



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 02:02 PM BST

PDB ID : 6R2W  
Title : Crystal structure of the super-active FVIIa variant VYT in complex with tissue factor  
Authors : Sorensen, A.B.; Svensson, L.A.; Gandhi, P.S.  
Deposited on : 2019-03-19  
Resolution : 1.25 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](mailto: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.

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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 : 2.13.1  
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) : 2.13.1

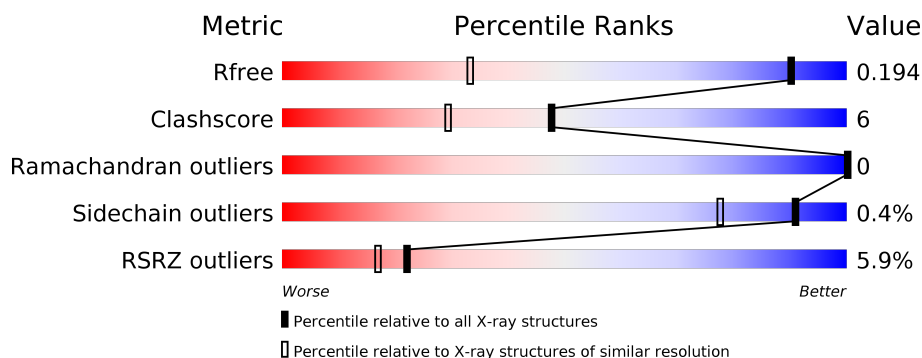
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.25 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	1023 (1.28-1.24)
Clashscore	141614	1060 (1.28-1.24)
Ramachandran outliers	138981	1029 (1.28-1.24)
Sidechain outliers	138945	1028 (1.28-1.24)
RSRZ outliers	127900	1004 (1.28-1.24)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	143	<div> <div>6%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
2	H	249	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
3	T	210	<div> <div>8%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
4	A	3	<div> <div></div> <div> <div>33%</div> <div>67%</div> </div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10616 atoms, of which 4859 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	1	0
			2156	694	1008	191	248	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	16	0
			4000	1284	1991	350	360	15			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	168	VAL	LEU	conflict	UNP P08709
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	174	GLU	LYS	engineered mutation	UNP P08709
H	175	ALA	VAL	engineered mutation	UNP P08709
H	176	SER	GLY	engineered mutation	UNP P08709
H	177	TYR	ASP	engineered mutation	UNP P08709
H	178	PRO	SER	engineered mutation	UNP P08709
H	179	GLY	PRO	engineered mutation	UNP P08709
H	180	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	9	0
			3350	1089	1633	275	348	5			

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

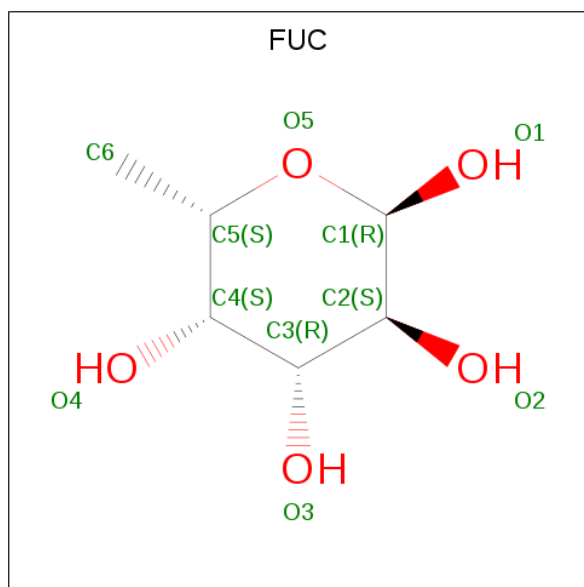


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	A	3	Total	C	H	O	0	0	0
			54	16	25	13			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

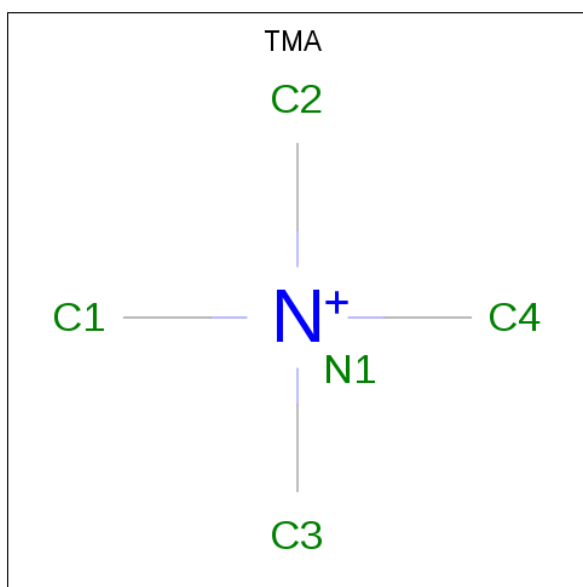
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Ca	0	0
			1	1		
5	L	8	Total	Ca	0	0
			8	8		

- Molecule 6 is alpha-L-fucopyranose (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



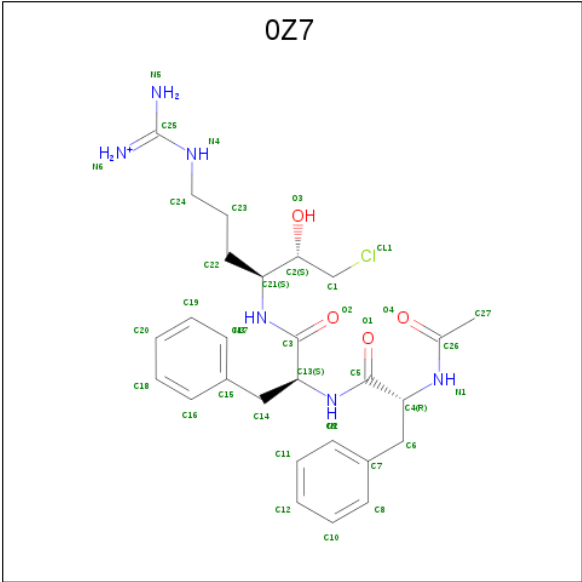
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	H	O	0	0
			20	6	10	4		

- Molecule 7 is TETRAMETHYLAMMONIUM ION (three-letter code: TMA) (formula: C<sub>4</sub>H<sub>12</sub>N).



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	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 (three-letter code: 0Z7) (formula: C<sub>27</sub>H<sub>38</sub>ClN<sub>6</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	H	1	Total	C	H	N	O	0	1
			143	53	72	11	7		

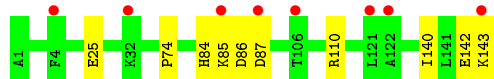
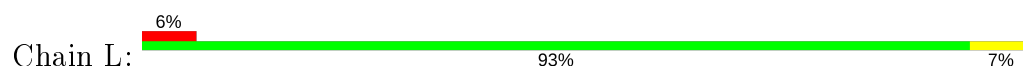
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	188	Total	O	0	0
			188	188		
9	H	283	Total	O	0	0
			283	283		
9	T	243	Total	O	0	0
			243	243		

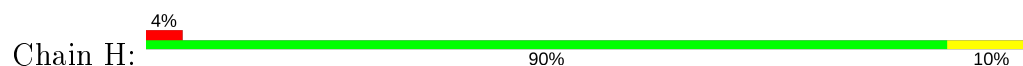
### 3 Residue-property plots [i](#)

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.

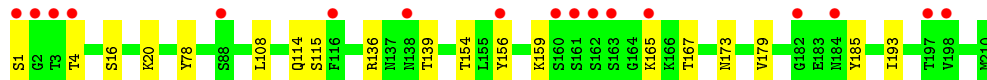
- Molecule 1: Coagulation factor VII



- 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, $\alpha$ , $\beta$ , $\gamma$	71.31Å 80.04Å 123.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.58 – 1.25 46.65 – 1.25	Depositor EDS
% Data completeness (in resolution range)	97.8 (36.58-1.25) 97.8 (46.65-1.25)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.00 (at 1.25Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, $R_{free}$	0.170 , 0.194 0.170 , 0.194	Depositor DCC
$R_{free}$ test set	9563 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.1	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 50.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	10616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BGC, 0Z7, TMA, XYS, FUC, CGU, CA

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	0.38	0/1045	0.60	0/1396
2	H	0.42	0/2096	0.69	0/2853
3	T	0.41	0/1781	0.69	0/2424
All	All	0.41	0/4922	0.67	0/6673

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	L	1148	1008	1011	12	0
2	H	2009	1991	2012	24	1
3	T	1717	1633	1692	21	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	25	60	60	3	0
7	L	5	12	12	0	0
7	T	20	48	48	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	71	72	61	4	0
9	H	283	0	0	9	1
9	L	188	0	0	4	1
9	T	243	0	0	5	0
All	All	5757	4859	4930	61	2

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 6.

All (61) 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	9:T:401:HOH:O	1.77	1.01
1:L:87:ASP:OD2	9:L:301:HOH:O	1.77	0.99
3:T:78:TYR:OH	7:T:302:TMA:H12	1.69	0.93
3:T:156[A]:TYR:OH	3:T:165:LYS:NZ	2.04	0.91
2:H:243[B]:GLU:OE2	9:H:401:HOH:O	1.93	0.86
1:L:74:PRO:O	1:L:85:LYS:HE2	1.81	0.81
2:H:164:ASN:HD22	7:H:306:TMA:H32	1.45	0.80
7:H:303:TMA:H11	9:H:634:HOH:O	1.87	0.75
2:H:101[A]:THR:HG21	9:H:558:HOH:O	1.88	0.74
2:H:90:GLN:OE1	2:H:259[B]:LEU:HD12	1.89	0.72
2:H:85:SER:OG	7:H:303:TMA:H12	1.89	0.71
3:T:115:SER:OG	7:T:304:TMA:H12	1.89	0.71
7:T:301:TMA:H32	9:T:423:HOH:O	1.91	0.71
2:H:49:ILE:HD11	2:H:114:PRO:HB3	1.71	0.71
3:T:173[B]:ASN:H	3:T:173[B]:ASN:HD22	1.40	0.70
3:T:114:GLN:OE1	7:T:304:TMA:H11	1.91	0.69
1:L:25:CGU:OE22	9:L:302:HOH:O	2.11	0.69
3:T:1:SER:OG	3:T:4:THR:OG1	2.08	0.69
7:T:302:TMA:H11	9:T:608:HOH:O	1.92	0.68
1:L:74:PRO:O	1:L:85:LYS:CE	2.44	0.64
2:H:101[A]:THR:HG23	9:H:443:HOH:O	2.01	0.59
3:T:156[A]:TYR:OH	3:T:165:LYS:CE	2.50	0.59
7:T:301:TMA:H31	9:T:574:HOH:O	2.03	0.59
2:H:49:ILE:CD1	2:H:114:PRO:HB3	2.34	0.58
2:H:35[B]:VAL:HG11	2:H:61:ILE:HD12	1.87	0.57
3:T:156[A]:TYR:OH	3:T:165:LYS:HD3	2.05	0.57
2:H:255:PRO:O	2:H:259[B]:LEU:HD21	2.06	0.56
3:T:78:TYR:HH	7:T:302:TMA:H12	1.71	0.54
3:T:159:LYS:HG2	3:T:185:TYR:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:302[B]:0Z7:C16	9:H:411:HOH:O	2.59	0.51
2:H:161[A]:MET:HE2	9:H:602:HOH:O	2.11	0.50
2:H:49:ILE:HG22	2:H:49:ILE:O	2.11	0.50
3:T:154[A]:THR:HG21	9:T:569:HOH:O	2.10	0.50
1:L:140[A]:ILE:HD11	2:H:26:GLU:HG3	1.94	0.49
1:L:140[A]:ILE:HD13	2:H:25:GLY:HA3	1.94	0.49
3:T:108:LEU:HD11	3:T:193[B]:ILE:HG12	1.93	0.49
8:H:302[B]:0Z7:H18	9:H:411:HOH:O	2.13	0.48
3:T:136:ARG:O	3:T:139:THR:HG22	2.12	0.48
1:L:140[A]:ILE:HD11	2:H:26:GLU:CG	2.45	0.47
3:T:156[B]:TYR:CD2	3:T:167:THR:HG22	2.49	0.47
2:H:56:HIS:CE1	2:H:202:SER:OG	2.69	0.46
3:T:179:VAL:HB	3:T:185:TYR:CE1	2.50	0.46
2:H:161[A]:MET:CE	9:H:602:HOH:O	2.63	0.46
1:L:142:GLU:OE2	9:L:303:HOH:O	2.21	0.45
2:H:168[A]:VAL:HG21	2:H:232:PHE:CE1	2.53	0.44
3:T:156[A]:TYR:OH	3:T:165:LYS:CD	2.66	0.44
3:T:16:SER:HA	3:T:20:LYS:O	2.18	0.44
3:T:159:LYS:HD3	3:T:185:TYR:OH	2.19	0.42
3:T:156[A]:TYR:CZ	3:T:165:LYS:HD3	2.54	0.42
1:L:84:HIS:CE1	1:L:86:ASP:OD1	2.72	0.42
2:H:35[A]:VAL:CG2	2:H:40:LEU:HD22	2.50	0.42
1:L:143:LYS:O	1:L:143:LYS:HG2	2.20	0.42
3:T:159:LYS:HG2	3:T:185:TYR:CE2	2.54	0.42
2:H:47[B]:ASN:CG	9:H:404:HOH:O	2.58	0.42
2:H:35[B]:VAL:HG11	2:H:61:ILE:CD1	2.49	0.41
2:H:102:THR:HA	8:H:302[A]:0Z7:H21	2.03	0.41
2:H:49:ILE:HD13	2:H:114:PRO:HA	2.02	0.41
1:L:86:ASP:O	1:L:86:ASP:OD1	2.39	0.41
1:L:142:GLU:HG3	9:L:303:HOH:O	2.19	0.41
2:H:48:THR:C	2:H:49:ILE:HD13	2.41	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:L:462:HOH:O	9:H:608:HOH:O[4_555]	2.11	0.09
2:H:80:ASP:O	2:H:254:ARG:HH12[4_454]	1.54	0.06

## 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	132/143 (92%)	124 (94%)	8 (6%)	0	100	100
2	H	261/249 (105%)	253 (97%)	8 (3%)	0	100	100
3	T	217/210 (103%)	212 (98%)	5 (2%)	0	100	100
All	All	610/602 (101%)	589 (97%)	21 (3%)	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	116/115 (101%)	115 (99%)	1 (1%)	78	47
2	H	224/210 (107%)	223 (100%)	1 (0%)	91	77
3	T	202/193 (105%)	202 (100%)	0	100	100
All	All	542/518 (105%)	540 (100%)	2 (0%)	91	77

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	110	ARG
2	H	29	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	164	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	20	1,5	3,11,12	1.16	0	1,14,16	0.98	0
1	CGU	L	25	1,5	3,11,12	1.15	0	1,14,16	0.32	0
1	CGU	L	19	1,5	3,11,12	1.07	0	1,14,16	0.57	0
1	CGU	L	26	1,5	3,11,12	0.94	0	1,14,16	0.19	0
1	CGU	L	14	1,5	3,11,12	1.04	0	1,14,16	0.98	0
1	CGU	L	6	1,5	3,11,12	0.97	0	1,14,16	1.32	0
1	CGU	L	29	1,5	3,11,12	1.36	0	1,14,16	0.84	0
1	CGU	L	35	1	3,11,12	1.24	0	1,14,16	1.19	0
1	CGU	L	16	1,5	3,11,12	1.11	0	1,14,16	0.00	0
1	CGU	L	7	1,5	3,11,12	1.05	0	1,14,16	0.29	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	20	1,5	-	0/5/14/16	-
1	CGU	L	25	1,5	-	0/5/14/16	-
1	CGU	L	19	1,5	-	0/5/14/16	-
1	CGU	L	26	1,5	-	0/5/14/16	-
1	CGU	L	14	1,5	-	0/5/14/16	-
1	CGU	L	6	1,5	-	2/5/14/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CGU	L	29	1,5	-	0/5/14/16	-
1	CGU	L	35	1	-	4/5/14/16	-
1	CGU	L	16	1,5	-	1/5/14/16	-
1	CGU	L	7	1,5	-	0/5/14/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) 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	35	CGU	N-CA-CB-CG
1	L	35	CGU	C-CA-CB-CG
1	L	35	CGU	CA-CB-CG-CD1
1	L	35	CGU	CA-CB-CG-CD2
1	L	16	CGU	O-C-CA-CB

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	1,4	11,11,12	0.80	0	15,15,17	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	XYS	A	2	4	9,9,10	1.04	1 (11%)	10,12,14	1.67	2 (20%)
4	XYS	A	3	4	9,9,10	0.99	1 (11%)	10,12,14	1.70	1 (10%)

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	1,4	-	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2	XYS	O5-C1	-2.76	1.37	1.42
4	A	3	XYS	O5-C1	-2.47	1.38	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3	XYS	C5-O5-C1	4.35	118.22	111.52
4	A	2	XYS	C5-O5-C1	3.38	116.72	111.52
4	A	2	XYS	C1-C2-C3	3.08	113.45	109.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry

Of 22 ligands modelled in this entry, 9 are monoatomic - leaving 13 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	304	-	4,4,4	1.21	0	6,6,6	0.30	0
7	TMA	H	305	-	4,4,4	1.19	0	6,6,6	0.08	0
7	TMA	L	213	-	4,4,4	1.22	0	6,6,6	0.04	0
7	TMA	T	303	-	4,4,4	1.19	0	6,6,6	0.13	0
7	TMA	H	304	-	4,4,4	1.18	0	6,6,6	0.12	0
8	0Z7	H	302[A]	2	37,38,39	4.30	12 (32%)	45,49,50	1.81	8 (17%)
7	TMA	H	303	-	4,4,4	1.16	0	6,6,6	0.34	0
7	TMA	H	307	-	4,4,4	1.21	0	6,6,6	0.10	0
6	FUC	L	212	1	10,10,11	0.97	1 (10%)	14,14,16	0.74	0
7	TMA	T	302	-	4,4,4	1.21	0	6,6,6	0.33	0
8	0Z7	H	302[B]	2	37,38,39	4.30	13 (35%)	45,49,50	2.04	11 (24%)
7	TMA	T	301	-	4,4,4	1.18	0	6,6,6	0.18	0
7	TMA	H	306	-	4,4,4	1.16	0	6,6,6	0.24	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
8	0Z7	H	302[B]	2	-	8/39/39/41	0/2/2/2
8	0Z7	H	302[A]	2	-	8/39/39/41	0/2/2/2
6	FUC	L	212	1	-	-	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	302[B]	0Z7	C27-C26	-17.75	1.13	1.50
8	H	302[A]	0Z7	C27-C26	-17.59	1.14	1.50
8	H	302[B]	0Z7	C26-N1	-9.37	1.02	1.34
8	H	302[A]	0Z7	C26-N1	-9.11	1.03	1.34
8	H	302[B]	0Z7	C3-N3	6.92	1.49	1.34
8	H	302[A]	0Z7	C3-N3	6.86	1.49	1.34
8	H	302[B]	0Z7	C25-N4	6.29	1.45	1.33
8	H	302[A]	0Z7	C25-N4	6.25	1.45	1.33
8	H	302[A]	0Z7	C13-N2	-6.02	1.33	1.45
8	H	302[B]	0Z7	C13-N2	-5.91	1.33	1.45
8	H	302[A]	0Z7	C6-C4	-5.60	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	302[B]	0Z7	C5-N2	5.18	1.45	1.34
8	H	302[A]	0Z7	C5-N2	5.11	1.45	1.34
8	H	302[B]	0Z7	C4-N1	-4.90	1.35	1.45
8	H	302[B]	0Z7	C14-C13	-4.79	1.42	1.54
8	H	302[A]	0Z7	C14-C13	-4.71	1.42	1.54
8	H	302[B]	0Z7	C6-C4	-4.31	1.43	1.54
8	H	302[B]	0Z7	O4-C26	-4.31	1.13	1.23
8	H	302[A]	0Z7	O4-C26	-4.21	1.13	1.23
8	H	302[A]	0Z7	C4-N1	-4.19	1.37	1.45
8	H	302[A]	0Z7	C21-N3	-4.08	1.39	1.46
8	H	302[B]	0Z7	C21-N3	-3.85	1.39	1.46
8	H	302[B]	0Z7	C4-C5	-2.61	1.46	1.52
8	H	302[A]	0Z7	O3-C2	-2.50	1.36	1.43
6	L	212	FUC	O5-C1	-2.41	1.39	1.43
8	H	302[B]	0Z7	O3-C2	-2.22	1.37	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	302[A]	0Z7	C27-C26-N1	7.39	128.60	116.10
8	H	302[B]	0Z7	C27-C26-N1	7.12	128.16	116.10
8	H	302[B]	0Z7	C6-C4-N1	-5.65	98.88	110.79
8	H	302[A]	0Z7	O4-C26-C27	-5.04	112.70	122.06
8	H	302[B]	0Z7	O4-C26-C27	-4.44	113.80	122.06
8	H	302[B]	0Z7	C22-C21-N3	-3.87	105.24	110.33
8	H	302[B]	0Z7	C7-C6-C4	3.47	122.96	113.39
8	H	302[A]	0Z7	C22-C21-N3	-2.85	106.58	110.33
8	H	302[A]	0Z7	O1-C5-C4	2.69	126.12	120.45
8	H	302[B]	0Z7	O2-C3-N3	-2.50	118.30	122.93
8	H	302[A]	0Z7	C6-C4-N1	2.50	116.05	110.79
8	H	302[A]	0Z7	C9-C7-C8	2.42	121.97	118.17
8	H	302[A]	0Z7	O2-C3-N3	-2.38	118.53	122.93
8	H	302[B]	0Z7	C5-C4-N1	2.29	117.40	111.16
8	H	302[A]	0Z7	O1-C5-N2	-2.27	118.72	122.93
8	H	302[B]	0Z7	O1-C5-N2	-2.21	118.84	122.93
8	H	302[B]	0Z7	O4-C26-N1	-2.14	118.02	121.95
8	H	302[B]	0Z7	O1-C5-C4	2.00	124.67	120.45
8	H	302[B]	0Z7	C14-C15-C16	-2.00	116.93	120.91

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	302[A]	0Z7	O3-C2-C21-C22
8	H	302[B]	0Z7	O3-C2-C21-C22
8	H	302[B]	0Z7	C3-C13-C14-C15
8	H	302[B]	0Z7	N2-C13-C14-C15
8	H	302[A]	0Z7	O4-C26-N1-C4
8	H	302[A]	0Z7	C27-C26-N1-C4
8	H	302[B]	0Z7	O4-C26-N1-C4
8	H	302[B]	0Z7	C27-C26-N1-C4
8	H	302[B]	0Z7	C13-C14-C15-C16
8	H	302[B]	0Z7	C13-C14-C15-C17
8	H	302[A]	0Z7	C1-C2-C21-C22
8	H	302[A]	0Z7	C6-C4-C5-O1
8	H	302[A]	0Z7	N1-C4-C5-O1
8	H	302[A]	0Z7	C6-C4-C5-N2
8	H	302[B]	0Z7	C1-C2-C21-C22
8	H	302[A]	0Z7	C1-C2-C21-N3

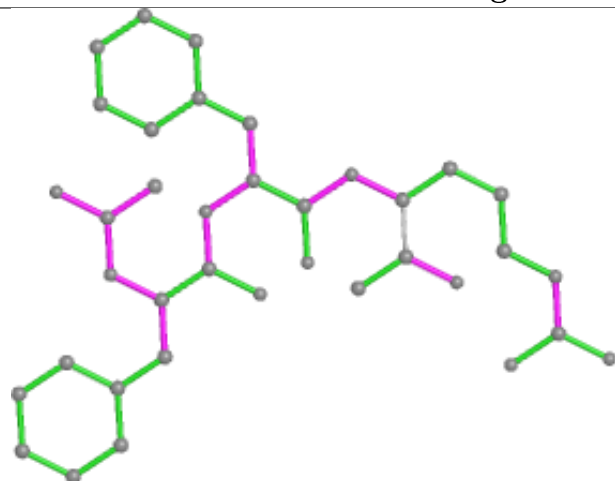
There are no ring outliers.

7 monomers are involved in 14 short contacts:

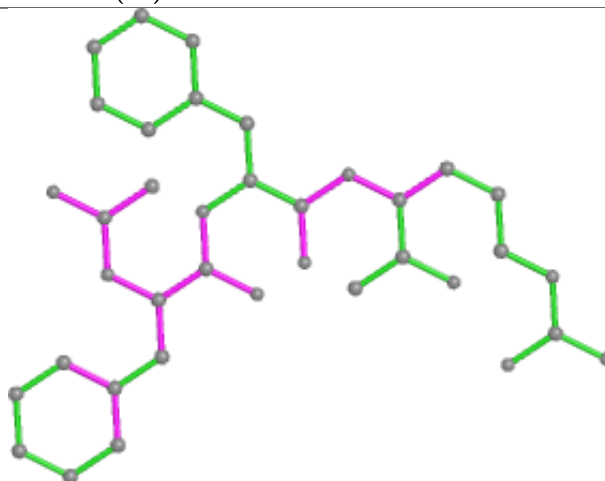
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	304	TMA	2	0
8	H	302[A]	0Z7	1	0
7	H	303	TMA	2	0
7	T	302	TMA	3	0
8	H	302[B]	0Z7	3	0
7	T	301	TMA	2	0
7	H	306	TMA	1	0

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

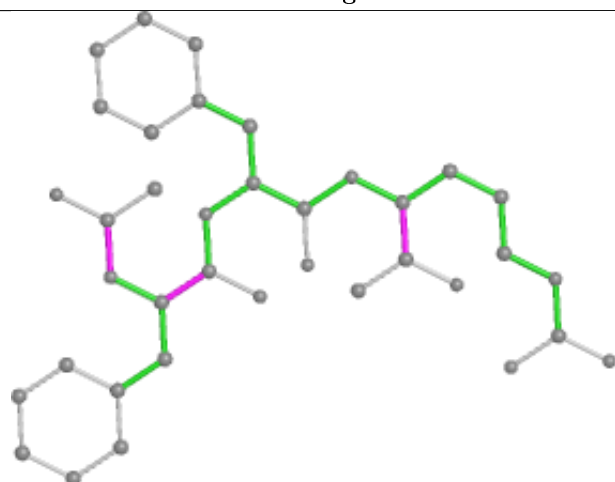
## Ligand 0Z7 H 302 (A)



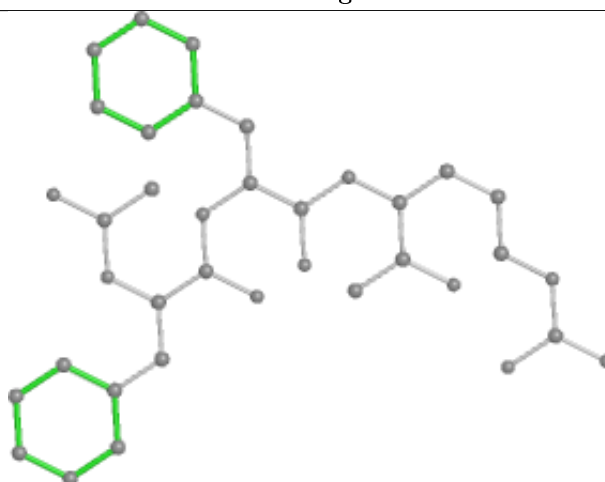
Bond lengths



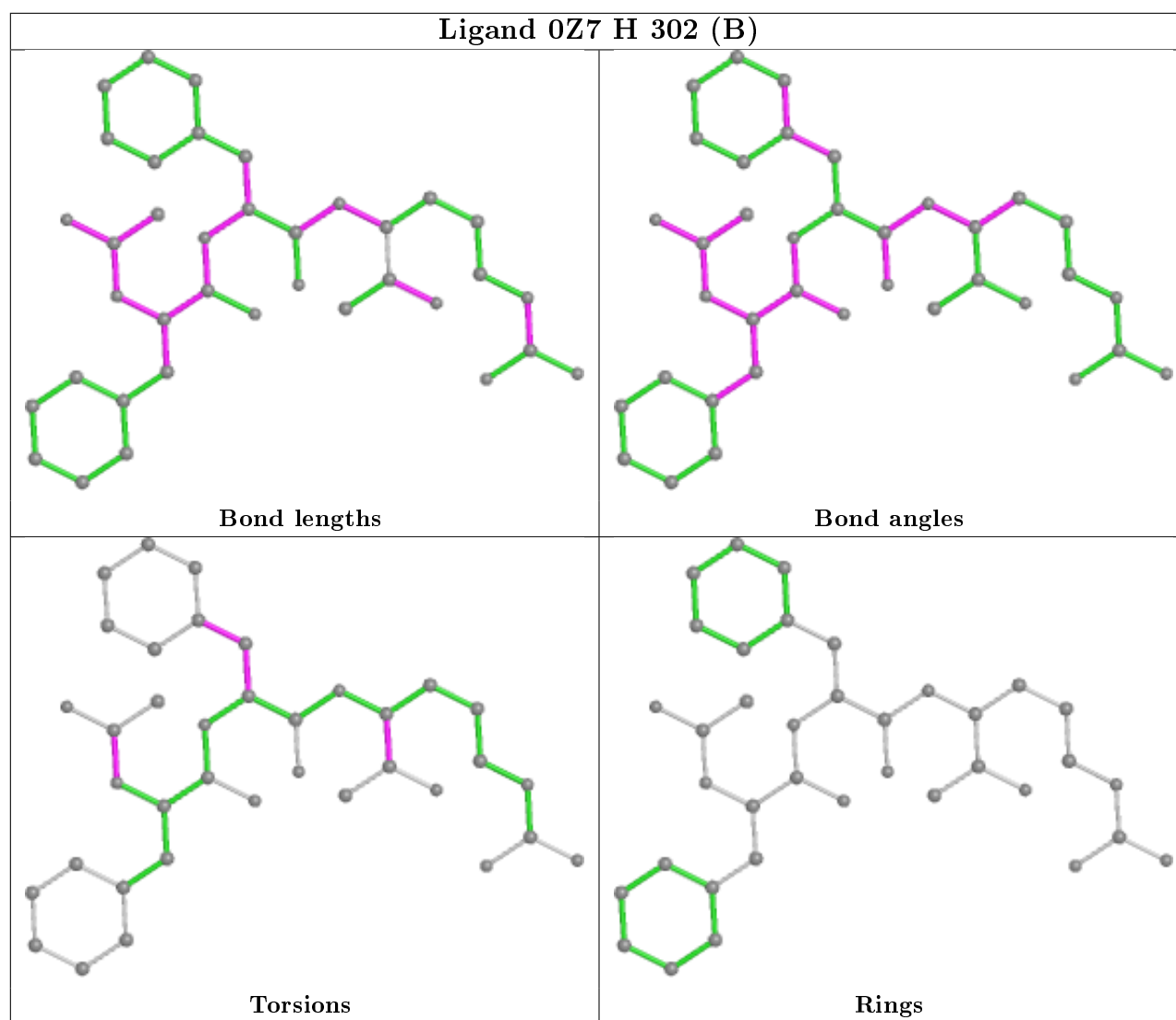
Bond angles



Torsions



Rings



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	L	133/143 (93%)	-0.04	8 (6%) 21 16	13, 27, 53, 79	0
2	H	249/249 (100%)	-0.21	10 (4%) 38 31	10, 15, 36, 80	0
3	T	210/210 (100%)	-0.17	17 (8%) 12 8	12, 19, 50, 85	0
All	All	592/602 (98%)	-0.16	35 (5%) 22 17	10, 19, 50, 85	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	1	SER	8.4
1	L	143	LYS	6.0
2	H	65	ARG	4.7
3	T	161	SER	4.5
2	H	62	LYS	3.9
1	L	122	ALA	3.8
3	T	162	SER	3.8
3	T	4	THR	3.8
3	T	165	LYS	3.7
1	L	4	PHE	3.6
2	H	63	ASN	3.4
3	T	2	GLY	3.3
1	L	106	THR	3.2
2	H	49	ILE	3.1
3	T	156[A]	TYR	3.1
3	T	116	PHE	3.1
1	L	87	ASP	3.0
2	H	36	ASN	3.0
3	T	182	GLY	2.9
2	H	252	GLU	2.8
2	H	64	TRP	2.7
3	T	3	THR	2.7
1	L	32	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	T	184	ASN	2.6
3	T	160	SER	2.6
2	H	61	ILE	2.4
3	T	163	SER	2.4
2	H	254	ARG	2.4
3	T	88	SER	2.2
1	L	85	LYS	2.2
3	T	198	VAL	2.2
3	T	138	ASN	2.1
1	L	121	LEU	2.1
2	H	255	PRO	2.1
3	T	197	THR	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CGU	L	25	12/13	0.87	0.14	28,34,39,41	0
1	CGU	L	19	12/13	0.90	0.14	35,44,48,51	0
1	CGU	L	35	12/13	0.92	0.11	35,66,77,80	0
1	CGU	L	14	12/13	0.94	0.17	26,39,43,46	0
1	CGU	L	29	12/13	0.96	0.08	26,30,35,35	0
1	CGU	L	20	12/13	0.96	0.08	29,32,39,39	0
1	CGU	L	6	12/13	0.97	0.05	21,23,27,29	0
1	CGU	L	26	12/13	0.98	0.05	22,25,28,30	0
1	CGU	L	16	12/13	0.98	0.05	19,21,24,26	0
1	CGU	L	7	12/13	0.98	0.06	20,22,28,28	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	XYS	A	2	9/10	0.82	0.15	33,36,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	XYS	A	3	9/10	0.87	0.20	31,33,39,40	0
4	BGC	A	1	11/12	0.96	0.06	37,43,52,54	0

## 6.4 Ligands

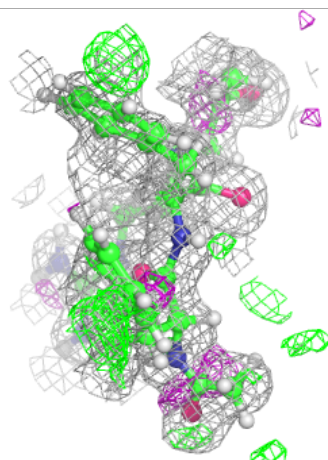
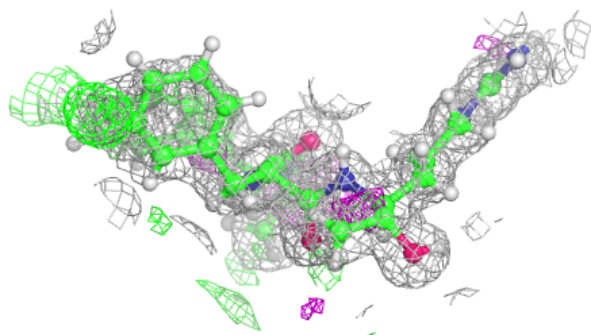
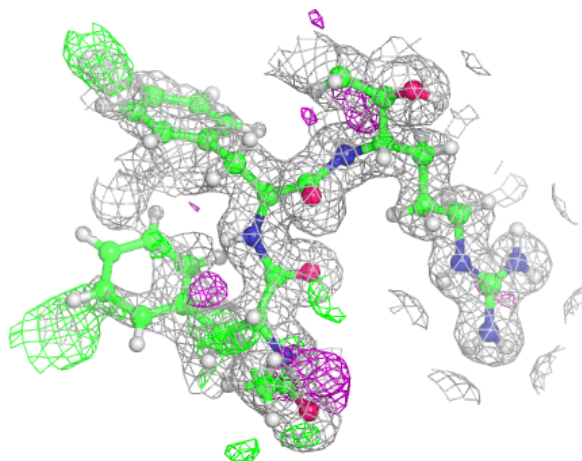
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
7	TMA	T	304	5/5	0.62	0.27	47,57,62,62	0
7	TMA	L	213	5/5	0.62	0.14	97,117,117,117	0
7	TMA	T	301	5/5	0.62	0.22	57,69,70,70	0
7	TMA	H	306	5/5	0.82	0.11	41,49,52,52	0
7	TMA	H	304	5/5	0.83	0.14	47,57,59,59	0
7	TMA	T	302	5/5	0.85	0.10	24,29,34,34	0
7	TMA	H	307	5/5	0.86	0.14	67,81,81,81	0
7	TMA	H	305	5/5	0.86	0.12	63,76,76,76	0
7	TMA	T	303	5/5	0.88	0.11	52,63,64,64	0
7	TMA	H	303	5/5	0.94	0.10	13,19,23,23	0
6	FUC	L	212	10/11	0.94	0.06	27,33,39,41	0
8	0Z7	H	302[B]	37/38	0.95	0.11	11,18,60,64	69
8	0Z7	H	302[A]	37/38	0.95	0.11	11,18,37,43	69
5	CA	L	208	1/1	0.97	0.04	28,28,28,28	1
5	CA	L	207	1/1	0.98	0.04	39,39,39,39	0
5	CA	L	206	1/1	0.98	0.12	49,49,49,49	0
5	CA	L	202	1/1	0.99	0.05	25,25,25,25	0
5	CA	L	203	1/1	1.00	0.03	20,20,20,20	0
5	CA	L	204	1/1	1.00	0.04	20,20,20,20	0
5	CA	H	301	1/1	1.00	0.07	12,12,12,12	0
5	CA	L	205	1/1	1.00	0.03	25,25,25,25	0
5	CA	L	201	1/1	1.00	0.04	27,27,27,27	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 302 (B):**

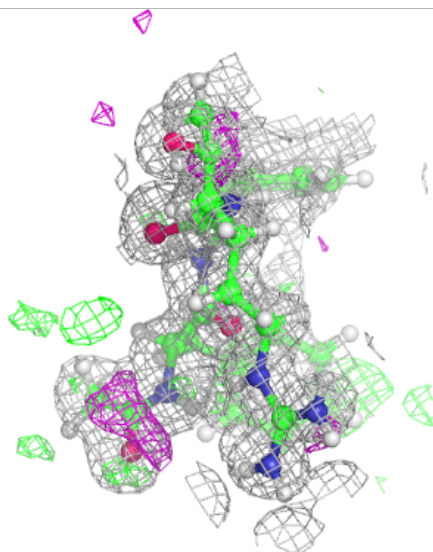
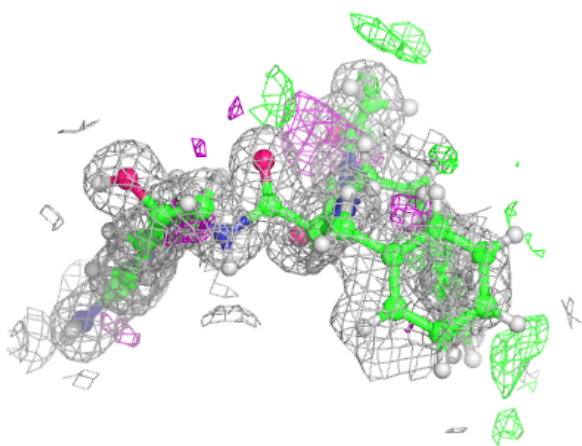
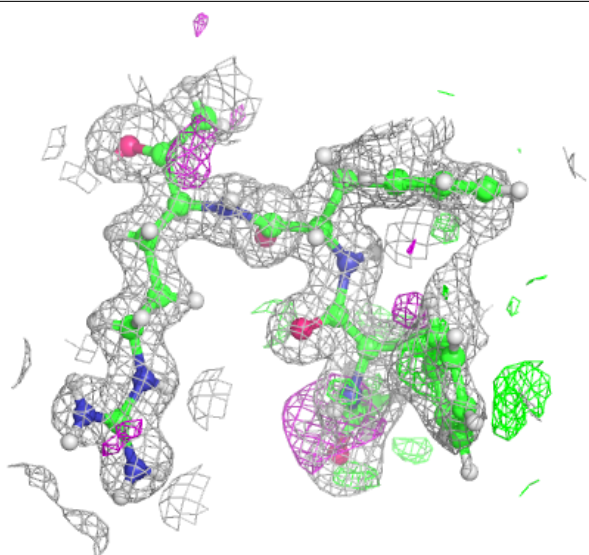
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around 0Z7 H 302 (A):**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.