Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2020 – 02:01 PM BST

PDB ID	:	2FIR
Title	:	Crystal structure of DFPR-VIIa/sTF
Authors	:	Bajaj, S.P.; Schmidt, A.E.; Padmanabhan, K.; Bajaj, M.S.; Prevost, D.; Schreuder, H.
Deposited on	:	2005-12-30
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

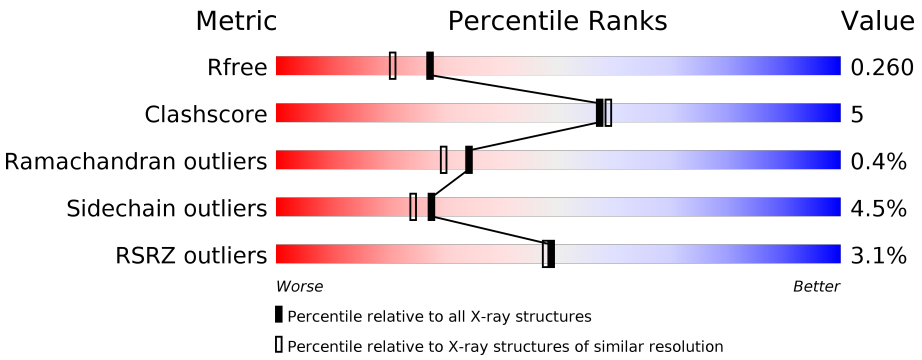
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 >=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 <=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% 85% 13% ••
2	H	254	2% 88% 11% •
3	T	205	4% 78% 14% • 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
7	CA	L	1005	-	-	-	X
7	CA	L	1006	-	-	-	X

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 5352 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

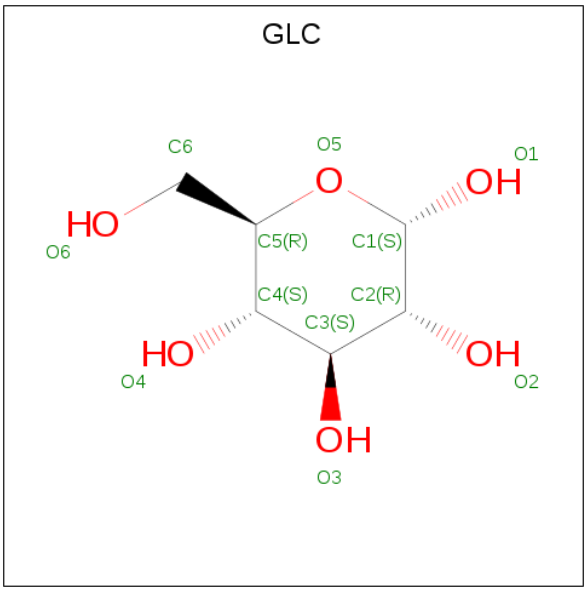
- Molecule 2 is a protein called Coagulation factor VII Heavy Chain (EC 3.4.21.21).

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.

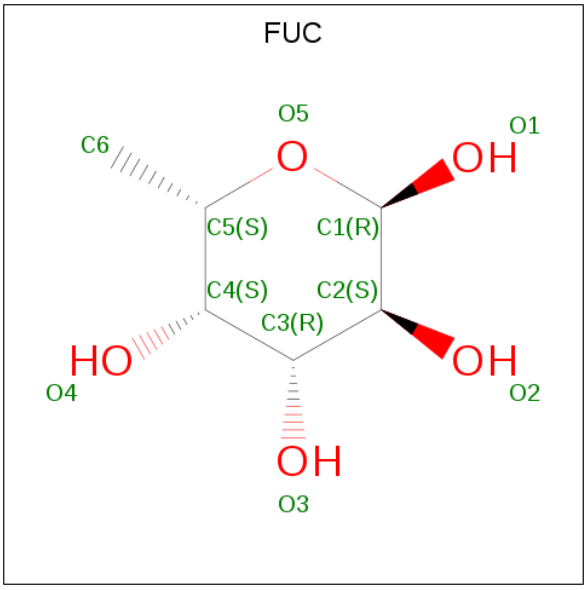
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	T	191	1551	987	250	309	5	0	0	0

- Molecule 4 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



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

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



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

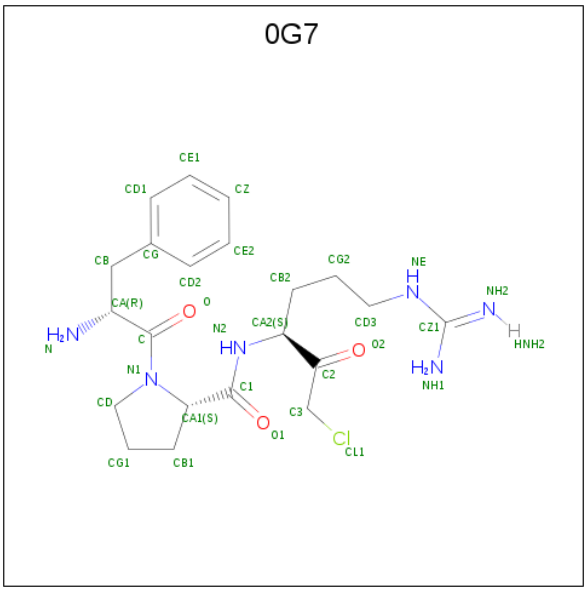
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 8 is D-phenylalanyl-N-[(3S)-6-carbamimidamido-1-chloro-2-oxohexan-3-yl]-L-proli namide (three-letter code: 0G7) (formula: $C_{21}H_{31}ClN_6O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	H	1	30	21	6	3	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 12 is water.

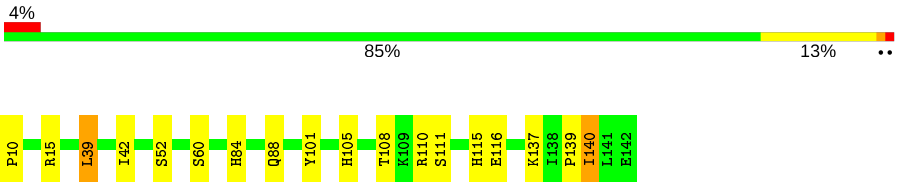
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
12	L	165	165	165	0	0
			Total	O		
12	H	281	281	281	0	0
			Total	O		
12	T	180	180	180	0	0

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.

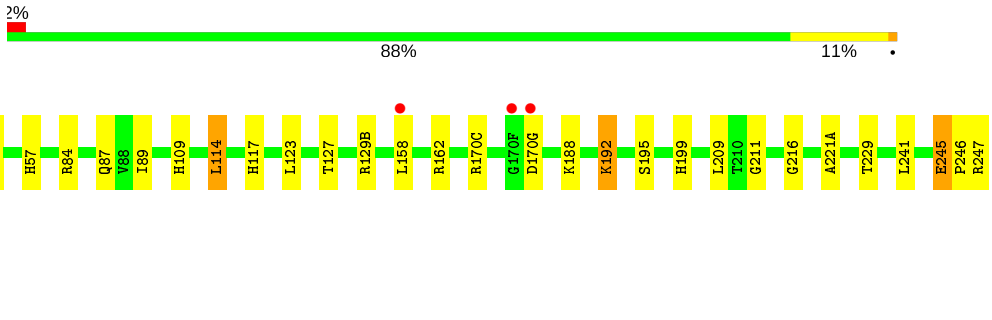
- Molecule 1: Coagulation factor VII Light chain

Chain L:



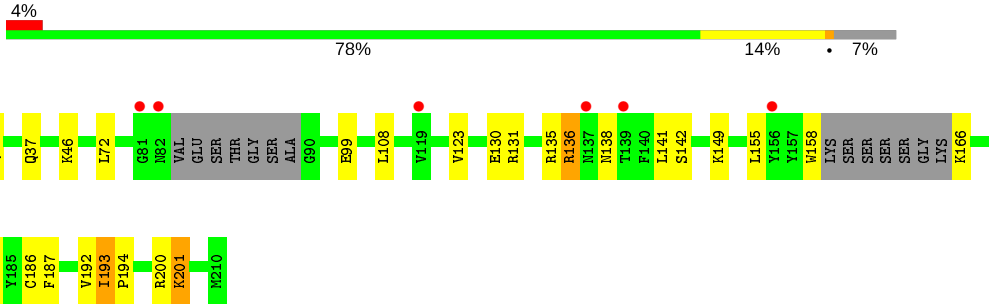
- Molecule 2: Coagulation factor VII Heavy Chain (EC 3.4.21.21)

Chain H:



- Molecule 3: Tissue factor

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.02Å 80.98Å 126.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 40.59 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.00) 84.2 (40.59-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.00Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.207 , 0.281 0.196 , 0.260	Depositor DCC
R_{free} test set	2113 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	21.0	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 78.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5352	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, 0G7, 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	0.55	0/1029	0.79	1/1374 (0.1%)
2	H	0.58	0/2024	0.80	3/2755 (0.1%)
3	T	0.60	0/1585	0.84	2/2156 (0.1%)
All	All	0.58	0/4638	0.81	6/6285 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	199	HIS	N-CA-C	-6.33	93.90	111.00
1	L	39	LEU	CA-CB-CG	5.77	128.57	115.30
3	T	20	LYS	N-CA-C	-5.14	97.12	111.00
2	H	162	ARG	NE-CZ-NH2	-5.12	117.74	120.30
3	T	193	ILE	N-CA-C	-5.07	97.32	111.00
2	H	123	LEU	N-CA-C	-5.03	97.41	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	1135	0	989	9	0
2	H	1974	0	1950	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	T	1551	0	1501	13	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	30	0	28	9	0
9	H	1	0	0	0	0
10	H	2	0	0	0	0
11	H	2	0	0	0	0
11	T	1	0	0	0	0
12	H	281	0	0	3	1
12	L	165	0	0	1	1
12	T	180	0	0	2	0
All	All	5352	0	4488	44	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 5.

All (44) 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)
8:H:701:0G7:CA1	8:H:701:0G7:N1	1.69	1.38
8:H:701:0G7:C	8:H:701:0G7:CA1	2.51	0.88
2:H:216:GLY:O	8:H:701:0G7:HB	1.76	0.84
2:H:57:HIS:CD2	8:H:701:0G7:C3	2.61	0.83
2:H:221(A):ALA:HA	12:H:1290:HOH:O	1.85	0.76
2:H:89:ILE:HG21	2:H:241:LEU:HD13	1.72	0.71
3:T:108:LEU:HD11	3:T:193:ILE:HG12	1.73	0.70
2:H:195:SER:OG	8:H:701:0G7:C2	2.42	0.68
1:L:52:SER:OG	4:L:801:GLC:C1	2.45	0.65
1:L:140:ILE:HD11	2:H:26:GLU:HG3	1.79	0.63
1:L:60:SER:OG	5:L:901:FUC:C1	2.47	0.61
2:H:117:HIS:HD2	12:H:1045:HOH:O	1.88	0.57
3:T:136:ARG:HB3	3:T:141:LEU:HD21	1.88	0.56
3:T:192:VAL:HG22	3:T:201:LYS:HB3	1.88	0.55
3:T:123:VAL:HG23	3:T:179:VAL:HG21	1.93	0.50
2:H:192:LYS:HE3	8:H:701:0G7:O1	2.12	0.50
2:H:57:HIS:NE2	8:H:701:0G7:C2	2.73	0.50
1:L:101:TYR:OH	1:L:115:HIS:HD2	1.95	0.50
2:H:49:THR:HG22	2:H:114:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:701:0G7:C1	8:H:701:0G7:N1	2.63	0.48
1:L:137:LYS:O	1:L:139:PRO:HD3	2.14	0.48
2:H:87:GLN:HE22	2:H:247:ARG:HB2	1.79	0.47
2:H:127:THR:O	2:H:129(B):ARG:HG2	2.15	0.46
2:H:211:GLY:HA2	2:H:229:THR:O	2.15	0.46
2:H:57:HIS:CE1	2:H:195:SER:OG	2.69	0.46
3:T:37:GLN:HA	3:T:46:LYS:O	2.16	0.46
3:T:158:TRP:CE2	3:T:186:CYS:HB2	2.51	0.45
2:H:170(C):ARG:NH1	12:H:1066:HOH:O	2.46	0.45
1:L:84:HIS:HE1	12:L:1083:HOH:O	2.00	0.44
1:L:105:HIS:HE1	1:L:111:SER:OG	2.01	0.44
3:T:131:ARG:HB3	12:T:1154:HOH:O	2.17	0.44
3:T:194:PRO:HA	3:T:200:ARG:HH21	1.82	0.44
2:H:158:LEU:HD11	2:H:188:LYS:HB3	2.00	0.43
3:T:72:LEU:HD23	3:T:99:GLU:HG2	1.98	0.43
2:H:158:LEU:HD11	2:H:188:LYS:HD3	2.01	0.43
2:H:84:ARG:HH11	2:H:109:HIS:CD2	2.36	0.43
3:T:29:PRO:HB2	3:T:32:GLN:O	2.19	0.43
3:T:155:LEU:HD11	3:T:187:PHE:HB3	2.01	0.42
1:L:4:PHE:CD1	1:L:4:PHE:C	2.93	0.41
3:T:130:GLU:O	3:T:142:SER:HA	2.20	0.41
3:T:149:LYS:HG2	12:T:1117:HOH:O	2.21	0.41
2:H:245:GLU:HA	2:H:246:PRO:HD3	1.85	0.41
1:L:10:PRO:O	1:L:15:ARG:NH2	2.53	0.41
2:H:195:SER:OG	8:H:701:0G7:O2	2.38	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:1173:HOH:O	12:H:1236:HOH:O[4_556]	0.52	1.68

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%)	120 (92%)	9 (7%)	1 (1%)	19	13
2	H	252/254 (99%)	243 (96%)	9 (4%)	0	100	100
3	T	185/205 (90%)	175 (95%)	9 (5%)	1 (0%)	29	23
All	All	567/601 (94%)	538 (95%)	27 (5%)	2 (0%)	34	30

All (2) Ramachandran outliers are listed below:

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

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%)	104 (91%)	10 (9%)	10	6
2	H	216/216 (100%)	210 (97%)	6 (3%)	43	44
3	T	178/189 (94%)	171 (96%)	7 (4%)	32	30
All	All	508/519 (98%)	485 (96%)	23 (4%)	27	24

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	PHE
1	L	5	LEU
1	L	9	ARG
1	L	39	LEU
1	L	42	ILE
1	L	88	GLN
1	L	108	THR
1	L	110	ARG

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Mol	Chain	Res	Type
1	L	116	GLU
1	L	140	ILE
2	H	29	TRP
2	H	114	LEU
2	H	170(G)	ASP
2	H	192	LYS
2	H	209	LEU
2	H	245	GLU
3	T	135	ARG
3	T	136	ARG
3	T	138	ASN
3	T	166	LYS
3	T	176	LEU
3	T	181	LYS
3	T	201	LYS

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

Mol	Chain	Res	Type
1	L	84	HIS
1	L	105	HIS
1	L	115	HIS
2	H	87	GLN
2	H	117	HIS
2	H	175	ASN
3	T	118	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	26	1,7,6	3,11,12	0.83	0	1,14,16	0.49	0
1	CGU	L	14	1,6	3,11,12	0.65	0	1,14,16	0.50	0
1	CGU	L	6	1,7	3,11,12	0.61	0	1,14,16	0.08	0
1	CGU	L	19	1,6	3,11,12	0.75	0	1,14,16	0.15	0
1	CGU	L	16	1,7,6	3,11,12	0.79	0	1,14,16	0.38	0
1	CGU	L	7	1	3,11,12	0.69	0	1,14,16	0.47	0
1	CGU	L	29	1,7,6	3,11,12	0.72	0	1,14,16	0.38	0
1	CGU	L	20	1,7	3,11,12	0.62	0	1,14,16	1.11	0
1	CGU	L	35	1	3,11,12	0.81	0	1,14,16	0.37	0
1	CGU	L	25	1,6	3,11,12	0.64	0	1,14,16	1.04	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	26	1,7,6	-	0/5/14/16	-
1	CGU	L	14	1,6	-	0/5/14/16	-
1	CGU	L	6	1,7	-	0/5/14/16	-
1	CGU	L	19	1,6	-	0/5/14/16	-
1	CGU	L	16	1,7,6	-	0/5/14/16	-
1	CGU	L	7	1	-	1/5/14/16	-
1	CGU	L	29	1,7,6	-	2/5/14/16	-
1	CGU	L	20	1,7	-	3/5/14/16	-
1	CGU	L	35	1	-	3/5/14/16	-
1	CGU	L	25	1,6	-	0/5/14/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	L	7	CGU	O-C-CA-CB
1	L	20	CGU	C-CA-CB-CG
1	L	35	CGU	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	L	35	CGU	CA-CB-CG-CD1
1	L	35	CGU	CA-CB-CG-CD2
1	L	20	CGU	CA-CB-CG-CD1
1	L	29	CGU	CA-CB-CG-CD2
1	L	20	CGU	N-CA-CB-CG
1	L	29	CGU	CA-CB-CG-CD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides 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	901	-	10,10,11	1.24	2 (20%)	14,14,16	0.71	0
4	GLC	L	801	-	11,11,12	1.70	3 (27%)	15,15,17	1.02	1 (6%)
8	0G7	H	701	2	31,31,32	4.14	6 (19%)	36,41,42	1.98	9 (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
5	FUC	L	901	-	-	-	0/1/1/1
4	GLC	L	801	-	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	0G7	H	701	2	-	5/31/41/43	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	701	0G7	CD-N1	-16.36	1.16	1.47
8	H	701	0G7	CA1-N1	11.29	1.69	1.47
8	H	701	0G7	O2-C2	8.30	1.43	1.21
8	H	701	0G7	CA2-C2	4.56	1.59	1.52
8	H	701	0G7	C3-C2	4.45	1.61	1.49
4	L	801	GLC	C4-C3	-3.79	1.42	1.52
8	H	701	0G7	O-C	2.46	1.26	1.22
4	L	801	GLC	O5-C1	-2.42	1.39	1.43
5	L	901	FUC	C1-C2	2.22	1.57	1.52
4	L	801	GLC	O4-C4	2.07	1.47	1.43
5	L	901	FUC	C2-C3	-2.04	1.49	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	701	0G7	O2-C2-C3	-4.85	112.53	121.15
8	H	701	0G7	CB1-CA1-N1	-4.45	96.42	103.03
8	H	701	0G7	C-CA-N	-4.14	93.80	109.21
8	H	701	0G7	CA1-N1-C	-3.70	108.65	121.41
8	H	701	0G7	CB-CA-C	3.21	116.97	109.27
8	H	701	0G7	CG1-CD-N1	3.19	108.84	103.25
8	H	701	0G7	CD-N1-C	2.98	136.29	125.88
4	L	801	GLC	C1-O5-C5	2.90	116.12	112.19
8	H	701	0G7	CB1-CA1-C1	2.87	117.35	111.22
8	H	701	0G7	CB2-CA2-N2	-2.84	105.14	110.88

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	801	GLC	O5-C5-C6-O6
8	H	701	0G7	CA-CB-CG-CD2
8	H	701	0G7	CA-CB-CG-CD1
4	L	801	GLC	C4-C5-C6-O6
8	H	701	0G7	C3-C2-CA2-CB2
8	H	701	0G7	O2-C2-CA2-CB2

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Mol	Chain	Res	Type	Atoms
8	H	701	0G7	N-CA-CB-CG

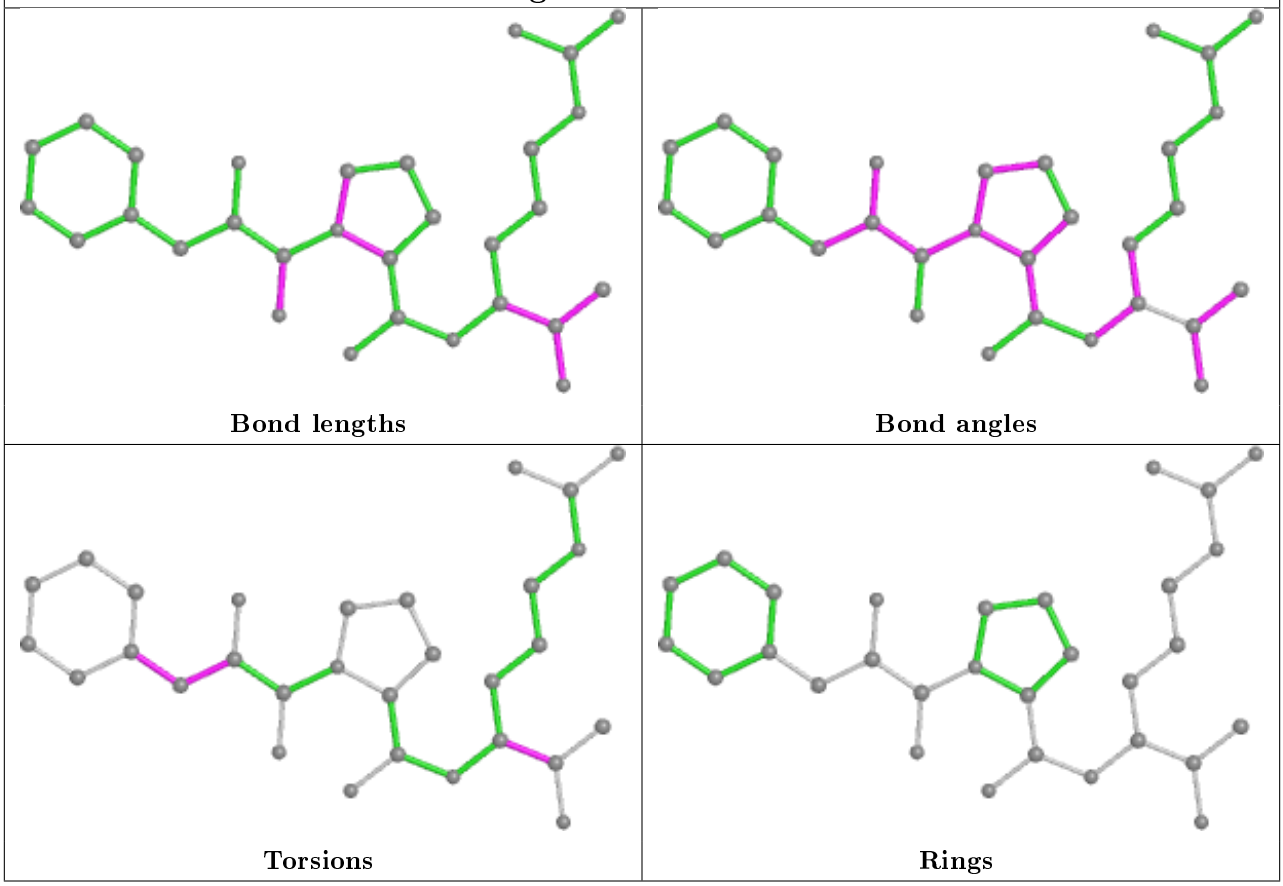
There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	901	FUC	1	0
4	L	801	GLC	1	0
8	H	701	0G7	9	0

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

Ligand 0G7 H 701



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 (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%)	0.14	5 (3%)	40	39	10, 25, 47, 71	0
2	H	254/254 (100%)	-0.15	5 (1%)	65	63	5, 14, 38, 54	0
3	T	191/205 (93%)	-0.07	8 (4%)	36	35	11, 20, 49, 70	0
All	All	577/601 (96%)	-0.06	18 (3%)	49	48	5, 19, 45, 71	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	82	ASN	7.7
1	L	3	ALA	6.8
1	L	1	ALA	6.5
3	T	119	VAL	5.6
1	L	2	ASN	4.6
3	T	137	ASN	4.4
1	L	4	PHE	3.7
1	L	9	ARG	3.6
3	T	81	GLY	3.6
3	T	181	LYS	3.5
3	T	156	TYR	3.0
2	H	248	PRO	2.5
2	H	170(G)	ASP	2.5
3	T	139	THR	2.4
2	H	16	ILE	2.3
3	T	6	THR	2.2
2	H	170(F)	GLY	2.1
2	H	158	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. 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	20	12/13	0.77	0.21	43,50,57,57	0
1	CGU	L	6	12/13	0.79	0.18	34,49,55,55	0
1	CGU	L	35	12/13	0.80	0.23	37,51,56,57	0
1	CGU	L	19	12/13	0.84	0.21	46,48,49,51	0
1	CGU	L	14	12/13	0.85	0.21	35,44,48,51	0
1	CGU	L	7	12/13	0.86	0.17	36,40,51,53	0
1	CGU	L	26	12/13	0.88	0.18	30,34,41,43	0
1	CGU	L	16	12/13	0.90	0.13	30,33,34,34	0
1	CGU	L	29	12/13	0.90	0.14	23,25,29,29	0
1	CGU	L	25	12/13	0.92	0.14	28,37,40,41	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
6	MG	L	1001	1/1	0.43	0.12	37,37,37,37	0
6	MG	L	1007	1/1	0.58	0.19	46,46,46,46	0
7	CA	L	1006	1/1	0.69	0.52	68,68,68,68	0
7	CA	L	1005	1/1	0.79	0.48	61,61,61,61	0
7	CA	L	1002	1/1	0.80	0.25	43,43,43,43	0
4	GLC	L	801	11/12	0.83	0.14	40,42,44,46	0
10	ZN	H	1012	1/1	0.84	0.30	42,42,42,42	0
5	FUC	L	901	10/11	0.85	0.15	34,38,39,40	0
7	CA	L	1003	1/1	0.85	0.44	77,77,77,77	0
6	MG	L	1004	1/1	0.88	0.06	36,36,36,36	0
8	0G7	H	701	30/31	0.90	0.18	10,21,30,33	0
11	CL	H	1013	1/1	0.95	0.12	41,41,41,41	0

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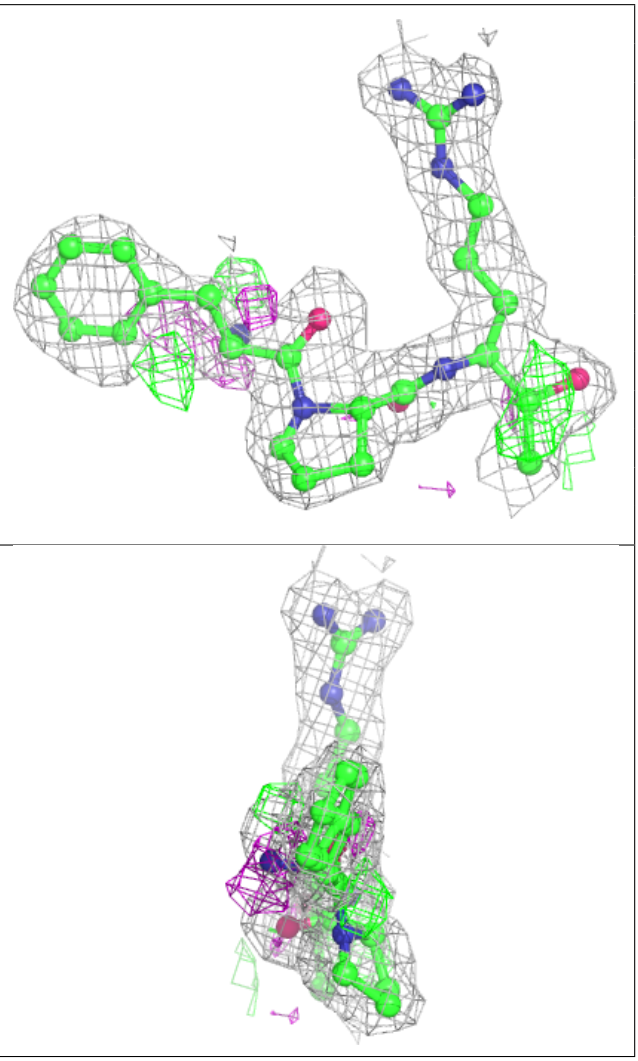
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	ZN	H	1011	1/1	0.96	0.42	49,49,49,49	0
7	CA	H	1009	1/1	0.97	0.04	28,28,28,28	0
11	CL	H	1014	1/1	0.98	0.06	20,20,20,20	0
9	NA	H	1010	1/1	0.99	0.09	27,27,27,27	0
11	CL	T	1015	1/1	0.99	0.07	21,21,21,21	0
7	CA	L	1008	1/1	0.99	0.04	23,23,23,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 0G7 H 701:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.