



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 08:24 pm GMT

PDB ID : 2A2Q  
Title : Complex of Active-site Inhibited Human Coagulation Factor VIIa with Human Soluble Tissue Factor in the Presence of Ca<sup>2+</sup>, Mg<sup>2+</sup>, Na<sup>+</sup>, and Zn<sup>2+</sup>  
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Deposited on : 2005-06-22  
Resolution : 1.80 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

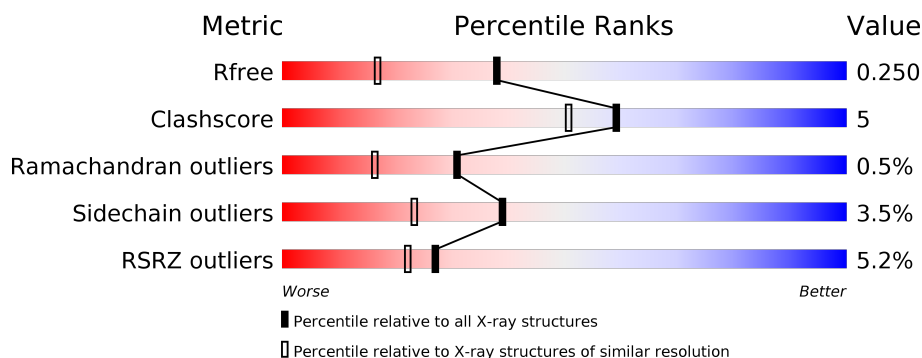
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	111664	5253 (1.80-1.80)
Clashscore	122126	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (1.80-1.80)
RSRZ outliers	108989	5157 (1.80-1.80)

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. 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>7%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>• • 7%</div> </div> </div>
2	H	254	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>•</div> </div> </div>
3	T	205	<div> <div>8%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>7%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GLC	L	201	X	-	-	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 5427 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 Coagulation factor VII.

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

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	6	CGU	GLU	MODIFIED RESIDUE	UNP P08709
L	7	CGU	GLU	MODIFIED RESIDUE	UNP P08709
L	14	CGU	GLU	MODIFIED RESIDUE	UNP P08709
L	16	CGU	GLU	MODIFIED RESIDUE	UNP P08709
L	19	CGU	GLU	MODIFIED RESIDUE	UNP P08709
L	20	CGU	GLU	MODIFIED RESIDUE	UNP P08709
L	25	CGU	GLU	MODIFIED RESIDUE	UNP P08709
L	26	CGU	GLU	MODIFIED RESIDUE	UNP P08709
L	29	CGU	GLU	MODIFIED RESIDUE	UNP P08709
L	35	CGU	GLU	MODIFIED RESIDUE	UNP P08709

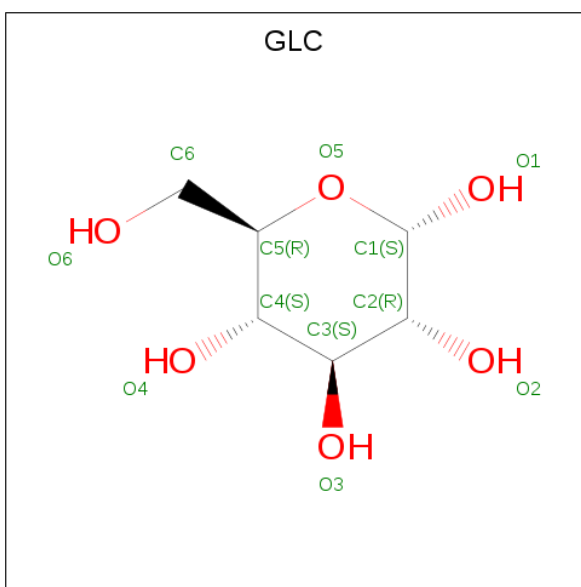
- Molecule 2 is a protein called Coagulation factor VII.

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

- Molecule 3 is a protein called Tissue factor.

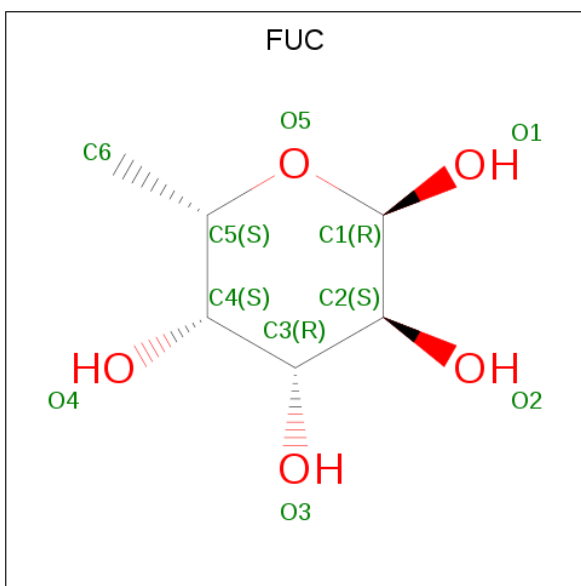
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	191	Total	C	N	O	S	0	0	0
			1551	987	250	309	5			

- Molecule 4 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	3	Total	Mg	0	0
			3	3		

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

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

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	1	Total	Na	0	0
			1	1		

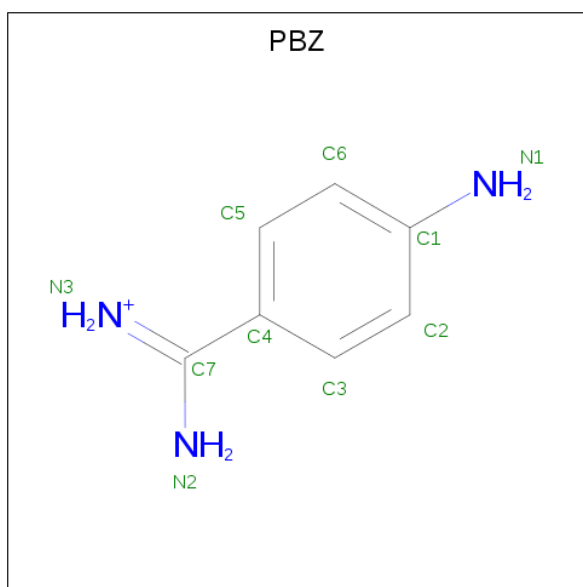
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	2	Total	Zn	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	H	2	Total	Cl	0	0
			2	2		
10	T	1	Total	Cl	0	0
			1	1		

- Molecule 11 is P-AMINO BENZAMIDINE (three-letter code: PBZ) (formula: C<sub>7</sub>H<sub>10</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	H	1	Total	C	N	0	0
			10	7	3		

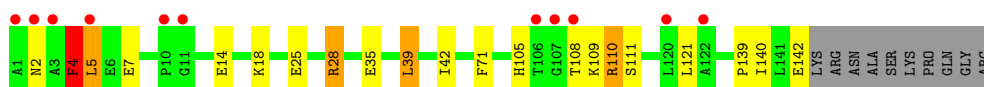
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	L	177	Total	O	0	0
			177	177		
12	H	329	Total	O	0	0
			329	329		
12	T	216	Total	O	0	0
			216	216		

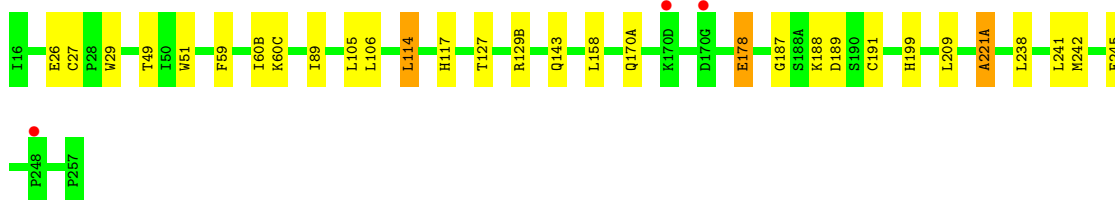
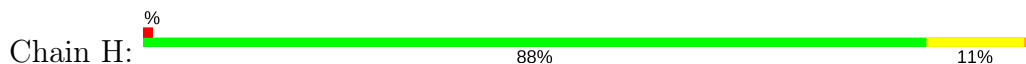
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

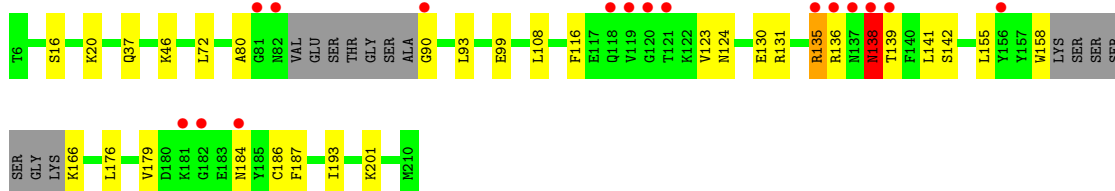
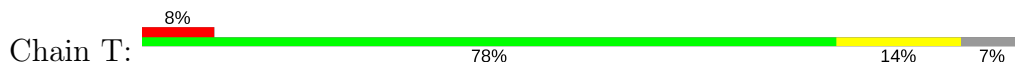
#### • Molecule 1: Coagulation factor VII



#### • 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, $\alpha$ , $\beta$ , $\gamma$	69.72Å 81.00Å 126.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.00 – 1.80 40.50 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (90.00-1.80) 89.8 (40.50-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 1.79Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.198 , 0.259 0.200 , 0.250	Depositor DCC
$R_{free}$ test set	5983 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.7	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 67.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5427	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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: MG, CL, NA, CA, GLC, ZN, PBZ, FUC, CGU

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	0.49	0/1028	0.73	1/1374 (0.1%)
2	H	0.55	1/2024 (0.0%)	0.80	1/2755 (0.0%)
3	T	0.54	0/1585	0.77	0/2156
All	All	0.53	1/4637 (0.0%)	0.77	2/6285 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	221(A)	ALA	C-O	5.36	1.33	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	199	HIS	N-CA-C	-6.87	92.46	111.00
1	L	4	PHE	N-CA-C	5.99	127.16	111.00

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	1134	0	987	15	0
2	H	1974	0	1950	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	T	1551	0	1501	18	0
4	L	11	0	10	0	0
5	L	10	0	10	0	0
6	L	3	0	0	0	0
7	H	1	0	0	0	0
7	L	5	0	0	0	0
8	H	1	0	0	0	0
9	H	2	0	0	0	0
10	H	2	0	0	0	0
10	T	1	0	0	0	0
11	H	10	0	10	0	0
12	H	329	0	0	6	0
12	L	177	0	0	0	0
12	T	216	0	0	4	0
All	All	5427	0	4468	47	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 (47) 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:187:GLY:HA2	2:H:221(A):ALA:O	1.90	0.72
3:T:108:LEU:HD11	3:T:193:ILE:HG12	1.71	0.71
1:L:105:HIS:HE1	1:L:111:SER:OG	1.76	0.69
1:L:35:CGU:O	1:L:39:LEU:HD23	1.97	0.65
2:H:188:LYS:O	2:H:189:ASP:HB2	1.98	0.64
2:H:117:HIS:HD2	12:H:1153:HOH:O	1.83	0.62
1:L:140:ILE:HD11	2:H:26:GLU:HG3	1.84	0.60
2:H:117:HIS:HE1	12:H:1157:HOH:O	1.85	0.59
1:L:140:ILE:HD11	2:H:26:GLU:CG	2.31	0.58
3:T:158:TRP:CE2	3:T:186:CYS:HB2	2.40	0.56
1:L:105:HIS:HB3	1:L:108:THR:HG23	1.87	0.56
3:T:72:LEU:HD23	3:T:99:GLU:HG2	1.87	0.56
3:T:138:ASN:ND2	3:T:139:THR:HG23	2.20	0.56
3:T:90:GLY:HA3	12:T:1156:HOH:O	2.05	0.56
3:T:155:LEU:HD11	3:T:187:PHE:HB3	1.89	0.55
2:H:170(A):GLN:NE2	12:H:1310:HOH:O	2.43	0.51
2:H:238:LEU:O	2:H:242:MET:HG3	2.11	0.51
3:T:166:LYS:HB2	12:T:1101:HOH:O	2.11	0.51
1:L:14:CGU:HA	1:L:18:LYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2:ASN:HB3	1:L:7:CGU:OE21	2.13	0.49
2:H:127:THR:O	2:H:129(B):ARG:HG2	2.11	0.49
3:T:80:ALA:HB2	12:T:1210:HOH:O	2.13	0.48
3:T:136:ARG:HB3	3:T:141:LEU:HD21	1.95	0.48
2:H:27:CYS:HB3	12:H:1246:HOH:O	2.14	0.48
2:H:158:LEU:HD12	12:H:1293:HOH:O	2.14	0.48
1:L:105:HIS:CB	1:L:108:THR:HG23	2.44	0.47
2:H:59:PHE:HA	2:H:60(B):ILE:HG12	1.97	0.47
3:T:130:GLU:O	3:T:142:SER:HA	2.15	0.47
1:L:139:PRO:HA	1:L:142:GLU:HG2	1.97	0.47
1:L:71:PHE:CE2	3:T:131:ARG:HG3	2.50	0.47
2:H:89:ILE:HG21	2:H:241:LEU:HD13	1.98	0.46
3:T:16:SER:HA	3:T:20:LYS:O	2.16	0.46
3:T:116:PHE:HA	3:T:124:ASN:O	2.17	0.45
3:T:123:VAL:HG23	3:T:179:VAL:HG21	1.98	0.45
3:T:37:GLN:HA	3:T:46:LYS:O	2.17	0.45
3:T:131:ARG:HB3	12:T:1180:HOH:O	2.16	0.44
1:L:140:ILE:HD11	2:H:26:GLU:HG2	1.98	0.44
12:H:1231:HOH:O	3:T:93:LEU:HG	2.18	0.44
2:H:49:THR:HG22	2:H:114:LEU:HD13	2.00	0.43
2:H:178:GLU:H	2:H:178:GLU:HG3	1.42	0.43
1:L:109:LYS:HG2	1:L:110:ARG:N	2.34	0.42
2:H:51:TRP:CE3	2:H:105:LEU:HG	2.55	0.42
1:L:25:CGU:OE21	1:L:28:ARG:NH1	2.53	0.42
1:L:110:ARG:C	1:L:110:ARG:HD2	2.40	0.41
2:H:143:GLN:HB2	2:H:191:CYS:SG	2.61	0.41
1:L:4:PHE:CE1	1:L:5:LEU:HD13	2.56	0.40
3:T:135:ARG:HA	3:T:139:THR:O	2.21	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%)	123 (95%)	6 (5%)	1 (1%)	21	8
2	H	252/254 (99%)	245 (97%)	7 (3%)	0	100	100
3	T	185/205 (90%)	177 (96%)	6 (3%)	2 (1%)	16	4
All	All	567/611 (93%)	545 (96%)	19 (3%)	3 (0%)	31	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	4	PHE
3	T	184	ASN
3	T	138	ASN

### 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	114/122 (93%)	107 (94%)	7 (6%)	20	7
2	H	216/216 (100%)	209 (97%)	7 (3%)	42	27
3	T	178/189 (94%)	174 (98%)	4 (2%)	55	42
All	All	508/527 (96%)	490 (96%)	18 (4%)	39	23

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	PHE
1	L	5	LEU
1	L	28	ARG
1	L	39	LEU
1	L	42	ILE
1	L	110	ARG
1	L	121	LEU
2	H	29	TRP
2	H	60(C)	LYS
2	H	106	LEU

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Mol	Chain	Res	Type
2	H	114	LEU
2	H	178	GLU
2	H	209	LEU
2	H	245	GLU
3	T	135	ARG
3	T	138	ASN
3	T	176	LEU
3	T	201	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	105	HIS
2	H	110	GLN
2	H	117	HIS
2	H	175	ASN
3	T	199	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	14	1,6	4,11,12	1.16	0	4,14,16	1.00	0
1	CGU	L	16	1,7,6	4,11,12	1.43	1 (25%)	4,14,16	1.70	1 (25%)
1	CGU	L	19	1,6	4,11,12	1.71	1 (25%)	4,14,16	0.98	0
1	CGU	L	20	1,7	4,11,12	1.49	1 (25%)	4,14,16	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CGU	L	25	1,6	4,11,12	1.33	1 (25%)	4,14,16	1.13	0
1	CGU	L	26	1,7,6	4,11,12	1.15	0	4,14,16	1.35	0
1	CGU	L	29	1,7,6	4,11,12	1.17	1 (25%)	4,14,16	0.87	0
1	CGU	L	35	1	4,11,12	0.64	0	4,14,16	1.14	0
1	CGU	L	6	1,7	4,11,12	0.43	0	4,14,16	1.24	0
1	CGU	L	7	1,7	4,11,12	1.75	1 (25%)	4,14,16	1.26	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	14	1,6	-	0/4/14/16	0/0/0/0
1	CGU	L	16	1,7,6	-	0/4/14/16	0/0/0/0
1	CGU	L	19	1,6	-	0/4/14/16	0/0/0/0
1	CGU	L	20	1,7	-	0/4/14/16	0/0/0/0
1	CGU	L	25	1,6	-	0/4/14/16	0/0/0/0
1	CGU	L	26	1,7,6	-	0/4/14/16	0/0/0/0
1	CGU	L	29	1,7,6	-	0/4/14/16	0/0/0/0
1	CGU	L	35	1	-	0/4/14/16	0/0/0/0
1	CGU	L	6	1,7	-	0/4/14/16	0/0/0/0
1	CGU	L	7	1,7	-	0/4/14/16	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	29	CGU	CA-C	2.02	1.52	1.50
1	L	25	CGU	CA-C	2.36	1.53	1.50
1	L	16	CGU	CA-C	2.63	1.53	1.50
1	L	20	CGU	CA-C	2.75	1.53	1.50
1	L	19	CGU	CA-C	3.14	1.54	1.50
1	L	7	CGU	CA-C	3.24	1.54	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	16	CGU	O-C-CA	-2.25	118.78	124.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L	14	CGU	1	0
1	L	25	CGU	1	0
1	L	35	CGU	1	0
1	L	7	CGU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 15 are monoatomic - leaving 3 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	$\# Z  > 2$
11	PBZ	H	1016	-	10,10,10	3.25	2 (20%)	11,13,13	1.35	1 (9%)
4	GLC	L	201	1	11,11,12	1.83	2 (18%)	15,15,17	1.13	2 (13%)
5	FUC	L	203	1	9,10,11	1.15	1 (11%)	13,14,16	0.85	1 (7%)

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
11	PBZ	H	1016	-	-	0/4/4/4	0/1/1/1
4	GLC	L	201	1	1/1/4/5	0/2/19/22	0/1/1/1
5	FUC	L	203	1	-	0/0/17/20	0/1/1/1

All (5) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	201	GLC	C4-C3	-4.32	1.41	1.52
11	H	1016	PBZ	C4-C7	-4.15	1.40	1.47
5	L	203	FUC	C1-C2	2.45	1.58	1.52
4	L	201	GLC	C2-C3	2.64	1.56	1.52
11	H	1016	PBZ	C3-C2	8.68	1.54	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	201	GLC	C1-C2-C3	-2.62	106.35	109.66
5	L	203	FUC	C2-C3-C4	-2.17	107.10	110.87
4	L	201	GLC	C1-O5-C5	2.27	115.31	112.19
11	H	1016	PBZ	C4-C7-N2	3.56	123.53	118.08

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	L	201	GLC	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	132/152 (86%)	0.31	11 (8%) <span>11</span> <span>9</span>	9, 19, 34, 53	0
2	H	254/254 (100%)	-0.06	3 (1%) <span>79</span> <span>76</span>	3, 10, 24, 40	0
3	T	191/205 (93%)	0.07	16 (8%) <span>11</span> <span>9</span>	8, 15, 38, 45	0
All	All	577/611 (94%)	0.07	30 (5%) <span>27</span> <span>22</span>	3, 14, 34, 53	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	1	ALA	10.9
3	T	137	ASN	6.4
3	T	82	ASN	6.2
1	L	2	ASN	5.8
1	L	3	ALA	4.6
2	H	170(G)	ASP	4.5
1	L	122	ALA	4.1
3	T	181	LYS	3.9
3	T	119	VAL	3.7
1	L	107	GLY	3.5
3	T	118	GLN	3.4
3	T	81	GLY	3.2
3	T	156	TYR	3.0
3	T	90	GLY	2.9
3	T	138	ASN	2.7
1	L	11	GLY	2.7
2	H	170(D)	LYS	2.6
1	L	108	THR	2.6
2	H	248	PRO	2.6
3	T	121	THR	2.5
3	T	184	ASN	2.4
3	T	135	ARG	2.4
3	T	136	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
3	T	182	GLY	2.4
3	T	139	THR	2.4
1	L	106	THR	2.2
1	L	10	PRO	2.2
3	T	120	GLY	2.1
1	L	120	LEU	2.1
1	L	5	LEU	2.1

## 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	35	12/13	0.71	0.31	32,42,44,45	0
1	CGU	L	20	12/13	0.74	0.26	34,45,47,49	0
1	CGU	L	19	12/13	0.78	0.25	36,41,43,44	0
1	CGU	L	6	12/13	0.82	0.17	24,33,37,37	0
1	CGU	L	14	12/13	0.84	0.19	27,34,36,36	0
1	CGU	L	29	12/13	0.87	0.13	23,23,25,25	0
1	CGU	L	7	12/13	0.87	0.14	25,29,31,33	0
1	CGU	L	26	12/13	0.87	0.14	22,26,29,29	0
1	CGU	L	16	12/13	0.88	0.12	20,23,26,26	0
1	CGU	L	25	12/13	0.90	0.10	23,26,30,30	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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(Å <sup>2</sup> )	Q<0.9
7	CA	L	1003	1/1	0.46	0.21	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	L	1007	1/1	0.63	0.24	41,41,41,41	0
5	FUC	L	203	10/11	0.63	0.20	28,29,31,32	0
4	GLC	L	201	11/12	0.64	0.23	40,41,41,41	0
7	CA	L	1006	1/1	0.68	0.27	53,53,53,53	0
7	CA	L	1002	1/1	0.70	0.16	55,55,55,55	0
9	ZN	H	1012	1/1	0.83	0.16	44,44,44,44	0
6	MG	L	1001	1/1	0.88	0.11	26,26,26,26	0
8	NA	H	1010	1/1	0.91	0.11	20,20,20,20	0
7	CA	L	1005	1/1	0.93	0.25	51,51,51,51	0
6	MG	L	1004	1/1	0.93	0.10	19,19,19,19	0
9	ZN	H	1011	1/1	0.93	0.45	41,41,41,41	0
10	CL	H	1013	1/1	0.94	0.11	45,45,45,45	0
11	PBZ	H	1016	10/10	0.95	0.11	6,9,10,10	0
10	CL	H	1014	1/1	0.98	0.06	17,17,17,17	0
7	CA	H	1009	1/1	0.98	0.04	21,21,21,21	0
10	CL	T	1015	1/1	0.98	0.06	13,13,13,13	0
7	CA	L	1008	1/1	0.99	0.04	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.