



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:01 AM UTC

PDB ID : 3TH2 / pdb_00003th2
Title : Mg²⁺ Is Required for Optimal Folding of the Gamma-Carboxyglutamic Acid (Gla) Domains of Vitamin K-Dependent Clotting Factors At Physiological Ca²⁺
Authors : Vadivel, K.; Agah, S.; Cascio, D.; Padmanabhan, K.; Bajaj, S.P.
Deposited on : 2011-08-18
Resolution : 1.72 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

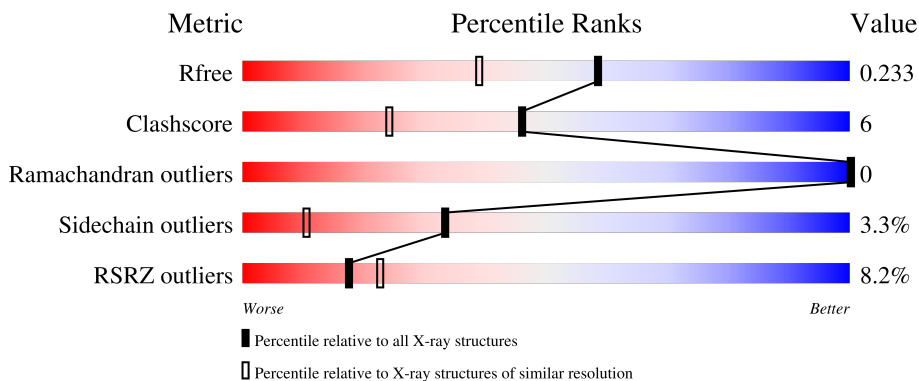
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	
2	H	254	
3	T	205	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5334 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 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	142	1135	683	189	248	15	0	0	0

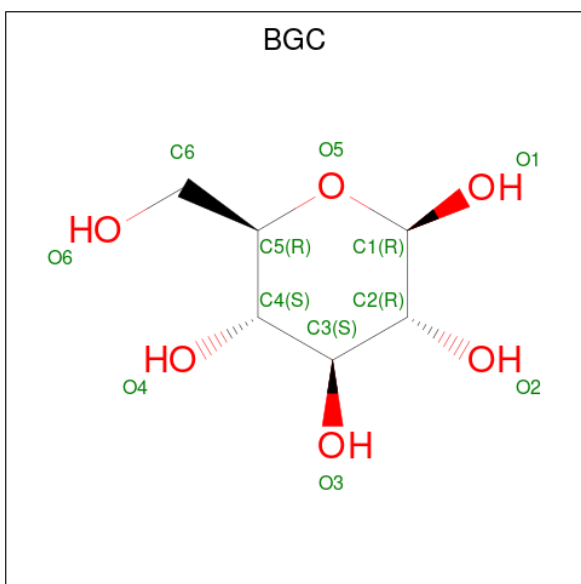
- Molecule 2 is a protein called Coagulation factor VII heavy chain.

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

- Molecule 3 is a protein called Tissue factor.

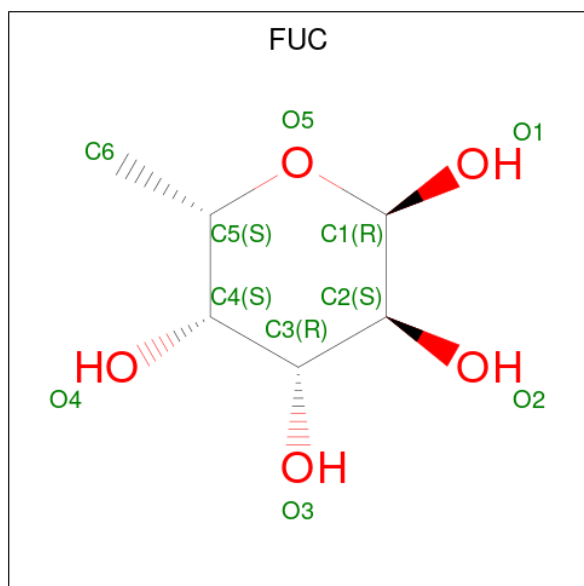
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	T	198	1597	1013	259	320	5	0	0	0

- Molecule 4 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



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	0	0
			10	6	4		

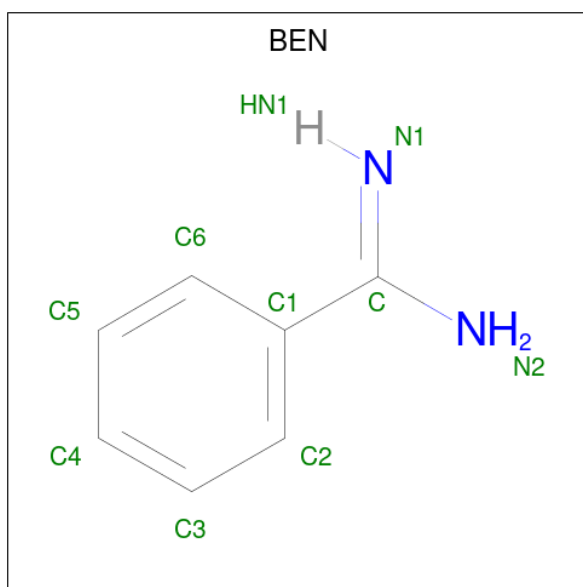
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

- Molecule 8 is BENZAMIDINE (CCD ID: BEN) (formula: $C_7H_8N_2$).



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

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

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

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

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

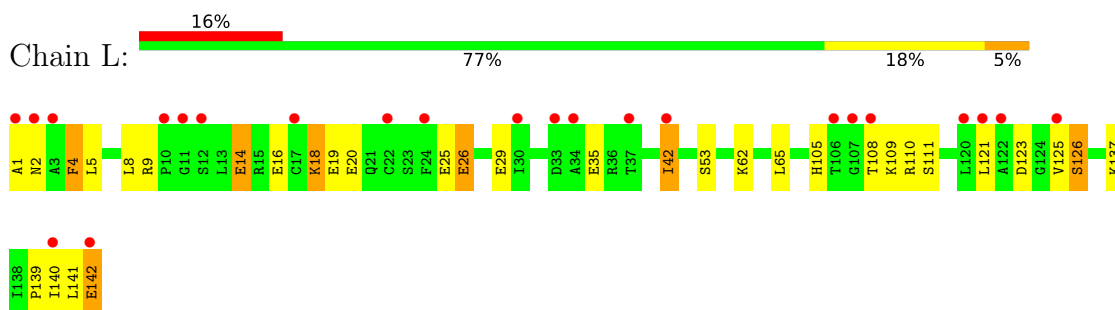
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	146	Total O 146 146	0	0
11	H	275	Total O 275 275	0	0
11	T	165	Total O 165 165	0	0

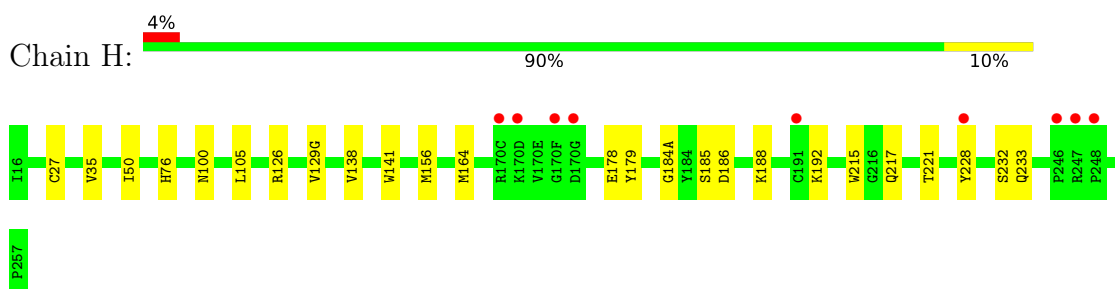
3 Residue-property plots [i](#)

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.

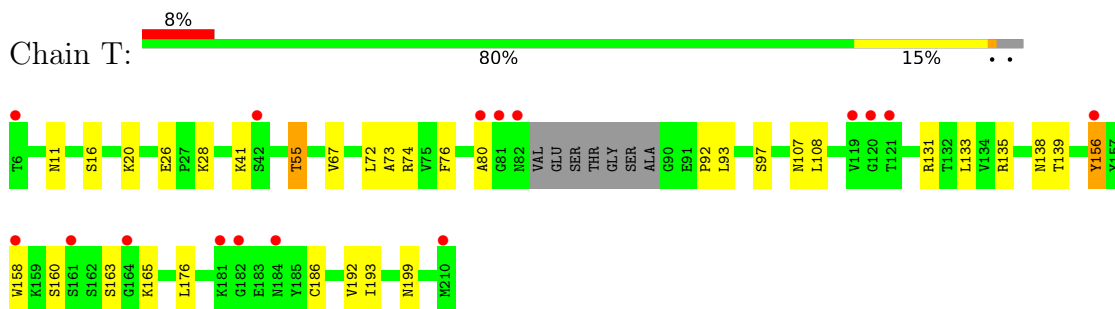
- Molecule 1: Coagulation factor VII light chain



- Molecule 2: Coagulation factor VII heavy chain



- Molecule 3: Tissue factor



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.94Å 80.87Å 126.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.20 – 1.72 61.20 – 1.72	Depositor EDS
% Data completeness (in resolution range)	96.2 (61.20-1.72) 96.1 (61.20-1.72)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 1.72Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.189 , 0.233 0.188 , 0.233	Depositor DCC
R_{free} test set	3695 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtrriage
Anisotropy	0.054	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5334	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.51% 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 i

5.1 Standard geometry i

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

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	1.24	1/1029 (0.1%)	1.23	5/1374 (0.4%)
2	H	1.48	13/2024 (0.6%)	1.27	5/2755 (0.2%)
3	T	1.41	2/1632 (0.1%)	1.24	4/2218 (0.2%)
All	All	1.40	16/4685 (0.3%)	1.25	14/6347 (0.2%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	50	ILE	CA-CB	7.35	1.63	1.54
2	H	184(A)	GLY	C-O	-6.44	1.20	1.24
2	H	188	LYS	N-CA	6.28	1.53	1.46
2	H	35	VAL	C-N	6.20	1.42	1.33
1	L	53	SER	C-O	-5.72	1.21	1.23
2	H	215	TRP	N-CA	5.66	1.52	1.46
3	T	192	VAL	CA-CB	5.59	1.62	1.54
2	H	129(G)	VAL	C-N	5.59	1.41	1.33
2	H	232	SER	N-CA	5.36	1.53	1.46
2	H	192	LYS	CA-C	5.27	1.59	1.52
2	H	217	GLN	C-N	5.21	1.40	1.33
2	H	185	SER	CA-CB	-5.18	1.44	1.53
2	H	141	TRP	N-CA	5.06	1.52	1.46
2	H	186	ASP	CA-C	5.05	1.61	1.52
2	H	179	TYR	N-CA	5.04	1.52	1.46
3	T	156	TYR	CA-C	-5.03	1.46	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	4	PHE	N-CA-C	8.62	120.67	111.28
2	H	105	LEU	CA-C-N	7.43	133.45	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	105	LEU	C-N-CA	7.43	133.45	123.05
1	L	2	ASN	N-CA-C	6.77	119.44	108.41
1	L	9	ARG	CA-C-N	-6.30	114.16	120.21
1	L	9	ARG	C-N-CA	-6.30	114.16	120.21
2	H	179	TYR	N-CA-C	-5.78	105.81	112.92
3	T	67	VAL	N-CA-C	5.73	120.15	111.89
1	L	125	VAL	N-CA-C	5.52	118.95	113.71
3	T	55	THR	N-CA-C	-5.33	105.22	112.26
3	T	74	ARG	CA-C-N	-5.25	116.11	123.10
3	T	74	ARG	C-N-CA	-5.25	116.11	123.10
2	H	186	ASP	CA-CB-CG	5.15	117.75	112.60
2	H	221	THR	N-CA-C	-5.01	101.55	109.96

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	1135	0	989	27	0
2	H	1974	0	1950	9	0
3	T	1597	0	1551	21	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	9	0	7	0	0
9	H	1	0	0	0	0
10	H	1	0	0	0	0
10	T	1	0	0	0	0
11	H	275	0	0	5	0
11	L	146	0	0	5	0
11	T	165	0	0	6	0
All	All	5334	0	4517	54	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 6.

All (54) 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:27:CYS:HB3	11:H:262:HOH:O	1.37	1.20
3:T:76:PHE:CD1	3:T:92:PRO:HG2	2.08	0.88
1:L:19:CGU:HA	11:L:572:HOH:O	1.74	0.86
1:L:42:ILE:HD11	1:L:65:LEU:HD11	1.58	0.85
3:T:156:TYR:CD2	11:T:269:HOH:O	2.33	0.82
1:L:1:ALA:HB1	1:L:20:CGU:OE22	1.81	0.80
3:T:135:ARG:HD3	11:T:576:HOH:O	1.83	0.79
1:L:141:LEU:O	1:L:142:GLU:HG3	1.83	0.78
1:L:105:HIS:HE1	1:L:111:SER:OG	1.68	0.76
3:T:72:LEU:HG	3:T:73:ALA:N	2.01	0.74
3:T:76:PHE:HD1	3:T:92:PRO:HG2	1.57	0.68
1:L:42:ILE:CD1	1:L:65:LEU:HD11	2.24	0.68
1:L:141:LEU:O	1:L:142:GLU:CG	2.42	0.68
3:T:156:TYR:CE2	11:T:269:HOH:O	2.50	0.63
1:L:62:LYS:HE3	3:T:131:ARG:HH21	1.64	0.62
1:L:105:HIS:CE1	1:L:111:SER:OG	2.52	0.62
2:H:156:MET:HE2	11:H:12:HOH:O	1.98	0.62
3:T:135:ARG:HD3	11:T:371:HOH:O	2.01	0.59
3:T:156:TYR:HD2	11:T:269:HOH:O	1.77	0.58
1:L:19:CGU:CA	11:L:572:HOH:O	2.40	0.57
3:T:108:LEU:HD11	3:T:193:ILE:HG12	1.86	0.57
1:L:105:HIS:O	1:L:108:THR:O	2.25	0.55
1:L:141:LEU:O	1:L:142:GLU:CD	2.49	0.55
1:L:14:CGU:HA	1:L:18:LYS:HG3	1.90	0.54
2:H:156:MET:HE1	11:H:447:HOH:O	2.07	0.54
3:T:156:TYR:CD1	3:T:165:LYS:NZ	2.77	0.53
3:T:16:SER:HA	3:T:20:LYS:O	2.12	0.49
3:T:80:ALA:HB2	11:T:254:HOH:O	2.12	0.49
2:H:126:ARG:NH2	2:H:233:GLN:OE1	2.46	0.49
1:L:14:CGU:HG	1:L:19:CGU:OE22	2.14	0.48
1:L:19:CGU:CD1	11:L:572:HOH:O	2.63	0.47
1:L:141:LEU:C	1:L:142:GLU:HG3	2.38	0.47
1:L:62:LYS:CE	3:T:131:ARG:HH21	2.26	0.47
2:H:76:HIS:CE1	11:H:590:HOH:O	2.67	0.46
1:L:42:ILE:HD11	1:L:65:LEU:CD1	2.37	0.46
3:T:72:LEU:HD11	3:T:97:SER:O	2.16	0.46
1:L:1:ALA:HB1	1:L:20:CGU:CD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:110:ARG:HD2	1:L:110:ARG:C	2.40	0.46
2:H:138:VAL:HG11	2:H:228:TYR:CE2	2.51	0.45
2:H:178:GLU:HB3	11:H:354:HOH:O	2.16	0.45
3:T:158:TRP:CE2	3:T:186:CYS:HB2	2.51	0.45
3:T:28:LYS:HD2	3:T:55:THR:HG21	1.98	0.45
1:L:26:CGU:HA	1:L:26:CGU:OE21	2.16	0.44
2:H:164:MET:HE1	3:T:76:PHE:HE1	1.84	0.43
1:L:1:ALA:N	11:L:433:HOH:O	2.51	0.42
3:T:11:ASN:ND2	3:T:26:GLU:OE1	2.49	0.42
1:L:108:THR:OG1	1:L:109:LYS:N	2.47	0.42
3:T:133:LEU:N	3:T:133:LEU:CD2	2.83	0.42
1:L:123:ASP:OD2	1:L:126:SER:HB2	2.20	0.42
2:H:228:TYR:CD1	2:H:228:TYR:N	2.88	0.41
1:L:19:CGU:CG	11:L:572:HOH:O	2.69	0.41
3:T:107:ASN:OD1	3:T:199:ASN:ND2	2.52	0.41
1:L:42:ILE:HG21	1:L:42:ILE:HD12	1.76	0.41
1:L:137:LYS:O	1:L:139:PRO:HD3	2.22	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	130/142 (92%)	124 (95%)	6 (5%)	0	100	100
2	H	252/254 (99%)	247 (98%)	5 (2%)	0	100	100
3	T	194/205 (95%)	191 (98%)	3 (2%)	0	100	100
All	All	576/601 (96%)	562 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	114/114 (100%)	105 (92%)	9 (8%)	11	1
2	H	216/216 (100%)	215 (100%)	1 (0%)	81	71
3	T	184/189 (97%)	177 (96%)	7 (4%)	29	8
All	All	514/519 (99%)	497 (97%)	17 (3%)	33	10

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	PHE
1	L	5	LEU
1	L	8	LEU
1	L	18	LYS
1	L	42	ILE
1	L	121	LEU
1	L	126	SER
1	L	140	ILE
1	L	142	GLU
2	H	100	ASN
3	T	41	LYS
3	T	93	LEU
3	T	138	ASN
3	T	139	THR
3	T	160	SER
3	T	163	SER
3	T	176	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	2	ASN
1	L	80	ASN
1	L	88	GLN
1	L	105	HIS

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Mol	Chain	Res	Type
2	H	76	HIS
2	H	100	ASN
2	H	159	ASN
2	H	175	ASN
2	H	239	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CGU	L	20	7,1	9,11,12	1.13	0	10,14,16	0.63	0
1	CGU	L	35	1	9,11,12	1.29	0	10,14,16	1.21	2 (20%)
1	CGU	L	14	6,1	9,11,12	2.69	3 (33%)	10,14,16	1.20	0
1	CGU	L	26	7,6,1	9,11,12	1.47	1 (11%)	10,14,16	1.46	1 (10%)
1	CGU	L	29	7,6,1	9,11,12	1.04	2 (22%)	10,14,16	0.55	0
1	CGU	L	19	6,1	9,11,12	1.09	0	10,14,16	0.56	0
1	CGU	L	6	1	9,11,12	1.29	0	10,14,16	0.64	0
1	CGU	L	25	6,1	9,11,12	1.07	2 (22%)	10,14,16	0.85	0
1	CGU	L	16	7,6,1	9,11,12	2.68	3 (33%)	10,14,16	1.21	0
1	CGU	L	7	1	9,11,12	1.05	0	10,14,16	0.80	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	20	7,1	-	4/13/14/16	-
1	CGU	L	35	1	-	7/13/14/16	-
1	CGU	L	14	6,1	-	4/13/14/16	-
1	CGU	L	26	7,6,1	-	6/13/14/16	-
1	CGU	L	29	7,6,1	-	4/13/14/16	-
1	CGU	L	19	6,1	-	1/13/14/16	-
1	CGU	L	6	1	-	2/13/14/16	-
1	CGU	L	25	6,1	-	0/13/14/16	-
1	CGU	L	16	7,6,1	-	5/13/14/16	-
1	CGU	L	7	1	-	1/13/14/16	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	14	CGU	OE11-CD1	6.20	1.40	1.22
1	L	16	CGU	OE11-CD1	6.17	1.40	1.22
1	L	14	CGU	OE12-CD1	-3.67	1.19	1.30
1	L	16	CGU	OE12-CD1	-3.66	1.19	1.30
1	L	16	CGU	OE22-CD2	3.09	1.40	1.30
1	L	26	CGU	OE22-CD2	-3.09	1.20	1.30
1	L	14	CGU	OE22-CD2	3.08	1.40	1.30
1	L	25	CGU	OE22-CD2	-2.16	1.23	1.30
1	L	25	CGU	OE12-CD1	-2.09	1.24	1.30
1	L	29	CGU	OE22-CD2	-2.02	1.24	1.30
1	L	29	CGU	OE12-CD1	-2.01	1.24	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	26	CGU	CB-CA-C	-3.75	105.22	110.99
1	L	35	CGU	CB-CG-CD2	2.45	118.09	113.11
1	L	35	CGU	CB-CG-CD1	2.03	117.23	113.11

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	L	7	CGU	O-C-CA-CB
1	L	16	CGU	O-C-CA-CB
1	L	20	CGU	N-CA-CB-CG
1	L	20	CGU	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	L	26	CGU	CA-CB-CG-CD2
1	L	29	CGU	O-C-CA-CB
1	L	35	CGU	OE12-CD1-CG-CD2
1	L	35	CGU	CA-CB-CG-CD1
1	L	26	CGU	N-CA-CB-CG
1	L	6	CGU	OE11-CD1-CG-CB
1	L	6	CGU	OE12-CD1-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	20	CGU	OE21-CD2-CG-CB
1	L	20	CGU	OE22-CD2-CG-CB
1	L	26	CGU	OE11-CD1-CG-CB
1	L	26	CGU	OE12-CD1-CG-CB
1	L	26	CGU	OE21-CD2-CG-CB
1	L	26	CGU	OE22-CD2-CG-CB
1	L	35	CGU	C-CA-CB-CG
1	L	19	CGU	CA-CB-CG-CD1
1	L	35	CGU	N-CA-CB-CG
1	L	14	CGU	OE11-CD1-CG-CB
1	L	14	CGU	OE21-CD2-CG-CB
1	L	14	CGU	OE22-CD2-CG-CB
1	L	29	CGU	OE11-CD1-CG-CB
1	L	29	CGU	OE12-CD1-CG-CB
1	L	35	CGU	OE21-CD2-CG-CB
1	L	35	CGU	OE22-CD2-CG-CB
1	L	14	CGU	OE11-CD1-CG-CD2
1	L	29	CGU	OE11-CD1-CG-CD2
1	L	35	CGU	OE11-CD1-CG-CD2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L	20	CGU	2	0
1	L	14	CGU	2	0
1	L	26	CGU	1	0
1	L	19	CGU	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 12 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
4	BGC	L	143	1	11,11,12	0.78	0	15,15,17	1.97	5 (33%)
5	FUC	L	144	1	10,10,11	0.43	0	14,14,16	0.99	0
8	BEN	H	1	-	9,9,9	1.24	0	7,11,11	3.10	5 (71%)

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	144	1	-	-	0/1/1/1
4	BGC	L	143	1	-	1/2/19/22	0/1/1/1
8	BEN	H	1	-	-	4/4/4/4	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1	BEN	C5-C6-C1	4.72	125.00	120.36
8	H	1	BEN	C4-C3-C2	4.53	125.83	120.24
4	L	143	BGC	O3-C3-C2	3.87	117.95	110.05
8	H	1	BEN	C5-C4-C3	-3.26	115.40	119.87
4	L	143	BGC	C1-O5-C5	2.93	116.11	112.19
4	L	143	BGC	C3-C4-C5	2.86	115.41	110.23
4	L	143	BGC	O4-C4-C3	-2.80	103.77	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1	BEN	C6-C1-C2	-2.67	115.17	118.57
4	L	143	BGC	O5-C5-C6	2.65	112.83	107.66
8	H	1	BEN	C1-C-N2	2.09	121.18	118.01

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	143	BGC	O5-C5-C6-O6
8	H	1	BEN	N2-C-C1-C2
8	H	1	BEN	N2-C-C1-C6
8	H	1	BEN	N1-C-C1-C2
8	H	1	BEN	N1-C-C1-C6

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, 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%)	1.09	23 (17%) 4 6	14, 27, 43, 61	0
2	H	254/254 (100%)	-0.15	9 (3%) 47 55	9, 16, 33, 54	0
3	T	198/205 (96%)	0.36	16 (8%) 18 23	13, 21, 45, 59	0
All	All	584/601 (97%)	0.31	48 (8%) 17 23	9, 20, 43, 61	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	1	ALA	9.1
1	L	3	ALA	7.2
1	L	108	THR	5.1
3	T	156	TYR	4.8
3	T	82	ASN	4.5
1	L	2	ASN	4.3
1	L	34	ALA	3.5
2	H	248	PRO	3.4
2	H	228	TYR	3.3
3	T	121	THR	3.3
1	L	24	PHE	3.3
1	L	106	THR	3.2
1	L	10	PRO	3.1
1	L	107	GLY	3.1
3	T	119	VAL	3.0
3	T	81	GLY	3.0
1	L	121	LEU	2.9
1	L	125	VAL	2.9
1	L	142	GLU	2.8
2	H	170(G)	ASP	2.8
1	L	11	GLY	2.8
2	H	170(D)	LYS	2.7
2	H	170(F)	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
3	T	120	GLY	2.6
3	T	182	GLY	2.6
1	L	120	LEU	2.5
1	L	30	ILE	2.5
3	T	158	TRP	2.5
1	L	42	ILE	2.5
2	H	246	PRO	2.4
2	H	170(C)	ARG	2.4
3	T	210	MET	2.4
1	L	122	ALA	2.3
3	T	80	ALA	2.3
1	L	12	SER	2.3
1	L	22	CYS	2.3
1	L	17	CYS	2.2
3	T	6	THR	2.2
3	T	42	SER	2.2
1	L	37	THR	2.2
2	H	247	ARG	2.1
3	T	184	ASN	2.1
3	T	161	SER	2.1
1	L	140	ILE	2.1
3	T	164	GLY	2.0
1	L	33	ASP	2.0
2	H	191	CYS	2.0
3	T	181	LYS	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, 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(Å ²)	Q<0.9
1	CGU	L	19	12/13	0.77	0.14	41,46,53,53	0
1	CGU	L	26	12/13	0.78	0.18	24,28,35,38	0
1	CGU	L	35	12/13	0.79	0.20	35,49,58,59	0
1	CGU	L	20	12/13	0.80	0.15	40,50,55,56	0
1	CGU	L	14	12/13	0.82	0.13	36,45,51,52	0
1	CGU	L	16	12/13	0.83	0.15	22,29,31,32	0
1	CGU	L	6	12/13	0.85	0.15	27,39,48,49	0
1	CGU	L	7	12/13	0.88	0.12	29,32,45,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CGU	L	29	12/13	0.89	0.12	27,28,29,31	0
1	CGU	L	25	12/13	0.91	0.11	28,31,37,38	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(\AA^2)	Q<0.9
7	CA	L	147	1/1	0.73	0.20	70,70,70,70	0
7	CA	L	149	1/1	0.82	0.15	73,73,73,73	0
4	BGC	L	143	11/12	0.88	0.11	34,38,40,42	0
7	CA	L	146	1/1	0.90	0.13	48,48,48,48	0
6	MG	L	151	1/1	0.93	0.08	55,55,55,55	0
6	MG	L	148	1/1	0.93	0.14	27,27,27,27	0
7	CA	L	150	1/1	0.94	0.08	57,57,57,57	0
5	FUC	L	144	10/11	0.95	0.07	24,31,35,37	0
6	MG	L	145	1/1	0.95	0.13	33,33,33,33	0
7	CA	L	152	1/1	0.97	0.05	22,22,22,22	0
7	CA	H	9	1/1	0.97	0.08	27,27,27,27	0
9	NA	H	10	1/1	0.97	0.07	25,25,25,25	0
8	BEN	H	1	9/9	0.98	0.06	11,15,17,17	0
10	CL	H	14	1/1	0.98	0.06	24,24,24,24	0
10	CL	T	211	1/1	0.98	0.03	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.