WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jul 6, 2022 – 04:09 am BST

PDB ID	:	7P32
Title	:	Crystal structure of human lysosomal acid-alpha-glucosidase, GAA, in complex with cyclosulfamidate 6
Authors	:	Roig-Zamboni, V.; Kok, K.; Overkleeft, H.; Artola, M.; Sulzenbacher, G.
Deposited on	:	2021-07-06
Resolution	:	1.82 Å(reported)

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	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 1.82 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	Percentile Ranks	Value
Clashscore		2
Ramachandran outliers		0.1%
Sidechain outliers		0.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	AAA	872	93% · ·
2	BBB	3	33% 67%
3	BcB	2	100%
4	BfB	3	100%
5	BiB	2	100%

2 Entry composition ⓘ

There are 13 unique types of molecules in this entry. The entry contains 7681 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lysosomal alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	847	Total 6764	C 4341	N 1137	O 1252	S 34	0	17	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	199	ARG	HIS	variant	UNP P10253
AAA	223	HIS	ARG	variant	UNP P10253
AAA	780	ILE	VAL	variant	UNP P10253

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

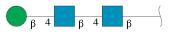| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	BBB	3	Total 38	C 22	N 2	O 14	0	0	0

- Molecule 3 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
3	BcB	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
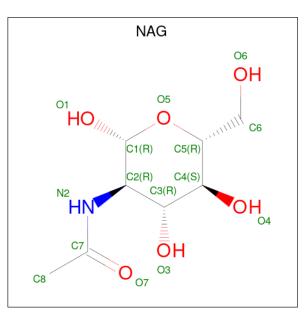
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	BfB	3	Total 39	C 22	N 2	O 15	0	0	0

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

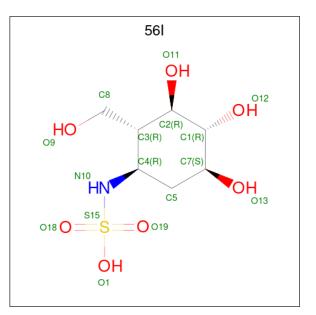| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	BiB	2	Total 24	C 14	N 1	O 9	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

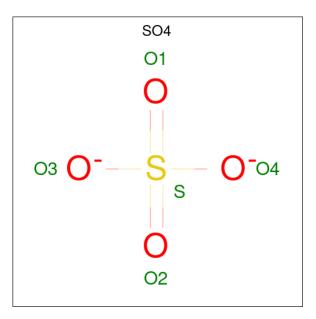| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 7 is [(1R,2R,3R,4R,5S)-2-(hydroxymethyl)-3,4,5-tris(oxidanyl)cyclohexyl]sulfamic acid (three-letter code: 56I) (formula: $C_7H_{15}NO_7S$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
7	AAA	1	16	7	1	7	1	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).
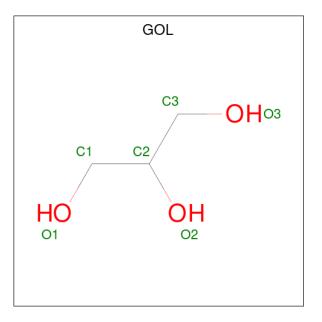
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	AAA	1	Total 5	O 4	S 1	0	0
8	AAA	1	Total 5	O 4	S 1	0	0
8	AAA	1	Total 5	O 4	S 1	0	0
8	AAA	1	Total 5	O 4	S 1	0	0
8	AAA	1	Total 5	O 4	S 1	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

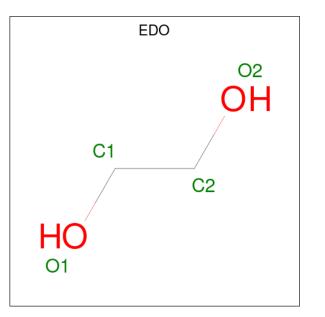| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	AAA	9	Total 9	Cl 9	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	AAA	1	Total 6	C 3	O 3	0	0
10	AAA	1	Total 6	C 3	O 3	0	0
10	AAA	1	Total 6	C 3	O 3	0	0

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	AAA	1	Total 4	C 2	O 2	0	0
11	AAA	1	Total 4	C 2	O 2	0	0
11	AAA	1	Total 4	C 2	O 2	0	0
11	AAA	1	Total 4	C 2	O 2	0	0

- Molecule 12 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$) (labeled as "Ligand of Interest" by depositor).

PGE

O4
OH

C5
C6

C4
O

O2
O3

C1
C3

C2

HO
O1

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

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	AAA	680	Total 680	O 680	0	0

3 Residue-property plots ⓘ

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. 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. 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.

Note EDS failed to run properly.

• Molecule 1: Lysosomal alpha-glucosidase

Chain AAA:

93%

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BBB:

33%   67%

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BcB:

100%

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

Chain BfB:

100%

• Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BiB:

100%

NAG1
FUC2

4 Data and refinement statistics ⓘ

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.04Å 102.61Å 129.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.00 – 1.82	Depositor
% Data completeness (in resolution range)	99.8 (47.00-1.82)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.150 , 0.175	Depositor
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.118	Xtriage
L-test for twinning[2]	$< \vert L \vert > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7681	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \vert L \vert >$, $< L^2 >$ 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: CL, NAG, BMA, GOL, 56I, FUC, EDO, PGE, CSO, SO4

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	0.65	0/6997	0.77	0/9554

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	6764	0	6572	26	0
2	BBB	38	0	34	0	0
3	BcB	28	0	25	0	0
4	BfB	39	0	34	0	0
5	BiB	24	0	22	0	0
6	AAA	14	0	13	0	0
7	AAA	16	0	0	0	0
8	AAA	25	0	0	0	0
9	AAA	9	0	0	0	0
10	AAA	18	0	24	0	0
11	AAA	16	0	24	3	0
12	AAA	10	0	14	0	0
13	AAA	680	0	0	4	0
All	All	7681	0	6762	27	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 27 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:393[A]:ARG:HG3	1:AAA:393[A]:ARG:HH21	1.36	0.90
1:AAA:393[A]:ARG:NH2	13:AAA:1101:HOH:O	2.15	0.77
1:AAA:393[A]:ARG:HH21	1:AAA:393[A]:ARG:CG	2.01	0.73
1:AAA:393[A]:ARG:HG3	1:AAA:393[A]:ARG:NH2	2.00	0.70
1:AAA:551:THR:OG1	1:AAA:553[B]:GLN:OE1	2.17	0.61

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	855/872 (98%)	835 (98%)	19 (2%)	1 (0%)	51	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	480	VAL

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	740/741 (100%)	734 (99%)	6 (1%)	81 77

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	440	MET
1	AAA	480	VAL
1	AAA	613	TRP
1	AAA	393[B]	ARG
1	AAA	393[A]	ARG

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)

1 non-standard protein/DNA/RNA residue is 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	$\#|Z| > 2$
1	CSO	AAA	938	1	3,6,7	0.72	0	0,6,8	-	-

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
1	CSO	AAA	938	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

10 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	BBB	1	1,2	14,14,15	0.69	0	17,19,21	1.13	1 (5%)
2	NAG	BBB	2	2	14,14,15	0.61	0	17,19,21	0.72	0
2	FUC	BBB	3	2	10,10,11	0.68	0	14,14,16	1.16	2 (14%)
3	NAG	BcB	1	3,1	14,14,15	0.69	0	17,19,21	1.23	2 (11%)
3	NAG	BcB	2	3	14,14,15	0.51	0	17,19,21	1.39	3 (17%)
4	NAG	BfB	1	4,1	14,14,15	0.64	0	17,19,21	1.11	1 (5%)
4	NAG	BfB	2	4	14,14,15	0.61	0	17,19,21	1.16	2 (11%)
4	BMA	BfB	3	4	11,11,12	0.55	0	15,15,17	1.37	2 (13%)
5	NAG	BiB	1	1,5	14,14,15	0.74	0	17,19,21	1.22	1 (5%)
5	FUC	BiB	2	5	10,10,11	0.62	0	14,14,16	1.42	3 (21%)

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	BBB	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	BBB	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUC	BBB	3	2	-	-	0/1/1/1
3	NAG	BcB	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	BcB	2	3	-	0/6/23/26	0/1/1/1
4	NAG	BfB	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	BfB	2	4	-	0/6/23/26	0/1/1/1
4	BMA	BfB	3	4	-	2/2/19/22	0/1/1/1
5	NAG	BiB	1	1,5	-	0/6/23/26	0/1/1/1
5	FUC	BiB	2	5	-	-	0/1/1/1

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	BfB	3	BMA	O5-C5-C6	3.78	113.14	107.20
2	BBB	1	NAG	O5-C1-C2	-3.63	105.55	111.29
5	BiB	2	FUC	O5-C5-C4	3.08	115.05	109.52
4	BfB	1	NAG	O5-C1-C2	-2.59	107.20	111.29
2	BBB	3	FUC	C1-O5-C5	2.39	118.19	112.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

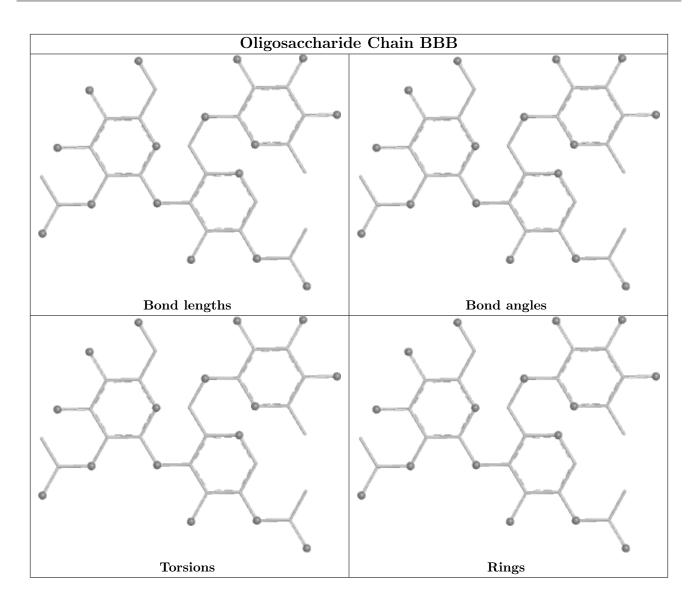| Mol	Chain	Res	Type	Atoms
4	BfB	3	BMA	O5-C5-C6-O6
4	BfB	3	BMA	C4-C5-C6-O6

There are no ring outliers.

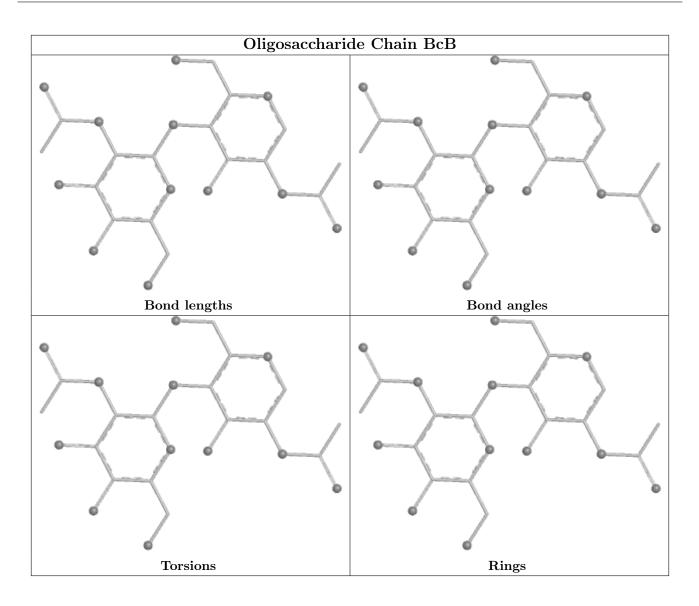No monomer is involved in short contacts.

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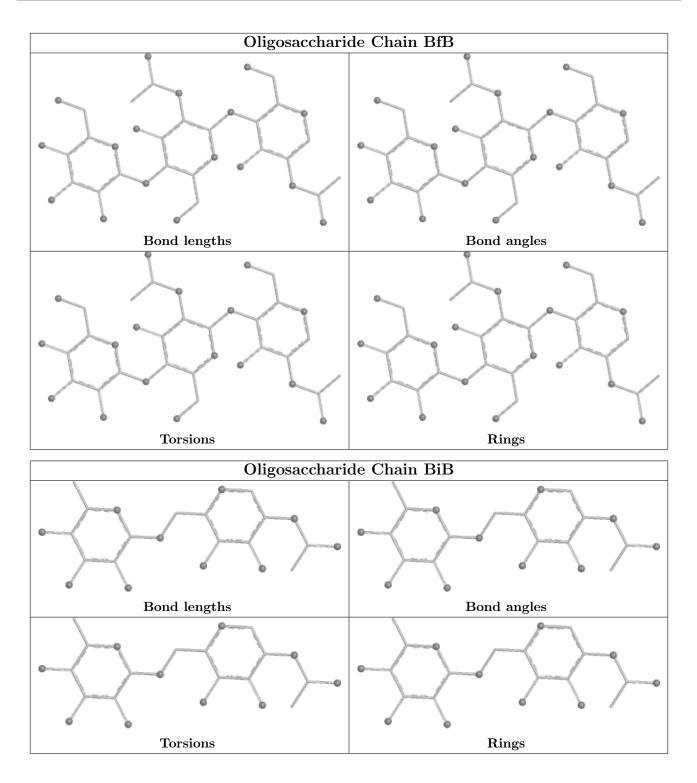
Oligosaccharide Chain BBB

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain BcB

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain BfB

Bond lengths	Bond angles

Torsions	Rings

Oligosaccharide Chain BiB

Bond lengths	Bond angles

Torsions	Rings

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 9 are monoatomic - leaving 15 for Mogul analysis.

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	$\#|Z| > 2$
8	SO4	AAA	1003	-	4,4,4	0.28	0	6,6,6	0.19	0
8	SO4	AAA	1004	-	4,4,4	0.27	0	6,6,6	0.15	0
11	EDO	AAA	1021	-	3,3,3	0.20	0	2,2,2	0.11	0
8	SO4	AAA	1006	-	4,4,4	0.41	0	6,6,6	0.22	0
8	SO4	AAA	1005	-	4,4,4	0.43	0	6,6,6	0.12	0
10	GOL	AAA	1018	-	5,5,5	0.21	0	5,5,5	0.62	0
11	EDO	AAA	1022	-	3,3,3	0.20	0	2,2,2	0.20	0
12	PGE	AAA	1024	-	9,9,9	0.23	0	8,8,8	0.13	0
10	GOL	AAA	1017	-	5,5,5	0.13	0	5,5,5	0.24	0
6	NAG	AAA	1001	1	14,14,15	0.66	0	17,19,21	1.56	4 (23%)
8	SO4	AAA	1007	-	4,4,4	0.31	0	6,6,6	0.38	0
10	GOL	AAA	1019	-	5,5,5	0.18	0	5,5,5	0.36	0
11	EDO	AAA	1020	-	3,3,3	0.13	0	2,2,2	0.50	0
11	EDO	AAA	1023	-	3,3,3	0.37	0	2,2,2	0.20	0
7	56I	AAA	1002	1	15,16,16	2.64	3 (20%)	18,24,24	1.67	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
11	EDO	AAA	1021	-	-	0/1/1/1	-
10	GOL	AAA	1018	-	-	2/4/4/4	-
11	EDO	AAA	1022	-	-	0/1/1/1	-
12	PGE	AAA	1024	-	-	1/7/7/7	-
10	GOL	AAA	1017	-	-	0/4/4/4	-
6	NAG	AAA	1001	1	-	0/6/23/26	0/1/1/1
10	GOL	AAA	1019	-	-	1/4/4/4	-
11	EDO	AAA	1020	-	-	1/1/1/1	-
11	EDO	AAA	1023	-	-	0/1/1/1	-
7	56I	AAA	1002	1	-	1/7/27/27	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	AAA	1002	56I	O19-S15	8.37	1.51	1.42
7	AAA	1002	56I	O18-S15	3.83	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	AAA	1002	56I	C3-C2	-3.26	1.49	1.53

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	AAA	1002	56I	O19-S15-O18	-4.77	108.90	120.16
6	AAA	1001	NAG	O5-C1-C2	-3.65	105.53	111.29
7	AAA	1002	56I	C5-C4-C3	3.45	115.45	111.49
6	AAA	1001	NAG	C3-C4-C5	-2.88	105.11	110.24
6	AAA	1001	NAG	O6-C6-C5	-2.32	103.32	111.29

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	AAA	1018	GOL	O1-C1-C2-O2
10	AAA	1018	GOL	O1-C1-C2-C3
7	AAA	1002	56I	C4-N10-S15-O19
11	AAA	1020	EDO	O1-C1-C2-O2
12	AAA	1024	PGE	O2-C3-C4-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	AAA	1021	EDO	1	0
11	AAA	1023	EDO	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.
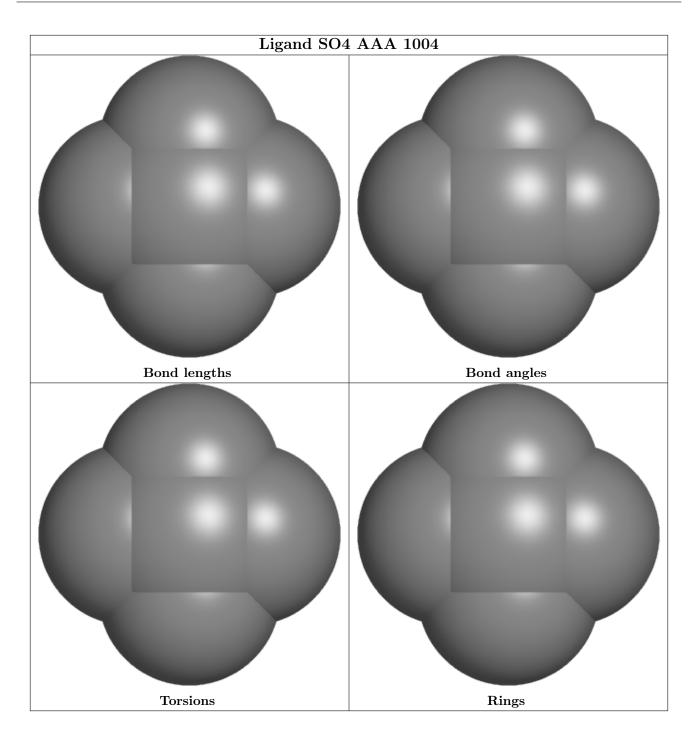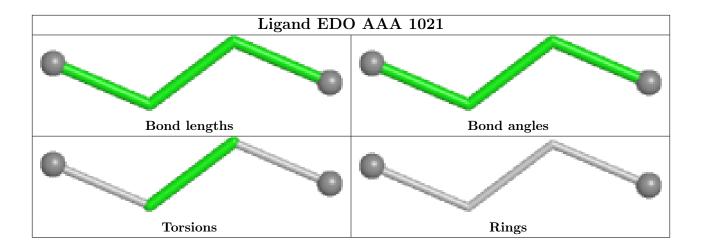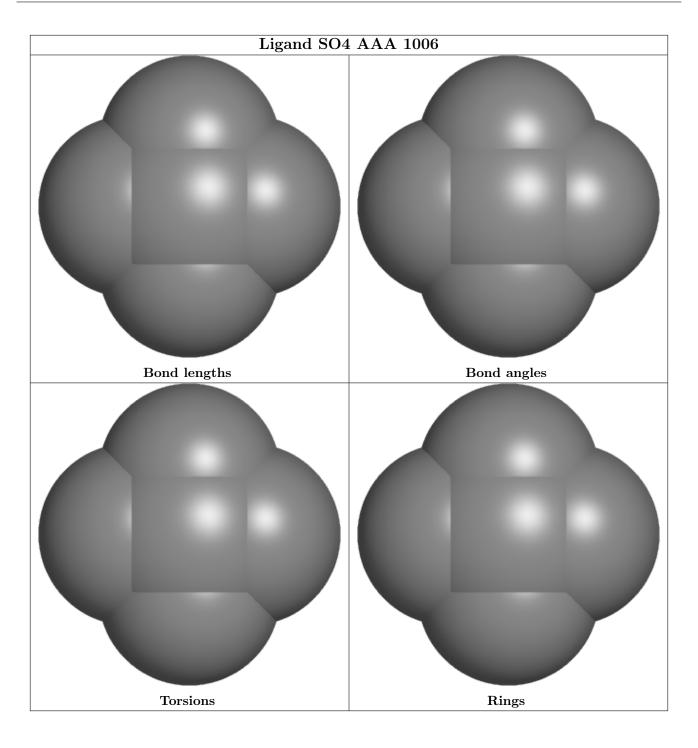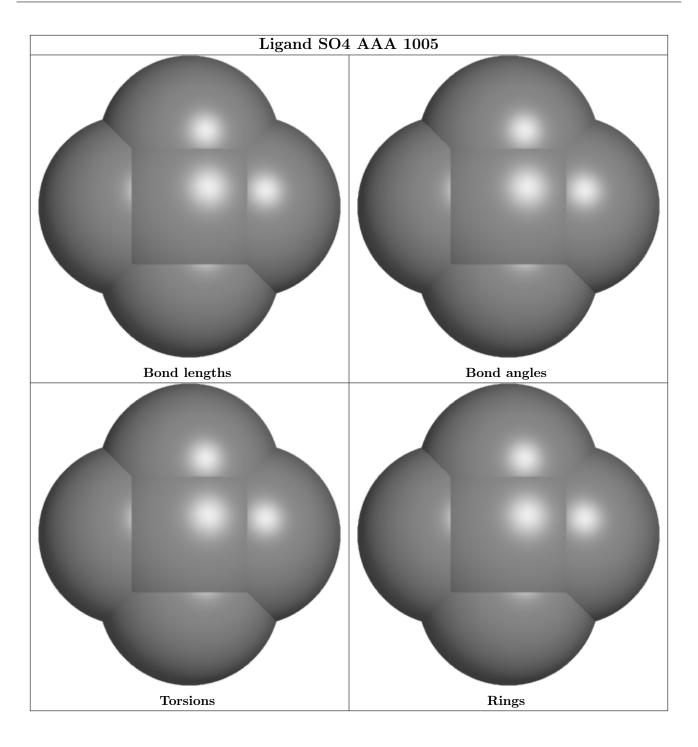
Ligand SO4 AAA 1003

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 AAA 1004

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO AAA 1021

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 AAA 1006

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 AAA 1005

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL AAA 1018

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO AAA 1022

Bond lengths

Bond angles

Torsions

Rings

Ligand PGE AAA 1024

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL AAA 1017

Bond lengths

Bond angles

Torsions

Rings

Ligand NAG AAA 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand SO4 AAA 1007

Bond lengths

Bond angles

Torsions

Rings

wwPDB X-ray Structure Validation Summary Report

Ligand GOL AAA 1019

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO AAA 1020

Bond lengths

Bond angles

Torsions

Rings

Ligand EDO AAA 1023

Bond lengths

Bond angles

Torsions

Rings

Ligand 56I AAA 1002

Bond lengths
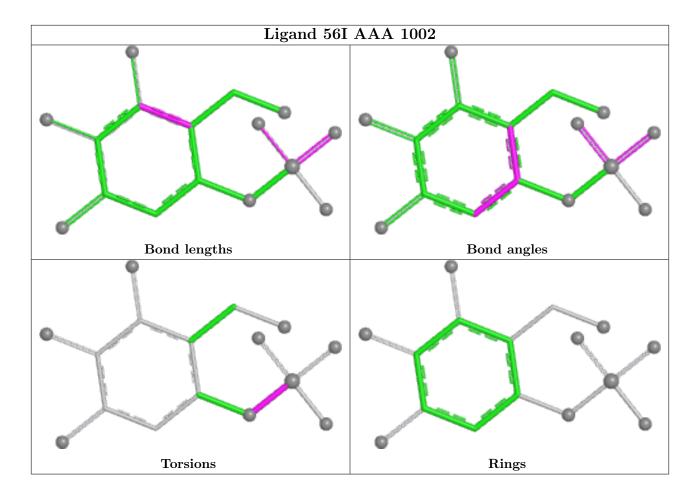

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.