



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 06:33 pm GMT

PDB ID : 4ZMA  
Title : Crystal Structure of a FVIIa-Trypsin Chimera (ST) in Complex with Soluble Tissue Factor  
Authors : Sorensen, A.B.; Svensson, L.A.; Gandhi, P.S.  
Deposited on : 2015-05-02  
Resolution : 2.30 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

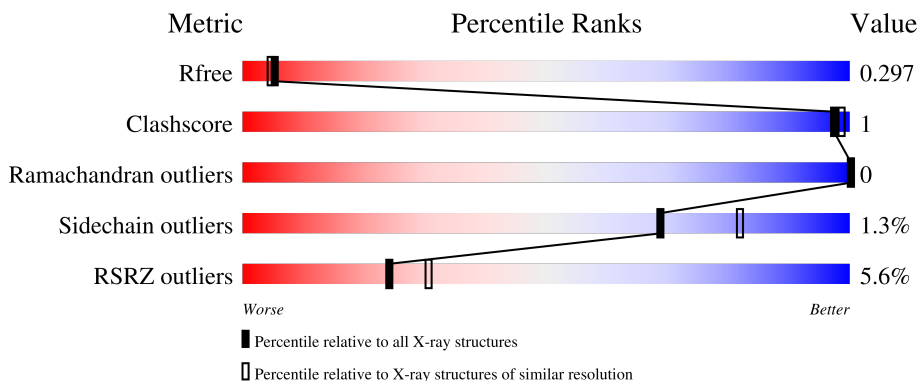
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


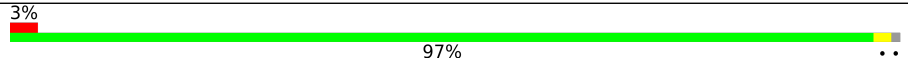
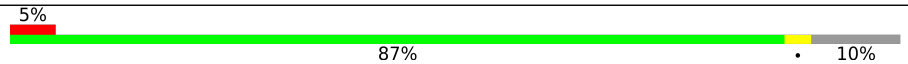
The reported resolution of this entry is 2.30 Å.

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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	152	
2	H	249	
3	T	219	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9129 atoms, of which 4295 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
			Total	C	H	N	O	S			
1	L	141	2009	656	919	182	237	15	0	0	0

- Molecule 2 is a protein called Coagulation factor VII.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	H	247	3735	1207	1845	325	342	16	0	3	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	169	GLU	LEU	engineered mutation	UNP P08709
H	170	ALA	GLN	engineered mutation	UNP P08709
H	171	SER	GLN	engineered mutation	UNP P08709
H	?	-	ARG	deletion	UNP P08709
H	?	-	LYS	deletion	UNP P08709
H	?	-	VAL	deletion	UNP P08709
H	?	-	GLY	deletion	UNP P08709
H	?	-	ASP	deletion	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

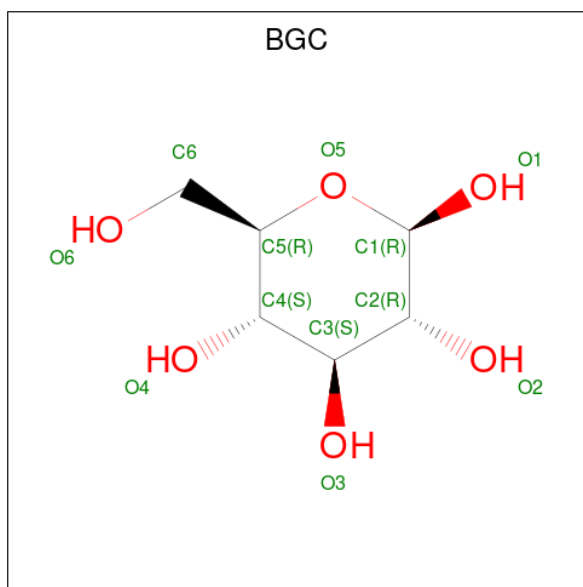
- Molecule 3 is a protein called Tissue factor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	T	198	3043	994	1477	249	316	7	0	2	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

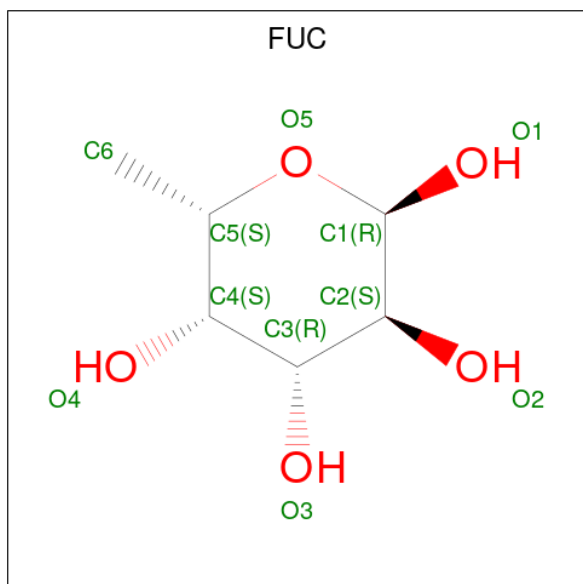
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	7	Total	Ca	0	0
			7	7		
4	H	1	Total	Ca	0	0
			1	1		

- Molecule 5 is beta-D-glucopyranose (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



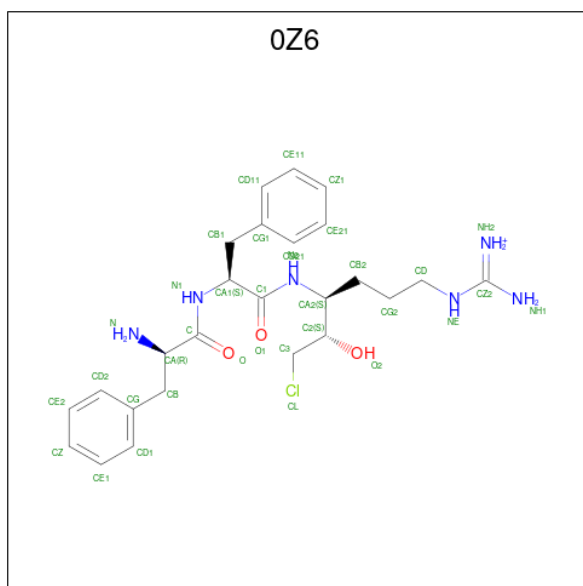
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	H	O	0	0
			21	6	10	5		

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



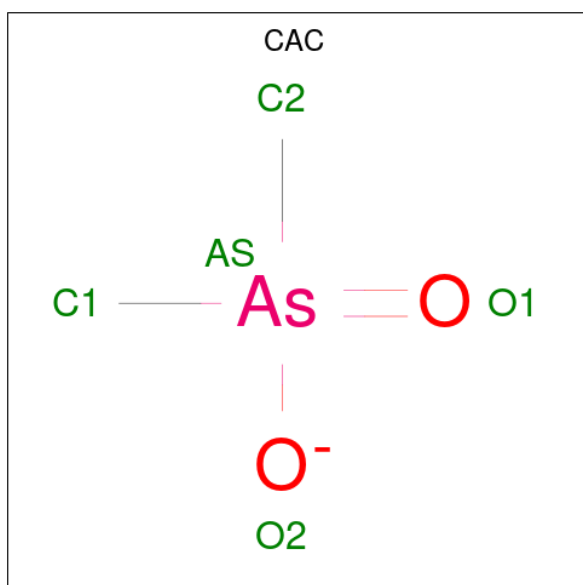
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	L	1	19	6	9	4	0	0

- Molecule 7 is D-phenylalanyl-N-[(2S,3S)-6-[[amino(iminio)methyl]amino]-1-chloro-2-hydroxyhexan-3-yl]-L-phenylalaninamide (three-letter code: 0Z6) (formula: C<sub>25</sub>H<sub>36</sub>ClN<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
7	H	1	69	25	35	6	3	0	0

- Molecule 8 is CACODYLATE ION (three-letter code: CAC) (formula: C<sub>2</sub>H<sub>6</sub>AsO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	H	1	Total	As	C	O	0	0
			5	1	2	2		
8	H	1	Total	As	C	O	0	0
			5	1	2	2		

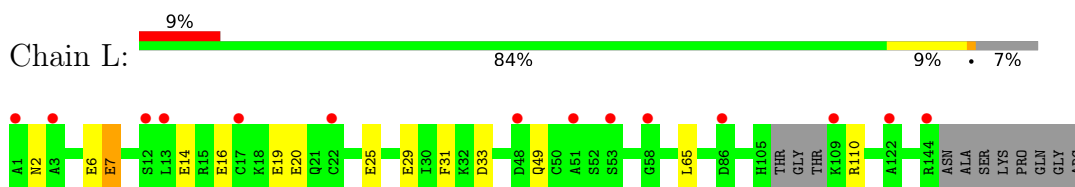
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	42	Total	O	0	0
			42	42		
9	H	115	Total	O	0	0
			115	115		
9	T	58	Total	O	0	0
			58	58		

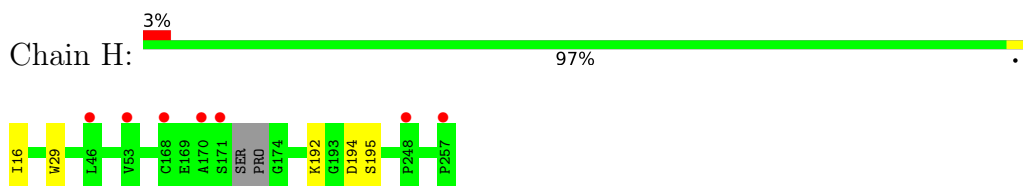
### 3 Residue-property plots [i](#)

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.

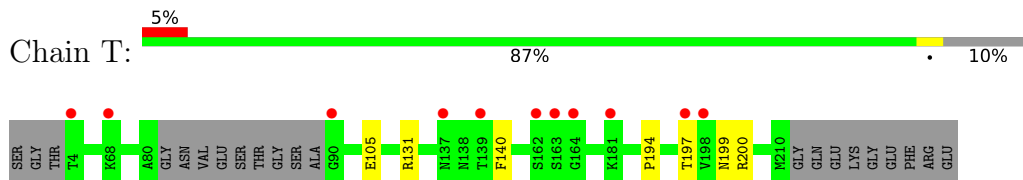
- Molecule 1: Coagulation factor VII



- Molecule 2: Coagulation factor VII



- Molecule 3: Tissue factor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.21Å 80.90Å 125.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 2.30 29.77 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.1 (29.77-2.30) 96.1 (29.77-2.30)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.31Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.240 , 0.295 0.243 , 0.297	Depositor DCC
$R_{free}$ test set	1500 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtrriage
Anisotropy	0.333	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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: FUC, OZ6, CAC, BGC, 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	0.22	0/988	0.35	0/1322
2	H	0.20	0/1947	0.37	0/2654
3	T	0.21	0/1607	0.37	0/2193
All	All	0.21	0/4542	0.37	0/6169

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	1090	919	916	3	0
2	H	1890	1845	1844	1	0
3	T	1566	1477	1476	3	0
4	H	1	0	0	0	0
4	L	7	0	0	0	0
5	L	11	10	10	0	0
6	L	10	9	10	0	0
7	H	34	35	30	0	0
8	H	10	0	0	0	0
9	H	115	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	42	0	0	0	0
9	T	58	0	0	0	0
All	All	4834	4295	4286	7	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 1.

All (7) 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:L:2:ASN:OD1	1:L:7:CGU:OE22	2.19	0.60
3:T:105:GLU:O	3:T:199:ASN:ND2	2.42	0.53
1:L:31:PHE:O	1:L:33:ASP:N	2.43	0.51
1:L:49:GLN:OE1	1:L:49:GLN:N	2.43	0.51
3:T:131:ARG:NH1	3:T:140:PHE:O	2.42	0.50
2:H:16:ILE:N	2:H:194:ASP:OD2	2.46	0.49
3:T:194:PRO:O	3:T:200:ARG:NH2	2.46	0.49

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	127/152 (84%)	118 (93%)	9 (7%)	0	100	100
2	H	246/249 (99%)	235 (96%)	11 (4%)	0	100	100
3	T	196/219 (90%)	186 (95%)	10 (5%)	0	100	100
All	All	569/620 (92%)	539 (95%)	30 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	104/122 (85%)	102 (98%)	2 (2%)	57	73
2	H	204/210 (97%)	201 (98%)	3 (2%)	65	79
3	T	176/200 (88%)	175 (99%)	1 (1%)	86	94
All	All	484/532 (91%)	478 (99%)	6 (1%)	69	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	65	LEU
1	L	110	ARG
2	H	29	TRP
2	H	192	LYS
2	H	195	SER
3	T	197	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	1,4	9,11,12	1.31	0	9,14,16	0.88	0
1	CGU	L	19	1,4	9,11,12	1.40	1 (11%)	9,14,16	0.88	0
1	CGU	L	14	1,4	9,11,12	1.46	2 (22%)	9,14,16	0.91	0
1	CGU	L	6	1,4	9,11,12	1.58	1 (11%)	9,14,16	0.82	0
1	CGU	L	16	1,4	9,11,12	1.66	2 (22%)	9,14,16	0.85	0
1	CGU	L	29	1,4	9,11,12	1.48	2 (22%)	9,14,16	0.81	0
1	CGU	L	25	1	9,11,12	1.45	1 (11%)	9,14,16	0.83	0
1	CGU	L	7	1,4	9,11,12	1.43	1 (11%)	9,14,16	0.75	0
1	CGU	L	35	1	3,4,12	1.08	0	2,4,16	1.08	0
1	CGU	L	20	1,4	9,11,12	1.47	1 (11%)	9,14,16	1.03	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	1,4	-	5/13/14/16	-
1	CGU	L	19	1,4	-	4/13/14/16	-
1	CGU	L	14	1,4	-	7/13/14/16	-
1	CGU	L	6	1,4	-	4/13/14/16	-
1	CGU	L	16	1,4	-	6/13/14/16	-
1	CGU	L	29	1,4	-	3/13/14/16	-
1	CGU	L	25	1	-	4/13/14/16	-
1	CGU	L	7	1,4	-	1/13/14/16	-
1	CGU	L	35	1	-	0/0/2/16	-
1	CGU	L	20	1,4	-	2/13/14/16	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	16	CGU	CG-CD2	2.77	1.55	1.52
1	L	6	CGU	CG-CD2	2.70	1.55	1.52
1	L	16	CGU	CG-CD1	2.42	1.55	1.52
1	L	7	CGU	CG-CD2	2.37	1.55	1.52
1	L	14	CGU	CG-CD2	2.29	1.55	1.52
1	L	20	CGU	CG-CD1	2.25	1.55	1.52
1	L	29	CGU	CG-CD1	2.17	1.54	1.52
1	L	19	CGU	CG-CD2	2.12	1.54	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	25	CGU	CG-CD2	2.08	1.54	1.52
1	L	14	CGU	CG-CD1	2.05	1.54	1.52
1	L	29	CGU	CG-CD2	2.03	1.54	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (36) 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	14	CGU	C-CA-CB-CG
1	L	14	CGU	CA-CB-CG-CD1
1	L	16	CGU	CA-CB-CG-CD2
1	L	16	CGU	OE12-CD1-CG-CD2
1	L	20	CGU	OE12-CD1-CG-CD2
1	L	25	CGU	C-CA-CB-CG
1	L	29	CGU	O-C-CA-CB
1	L	29	CGU	C-CA-CB-CG
1	L	6	CGU	OE21-CD2-CG-CB
1	L	6	CGU	OE22-CD2-CG-CB
1	L	14	CGU	OE11-CD1-CG-CB
1	L	14	CGU	OE12-CD1-CG-CB
1	L	14	CGU	OE21-CD2-CG-CB
1	L	14	CGU	OE22-CD2-CG-CB
1	L	16	CGU	OE11-CD1-CG-CB
1	L	16	CGU	OE12-CD1-CG-CB
1	L	19	CGU	OE11-CD1-CG-CB
1	L	19	CGU	OE12-CD1-CG-CB
1	L	19	CGU	OE21-CD2-CG-CB
1	L	19	CGU	OE22-CD2-CG-CB
1	L	25	CGU	OE21-CD2-CG-CB
1	L	26	CGU	OE11-CD1-CG-CB
1	L	26	CGU	OE12-CD1-CG-CB
1	L	26	CGU	OE21-CD2-CG-CB
1	L	26	CGU	OE22-CD2-CG-CB
1	L	16	CGU	OE11-CD1-CG-CD2
1	L	20	CGU	OE11-CD1-CG-CD2
1	L	14	CGU	N-CA-CB-CG
1	L	25	CGU	N-CA-CB-CG
1	L	25	CGU	OE22-CD2-CG-CB

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Mol	Chain	Res	Type	Atoms
1	L	29	CGU	N-CA-CB-CG
1	L	7	CGU	OE12-CD1-CG-CD2
1	L	16	CGU	OE21-CD2-CG-CD1
1	L	26	CGU	OE12-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	7	CGU	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	CAC	H	503	2	0,4,4	-	-	0,6,6	-	-
8	CAC	H	504	-	0,4,4	-	-	0,6,6	-	-
6	FUC	L	209	1	10,10,11	0.72	0	14,14,16	0.82	0
7	OZ6	H	501	2	34,35,36	1.83	4 (11%)	41,45,46	0.95	1 (2%)
5	BGC	L	208	1	11,11,12	0.83	0	15,15,17	0.82	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
7	OZ6	H	501	2	-	6/35/35/37	0/2/2/2
5	BGC	L	208	1	-	2/2/19/22	0/1/1/1
6	FUC	L	209	1	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	501	OZ6	CZ2-NE	6.47	1.46	1.33
7	H	501	OZ6	C1-N2	5.56	1.46	1.34
7	H	501	OZ6	C-N1	4.97	1.45	1.34
7	H	501	OZ6	CZ2-NH1	2.04	1.43	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	501	OZ6	CA-C-N1	3.26	120.67	116.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

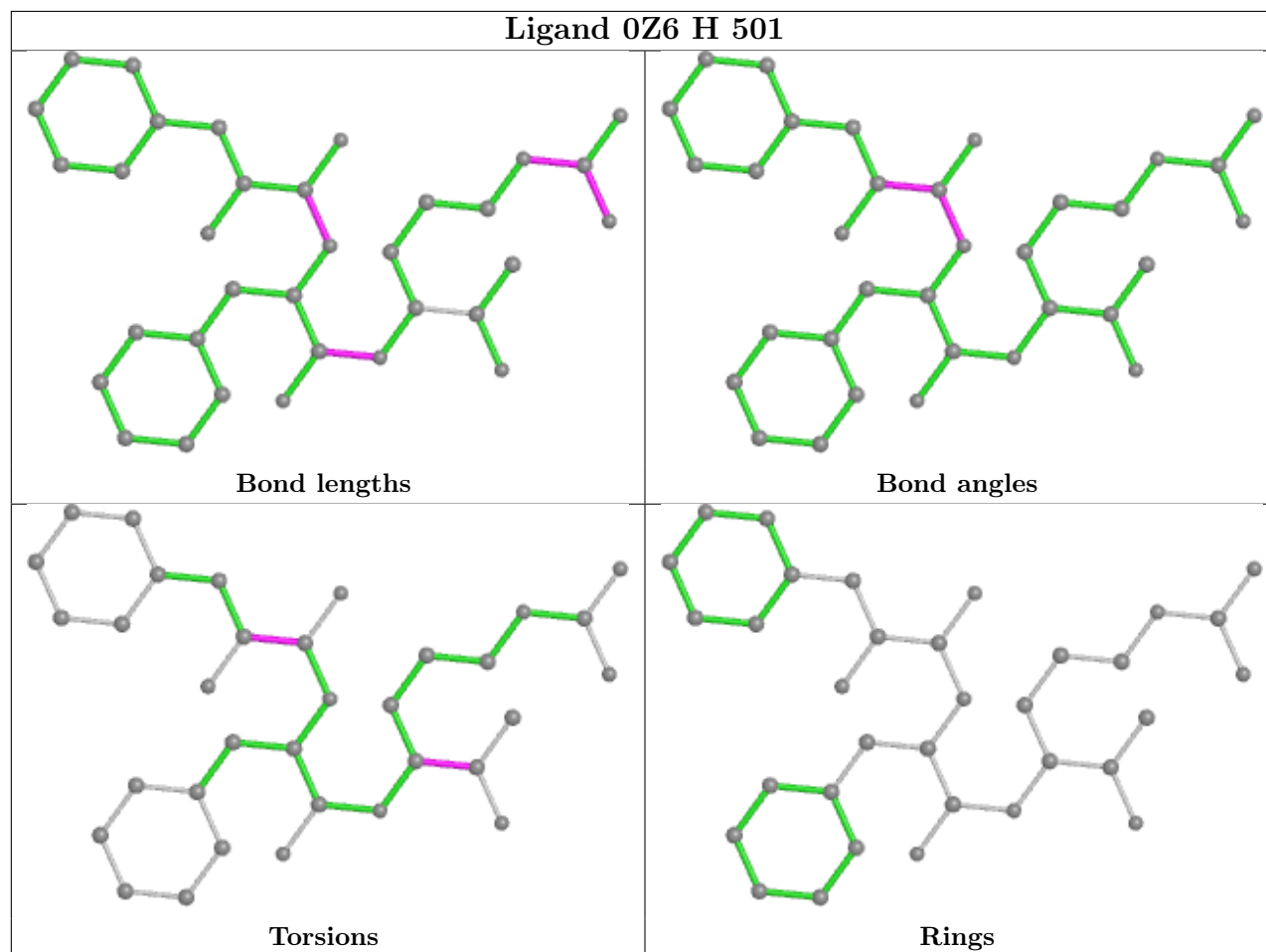
Mol	Chain	Res	Type	Atoms
7	H	501	OZ6	O-C-CA-CB
7	H	501	OZ6	N1-C-CA-CB
7	H	501	OZ6	O2-C2-CA2-N2
7	H	501	OZ6	C3-C2-CA2-N2
7	H	501	OZ6	O2-C2-CA2-CB2
7	H	501	OZ6	C3-C2-CA2-CB2
5	L	208	BGC	O5-C5-C6-O6
5	L	208	BGC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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, 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	131/152 (86%)	0.72	14 (10%) <b>6</b> <b>8</b>	26, 50, 61, 67	0
2	H	247/249 (99%)	0.44	7 (2%) 53 60	16, 29, 45, 61	0
3	T	198/219 (90%)	0.43	11 (5%) <b>24</b> <b>30</b>	26, 39, 59, 67	0
All	All	576/620 (92%)	0.50	32 (5%) <b>24</b> <b>30</b>	16, 37, 58, 67	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	248	PRO	7.4
3	T	164	GLY	5.9
1	L	51	ALA	4.7
3	T	4	THR	4.3
1	L	17	CYS	4.1
1	L	53	SER	4.0
2	H	170	ALA	3.9
2	H	171	SER	3.8
2	H	257	PRO	3.7
3	T	181	LYS	3.4
1	L	13	LEU	3.4
3	T	137	ASN	3.4
1	L	1	ALA	3.2
1	L	58	GLY	3.1
1	L	48	ASP	3.0
3	T	139	THR	3.0
1	L	144	ARG	2.8
3	T	90	GLY	2.8
3	T	162	SER	2.7
3	T	163	SER	2.6
1	L	86	ASP	2.6
1	L	109	LYS	2.6
1	L	3	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	22	CYS	2.5
2	H	168[A]	CYS	2.5
1	L	122	ALA	2.4
3	T	198	VAL	2.3
2	H	53	VAL	2.2
2	H	46	LEU	2.0
3	T	68	LYS	2.0
1	L	12	SER	2.0
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	20	12/13	0.68	0.31	59,66,81,81	0
1	CGU	L	26	12/13	0.75	0.17	47,54,60,64	0
1	CGU	L	19	12/13	0.77	0.38	60,69,79,81	0
1	CGU	L	14	12/13	0.78	0.24	51,61,72,74	0
1	CGU	L	6	12/13	0.78	0.22	48,58,67,70	0
1	CGU	L	7	12/13	0.80	0.17	38,51,62,65	0
1	CGU	L	25	12/13	0.82	0.20	42,53,65,65	0
1	CGU	L	16	12/13	0.84	0.22	52,58,77,77	0
1	CGU	L	29	12/13	0.86	0.19	40,48,63,64	0
1	CGU	L	35	5/13	0.89	0.23	55,58,69,70	0

## 6.3 Carbohydrates [i](#)

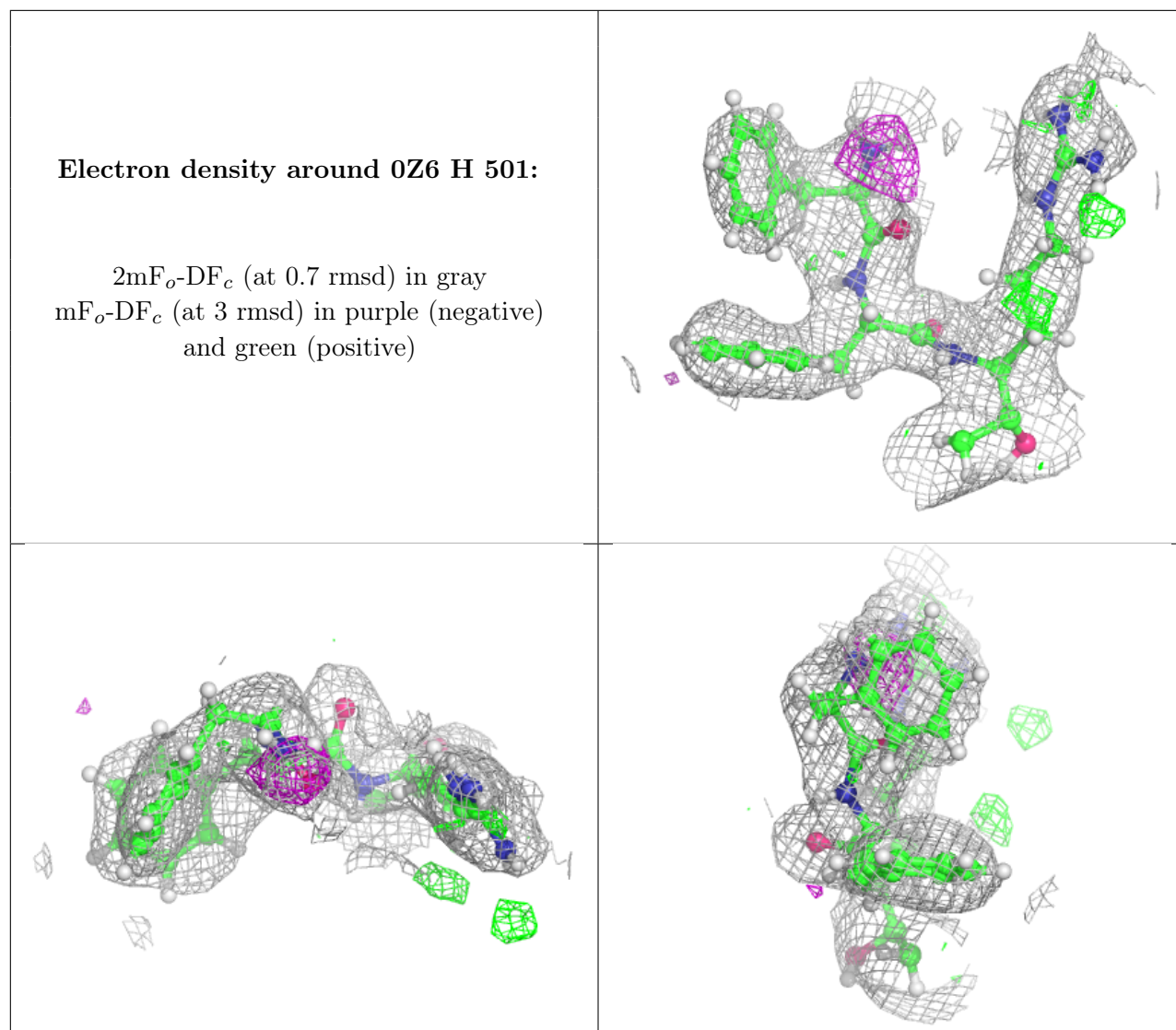
There are no monosaccharides in this entry.

## 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, 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
4	CA	L	204	1/1	0.04	0.14	64,64,64,64	0
4	CA	L	205	1/1	0.41	0.08	57,57,57,57	0
4	CA	L	206	1/1	0.68	0.12	70,70,70,70	0
4	CA	L	207	1/1	0.68	0.12	73,73,73,73	0
4	CA	L	202	1/1	0.71	0.09	43,43,43,43	0
4	CA	L	201	1/1	0.79	0.10	52,52,52,52	0
5	BGC	L	208	11/12	0.80	0.17	45,54,62,75	0
6	FUC	L	209	10/11	0.85	0.24	49,55,66,66	0
7	0Z6	H	501	34/35	0.85	0.16	26,36,47,52	0
4	CA	L	203	1/1	0.86	0.06	47,47,47,47	0
8	CAC	H	503	5/5	0.89	0.15	46,50,57,81	0
4	CA	H	502	1/1	0.91	0.12	32,32,32,32	0
8	CAC	H	504	5/5	0.98	0.19	47,52,66,67	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.