	0.54	0.14	103,103,107,108	0
3	NAG	BBB	503	14/15	0.67	0.16	70,78,81,82	3
6	SO4	BBB	510	5/5	0.70	0.16	79,84,86,91	0
3	NAG	AAA	503	14/15	0.75	0.15	44,50,55,66	3
8	GOL	BBB	521	6/6	0.76	0.20	41,47,53,56	2
7	EDO	AAA	514	4/4	0.79	0.18	46,46,53,53	1
7	EDO	AAA	520	4/4	0.80	0.21	51,53,54,55	1
10	ACT	BBB	504	4/4	0.80	0.21	53,53,54,55	0
8	GOL	BBB	522	6/6	0.81	0.22	58,64,64,65	2
6	SO4	AAA	511	5/5	0.81	0.13	67,67,71,79	0
8	GOL	BBB	520	6/6	0.82	0.19	55,59,61,61	2
7	EDO	AAA	521	4/4	0.82	0.20	59,63,66,67	1
7	EDO	AAA	518	4/4	0.83	0.19	68,71,72,73	1

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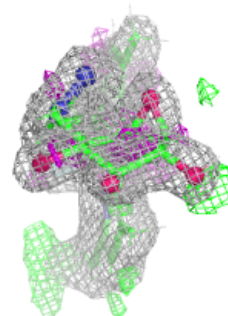
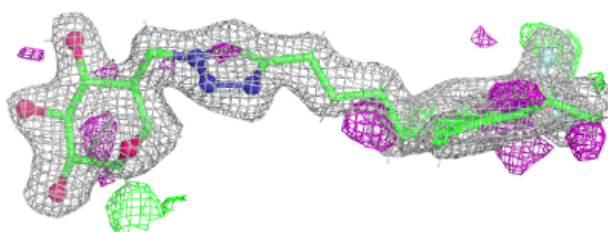
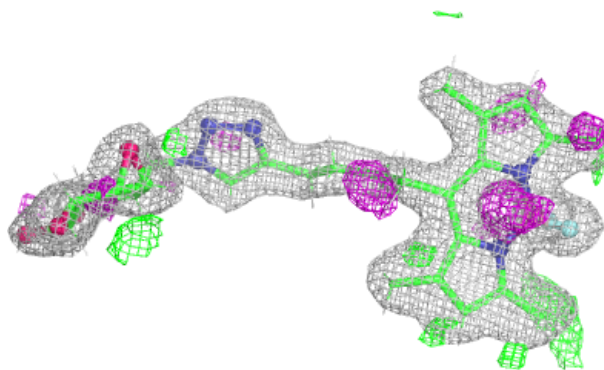
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	AAA	519	4/4	0.83	0.19	52,54,55,55	1
7	EDO	AAA	517	4/4	0.84	0.19	43,44,47,47	1
8	GOL	AAA	522	6/6	0.84	0.15	28,38,44,44	2
7	EDO	AAA	515	4/4	0.84	0.17	36,42,48,48	1
7	EDO	BBB	516	4/4	0.85	0.17	61,65,66,66	1
7	EDO	AAA	516	4/4	0.85	0.16	48,52,53,53	1
6	SO4	BBB	511	5/5	0.85	0.10	61,65,69,71	0
4	Q65	AAA	504	38/38	0.86	0.13	28,36,46,48	6
7	EDO	AAA	513	4/4	0.87	0.18	56,59,60,60	1
8	GOL	AAA	523	6/6	0.87	0.18	40,46,51,51	2
7	EDO	BBB	517	4/4	0.87	0.17	54,55,57,57	1
7	EDO	BBB	513	4/4	0.88	0.16	48,50,51,51	1
7	EDO	BBB	514	4/4	0.88	0.20	51,55,57,58	1
6	SO4	BBB	509	5/5	0.88	0.12	49,51,55,58	0
6	SO4	BBB	508	5/5	0.88	0.12	54,57,61,63	0
7	EDO	AAA	512	4/4	0.88	0.21	50,54,55,55	1
7	EDO	BBB	515	4/4	0.89	0.14	37,40,41,42	1
7	EDO	BBB	518	4/4	0.89	0.15	50,51,51,52	1
6	SO4	AAA	510	5/5	0.90	0.10	43,52,54,57	0
8	GOL	BBB	519	6/6	0.90	0.14	36,44,48,48	2
6	SO4	AAA	509	5/5	0.93	0.09	55,56,59,60	0
9	GAI	AAA	524	4/4	0.94	0.10	30,34,34,35	4
6	SO4	BBB	506	5/5	0.95	0.08	39,41,42,42	0
6	SO4	AAA	508	5/5	0.95	0.07	44,47,50,52	0
6	SO4	AAA	507	5/5	0.95	0.08	39,40,42,42	0
5	K35	BBB	505	18/19	0.96	0.10	17,26,50,50	4
5	K35	AAA	505	18/19	0.97	0.08	17,18,42,43	4
6	SO4	BBB	507	5/5	0.99	0.04	25,26,27,29	0
6	SO4	AAA	506	5/5	0.99	0.06	27,27,29,32	0

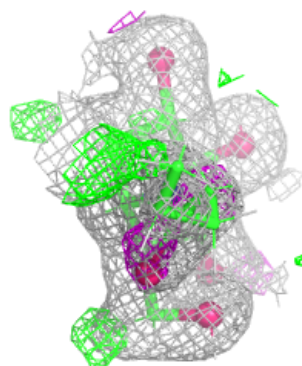
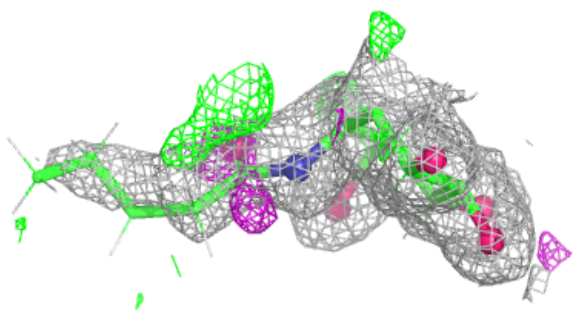
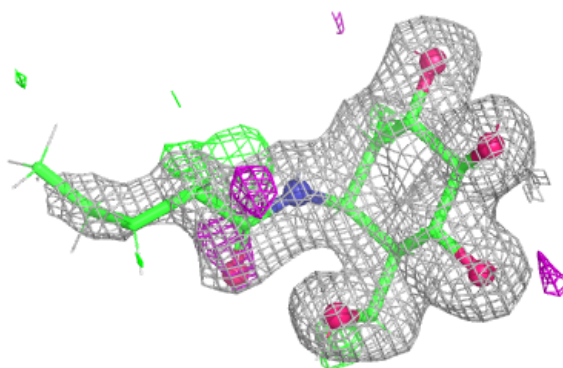
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around Q65 AAA 504:

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

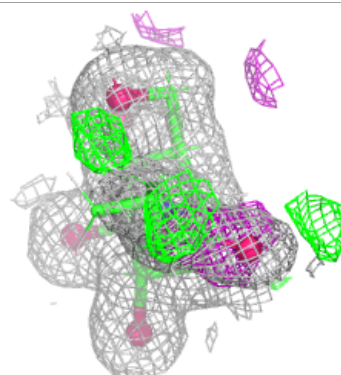
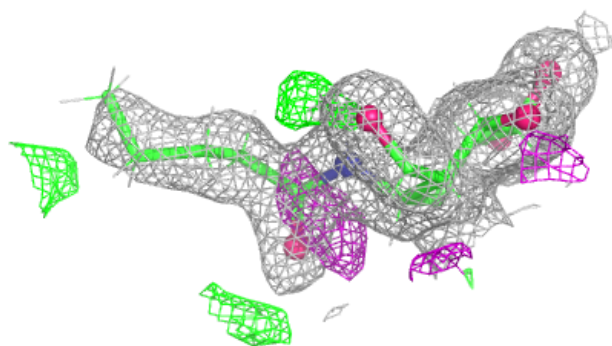
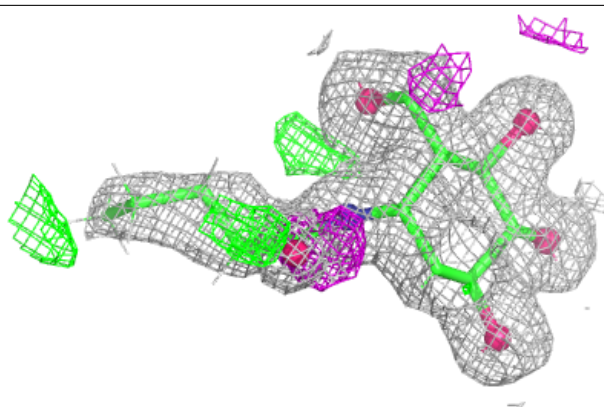
**Electron density around K35 BBB 505:**

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



Electron density around K35 AAA 505:

$2mF_o-DF_c$ (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.