



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2020 – 11:29 am GMT

PDB ID : 6T13
Title : CRYSTAL STRUCTURE OF GLUCOCEREBROSIDASE IN COMPLEX WITH A PYRROLOPYRAZINE
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Deposited on : 2019-10-03
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.15.1
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) : 2.15.1

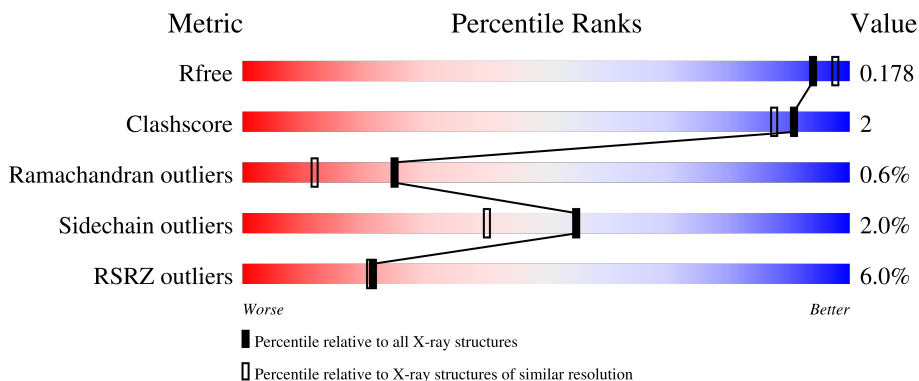
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	A	536	
1	B	536	
1	C	536	
1	D	536	
2	E	2	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 17443 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 Glucosylceramidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	497	Total 3929	C 2532	N 671	O 710	S 16	0	0	0
1	B	497	Total 3929	C 2532	N 671	O 710	S 16	0	0	0
1	C	497	Total 3947	C 2542	N 675	O 714	S 16	0	2	0
1	D	494	Total 3908	C 2518	N 668	O 706	S 16	0	0	0

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



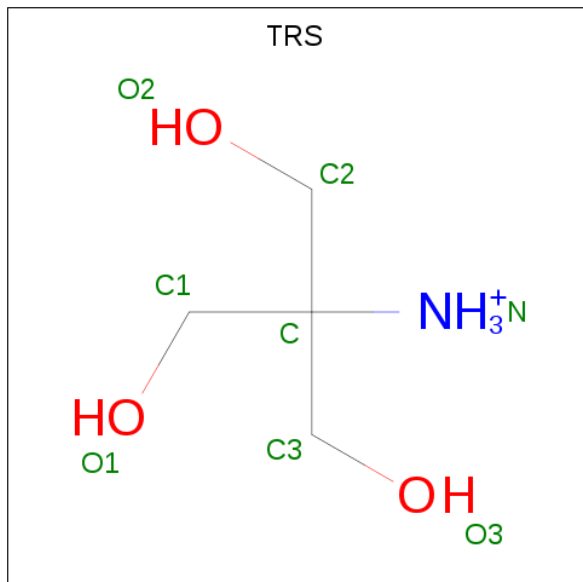
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	2	Total 28	C 16	N 2	O 10	0	0	0

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



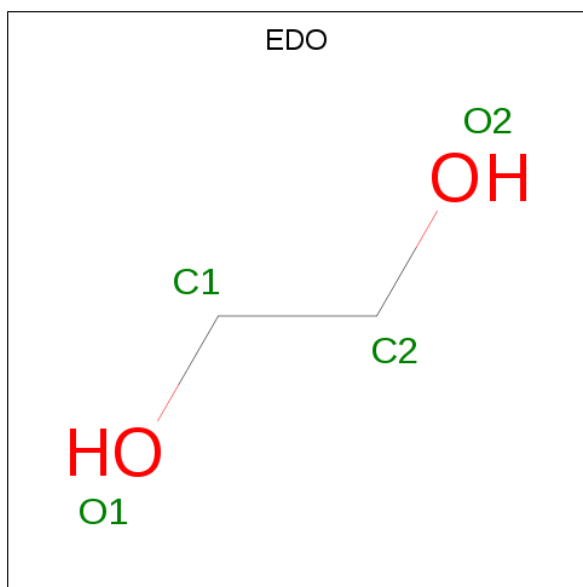
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



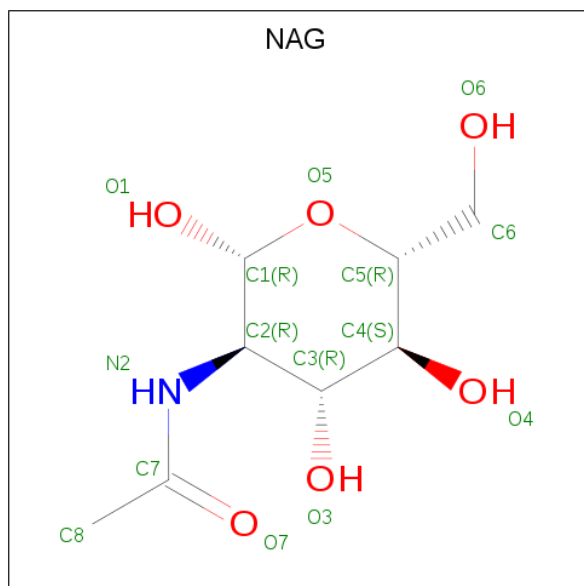
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	8	4	1	3	0	0
4	B	1	8	4	1	3	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



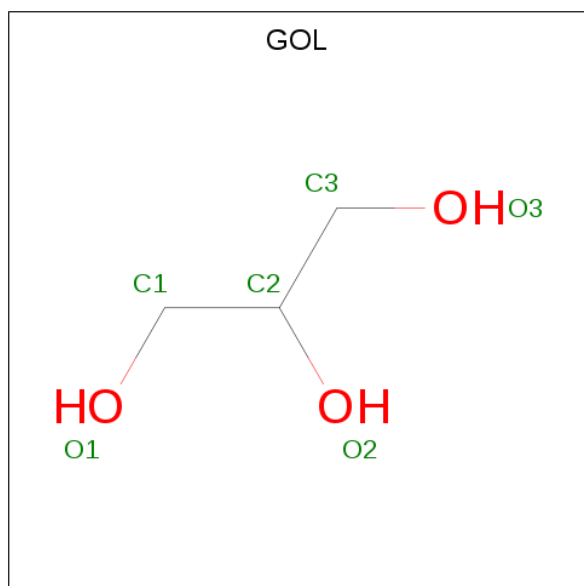
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



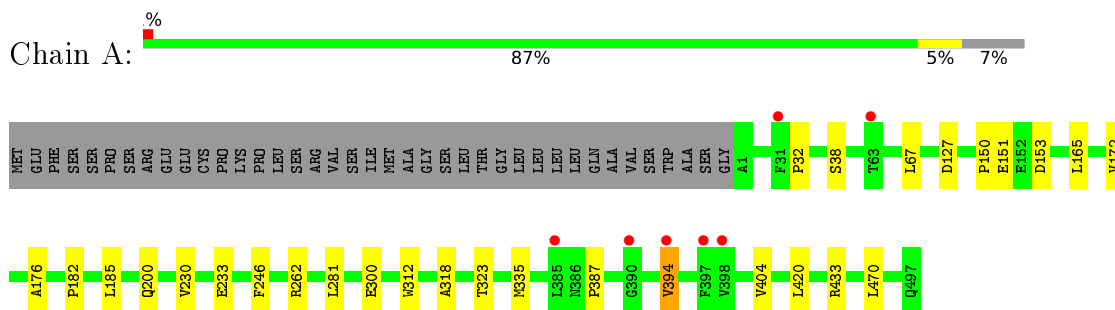
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	B	1	6	3	3	0	0

- Molecule 8 is 1-[4-[2-(4-methoxyphenyl)-5-methyl-pyrrolo[2,3-b]pyrazin-6-yl]piperidin-1-yl] ethanone (three-letter code: M7H) (formula: C₂₁H₂₄N₄O₂) (labeled as "Ligand of Interest" by depositor).

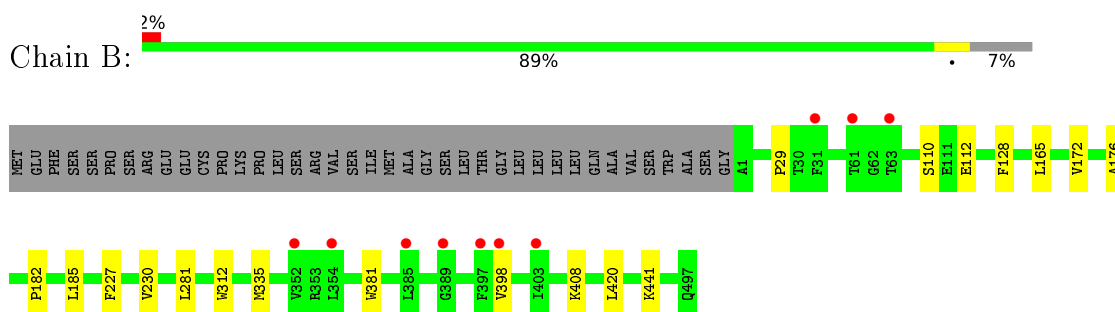
3 Residue-property plots [i](#)

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.

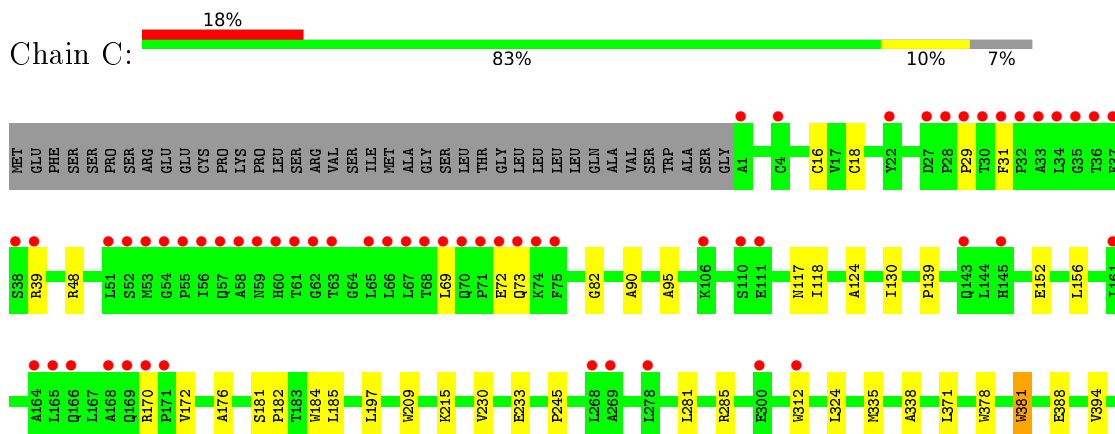
- Molecule 1: Glucosylceramidase

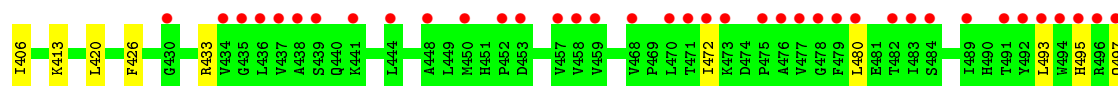


- Molecule 1: Glucosylceramidase

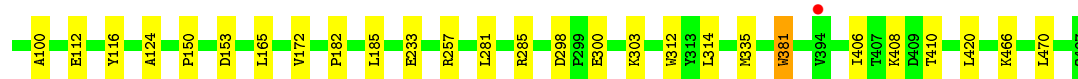
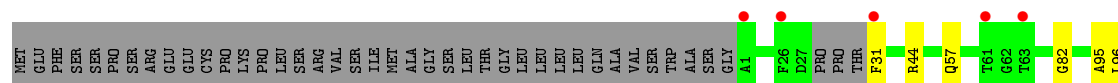
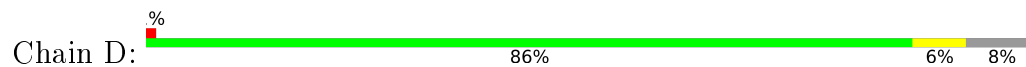


- Molecule 1: Glucosylceramidase





- Molecule 1: Glucosylceramidase



- 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	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.85Å 135.41Å 191.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.71 – 1.85 47.85 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.71-1.85) 99.9 (47.85-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.86Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.174 , 0.204 0.179 , 0.178	Depositor DCC
R_{free} test set	9940 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtrriage
Anisotropy	0.599	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17443	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: GOL, NAG, CL, EDO, SO4, TRS, M7H

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	A	0.54	0/4050	0.66	0/5523
1	B	0.54	0/4050	0.64	0/5523
1	C	0.45	0/4068	0.64	0/5547
1	D	0.49	0/4026	0.64	0/5486
All	All	0.51	0/16194	0.64	0/22079

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 [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	A	3929	0	3843	11	0
1	B	3929	0	3843	8	0
1	C	3947	0	3857	23	0
1	D	3908	0	3821	11	0
2	E	28	0	25	0	0
3	A	20	0	0	0	0
3	B	20	0	0	0	0
3	C	10	0	0	0	0
3	D	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	8	0	12	2	0
4	B	8	0	12	0	0
5	A	12	0	18	0	0
5	B	20	0	30	1	0
5	D	4	0	6	0	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
6	D	14	0	13	0	0
7	B	6	0	8	1	0
8	C	27	0	0	0	0
8	D	27	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	478	0	0	0	0
10	B	463	0	0	0	0
10	C	195	0	0	1	0
10	D	340	0	0	2	0
All	All	17443	0	15514	54	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.

All (54) 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:C:394:VAL:O	1:C:394:VAL:HG12	1.96	0.66
1:D:312:TRP:HD1	1:D:314:LEU:HD23	1.60	0.65
1:C:182:PRO:HD2	1:C:185:LEU:HD12	1.83	0.59
1:B:176:ALA:HB3	1:B:230:VAL:HG12	1.86	0.58
1:A:165:LEU:HD22	1:A:172:VAL:HB	1.86	0.57
1:B:165:LEU:HD22	1:B:172:VAL:HB	1.87	0.56
4:A:507:TRS:H32	10:D:790:HOH:O	2.06	0.55
1:A:67:LEU:HG	1:A:470:LEU:HD11	1.88	0.55
1:B:110:SER:OG	1:B:112:GLU:HG2	2.06	0.55
1:D:408:LYS:O	1:D:410:THR:HG23	2.06	0.55
1:A:176:ALA:HB3	1:A:230:VAL:HG12	1.88	0.54
1:D:182:PRO:HD2	1:D:185:LEU:HD12	1.89	0.53
1:C:312:TRP:HZ2	1:C:324:LEU:HD11	1.73	0.53
1:C:245:PRO:HB2	1:C:394:VAL:HG11	1.91	0.53
1:C:176:ALA:HB3	1:C:230:VAL:HG12	1.92	0.52
1:C:426:PHE:HB3	1:C:493:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:CYS:SG	1:C:413:LYS:HD2	2.52	0.50
1:A:127:ASP:HB3	1:A:246:PHE:CD2	2.47	0.49
1:A:246:PHE:HD2	1:A:394:VAL:HG21	1.77	0.49
1:A:318:ALA:HB1	1:A:323:THR:HG21	1.95	0.48
1:C:472:ILE:HB	1:C:480:LEU:HB2	1.96	0.47
1:C:16:CYS:SG	1:C:48:ARG:HG3	2.54	0.47
1:C:95:ALA:HB1	1:C:406:ILE:HD12	1.96	0.47
4:A:507:TRS:C3	10:D:790:HOH:O	2.63	0.46
1:C:197:LEU:HD11	1:C:209:TRP:CD1	2.50	0.46
1:C:371:LEU:O	1:C:433:ARG:HD2	2.16	0.46
1:C:394:VAL:CG1	1:C:394:VAL:O	2.63	0.45
1:D:300:GLU:HA	1:D:303:LYS:HE2	1.99	0.45
1:C:117:ASN:HA	1:C:172:VAL:HG22	1.98	0.45
1:C:152:GLU:HA	1:C:156:LEU:HD12	1.99	0.45
1:B:29:PRO:HB3	7:B:502:GOL:H2	1.99	0.44
1:D:165:LEU:HD23	1:D:172:VAL:HB	1.97	0.44
1:B:128:PHE:CZ	1:B:398:VAL:HG22	2.53	0.43
1:D:165:LEU:CD2	1:D:172:VAL:HB	2.49	0.43
1:A:182:PRO:HD2	1:A:185:LEU:HD12	2.01	0.43
1:B:408:LYS:HE3	5:B:509:EDO:H11	2.01	0.42
1:D:82:GLY:HA2	1:D:116:TYR:CD1	2.53	0.42
1:D:95:ALA:HB1	1:D:406:ILE:HD12	2.01	0.42
1:C:39:ARG:HD2	10:C:605:HOH:O	2.18	0.42
1:B:176:ALA:HB2	1:B:227:PHE:CE2	2.55	0.42
1:C:31:PHE:HB3	1:C:495:HIS:CE1	2.55	0.42
1:A:32:PRO:HG2	1:A:38:SER:OG	2.20	0.42
1:A:150:PRO:HD2	1:A:153:ASP:OD2	2.20	0.41
1:B:182:PRO:HD2	1:B:185:LEU:HD12	2.01	0.41
1:D:257:ARG:HD2	1:D:298:ASP:HB2	2.03	0.41
1:C:90:ALA:HB1	1:C:156:LEU:HB3	2.02	0.41
1:D:96:LEU:HB3	1:D:100:ALA:HB3	2.02	0.41
1:D:150:PRO:HD2	1:D:153:ASP:OD2	2.20	0.41
1:C:181:SER:HA	1:C:209:TRP:CZ3	2.56	0.41
1:C:139:PRO:HA	1:C:184:TRP:CD1	2.57	0.40
1:A:387:PRO:HD3	1:A:404:VAL:O	2.20	0.40
1:C:338:ALA:HB3	1:C:378:TRP:HA	2.03	0.40
1:C:82:GLY:HA3	1:C:118:ILE:O	2.21	0.40
1:A:151:GLU:HB2	1:C:130:ILE:HD11	2.03	0.40

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	A	495/536 (92%)	477 (96%)	16 (3%)	2 (0%)	34	19
1	B	495/536 (92%)	476 (96%)	18 (4%)	1 (0%)	47	33
1	C	497/536 (93%)	469 (94%)	23 (5%)	5 (1%)	15	5
1	D	490/536 (91%)	470 (96%)	16 (3%)	4 (1%)	19	7
All	All	1977/2144 (92%)	1892 (96%)	73 (4%)	12 (1%)	25	12

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	124	ALA
1	D	233	GLU
1	A	233	GLU
1	D	381	TRP
1	A	281	LEU
1	B	281	LEU
1	C	29	PRO
1	C	124	ALA
1	C	233	GLU
1	C	381	TRP
1	D	281	LEU
1	C	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	A	424/457 (93%)	416 (98%)	8 (2%)	57	43
1	B	424/457 (93%)	419 (99%)	5 (1%)	71	62
1	C	426/457 (93%)	414 (97%)	12 (3%)	43	27
1	D	421/457 (92%)	411 (98%)	10 (2%)	49	33
All	All	1695/1828 (93%)	1660 (98%)	35 (2%)	55	38

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	GLN
1	A	262	ARG
1	A	300	GLU
1	A	312	TRP
1	A	335	MET
1	A	394	VAL
1	A	420	LEU
1	A	433	ARG
1	B	312	TRP
1	B	335	MET
1	B	381	TRP
1	B	420	LEU
1	B	441	LYS
1	C	69	LEU
1	C	72	GLU
1	C	73[A]	GLN
1	C	73[B]	GLN
1	C	170	ARG
1	C	215	LYS
1	C	285	ARG
1	C	335	MET
1	C	381	TRP
1	C	388	GLU
1	C	420	LEU
1	C	497	GLN
1	D	31	PHE
1	D	44	ARG
1	D	57	GLN
1	D	112	GLU
1	D	285	ARG
1	D	335	MET
1	D	381	TRP
1	D	420	LEU

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Mol	Chain	Res	Type
1	D	466	LYS
1	D	470	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	A	350	GLN
1	A	495	HIS
1	B	497	GLN
1	C	169	GLN
1	C	284	GLN
1	D	284	GLN
1	D	374	HIS
1	D	497	GLN

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](#)

2 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	E	1	1,2	14,14,15	0.29	0	17,19,21	0.43	0
2	NAG	E	2	2	14,14,15	0.33	0	17,19,21	0.75	1 (5%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-O5-C5	2.69	115.83	112.19

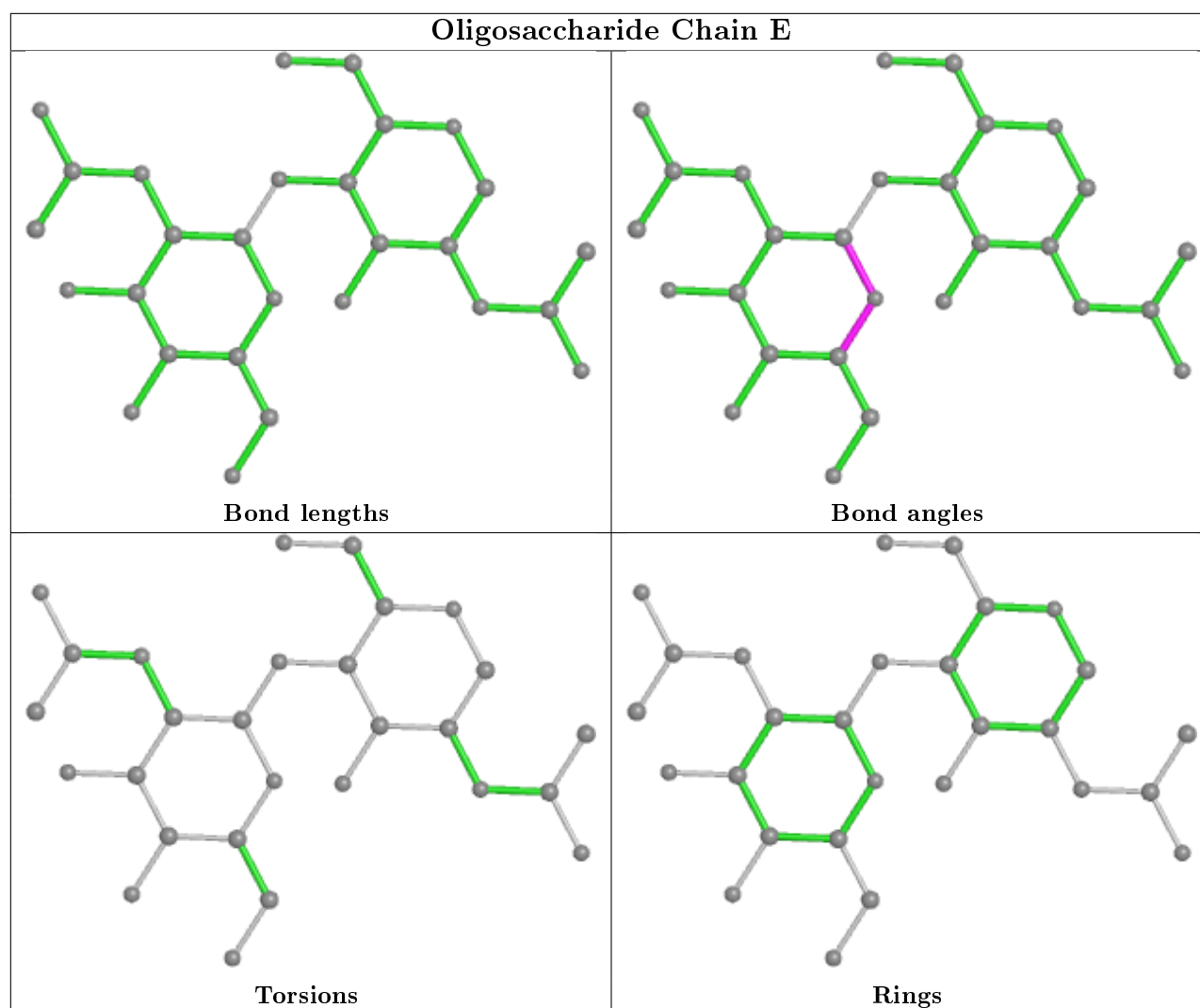
There are no chirality outliers.

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](#)

Of 33 ligands modelled in this entry, 2 are monoatomic - leaving 31 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	$\# Z > 2$
5	EDO	A	509	-	3,3,3	0.52	0	2,2,2	0.45	0
3	SO4	C	504	-	4,4,4	0.20	0	6,6,6	0.16	0
6	NAG	C	501	1	14,14,15	0.28	0	17,19,21	0.46	0
5	EDO	B	510	-	3,3,3	0.42	0	2,2,2	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	504	-	4,4,4	0.15	0	6,6,6	0.20	0
3	SO4	D	503	-	4,4,4	0.26	0	6,6,6	0.35	0
4	TRS	B	507	-	7,7,7	0.27	0	9,9,9	0.31	0
5	EDO	B	512	-	3,3,3	0.42	0	2,2,2	0.46	0
3	SO4	D	505	-	4,4,4	0.17	0	6,6,6	0.19	0
3	SO4	D	506	-	4,4,4	0.25	0	6,6,6	0.18	0
5	EDO	B	511	-	3,3,3	0.49	0	2,2,2	0.44	0
5	EDO	B	509	-	3,3,3	0.34	0	2,2,2	0.64	0
8	M7H	D	502	-	28,30,30	0.81	1 (3%)	36,43,43	1.30	5 (13%)
3	SO4	A	503	-	4,4,4	0.35	0	6,6,6	0.24	0
7	GOL	B	502	-	5,5,5	0.06	0	5,5,5	0.11	0
3	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.21	0
3	SO4	B	506	-	4,4,4	0.18	0	6,6,6	0.17	0
3	SO4	B	505	-	4,4,4	0.12	0	6,6,6	0.30	0
6	NAG	B	501	1	14,14,15	0.44	0	17,19,21	1.45	4 (23%)
3	SO4	C	503	-	4,4,4	0.23	0	6,6,6	0.25	0
3	SO4	B	503	-	4,4,4	0.34	0	6,6,6	0.30	0
3	SO4	B	504	-	4,4,4	0.15	0	6,6,6	0.37	0
3	SO4	A	505	-	4,4,4	0.16	0	6,6,6	0.23	0
5	EDO	A	508	-	3,3,3	0.57	0	2,2,2	0.19	0
5	EDO	A	510	-	3,3,3	0.63	0	2,2,2	0.23	0
3	SO4	A	504	-	4,4,4	0.23	0	6,6,6	0.17	0
5	EDO	B	508	-	3,3,3	1.03	0	2,2,2	0.23	0
8	M7H	C	502	-	28,30,30	0.78	0	36,43,43	1.25	4 (11%)
6	NAG	D	501	1	14,14,15	0.32	0	17,19,21	0.39	0
4	TRS	A	507	-	7,7,7	0.25	0	9,9,9	0.35	0
5	EDO	D	508	-	3,3,3	0.50	0	2,2,2	0.57	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
6	NAG	D	501	1	-	0/6/23/26	0/1/1/1
5	EDO	A	509	-	-	1/1/1/1	-
4	TRS	A	507	-	-	0/9/9/9	-
6	NAG	C	501	1	-	0/6/23/26	0/1/1/1
7	GOL	B	502	-	-	0/4/4/4	-
5	EDO	B	510	-	-	0/1/1/1	-
5	EDO	B	509	-	-	1/1/1/1	-
4	TRS	B	507	-	-	2/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	508	-	-	0/1/1/1	-
5	EDO	B	512	-	-	0/1/1/1	-
5	EDO	D	508	-	-	0/1/1/1	-
8	M7H	D	502	-	-	2/14/24/24	0/4/4/4
5	EDO	A	510	-	-	1/1/1/1	-
6	NAG	B	501	1	-	1/6/23/26	0/1/1/1
5	EDO	B	508	-	-	0/1/1/1	-
5	EDO	B	511	-	-	0/1/1/1	-
8	M7H	C	502	-	-	1/14/24/24	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	502	M7H	C10-N6	2.15	1.36	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	502	M7H	C10-N6-C5	-3.70	115.31	118.06
6	B	501	NAG	C1-C2-N2	3.68	116.78	110.49
8	C	502	M7H	C10-N6-C5	-3.50	115.47	118.06
8	C	502	M7H	C12-N7-C3	-2.98	112.92	116.73
8	D	502	M7H	C12-N7-C3	-2.93	112.98	116.73
6	B	501	NAG	C1-O5-C5	2.78	115.96	112.19
8	C	502	M7H	C4-C2-N1	2.77	109.08	105.65
8	D	502	M7H	C18-C11-C2	2.70	115.44	112.06
8	C	502	M7H	C17-C11-C2	2.64	115.37	112.06
8	D	502	M7H	C4-C2-N1	2.49	108.74	105.65
6	B	501	NAG	C2-N2-C7	2.48	126.43	122.90
6	B	501	NAG	O5-C1-C2	2.45	115.16	111.29
8	D	502	M7H	C21-N1-C2	2.28	126.32	124.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	501	NAG	C1-C2-N2-C7
5	A	510	EDO	O1-C1-C2-O2
4	B	507	TRS	N-C-C1-O1
5	A	509	EDO	O1-C1-C2-O2
4	B	507	TRS	C2-C-C1-O1

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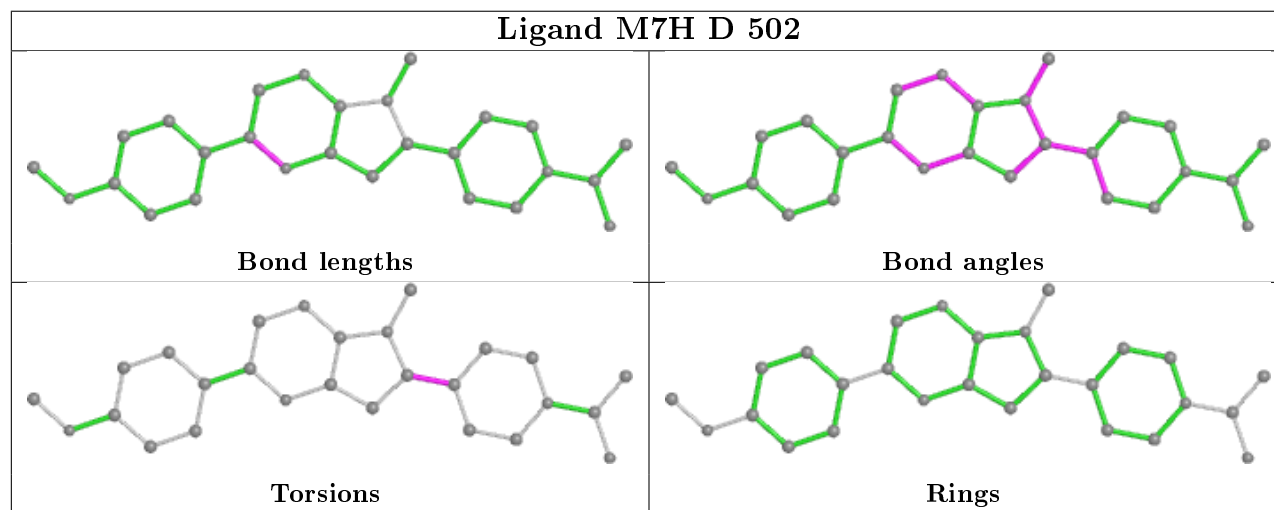
Mol	Chain	Res	Type	Atoms
8	D	502	M7H	C18-C11-C2-C4
8	D	502	M7H	C18-C11-C2-N1
8	C	502	M7H	C18-C11-C2-C4
5	B	509	EDO	O1-C1-C2-O2

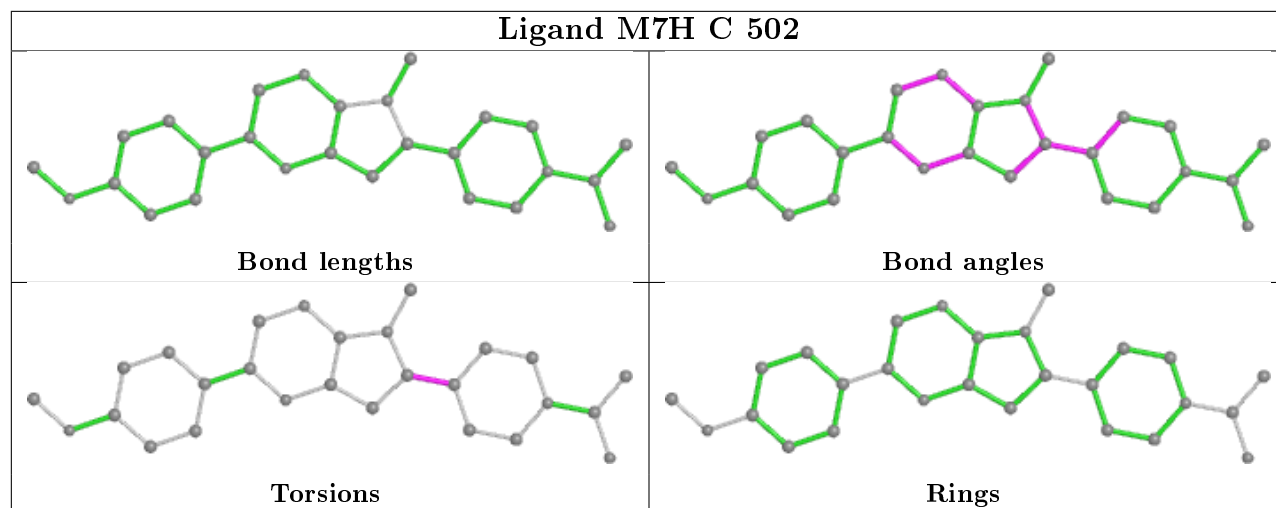
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	509	EDO	1	0
7	B	502	GOL	1	0
4	A	507	TRS	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	497/536 (92%)	-0.17	7 (1%) 75 76	23, 37, 59, 75	0
1	B	497/536 (92%)	-0.11	10 (2%) 65 64	25, 40, 62, 82	0
1	C	497/536 (92%)	1.05	96 (19%) 1 1	36, 74, 151, 181	0
1	D	494/536 (92%)	-0.10	6 (1%) 79 79	31, 48, 72, 96	0
All	All	1985/2144 (92%)	0.17	119 (5%) 21 21	23, 46, 106, 181	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	31	PHE	13.5
1	C	472	ILE	8.6
1	C	470	LEU	8.1
1	C	69	LEU	7.5
1	C	437	VAL	7.5
1	C	450	MET	7.4
1	C	29	PRO	7.4
1	C	434	VAL	7.3
1	C	58	ALA	7.1
1	C	32	PRO	6.8
1	C	480	LEU	6.7
1	C	493	LEU	6.6
1	C	62	GLY	6.6
1	C	492	TYR	6.4
1	C	36	THR	6.4
1	C	68	THR	6.4
1	C	67	LEU	6.2
1	B	31	PHE	6.0
1	C	59	ASN	6.0
1	C	477	VAL	5.8
1	C	483	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	1	ALA	5.6
1	C	56	ILE	5.6
1	C	479	PHE	5.6
1	C	37	PHE	5.6
1	D	63	THR	5.5
1	C	478	GLY	5.3
1	C	73[A]	GLN	5.2
1	C	60	HIS	5.0
1	C	494	TRP	5.0
1	C	61	THR	4.9
1	C	57[A]	GLN	4.9
1	C	435	GLY	4.8
1	C	473	LYS	4.6
1	C	452	PRO	4.5
1	C	72	GLU	4.3
1	C	495	HIS	4.2
1	C	471	THR	4.1
1	C	33	ALA	4.1
1	B	63	THR	4.0
1	A	31	PHE	4.0
1	C	30	THR	4.0
1	C	476	ALA	4.0
1	C	54	GLY	4.0
1	C	497	GLN	4.0
1	C	22	TYR	3.9
1	D	61	THR	3.9
1	C	468	VAL	3.8
1	C	436	LEU	3.8
1	C	35	GLY	3.5
1	C	74	LYS	3.5
1	C	55	PRO	3.4
1	C	458	VAL	3.3
1	C	300	GLU	3.2
1	C	169	GLN	3.1
1	C	171	PRO	3.1
1	C	34	LEU	3.1
1	C	71	PRO	3.1
1	C	269	ALA	3.1
1	C	65	LEU	3.1
1	B	61	THR	3.0
1	C	168	ALA	3.0
1	C	489	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	38	SER	3.0
1	A	397	PHE	3.0
1	C	312	TRP	3.0
1	C	70	GLN	2.9
1	C	75	PHE	2.9
1	C	63	THR	2.9
1	C	491	THR	2.8
1	C	28	PRO	2.8
1	C	51	LEU	2.8
1	C	482	THR	2.7
1	C	39	ARG	2.7
1	B	397	PHE	2.6
1	C	496	ARG	2.6
1	D	1	ALA	2.6
1	C	4	CYS	2.6
1	C	444	LEU	2.6
1	C	268	LEU	2.6
1	A	63	THR	2.6
1	D	26	PHE	2.5
1	C	27	ASP	2.5
1	C	52	SER	2.5
1	B	398	VAL	2.5
1	C	143	GLN	2.5
1	A	398	VAL	2.5
1	C	145	HIS	2.4
1	C	165	LEU	2.4
1	B	389	GLY	2.4
1	C	430	GLY	2.4
1	C	439	SER	2.4
1	B	352	VAL	2.4
1	C	457	VAL	2.4
1	B	354	LEU	2.4
1	C	278	LEU	2.4
1	A	394	VAL	2.3
1	C	164	ALA	2.3
1	C	475	PRO	2.3
1	C	66	LEU	2.3
1	C	110	SER	2.3
1	C	453	ASP	2.3
1	C	448	ALA	2.3
1	C	441	LYS	2.3
1	D	31	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	438	ALA	2.2
1	D	394	VAL	2.2
1	C	484	SER	2.2
1	B	385	LEU	2.2
1	B	403	ILE	2.2
1	C	161	ILE	2.2
1	C	53	MET	2.2
1	A	390	GLY	2.2
1	C	459	VAL	2.1
1	A	385	LEU	2.1
1	C	106	LYS	2.1
1	C	111	GLU	2.1
1	C	170	ARG	2.1
1	C	166	GLN	2.0

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

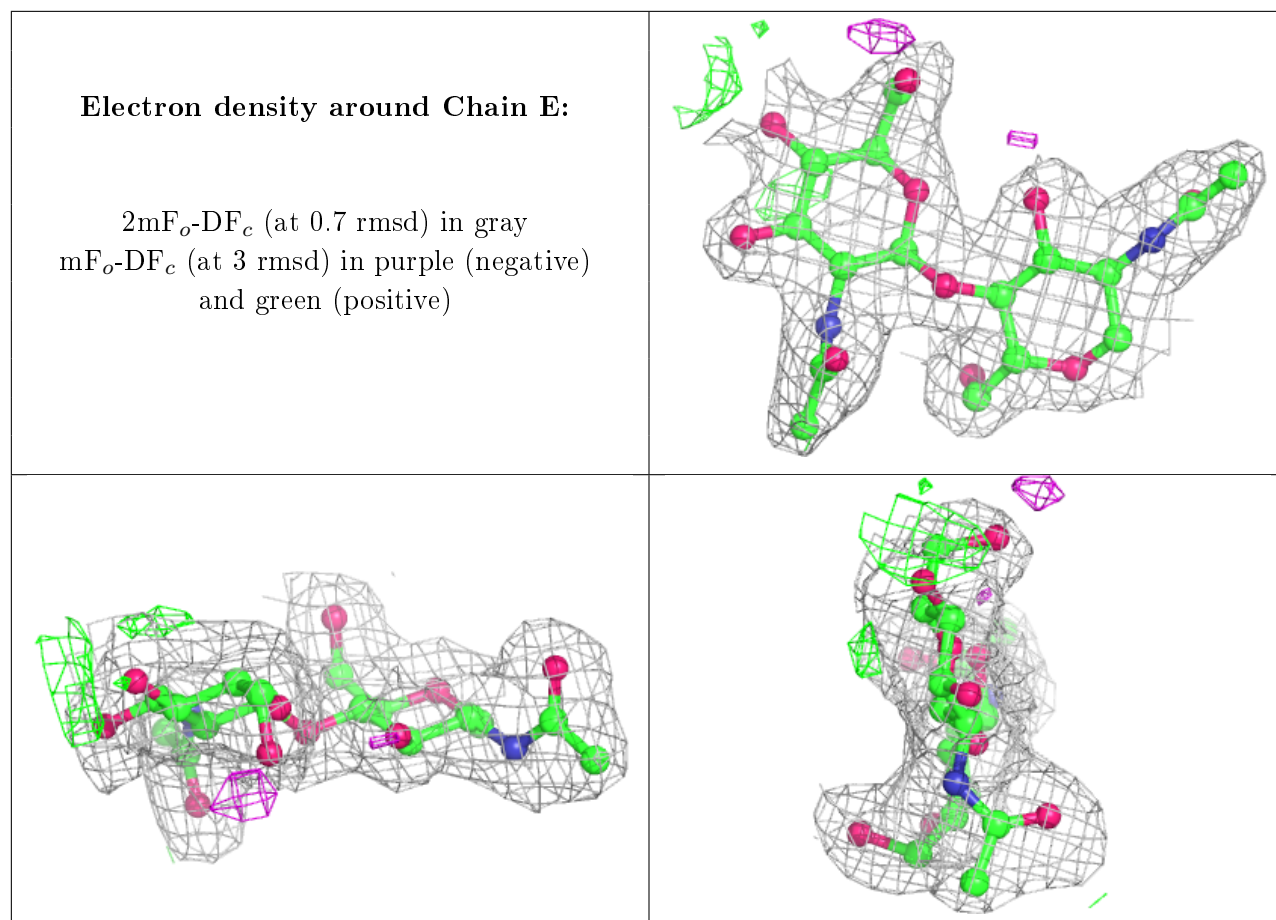
There are no non-standard protein/DNA/RNA residues in this entry.

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	E	2	14/15	0.92	0.14	46,53,63,68	0
2	NAG	E	1	14/15	0.95	0.08	40,43,48,52	0

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(Å ²)	Q<0.9
6	NAG	B	501	14/15	0.74	0.17	52,58,61,64	0
7	GOL	B	502	6/6	0.77	0.17	83,83,84,84	0
4	TRS	A	507	8/8	0.79	0.26	54,62,69,72	0
5	EDO	A	509	4/4	0.84	0.16	45,48,55,57	0
5	EDO	B	509	4/4	0.87	0.21	50,54,56,57	0
3	SO4	A	506	5/5	0.87	0.13	111,111,111,112	0
4	TRS	B	507	8/8	0.88	0.15	39,48,51,53	0
3	SO4	C	504	5/5	0.88	0.18	110,110,112,112	0
6	NAG	C	501	14/15	0.89	0.13	96,99,103,106	0
6	NAG	D	501	14/15	0.89	0.11	66,68,74,75	0
3	SO4	B	506	5/5	0.89	0.12	124,125,125,125	0
5	EDO	A	510	4/4	0.91	0.19	52,56,62,67	0

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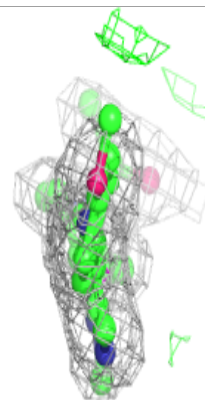
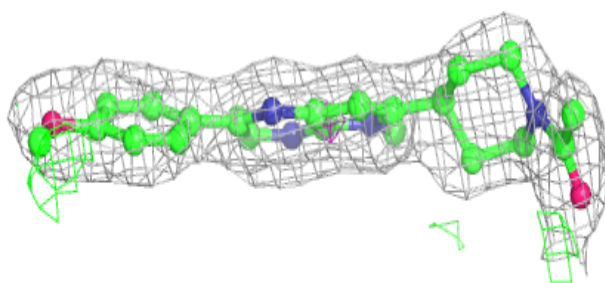
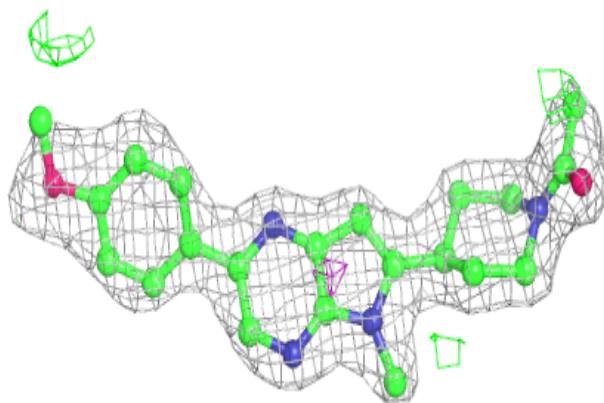
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	D	508	4/4	0.91	0.24	56,58,59,60	0
8	M7H	C	502	27/27	0.92	0.12	42,45,51,56	0
5	EDO	A	508	4/4	0.92	0.09	62,63,65,67	0
3	SO4	D	506	5/5	0.93	0.13	75,77,81,82	0
5	EDO	B	508	4/4	0.93	0.16	35,37,38,45	0
3	SO4	B	505	5/5	0.93	0.18	79,81,82,83	0
3	SO4	A	505	5/5	0.94	0.13	81,82,86,87	0
5	EDO	B	512	4/4	0.94	0.14	49,54,59,62	0
5	EDO	B	510	4/4	0.94	0.25	43,48,52,55	0
5	EDO	B	511	4/4	0.94	0.18	45,48,54,58	0
3	SO4	D	504	5/5	0.95	0.10	72,76,77,79	0
9	CL	C	505	1/1	0.95	0.08	53,53,53,53	0
3	SO4	D	505	5/5	0.96	0.10	82,83,85,85	0
8	M7H	D	502	27/27	0.96	0.13	30,35,44,54	0
9	CL	D	507	1/1	0.97	0.09	37,37,37,37	0
3	SO4	B	504	5/5	0.98	0.09	57,57,59,60	0
3	SO4	D	503	5/5	0.99	0.09	41,42,43,43	0
3	SO4	C	503	5/5	0.99	0.08	57,60,62,63	0
3	SO4	A	504	5/5	0.99	0.12	61,61,62,64	0
3	SO4	B	503	5/5	0.99	0.12	37,37,43,43	0
3	SO4	A	503	5/5	1.00	0.13	30,31,34,40	0

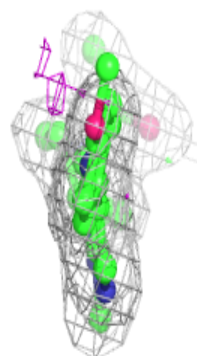
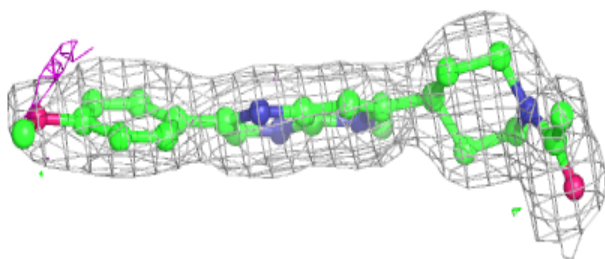
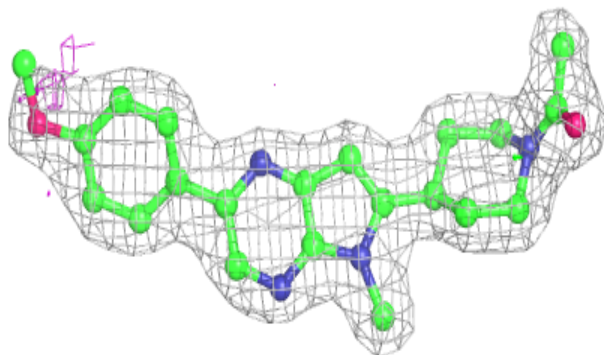
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around M7H C 502:

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

**Electron density around M7H D 502:**

$2mF_o-DF_c$ (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.