



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:21 pm GMT

PDB ID : 2EC9  
Title : Crystal structure analysis of human Factor VIIa , Soluble tissue factor complexed with BCX-3607  
Authors : Raman, K.; Yarlagadda, B.  
Deposited on : 2007-02-13  
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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

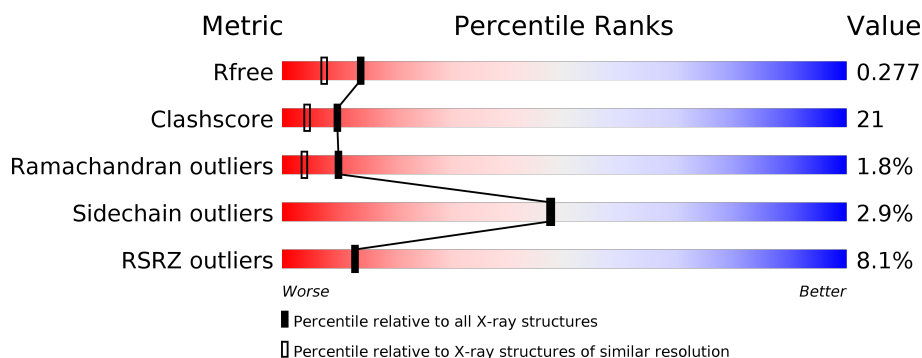
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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 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	142	<div> <div>13%</div> <div>60%</div> <div>34%</div> <div>• •</div> </div>
2	H	254	<div> <div>5%</div> <div>73%</div> <div>25%</div> <div>•</div> </div>
3	T	75	<div> <div>%</div> <div>68%</div> <div>32%</div> <div></div> </div>
4	U	120	<div> <div>12%</div> <div>63%</div> <div>33%</div> <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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CGU	L	16	X	-	-	-
1	CGU	L	19	X	-	-	-
1	CGU	L	29	X	-	X	-
5	ASO	L	1052	X	-	-	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4952 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
			1135	683	189	248	15			

- 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			

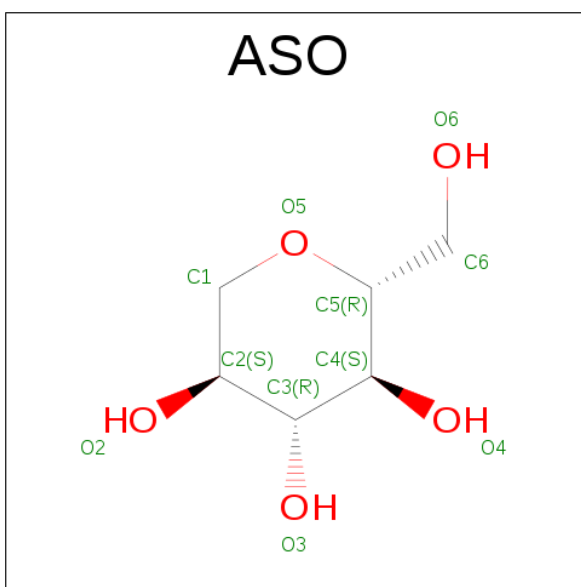
- Molecule 3 is a protein called Tissue factor.

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

- Molecule 4 is a protein called Tissue factor.

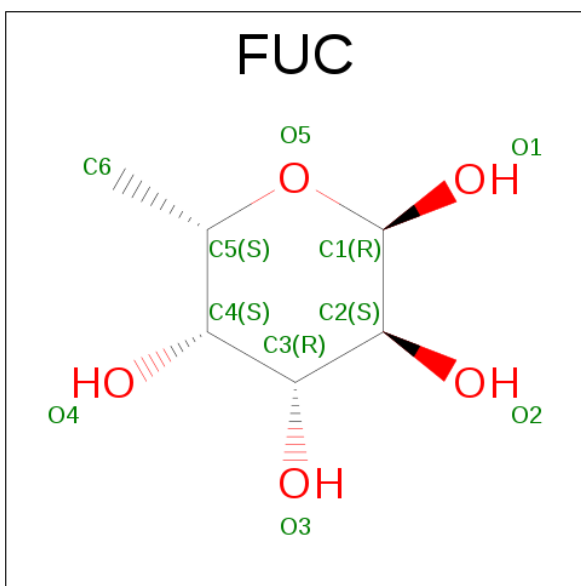
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	U	116	Total	C	N	O	S	0	0	0
			940	593	155	189	3			

- Molecule 5 is SUGAR (1,5-ANHYDROSORBITOL) (three-letter code: ASO) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



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

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

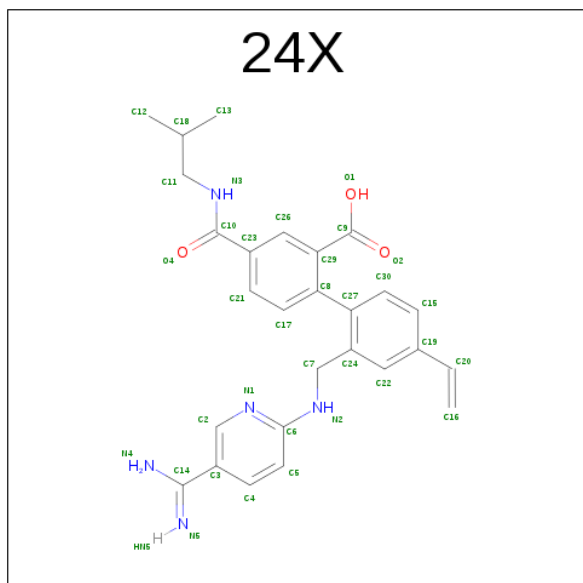


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			10	6	4		

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

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

- Molecule 8 is 2'-((5-CARBAMIMIDOYLPYRIDIN-2-YLAMINO)METHYL)-4-(ISOBUTYL CARBAMOYL)-4'-VINYLBIIPHENYL-2-CARBOXYLIC ACID (three-letter code: 24X) (formula: C<sub>27</sub>H<sub>29</sub>N<sub>5</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total C N O 35 27 5 3	0	0

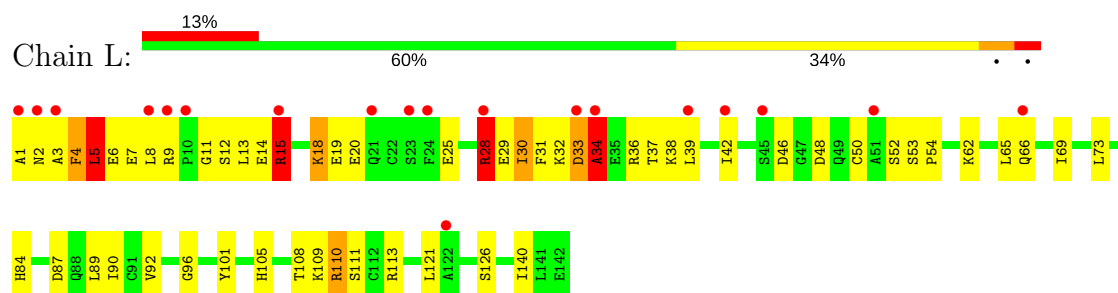
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	44	Total O 44 44	0	0
9	H	121	Total O 121 121	0	0
9	T	31	Total O 31 31	0	0
9	U	28	Total O 28 28	0	0

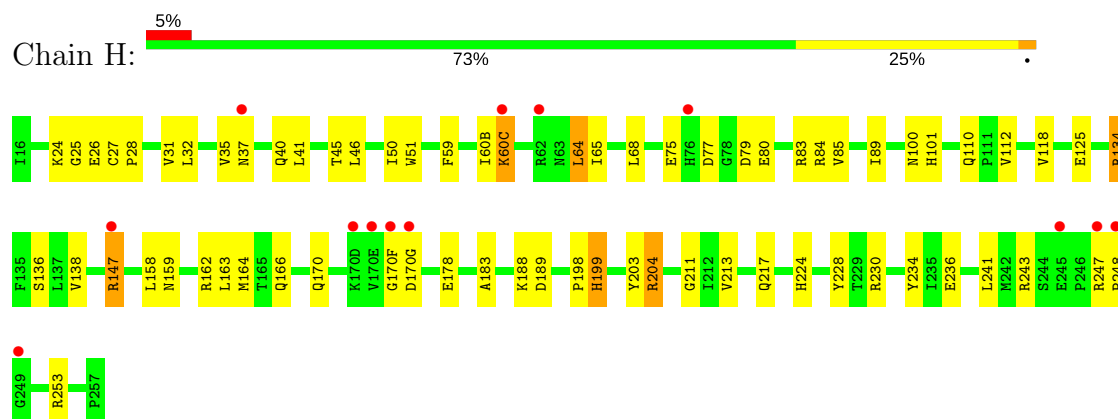
### 3 Residue-property plots

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.

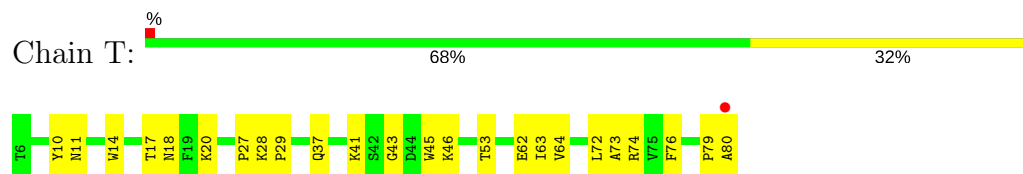
#### • Molecule 1: Coagulation factor VII



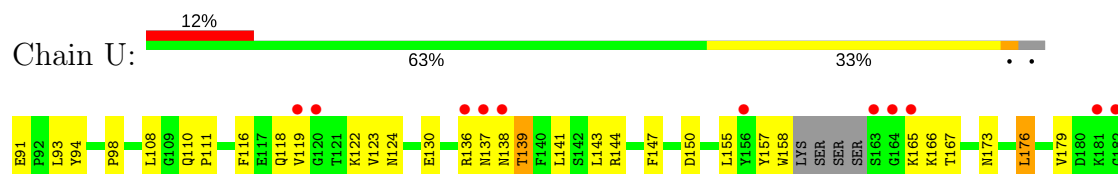
#### • Molecule 2: Coagulation factor VII

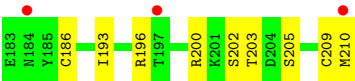


#### • Molecule 3: Tissue factor



#### • Molecule 4: Tissue factor







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.78Å 81.41Å 125.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 24.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.00) 98.8 (24.90-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 1.99Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.242 , 0.282 0.236 , 0.277	Depositor DCC
$R_{free}$ test set	4890 reflections (11.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4952	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: ASO, CA, CGU, FUC, 24X

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	0.29	0/1029	0.57	0/1374
2	H	0.33	0/2024	0.71	1/2755 (0.0%)
3	T	0.33	0/630	0.69	1/860 (0.1%)
4	U	0.31	0/958	0.65	0/1299
All	All	0.31	0/4641	0.67	2/6288 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	3	9

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	199	HIS	N-CA-C	-7.47	90.83	111.00
3	T	20	LYS	N-CA-C	-5.90	95.07	111.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	L	16	CGU	CA
1	L	19	CGU	CA
1	L	29	CGU	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	13	LEU	Mainchain
1	L	15	ARG	Mainchain,Peptide
1	L	18	LYS	Peptide
1	L	28	ARG	Mainchain,Peptide
1	L	34	ALA	Mainchain,Peptide
1	L	5	LEU	Mainchain

## 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	1135	0	1012	74	0
2	H	1974	0	1950	72	0
3	T	614	0	598	27	0
4	U	940	0	912	42	0
5	L	11	0	12	2	0
6	L	10	0	10	1	0
7	H	1	0	0	0	0
7	L	8	0	0	0	0
8	H	35	0	28	0	0
9	H	121	0	0	12	0
9	L	44	0	0	8	0
9	T	31	0	0	4	0
9	U	28	0	0	3	0
All	All	4952	0	4522	198	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 21.

All (198) 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)
4:U:136:ARG:NH2	4:U:136:ARG:HB3	1.71	1.06
2:H:147:ARG:HB2	2:H:147:ARG:HH21	1.22	1.05
4:U:130:GLU:OE1	4:U:143:LEU:HD22	1.61	1.00
4:U:136:ARG:HH21	4:U:141:LEU:HD21	1.31	0.94
2:H:68:LEU:HD12	2:H:112:VAL:HG11	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:213:VAL:HA	9:H:1017:HOH:O	1.69	0.91
1:L:25:CGU:OE21	1:L:28:ARG:HD3	1.71	0.89
2:H:50:ILE:HG13	2:H:51:TRP:CD1	2.11	0.86
2:H:183:ALA:HB2	9:H:1024:HOH:O	1.75	0.85
2:H:147:ARG:NH2	2:H:147:ARG:HB2	1.91	0.84
3:T:74:ARG:HD3	3:T:76:PHE:CZ	2.15	0.81
4:U:136:ARG:HH21	4:U:136:ARG:HB3	1.45	0.80
1:L:113:ARG:NH1	2:H:125:GLU:OE2	2.15	0.80
2:H:65:ILE:CD1	2:H:84:ARG:HD3	2.12	0.79
1:L:1:ALA:HB3	1:L:20:CGU:HG	1.66	0.78
1:L:38:LYS:O	1:L:42:ILE:HG13	1.85	0.77
1:L:25:CGU:O	1:L:28:ARG:HB3	1.85	0.76
1:L:33:ASP:CG	1:L:36:ARG:HD3	2.04	0.76
1:L:29:CGU:O	1:L:30:ILE:HG13	1.85	0.75
1:L:96:GLY:O	1:L:110:ARG:NH2	2.21	0.74
1:L:15:ARG:HG2	1:L:15:ARG:HH21	1.53	0.73
1:L:140:ILE:HD11	2:H:26:GLU:HG3	1.68	0.73
2:H:147:ARG:HH21	2:H:147:ARG:CB	1.98	0.73
1:L:113:ARG:HH12	2:H:125:GLU:CD	1.92	0.72
1:L:28:ARG:NH1	1:L:29:CGU:HB2	2.05	0.72
1:L:33:ASP:HB2	1:L:36:ARG:HB2	1.72	0.72
1:L:6:CGU:HG	1:L:9:ARG:HG3	1.71	0.71
2:H:46:LEU:HD13	2:H:68:LEU:HD11	1.73	0.70
4:U:119:VAL:HG23	4:U:119:VAL:O	1.90	0.70
3:T:63:ILE:HD12	3:T:64:VAL:N	2.06	0.69
2:H:35:VAL:CG2	2:H:41:LEU:HD22	2.22	0.69
1:L:110:ARG:C	1:L:110:ARG:HD2	2.13	0.69
4:U:136:ARG:HH21	4:U:136:ARG:CB	2.05	0.69
2:H:236:GLU:HG3	9:H:1062:HOH:O	1.92	0.69
2:H:31:VAL:HG22	2:H:68:LEU:HD21	1.75	0.68
4:U:136:ARG:NH2	4:U:141:LEU:HD21	2.06	0.68
2:H:35:VAL:HG22	2:H:64:LEU:CD1	2.24	0.68
2:H:75:GLU:HB3	9:H:1080:HOH:O	1.95	0.67
1:L:89:LEU:HD11	1:L:110:ARG:HH22	1.59	0.67
3:T:79:PRO:O	3:T:80:ALA:HB3	1.95	0.67
2:H:35:VAL:HG23	2:H:41:LEU:HB2	1.75	0.67
1:L:33:ASP:CB	1:L:36:ARG:HD3	2.24	0.66
2:H:65:ILE:HD11	2:H:84:ARG:HD3	1.78	0.66
1:L:4:PHE:O	1:L:5:LEU:CB	2.44	0.64
4:U:136:ARG:CZ	4:U:136:ARG:HB3	2.26	0.64
1:L:48:ASP:OD1	1:L:50:CYS:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:8:LEU:H	1:L:8:LEU:HD12	1.61	0.64
4:U:196:ARG:HD2	9:U:218:HOH:O	1.99	0.63
4:U:136:ARG:HH21	4:U:141:LEU:CD2	2.06	0.63
2:H:203:TYR:CE2	2:H:204:ARG:HG3	2.34	0.63
1:L:101:TYR:CZ	2:H:125:GLU:HG3	2.34	0.63
2:H:24:LYS:NZ	2:H:79:ASP:OD2	2.33	0.62
2:H:243:ARG:HG3	2:H:243:ARG:HH21	1.64	0.61
1:L:108:THR:CG2	1:L:109:LYS:N	2.63	0.61
2:H:162:ARG:HG3	2:H:163:LEU:N	2.13	0.61
3:T:46:LYS:HE2	3:T:62:GLU:OE1	2.00	0.61
4:U:136:ARG:NH2	4:U:141:LEU:CD2	2.64	0.60
1:L:110:ARG:HD2	1:L:111:SER:N	2.16	0.59
3:T:29:PRO:HG3	3:T:53:THR:O	2.02	0.59
2:H:60(C):LYS:CB	2:H:60(C):LYS:NZ	2.65	0.58
2:H:83:ARG:NH1	9:H:1019:HOH:O	2.34	0.58
1:L:28:ARG:HG3	9:L:1065:HOH:O	2.04	0.57
3:T:45:TRP:HH2	3:T:72:LEU:HD12	1.70	0.57
2:H:35:VAL:HG21	2:H:41:LEU:HD22	1.86	0.57
1:L:28:ARG:HH11	1:L:29:CGU:HB2	1.68	0.56
3:T:63:ILE:C	3:T:63:ILE:HD12	2.26	0.56
3:T:79:PRO:O	3:T:80:ALA:CB	2.53	0.56
1:L:12:SER:HB3	1:L:15:ARG:HB3	1.86	0.56
2:H:162:ARG:HD2	9:U:215:HOH:O	2.06	0.56
2:H:89:ILE:HG21	2:H:241:LEU:HD13	1.86	0.56
2:H:217:GLN:HG3	2:H:224:HIS:CE1	2.40	0.56
2:H:45:THR:OG1	2:H:198:PRO:HB3	2.05	0.56
2:H:77:ASP:O	2:H:80:GLU:OE1	2.24	0.56
1:L:12:SER:HB3	1:L:15:ARG:CB	2.36	0.55
3:T:74:ARG:NE	9:T:111:HOH:O	2.39	0.55
1:L:5:LEU:HA	1:L:8:LEU:HD13	1.88	0.54
2:H:60(C):LYS:HZ2	2:H:60(C):LYS:HB2	1.72	0.54
1:L:30:ILE:N	9:L:1064:HOH:O	2.41	0.54
1:L:4:PHE:O	1:L:5:LEU:HB2	2.06	0.54
2:H:164:MET:CE	4:U:91:GLU:HB3	2.37	0.54
3:T:74:ARG:HD3	3:T:76:PHE:CE2	2.42	0.54
4:U:118:GLN:HG2	4:U:123:VAL:HG22	1.89	0.54
1:L:14:CGU:HG	1:L:19:CGU:OE21	2.08	0.54
3:T:37:GLN:OE1	3:T:74:ARG:HD2	2.08	0.54
4:U:130:GLU:CD	9:U:211:HOH:O	2.45	0.54
1:L:1:ALA:HA	9:L:1068:HOH:O	2.08	0.54
2:H:134:ARG:HD2	3:T:43:GLY:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:LEU:O	1:L:66:GLN:HB2	2.08	0.54
3:T:37:GLN:HB2	3:T:74:ARG:HG3	1.90	0.54
2:H:228:TYR:CD2	9:H:1017:HOH:O	2.54	0.53
1:L:105:HIS:O	1:L:108:THR:O	2.27	0.53
1:L:8:LEU:N	1:L:8:LEU:HD12	2.23	0.53
4:U:144:ARG:NH2	4:U:173:ASN:OD1	2.41	0.53
1:L:108:THR:HG22	1:L:109:LYS:N	2.23	0.52
1:L:101:TYR:CE2	2:H:125:GLU:HG3	2.45	0.52
3:T:18:ASN:HD21	4:U:130:GLU:HG2	1.75	0.52
2:H:158:LEU:HD11	2:H:188:LYS:HB3	1.91	0.52
2:H:65:ILE:HD11	2:H:84:ARG:HH21	1.73	0.52
1:L:140:ILE:HD11	2:H:26:GLU:CG	2.38	0.52
1:L:15:ARG:HH21	1:L:15:ARG:CG	2.23	0.52
1:L:28:ARG:C	1:L:30:ILE:H	2.13	0.52
2:H:162:ARG:HD3	9:H:1024:HOH:O	2.10	0.52
2:H:243:ARG:HG3	2:H:243:ARG:NH2	2.23	0.51
1:L:15:ARG:O	1:L:19:CGU:HA	2.10	0.51
4:U:136:ARG:NH2	4:U:136:ARG:CB	2.56	0.51
1:L:5:LEU:O	1:L:5:LEU:HD13	2.11	0.51
1:L:54:PRO:HB3	5:L:1052:ASO:H2	1.93	0.51
4:U:123:VAL:HG23	4:U:179:VAL:HG21	1.93	0.51
1:L:92:VAL:HG22	1:L:92:VAL:O	2.11	0.50
3:T:72:LEU:HD13	3:T:73:ALA:N	2.27	0.50
1:L:46:ASP:OD2	1:L:65:LEU:HA	2.11	0.50
1:L:29:CGU:C	1:L:30:ILE:HG13	2.42	0.50
2:H:162:ARG:HA	9:H:1024:HOH:O	2.12	0.49
1:L:3:ALA:O	1:L:4:PHE:C	2.50	0.49
1:L:3:ALA:O	1:L:4:PHE:O	2.29	0.49
3:T:18:ASN:HD21	4:U:130:GLU:CG	2.26	0.49
4:U:116:PHE:HA	4:U:124:ASN:O	2.11	0.49
4:U:93:LEU:HD12	4:U:93:LEU:N	2.28	0.49
2:H:35:VAL:HG22	2:H:64:LEU:HD11	1.95	0.49
1:L:110:ARG:C	1:L:110:ARG:CD	2.80	0.49
1:L:33:ASP:HB2	1:L:36:ARG:HD3	1.93	0.49
1:L:15:ARG:HG2	1:L:15:ARG:NH2	2.26	0.49
2:H:31:VAL:HG22	2:H:68:LEU:CD2	2.41	0.49
1:L:29:CGU:O	1:L:30:ILE:CG1	2.60	0.49
3:T:28:LYS:NZ	9:T:85:HOH:O	2.46	0.49
3:T:37:GLN:HB2	3:T:74:ARG:CG	2.42	0.49
2:H:64:LEU:HB3	2:H:85:VAL:HB	1.93	0.48
2:H:60(C):LYS:HB2	2:H:60(C):LYS:NZ	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:52:SER:O	1:L:53:SER:C	2.52	0.48
2:H:27:CYS:N	2:H:28:PRO:CD	2.76	0.48
4:U:158:TRP:CE2	4:U:186:CYS:HB2	2.50	0.47
4:U:157:TYR:CZ	4:U:166:LYS:HB3	2.49	0.47
1:L:52:SER:OG	5:L:1052:ASO:H11	2.15	0.47
2:H:162:ARG:C	2:H:163:LEU:HD12	2.35	0.47
2:H:138:VAL:HA	2:H:198:PRO:O	2.15	0.47
4:U:108:LEU:HD22	4:U:143:LEU:HD21	1.97	0.47
1:L:28:ARG:CZ	9:L:1063:HOH:O	2.60	0.47
1:L:8:LEU:CD1	1:L:8:LEU:H	2.27	0.47
1:L:28:ARG:CG	9:L:1065:HOH:O	2.63	0.47
2:H:166:GLN:O	2:H:170:GLN:HG3	2.14	0.46
2:H:35:VAL:HG22	2:H:64:LEU:HD12	1.96	0.46
2:H:199:HIS:HB3	2:H:211:GLY:CA	2.46	0.46
1:L:2:ASN:HD21	1:L:7:CGU:HA	1.80	0.46
4:U:138:ASN:O	4:U:139:THR:HB	2.16	0.46
4:U:186:CYS:HA	4:U:209:CYS:HA	1.98	0.46
2:H:68:LEU:HD13	2:H:118:VAL:HG13	1.97	0.46
1:L:39:LEU:HD22	4:U:165:LYS:NZ	2.31	0.46
1:L:73:LEU:HD23	6:L:1060:FUC:H62	1.97	0.45
2:H:101:HIS:HA	2:H:234:TYR:OH	2.17	0.45
1:L:34:ALA:O	1:L:37:THR:HB	2.16	0.45
3:T:76:PHE:CD1	4:U:94:TYR:HB3	2.51	0.45
2:H:59:PHE:HA	2:H:60(B):ILE:HG12	1.98	0.45
3:T:10:TYR:CD1	3:T:11:ASN:ND2	2.85	0.45
4:U:193:ILE:CG2	4:U:196:ARG:HD3	2.46	0.45
1:L:140:ILE:CD1	2:H:26:GLU:HG3	2.44	0.44
2:H:178:GLU:O	2:H:230:ARG:HD3	2.17	0.44
1:L:15:ARG:NH2	1:L:15:ARG:CG	2.80	0.44
2:H:46:LEU:HD22	2:H:68:LEU:CD1	2.48	0.44
4:U:110:GLN:HB2	4:U:203:THR:CG2	2.47	0.44
2:H:228:TYR:N	2:H:228:TYR:CD1	2.85	0.43
1:L:69:ILE:HD11	3:T:17:THR:CG2	2.47	0.43
4:U:122:LYS:HB3	4:U:176:LEU:CD2	2.48	0.43
4:U:136:ARG:HB2	4:U:141:LEU:HD21	1.99	0.43
2:H:166:GLN:HB3	4:U:94:TYR:OH	2.18	0.43
1:L:62:LYS:HE2	9:L:1097:HOH:O	2.17	0.43
9:T:95:HOH:O	4:U:93:LEU:HD13	2.19	0.43
3:T:72:LEU:HD13	3:T:72:LEU:C	2.39	0.43
2:H:136:SER:CB	2:H:199:HIS:CE1	3.02	0.43
4:U:108:LEU:HB2	4:U:202:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:111:PRO:HG2	4:U:205:SER:HB3	2.01	0.42
2:H:162:ARG:HB2	9:H:1024:HOH:O	2.19	0.42
3:T:41:LYS:HB2	9:T:102:HOH:O	2.19	0.42
1:L:140:ILE:HG12	9:H:1015:HOH:O	2.19	0.42
1:L:84:HIS:HB2	1:L:87:ASP:OD2	2.20	0.42
3:T:45:TRP:CH2	3:T:72:LEU:HD12	2.52	0.42
4:U:147:PHE:O	4:U:150:ASP:HB2	2.19	0.42
3:T:14:TRP:CD1	4:U:98:PRO:HG2	2.54	0.42
1:L:29:CGU:C	9:L:1064:HOH:O	2.67	0.42
1:L:140:ILE:HD13	2:H:25:GLY:HA3	2.02	0.42
4:U:116:PHE:CE2	4:U:210:MET:HA	2.55	0.41
1:L:121:LEU:HD12	1:L:126:SER:CB	2.50	0.41
2:H:68:LEU:HD13	2:H:118:VAL:CG1	2.50	0.41
2:H:32:LEU:HD11	2:H:40:GLN:HG3	2.03	0.41
1:L:31:PHE:O	1:L:32:LYS:HB2	2.21	0.41
2:H:170(G):ASP:N	2:H:170(G):ASP:OD1	2.54	0.41
2:H:188:LYS:O	2:H:189:ASP:HB2	2.21	0.41
3:T:46:LYS:CE	3:T:62:GLU:OE1	2.67	0.41
4:U:155:LEU:O	4:U:167:THR:HA	2.21	0.41
2:H:110:GLN:HA	2:H:110:GLN:NE2	2.36	0.40
2:H:247:ARG:HB3	2:H:248:PRO:HD2	2.03	0.40
1:L:25:CGU:HG	9:L:1063:HOH:O	2.21	0.40
4:U:193:ILE:HB	4:U:196:ARG:HD3	2.03	0.40
2:H:253:ARG:HD2	9:H:1007:HOH:O	2.20	0.40
1:L:25:CGU:OE22	1:L:28:ARG:NH2	2.53	0.40
2:H:125:GLU:HB2	9:H:1025:HOH:O	2.20	0.40
3:T:37:GLN:HA	3:T:46:LYS:O	2.21	0.40
1:L:90:ILE:CD1	1:L:92:VAL:CG1	3.00	0.40
4:U:193:ILE:HG21	4:U:196:ARG:HD3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	130/142 (92%)	114 (88%)	8 (6%)	8 (6%)	2	0
2	H	252/254 (99%)	239 (95%)	12 (5%)	1 (0%)	38	33
3	T	73/75 (97%)	69 (94%)	4 (6%)	0	100	100
4	U	112/120 (93%)	104 (93%)	7 (6%)	1 (1%)	20	12
All	All	567/591 (96%)	526 (93%)	31 (6%)	10 (2%)	10	4

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	4	PHE
1	L	15	ARG
1	L	28	ARG
1	L	34	ALA
2	H	170(F)	GLY
4	U	139	THR
1	L	5	LEU
1	L	18	LYS
1	L	30	ILE
1	L	11	GLY

### 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	114/114 (100%)	111 (97%)	3 (3%)	51	52
2	H	216/216 (100%)	208 (96%)	8 (4%)	39	36
3	T	70/70 (100%)	69 (99%)	1 (1%)	71	76
4	U	109/113 (96%)	106 (97%)	3 (3%)	49	49
All	All	509/513 (99%)	494 (97%)	15 (3%)	48	47

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	LEU

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Mol	Chain	Res	Type
1	L	33	ASP
1	L	110	ARG
2	H	37	ASN
2	H	60(C)	LYS
2	H	64	LEU
2	H	100	ASN
2	H	134	ARG
2	H	147	ARG
2	H	159	ASN
2	H	204	ARG
3	T	27	PRO
4	U	137	ASN
4	U	176	LEU
4	U	200	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	56	GLN
2	H	37	ASN
2	H	100	ASN
2	H	110	GLN
2	H	143	GLN
2	H	159	ASN
2	H	217	GLN
2	H	224	HIS
3	T	11	ASN
3	T	18	ASN
4	U	110	GLN
4	U	137	ASN
4	U	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	1,7	5,11,12	1.09	1 (20%)	4,14,16	1.87	1 (25%)
1	CGU	L	16	1,7	5,11,12	0.88	0	4,14,16	0.60	0
1	CGU	L	19	1,7	5,11,12	1.18	1 (20%)	4,14,16	1.07	0
1	CGU	L	20	1	5,11,12	0.76	0	4,14,16	2.58	2 (50%)
1	CGU	L	25	1	5,11,12	0.81	0	4,14,16	1.52	1 (25%)
1	CGU	L	26	1,7	5,11,12	0.55	0	4,14,16	1.22	0
1	CGU	L	29	1,7	5,11,12	1.84	2 (40%)	4,14,16	3.02	2 (50%)
1	CGU	L	35	1	5,11,12	0.80	0	4,14,16	1.04	0
1	CGU	L	6	1	5,11,12	1.33	1 (20%)	4,14,16	1.33	1 (25%)
1	CGU	L	7	1	5,11,12	1.95	2 (40%)	4,14,16	1.88	1 (25%)

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	1,7	-	0/4/14/16	0/0/0/0
1	CGU	L	16	1,7	1/1/4/5	0/4/14/16	0/0/0/0
1	CGU	L	19	1,7	1/1/4/5	0/4/14/16	0/0/0/0
1	CGU	L	20	1	-	0/4/14/16	0/0/0/0
1	CGU	L	25	1	-	0/4/14/16	0/0/0/0
1	CGU	L	26	1,7	-	0/4/14/16	0/0/0/0
1	CGU	L	29	1,7	1/1/4/5	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	-	0/4/14/16	0/0/0/0
1	CGU	L	7	1	-	0/4/14/16	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	14	CGU	CA-C	2.14	1.53	1.50
1	L	19	CGU	CA-C	2.49	1.53	1.50
1	L	29	CGU	CB-CG	2.71	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	6	CGU	CA-C	2.79	1.53	1.50
1	L	29	CGU	CA-C	2.80	1.53	1.50
1	L	7	CGU	CA-C	2.83	1.54	1.50
1	L	7	CGU	CB-CG	2.84	1.59	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	6	CGU	O-C-CA	-2.44	118.27	125.02
1	L	25	CGU	CB-CG-CD2	-2.39	108.22	112.81
1	L	29	CGU	CB-CG-CD1	2.42	117.46	112.81
1	L	7	CGU	CB-CG-CD2	2.76	118.10	112.81
1	L	20	CGU	CB-CG-CD2	3.27	119.09	112.81
1	L	14	CGU	CB-CG-CD1	3.44	119.41	112.81
1	L	20	CGU	CB-CG-CD1	3.71	119.93	112.81
1	L	29	CGU	CB-CG-CD2	5.30	122.99	112.81

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	L	29	CGU	CA
1	L	16	CGU	CA
1	L	19	CGU	CA

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L	14	CGU	1	0
1	L	19	CGU	2	0
1	L	20	CGU	1	0
1	L	25	CGU	4	0
1	L	29	CGU	6	0
1	L	6	CGU	1	0
1	L	7	CGU	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 9 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	$\# Z  > 2$
8	24X	H	999	-	34,37,37	2.52	9 (26%)	43,51,51	1.73	4 (9%)
5	ASO	L	1052	-	11,11,11	0.76	0	13,15,15	1.09	0
6	FUC	L	1060	-	9,9,11	0.52	0	10,11,16	1.97	3 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	24X	H	999	-	-	0/24/28/28	0/3/3/3
5	ASO	L	1052	-	2/2/4/4	0/2/19/19	0/1/1/1
6	FUC	L	1060	-	-	0/12/12/20	0/0/0/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	999	24X	C27-C8	-3.65	1.44	1.49
8	H	999	24X	C4-C3	2.18	1.42	1.39
8	H	999	24X	C14-N5	2.69	1.38	1.28
8	H	999	24X	C2-C3	2.73	1.43	1.39
8	H	999	24X	C2-N1	2.98	1.40	1.34
8	H	999	24X	C16-C20	3.65	1.54	1.28
8	H	999	24X	C6-N1	4.15	1.42	1.34
8	H	999	24X	C10-N3	6.22	1.47	1.33
8	H	999	24X	O4-C10	8.73	1.41	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	999	24X	C11-N3-C10	-7.26	108.09	122.26
8	H	999	24X	C3-C2-N1	-3.29	118.84	123.64
6	L	1060	FUC	C4-C3-C2	2.78	119.39	113.41
6	L	1060	FUC	C1-C2-C3	3.00	119.10	112.41
8	H	999	24X	N2-C6-N1	3.34	121.80	117.00
8	H	999	24X	C4-C3-C2	3.38	121.54	117.66
6	L	1060	FUC	O4-C4-C5	3.52	115.60	109.28

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1052	ASO	C2
5	L	1052	ASO	C4

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	1052	ASO	2	0
6	L	1060	FUC	1	0

## 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	132/142 (92%)	0.75	19 (14%) <b>3</b> <b>3</b>	16, 29, 60, 77	0
2	H	254/254 (100%)	0.16	13 (5%) <b>29</b> <b>29</b>	12, 18, 41, 56	0
3	T	75/75 (100%)	0.13	1 (1%) <b>77</b> <b>77</b>	16, 23, 41, 45	0
4	U	116/120 (96%)	0.68	14 (12%) <b>5</b> <b>5</b>	18, 31, 59, 69	0
All	All	577/591 (97%)	0.40	47 (8%) <b>13</b> <b>13</b>	12, 24, 53, 77	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	1	ALA	9.8
4	U	137	ASN	7.7
4	U	181	LYS	5.4
2	H	170(F)	GLY	5.4
4	U	138	ASN	4.8
2	H	248	PRO	4.8
1	L	28	ARG	4.6
1	L	42	ILE	4.5
1	L	2	ASN	4.5
4	U	182	GLY	4.3
1	L	15	ARG	3.8
1	L	3	ALA	3.8
1	L	21	GLN	3.8
1	L	51	ALA	3.8
4	U	164	GLY	3.7
2	H	247	ARG	3.6
2	H	147	ARG	3.4
4	U	120	GLY	3.4
4	U	136	ARG	3.3
1	L	34	ALA	3.2
2	H	76	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	L	122	ALA	2.9
2	H	170(E)	VAL	2.8
1	L	33	ASP	2.8
2	H	170(G)	ASP	2.8
4	U	165	LYS	2.7
1	L	66	GLN	2.7
4	U	184	ASN	2.7
3	T	80	ALA	2.7
2	H	37	ASN	2.7
4	U	119	VAL	2.6
4	U	197	THR	2.6
2	H	60(C)	LYS	2.6
1	L	10	PRO	2.6
2	H	245	GLU	2.5
4	U	210	MET	2.5
1	L	45	SER	2.4
4	U	156	TYR	2.4
1	L	39	LEU	2.2
1	L	9	ARG	2.2
2	H	62	ARG	2.2
4	U	163	SER	2.2
2	H	249	GLY	2.2
2	H	170(D)	LYS	2.1
1	L	24	PHE	2.1
1	L	23	SER	2.0
1	L	8	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CGU	L	29	12/13	0.48	0.51	-	55,62,63,64	0
1	CGU	L	26	12/13	0.86	0.21	-	41,44,46,49	0
1	CGU	L	16	12/13	0.88	0.14	-	47,50,53,54	0
1	CGU	L	35	12/13	0.60	0.40	-	52,65,70,72	0
1	CGU	L	20	12/13	0.82	0.27	-	54,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CGU	L	7	12/13	0.49	0.31	-	60,66,68,68	0
1	CGU	L	19	12/13	0.83	0.27	-	59,64,68,69	0
1	CGU	L	6	12/13	0.50	0.37	-	53,60,65,65	0
1	CGU	L	14	12/13	0.81	0.29	-	52,63,66,68	0
1	CGU	L	25	12/13	0.61	0.30	-	40,49,56,56	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	FUC	L	1060	10/11	0.77	0.19	1.33	38,46,51,53	0
5	ASO	L	1052	11/11	0.81	0.23	1.19	49,52,55,58	0
8	24X	H	999	35/35	0.92	0.13	0.97	12,17,41,46	0
7	CA	H	1001	1/1	0.90	0.18	0.25	60,60,60,60	0
7	CA	L	1002	1/1	0.89	0.08	-2.04	64,64,64,64	0
7	CA	L	1006	1/1	0.88	0.15	-	68,68,68,68	0
7	CA	L	1009	1/1	0.95	0.12	-	68,68,68,68	0
7	CA	L	1003	1/1	0.65	0.21	-	97,97,97,97	0
7	CA	L	1004	1/1	0.78	0.31	-	121,121,121,121	0
7	CA	L	1005	1/1	0.86	0.10	-	70,70,70,70	0
7	CA	L	1008	1/1	0.49	0.34	-	97,97,97,97	0
7	CA	L	1007	1/1	0.60	0.20	-	84,84,84,84	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.