



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2025 – 10:27 PM EDT

PDB ID : 1DAN  
Title : Complex of active site inhibited human blood coagulation factor VIIA with human recombinant soluble tissue factor  
Authors : Banner, D.W.  
Deposited on : 1997-03-05  
Resolution : 2.00 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

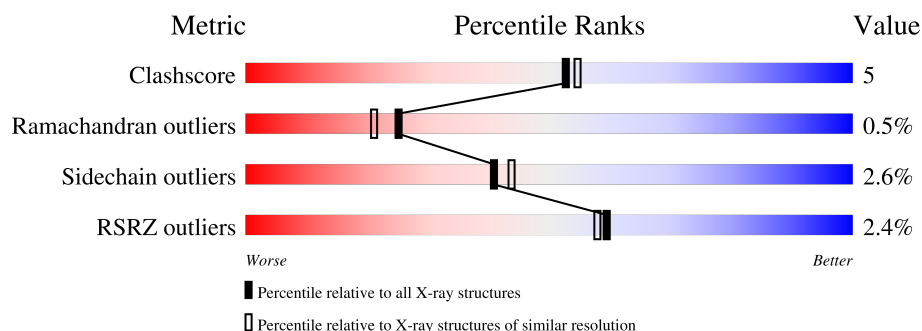
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>80%</span> <span>13%</span> <span>7%</span> </div> </div>
2	H	254	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>89%</span> <span>10%</span> </div> </div>
3	T	80	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>81%</span> <span>11%</span> <span>6%</span> </div> </div>
4	U	121	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>7%</span> <span>82%</span> <span>12%</span> </div> </div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 4971 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BLOOD COAGULATION FACTOR VIIA light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	142	Total	C	N	O	S	46	0	0
			1134	683	189	247	15			

- Molecule 2 is a protein called BLOOD COAGULATION FACTOR VIIA heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	254	Total	C	N	O	S	75	0	0
			1974	1253	351	357	13			

- Molecule 3 is a protein called SOLUBLE TISSUE FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	75	Total	C	N	O	S	7	0	0
			614	397	95	120	2			

- Molecule 4 is a protein called SOLUBLE TISSUE FACTOR.

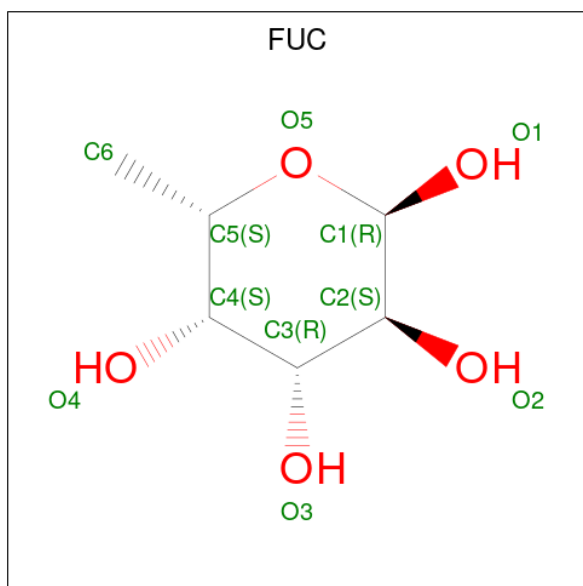
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	U	116	Total	C	N	O	S	39	0	0
			940	593	155	189	3			

- 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	O	0	0
			11	6	5		

- Molecule 6 is alpha-L-fucopyranose (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).

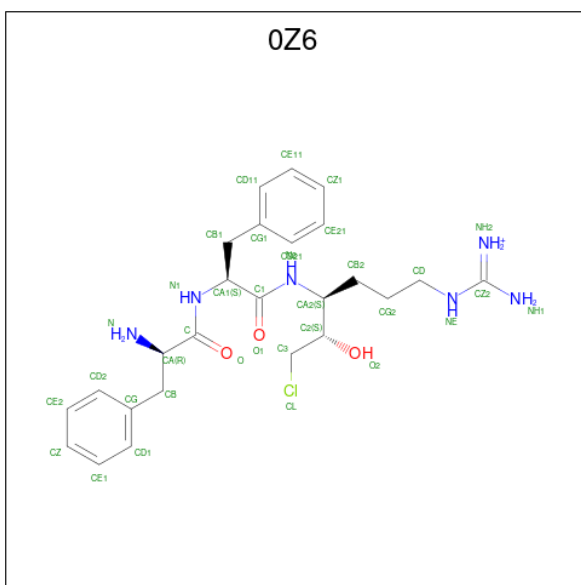


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

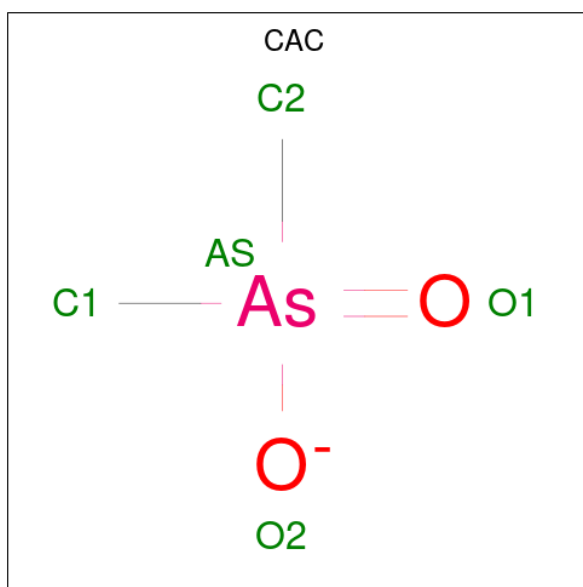
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	8	Total Ca 8 8	0	0
7	H	1	Total Ca 1 1	0	0

- Molecule 8 is D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-phenylalaninamide (three-letter code: 0Z6) (formula:  $C_{25}H_{36}ClN_6O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	H	1	Total	C	N	O	0	0
			34	25	6	3		

- Molecule 9 is CACODYLATE ION (three-letter code: CAC) (formula:  $\text{C}_2\text{H}_6\text{AsO}_2$ ).



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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	H	1	Total	Cl	0	0
			1	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	47	Total	O	0	0
			47	47		
11	H	106	Total	O	0	0
			106	106		
11	T	40	Total	O	0	0
			40	40		
11	U	46	Total	O	0	0
			46	46		

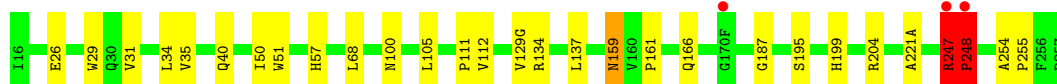
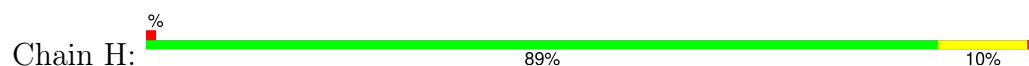
### 3 Residue-property plots

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.

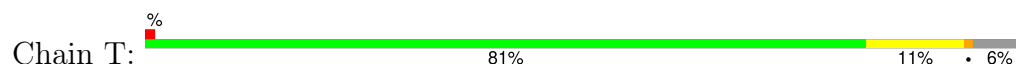
- Molecule 1: BLOOD COAGULATION FACTOR VIIA light chain



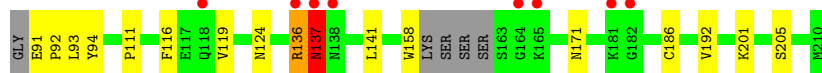
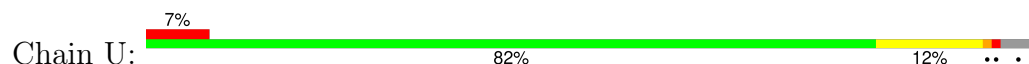
- Molecule 2: BLOOD COAGULATION FACTOR VIIA heavy chain



- Molecule 3: SOLUBLE TISSUE FACTOR



- Molecule 4: SOLUBLE TISSUE FACTOR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.65Å 82.55Å 126.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-2.00) 98.0 (20.00-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.50 (at 2.01Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.187 , 0.218 0.189 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4971	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CGU, CAC, CL, OZ6, BGC, CA, FUC

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	0.40	0/1028	0.64	0/1374
2	H	0.41	0/2024	0.76	3/2755 (0.1%)
3	T	0.43	0/630	0.73	0/860
4	U	0.43	0/958	0.73	1/1299 (0.1%)
All	All	0.41	0/4640	0.73	4/6288 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	248	PRO	N-CA-C	6.82	129.83	112.10
2	H	199	HIS	N-CA-C	-6.39	93.74	111.00
2	H	129(G)	VAL	N-CA-C	-5.13	97.14	111.00
4	U	136	ARG	N-CA-C	-5.11	97.21	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1134	0	987	6	0
2	H	1974	0	1949	20	0
3	T	614	0	598	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	U	940	0	912	12	0
5	L	11	0	10	1	0
6	L	10	0	10	0	0
7	H	1	0	0	0	0
7	L	8	0	0	0	0
8	H	34	0	32	0	0
9	H	5	0	0	0	0
10	H	1	0	0	0	0
11	H	106	0	0	0	0
11	L	47	0	0	1	0
11	T	40	0	0	1	0
11	U	46	0	0	0	0
All	All	4971	0	4498	43	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 (43) 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)
2:H:68:LEU:HD12	2:H:112:VAL:HG11	1.47	0.94
2:H:31:VAL:HG22	2:H:68:LEU:HD21	1.56	0.85
2:H:68:LEU:CD1	2:H:112:VAL:HG11	2.18	0.74
2:H:247:ARG:HB3	2:H:248:PRO:CD	2.17	0.74
3:T:45:TRP:HH2	3:T:72:LEU:HD12	1.60	0.66
2:H:34:LEU:HD23	2:H:40:GLN:HA	1.79	0.64
2:H:50:ILE:HG22	2:H:111:PRO:HB3	1.82	0.59
4:U:136:ARG:HE	4:U:141:LEU:HD21	1.69	0.57
3:T:76:PHE:CD1	4:U:94:TYR:HB3	2.40	0.56
2:H:247:ARG:HB3	2:H:248:PRO:HD3	1.86	0.56
3:T:69:GLN:NE2	3:T:69:GLN:HA	2.21	0.54
2:H:187:GLY:HA2	2:H:221(A):ALA:O	2.08	0.54
3:T:29:PRO:HB2	3:T:32:GLN:O	2.08	0.53
1:L:137:LYS:O	1:L:139:PRO:HD3	2.08	0.53
1:L:101:TYR:OH	1:L:115:HIS:HD2	1.93	0.50
3:T:69:GLN:HA	3:T:69:GLN:HE21	1.76	0.50
1:L:98:CYS:O	2:H:204:ARG:NH1	2.45	0.49
4:U:111:PRO:HG2	4:U:205:SER:HB3	1.94	0.48
4:U:192:VAL:HG22	4:U:201:LYS:HG2	1.95	0.47
5:L:153:BGC:H6C1	11:L:170:HOH:O	2.14	0.47
2:H:50:ILE:HG13	2:H:51:TRP:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:116:PHE:HA	4:U:124:ASN:O	2.16	0.47
1:L:140:ILE:HD11	2:H:26:GLU:HG3	1.96	0.46
3:T:46:LYS:HE2	11:T:119:HOH:O	2.14	0.46
3:T:45:TRP:CH2	3:T:72:LEU:HD12	2.46	0.46
2:H:51:TRP:CE3	2:H:105:LEU:HG	2.50	0.45
1:L:36:ARG:HD3	4:U:158:TRP:CD1	2.51	0.45
3:T:16:SER:HA	3:T:20:LYS:O	2.17	0.44
4:U:158:TRP:CE2	4:U:186:CYS:HB2	2.53	0.44
2:H:137:LEU:HD23	2:H:159:ASN:HD22	1.82	0.43
4:U:119:VAL:HG23	4:U:119:VAL:O	2.19	0.43
1:L:110:ARG:HD2	1:L:110:ARG:C	2.38	0.43
2:H:57:HIS:CE1	2:H:195:SER:OG	2.71	0.43
2:H:254:ALA:HA	2:H:255:PRO:HD3	1.92	0.43
4:U:91:GLU:HA	4:U:92:PRO:HD3	1.82	0.43
2:H:35:VAL:O	2:H:35:VAL:HG23	2.20	0.42
4:U:136:ARG:O	4:U:137:ASN:C	2.58	0.42
2:H:166:GLN:HB3	4:U:94:TYR:OH	2.19	0.41
4:U:158:TRP:NE1	4:U:186:CYS:HB2	2.34	0.41
3:T:72:LEU:HD13	3:T:73:ALA:N	2.35	0.41
2:H:134:ARG:O	2:H:161:PRO:HA	2.21	0.41
2:H:31:VAL:HG22	2:H:68:LEU:CD2	2.38	0.41
2:H:50:ILE:CG2	2:H:111:PRO:HB3	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	130/152 (86%)	121 (93%)	9 (7%)	0	100	100
2	H	252/254 (99%)	238 (94%)	12 (5%)	2 (1%)	16	12
3	T	73/80 (91%)	70 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	U	112/121 (93%)	106 (95%)	5 (4%)	1 (1%)	14	10
All	All	567/607 (93%)	535 (94%)	29 (5%)	3 (0%)	25	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	247	ARG
4	U	137	ASN
2	H	248	PRO

### 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	114/122 (93%)	109 (96%)	5 (4%)	24	22
2	H	216/216 (100%)	212 (98%)	4 (2%)	52	57
3	T	70/74 (95%)	69 (99%)	1 (1%)	62	68
4	U	109/113 (96%)	106 (97%)	3 (3%)	38	40
All	All	509/525 (97%)	496 (97%)	13 (3%)	41	44

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	52	SER
1	L	86	ASP
1	L	103	SER
1	L	106	THR
1	L	110	ARG
2	H	29	TRP
2	H	100	ASN
2	H	159	ASN
2	H	247	ARG
3	T	69	GLN
4	U	93	LEU

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Mol	Chain	Res	Type
4	U	137	ASN
4	U	171	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	80	ASN
1	L	115	HIS
2	H	100	ASN
2	H	110	GLN
2	H	143	GLN
2	H	159	ASN
4	U	171	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	6	1,7	9,11,12	1.19	1 (11%)	10,14,16	1.28	1 (10%)
1	CGU	L	19	1,7	9,11,12	1.55	1 (11%)	10,14,16	1.16	1 (10%)
1	CGU	L	25	1,7	9,11,12	1.48	1 (11%)	10,14,16	1.09	1 (10%)
1	CGU	L	16	1,7	9,11,12	1.03	0	10,14,16	0.93	1 (10%)
1	CGU	L	26	1,7	9,11,12	1.28	1 (11%)	10,14,16	1.35	2 (20%)
1	CGU	L	29	1,7	9,11,12	1.37	1 (11%)	10,14,16	1.18	1 (10%)
1	CGU	L	35	1	9,11,12	1.09	1 (11%)	10,14,16	1.04	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CGU	L	20	1,7	9,11,12	1.08	0	10,14,16	1.53	2 (20%)
1	CGU	L	14	1,7	9,11,12	1.02	0	10,14,16	0.72	0
1	CGU	L	7	1,7	9,11,12	1.64	2 (22%)	10,14,16	1.10	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	6	1,7	-	3/13/14/16	-
1	CGU	L	19	1,7	-	0/13/14/16	-
1	CGU	L	25	1,7	-	0/13/14/16	-
1	CGU	L	16	1,7	-	4/13/14/16	-
1	CGU	L	26	1,7	-	2/13/14/16	-
1	CGU	L	29	1,7	-	0/13/14/16	-
1	CGU	L	35	1	-	3/13/14/16	-
1	CGU	L	20	1,7	-	0/13/14/16	-
1	CGU	L	14	1,7	-	0/13/14/16	-
1	CGU	L	7	1,7	-	2/13/14/16	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	7	CGU	CG-CD2	-3.12	1.48	1.52
1	L	25	CGU	CG-CD2	3.06	1.56	1.52
1	L	19	CGU	CG-CD2	3.05	1.56	1.52
1	L	6	CGU	OE22-CD2	-2.40	1.23	1.30
1	L	7	CGU	CG-CD1	2.32	1.55	1.52
1	L	26	CGU	OE22-CD2	-2.13	1.23	1.30
1	L	29	CGU	OE22-CD2	-2.11	1.23	1.30
1	L	35	CGU	OE22-CD2	-2.11	1.23	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	20	CGU	CB-CG-CD2	-3.72	105.56	113.11
1	L	6	CGU	CB-CG-CD2	-2.74	107.54	113.11
1	L	26	CGU	OE22-CD2-CG	2.47	124.92	116.50
1	L	20	CGU	CB-CA-C	-2.42	107.27	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	26	CGU	OE22-CD2-OE21	-2.31	118.84	124.08
1	L	29	CGU	OE22-CD2-OE21	-2.29	118.88	124.08
1	L	19	CGU	CB-CG-CD2	-2.23	108.57	113.11
1	L	35	CGU	OE21-CD2-CG	-2.21	112.81	120.19
1	L	25	CGU	CB-CG-CD2	-2.16	108.73	113.11
1	L	16	CGU	CB-CG-CD2	-2.14	108.77	113.11

There are no chirality outliers.

All (14) 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	6	CGU	OE21-CD2-CG-CD1
1	L	26	CGU	OE21-CD2-CG-CB
1	L	26	CGU	OE22-CD2-CG-CB
1	L	35	CGU	N-CA-CB-CG
1	L	35	CGU	C-CA-CB-CG
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	16	CGU	OE21-CD2-CG-CD1
1	L	16	CGU	OE22-CD2-CG-CD1
1	L	35	CGU	OE11-CD1-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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	0Z6	H	1	2	34,35,36	1.31	2 (5%)	41,45,46	0.74	2 (4%)
6	FUC	L	154	1	10,10,11	1.06	1 (10%)	14,14,16	0.92	0
5	BGC	L	153	1	11,11,12	1.23	1 (9%)	15,15,17	1.71	1 (6%)
9	CAC	H	259	-	2,4,4	0.56	0	2,6,6	0.72	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	0Z6	H	1	2	-	1/35/35/37	0/2/2/2
6	FUC	L	154	1	-	-	0/1/1/1
5	BGC	L	153	1	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	1	0Z6	O2-C2	-6.92	1.24	1.43
5	L	153	BGC	C2-C3	2.67	1.56	1.52
8	H	1	0Z6	C3-C2	2.11	1.57	1.51
6	L	154	FUC	C1-C2	2.04	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	153	BGC	C1-O5-C5	5.89	120.08	112.19
8	H	1	0Z6	C1-CA1-N1	-2.66	103.91	111.11
8	H	1	0Z6	C2-CA2-N2	2.24	114.97	110.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	1	0Z6	O2-C2-CA2-CB2

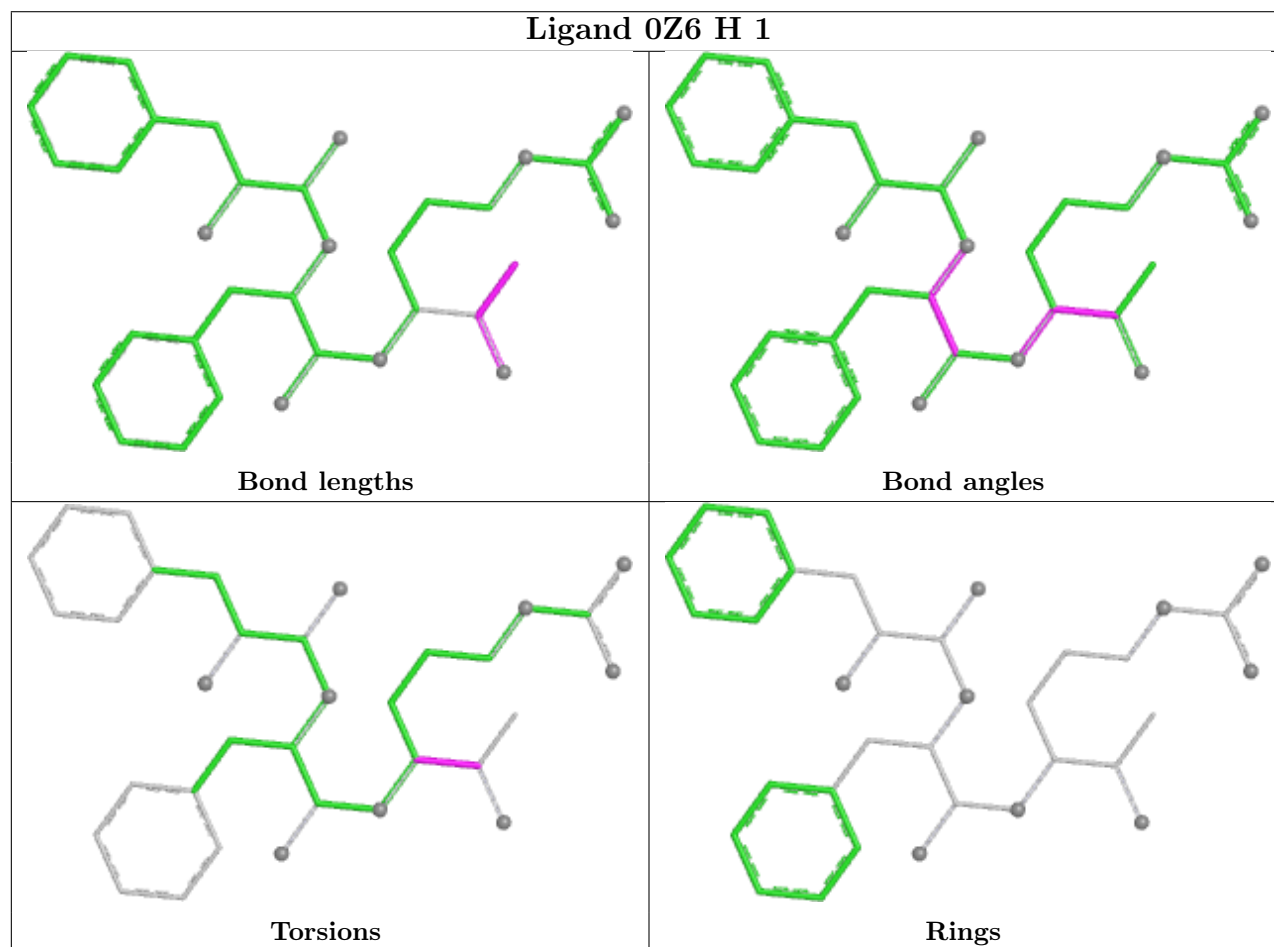


There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	153	BGC	1	0

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



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 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	132/152 (86%)	0.29	2 (1%) 71 70	18, 38, 54, 68	10 (7%)
2	H	254/254 (100%)	-0.40	3 (1%) 76 75	12, 23, 50, 72	23 (9%)
3	T	75/80 (93%)	-0.44	1 (1%) 74 73	15, 25, 50, 62	4 (5%)
4	U	116/121 (95%)	0.33	8 (6%) 24 22	9, 32, 58, 69	21 (18%)
All	All	577/607 (95%)	-0.10	14 (2%) 59 58	9, 29, 54, 72	58 (10%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	U	181	LYS	5.6
4	U	165	LYS	4.5
4	U	137	ASN	4.3
3	T	80	ALA	3.9
4	U	182	GLY	3.7
4	U	118	GLN	3.6
1	L	107	GLY	3.1
2	H	170(F)	GLY	3.0
1	L	36	ARG	2.9
4	U	138	ASN	2.9
4	U	164	GLY	2.6
4	U	136	ARG	2.6
2	H	248	PRO	2.4
2	H	247	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, 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
1	CGU	L	35	12/13	0.73	0.11	58,70,96,99	7
1	CGU	L	19	12/13	0.80	0.11	44,59,68,70	1
1	CGU	L	14	12/13	0.83	0.11	39,61,70,72	0
1	CGU	L	25	12/13	0.84	0.13	36,63,72,72	0
1	CGU	L	20	12/13	0.89	0.10	38,43,47,55	0
1	CGU	L	29	12/13	0.92	0.07	31,36,47,50	0
1	CGU	L	7	12/13	0.93	0.07	23,31,36,40	0
1	CGU	L	26	12/13	0.93	0.10	28,34,40,45	0
1	CGU	L	6	12/13	0.95	0.07	26,32,40,48	0
1	CGU	L	16	12/13	0.95	0.07	19,34,38,38	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

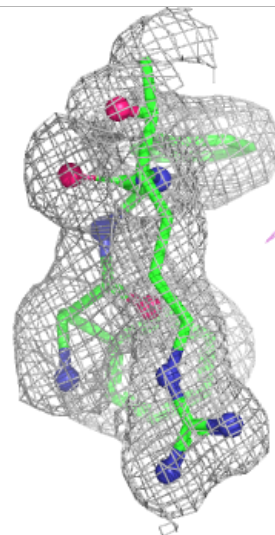
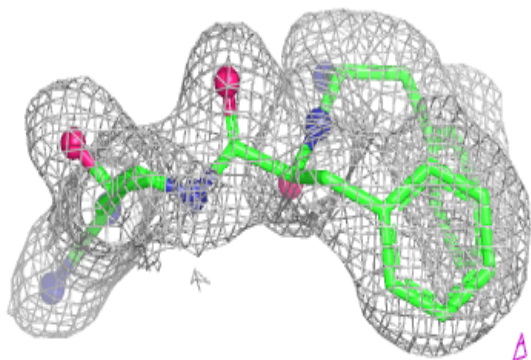
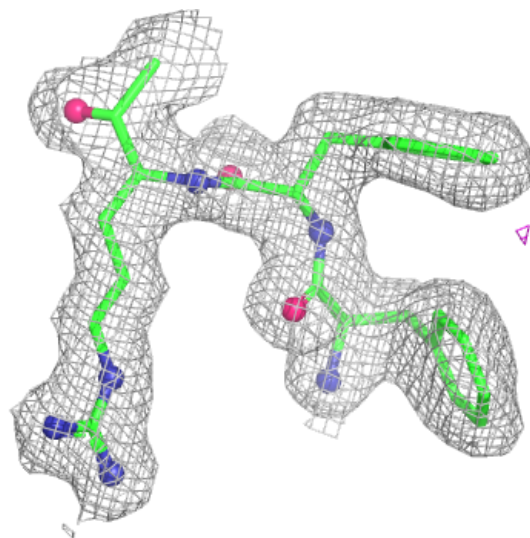
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	BGC	L	153	11/12	0.84	0.14	54,59,74,81	0
7	CA	L	161	1/1	0.88	0.13	62,62,62,62	0
6	FUC	L	154	10/11	0.89	0.09	53,56,57,59	0
7	CA	L	162	1/1	0.89	0.10	62,62,62,62	0
7	CA	L	160	1/1	0.93	0.06	76,76,76,76	0
7	CA	L	155	1/1	0.96	0.04	41,41,41,41	0
7	CA	H	258	1/1	0.96	0.05	30,30,30,30	0
8	OZ6	H	1	34/35	0.96	0.06	9,24,34,35	0
7	CA	L	159	1/1	0.97	0.04	34,34,34,34	0
7	CA	L	156	1/1	0.98	0.04	31,31,31,31	0
7	CA	L	157	1/1	0.98	0.04	31,31,31,31	0
7	CA	L	158	1/1	0.98	0.03	29,29,29,29	0
10	CL	H	260	1/1	0.98	0.04	27,27,27,27	0
9	CAC	H	259	5/5	0.99	0.08	29,32,36,44	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 0Z6 H 1:**

$2mF_o-DF_c$  (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.