



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:47 PM UTC

PDB ID : 4YLQ / pdb_00004ylq
Title : Crystal Structure of a FVIIa-Trypsin Chimera (FT) in Complex with Soluble Tissue Factor
Authors : Sorensen, A.B.; Svensson, L.A.; Gandhi, P.S.
Deposited on : 2015-03-05
Resolution : 1.40 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

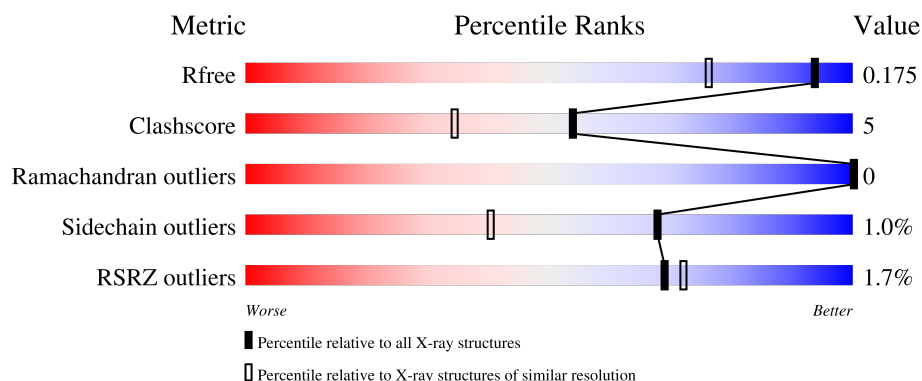
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

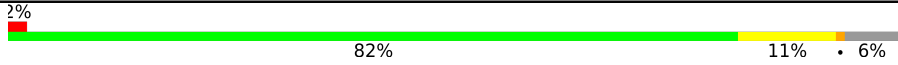
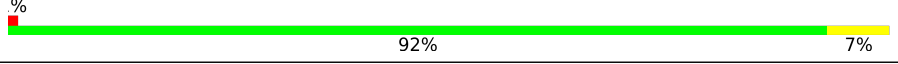
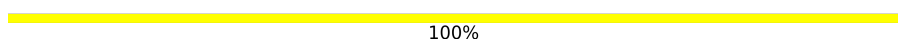
The reported resolution of this entry is 1.40 Å.

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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	L	152	
2	H	249	
3	T	219	
4	A	3	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 10324 atoms, of which 4784 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 Coagulation factor VII.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	143	Total	C	H	N	O	S	0	3	0
			2128	697	985	189	242	15			

- Molecule 2 is a protein called Coagulation factor VII.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	249	Total	C	H	N	O	S	0	8	0
			3802	1244	1863	335	345	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	LEU	deletion	UNP P08709
H	?	-	GLN	deletion	UNP P08709
H	?	-	GLN	deletion	UNP P08709
H	?	-	SER	deletion	UNP P08709
H	?	-	ARG	deletion	UNP P08709
H	169	GLU	LYS	engineered mutation	UNP P08709
H	170	ALA	VAL	engineered mutation	UNP P08709
H	171	SER	GLY	engineered mutation	UNP P08709
H	172	PHE	ASP	engineered mutation	UNP P08709
H	173	PRO	SER	engineered mutation	UNP P08709
H	174	GLY	PRO	engineered mutation	UNP P08709
H	175	LYS	ASN	engineered mutation	UNP P08709

- Molecule 3 is a protein called Tissue factor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	T	210	Total	C	H	N	O	S	0	5	0
			3276	1065	1592	271	343	5			

- Molecule 4 is an oligosaccharide called alpha-D-xylopyranose-(1-3)-alpha-D-xylopyranose-(1

-3)-beta-D-glucopyranose.

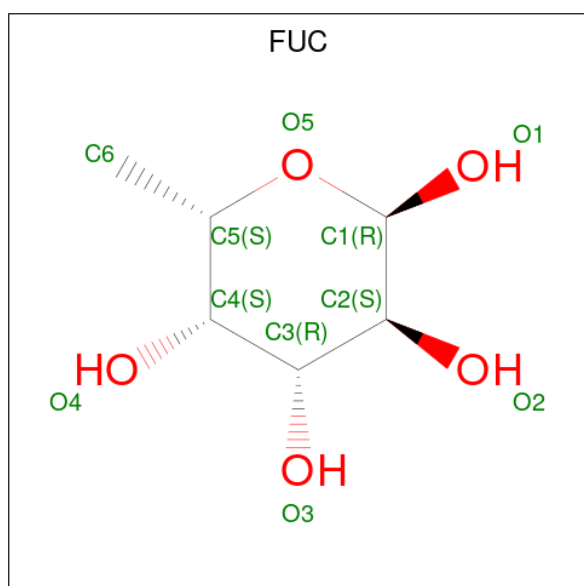


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	A	3	Total	C	H	O	0	0	0
			54	16	25	13			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

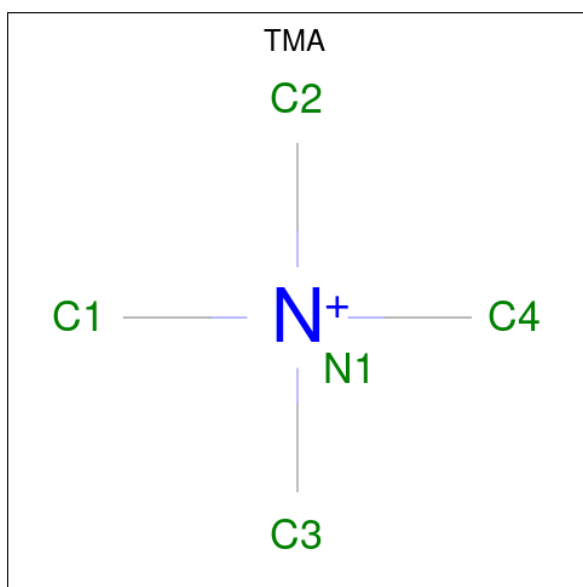
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	8	Total	Ca	0	0
			8	8		
5	H	1	Total	Ca	0	0
			1	1		

- Molecule 6 is alpha-L-fucopyranose (CCD ID: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	H	O	0	0
			20	6	10	4		

- Molecule 7 is TETRAMETHYLAMMONIUM ION (CCD ID: TMA) (formula: C₄H₁₂N).



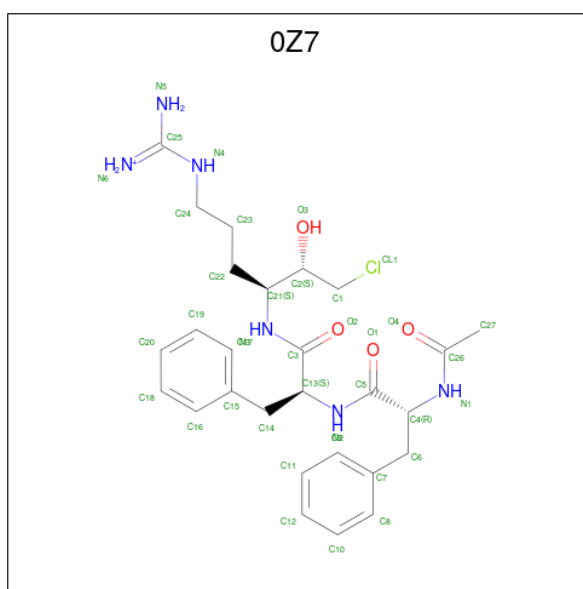
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	H	N	0	0
			17	4	12	1		
7	H	1	Total	C	H	N	0	0
			17	4	12	1		
7	H	1	Total	C	H	N	0	0
			17	4	12	1		
7	H	1	Total	C	H	N	0	0
			17	4	12	1		
7	H	1	Total	C	H	N	0	0
			17	4	12	1		
7	H	1	Total	C	H	N	0	0
			17	4	12	1		
7	H	1	Total	C	H	N	0	0
			17	4	12	1		
7	H	1	Total	C	H	N	0	0
			17	4	12	1		
7	T	1	Total	C	H	N	0	0
			17	4	12	1		
7	T	1	Total	C	H	N	0	0
			17	4	12	1		
7	T	1	Total	C	H	N	0	0
			17	4	12	1		
7	T	1	Total	C	H	N	0	0
			17	4	12	1		

Continued on next page...

Continued from previous page...

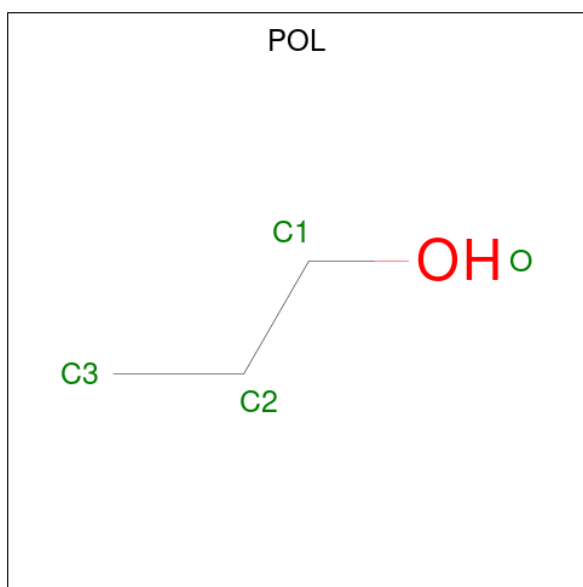
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	T	1	Total	C	H	N	0	0
			17	4	12	1		
7	T	1	Total	C	H	N	0	0
			17	4	12	1		
7	T	1	Total	C	H	N	0	0
			17	4	12	1		
7	T	1	Total	C	H	N	0	0
			17	4	12	1		
7	T	1	Total	C	H	N	0	0
			17	4	12	1		
7	T	1	Total	C	H	N	0	0
			17	4	12	1		
7	T	1	Total	C	H	N	0	0
			17	4	12	1		

- Molecule 8 is N-acetyl-D-phenylalanyl-N-[(2S,3S)-6-carbamimidamido-1-chloro-2-hydroxyhexan-3-yl]-L-phenylalaninamide (CCD ID: 0Z7) (formula: $C_{27}H_{38}ClN_6O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	H	1	Total	C	H	N	O	0	0
			74	27	37	6	4		

- Molecule 9 is N-PROPANOL (CCD ID: POL) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	H	1	Total	C	H	O	0	0
			12	3	8	1		

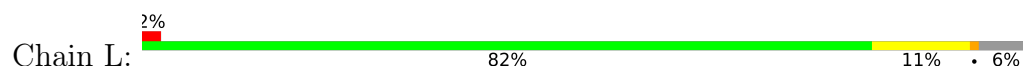
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	143	Total	O	0	0
			143	143		
10	H	242	Total	O	0	0
			242	242		
10	T	190	Total	O	0	0
			190	190		

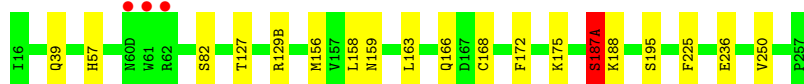
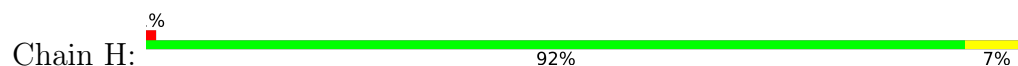
3 Residue-property plots [i](#)

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.

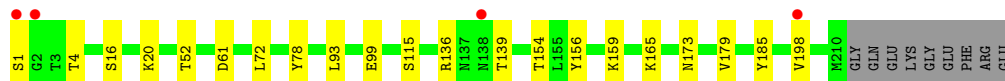
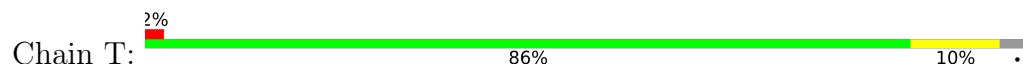
- Molecule 1: Coagulation factor VII



- Molecule 2: Coagulation factor VII



- Molecule 3: Tissue factor



- Molecule 4: alpha-D-xylopyranose-(1-3)-alpha-D-xylopyranose-(1-3)-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	71.31Å 80.04Å 123.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.25 – 1.40 34.25 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.25-1.40) 99.8 (34.25-1.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.140 , 0.174 0.142 , 0.175	Depositor DCC
R_{free} test set	6918 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10324	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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: FUC, POL, TMA, XYS, BGC, CA, CGU, OZ7

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	L	0.82	0/1048	0.90	1/1403 (0.1%)
2	H	1.01	2/2008 (0.1%)	0.97	1/2737 (0.0%)
3	T	0.94	0/1735	0.91	0/2364
All	All	0.95	2/4791 (0.0%)	0.93	2/6504 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	39	GLN	CB-CG	-5.76	1.35	1.52
2	H	250	VAL	C-O	-5.18	1.17	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	187(A)	SER	CA-C-O	5.65	126.51	120.24
1	L	28	ARG	CD-NE-CZ	-5.17	117.16	124.40

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	L	1143	985	992	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1939	1863	1906	19	0
3	T	1684	1592	1637	18	0
4	A	29	25	24	0	0
5	H	1	0	0	0	0
5	L	8	0	0	0	0
6	L	10	10	10	0	0
7	H	45	108	108	9	0
7	L	5	12	12	0	0
7	T	60	144	144	9	0
8	H	37	37	31	0	0
9	H	4	8	8	0	0
10	H	242	0	0	8	0
10	L	143	0	0	0	0
10	T	190	0	0	6	0
All	All	5540	4784	4872	48	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 5.

All (48) 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)
3:T:173[B]:ASN:OD1	10:T:401:HOH:O	1.86	0.92
3:T:78:TYR:OH	7:T:302:TMA:H12	1.81	0.80
3:T:165:LYS:HE3	7:T:309:TMA:C3	2.15	0.76
3:T:165:LYS:HE3	7:T:309:TMA:H33	1.72	0.70
2:H:129(B):ARG:NH2	10:H:601:HOH:O	2.25	0.69
2:H:82:SER:OG	7:H:503:TMA:H33	1.93	0.67
3:T:115:SER:OG	7:T:304:TMA:H12	1.96	0.65
2:H:156[B]:MET:HE2	10:H:788:HOH:O	2.01	0.61
7:H:503:TMA:H32	10:H:811:HOH:O	2.02	0.59
3:T:165:LYS:HE3	7:T:309:TMA:H31	1.85	0.59
7:H:510:TMA:H32	10:H:728:HOH:O	2.04	0.58
3:T:1:SER:OG	3:T:4:THR:OG1	2.20	0.58
3:T:52:THR:OG1	7:T:312:TMA:H33	2.05	0.57
7:H:510:TMA:H31	10:H:784:HOH:O	2.04	0.56
3:T:173[B]:ASN:ND2	10:T:402:HOH:O	2.28	0.56
2:H:166:GLN:HE21	7:H:511:TMA:H31	1.73	0.54
2:H:159:ASN:HD22	7:H:506:TMA:H32	1.73	0.54
2:H:187(A):SER:C	2:H:188:LYS:HG3	2.35	0.51
2:H:158:LEU:HD11	2:H:188:LYS:HB3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:156:TYR:HD1	3:T:165:LYS:HD3	1.77	0.49
2:H:158:LEU:HD11	2:H:188:LYS:HE3	1.94	0.49
7:T:310:TMA:H32	10:T:569:HOH:O	2.13	0.49
3:T:156:TYR:CD1	3:T:165:LYS:HD3	2.49	0.48
2:H:127:THR:HB	10:H:700:HOH:O	2.12	0.48
1:L:85:LYS:NZ	3:T:61:ASP:OD2	2.46	0.46
3:T:154[A]:THR:HG21	10:T:541:HOH:O	2.15	0.46
3:T:16:SER:HA	3:T:20:LYS:O	2.15	0.46
7:T:301:TMA:H32	10:T:412:HOH:O	2.15	0.46
2:H:158:LEU:CD1	2:H:188:LYS:HE3	2.46	0.45
2:H:163:LEU:HD22	2:H:168[B]:CYS:HB3	1.99	0.45
2:H:172[A]:PHE:HB3	2:H:175:LYS:HB2	1.98	0.44
2:H:127:THR:HG21	2:H:129(B):ARG:CZ	2.48	0.44
2:H:163:LEU:HD21	2:H:225:PHE:CZ	2.52	0.44
1:L:4[B]:PHE:CZ	1:L:5:LEU:CD1	3.01	0.43
1:L:25:CGU:OE22	1:L:28:ARG:NH2	2.39	0.43
2:H:166:GLN:HE21	7:H:511:TMA:C3	2.30	0.43
1:L:121:LEU:HD12	1:L:126:SER:HB2	2.02	0.42
3:T:179:VAL:HB	3:T:185:TYR:CE1	2.55	0.42
3:T:72:LEU:CD2	3:T:99:GLU:HG2	2.50	0.42
2:H:57:HIS:CE1	2:H:195:SER:OG	2.74	0.41
3:T:136:ARG:O	3:T:139:THR:HG22	2.21	0.41
2:H:236:GLU:HG2	10:H:699:HOH:O	2.20	0.41
3:T:1:SER:HG	3:T:4:THR:HG1	1.49	0.41
1:L:33:ASP:HB3	1:L:36:ARG:HD2	2.03	0.41
2:H:127:THR:CG2	2:H:129(B):ARG:CZ	2.99	0.41
7:T:301:TMA:H31	10:T:548:HOH:O	2.20	0.40
2:H:82:SER:HG	7:H:503:TMA:H33	1.85	0.40
7:H:504:TMA:H12	10:H:612:HOH:O	2.21	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	L	134/152 (88%)	129 (96%)	5 (4%)	0	100	100
2	H	253/249 (102%)	248 (98%)	5 (2%)	0	100	100
3	T	213/219 (97%)	208 (98%)	5 (2%)	0	100	100
All	All	600/620 (97%)	585 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	L	112/122 (92%)	111 (99%)	1 (1%)	70	44
2	H	208/210 (99%)	207 (100%)	1 (0%)	81	61
3	T	195/200 (98%)	192 (98%)	3 (2%)	57	26
All	All	515/532 (97%)	510 (99%)	5 (1%)	68	40

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	140	ILE
2	H	187(A)	SER
3	T	93	LEU
3	T	159	LYS
3	T	198	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	56	GLN
2	H	87	GLN
2	H	117	HIS
2	H	159	ASN
2	H	166	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	T	137	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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
1	CGU	L	26	5,1	9,11,12	1.86	3 (33%)	10,14,16	1.39	1 (10%)
1	CGU	L	25	5,1	9,11,12	4.30	4 (44%)	10,14,16	3.43	5 (50%)
1	CGU	L	7	5,1	9,11,12	1.28	1 (11%)	10,14,16	1.13	1 (10%)
1	CGU	L	6	5,1	9,11,12	1.25	0	10,14,16	1.01	1 (10%)
1	CGU	L	35	1	9,11,12	2.01	2 (22%)	10,14,16	1.58	2 (20%)
1	CGU	L	16	5,1	9,11,12	0.98	0	10,14,16	1.46	2 (20%)
1	CGU	L	20	5,1	9,11,12	1.22	0	10,14,16	1.22	1 (10%)
1	CGU	L	29	5,1	9,11,12	1.58	0	10,14,16	0.87	0
1	CGU	L	14	5,1	9,11,12	1.83	3 (33%)	10,14,16	0.86	0
1	CGU	L	19	5,1	9,11,12	1.43	1 (11%)	10,14,16	0.94	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
1	CGU	L	26	5,1	-	3/13/14/16	-
1	CGU	L	25	5,1	-	1/13/14/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CGU	L	7	5,1	-	4/13/14/16	-
1	CGU	L	6	5,1	-	6/13/14/16	-
1	CGU	L	35	1	-	6/13/14/16	-
1	CGU	L	16	5,1	-	2/13/14/16	-
1	CGU	L	20	5,1	-	5/13/14/16	-
1	CGU	L	29	5,1	-	0/13/14/16	-
1	CGU	L	14	5,1	-	0/13/14/16	-
1	CGU	L	19	5,1	-	3/13/14/16	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	25	CGU	CG-CD2	10.87	1.66	1.52
1	L	25	CGU	OE21-CD2	4.64	1.35	1.22
1	L	35	CGU	CG-CD2	3.85	1.57	1.52
1	L	26	CGU	CG-CD2	3.31	1.56	1.52
1	L	35	CGU	CG-CD1	-3.05	1.48	1.52
1	L	14	CGU	CG-CD2	3.00	1.56	1.52
1	L	19	CGU	CG-CD2	2.67	1.55	1.52
1	L	25	CGU	OE11-CD1	2.50	1.29	1.22
1	L	25	CGU	CG-CD1	2.48	1.55	1.52
1	L	14	CGU	OE11-CD1	2.35	1.29	1.22
1	L	26	CGU	OE11-CD1	2.25	1.28	1.22
1	L	14	CGU	CG-CD1	2.25	1.55	1.52
1	L	26	CGU	OE12-CD1	-2.09	1.24	1.30
1	L	7	CGU	OE21-CD2	2.04	1.28	1.22

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	25	CGU	CB-CG-CD2	8.01	129.38	113.11
1	L	25	CGU	OE11-CD1-CG	-4.05	106.68	120.19
1	L	25	CGU	OE12-CD1-CG	3.92	129.84	116.50
1	L	35	CGU	CB-CG-CD2	3.29	119.79	113.11
1	L	26	CGU	CB-CG-CD2	-2.94	107.14	113.11
1	L	25	CGU	OE21-CD2-CG	2.90	129.88	120.19
1	L	20	CGU	CB-CA-C	-2.80	106.67	110.99
1	L	35	CGU	CB-CG-CD1	-2.67	107.69	113.11
1	L	25	CGU	OE22-CD2-OE21	-2.27	118.93	124.08
1	L	16	CGU	CB-CA-C	-2.15	107.67	110.99
1	L	6	CGU	CB-CA-C	-2.12	107.73	110.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	7	CGU	CB-CG-CD1	-2.09	108.86	113.11
1	L	16	CGU	OE22-CD2-CG	2.03	123.39	116.50

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	L	6	CGU	CA-CB-CG-CD1
1	L	6	CGU	CA-CB-CG-CD2
1	L	25	CGU	CA-CB-CG-CD2
1	L	35	CGU	N-CA-CB-CG
1	L	35	CGU	CA-CB-CG-CD1
1	L	35	CGU	CA-CB-CG-CD2
1	L	6	CGU	OE21-CD2-CG-CB
1	L	6	CGU	OE22-CD2-CG-CB
1	L	7	CGU	OE21-CD2-CG-CB
1	L	7	CGU	OE22-CD2-CG-CB
1	L	16	CGU	OE21-CD2-CG-CB
1	L	16	CGU	OE22-CD2-CG-CB
1	L	19	CGU	OE11-CD1-CG-CB
1	L	20	CGU	OE21-CD2-CG-CB
1	L	26	CGU	OE21-CD2-CG-CB
1	L	26	CGU	OE22-CD2-CG-CB
1	L	35	CGU	OE21-CD2-CG-CB
1	L	35	CGU	OE22-CD2-CG-CB
1	L	6	CGU	OE21-CD2-CG-CD1
1	L	6	CGU	OE22-CD2-CG-CD1
1	L	7	CGU	OE21-CD2-CG-CD1
1	L	7	CGU	OE22-CD2-CG-CD1
1	L	19	CGU	OE11-CD1-CG-CD2
1	L	20	CGU	OE21-CD2-CG-CD1
1	L	35	CGU	C-CA-CB-CG
1	L	19	CGU	OE12-CD1-CG-CB
1	L	20	CGU	OE11-CD1-CG-CB
1	L	20	CGU	OE22-CD2-CG-CB
1	L	20	CGU	OE22-CD2-CG-CD1
1	L	26	CGU	OE11-CD1-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L	25	CGU	1	0

5.5 Carbohydrates

3 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
4	BGC	A	1	4,1	11,11,12	2.24	2 (18%)	15,15,17	1.45	3 (20%)
4	XYS	A	2	4	9,9,10	1.09	1 (11%)	10,12,14	1.58	2 (20%)
4	XYS	A	3	4	9,9,10	0.76	0	10,12,14	2.01	3 (30%)

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
4	BGC	A	1	4,1	-	0/2/19/22	0/1/1/1
4	XYS	A	2	4	-	-	0/1/1/1
4	XYS	A	3	4	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	BGC	O5-C1	5.73	1.53	1.43
4	A	2	XYS	O5-C1	-2.80	1.37	1.43
4	A	1	BGC	O5-C5	2.42	1.48	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3	XYS	O4-C4-C3	3.47	117.34	110.15
4	A	1	BGC	O5-C1-C2	-3.45	102.57	110.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2	XYS	C5-O5-C1	3.31	116.77	111.42
4	A	3	XYS	C5-O5-C1	3.28	116.71	111.42
4	A	1	BGC	C6-C5-C4	-2.45	106.99	113.02
4	A	3	XYS	O3-C3-C4	2.24	114.62	110.05
4	A	1	BGC	C3-C4-C5	2.22	114.25	110.23
4	A	2	XYS	C1-C2-C3	2.16	112.80	109.64

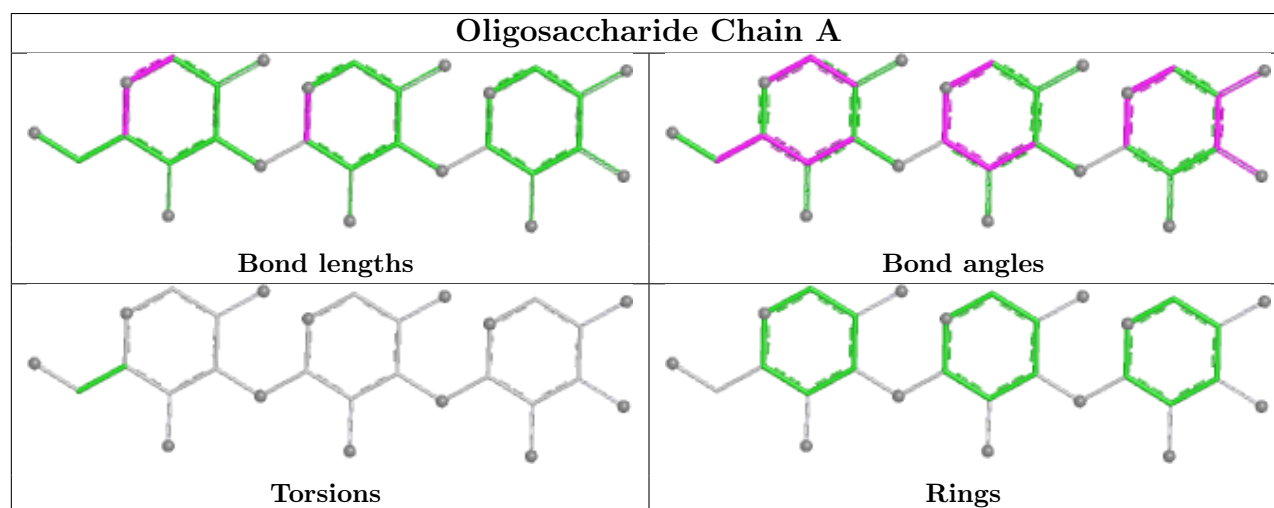
There are no chirality outliers.

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 34 ligands modelled in this entry, 9 are monoatomic - leaving 25 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
7	TMA	T	301	-	4,4,4	1.20	0	6,6,6	0.53	0
7	TMA	T	304	-	4,4,4	1.26	0	6,6,6	0.39	0
7	TMA	H	504	-	4,4,4	1.32	0	6,6,6	0.30	0
7	TMA	T	303	-	4,4,4	1.25	0	6,6,6	0.28	0
7	TMA	H	505	-	4,4,4	1.24	0	6,6,6	0.20	0
7	TMA	T	312	-	4,4,4	1.18	0	6,6,6	0.36	0
7	TMA	T	309	-	4,4,4	1.22	0	6,6,6	0.25	0
7	TMA	H	512	-	4,4,4	1.16	0	6,6,6	0.24	0
7	TMA	T	310	-	4,4,4	0.92	0	6,6,6	0.43	0
7	TMA	T	308	-	4,4,4	1.31	0	6,6,6	0.22	0
8	0Z7	H	501	2	37,38,39	3.61	12 (32%)	45,49,50	1.98	9 (20%)
7	TMA	T	306	-	4,4,4	1.28	0	6,6,6	0.66	0
7	TMA	L	213	-	4,4,4	1.14	0	6,6,6	0.34	0
7	TMA	H	508	-	4,4,4	1.34	0	6,6,6	0.15	0
7	TMA	T	305	-	4,4,4	1.29	0	6,6,6	0.26	0
9	POL	H	509	-	3,3,3	0.42	0	2,2,2	0.48	0
7	TMA	H	506	-	4,4,4	1.19	0	6,6,6	0.23	0
7	TMA	H	511	-	4,4,4	1.24	0	6,6,6	0.18	0
7	TMA	H	507	-	4,4,4	1.31	0	6,6,6	0.34	0
7	TMA	H	503	-	4,4,4	1.53	1 (25%)	6,6,6	0.37	0
7	TMA	T	302	-	4,4,4	1.48	1 (25%)	6,6,6	0.52	0
7	TMA	H	510	-	4,4,4	0.91	0	6,6,6	0.36	0
7	TMA	T	311	-	4,4,4	0.95	0	6,6,6	0.38	0
7	TMA	T	307	-	4,4,4	1.25	0	6,6,6	0.18	0
6	FUC	L	212	1	10,10,11	0.99	1 (10%)	14,14,16	0.63	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
9	POL	H	509	-	-	0/1/1/1	-
8	0Z7	H	501	2	-	10/39/39/41	0/2/2/2
6	FUC	L	212	1	-	-	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	501	OZ7	C27-C26	-15.59	1.18	1.50
8	H	501	OZ7	C26-N1	-8.05	1.08	1.34
8	H	501	OZ7	C25-N4	5.28	1.43	1.33
8	H	501	OZ7	C5-N2	5.06	1.44	1.34
8	H	501	OZ7	C3-N3	4.90	1.44	1.34
8	H	501	OZ7	C13-N2	-4.51	1.36	1.45
8	H	501	OZ7	C14-C13	-3.68	1.45	1.54
8	H	501	OZ7	C6-C4	-3.52	1.45	1.54
8	H	501	OZ7	C4-N1	-3.25	1.39	1.45
7	H	503	TMA	C3-N1	-2.50	1.36	1.48
7	T	302	TMA	C1-N1	-2.31	1.37	1.48
8	H	501	OZ7	C4-C5	-2.28	1.47	1.52
8	H	501	OZ7	C21-N3	-2.25	1.42	1.46
6	L	212	FUC	O5-C1	-2.23	1.39	1.43
8	H	501	OZ7	C13-C3	-2.19	1.47	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	501	OZ7	C27-C26-N1	7.05	127.81	116.12
8	H	501	OZ7	O4-C26-C27	-6.18	111.05	122.05
8	H	501	OZ7	C22-C21-N3	-3.40	105.89	110.30
8	H	501	OZ7	C23-C24-N4	-2.91	104.03	112.20
8	H	501	OZ7	C15-C14-C13	2.81	120.83	113.36
8	H	501	OZ7	C4-N1-C26	2.61	128.90	121.58
8	H	501	OZ7	O1-C5-N2	-2.53	118.42	122.96
8	H	501	OZ7	C10-C8-C7	2.14	123.62	120.61
8	H	501	OZ7	O1-C5-C4	2.13	124.94	120.48

There are no chirality outliers.

All (10) torsion outliers are listed below:

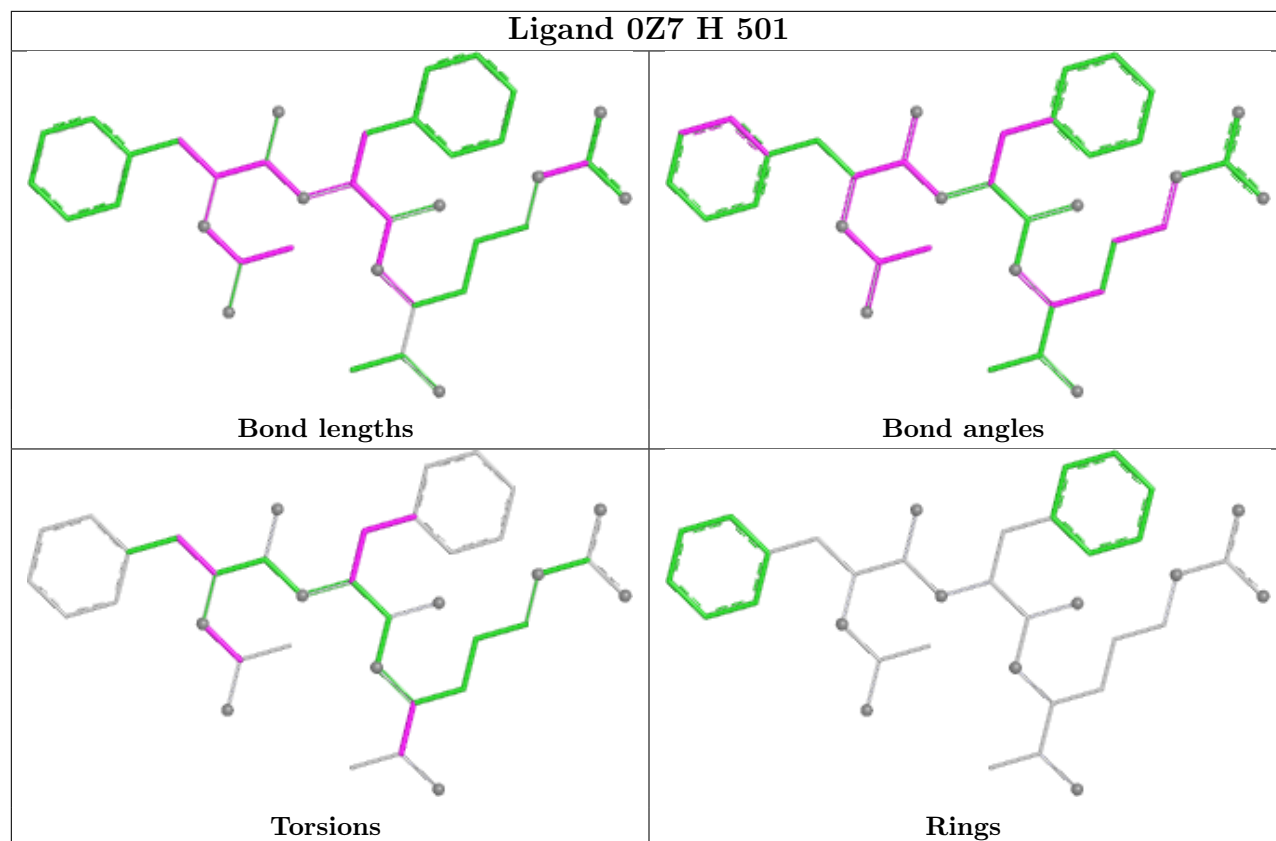
Mol	Chain	Res	Type	Atoms
8	H	501	OZ7	O4-C26-N1-C4
8	H	501	OZ7	C27-C26-N1-C4
8	H	501	OZ7	N2-C13-C14-C15
8	H	501	OZ7	C3-C13-C14-C15
8	H	501	OZ7	O3-C2-C21-C22
8	H	501	OZ7	C13-C14-C15-C16
8	H	501	OZ7	C1-C2-C21-C22
8	H	501	OZ7	C1-C2-C21-N3
8	H	501	OZ7	C13-C14-C15-C17
8	H	501	OZ7	N1-C4-C6-C7

There are no ring outliers.

11 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	301	TMA	2	0
7	T	304	TMA	1	0
7	H	504	TMA	1	0
7	T	312	TMA	1	0
7	T	309	TMA	3	0
7	T	310	TMA	1	0
7	H	506	TMA	1	0
7	H	511	TMA	2	0
7	H	503	TMA	3	0
7	T	302	TMA	1	0
7	H	510	TMA	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	L	133/152 (87%)	-0.24	3 (2%) 61 63	13, 30, 45, 59	3 (2%)
2	H	249/249 (100%)	-0.73	3 (1%) 76 80	8, 17, 42, 59	6 (2%)
3	T	210/219 (95%)	-0.52	4 (1%) 66 69	9, 22, 49, 68	5 (2%)
All	All	592/620 (95%)	-0.55	10 (1%) 69 72	8, 22, 47, 68	14 (2%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	143	LYS	3.4
3	T	1	SER	3.0
3	T	2	GLY	2.8
3	T	138	ASN	2.5
2	H	60(D)	ASN	2.5
1	L	84[A]	HIS	2.4
2	H	61	TRP	2.3
1	L	85	LYS	2.2
3	T	198	VAL	2.0
2	H	62	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CGU	L	35	12/13	0.87	0.12	31,58,63,68	0
1	CGU	L	25	12/13	0.94	0.09	22,30,36,36	0
1	CGU	L	19	12/13	0.95	0.08	32,41,46,49	0

Continued on next page...

Continued from previous page...

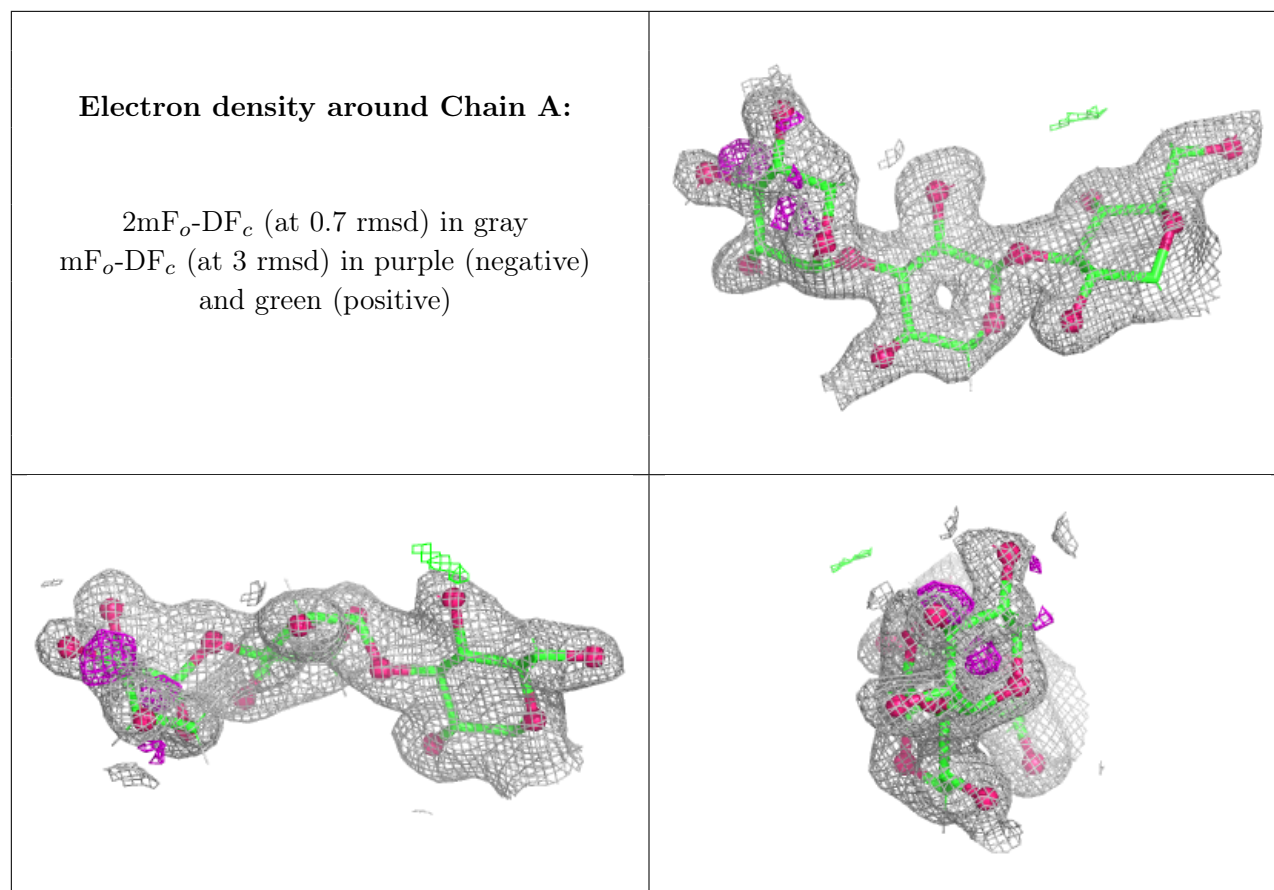
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CGU	L	14	12/13	0.96	0.06	26,39,43,46	0
1	CGU	L	20	12/13	0.97	0.06	26,30,35,36	0
1	CGU	L	6	12/13	0.98	0.05	20,24,28,29	0
1	CGU	L	26	12/13	0.98	0.04	20,23,26,28	0
1	CGU	L	29	12/13	0.98	0.05	21,24,29,30	0
1	CGU	L	16	12/13	0.98	0.04	18,21,24,25	0
1	CGU	L	7	12/13	0.99	0.04	18,19,23,23	0

6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BGC	A	1	11/12	-	-	38,45,55,57	0
4	XYS	A	2	9/10	-	-	40,43,51,52	0
4	XYS	A	3	9/10	-	-	41,43,51,52	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 ⓘ

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	TMA	T	311	5/5	0.75	0.17	41,49,53,53	0
7	TMA	T	301	5/5	0.77	0.21	50,61,64,64	0
7	TMA	T	312	5/5	0.78	0.15	37,44,48,48	0
7	TMA	H	512	5/5	0.79	0.22	66,79,80,80	0
7	TMA	T	309	5/5	0.80	0.14	42,50,52,52	0
7	TMA	H	511	5/5	0.81	0.21	55,67,68,68	0
9	POL	H	509	4/4	0.81	0.19	55,66,68,70	0
7	TMA	H	510	5/5	0.82	0.17	37,44,49,49	0
7	TMA	L	213	5/5	0.82	0.23	63,76,77,77	0
7	TMA	H	506	5/5	0.83	0.21	61,74,74,74	0
7	TMA	T	306	5/5	0.83	0.19	48,58,61,61	0
7	TMA	T	303	5/5	0.84	0.17	56,68,68,68	0
7	TMA	T	308	5/5	0.84	0.23	69,83,84,84	0

Continued on next page...

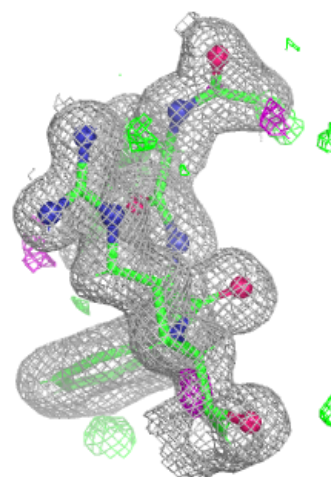
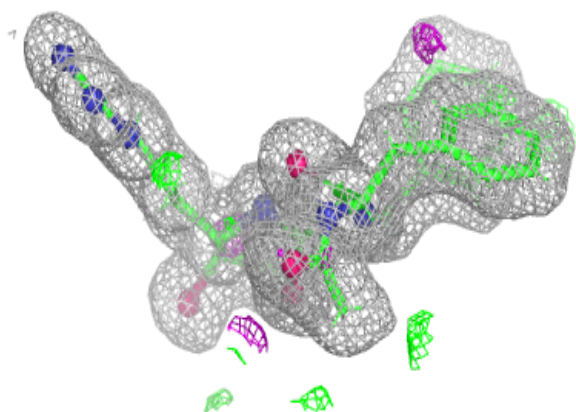
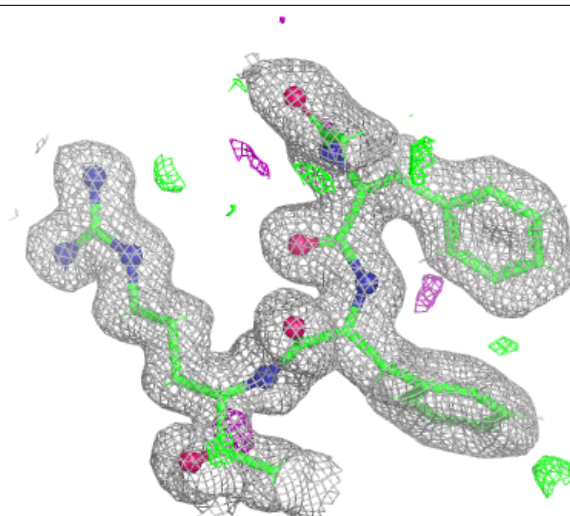
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	TMA	T	305	5/5	0.86	0.16	50,60,61,61	0
7	TMA	T	310	5/5	0.87	0.13	38,46,47,47	0
7	TMA	H	507	5/5	0.88	0.17	58,70,71,71	0
7	TMA	T	304	5/5	0.88	0.12	40,48,57,57	0
7	TMA	T	307	5/5	0.88	0.15	51,62,63,63	0
7	TMA	H	505	5/5	0.89	0.11	44,53,55,55	0
7	TMA	H	504	5/5	0.91	0.11	36,43,47,47	0
7	TMA	T	302	5/5	0.93	0.10	27,33,39,39	0
7	TMA	H	508	5/5	0.93	0.13	55,66,68,68	0
6	FUC	L	212	10/11	0.96	0.06	33,38,43,46	0
8	0Z7	H	501	37/38	0.98	0.05	15,20,29,32	0
7	TMA	H	503	5/5	0.98	0.05	14,23,27,27	0
5	CA	L	207	1/1	0.99	0.04	44,44,44,44	0
5	CA	L	208	1/1	0.99	0.04	27,27,27,27	0
5	CA	L	206	1/1	0.99	0.04	35,35,35,35	0
5	CA	L	205	1/1	1.00	0.02	25,25,25,25	0
5	CA	L	201	1/1	1.00	0.02	28,28,28,28	0
5	CA	L	202	1/1	1.00	0.01	22,22,22,22	0
5	CA	L	203	1/1	1.00	0.02	19,19,19,19	0
5	CA	H	502	1/1	1.00	0.01	13,13,13,13	0
5	CA	L	204	1/1	1.00	0.02	20,20,20,20	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 0Z7 H 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.