Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 12:39 AM GMT

PDB ID	:	2B8O
Title	:	Crystal Structure of Glu-Gly-Arg-Chloromethyl Ketone-Factor VIIa/Soluble Tissue Factor Complex
Authors	:	Bajaj, S.P.; Schmidt, A.E.; Padmanabhan, K.
Deposited on	:	2005-10-08
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

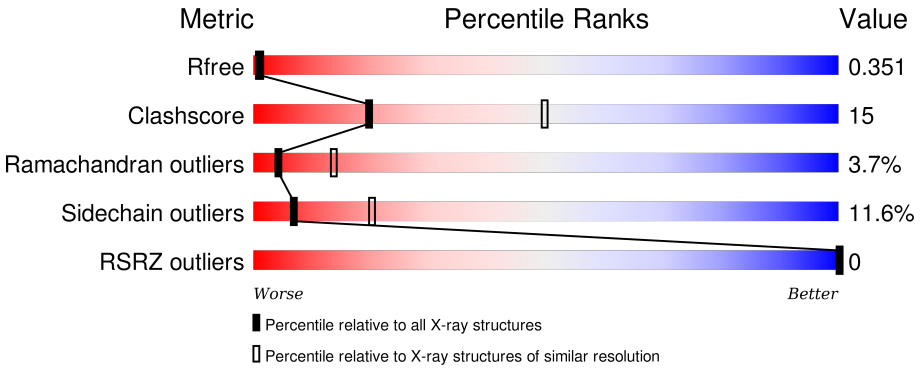
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	59% 35% 6%
2	H	254	64% 30% 6%
3	T	205	57% 32% • • 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	ZN	H	513	-	-	-	X
11	CL	H	514	-	-	X	-
11	CL	H	515	-	-	X	-
4	GLC	L	501	X	-	-	-
5	FUC	L	502	X	-	-	-
8	0GJ	H	1	-	-	-	X
9	NA	H	511	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 4959 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
1	L	142	Total	C	N	O	S	0	0	0
			1135	683	189	248	15			

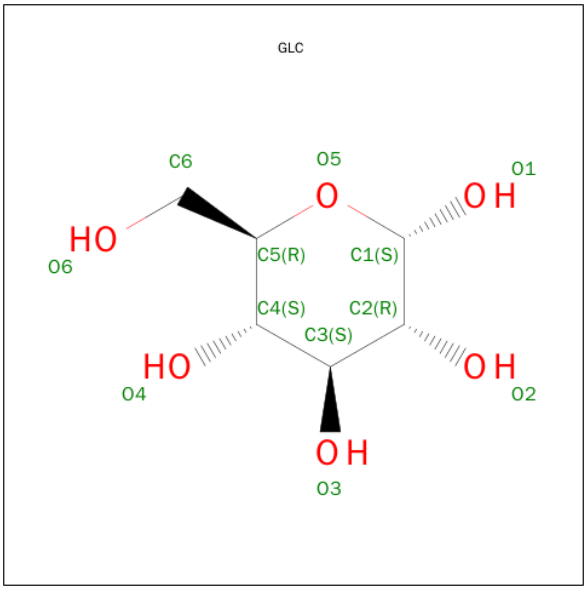
- Molecule 2 is a protein called Coagulation factor VII heavy chain.

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

- Molecule 3 is a protein called Tissue factor.

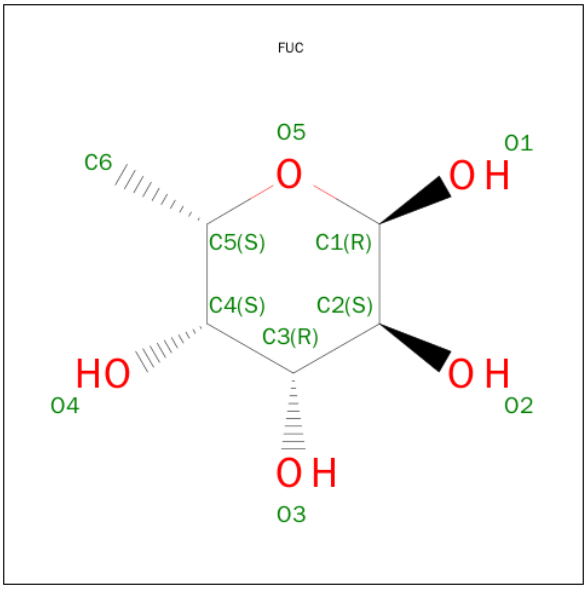
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	191	Total	C	N	O	S	0	0	0
			1551	987	250	309	5			

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



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

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



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

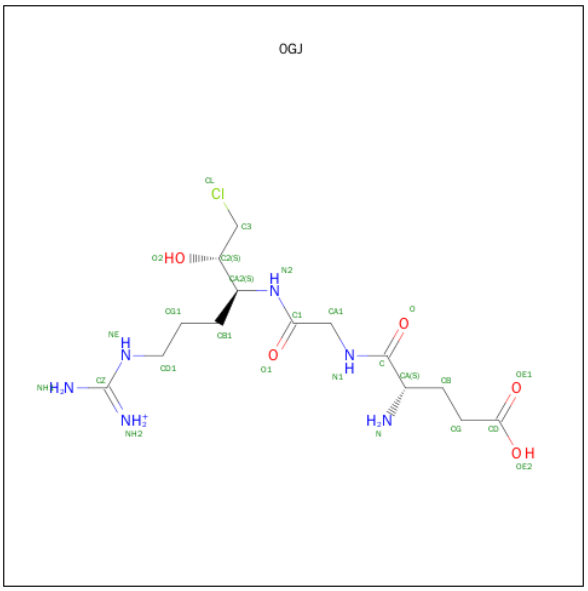
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	2	Total Mg 2 2	0	0

- Molecule 8 is L-ALPHA-GLUTAMYL-N-{(1S)-4-{[AMINO(IMINIO)METHYL]AMINO}-1-[(1S)-2-CHLORO-1-HYDROXYETHYL]BUTYL}GLYCINAMIDE (three-letter code: 0GJ) (formula: $C_{14}H_{28}ClN_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total C N O 25 14 6 5	0	0

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

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

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

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

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

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

- Molecule 12 is water.

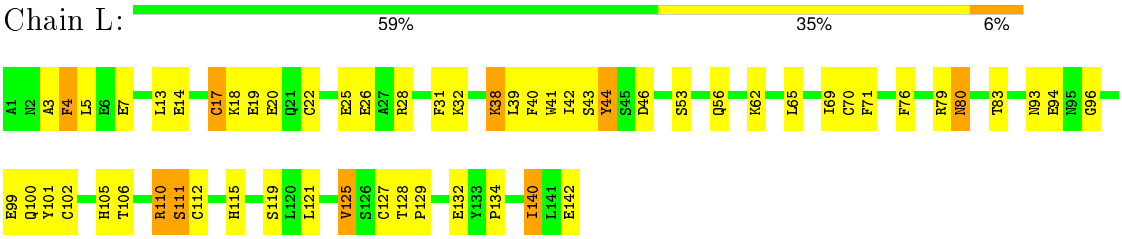
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	L	66	Total O 66 66	0	0
12	H	91	Total O 91 91	0	0
12	T	82	Total O 82 82	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

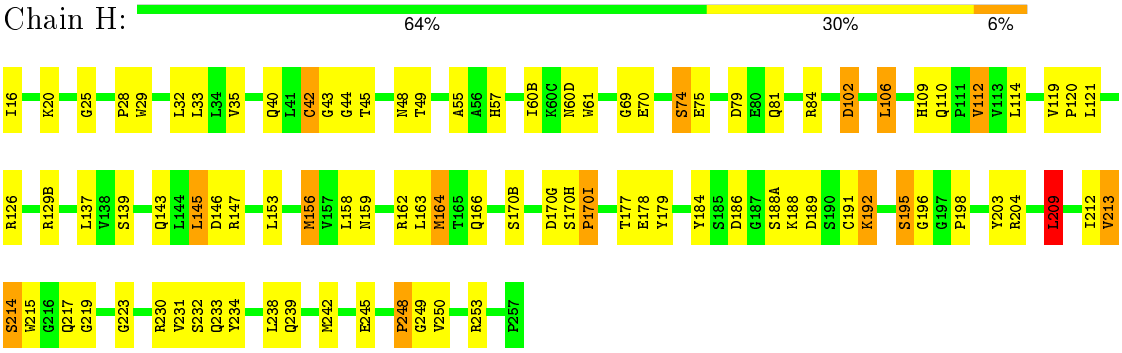
- Molecule 1: Coagulation factor VII light chain

Chain L:



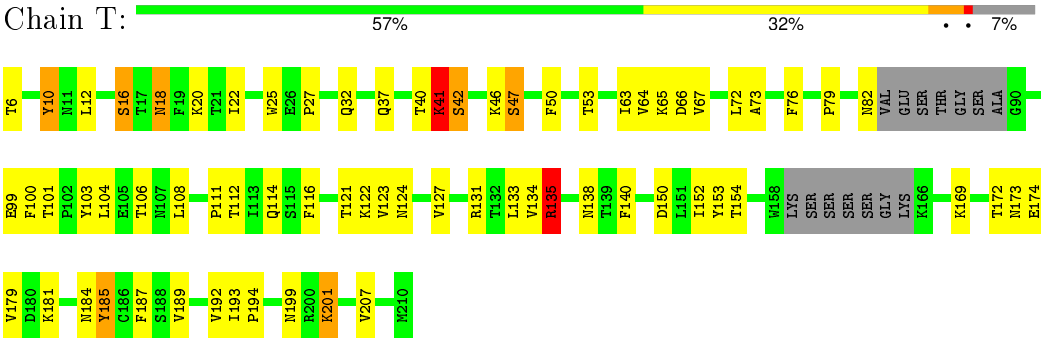
- Molecule 2: Coagulation factor VII heavy chain

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	70.28Å 81.11Å 126.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 40.72 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.80) 54.3 (40.72-2.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.73 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.225 , 0.285 0.211 , 0.351	Depositor DCC
R_{free} test set	1582 reflections (9.76%)	DCC
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.944	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 20351 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4959	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, CL, NA, CA, GLC, 0GJ, MG, 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	0.64	0/1029	0.93	1/1374 (0.1%)
2	H	0.72	0/2024	0.99	1/2755 (0.0%)
3	T	0.72	0/1585	0.99	3/2156 (0.1%)
All	All	0.70	0/4638	0.97	5/6285 (0.1%)

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	0	1
3	T	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	135	ARG	NE-CZ-NH1	6.15	123.37	120.30
3	T	20	LYS	N-CA-C	-5.21	96.93	111.00
1	L	17	CYS	CA-CB-SG	5.15	123.26	114.00
2	H	209	LEU	CA-CB-CG	5.07	126.96	115.30
3	T	66	ASP	N-CA-C	-5.04	97.39	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	44	TYR	Sidechain
3	T	103	TYR	Sidechain

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	987	38	0
2	H	1974	0	1950	60	0
3	T	1551	0	1501	46	0
4	L	11	0	10	0	0
5	L	10	0	10	3	0
6	H	1	0	0	0	0
6	L	5	0	0	0	0
7	L	2	0	0	0	0
8	H	25	0	25	8	0
9	H	1	0	0	0	0
10	H	2	0	0	0	0
11	H	2	0	0	4	0
11	T	1	0	0	1	0
12	H	91	0	0	1	0
12	L	66	0	0	0	0
12	T	82	0	0	3	0
All	All	4959	0	4483	137	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 15.

All (137) 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:1:0GJ:HB3	11:H:514:CL:CL	2.03	0.94
2:H:196:GLY:HA2	2:H:212:ILE:HG23	1.57	0.84
2:H:81:GLN:OE1	2:H:112:VAL:HG12	1.77	0.83
3:T:10:TYR:HD1	3:T:10:TYR:H	1.31	0.79
2:H:44:GLY:HA2	2:H:196:GLY:O	1.86	0.75
3:T:172:THR:HG22	3:T:173:ASN:H	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:101:TYR:OH	1:L:115:HIS:HD2	1.70	0.73
1:L:38:LYS:HD3	1:L:39:LEU:HD22	1.72	0.71
1:L:79:ARG:HE	3:T:22:ILE:HD13	1.55	0.70
2:H:57:HIS:NE2	8:H:1:0GJ:H27	2.06	0.69
3:T:135:ARG:O	3:T:135:ARG:HG3	1.90	0.69
3:T:152:ILE:O	3:T:152:ILE:HG13	1.94	0.68
3:T:192:VAL:HG22	3:T:201:LYS:HB3	1.77	0.67
1:L:99:GLU:HA	2:H:204:ARG:HD2	1.77	0.66
1:L:41:TRP:CZ3	1:L:44:TYR:HD2	2.13	0.65
2:H:143:GLN:HG3	2:H:192:LYS:HG3	1.82	0.61
1:L:13:LEU:HB2	1:L:17:CYS:SG	2.41	0.60
1:L:93:ASN:HB2	3:T:50:PHE:CZ	2.36	0.60
2:H:195:SER:OG	8:H:1:0GJ:C2	2.49	0.60
1:L:79:ARG:HG2	1:L:80:ASN:OD1	2.02	0.60
2:H:32:LEU:HD22	2:H:70:GLU:HG2	1.84	0.59
2:H:162:ARG:HH21	2:H:230:ARG:NH1	1.99	0.59
1:L:62:LYS:HD2	12:T:594:HOH:O	2.02	0.59
5:L:502:FUC:C6	3:T:140:PHE:HE2	2.16	0.58
3:T:76:PHE:HD1	3:T:94:TYR:HB3	1.68	0.57
1:L:17:CYS:O	1:L:20:CGU:O	2.23	0.56
2:H:146:ASP:O	2:H:147:ARG:HB2	2.05	0.56
2:H:231:VAL:HG12	2:H:231:VAL:O	2.05	0.56
1:L:14:CGU:HA	1:L:18:LYS:HB2	1.88	0.55
2:H:110:GLN:HB2	11:H:515:CL:CL	2.43	0.55
1:L:140:ILE:O	1:L:140:ILE:HG12	2.06	0.55
2:H:170(B):SER:HA	2:H:223:GLY:O	2.07	0.55
2:H:239:GLN:HA	2:H:242:MET:HE3	1.88	0.55
3:T:12:LEU:HG	3:T:25:TRP:HB3	1.89	0.55
3:T:123:VAL:HG23	3:T:179:VAL:HG21	1.88	0.54
2:H:203:TYR:CE2	2:H:204:ARG:HG3	2.42	0.54
3:T:47:SER:HB3	3:T:50:PHE:HE1	1.71	0.54
3:T:82:ASN:HB2	12:T:575:HOH:O	2.08	0.54
2:H:234:TYR:O	2:H:238:LEU:HD12	2.08	0.53
1:L:25:CGU:O	1:L:26:CGU:C	2.56	0.53
2:H:55:ALA:HB1	2:H:102:ASP:OD1	2.08	0.53
2:H:184:TYR:CD2	2:H:184:TYR:N	2.77	0.53
1:L:132:GLU:O	1:L:134:PRO:HD3	2.09	0.53
5:L:502:FUC:H61	3:T:140:PHE:CE2	2.43	0.53
3:T:122:LYS:HE2	3:T:176:LEU:HD13	1.91	0.53
2:H:35:VAL:HG13	2:H:35:VAL:O	2.09	0.53
2:H:69:GLY:HA3	2:H:79:ASP:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:116:PHE:HA	3:T:124:ASN:O	2.10	0.52
3:T:18:ASN:O	3:T:133:LEU:HD23	2.09	0.51
2:H:126:ARG:HG3	2:H:232:SER:O	2.10	0.51
3:T:153:TYR:OH	11:T:516:CL:CL	2.53	0.51
2:H:162:ARG:C	2:H:163:LEU:HD12	2.31	0.51
3:T:127:VAL:HG23	3:T:173:ASN:O	2.11	0.51
2:H:158:LEU:HD11	2:H:188:LYS:HB3	1.93	0.50
2:H:162:ARG:NH2	2:H:230:ARG:NH1	2.60	0.50
1:L:110:ARG:C	1:L:110:ARG:HD2	2.32	0.50
3:T:97:SER:HB2	3:T:98:PRO:HD2	1.93	0.50
3:T:10:TYR:O	3:T:12:LEU:HD12	2.12	0.49
2:H:209:LEU:HD13	2:H:231:VAL:HG11	1.94	0.49
2:H:16:ILE:HG13	2:H:156:MET:O	2.10	0.49
3:T:122:LYS:HE3	3:T:178:ASP:OD1	2.12	0.49
2:H:49:THR:O	2:H:112:VAL:HG23	2.12	0.49
5:L:502:FUC:C6	3:T:140:PHE:CE2	2.96	0.49
3:T:40:THR:O	3:T:42:SER:N	2.46	0.49
1:L:112:CYS:SG	1:L:125:VAL:HG12	2.53	0.49
2:H:195:SER:HA	2:H:213:VAL:HB	1.94	0.49
8:H:1:0GJ:CB	11:H:514:CL:CL	2.90	0.48
2:H:195:SER:HG	8:H:1:0GJ:C2	2.26	0.48
1:L:38:LYS:O	1:L:40:PHE:N	2.47	0.48
1:L:56:GLN:HG3	1:L:80:ASN:O	2.14	0.48
2:H:74:SER:HB3	2:H:153:LEU:HD22	1.96	0.48
1:L:14:CGU:O	1:L:19:CGU:HB3	2.14	0.47
3:T:108:LEU:HD11	3:T:193:ILE:HG12	1.97	0.47
2:H:212:ILE:O	2:H:214:SER:N	2.46	0.47
3:T:111:PRO:HB2	3:T:189:VAL:HG23	1.95	0.47
1:L:102:CYS:O	2:H:129(B):ARG:NH2	2.48	0.47
2:H:177:THR:C	2:H:179:TYR:H	2.17	0.47
3:T:187:PHE:O	3:T:207:VAL:HG13	2.15	0.47
2:H:45:THR:OG1	2:H:198:PRO:HG3	2.15	0.47
3:T:185:TYR:CD1	3:T:185:TYR:N	2.82	0.47
1:L:46:ASP:OD1	1:L:65:LEU:HD22	2.15	0.47
2:H:238:LEU:O	2:H:242:MET:HG3	2.15	0.47
2:H:178:GLU:O	2:H:233:GLN:NE2	2.48	0.46
2:H:214:SER:OG	2:H:215:TRP:HD1	1.98	0.46
2:H:33:LEU:HD11	2:H:106:LEU:HD11	1.98	0.46
2:H:162:ARG:O	2:H:163:LEU:HD12	2.16	0.46
2:H:166:GLN:NE2	3:T:94:TYR:CE1	2.83	0.46
3:T:135:ARG:O	3:T:135:ARG:CG	2.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:105:HIS:CE1	1:L:111:SER:OG	2.69	0.45
1:L:71:PHE:CE2	3:T:131:ARG:HG3	2.51	0.45
3:T:6:THR:HG22	3:T:32:GLN:HG2	1.98	0.45
2:H:195:SER:OG	8:H:1:0GJ:O2	2.35	0.45
1:L:76:PHE:HA	1:L:83:THR:O	2.17	0.45
2:H:61:TRP:O	2:H:250:VAL:HG21	2.16	0.45
1:L:31:PHE:O	1:L:32:LYS:HB2	2.17	0.44
3:T:67:VAL:HG22	12:T:545:HOH:O	2.16	0.44
3:T:100:PHE:CD2	3:T:100:PHE:O	2.71	0.44
1:L:3:ALA:H	1:L:7:CGU:CD2	2.30	0.44
2:H:109:HIS:CD2	11:H:515:CL:CL	3.08	0.44
1:L:28:ARG:O	1:L:32:LYS:N	2.49	0.43
1:L:70:CYS:HB2	1:L:79:ARG:O	2.19	0.43
2:H:164:MET:HE2	3:T:94:TYR:CE1	2.53	0.43
2:H:184:TYR:HB3	2:H:186:ASP:OD1	2.19	0.43
3:T:16:SER:HB3	3:T:106:THR:HA	2.00	0.43
3:T:41:LYS:O	3:T:42:SER:HB3	2.18	0.43
2:H:143:GLN:HB3	2:H:145:LEU:O	2.19	0.43
1:L:38:LYS:O	1:L:39:LEU:C	2.57	0.42
2:H:60(B):ILE:HD13	12:H:594:HOH:O	2.19	0.42
2:H:188:LYS:O	2:H:189:ASP:HB2	2.20	0.42
1:L:80:ASN:N	1:L:80:ASN:OD1	2.52	0.42
3:T:192:VAL:HG22	3:T:201:LYS:CB	2.47	0.42
2:H:137:LEU:HA	2:H:158:LEU:O	2.19	0.42
1:L:140:ILE:HD12	2:H:25:GLY:HA3	2.00	0.42
2:H:170(H):SER:HA	2:H:170(I):PRO:HD3	1.84	0.42
1:L:128:THR:HA	1:L:129:PRO:HD3	1.85	0.42
1:L:71:PHE:CZ	3:T:131:ARG:HG3	2.55	0.42
3:T:72:LEU:HD13	3:T:73:ALA:N	2.34	0.41
3:T:140:PHE:CD2	3:T:140:PHE:N	2.88	0.41
2:H:231:VAL:O	2:H:231:VAL:CG1	2.68	0.41
2:H:45:THR:HG21	2:H:121:LEU:HD23	2.03	0.41
1:L:69:ILE:HG22	1:L:71:PHE:CE1	2.55	0.41
3:T:185:TYR:HD1	3:T:185:TYR:N	2.18	0.41
2:H:195:SER:OG	8:H:1:0GJ:H27	2.21	0.41
2:H:219:GLY:O	8:H:1:0GJ:NH1	2.47	0.41
2:H:188(A):SER:C	2:H:188:LYS:HG2	2.41	0.41
3:T:150:ASP:O	3:T:194:PRO:HD2	2.19	0.41
3:T:63:ILE:C	3:T:65:LYS:H	2.24	0.41
1:L:25:CGU:O	1:L:28:ARG:N	2.54	0.41
1:L:110:ARG:O	1:L:110:ARG:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:154:THR:HG22	3:T:169:LYS:HG2	2.03	0.41
1:L:119:SER:O	1:L:127:CYS:HA	2.20	0.41
2:H:162:ARG:NH2	2:H:230:ARG:HH11	2.19	0.41
2:H:57:HIS:CE1	2:H:195:SER:OG	2.74	0.40
1:L:41:TRP:CZ3	1:L:44:TYR:CD2	3.00	0.40
2:H:119:VAL:HA	2:H:120:PRO:HD3	1.89	0.40
2:H:42:CYS:HB3	2:H:43:GLY:H	1.72	0.40
3:T:37:GLN:HA	3:T:46:LYS:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	130/142 (92%)	108 (83%)	18 (14%)	4 (3%)	5 17
2	H	252/254 (99%)	220 (87%)	23 (9%)	9 (4%)	4 14
3	T	185/205 (90%)	160 (86%)	17 (9%)	8 (4%)	3 10
All	All	567/601 (94%)	488 (86%)	58 (10%)	21 (4%)	4 14

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	48	ASN
2	H	195	SER
2	H	248	PRO
3	T	41	LYS
3	T	42	SER
3	T	138	ASN
1	L	4	PHE
2	H	213	VAL
2	H	214	SER

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Mol	Chain	Res	Type
3	T	135	ARG
1	L	106	THR
3	T	184	ASN
1	L	38	LYS
2	H	74	SER
2	H	170(I)	PRO
2	H	102	ASP
3	T	79	PRO
3	T	64	VAL
1	L	96	GLY
2	H	249	GLY
3	T	134	VAL

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%)	99 (87%)	15 (13%)	5	14
2	H	216/216 (100%)	192 (89%)	24 (11%)	8	23
3	T	178/189 (94%)	158 (89%)	20 (11%)	7	22
All	All	508/519 (98%)	449 (88%)	59 (12%)	7	20

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	PHE
1	L	5	LEU
1	L	22	CYS
1	L	42	ILE
1	L	43	SER
1	L	53	SER
1	L	80	ASN
1	L	94	GLU
1	L	100	GLN
1	L	110	ARG

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Mol	Chain	Res	Type
1	L	111	SER
1	L	121	LEU
1	L	125	VAL
1	L	140	ILE
1	L	142	GLU
2	H	20	LYS
2	H	28	PRO
2	H	29	TRP
2	H	40	GLN
2	H	42	CYS
2	H	60(D)	ASN
2	H	75	GLU
2	H	84	ARG
2	H	106	LEU
2	H	112	VAL
2	H	114	LEU
2	H	139	SER
2	H	145	LEU
2	H	156	MET
2	H	159	ASN
2	H	164	MET
2	H	170(G)	ASP
2	H	191	CYS
2	H	192	LYS
2	H	209	LEU
2	H	217	GLN
2	H	245	GLU
2	H	248	PRO
2	H	253	ARG
3	T	10	TYR
3	T	16	SER
3	T	18	ASN
3	T	27	PRO
3	T	41	LYS
3	T	47	SER
3	T	53	THR
3	T	99	GLU
3	T	101	THR
3	T	104	LEU
3	T	112	THR
3	T	114	GLN
3	T	121	THR

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Mol	Chain	Res	Type
3	T	135	ARG
3	T	174	GLU
3	T	176	LEU
3	T	181	LYS
3	T	185	TYR
3	T	199	ASN
3	T	201	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	88	GLN
1	L	115	HIS
2	H	37	ASN
2	H	40	GLN
2	H	63	ASN
2	H	109	HIS
2	H	117	HIS
2	H	143	GLN
2	H	175	ASN
3	T	96	ASN

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	14	1,7	4,11,12	0.84	0	4,14,16	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	CGU	L	16	1,7,6	4,11,12	0.93	0	4,14,16	2.04	2 (50%)
1	CGU	L	19	1,7	4,11,12	0.66	0	4,14,16	0.88	0
1	CGU	L	20	1	4,11,12	0.87	0	4,14,16	1.22	0
1	CGU	L	25	1,6	4,11,12	0.44	0	4,14,16	1.55	1 (25%)
1	CGU	L	26	1,7	4,11,12	0.54	0	4,14,16	1.03	0
1	CGU	L	29	1,6	4,11,12	0.93	0	4,14,16	0.90	0
1	CGU	L	35	1	4,11,12	0.51	0	4,14,16	1.33	1 (25%)
1	CGU	L	6	1,6	4,11,12	0.66	0	4,14,16	0.90	0
1	CGU	L	7	1,6	4,11,12	0.75	0	4,14,16	1.67	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	1,7,6	-	0/4/14/16	0/0/0/0
1	CGU	L	19	1,7	-	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	1,6	-	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	1,6	-	0/4/14/16	0/0/0/0
1	CGU	L	35	1	-	0/4/14/16	0/0/0/0
1	CGU	L	6	1,6	-	0/4/14/16	0/0/0/0
1	CGU	L	7	1,6	-	0/4/14/16	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	16	CGU	O-C-CA	-2.98	117.72	125.49
1	L	7	CGU	CB-CG-CD2	-2.97	106.77	112.83
1	L	16	CGU	CB-CG-CD2	-2.57	107.59	112.83
1	L	25	CGU	O-C-CA	-2.49	119.00	125.49
1	L	35	CGU	O-C-CA	-2.04	120.17	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L	14	CGU	2	0
1	L	19	CGU	1	0
1	L	20	CGU	1	0
1	L	25	CGU	2	0
1	L	26	CGU	1	0
1	L	7	CGU	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 14 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	0GJ	H	1	-	17,24,25	1.66	5 (29%)	20,30,31	1.55	4 (20%)
4	GLC	L	501	1	11,11,12	1.71	3 (27%)	14,15,17	1.46	1 (7%)
5	FUC	L	502	1	10,10,11	1.23	2 (20%)	14,14,16	0.75	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
8	0GJ	H	1	-	-	0/25/29/31	0/0/0/0
4	GLC	L	501	1	1/1/4/5	0/2/19/22	0/1/1/1
5	FUC	L	502	1	1/1/4/5	0/0/17/20	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	1	0GJ	CA1-C1	-3.10	1.42	1.52
4	L	501	GLC	O4-C4	2.00	1.47	1.43
8	H	1	0GJ	CB1-CA2	2.08	1.56	1.52
5	L	502	FUC	C1-C2	2.14	1.57	1.52
5	L	502	FUC	C4-C5	2.22	1.57	1.52
8	H	1	0GJ	C1-N2	2.24	1.38	1.34
4	L	501	GLC	C1-C2	2.34	1.57	1.52
8	H	1	0GJ	CA2-N2	2.41	1.50	1.46
8	H	1	0GJ	O2-C2	2.50	1.48	1.43
4	L	501	GLC	C2-C3	3.79	1.57	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	1	0GJ	C2-CA2-N2	-2.49	105.45	110.11
8	H	1	0GJ	O-C-N1	-2.09	118.90	123.08
8	H	1	0GJ	CB1-CA2-N2	-2.04	107.51	110.41
8	H	1	0GJ	CB-CA-N	3.85	117.88	109.81
4	L	501	GLC	C1-O5-C5	4.28	117.67	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	502	FUC	C1
4	L	501	GLC	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	1	0GJ	8	0
5	L	502	FUC	3	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^{th} 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%)	-0.75	0	100	100	3, 20, 38, 40	0
2	H	254/254 (100%)	-0.74	0	100	100	2, 12, 28, 47	0
3	T	191/205 (93%)	-0.90	0	100	100	3, 17, 34, 40	0
All	All	577/601 (96%)	-0.79	0	100	100	2, 15, 33, 47	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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^{th} 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^2)	Q<0.9
1	CGU	L	25	12/13	0.79	0.18	-	20,33,37,42	0
1	CGU	L	6	12/13	0.71	0.22	-	27,32,39,40	0
1	CGU	L	35	12/13	0.68	0.22	-	40,46,50,51	0
1	CGU	L	14	12/13	0.81	0.14	-	26,41,43,43	0
1	CGU	L	26	12/13	0.87	0.12	-	22,27,36,37	0
1	CGU	L	19	12/13	0.84	0.14	-	29,38,46,47	0
1	CGU	L	16	12/13	0.85	0.10	-	9,12,26,28	0
1	CGU	L	20	12/13	0.78	0.15	-	30,37,45,45	0
1	CGU	L	7	12/13	0.86	0.15	-	21,27,29,30	0
1	CGU	L	29	12/13	0.82	0.12	-	18,22,26,26	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^{th} 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^2)	Q<0.9
10	ZN	H	513	1/1	0.92	0.46	14.65	57,57,57,57	0
9	NA	H	511	1/1	0.59	0.43	10.86	49,49,49,49	0
8	0GJ	H	1	25/26	0.76	0.26	2.77	20,27,34,34	0
5	FUC	L	502	10/11	0.86	0.20	1.45	34,36,38,39	0
6	CA	H	510	1/1	0.96	0.14	1.01	35,35,35,35	0
11	CL	T	516	1/1	0.94	0.11	-0.45	23,23,23,23	0
6	CA	L	509	1/1	0.93	0.05	-2.56	29,29,29,29	0
7	MG	L	508	1/1	0.88	0.06	-	38,38,38,38	0
7	MG	L	505	1/1	0.89	0.14	-	25,25,25,25	0
4	GLC	L	501	11/12	0.54	0.36	-	44,48,51,51	0
11	CL	H	515	1/1	0.98	0.04	-	27,27,27,27	0
6	CA	L	504	1/1	0.67	0.16	-	60,60,60,60	0
11	CL	H	514	1/1	0.87	0.33	-	49,49,49,49	0
6	CA	L	506	1/1	0.90	0.04	-	55,55,55,55	0
6	CA	L	503	1/1	0.74	0.13	-	50,50,50,50	0
6	CA	L	507	1/1	0.81	0.18	-	66,66,66,66	0
10	ZN	H	512	1/1	0.96	0.21	-	44,44,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.