



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:54 PM UTC

PDB ID : 6T13 / pdb_00006t13
Title : CRYSTAL STRUCTURE OF GLUCOCEREBROSIDASE IN COMPLEX WITH A PYRROLOPYRAZINE
Authors : Benz, J.; Ehler, A.; Hug, M.; Huber, S.; Rufer, A.C.; Guba, W.; Jagasia, R.; Hofmann, E.C.; Rodriguez Sarmiento, R.M.
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 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

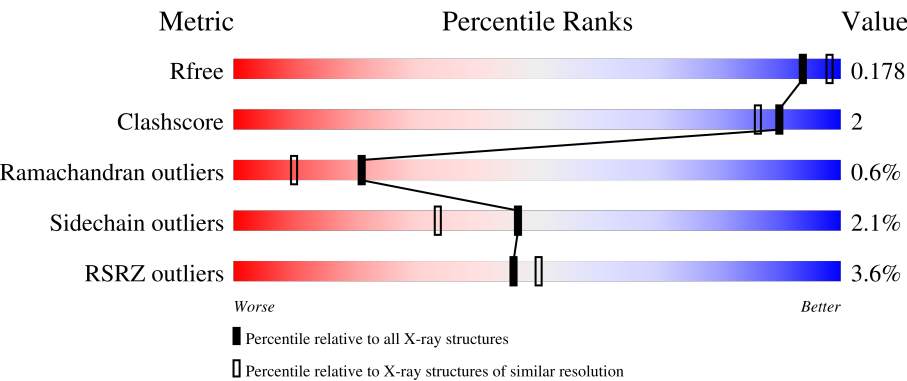
1 Overall quality at a glance i

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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (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	% 86%6%7%
1	B	536	88%5%7%
1	C	536	11% 81%11%7%
1	D	536	% 85%7%8%

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Mol	Chain	Length	Quality of chain
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
1	A	497	Total	C	N	O	S	0	0	0
			3929	2532	671	710	16			
1	B	497	Total	C	N	O	S	0	0	0
			3929	2532	671	710	16			
1	C	497	Total	C	N	O	S	0	2	0
			3947	2542	675	714	16			
1	D	494	Total	C	N	O	S	0	0	0
			3908	2518	668	706	16			

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



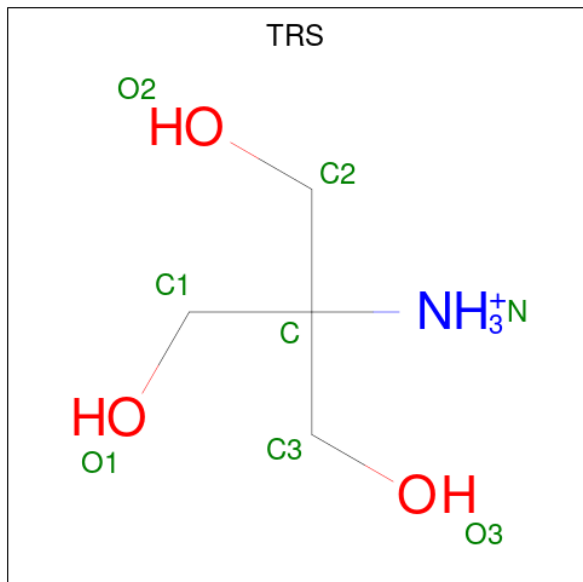
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



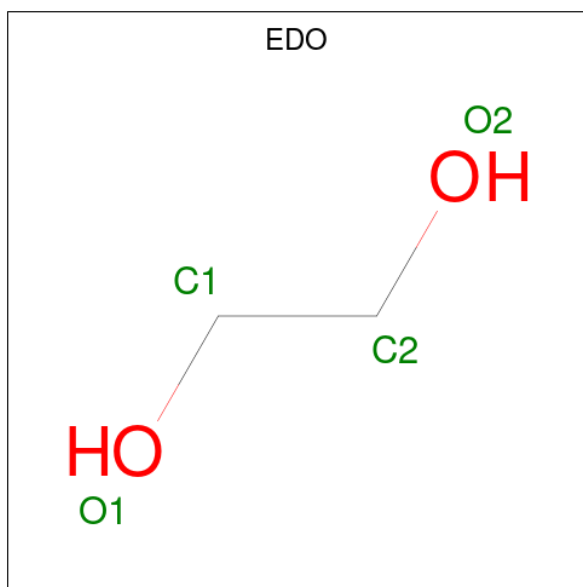
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	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 (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



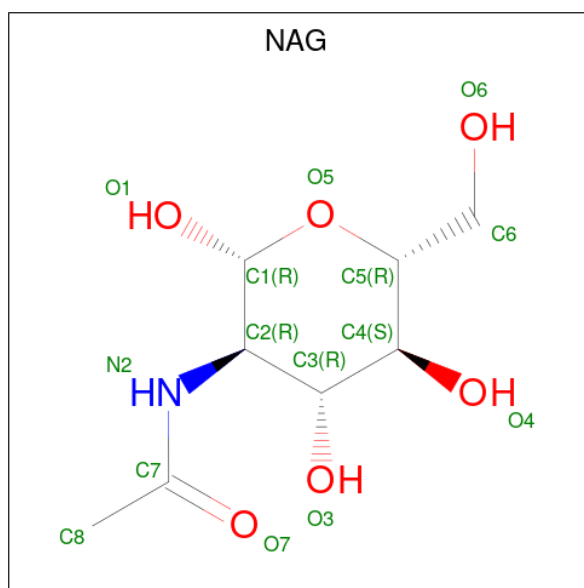
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: 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	D	1	Total C O 4 2 2	0	0

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



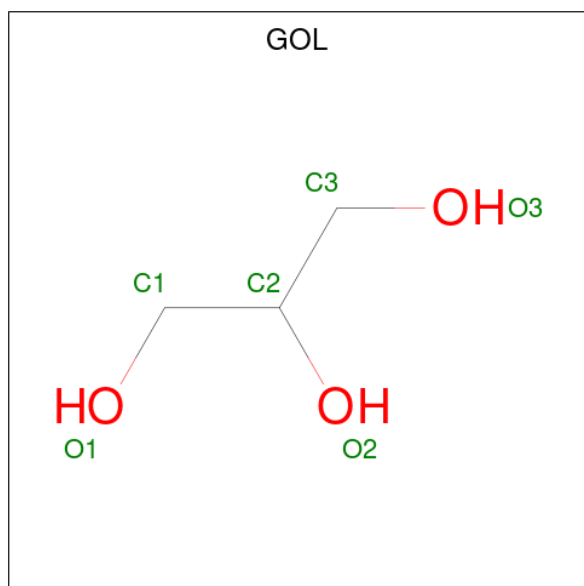
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0

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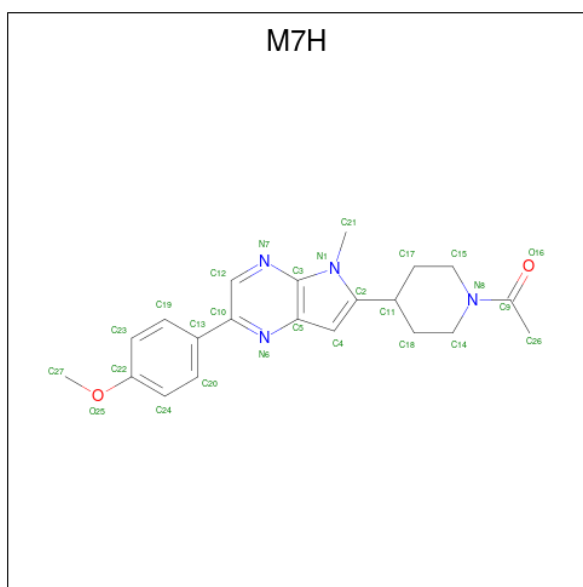
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is 1-[4-[2-(4-methoxyphenyl)-5-methyl-pyrrolo[2,3-b]pyrazin-6-yl]piperidin-1-yl]ethanone (CCD ID: M7H) (formula: $C_{21}H_{24}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			27	21	4	2		
8	D	1	Total	C	N	O	0	0
			27	21	4	2		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Cl	0	0
			1	1		
9	D	1	Total	Cl	0	0
			1	1		

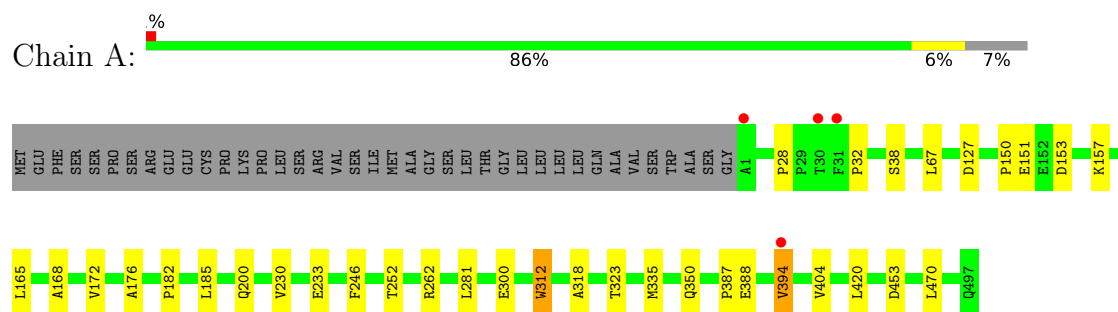
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	478	Total	O	0	0
			478	478		
10	B	463	Total	O	0	0
			463	463		
10	C	195	Total	O	0	0
			195	195		
10	D	340	Total	O	0	0
			340	340		

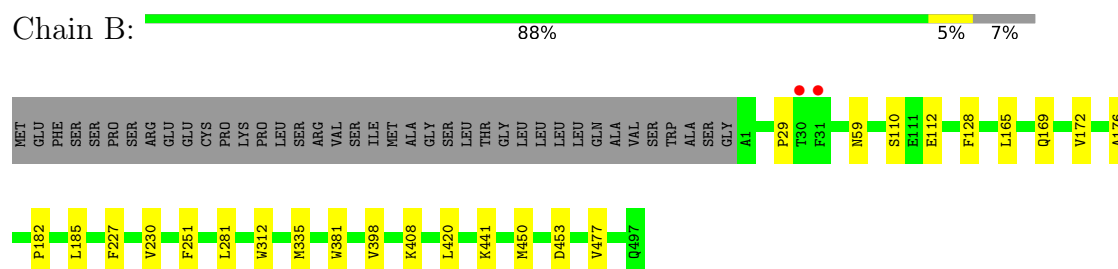
3 Residue-property plots [i](#)

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.

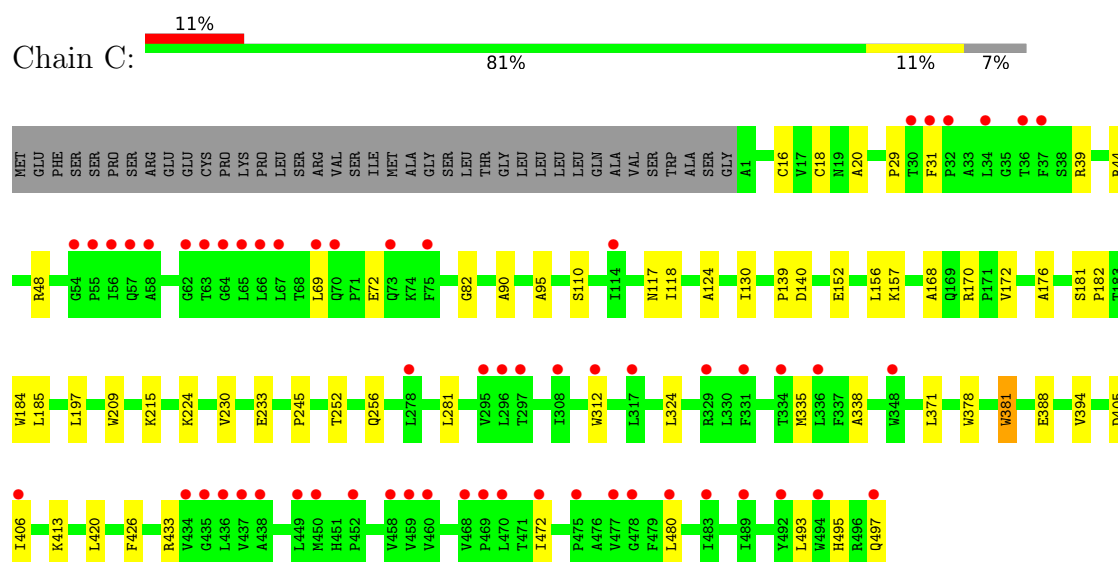
• Molecule 1: Glucosylceramidase



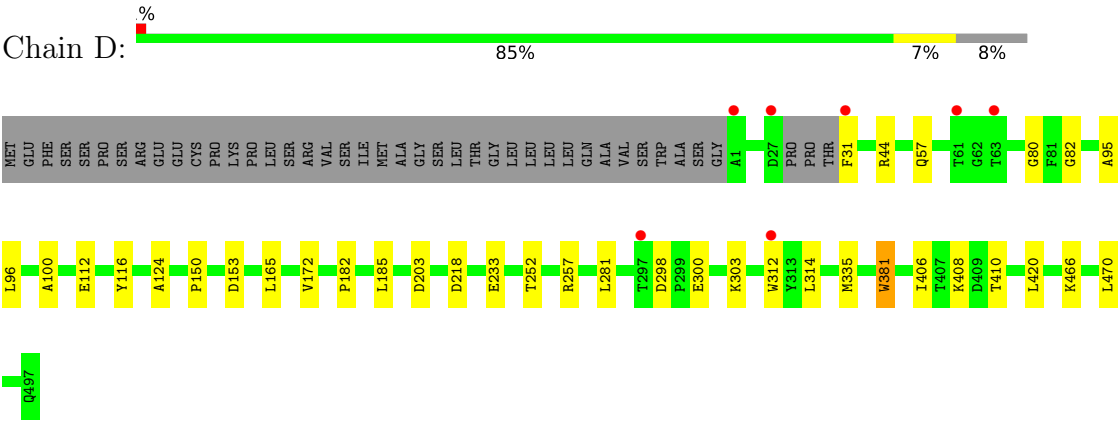
• Molecule 1: Glucosylceramidase



• 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 48.71 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.71-1.85) 99.9 (48.71-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.86Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.174 , 0.204 0.180 , 0.178	Depositor DCC
R_{free} test set	9940 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.599	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	17443	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, GOL, M7H, SO4, NAG, TRS, CL

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	0.85	1/4050 (0.0%)	1.12	8/5523 (0.1%)
1	B	0.86	0/4050	1.10	3/5523 (0.1%)
1	C	0.78	0/4068	1.22	13/5547 (0.2%)
1	D	0.81	0/4026	1.13	4/5486 (0.1%)
All	All	0.83	1/16194 (0.0%)	1.14	28/22079 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	PRO	CA-C	5.22	1.54	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	ALA	CA-C-N	7.65	130.75	120.65
1	A	168	ALA	C-N-CA	7.65	130.75	120.65
1	C	405	ASP	CA-C-N	6.36	128.80	120.60
1	C	405	ASP	C-N-CA	6.36	128.80	120.60
1	D	252	THR	N-CA-C	-6.20	101.09	110.39
1	D	203	ASP	CA-CB-CG	6.18	118.78	112.60
1	C	110	SER	CA-C-N	6.12	128.47	120.28
1	C	110	SER	C-N-CA	6.12	128.47	120.28
1	C	168	ALA	CA-C-N	6.01	128.61	120.44
1	C	168	ALA	C-N-CA	6.01	128.61	120.44
1	A	252	THR	N-CA-C	-5.57	101.94	110.07
1	A	350	GLN	N-CA-C	-5.53	101.67	109.96
1	C	252	THR	N-CA-C	-5.50	102.29	110.20
1	A	157	LYS	CA-C-N	5.44	124.68	120.33
1	A	157	LYS	C-N-CA	5.44	124.68	120.33
1	A	453	ASP	CA-CB-CG	5.41	118.01	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	ASN	CA-CB-CG	5.30	117.90	112.60
1	B	453	ASP	CA-CB-CG	5.26	117.86	112.60
1	C	256	GLN	CA-C-N	5.24	127.61	120.54
1	C	256	GLN	C-N-CA	5.24	127.61	120.54
1	D	80	GLY	N-CA-C	5.22	117.07	110.38
1	C	157	LYS	CA-C-N	5.18	124.47	120.33
1	C	157	LYS	C-N-CA	5.18	124.47	120.33
1	B	251	PHE	CA-CB-CG	5.12	118.92	113.80
1	C	20	ALA	CA-C-N	5.10	130.63	121.66
1	C	20	ALA	C-N-CA	5.10	130.63	121.66
1	A	388	GLU	CB-CG-CD	5.07	121.23	112.60
1	D	218	ASP	CA-CB-CG	5.07	117.67	112.60

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	A	3929	0	3843	12	0
1	B	3929	0	3843	9	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	56	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 (56) 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:HG12	1:C:394:VAL:O	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:C:394:VAL:CG1	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:A:312:TRP:CD1	1:A:312:TRP:C	2.99	0.40
1:C:139:PRO:HA	1:C:184:TRP:CD1	2.57	0.40
1:B:450:MET:HE3	1:B:450:MET:HB2	1.96	0.40
1:A:387:PRO:HD3	1:A:404:VAL:O	2.20	0.40
1:C:82:GLY:HA3	1:C:118:ILE:O	2.21	0.40
1:C:338:ALA:HB3	1:C:378:TRP:HA	2.03	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 ⓘ

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	A	495/536 (92%)	477 (96%)	16 (3%)	2 (0%)	30	17
1	B	495/536 (92%)	476 (96%)	18 (4%)	1 (0%)	43	31
1	C	497/536 (93%)	469 (94%)	23 (5%)	5 (1%)	12	4
1	D	490/536 (91%)	470 (96%)	16 (3%)	4 (1%)	16	6
All	All	1977/2144 (92%)	1892 (96%)	73 (4%)	12 (1%)	21	10

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 ⓘ

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%)	417 (98%)	7 (2%)	53	42
1	B	424/457 (93%)	417 (98%)	7 (2%)	53	42
1	C	426/457 (93%)	414 (97%)	12 (3%)	38	23
1	D	421/457 (92%)	412 (98%)	9 (2%)	47	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1695/1828 (93%)	1660 (98%)	35 (2%)	47 33

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	B	169	GLN
1	B	312	TRP
1	B	335	MET
1	B	381	TRP
1	B	420	LEU
1	B	441	LYS
1	B	477	VAL
1	C	44	ARG
1	C	69	LEU
1	C	72	GLU
1	C	140	ASP
1	C	170	ARG
1	C	215	LYS
1	C	224	LYS
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	335	MET
1	D	381	TRP
1	D	420	LEU
1	D	466	LYS
1	D	470	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	200	GLN
1	A	223	HIS
1	A	350	GLN
1	A	365	HIS
1	A	495	HIS
1	B	57	GLN
1	B	145	HIS
1	B	223	HIS
1	B	497	GLN
1	C	59	ASN
1	C	169	GLN
1	C	306	HIS
1	C	440	GLN
1	C	442	ASN
1	D	223	HIS
1	D	432	GLN
1	D	440	GLN
1	D	497	GLN

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 ⓘ

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	0.44	0
2	NAG	E	2	2	14,14,15	0.34	0	17,19,21	0.77	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	2.72	115.83	112.19

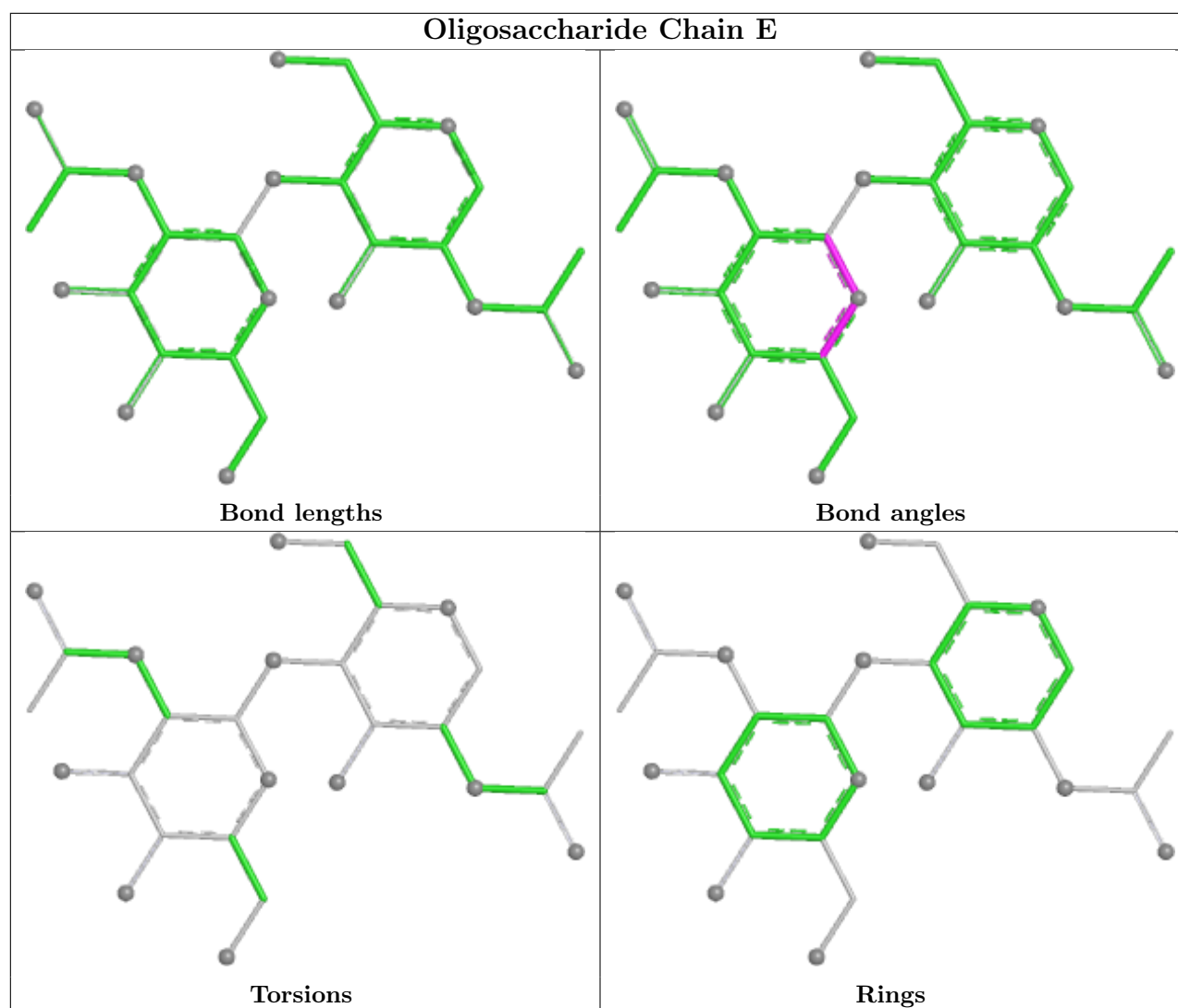
There are no chirality outliers.

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	$\# Z > 2$
3	SO4	B	505	-	4,4,4	0.18	0	6,6,6	0.30	0
3	SO4	A	505	-	4,4,4	0.27	0	6,6,6	0.20	0
5	EDO	B	511	-	3,3,3	0.44	0	2,2,2	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	M7H	D	502	-	29,30,30	0.45	0	36,43,43	0.89	1 (2%)
4	TRS	B	507	-	7,7,7	0.32	0	9,9,9	0.37	0
5	EDO	A	508	-	3,3,3	0.51	0	2,2,2	0.24	0
3	SO4	D	505	-	4,4,4	0.29	0	6,6,6	0.15	0
3	SO4	A	506	-	4,4,4	0.26	0	6,6,6	0.24	0
3	SO4	B	503	-	4,4,4	0.42	0	6,6,6	0.29	0
5	EDO	B	508	-	3,3,3	0.95	0	2,2,2	0.25	0
5	EDO	B	510	-	3,3,3	0.38	0	2,2,2	0.46	0
5	EDO	B	512	-	3,3,3	0.38	0	2,2,2	0.50	0
5	EDO	D	508	-	3,3,3	0.45	0	2,2,2	0.59	0
3	SO4	C	504	-	4,4,4	0.31	0	6,6,6	0.18	0
3	SO4	A	504	-	4,4,4	0.28	0	6,6,6	0.18	0
8	M7H	C	502	-	29,30,30	0.45	0	36,43,43	0.86	2 (5%)
3	SO4	D	503	-	4,4,4	0.20	0	6,6,6	0.33	0
3	SO4	C	503	-	4,4,4	0.28	0	6,6,6	0.24	0
6	NAG	D	501	1	14,14,15	0.33	0	17,19,21	0.41	0
6	NAG	B	501	1	14,14,15	0.45	0	17,19,21	1.53	4 (23%)
5	EDO	A	509	-	3,3,3	0.49	0	2,2,2	0.46	0
3	SO4	B	506	-	4,4,4	0.28	0	6,6,6	0.19	0
4	TRS	A	507	-	7,7,7	0.31	0	9,9,9	0.43	0
3	SO4	A	503	-	4,4,4	0.32	0	6,6,6	0.23	0
6	NAG	C	501	1	14,14,15	0.29	0	17,19,21	0.47	0
5	EDO	B	509	-	3,3,3	0.32	0	2,2,2	0.67	0
3	SO4	B	504	-	4,4,4	0.25	0	6,6,6	0.38	0
3	SO4	D	504	-	4,4,4	0.25	0	6,6,6	0.24	0
3	SO4	D	506	-	4,4,4	0.35	0	6,6,6	0.16	0
5	EDO	A	510	-	3,3,3	0.56	0	2,2,2	0.25	0
7	GOL	B	502	-	5,5,5	0.06	0	5,5,5	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	510	-	-	0/1/1/1	-
4	TRS	A	507	-	-	1/9/9/9	-
6	NAG	C	501	1	-	0/6/23/26	0/1/1/1
5	EDO	B	509	-	-	1/1/1/1	-
5	EDO	B	511	-	-	0/1/1/1	-
8	M7H	D	502	-	-	2/14/24/24	0/4/4/4
7	GOL	B	502	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	501	1	-	0/6/23/26	0/1/1/1
4	TRS	B	507	-	-	2/9/9/9	-
5	EDO	A	508	-	-	0/1/1/1	-
5	EDO	D	508	-	-	0/1/1/1	-
6	NAG	B	501	1	-	1/6/23/26	0/1/1/1
8	M7H	C	502	-	-	0/14/24/24	0/4/4/4
5	EDO	B	508	-	-	0/1/1/1	-
5	EDO	B	512	-	-	0/1/1/1	-
5	EDO	A	510	-	-	1/1/1/1	-
5	EDO	A	509	-	-	1/1/1/1	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	NAG	C1-C2-N2	4.03	116.78	110.43
6	B	501	NAG	C1-O5-C5	2.82	115.96	112.19
6	B	501	NAG	C2-N2-C7	2.63	126.43	122.90
6	B	501	NAG	O5-C1-C2	2.50	115.16	111.29
8	D	502	M7H	C18-C11-C2	2.14	115.44	111.78
8	C	502	M7H	C17-C11-C2	2.10	115.37	111.78
8	C	502	M7H	C21-N1-C3	2.06	127.45	124.69

There are no chirality outliers.

All (9) torsion outliers are listed below:

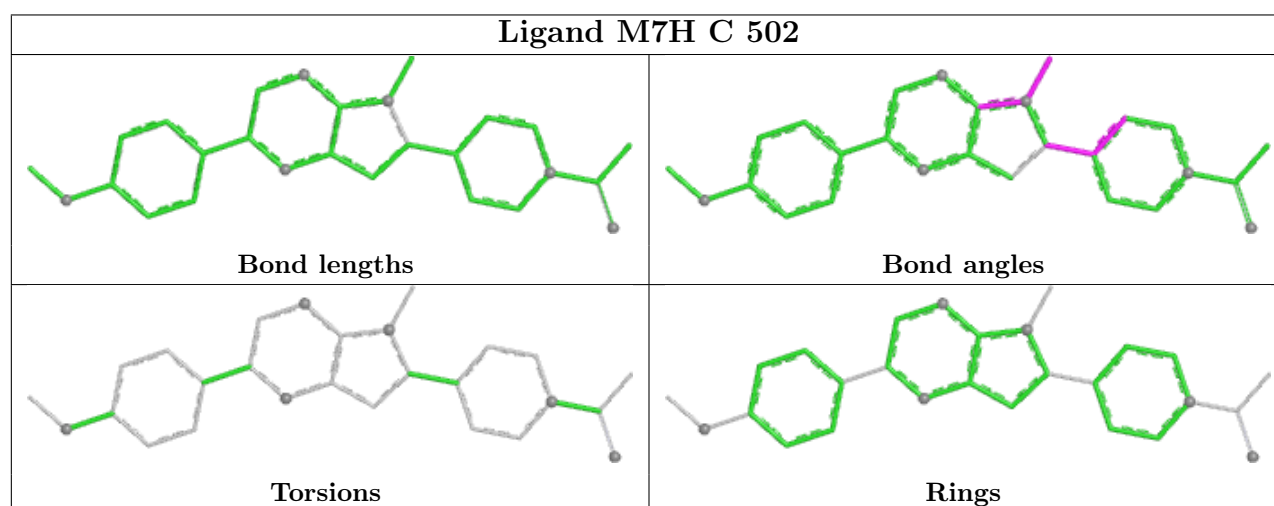
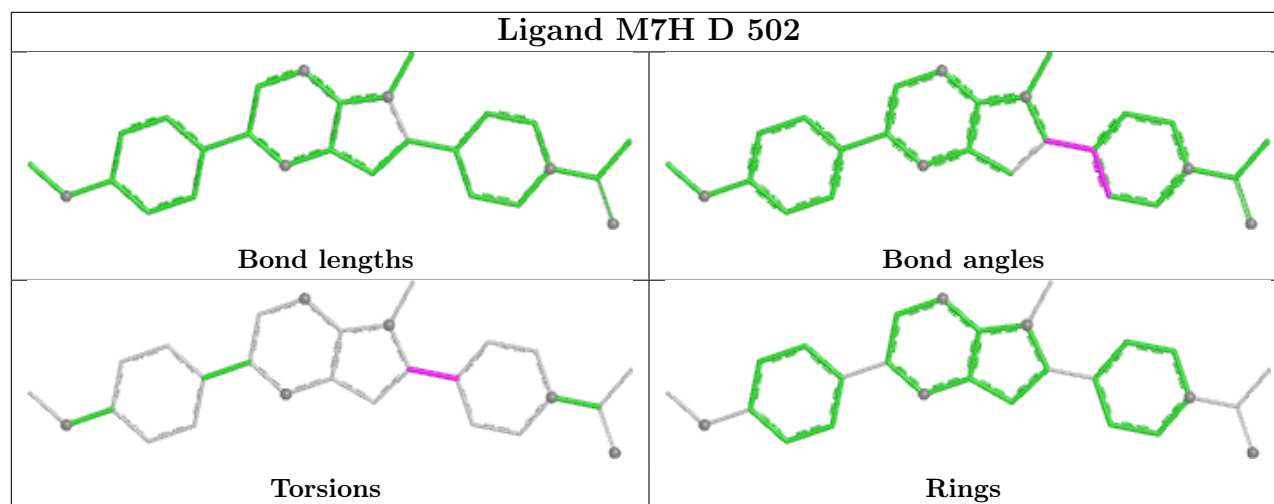
Mol	Chain	Res	Type	Atoms
6	B	501	NAG	C1-C2-N2-C7
4	B	507	TRS	N-C-C1-O1
8	D	502	M7H	C18-C11-C2-N1
5	A	510	EDO	O1-C1-C2-O2
4	B	507	TRS	C2-C-C1-O1
5	A	509	EDO	O1-C1-C2-O2
4	A	507	TRS	C1-C-C3-O3
5	B	509	EDO	O1-C1-C2-O2
8	D	502	M7H	C18-C11-C2-C4

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	507	TRS	2	0
5	B	509	EDO	1	0
7	B	502	GOL	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.33	4 (0%) 82 86	23, 37, 59, 75	0
1	B	497/536 (92%)	-0.31	2 (0%) 88 91	25, 40, 62, 82	0
1	C	497/536 (92%)	0.83	59 (11%) 9 8	36, 74, 151, 181	2 (0%)
1	D	494/536 (92%)	-0.03	7 (1%) 73 77	31, 48, 72, 96	0
All	All	1985/2144 (92%)	0.04	72 (3%) 46 50	23, 46, 106, 181	2 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	67	LEU	4.8
1	B	31	PHE	4.2
1	C	69	LEU	4.2
1	C	312	TRP	3.9
1	D	27	ASP	3.9
1	C	472	ILE	3.8
1	C	31	PHE	3.8
1	C	34	LEU	3.6
1	A	31	PHE	3.4
1	C	65	LEU	3.4
1	C	494	TRP	3.3
1	B	30	THR	3.3
1	C	66	LEU	3.2
1	C	55	PRO	3.1
1	C	470	LEU	3.1
1	C	73[A]	GLN	3.0
1	C	64	GLY	3.0
1	C	348	TRP	2.9
1	C	36	THR	2.9
1	D	31	PHE	2.8
1	C	406	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	30	THR	2.8
1	C	32	PRO	2.8
1	C	62	GLY	2.7
1	C	63	THR	2.7
1	C	458	VAL	2.7
1	C	58	ALA	2.6
1	C	308	ILE	2.6
1	D	61	THR	2.6
1	C	435	GLY	2.6
1	C	437	VAL	2.6
1	C	459	VAL	2.6
1	C	331	PHE	2.5
1	C	278	LEU	2.5
1	C	492	TYR	2.5
1	C	70	GLN	2.5
1	C	30	THR	2.5
1	C	57[A]	GLN	2.4
1	D	1	ALA	2.4
1	C	497	GLN	2.4
1	C	56	ILE	2.4
1	C	483	ILE	2.4
1	C	449	LEU	2.4
1	C	434	VAL	2.4
1	C	468	VAL	2.4
1	D	312	TRP	2.4
1	C	436	LEU	2.3
1	C	75	PHE	2.3
1	C	297	THR	2.3
1	C	450	MET	2.3
1	C	480	LEU	2.3
1	A	1	ALA	2.2
1	C	438	ALA	2.2
1	C	114	ILE	2.2
1	C	489	ILE	2.2
1	C	317	LEU	2.2
1	C	334	THR	2.2
1	C	478	GLY	2.2
1	C	37	PHE	2.1
1	C	329	ARG	2.1
1	C	460	VAL	2.1
1	C	296	LEU	2.1
1	C	452	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	475	PRO	2.1
1	D	63	THR	2.1
1	C	54	GLY	2.0
1	A	394	VAL	2.0
1	C	295	VAL	2.0
1	C	336	LEU	2.0
1	D	297	THR	2.0
1	C	469	PRO	2.0
1	C	477	VAL	2.0

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

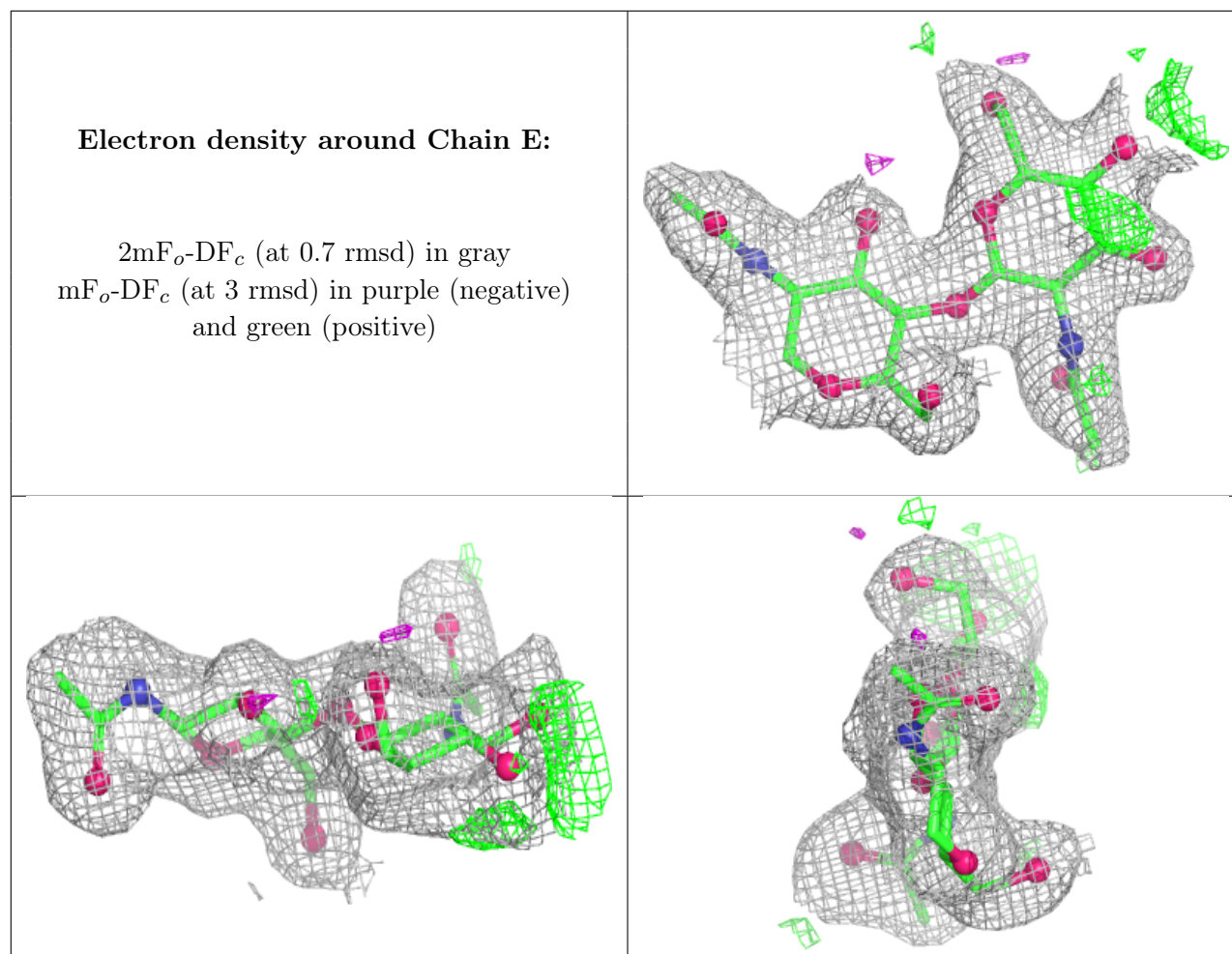
There are no non-standard protein/DNA/RNA residues in this entry.

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	0.84	0.10	46,53,63,68	0
2	NAG	E	1	14/15	0.95	0.06	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
7	GOL	B	502	6/6	0.75	0.20	83,83,84,84	0
3	SO4	C	504	5/5	0.79	0.11	110,110,112,112	0
3	SO4	A	506	5/5	0.79	0.15	111,111,111,112	0
4	TRS	A	507	8/8	0.80	0.20	54,62,69,72	0
6	NAG	B	501	14/15	0.81	0.14	52,58,61,64	0
3	SO4	B	506	5/5	0.83	0.13	124,125,125,125	0
6	NAG	C	501	14/15	0.84	0.11	96,99,103,106	0
5	EDO	A	509	4/4	0.85	0.17	45,48,55,57	0
3	SO4	D	506	5/5	0.87	0.09	75,77,81,82	0
4	TRS	B	507	8/8	0.87	0.12	39,48,51,53	0

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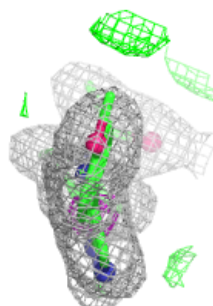
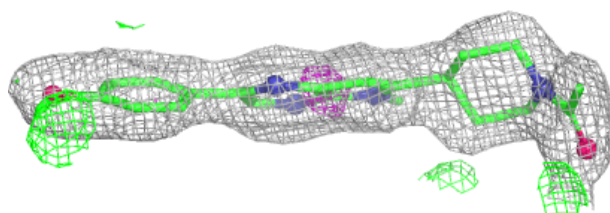
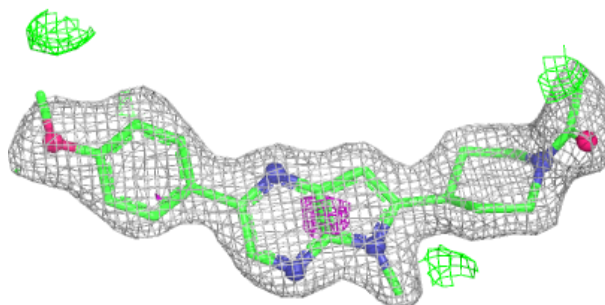
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	D	505	5/5	0.88	0.09	82,83,85,85	0
3	SO4	D	504	5/5	0.88	0.10	72,76,77,79	0
5	EDO	B	509	4/4	0.89	0.16	50,54,56,57	0
3	SO4	A	505	5/5	0.89	0.10	81,82,86,87	0
3	SO4	B	505	5/5	0.89	0.09	79,81,82,83	0
5	EDO	A	510	4/4	0.89	0.14	52,56,62,67	0
5	EDO	B	510	4/4	0.90	0.13	43,48,52,55	0
5	EDO	B	512	4/4	0.90	0.10	49,54,59,62	0
6	NAG	D	501	14/15	0.90	0.08	66,68,74,75	0
5	EDO	D	508	4/4	0.90	0.10	56,58,59,60	0
5	EDO	B	508	4/4	0.91	0.15	35,37,38,45	0
5	EDO	A	508	4/4	0.92	0.12	62,63,65,67	0
5	EDO	B	511	4/4	0.92	0.09	45,48,54,58	0
8	M7H	C	502	27/27	0.92	0.10	42,45,51,56	0
3	SO4	A	504	5/5	0.94	0.07	61,61,62,64	0
3	SO4	B	504	5/5	0.94	0.07	57,57,59,60	0
9	CL	C	505	1/1	0.94	0.12	53,53,53,53	0
8	M7H	D	502	27/27	0.95	0.07	30,35,44,54	0
3	SO4	B	503	5/5	0.97	0.06	37,37,43,43	0
3	SO4	C	503	5/5	0.97	0.05	57,60,62,63	0
9	CL	D	507	1/1	0.97	0.10	37,37,37,37	0
3	SO4	D	503	5/5	0.98	0.05	41,42,43,43	0
3	SO4	A	503	5/5	0.99	0.03	30,31,34,40	0

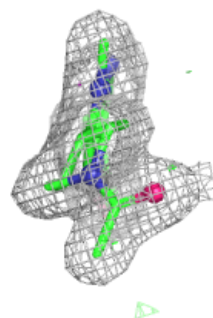
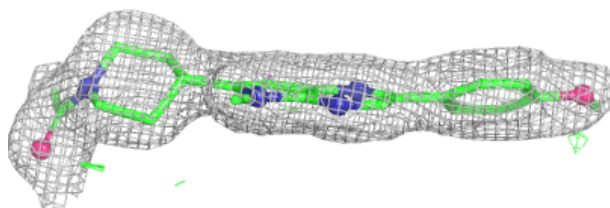
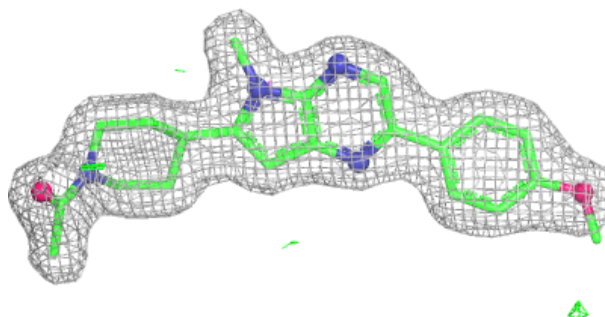
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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