Full wwPDB X-ray Structure Validation Report

Aug 21, 2023 – 02:37 PM EDT

PDB ID	:	2PUQ
Title	:	Crystal structure of active site inhibited coagulation factor VIIA in complex with soluble tissue factor
Authors	:	Bjelke, J.R.; Rasmussen, H.B.
Deposited on	:	2007-05-09
Resolution	:	2.05 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:

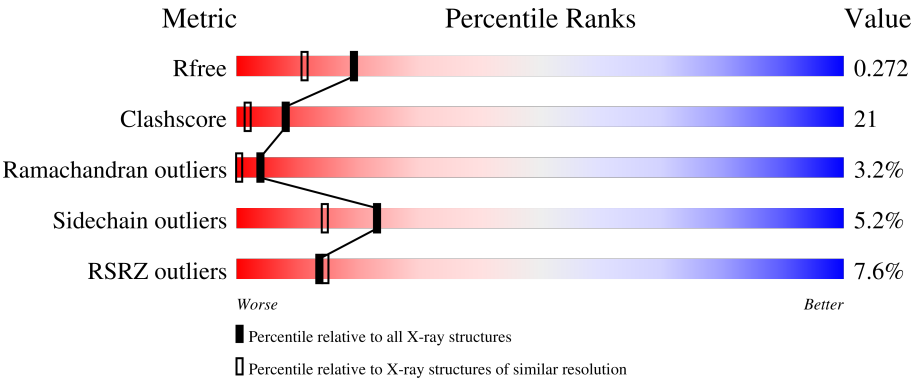
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 <=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	94	5% 71% 22% 5%
2	H	254	2% 67% 24% 8%
3	T	204	16% 56% 30% 6% 7%
4	I	5	20% 20% 40% 20%

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
5	BGC	L	143	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 4306 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	94	Total	C	N	O	S	0	0	0
			695	417	121	144	13			

- 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
			1917	1219	335	350	13			

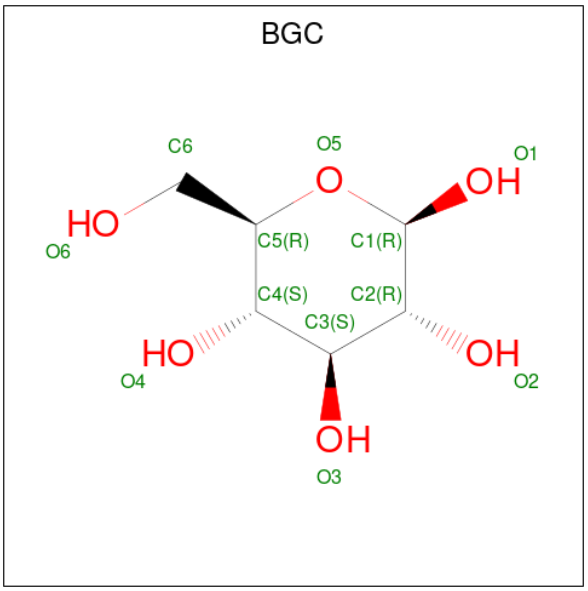
- Molecule 3 is a protein called Tissue factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	190	Total	C	N	O	S	1	0	0
			1454	921	233	296	4			

- Molecule 4 is a protein called TRP-TYR-THR-ARG CHLOROMETHYLKETONE INHIBITOR.

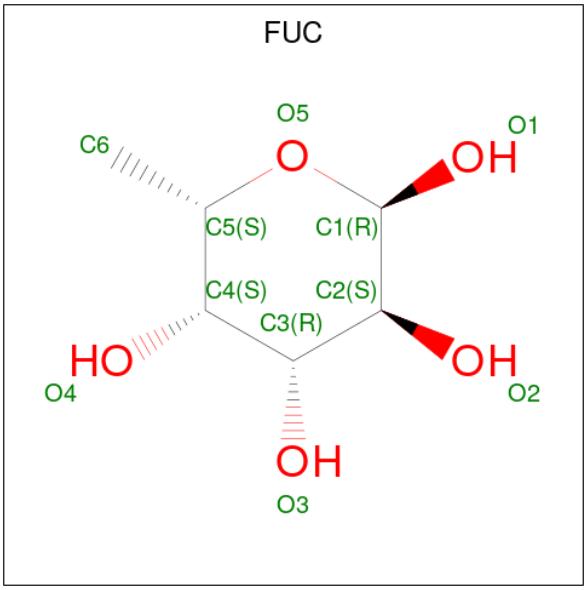
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	4	Total	C	N	O	0	0	1
			31	20	6	5			

- Molecule 5 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



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

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



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

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

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

- Molecule 8 is water.

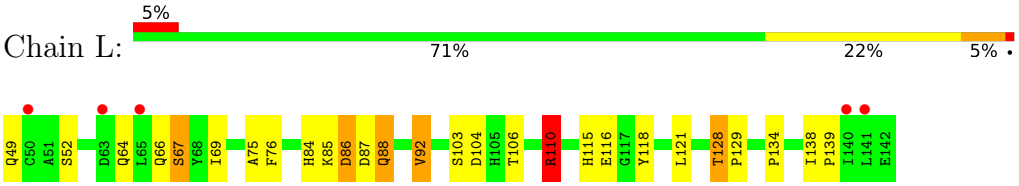
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	27	Total O 27 27	0	0
8	H	103	Total O 103 103	0	0
8	T	56	Total O 56 56	0	0
8	I	1	Total O 1 1	0	0

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.

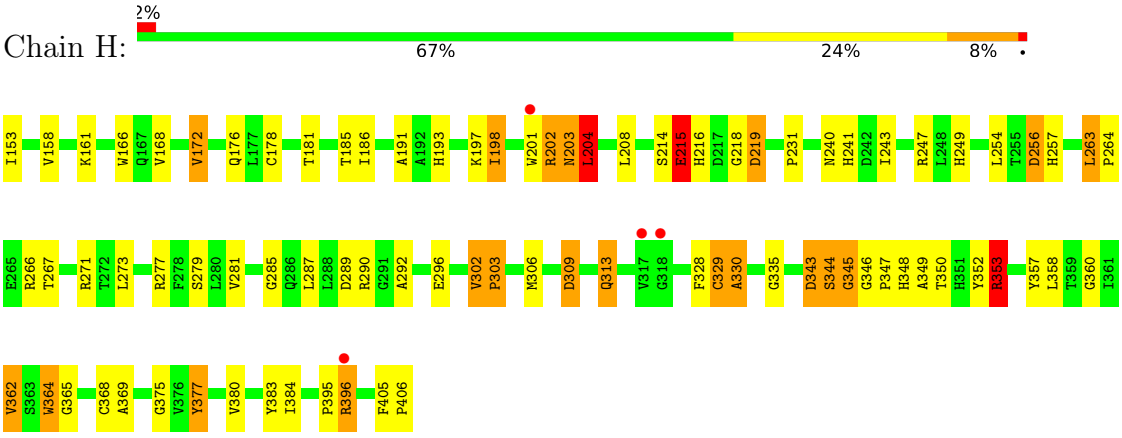
• Molecule 1: Coagulation factor VII

Chain L:



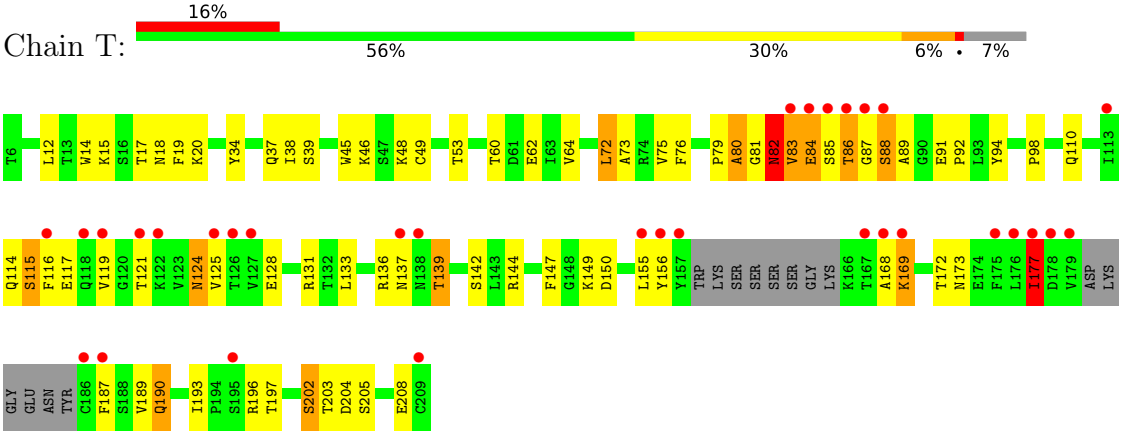
• Molecule 2: Coagulation factor VII

Chain H:



• Molecule 3: Tissue factor

Chain T:



• Molecule 4: TRP-TYR-THR-ARG CHLOROMETHYLKETONE INHIBITOR

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.31Å 68.83Å 78.73Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	39.15 – 2.05 39.15 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.15-2.05) 99.6 (39.15-2.05)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.228 , 0.273 0.229 , 0.272	Depositor DCC
R_{free} test set	2626 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.5	Xtriage
Anisotropy	0.891	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 63.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.036 for h,-k,-l 0.008 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4306	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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: AR7, CA, FUC, 0QE, 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	1.10	1/708 (0.1%)	0.97	3/956 (0.3%)
2	H	1.55	21/1966 (1.1%)	1.41	31/2683 (1.2%)
3	T	1.13	3/1484 (0.2%)	0.99	3/2027 (0.1%)
4	I	1.00	0/19	1.25	0/25
All	All	1.34	25/4177 (0.6%)	1.20	37/5691 (0.7%)

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
2	H	1	5
3	T	0	2
All	All	1	8

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	377	TYR	CD1-CE1	15.02	1.61	1.39
3	T	15	LYS	CE-NZ	-14.46	1.12	1.49
2	H	362	VAL	CB-CG2	13.51	1.81	1.52
2	H	330	ALA	N-CA	12.74	1.71	1.46
2	H	302	VAL	CA-CB	11.63	1.79	1.54
3	T	49	CYS	CB-SG	8.54	1.96	1.82
2	H	329	CYS	CB-SG	7.41	1.94	1.82
2	H	346	GLY	N-CA	7.35	1.57	1.46
2	H	330	ALA	C-O	7.28	1.37	1.23
2	H	303	PRO	CA-CB	-7.20	1.39	1.53
2	H	302	VAL	CB-CG2	-6.87	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	296	GLU	CB-CG	-6.33	1.40	1.52
2	H	313	GLN	CB-CG	-6.16	1.35	1.52
1	L	116	GLU	CD-OE2	5.91	1.32	1.25
2	H	349	ALA	CA-CB	5.76	1.64	1.52
2	H	362	VAL	CA-CB	-5.64	1.43	1.54
2	H	350	THR	CB-OG1	5.54	1.54	1.43
2	H	344	SER	CA-CB	5.43	1.61	1.52
2	H	303	PRO	N-CD	-5.34	1.40	1.47
2	H	178	CYS	CB-SG	5.25	1.91	1.82
2	H	285	GLY	C-O	5.17	1.31	1.23
3	T	75	VAL	CB-CG2	5.13	1.63	1.52
2	H	329	CYS	CA-C	5.09	1.66	1.52
2	H	357	TYR	CE1-CZ	-5.03	1.32	1.38
2	H	328	PHE	CD1-CE1	5.02	1.49	1.39

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	281	VAL	CG1-CB-CG2	-8.77	96.88	110.90
2	H	330	ALA	N-CA-C	-8.59	87.81	111.00
2	H	330	ALA	N-CA-CB	-8.08	98.78	110.10
2	H	343	ASP	CB-CG-OD2	7.29	124.86	118.30
2	H	289	ASP	C-N-CA	-7.13	103.87	121.70
2	H	178	CYS	CA-CB-SG	-6.73	101.89	114.00
2	H	273	LEU	CB-CG-CD1	-6.53	99.89	111.00
2	H	329	CYS	O-C-N	6.40	132.94	122.70
2	H	303	PRO	O-C-N	6.23	132.67	122.70
3	T	72	LEU	CB-CG-CD1	6.18	121.50	111.00
2	H	309	ASP	CB-CG-OD2	6.17	123.85	118.30
2	H	219	ASP	CB-CG-OD2	6.07	123.76	118.30
2	H	329	CYS	CB-CA-C	-6.01	98.38	110.40
2	H	345	GLY	N-CA-C	-5.98	98.15	113.10
2	H	204	LEU	N-CA-C	5.92	126.97	111.00
3	T	80	ALA	N-CA-C	5.86	126.82	111.00
1	L	104	ASP	CB-CG-OD1	5.72	123.45	118.30
2	H	362	VAL	CG1-CB-CG2	-5.72	101.75	110.90
1	L	110	ARG	NE-CZ-NH1	-5.71	117.45	120.30
2	H	266	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	H	343	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	L	92	VAL	CG1-CB-CG2	-5.57	101.98	110.90
2	H	216	HIS	N-CA-C	-5.53	96.08	111.00
2	H	216	HIS	N-CA-CB	5.50	120.50	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	290	ARG	CB-CA-C	5.43	121.25	110.40
2	H	328	PHE	N-CA-CB	-5.36	100.95	110.60
2	H	345	GLY	C-N-CA	-5.33	111.11	122.30
2	H	302	VAL	C-N-CD	-5.29	108.95	120.60
2	H	263	LEU	N-CA-C	-5.20	96.96	111.00
2	H	329	CYS	N-CA-CB	-5.17	101.30	110.60
3	T	88	SER	N-CA-C	5.16	124.93	111.00
2	H	302	VAL	CA-CB-CG1	-5.15	103.17	110.90
2	H	257	HIS	N-CA-CB	5.14	119.85	110.60
2	H	303	PRO	CB-CA-C	-5.13	99.18	112.00
2	H	353	ARG	N-CA-CB	-5.12	101.39	110.60
2	H	303	PRO	CA-C-O	-5.11	107.94	120.20
2	H	186	ILE	CG1-CB-CG2	-5.09	100.21	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	290	ARG	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	203	ASN	Peptide
2	H	215	GLU	Peptide
2	H	218	GLY	Peptide
2	H	256	ASP	Peptide
2	H	364	TRP	Peptide
1	L	86	ASP	Peptide
3	T	79	PRO	Peptide
3	T	82	ASN	Peptide

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	695	0	610	25	0
2	H	1917	0	1840	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	T	1454	0	1359	79	0
4	I	31	0	30	3	0
5	L	11	0	10	1	0
6	L	10	0	10	1	0
7	H	1	0	0	0	0
8	H	103	0	0	4	0
8	I	1	0	0	0	0
8	L	27	0	0	1	0
8	T	56	0	0	5	0
All	All	4306	0	3859	170	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (170) 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:302:VAL:CA	2:H:302:VAL:CB	1.79	1.60
2:H:362:VAL:CB	2:H:362:VAL:CG2	1.81	1.55
2:H:330:ALA:N	2:H:330:ALA:CA	1.71	1.50
2:H:214:SER:O	2:H:215:GLU:HB3	1.57	1.03
3:T:84:GLU:HG3	3:T:85:SER:HB2	1.02	1.01
2:H:365:GLY:O	4:I:1:TYR:HB2	1.61	1.01
2:H:353:ARG:NH2	8:H:1075:HOH:O	1.96	0.98
2:H:158:VAL:O	8:H:1082:HOH:O	1.80	0.98
3:T:114:GLN:HG2	3:T:128:GLU:HB2	1.46	0.95
3:T:84:GLU:CG	3:T:85:SER:HB2	1.96	0.94
3:T:84:GLU:HG3	3:T:85:SER:CB	1.96	0.93
3:T:124:ASN:O	3:T:124:ASN:ND2	2.03	0.92
2:H:330:ALA:N	2:H:330:ALA:C	2.24	0.90
2:H:302:VAL:CA	2:H:302:VAL:CG2	2.53	0.86
3:T:87:GLY:H	3:T:88:SER:HB2	1.39	0.86
3:T:46:LYS:HD3	3:T:62:GLU:OE2	1.76	0.85
2:H:302:VAL:CA	2:H:302:VAL:CG1	2.56	0.83
1:L:64:GLN:N	1:L:67:SER:O	2.12	0.82
3:T:86:THR:HG22	3:T:89:ALA:H	1.42	0.82
2:H:405:PHE:HA	2:H:406:PRO:C	2.02	0.80
1:L:76:PHE:HE1	1:L:84:HIS:CD2	1.99	0.80
2:H:330:ALA:N	2:H:330:ALA:CB	2.43	0.80
2:H:362:VAL:CG2	2:H:362:VAL:CG1	2.58	0.80
1:L:49:GLN:O	5:L:143:BGC:O6	1.99	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:87:GLY:N	3:T:88:SER:HB2	1.98	0.78
3:T:91:GLU:HB3	3:T:92:PRO:HD2	1.65	0.77
3:T:86:THR:HG23	3:T:88:SER:HB2	1.68	0.75
3:T:83:VAL:O	3:T:84:GLU:HB3	1.87	0.74
3:T:187:PHE:HB2	3:T:208:GLU:O	1.86	0.74
3:T:83:VAL:O	3:T:84:GLU:CB	2.35	0.74
2:H:214:SER:O	2:H:215:GLU:CB	2.33	0.73
2:H:362:VAL:CG2	2:H:362:VAL:CA	2.64	0.73
3:T:80:ALA:HB3	3:T:81:GLY:HA3	1.69	0.73
3:T:80:ALA:CB	3:T:81:GLY:HA3	2.19	0.73
2:H:329:CYS:C	2:H:330:ALA:CA	2.57	0.72
3:T:86:THR:HG22	3:T:89:ALA:N	2.05	0.71
3:T:82:ASN:HA	3:T:83:VAL:HG22	1.73	0.71
1:L:49:GLN:NE2	1:L:67:SER:HA	2.05	0.71
3:T:147:PHE:O	3:T:150:ASP:HB2	1.91	0.70
3:T:202:SER:OG	3:T:203:THR:N	2.21	0.70
2:H:303:PRO:O	2:H:330:ALA:HA	1.92	0.70
3:T:86:THR:CG2	3:T:88:SER:HB2	2.23	0.69
2:H:335:GLY:HA2	2:H:369:ALA:O	1.93	0.69
3:T:48:LYS:HE3	3:T:62:GLU:CG	2.22	0.69
2:H:191:ALA:HB2	2:H:345:GLY:HA2	1.76	0.67
1:L:92:VAL:HG12	1:L:92:VAL:O	1.95	0.66
2:H:302:VAL:CB	2:H:302:VAL:N	2.54	0.66
3:T:86:THR:N	3:T:91:GLU:O	2.28	0.66
3:T:81:GLY:C	3:T:82:ASN:HD22	1.99	0.65
2:H:330:ALA:N	2:H:330:ALA:O	2.29	0.65
3:T:86:THR:CG2	3:T:88:SER:CB	2.75	0.65
2:H:153:ILE:N	2:H:343:ASP:OD2	2.30	0.64
3:T:137:ASN:O	3:T:139:THR:HG23	1.98	0.64
2:H:279:SER:HB2	2:H:348:HIS:CE1	2.32	0.64
3:T:189:VAL:HG23	3:T:205:SER:HB3	1.78	0.64
2:H:309:ASP:O	2:H:313:GLN:HG3	1.98	0.64
3:T:88:SER:OG	8:T:265:HOH:O	2.09	0.63
2:H:368:CYS:O	2:H:369:ALA:HB3	1.97	0.63
2:H:302:VAL:CB	2:H:302:VAL:C	2.66	0.63
2:H:396:ARG:HH11	2:H:396:ARG:HB3	1.63	0.63
3:T:34:TYR:HA	3:T:76:PHE:O	1.99	0.63
1:L:139:PRO:HD2	8:H:1043:HOH:O	1.99	0.62
3:T:86:THR:OG1	8:T:229:HOH:O	2.07	0.61
3:T:18:ASN:O	3:T:19:PHE:HB2	2.01	0.61
3:T:60:THR:O	3:T:64:VAL:HG22	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:329:CYS:HA	2:H:375:GLY:O	2.00	0.61
2:H:267:THR:O	2:H:271:ARG:HB2	2.00	0.61
1:L:115:HIS:O	1:L:118:TYR:HB2	2.02	0.60
3:T:82:ASN:HD22	3:T:82:ASN:N	2.00	0.60
3:T:86:THR:HG23	3:T:88:SER:CB	2.32	0.59
1:L:76:PHE:CE1	1:L:84:HIS:CD2	2.88	0.59
3:T:20:LYS:HB2	3:T:133:LEU:CD2	2.33	0.58
2:H:176:GLN:OE1	8:H:1020:HOH:O	2.17	0.58
3:T:114:GLN:CG	3:T:128:GLU:HB2	2.28	0.58
2:H:365:GLY:O	4:I:1:TYR:CB	2.45	0.57
2:H:193:HIS:CE1	2:H:344:SER:OG	2.55	0.57
1:L:92:VAL:HG22	2:H:271:ARG:HG2	1.85	0.57
2:H:264:PRO:O	2:H:384:ILE:HD13	2.05	0.57
1:L:129:PRO:HB3	1:L:134:PRO:HG3	1.88	0.56
3:T:37:GLN:O	3:T:73:ALA:HA	2.06	0.55
2:H:279:SER:CB	2:H:348:HIS:CE1	2.89	0.55
3:T:46:LYS:CD	3:T:62:GLU:OE2	2.51	0.55
2:H:405:PHE:CG	2:H:406:PRO:HA	2.42	0.55
3:T:168:ALA:O	3:T:169:LYS:HB2	2.06	0.55
2:H:302:VAL:H	2:H:302:VAL:HG22	1.71	0.55
3:T:39:SER:HB3	3:T:45:TRP:CE3	2.42	0.55
2:H:405:PHE:CD1	2:H:406:PRO:HA	2.41	0.54
2:H:306:MET:CE	3:T:91:GLU:HB3	2.38	0.54
3:T:48:LYS:HE3	3:T:62:GLU:HG2	1.89	0.53
3:T:114:GLN:O	3:T:115:SER:HB3	2.08	0.53
3:T:80:ALA:CB	3:T:81:GLY:CA	2.86	0.52
2:H:364:TRP:HE3	2:H:365:GLY:H	1.57	0.52
3:T:86:THR:HG22	3:T:88:SER:CB	2.39	0.52
3:T:86:THR:CG2	3:T:88:SER:HB3	2.39	0.52
3:T:48:LYS:HE3	3:T:62:GLU:CD	2.31	0.52
1:L:92:VAL:HG13	8:L:157:HOH:O	2.09	0.52
2:H:302:VAL:CG2	2:H:302:VAL:N	2.73	0.51
3:T:155:LEU:HD23	3:T:177:ILE:HD11	1.92	0.51
1:L:110:ARG:HD2	1:L:110:ARG:C	2.31	0.51
2:H:181:THR:OG1	2:H:347:PRO:HG3	2.11	0.51
2:H:185:THR:HG22	2:H:254:LEU:HD21	1.91	0.51
1:L:92:VAL:O	1:L:92:VAL:CG1	2.59	0.50
1:L:121:LEU:HD21	1:L:128:THR:HB	1.93	0.50
2:H:201:TRP:O	2:H:203:ASN:N	2.44	0.50
2:H:358:LEU:HG	2:H:380:VAL:HG21	1.93	0.50
3:T:76:PHE:CE1	3:T:92:PRO:HG2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:377:TYR:CD1	2:H:377:TYR:N	2.80	0.50
1:L:85:LYS:O	1:L:87:ASP:N	2.41	0.50
3:T:116:PHE:O	3:T:117:GLU:C	2.50	0.50
2:H:306:MET:HE1	3:T:92:PRO:HD2	1.95	0.49
3:T:86:THR:CG2	8:T:229:HOH:O	2.60	0.49
3:T:82:ASN:CA	3:T:83:VAL:HG22	2.43	0.49
3:T:114:GLN:HG2	3:T:128:GLU:CB	2.31	0.49
3:T:189:VAL:O	3:T:204:ASP:HA	2.13	0.49
1:L:85:LYS:C	1:L:87:ASP:H	2.16	0.48
1:L:85:LYS:HA	1:L:88:GLN:HE21	1.78	0.48
3:T:72:LEU:HD13	3:T:73:ALA:O	2.13	0.48
3:T:86:THR:HG21	8:T:229:HOH:O	2.12	0.48
1:L:110:ARG:HD2	1:L:110:ARG:O	2.14	0.48
3:T:144:ARG:HG3	3:T:173:ASN:HD21	1.77	0.48
1:L:69:ILE:HD11	3:T:17:THR:HB	1.96	0.47
3:T:114:GLN:O	3:T:115:SER:CB	2.61	0.47
2:H:343:ASP:O	2:H:344:SER:C	2.52	0.47
2:H:352:TYR:CE2	2:H:353:ARG:HG3	2.49	0.47
2:H:302:VAL:N	2:H:302:VAL:HG22	2.30	0.47
3:T:12:LEU:N	3:T:12:LEU:HD12	2.29	0.47
1:L:138:ILE:HA	1:L:139:PRO:HD3	1.76	0.46
2:H:161:LYS:CE	2:H:219:ASP:OD2	2.64	0.46
2:H:153:ILE:HG12	2:H:343:ASP:OD2	2.15	0.46
2:H:247:ARG:NH1	2:H:395:PRO:HG3	2.31	0.46
3:T:124:ASN:ND2	3:T:124:ASN:C	2.69	0.46
2:H:201:TRP:O	2:H:202:ARG:C	2.54	0.46
3:T:76:PHE:HD1	3:T:92:PRO:HB2	1.81	0.46
3:T:114:GLN:O	3:T:114:GLN:CD	2.54	0.45
3:T:144:ARG:HG3	3:T:173:ASN:ND2	2.32	0.45
3:T:53:THR:HG22	8:T:215:HOH:O	2.17	0.45
1:L:66:GLN:O	1:L:67:SER:HB3	2.16	0.45
1:L:69:ILE:O	1:L:69:ILE:HG22	2.16	0.45
2:H:240:ASN:O	2:H:241:HIS:HB2	2.18	0.44
2:H:263:LEU:HD12	2:H:263:LEU:HA	1.62	0.44
2:H:279:SER:HB2	2:H:348:HIS:NE2	2.33	0.44
2:H:168:VAL:HG22	2:H:208:LEU:HD11	1.99	0.44
3:T:14:TRP:CD1	3:T:98:PRO:HG2	2.54	0.43
2:H:193:HIS:CD2	4:I:2:THR:HG23	2.54	0.43
3:T:189:VAL:HB	3:T:190:GLN:H	1.64	0.43
3:T:190:GLN:HE21	3:T:190:GLN:HB2	1.49	0.43
3:T:81:GLY:CA	3:T:82:ASN:HD22	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:144:FUC:C1	3:T:131:ARG:HH22	2.32	0.42
3:T:76:PHE:CD1	3:T:94:TYR:HB3	2.54	0.42
3:T:136:ARG:O	3:T:137:ASN:HB2	2.19	0.42
3:T:82:ASN:N	3:T:82:ASN:ND2	2.68	0.42
3:T:110:GLN:HB2	3:T:203:THR:HG23	2.01	0.42
2:H:302:VAL:CG1	2:H:302:VAL:N	2.81	0.42
2:H:172:VAL:HG11	2:H:198:ILE:CD1	2.50	0.42
2:H:197:LYS:O	2:H:198:ILE:C	2.58	0.42
2:H:303:PRO:O	2:H:330:ALA:CA	2.66	0.42
3:T:156:TYR:CD2	3:T:156:TYR:N	2.88	0.41
2:H:302:VAL:CG2	2:H:302:VAL:H	2.32	0.41
3:T:38:ILE:HG12	3:T:39:SER:N	2.35	0.41
3:T:86:THR:HG22	3:T:88:SER:HB3	2.01	0.41
1:L:75:ALA:O	1:L:85:LYS:HB2	2.21	0.41
1:L:129:PRO:HB3	1:L:134:PRO:CG	2.50	0.41
3:T:193:ILE:HB	3:T:196:ARG:HD2	2.02	0.41
2:H:360:GLY:HA2	2:H:380:VAL:HG23	2.02	0.41
1:L:85:LYS:C	1:L:87:ASP:N	2.74	0.41
2:H:231:PRO:HD3	2:H:243:ILE:O	2.21	0.41
2:H:287:LEU:HD12	2:H:292:ALA:O	2.21	0.40
2:H:201:TRP:C	2:H:203:ASN:N	2.74	0.40
2:H:241:HIS:HA	2:H:383:TYR:OH	2.22	0.40
2:H:277:ARG:O	2:H:303:PRO:HA	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	92/94 (98%)	83 (90%)	6 (6%)	3 (3%)	4 0
2	H	252/254 (99%)	228 (90%)	18 (7%)	6 (2%)	6 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	T	184/204 (90%)	155 (84%)	21 (11%)	8 (4%)	2 0
4	I	1/5 (20%)	1 (100%)	0	0	100 100
All	All	529/557 (95%)	467 (88%)	45 (8%)	17 (3%)	4 0

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	198	ILE
2	H	215	GLU
2	H	256	ASP
3	T	83	VAL
3	T	84	GLU
3	T	115	SER
3	T	202	SER
1	L	86	ASP
2	H	202	ARG
2	H	353	ARG
3	T	169	LYS
1	L	67	SER
3	T	149	LYS
1	L	106	THR
2	H	204	LEU
3	T	119	VAL
3	T	177	ILE

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	78/82 (95%)	73 (94%)	5 (6%)	17 9
2	H	203/216 (94%)	198 (98%)	5 (2%)	47 40
3	T	161/188 (86%)	150 (93%)	11 (7%)	16 8
4	I	2/3 (67%)	0	2 (100%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	444/489 (91%)	421 (95%)	23 (5%)	23 14

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

Mol	Chain	Res	Type
1	L	52	SER
1	L	88	GLN
1	L	103	SER
1	L	110	ARG
1	L	128	THR
2	H	166	TRP
2	H	172	VAL
2	H	204	LEU
2	H	249	HIS
2	H	396	ARG
3	T	82	ASN
3	T	86	THR
3	T	121	THR
3	T	124	ASN
3	T	125	VAL
3	T	139	THR
3	T	142	SER
3	T	172	THR
3	T	177	ILE
3	T	190	GLN
3	T	197	THR
4	I	1	TYR
4	I	2	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	49	GLN
1	L	80	ASN
1	L	84	HIS
1	L	88	GLN
1	L	115	HIS
2	H	176	GLN
2	H	286	GLN
2	H	308	GLN
2	H	373	HIS

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Mol	Chain	Res	Type
3	T	82	ASN
3	T	173	ASN
3	T	190	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)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
4	AR7	I	3	2,4	10,10,11	1.87	3 (30%)	9,11,13	1.81	1 (11%)

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
4	AR7	I	3	2,4	-	1/9/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	3	AR7	C-CA	4.19	1.59	1.52
4	I	3	AR7	O-C	-3.10	1.29	1.42
4	I	3	AR7	CB-CA	2.40	1.56	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	3	AR7	CB-CA-C	-4.93	105.51	112.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	3	AR7	O-C-CA-N

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
6	FUC	L	144	1	10,10,11	0.72	0	14,14,16	1.51	2 (14%)
5	BGC	L	143	1	11,11,12	0.80	0	15,15,17	1.92	4 (26%)

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
6	FUC	L	144	1	-	-	0/1/1/1
5	BGC	L	143	1	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	143	BGC	O5-C5-C6	3.73	113.05	107.20
6	L	144	FUC	C2-C3-C4	-3.53	104.78	110.89
5	L	143	BGC	C1-O5-C5	3.30	116.66	112.19
5	L	143	BGC	O4-C4-C5	2.85	116.38	109.30
6	L	144	FUC	O5-C5-C6	2.16	111.97	107.33
5	L	143	BGC	O5-C5-C4	-2.06	105.81	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	143	BGC	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	144	FUC	1	0
5	L	143	BGC	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	94/94 (100%)	0.23	5 (5%) 26 28	15, 38, 73, 84	0
2	H	254/254 (100%)	0.21	4 (1%) 72 74	4, 28, 62, 82	4 (1%)
3	T	190/204 (93%)	0.96	32 (16%) 1 1	12, 50, 99, 112	6 (3%)
4	I	2/5 (40%)	0.77	0 100 100	33, 33, 33, 49	0
All	All	540/557 (96%)	0.48	41 (7%) 13 14	4, 34, 88, 112	10 (1%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	T	119	VAL	8.7
3	T	186	CYS	8.7
3	T	209	CYS	8.5
3	T	116	PHE	5.6
3	T	87	GLY	5.0
3	T	157	TYR	4.7
3	T	179	VAL	4.6
3	T	125	VAL	4.5
3	T	121	THR	4.2
3	T	83	VAL	4.1
3	T	88	SER	4.1
3	T	178	ASP	4.0
3	T	187	PHE	3.8
1	L	50	CYS	3.7
1	L	65	LEU	3.6
2	H	396	ARG	3.5
3	T	85	SER	3.4
3	T	86	THR	3.4
3	T	156	TYR	3.3
3	T	113	ILE	3.2
2	H	201	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
3	T	126	THR	2.9
3	T	138	ASN	2.8
3	T	168	ALA	2.8
2	H	318	GLY	2.7
3	T	177	ILE	2.7
3	T	175	PHE	2.6
3	T	155	LEU	2.6
1	L	63	ASP	2.6
3	T	195	SER	2.6
3	T	127	VAL	2.5
3	T	118	GLN	2.5
3	T	167	THR	2.4
3	T	137	ASN	2.4
3	T	122	LYS	2.4
3	T	84	GLU	2.4
3	T	176	LEU	2.3
1	L	140	ILE	2.3
2	H	317	VAL	2.3
3	T	169	LYS	2.2
1	L	141	LEU	2.2

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, 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	B-factors(Å^2)	Q<0.9
4	AR7	I	3	11/12	0.91	0.15	22,24,30,31	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, 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	B-factors(Å^2)	Q<0.9
5	BGC	L	143	11/12	0.75	0.21	71,72,74,76	0
6	FUC	L	144	10/11	0.94	0.10	64,66,66,66	0
7	CA	H	1001	1/1	0.99	0.07	60,60,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.