



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:27 AM UTC

PDB ID : 2AER / pdb_00002aer
Title : Crystal Structure of Benzamidine-Factor VIIa/Soluble Tissue Factor complex.
Authors : Bajaj, S.P.; Schmidt, A.E.; Padmanabhan, K.; Bajaj, M.S.; Liesum, A.; Dumas, J.; Prevost, D.; Schreuder, H.
Deposited on : 2005-07-23
Resolution : 1.87 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

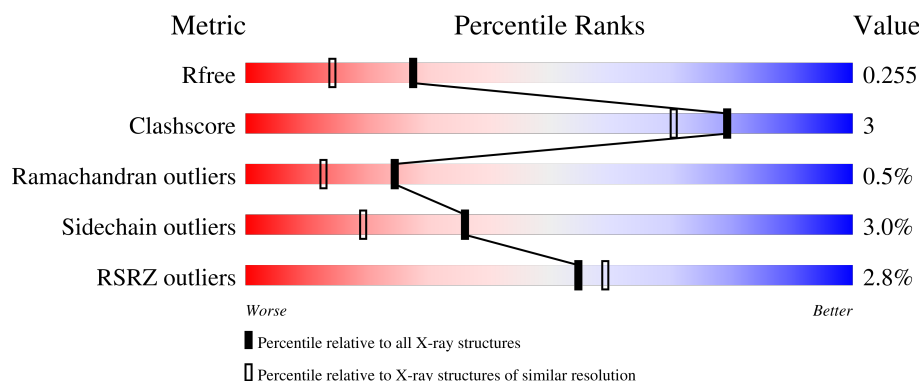
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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 ≥ 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	142	4% 78% 20% ..
2	H	254	% 92% 7% .
3	T	206	3% 81% 12% 7%

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
10	CL	H	3013	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 5425 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			

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			

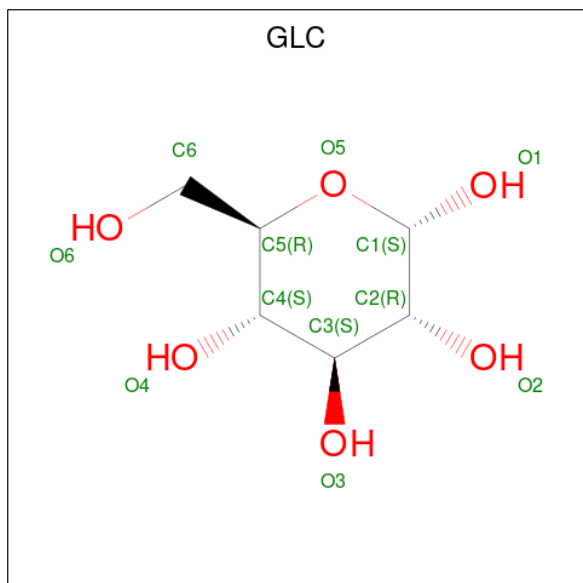
- Molecule 3 is a protein called Tissue factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	192	Total	C	N	O	S	0	0	0
			1556	990	251	310	5			

There is a discrepancy between the modelled and reference sequences:

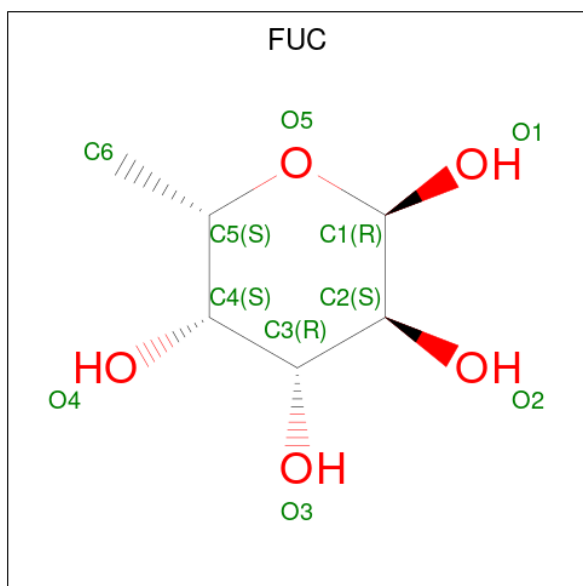
Chain	Residue	Modelled	Actual	Comment	Reference
T	5	ALA	-	cloning artifact	UNP P13726

- Molecule 4 is alpha-D-glucopyranose (CCD ID: GLC) (formula: $C_6H_{12}O_6$).



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

- Molecule 5 is alpha-L-fucopyranose (CCD ID: FUC) (formula: $C_6H_{12}O_5$).



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

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

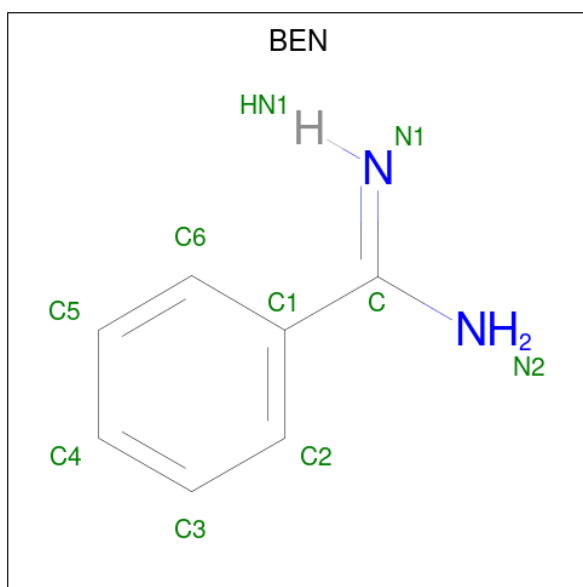
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 11 is BENZAMIDINE (CCD ID: BEN) (formula: C₇H₈N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	H	1	Total	C	N	0	0
			9	7	2		

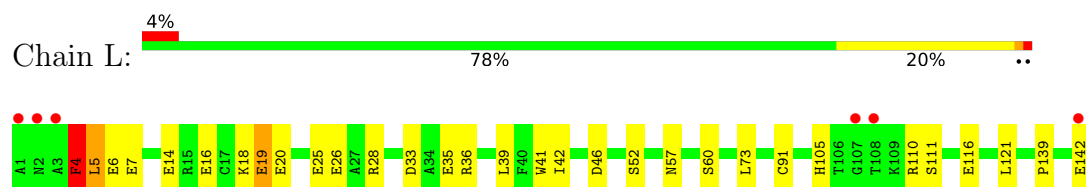
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	L	159	Total	O	0	0
			159	159		
12	H	333	Total	O	0	0
			333	333		
12	T	223	Total	O	0	0
			223	223		

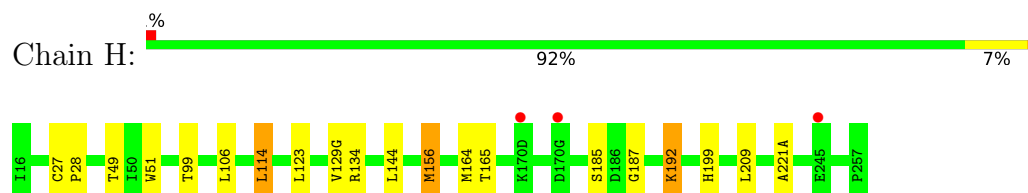
3 Residue-property plots [i](#)

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.

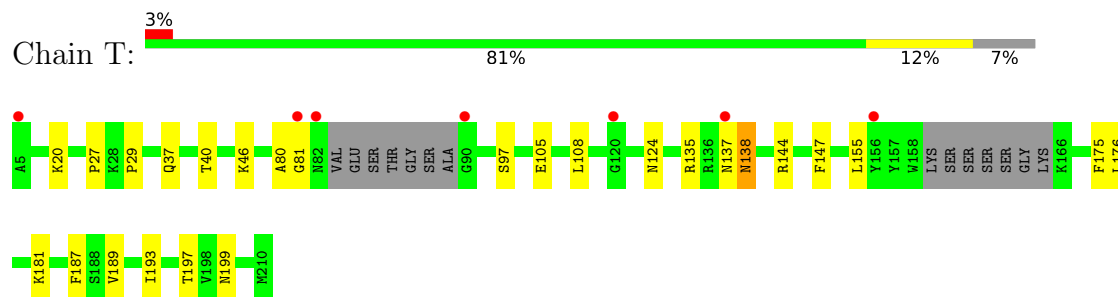
- Molecule 1: Coagulation factor VII



- 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, α , β , γ	69.90Å 81.20Å 125.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.87 8.00 – 1.87	Depositor EDS
% Data completeness (in resolution range)	98.7 (8.00-1.87) 95.9 (8.00-1.87)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 1.87Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.191 , 0.256 0.196 , 0.255	Depositor DCC
R_{free} test set	5992 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 89.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5425	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CL, ZN, MG, NA, FUC, GLC, CA, BEN, 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	0.59	0/1029	1.03	5/1374 (0.4%)
2	H	0.72	2/2024 (0.1%)	1.01	11/2755 (0.4%)
3	T	0.63	0/1590	1.02	10/2163 (0.5%)
All	All	0.66	2/4643 (0.0%)	1.02	26/6292 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	185	SER	C-O	-6.91	1.14	1.24
2	H	156	MET	SD-CE	-5.46	1.65	1.79

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	4	PHE	N-CA-C	7.58	126.94	110.80
2	H	199	HIS	N-CA-C	-6.81	94.00	107.69
2	H	51	TRP	N-CA-C	6.81	120.55	109.59
2	H	123	LEU	N-CA-C	-6.23	100.20	109.42
2	H	27	CYS	N-CA-C	-6.01	100.18	109.79
2	H	99	THR	N-CA-C	5.92	120.64	113.41
3	T	40	THR	N-CA-C	-5.85	101.36	110.42
3	T	20	LYS	N-CA-C	-5.84	99.61	108.67
3	T	138	ASN	N-CA-C	-5.77	106.19	113.23
3	T	197	THR	N-CA-C	-5.76	106.39	113.41
2	H	28	PRO	N-CA-C	5.74	121.08	114.03
2	H	134	ARG	N-CA-C	5.70	117.18	110.97
3	T	97	SER	CA-C-N	-5.68	114.74	120.31
3	T	97	SER	C-N-CA	-5.68	114.74	120.31
2	H	165	THR	N-CA-C	5.66	118.18	111.33
2	H	164	MET	N-CA-C	-5.56	102.66	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	192	LYS	N-CA-C	5.36	120.21	111.37
3	T	147	PHE	N-CA-C	5.34	118.96	112.23
2	H	129(G)	VAL	N-CA-C	-5.27	100.74	108.54
1	L	41	TRP	N-CA-C	5.27	117.02	111.28
1	L	73	LEU	N-CA-C	-5.26	102.63	110.20
3	T	29	PRO	N-CA-C	5.17	119.30	111.19
3	T	105	GLU	N-CA-C	5.14	120.55	113.97
1	L	57	ASN	N-CA-C	5.04	118.40	111.54
1	L	91	CYS	N-CA-C	5.03	117.49	111.71
3	T	189	VAL	N-CA-C	5.02	116.82	108.99

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	1135	0	989	11	0
2	H	1974	0	1950	7	0
3	T	1556	0	1506	6	0
4	L	11	0	10	1	0
5	L	10	0	10	1	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	2	0
10	T	1	0	0	0	0
11	H	9	0	7	1	0
12	H	333	0	0	4	0
12	L	159	0	0	0	1
12	T	223	0	0	0	1
All	All	5425	0	4472	25	1

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 3.

All (25) 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:192:LYS:HE2	10:H:3013:CL:CL	2.03	0.95
1:L:60:SER:OG	5:L:2003:FUC:C1	2.40	0.69
1:L:33:ASP:HB3	1:L:36:ARG:HD2	1.75	0.68
1:L:52:SER:OG	4:L:2001:GLC:C1	2.42	0.67
2:H:156:MET:SD	12:H:3320:HOH:O	2.54	0.65
10:H:3013:CL:CL	12:H:3317:HOH:O	2.52	0.65
1:L:105:HIS:HE1	1:L:111:SER:OG	1.80	0.64
3:T:108:LEU:HD11	3:T:193:ILE:HG12	1.81	0.62
1:L:4:PHE:CE1	1:L:5:LEU:HD13	2.47	0.49
1:L:139:PRO:HD2	12:H:3016:HOH:O	2.14	0.48
1:L:105:HIS:CE1	1:L:111:SER:OG	2.65	0.47
2:H:192:LYS:HG3	11:H:1001:BEN:H3	1.98	0.46
1:L:110:ARG:HD2	1:L:110:ARG:C	2.42	0.45
1:L:14:CGU:O	1:L:19:CGU:HB3	2.17	0.44
3:T:155:LEU:HD11	3:T:187:PHE:HB3	2.00	0.44
3:T:137:ASN:O	3:T:138:ASN:HB3	2.17	0.43
3:T:124:ASN:HA	3:T:175:PHE:O	2.19	0.43
2:H:187:GLY:HA2	2:H:221(A):ALA:O	2.19	0.43
3:T:37:GLN:HA	3:T:46:LYS:O	2.20	0.42
3:T:144:ARG:HH11	3:T:144:ARG:HG3	1.84	0.42
2:H:156:MET:HE2	12:H:3060:HOH:O	2.19	0.42
1:L:14:CGU:HA	1:L:18:LYS:HB2	2.02	0.42
1:L:42:ILE:O	1:L:46:ASP:HB2	2.20	0.42
2:H:144:LEU:HD21	2:H:156:MET:HE3	2.01	0.42
2:H:49:THR:HG22	2:H:114:LEU:HD13	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:3152:HOH:O	12:T:3088:HOH:O[4_556]	0.16	2.04

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%)	124 (95%)	5 (4%)	1 (1%)	16	5
2	H	252/254 (99%)	245 (97%)	7 (3%)	0	100	100
3	T	186/206 (90%)	177 (95%)	7 (4%)	2 (1%)	11	3
All	All	568/602 (94%)	546 (96%)	19 (3%)	3 (0%)	24	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	4	PHE
3	T	81	GLY
3	T	80	ALA

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%)	107 (94%)	7 (6%)	17	4
2	H	216/216 (100%)	213 (99%)	3 (1%)	59	48
3	T	178/189 (94%)	173 (97%)	5 (3%)	38	22
All	All	508/519 (98%)	493 (97%)	15 (3%)	36	19

All (15) 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	116	GLU
1	L	121	LEU
1	L	142	GLU
2	H	106	LEU
2	H	114	LEU
2	H	209	LEU
3	T	27	PRO
3	T	135	ARG
3	T	176	LEU
3	T	181	LYS
3	T	199	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	105	HIS
2	H	117	HIS
2	H	170(A)	GLN
2	H	175	ASN
3	T	137	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	6,1	9,11,12	1.07	0	10,14,16	0.73	0
1	CGU	L	20	7,1	9,11,12	1.43	1 (11%)	10,14,16	1.06	0
1	CGU	L	6	7,1	9,11,12	1.50	2 (22%)	10,14,16	0.96	1 (10%)
1	CGU	L	26	7,6,1	9,11,12	1.38	1 (11%)	10,14,16	0.93	0
1	CGU	L	25	6,1	9,11,12	1.28	1 (11%)	10,14,16	0.85	0
1	CGU	L	35	1	9,11,12	1.54	1 (11%)	10,14,16	0.82	0
1	CGU	L	16	7,6,1	9,11,12	1.39	1 (11%)	10,14,16	1.19	1 (10%)
1	CGU	L	7	7,1	9,11,12	1.42	2 (22%)	10,14,16	0.74	0
1	CGU	L	29	7,6,1	9,11,12	1.24	0	10,14,16	0.82	0
1	CGU	L	19	6,1	9,11,12	1.37	1 (11%)	10,14,16	1.43	2 (20%)

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	6,1	-	4/13/14/16	-
1	CGU	L	20	7,1	-	7/13/14/16	-
1	CGU	L	6	7,1	-	3/13/14/16	-
1	CGU	L	26	7,6,1	-	4/13/14/16	-
1	CGU	L	25	6,1	-	0/13/14/16	-
1	CGU	L	35	1	-	4/13/14/16	-
1	CGU	L	16	7,6,1	-	4/13/14/16	-
1	CGU	L	7	7,1	-	0/13/14/16	-
1	CGU	L	29	7,6,1	-	1/13/14/16	-
1	CGU	L	19	6,1	-	6/13/14/16	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	35	CGU	CG-CD1	2.83	1.55	1.52
1	L	20	CGU	CG-CD2	2.66	1.55	1.52
1	L	19	CGU	CG-CD1	2.42	1.55	1.52
1	L	25	CGU	CG-CD2	2.24	1.55	1.52
1	L	16	CGU	CG-CD1	2.14	1.54	1.52
1	L	6	CGU	CG-CD2	2.13	1.54	1.52
1	L	6	CGU	CG-CD1	2.08	1.54	1.52
1	L	7	CGU	CG-CD2	2.06	1.54	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	7	CGU	CG-CD1	2.04	1.54	1.52
1	L	26	CGU	CG-CD2	2.01	1.54	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	19	CGU	CB-CG-CD2	-3.01	107.00	113.11
1	L	6	CGU	CB-CA-C	-2.34	107.39	110.99
1	L	19	CGU	OE12-CD1-OE11	-2.22	119.05	124.08
1	L	16	CGU	CB-CG-CD2	-2.02	109.01	113.11

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	L	14	CGU	CA-CB-CG-CD1
1	L	14	CGU	CA-CB-CG-CD2
1	L	19	CGU	C-CA-CB-CG
1	L	19	CGU	OE22-CD2-CG-CB
1	L	19	CGU	OE22-CD2-CG-CD1
1	L	20	CGU	N-CA-CB-CG
1	L	20	CGU	C-CA-CB-CG
1	L	20	CGU	CA-CB-CG-CD1
1	L	20	CGU	OE21-CD2-CG-CB
1	L	20	CGU	OE22-CD2-CG-CB
1	L	26	CGU	OE21-CD2-CG-CB
1	L	26	CGU	OE22-CD2-CG-CB
1	L	29	CGU	O-C-CA-CB
1	L	6	CGU	N-CA-CB-CG
1	L	6	CGU	OE11-CD1-CG-CB
1	L	6	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	16	CGU	OE21-CD2-CG-CB
1	L	16	CGU	OE22-CD2-CG-CB
1	L	19	CGU	OE21-CD2-CG-CB
1	L	20	CGU	OE11-CD1-CG-CB
1	L	20	CGU	OE12-CD1-CG-CB
1	L	26	CGU	OE11-CD1-CG-CB
1	L	26	CGU	OE12-CD1-CG-CB

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Mol	Chain	Res	Type	Atoms
1	L	35	CGU	OE21-CD2-CG-CB
1	L	35	CGU	OE22-CD2-CG-CB
1	L	19	CGU	OE21-CD2-CG-CD1
1	L	19	CGU	N-CA-CB-CG
1	L	35	CGU	OE21-CD2-CG-CD1
1	L	35	CGU	OE22-CD2-CG-CD1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L	14	CGU	2	0
1	L	19	CGU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
5	FUC	L	2003	-	10,10,11	1.53	3 (30%)	14,14,16	0.84	0
11	BEN	H	1001	-	9,9,9	1.58	2 (22%)	7,11,11	0.72	0
4	GLC	L	2001	-	11,11,12	0.91	0	15,15,17	1.12	1 (6%)

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
5	FUC	L	2003	-	-	-	0/1/1/1
11	BEN	H	1001	-	-	4/4/4/4	0/1/1/1
4	GLC	L	2001	-	-	1/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	1001	BEN	C6-C1	3.09	1.44	1.39
5	L	2003	FUC	C1-C2	2.57	1.58	1.52
5	L	2003	FUC	O5-C5	2.33	1.48	1.43
11	H	1001	BEN	C1-C	-2.18	1.43	1.47
5	L	2003	FUC	C4-C5	2.10	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	2001	GLC	C1-O5-C5	3.22	116.51	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	H	1001	BEN	N2-C-C1-C2
11	H	1001	BEN	N2-C-C1-C6
4	L	2001	GLC	O5-C5-C6-O6
11	H	1001	BEN	N1-C-C1-C2
11	H	1001	BEN	N1-C-C1-C6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	2003	FUC	1	0
11	H	1001	BEN	1	0
4	L	2001	GLC	1	0

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, 95th 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 ²)	Q<0.9
1	L	132/142 (92%)	0.18	6 (4%) 38 41	11, 21, 48, 65	0
2	H	254/254 (100%)	-0.56	3 (1%) 76 81	7, 12, 28, 43	0
3	T	192/206 (93%)	-0.06	7 (3%) 46 50	10, 20, 46, 62	0
All	All	578/602 (96%)	-0.23	16 (2%) 55 59	7, 17, 43, 65	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	1	ALA	7.6
3	T	5	ALA	5.9
3	T	82	ASN	5.4
1	L	3	ALA	5.2
1	L	2	ASN	4.8
3	T	137	ASN	4.6
2	H	170(G)	ASP	4.2
1	L	108	THR	3.2
3	T	120	GLY	3.1
3	T	81	GLY	3.0
3	T	156	TYR	2.7
1	L	142	GLU	2.7
1	L	107	GLY	2.5
3	T	90	GLY	2.5
2	H	170(D)	LYS	2.4
2	H	245	GLU	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, 95th 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	20	12/13	0.60	0.14	53,61,64,64	0
1	CGU	L	6	12/13	0.63	0.14	28,42,45,46	0
1	CGU	L	35	12/13	0.64	0.12	45,53,54,55	0
1	CGU	L	19	12/13	0.71	0.13	52,59,60,62	0
1	CGU	L	14	12/13	0.75	0.13	41,50,54,54	0
1	CGU	L	29	12/13	0.77	0.11	28,30,30,31	0
1	CGU	L	7	12/13	0.78	0.10	30,34,37,37	0
1	CGU	L	26	12/13	0.81	0.10	26,31,35,36	0
1	CGU	L	16	12/13	0.82	0.10	36,37,39,39	0
1	CGU	L	25	12/13	0.88	0.08	26,28,33,33	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CA	L	3003	1/1	0.37	0.25	69,69,69,69	0
7	CA	L	3006	1/1	0.47	0.30	76,76,76,76	0
5	FUC	L	2003	10/11	0.61	0.17	39,42,43,44	0
7	CA	L	3002	1/1	0.65	0.14	67,67,67,67	0
6	MG	L	3007	1/1	0.66	0.11	51,51,51,51	0
4	GLC	L	2001	11/12	0.67	0.12	37,38,39,41	0
8	NA	H	3010	1/1	0.79	0.10	22,22,22,22	0
6	MG	L	3004	1/1	0.81	0.07	37,37,37,37	0
6	MG	L	3001	1/1	0.82	0.09	33,33,33,33	0
7	CA	L	3005	1/1	0.84	0.16	60,60,60,60	0
10	CL	H	3013	1/1	0.86	0.13	43,43,43,43	0
7	CA	H	3009	1/1	0.88	0.06	29,29,29,29	0
11	BEN	H	1001	9/9	0.94	0.05	9,11,12,13	0
9	ZN	H	3012	1/1	0.95	0.13	55,55,55,55	0
7	CA	L	3008	1/1	0.96	0.04	25,25,25,25	0
9	ZN	H	3011	1/1	0.97	0.17	62,62,62,62	0
10	CL	T	3015	1/1	0.99	0.02	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	CL	H	3014	1/1	0.99	0.02	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.