Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2023 – 05:10 PM EDT

PDB ID	:	6W9R
Title	:	Crystal structure of an OTU deubiquitinase from Wolbachia pipientis wMel bound to ubiquitin
Authors	:	Schubert, A.F.; Pruneda, J.N.; Komander, D.
Deposited on	:	2020-03-23
Resolution	:	1.82 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:

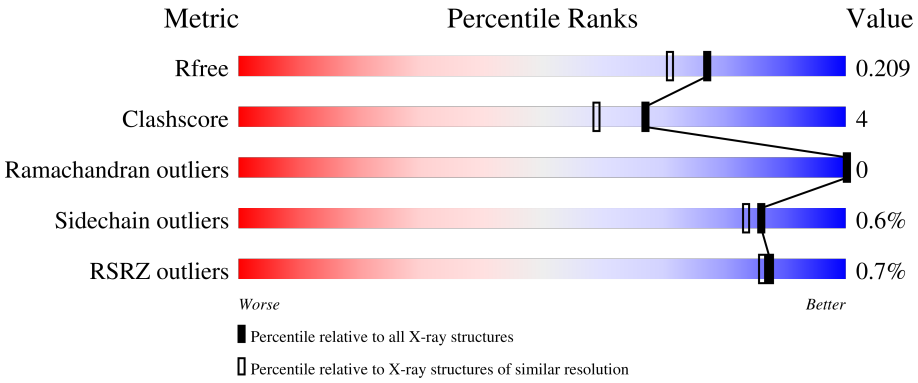
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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 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	M	78	95% . .
1	N	78	94% . .
1	O	78	88% 9% .
1	P	78	91% 6% .
1	Q	78	91% 6% .

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Mol	Chain	Length	Quality of chain
1	R	78	91% 6%
1	S	78	94%
1	T	78	94%
1	U	78	4% 85% 13%
1	V	78	96%
1	W	78	5% 73% 24%
1	X	78	91% 6%
2	A	168	86% 10%
2	B	168	90% 7%
2	C	168	88% 8%
2	D	168	90% 6%
2	E	168	88% 8%
2	F	168	89% 7%
2	G	168	88% 8%
2	H	168	89% 7%
2	I	168	80% 15%
2	J	168	89% 8%
2	K	168	83% 12%
2	L	168	89% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26594 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 Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	76	Total	C	N	O	S	0	1	0
			599	377	104	117	1			
1	N	76	Total	C	N	O	S	0	0	0
			600	378	105	116	1			
1	O	76	Total	C	N	O	S	0	0	0
			592	373	103	115	1			
1	P	76	Total	C	N	O	S	0	0	0
			600	378	105	116	1			
1	Q	76	Total	C	N	O	S	0	1	0
			603	380	105	117	1			
1	R	76	Total	C	N	O	S	0	1	0
			601	379	104	117	1			
1	S	76	Total	C	N	O	S	0	0	0
			596	375	104	116	1			
1	T	76	Total	C	N	O	S	0	0	0
			592	372	103	116	1			
1	U	76	Total	C	N	O	S	0	0	0
			592	373	104	114	1			
1	V	76	Total	C	N	O	S	0	0	0
			600	378	105	116	1			
1	W	76	Total	C	N	O	S	0	0	0
			584	368	103	112	1			
1	X	76	Total	C	N	O	S	0	0	0
			596	375	104	116	1			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-1	GLY	-	expression tag	UNP P0CG48
M	0	PRO	-	expression tag	UNP P0CG48
M	76	NEH	-	amidation	UNP P0CG48
N	-1	GLY	-	expression tag	UNP P0CG48
N	0	PRO	-	expression tag	UNP P0CG48

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Chain	Residue	Modelled	Actual	Comment	Reference
N	76	NEH	-	amidation	UNP P0CG48
O	-1	GLY	-	expression tag	UNP P0CG48
O	0	PRO	-	expression tag	UNP P0CG48
O	76	NEH	-	amidation	UNP P0CG48
P	-1	GLY	-	expression tag	UNP P0CG48
P	0	PRO	-	expression tag	UNP P0CG48
P	76	NEH	-	amidation	UNP P0CG48
Q	-1	GLY	-	expression tag	UNP P0CG48
Q	0	PRO	-	expression tag	UNP P0CG48
Q	76	NEH	-	amidation	UNP P0CG48
R	-1	GLY	-	expression tag	UNP P0CG48
R	0	PRO	-	expression tag	UNP P0CG48
R	76	NEH	-	amidation	UNP P0CG48
S	-1	GLY	-	expression tag	UNP P0CG48
S	0	PRO	-	expression tag	UNP P0CG48
S	76	NEH	-	amidation	UNP P0CG48
T	-1	GLY	-	expression tag	UNP P0CG48
T	0	PRO	-	expression tag	UNP P0CG48
T	76	NEH	-	amidation	UNP P0CG48
U	-1	GLY	-	expression tag	UNP P0CG48
U	0	PRO	-	expression tag	UNP P0CG48
U	76	NEH	-	amidation	UNP P0CG48
V	-1	GLY	-	expression tag	UNP P0CG48
V	0	PRO	-	expression tag	UNP P0CG48
V	76	NEH	-	amidation	UNP P0CG48
W	-1	GLY	-	expression tag	UNP P0CG48
W	0	PRO	-	expression tag	UNP P0CG48
W	76	NEH	-	amidation	UNP P0CG48
X	-1	GLY	-	expression tag	UNP P0CG48
X	0	PRO	-	expression tag	UNP P0CG48
X	76	NEH	-	amidation	UNP P0CG48

- Molecule 2 is a protein called OTU domain-containing protein wMelOTU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	162	Total	C	N	O	S	0	3	0
			1309	806	238	261	4			
2	B	163	Total	C	N	O	S	0	4	0
			1317	810	239	264	4			
2	C	163	Total	C	N	O	S	0	2	0
			1306	804	236	262	4			
2	D	162	Total	C	N	O	S	0	2	0
			1307	804	236	263	4			

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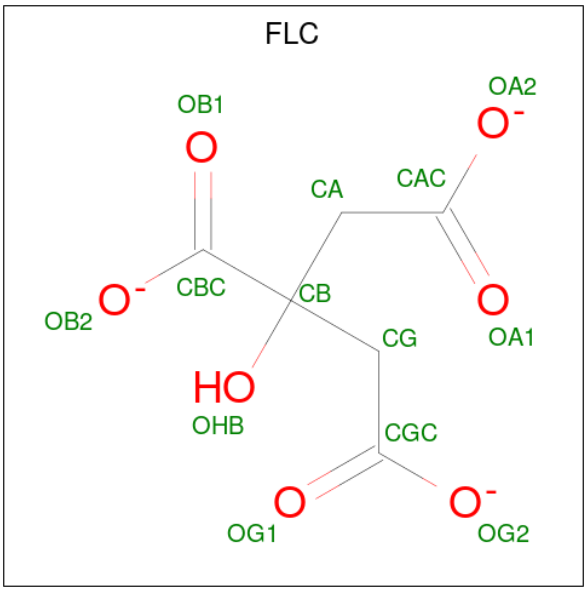
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	162	Total	C	N	O	S	0	2	0
			1305	804	238	259	4			
2	F	161	Total	C	N	O	S	0	3	0
			1304	802	237	261	4			
2	G	163	Total	C	N	O	S	0	2	0
			1302	800	239	259	4			
2	H	162	Total	C	N	O	S	0	2	0
			1303	801	237	261	4			
2	I	161	Total	C	N	O	S	0	2	0
			1298	799	234	261	4			
2	J	163	Total	C	N	O	S	0	3	0
			1310	805	238	263	4			
2	K	161	Total	C	N	O	S	0	2	0
			1283	792	230	257	4			
2	L	163	Total	C	N	O	S	0	3	0
			1308	806	239	259	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLY	-	expression tag	UNP Q73HU7
B	38	GLY	-	expression tag	UNP Q73HU7
C	38	GLY	-	expression tag	UNP Q73HU7
D	38	GLY	-	expression tag	UNP Q73HU7
E	38	GLY	-	expression tag	UNP Q73HU7
F	38	GLY	-	expression tag	UNP Q73HU7
G	38	GLY	-	expression tag	UNP Q73HU7
H	38	GLY	-	expression tag	UNP Q73HU7
I	38	GLY	-	expression tag	UNP Q73HU7
J	38	GLY	-	expression tag	UNP Q73HU7
K	38	GLY	-	expression tag	UNP Q73HU7
L	38	GLY	-	expression tag	UNP Q73HU7

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total C O 13 6 7	0	0
3	N	1	Total C O 13 6 7	0	0
3	O	1	Total C O 13 6 7	0	0
3	P	1	Total C O 13 6 7	0	0
3	Q	1	Total C O 13 6 7	0	0
3	R	1	Total C O 13 6 7	0	0
3	S	1	Total C O 13 6 7	0	0
3	T	1	Total C O 13 6 7	0	0
3	U	1	Total C O 13 6 7	0	0
3	V	1	Total C O 13 6 7	0	0
3	W	1	Total C O 13 6 7	0	0
3	X	1	Total C O 13 6 7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	100	Total O 100 100	0	0
4	N	95	Total O 95 95	0	0
4	O	89	Total O 89 89	0	0
4	P	104	Total O 104 104	0	0
4	Q	79	Total O 79 79	0	0
4	R	97	Total O 97 97	0	0
4	S	56	Total O 56 56	0	0
4	T	67	Total O 67 67	0	0
4	U	64	Total O 64 64	0	0
4	V	97	Total O 97 97	0	0
4	W	58	Total O 58 58	0	0
4	X	75	Total O 75 75	0	0
4	A	230	Total O 230 230	0	0
4	B	275	Total O 275 275	0	0
4	C	241	Total O 241 241	0	0
4	D	255	Total O 255 255	0	0
4	E	206	Total O 206 206	0	0
4	F	226	Total O 226 226	0	0
4	G	192	Total O 192 192	0	0
4	H	234	Total O 234 234	0	0
4	I	185	Total O 185 185	0	0
4	J	245	Total O 245 245	0	0

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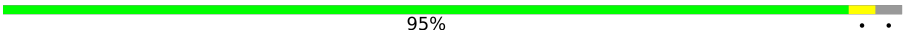
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	137	Total O 137 137	0	0
4	L	224	Total O 224 224	0	0

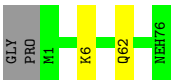
3 Residue-property plots (i)

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: Ubiquitin

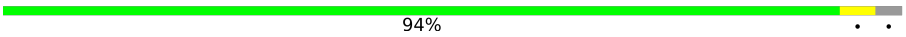
Chain M:





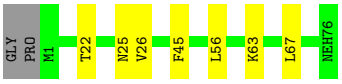
- Molecule 1: Ubiquitin

Chain N:



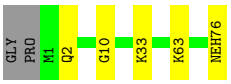
- Molecule 1: Ubiquitin

Chain O:



- Molecule 1: Ubiquitin

Chain P:

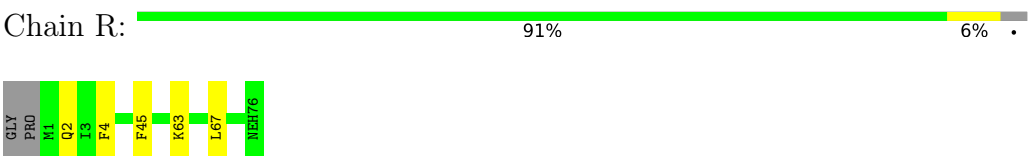


- Molecule 1: Ubiquitin

Chain Q:

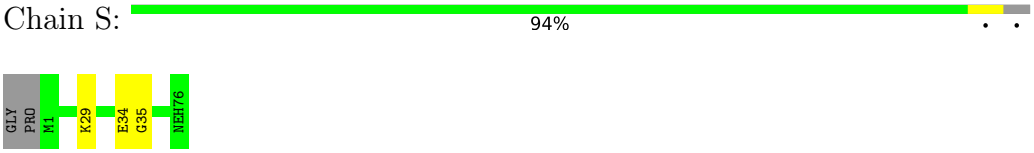
- Molecule 1: Ubiquitin

Chain R:



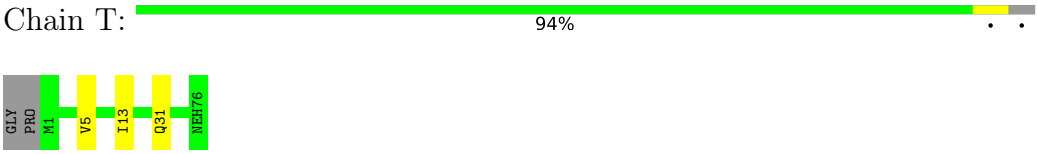
• Molecule 1: Ubiquitin

Chain S:



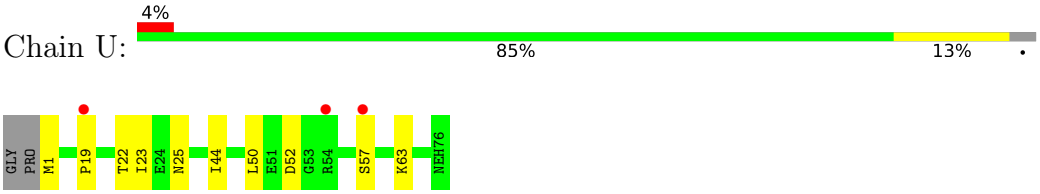
• Molecule 1: Ubiquitin

Chain T:



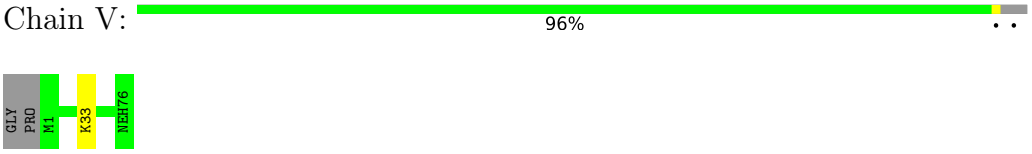
• Molecule 1: Ubiquitin

Chain U:



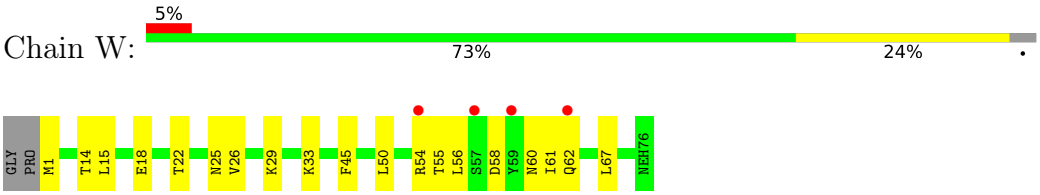
• Molecule 1: Ubiquitin

Chain V:



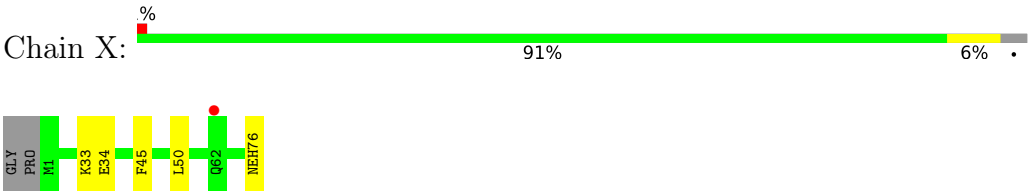
• Molecule 1: Ubiquitin

Chain W:



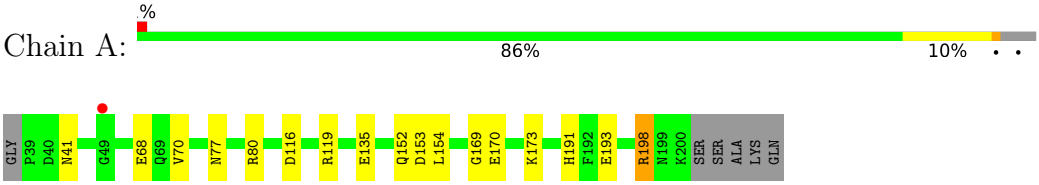
• Molecule 1: Ubiquitin

Chain X:



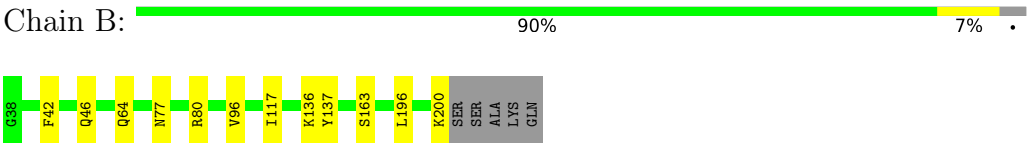
• Molecule 2: OTU domain-containing protein wMelOTU

Chain A:



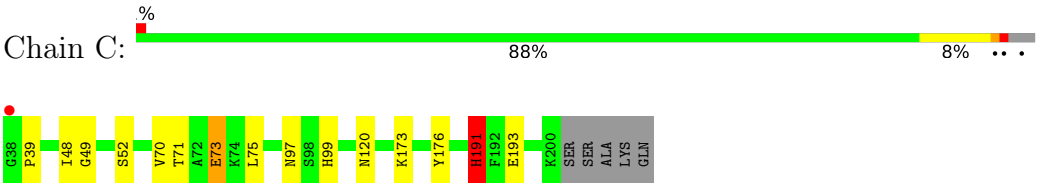
• Molecule 2: OTU domain-containing protein wMelOTU

Chain B:



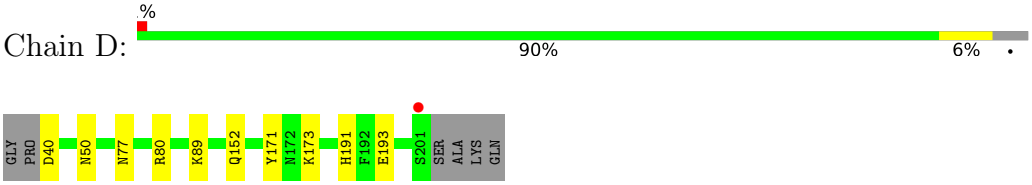
• Molecule 2: OTU domain-containing protein wMelOTU

Chain C:



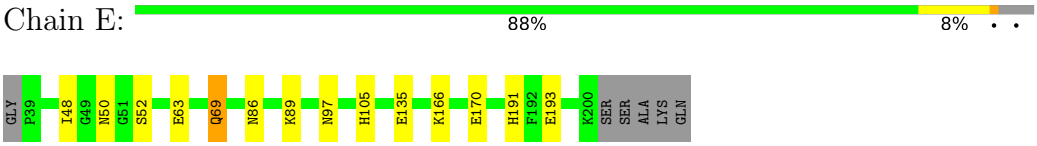
• Molecule 2: OTU domain-containing protein wMelOTU

Chain D:



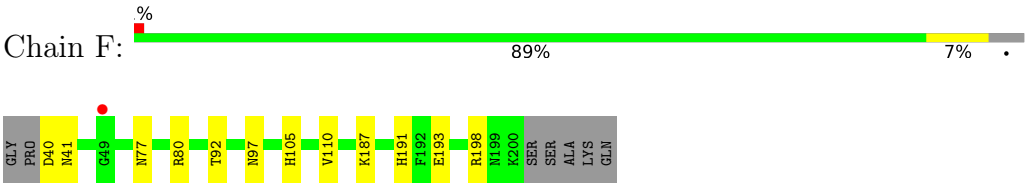
• Molecule 2: OTU domain-containing protein wMelOTU

Chain E:



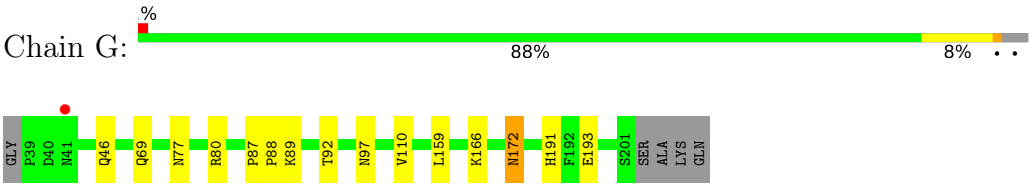
• Molecule 2: OTU domain-containing protein wMelOTU

Chain F:



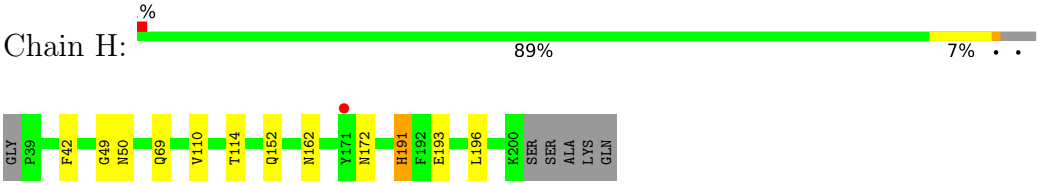
• Molecule 2: OTU domain-containing protein wMelOTU

Chain G:



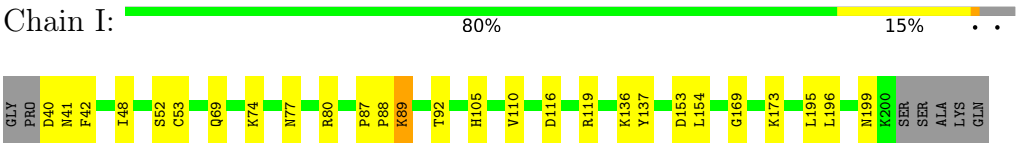
• Molecule 2: OTU domain-containing protein wMelOTU

Chain H:



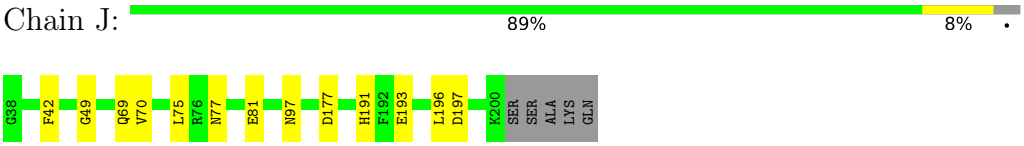
• Molecule 2: OTU domain-containing protein wMelOTU

Chain I:



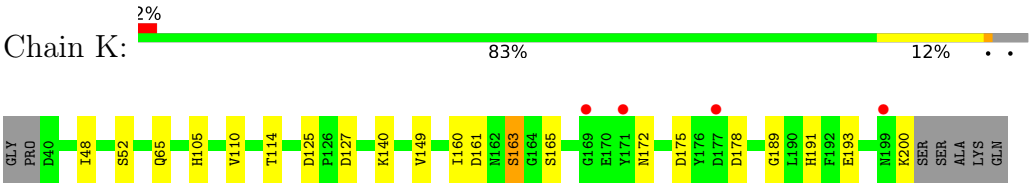
• Molecule 2: OTU domain-containing protein wMelOTU

Chain J:



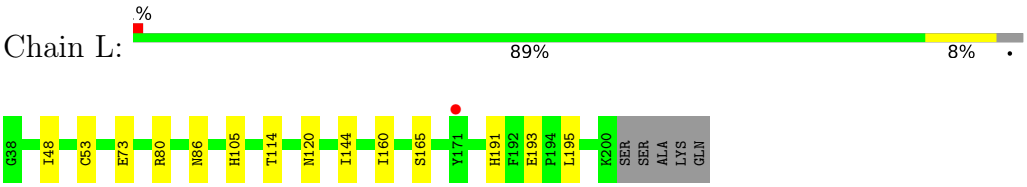
• Molecule 2: OTU domain-containing protein wMelOTU

Chain K:



• Molecule 2: OTU domain-containing protein wMelOTU

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	136.93Å 78.20Å 280.43Å 90.00° 91.57° 90.00°	Depositor
Resolution (Å)	27.29 – 1.82 27.29 – 1.82	Depositor EDS
% Data completeness (in resolution range)	92.2 (27.29-1.82) 92.3 (27.29-1.82)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.166 , 0.208 0.168 , 0.209	Depositor DCC
R_{free} test set	12304 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	15.7	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.000 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.033 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26594	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7078e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: NEH, FLC

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	M	0.44	0/605	0.58	0/815
1	N	0.43	0/603	0.63	0/811
1	O	0.41	0/595	0.57	0/802
1	P	0.43	0/603	0.63	0/811
1	Q	0.41	0/609	0.57	0/819
1	R	0.45	0/607	0.61	0/817
1	S	0.38	0/599	0.55	0/807
1	T	0.39	0/595	0.58	0/803
1	U	0.33	0/595	0.54	0/802
1	V	0.44	0/603	0.60	0/811
1	W	0.34	0/587	0.55	0/793
1	X	0.41	0/599	0.58	0/807
2	A	0.48	0/1346	0.58	0/1820
2	B	0.48	0/1357	0.61	0/1835
2	C	0.53	2/1340 (0.1%)	0.65	2/1813 (0.1%)
2	D	0.49	0/1340	0.62	0/1811
2	E	0.46	0/1339	0.58	0/1810
2	F	0.48	0/1340	0.61	0/1811
2	G	0.45	0/1335	0.55	0/1805
2	H	0.51	0/1337	0.60	0/1809
2	I	0.45	1/1331 (0.1%)	0.56	0/1799
2	J	0.49	0/1347	0.60	0/1823
2	K	0.44	0/1316	0.55	0/1781
2	L	0.49	0/1345	0.57	0/1819
All	All	0.46	3/23273 (0.0%)	0.59	2/31434 (0.0%)

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
2	C	0	2
2	F	0	2
2	H	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	191[A]	HIS	CA-C	6.14	1.69	1.52
2	C	191[B]	HIS	CA-C	6.14	1.69	1.52
2	I	53	CYS	CB-SG	5.67	1.91	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	191[A]	HIS	CA-C-O	-5.33	108.92	120.10
2	C	191[B]	HIS	CA-C-O	-5.33	108.92	120.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	191[A]	HIS	Mainchain
2	C	191[B]	HIS	Mainchain
2	F	191[A]	HIS	Mainchain
2	F	191[B]	HIS	Mainchain
2	H	191[A]	HIS	Mainchain
2	H	191[B]	HIS	Mainchain

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	M	599	0	624	2	0
1	N	600	0	630	2	0
1	O	592	0	613	4	0
1	P	600	0	630	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	603	0	635	3	1
1	R	601	0	628	3	0
1	S	596	0	619	3	0
1	T	592	0	608	2	0
1	U	592	0	615	6	0
1	V	600	0	630	1	0
1	W	584	0	600	14	0
1	X	596	0	619	3	0
2	A	1309	0	1218	16	0
2	B	1317	0	1227	13	0
2	C	1306	0	1208	12	0
2	D	1307	0	1213	8	0
2	E	1305	0	1215	11	1
2	F	1304	0	1214	7	0
2	G	1302	0	1208	10	0
2	H	1303	0	1204	9	0
2	I	1298	0	1205	18	0
2	J	1310	0	1211	8	0
2	K	1283	0	1177	16	0
2	L	1308	0	1218	10	0
3	M	13	0	5	0	0
3	N	13	0	5	0	0
3	O	13	0	5	1	0
3	P	13	0	5	0	0
3	Q	13	0	5	0	0
3	R	13	0	5	0	0
3	S	13	0	5	0	0
3	T	13	0	5	0	0
3	U	13	0	5	0	0
3	V	13	0	5	0	0
3	W	13	0	5	0	0
3	X	13	0	5	0	0
4	A	230	0	0	3	1
4	B	275	0	0	5	2
4	C	241	0	0	2	2
4	D	255	0	0	2	1
4	E	206	0	0	1	3
4	F	226	0	0	3	1
4	G	192	0	0	3	1
4	H	234	0	0	3	1
4	I	185	0	0	2	2
4	J	245	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	137	0	0	2	0
4	L	224	0	0	2	0
4	M	100	0	0	2	0
4	N	95	0	0	1	0
4	O	89	0	0	1	0
4	P	104	0	0	2	0
4	Q	79	0	0	1	0
4	R	97	0	0	1	0
4	S	56	0	0	4	0
4	T	67	0	0	1	0
4	U	64	0	0	2	0
4	V	97	0	0	1	0
4	W	58	0	0	3	0
4	X	75	0	0	0	0
All	All	26594	0	22029	176	9

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 4.

All (176) 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:K:191[B]:HIS:CD2	2:K:193:GLU:OE2	2.21	0.92
2:B:46:GLN:NE2	4:B:302:HOH:O	2.05	0.89
2:L:120:ASN:OD1	4:L:301:HOH:O	1.91	0.88
2:E:191[B]:HIS:HD2	2:E:193:GLU:OE2	1.59	0.85
2:K:140:LYS:HD2	2:K:161:ASP:HB3	1.58	0.84
2:B:77:ASN:OD1	4:B:301:HOH:O	1.94	0.83
2:A:152:GLN:NE2	2:A:154:LEU:HD21	1.99	0.77
2:K:191[B]:HIS:HD2	2:K:193:GLU:OE2	1.63	0.77
2:C:191[A]:HIS:CD2	2:C:193:GLU:OE1	2.37	0.77
1:U:25:ASN:ND2	4:U:201:HOH:O	2.17	0.77
1:W:1:MET:SD	4:W:247:HOH:O	2.44	0.75
2:B:77:ASN:HD22	2:B:80:ARG:HE	1.36	0.74
2:E:191[B]:HIS:CD2	2:E:193:GLU:OE2	2.40	0.74
2:C:191[A]:HIS:HD2	2:C:193:GLU:OE1	1.70	0.74
1:S:29:LYS:NZ	4:S:202:HOH:O	2.21	0.73
2:K:65:GLN:NE2	4:K:301:HOH:O	2.20	0.73
2:L:80:ARG:NH2	4:L:302:HOH:O	2.22	0.71
1:Q:48:LYS:HD2	1:Q:49:GLN:N	2.04	0.71
1:T:31:GLN:OE1	4:T:201:HOH:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:191[A]:HIS:CD2	2:L:193:GLU:OE2	2.46	0.69
2:D:152:GLN:NE2	4:D:303:HOH:O	2.25	0.68
2:G:46:GLN:NE2	4:G:302:HOH:O	2.27	0.68
2:K:172:ASN:ND2	4:K:302:HOH:O	2.27	0.68
2:B:77:ASN:ND2	2:B:80:ARG:HE	1.94	0.66
2:F:40:ASP:O	2:F:198:ARG:NH1	2.28	0.66
2:C:120:ASN:OD1	4:C:301:HOH:O	2.13	0.66
2:D:191[B]:HIS:CD2	2:D:193:GLU:OE1	2.49	0.65
2:D:191[B]:HIS:HD2	2:D:193:GLU:OE1	1.79	0.65
1:S:34:GLU:OE2	4:S:201:HOH:O	2.15	0.64
2:A:135:GLU:OE2	4:A:302:HOH:O	2.15	0.64
2:J:49:GLY:HA2	2:J:191[A]:HIS:HE1	1.63	0.64
2:A:152:GLN:OE1	4:A:303:HOH:O	2.15	0.63
2:J:197:ASP:OD2	4:J:301:HOH:O	2.15	0.63
2:K:160:ILE:HG12	2:K:165:SER:HB2	1.81	0.62
1:S:35:GLY:O	2:E:97:ASN:ND2	2.31	0.61
2:K:175:ASP:OD1	2:K:178:ASP:HB2	2.00	0.61
2:F:193:GLU:OE1	4:F:301:HOH:O	2.16	0.60
2:C:49:GLY:HA2	2:C:191[A]:HIS:HE1	1.65	0.60
2:A:191[A]:HIS:CD2	2:A:193[A]:GLU:OE1	2.54	0.60
2:H:191[A]:HIS:CD2	2:H:193:GLU:OE2	2.55	0.60
2:A:152:GLN:NE2	2:A:154:LEU:CD2	2.64	0.59
2:L:160:ILE:HG12	2:L:165:SER:HB2	1.84	0.59
1:Q:48:LYS:HD2	1:Q:49:GLN:H	1.67	0.59
1:W:18:GLU:OE2	2:I:89:LYS:HE2	2.03	0.59
2:C:71:THR:OG1	2:C:73:GLU:HG3	2.03	0.59
1:P:63:LYS:NZ	4:P:203:HOH:O	2.35	0.58
1:Q:16:GLU:O	1:Q:29:LYS:HE2	2.03	0.58
1:W:60:ASN:OD1	1:W:62:GLN:NE2	2.37	0.58
2:E:48:ILE:HD13	2:E:50:ASN:OD1	2.04	0.58
2:E:135:GLU:OE1	4:E:301:HOH:O	2.17	0.57
2:G:97:ASN:ND2	4:G:308:HOH:O	2.36	0.57
2:G:89:LYS:HE3	2:J:177:ASP:OD2	2.05	0.57
2:I:92:THR:HG22	2:I:110:VAL:HG21	1.86	0.57
2:H:152:GLN:NE2	4:H:303:HOH:O	2.33	0.56
2:L:144:ILE:HD12	2:L:195:LEU:HD11	1.88	0.56
2:A:170:GLU:O	2:A:173:LYS:HD3	2.07	0.55
2:H:49:GLY:HA2	2:H:191[A]:HIS:HE1	1.72	0.54
2:L:191[A]:HIS:HD2	2:L:193:GLU:OE2	1.88	0.54
3:O:101:FLC:OB2	2:F:105[B]:HIS:NE2	2.40	0.54
1:N:6:LYS:HE2	1:N:10:GLY:HA2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:189:GLY:O	2:K:191[A]:HIS:HD2	1.90	0.53
1:O:45:PHE:HB2	1:O:67:LEU:HD22	1.91	0.52
1:T:5:VAL:HB	1:T:13:ILE:HG12	1.90	0.52
2:A:77:ASN:OD1	2:A:80:ARG:NH1	2.26	0.52
2:F:187:LYS:NZ	4:F:304:HOH:O	2.32	0.52
2:A:191[A]:HIS:HD2	2:A:193[A]:GLU:OE1	1.93	0.52
2:A:191[A]:HIS:HD2	4:A:310:HOH:O	1.93	0.52
2:H:69:GLN:NE2	4:H:302:HOH:O	2.29	0.51
2:J:193:GLU:OE2	4:J:302:HOH:O	2.19	0.51
2:F:92:THR:HG22	2:F:110:VAL:HG21	1.93	0.51
2:D:171:TYR:O	2:D:173:LYS:HD2	2.11	0.51
2:A:41:ASN:O	2:A:198:ARG:HG2	2.10	0.50
2:E:48:ILE:HD12	2:E:48:ILE:O	2.11	0.50
1:W:56:LEU:HD22	1:W:61:ILE:HD12	1.93	0.50
1:M:62:GLN:NE2	4:M:204:HOH:O	2.44	0.50
2:B:64:GLN:NE2	4:B:315:HOH:O	2.42	0.50
1:W:61:ILE:HD13	1:W:67:LEU:HD21	1.94	0.49
2:L:48:ILE:HG22	2:L:53:CYS:HA	1.93	0.49
2:G:69:GLN:OE1	4:G:301:HOH:O	2.20	0.49
1:U:1:MET:HE2	1:U:63:LYS:HA	1.93	0.49
1:U:23:ILE:HD12	1:U:50:LEU:HD23	1.93	0.49
2:H:42:PHE:HA	2:H:196:LEU:O	2.13	0.49
1:R:2:GLN:HE21	1:R:4:PHE:HZ	1.60	0.48
2:G:77:ASN:OD1	2:G:80:ARG:NH1	2.43	0.48
1:W:22:THR:O	1:W:26:VAL:HG23	2.14	0.48
2:B:136:LYS:HD3	2:B:137:TYR:CE2	2.49	0.47
4:Q:206:HOH:O	2:I:105[A]:HIS:HE1	1.97	0.47
2:H:191[A]:HIS:HD2	2:H:193:GLU:OE2	1.98	0.47
2:I:41:ASN:OD1	2:I:199:ASN:ND2	2.47	0.47
2:B:77:ASN:HD22	2:B:80:ARG:NE	2.09	0.47
2:B:96:VAL:HG13	4:B:438:HOH:O	2.15	0.47
2:G:191[A]:HIS:CD2	2:G:193:GLU:OE2	2.68	0.47
2:K:48:ILE:HD11	2:K:52:SER:HB2	1.97	0.47
2:F:97:ASN:ND2	4:F:303:HOH:O	2.27	0.47
2:D:40:ASP:HB3	4:D:427:HOH:O	2.14	0.46
2:I:88:PRO:HG2	4:I:430:HOH:O	2.15	0.46
2:I:42:PHE:HA	2:I:196:LEU:O	2.16	0.46
2:A:152:GLN:CD	2:A:154:LEU:HD21	2.34	0.46
1:W:55:THR:O	1:W:58:ASP:HB2	2.16	0.46
2:I:69:GLN:NE2	4:I:301:HOH:O	2.19	0.46
2:E:170:GLU:OE2	2:E:170:GLU:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:40:ASP:OD2	2:I:41:ASN:N	2.41	0.46
2:J:77:ASN:O	2:J:81:GLU:HG3	2.16	0.45
2:I:48:ILE:HD11	2:I:52:SER:HB2	1.98	0.45
1:W:25:ASN:O	1:W:29:LYS:HG3	2.16	0.45
2:I:169:GLY:O	2:I:173:LYS:HE2	2.16	0.45
4:S:205:HOH:O	2:E:166:LYS:NZ	2.49	0.45
2:K:161:ASP:OD1	2:K:163:SER:HB3	2.16	0.45
2:C:120:ASN:ND2	4:C:308:HOH:O	2.50	0.45
1:X:33:LYS:HG3	1:X:34:GLU:HG2	1.98	0.45
1:X:45:PHE:HB3	1:X:50:LEU:HD21	1.98	0.45
2:G:92:THR:HG23	2:G:110:VAL:HG23	1.98	0.45
1:O:22:THR:O	1:O:25:ASN:HB2	2.17	0.44
2:H:162:ASN:ND2	4:H:317:HOH:O	2.50	0.44
1:W:45:PHE:HB3	1:W:50:LEU:HD21	1.97	0.44
2:F:77:ASN:CG	2:F:80:ARG:HH11	2.19	0.44
2:D:89:LYS:HB3	2:D:89:LYS:HE2	1.62	0.44
1:M:6:LYS:HD3	4:M:224:HOH:O	2.17	0.44
1:R:45:PHE:HB2	1:R:67:LEU:HD22	2.00	0.44
2:B:42:PHE:HA	2:B:196:LEU:O	2.17	0.44
2:C:70:VAL:HG21	2:C:75:LEU:HD21	1.99	0.44
4:S:212:HOH:O	2:E:105[A]:HIS:HE1	2.01	0.43
1:V:33:LYS:HE2	2:B:163[A]:SER:HB3	2.00	0.43
1:W:15:LEU:HD12	4:W:214:HOH:O	2.18	0.43
1:W:14:THR:O	1:W:33:LYS:NZ	2.51	0.43
2:I:153:ASP:O	2:I:154:LEU:HD13	2.17	0.43
1:N:54:ARG:NH2	4:N:207:HOH:O	2.49	0.43
2:I:42:PHE:HB3	2:I:195:LEU:HG	2.00	0.43
2:I:136:LYS:HG2	2:I:137:TYR:CE2	2.53	0.43
1:P:76:NEH:HB1	2:D:50:ASN:O	2.18	0.43
1:U:44:ILE:HG13	2:K:149:VAL:HG21	1.99	0.43
2:C:49:GLY:HA2	2:C:191[A]:HIS:CE1	2.51	0.43
2:E:63:GLU:CD	2:E:69:GLN:HG3	2.38	0.43
1:X:76:NEH:HB1	2:H:50:ASN:O	2.19	0.43
2:A:68:GLU:HG2	2:A:70:VAL:HG23	2.00	0.43
2:A:169:GLY:O	2:A:173:LYS:HD2	2.18	0.43
2:L:191[A]:HIS:CD2	2:L:193:GLU:CD	2.92	0.43
1:W:15:LEU:HD21	1:W:29:LYS:HB2	2.01	0.43
2:C:48:ILE:HD11	2:C:52:SER:HB2	2.01	0.42
2:G:166:LYS:HE3	2:G:172:ASN:OD1	2.19	0.42
2:I:74:LYS:HE3	2:J:69:GLN:NE2	2.34	0.42
1:U:19:PRO:O	1:U:57:SER:OG	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:249:HOH:O	2:L:105[A]:HIS:HE1	2.02	0.42
1:W:18:GLU:HG2	4:W:212:HOH:O	2.19	0.42
2:A:191[A]:HIS:CD2	2:A:193[A]:GLU:CD	2.93	0.42
2:A:116:ASP:HA	2:A:119:ARG:NH1	2.35	0.42
2:K:110:VAL:O	2:K:114:THR:HG23	2.18	0.42
1:P:33:LYS:HE3	1:P:33:LYS:HB2	1.90	0.42
4:U:218:HOH:O	2:K:105[B]:HIS:HE1	2.02	0.42
2:I:116:ASP:HA	2:I:119:ARG:NH1	2.34	0.42
1:P:10:GLY:HA2	4:P:267:HOH:O	2.20	0.42
2:J:42:PHE:HA	2:J:196:LEU:O	2.19	0.42
2:E:48:ILE:HD11	2:E:52:SER:C	2.40	0.41
1:O:63:LYS:NZ	4:O:3702:HOH:O	2.41	0.41
2:L:80:ARG:HG3	2:L:114:THR:O	2.21	0.41
2:B:117:ILE:HD12	2:B:117:ILE:HA	1.94	0.41
2:I:87:PRO:HA	2:I:88:PRO:HD3	1.92	0.41
2:J:70:VAL:HG21	2:J:75:LEU:HD21	2.02	0.41
2:A:153:ASP:O	2:A:154:LEU:HD23	2.21	0.41
2:K:200:LYS:HD3	2:K:200:LYS:N	2.36	0.41
1:O:26:VAL:HG21	1:O:56:LEU:HD21	2.03	0.41
2:C:39:PRO:HG3	2:C:176:TYR:CE2	2.56	0.41
2:C:173:LYS:HB3	2:C:173:LYS:HE3	1.81	0.41
2:C:97:ASN:OD1	2:C:99:HIS:NE2	2.53	0.41
2:D:77:ASN:CG	2:D:80:ARG:HH11	2.23	0.41
2:G:159:LEU:HD23	2:G:159:LEU:HA	1.92	0.41
2:I:77:ASN:OD1	2:I:80:ARG:NH1	2.37	0.41
2:K:125:ASP:HB3	2:K:127:ASP:OD1	2.20	0.41
1:U:22:THR:H	1:U:25:ASN:ND2	2.19	0.41
2:B:77:ASN:HD22	2:B:80:ARG:HH11	1.68	0.40
2:K:189:GLY:O	2:K:191[A]:HIS:CD2	2.71	0.40
2:B:200:LYS:NZ	4:B:321:HOH:O	2.54	0.40
1:W:18:GLU:CD	2:I:89:LYS:HE2	2.41	0.40
2:G:87:PRO:HA	2:G:88:PRO:HD3	1.94	0.40
1:R:63:LYS:NZ	4:R:210:HOH:O	2.55	0.40
2:H:110:VAL:O	2:H:114:THR:HG23	2.20	0.40

All (9) 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)
4:B:492:HOH:O	4:D:340:HOH:O[3_545]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:18:GLU:OE1	2:E:89:LYS:NZ[2_555]	2.01	0.19
4:B:312:HOH:O	4:B:458:HOH:O[2_556]	2.01	0.19
4:E:407:HOH:O	4:I:345:HOH:O[3_555]	2.04	0.16
4:E:344:HOH:O	4:G:304:HOH:O[3_545]	2.06	0.14
4:F:467:HOH:O	4:J:529:HOH:O[3_455]	2.08	0.12
4:A:511:HOH:O	4:C:535:HOH:O[3_445]	2.10	0.10
4:E:479:HOH:O	4:I:454:HOH:O[3_555]	2.16	0.04
4:C:462:HOH:O	4:H:391:HOH:O[3_545]	2.19	0.01

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	M	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
1	N	74/78 (95%)	74 (100%)	0	0	100	100
1	O	74/78 (95%)	73 (99%)	1 (1%)	0	100	100
1	P	74/78 (95%)	74 (100%)	0	0	100	100
1	Q	75/78 (96%)	75 (100%)	0	0	100	100
1	R	75/78 (96%)	75 (100%)	0	0	100	100
1	S	74/78 (95%)	74 (100%)	0	0	100	100
1	T	74/78 (95%)	74 (100%)	0	0	100	100
1	U	74/78 (95%)	74 (100%)	0	0	100	100
1	V	74/78 (95%)	74 (100%)	0	0	100	100
1	W	74/78 (95%)	73 (99%)	1 (1%)	0	100	100
1	X	74/78 (95%)	74 (100%)	0	0	100	100
2	A	163/168 (97%)	158 (97%)	5 (3%)	0	100	100
2	B	165/168 (98%)	161 (98%)	4 (2%)	0	100	100
2	C	163/168 (97%)	158 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	162/168 (96%)	156 (96%)	6 (4%)	0	100	100
2	E	162/168 (96%)	156 (96%)	6 (4%)	0	100	100
2	F	162/168 (96%)	155 (96%)	7 (4%)	0	100	100
2	G	163/168 (97%)	159 (98%)	4 (2%)	0	100	100
2	H	162/168 (96%)	157 (97%)	5 (3%)	0	100	100
2	I	161/168 (96%)	157 (98%)	4 (2%)	0	100	100
2	J	164/168 (98%)	160 (98%)	4 (2%)	0	100	100
2	K	161/168 (96%)	157 (98%)	4 (2%)	0	100	100
2	L	164/168 (98%)	159 (97%)	5 (3%)	0	100	100
All	All	2843/2952 (96%)	2781 (98%)	62 (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	M	68/69 (99%)	68 (100%)	0	100	100
1	N	68/69 (99%)	68 (100%)	0	100	100
1	O	66/69 (96%)	66 (100%)	0	100	100
1	P	68/69 (99%)	67 (98%)	1 (2%)	65	55
1	Q	69/69 (100%)	69 (100%)	0	100	100
1	R	68/69 (99%)	68 (100%)	0	100	100
1	S	67/69 (97%)	67 (100%)	0	100	100
1	T	66/69 (96%)	66 (100%)	0	100	100
1	U	66/69 (96%)	65 (98%)	1 (2%)	65	55
1	V	68/69 (99%)	68 (100%)	0	100	100
1	W	64/69 (93%)	63 (98%)	1 (2%)	62	53
1	X	67/69 (97%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	145/149 (97%)	144 (99%)	1 (1%)	84 80
2	B	147/149 (99%)	147 (100%)	0	100 100
2	C	144/149 (97%)	143 (99%)	1 (1%)	84 80
2	D	145/149 (97%)	145 (100%)	0	100 100
2	E	144/149 (97%)	142 (99%)	2 (1%)	67 58
2	F	145/149 (97%)	144 (99%)	1 (1%)	84 80
2	G	143/149 (96%)	142 (99%)	1 (1%)	84 80
2	H	144/149 (97%)	143 (99%)	1 (1%)	84 80
2	I	144/149 (97%)	143 (99%)	1 (1%)	84 80
2	J	145/149 (97%)	144 (99%)	1 (1%)	84 80
2	K	139/149 (93%)	138 (99%)	1 (1%)	84 80
2	L	144/149 (97%)	142 (99%)	2 (1%)	67 58
All	All	2534/2616 (97%)	2519 (99%)	15 (1%)	86 83

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	2	GLN
1	U	52	ASP
1	W	54	ARG
2	A	198	ARG
2	C	73	GLU
2	E	69	GLN
2	E	86	ASN
2	F	41	ASN
2	G	172	ASN
2	H	172	ASN
2	I	89	LYS
2	J	97	ASN
2	K	163	SER
2	L	73	GLU
2	L	86	ASN

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

Mol	Chain	Res	Type
1	O	60	ASN

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Mol	Chain	Res	Type
1	T	25	ASN
2	B	77	ASN
2	B	104	GLN
2	H	172	ASN
2	J	69	GLN
2	J	86	ASN
2	J	97	ASN
2	K	65	GLN
2	K	69	GLN
2	K	77	ASN
2	K	97	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

12 ligands 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	$\#\|Z\| > 2$
3	FLC	X	101	-	12,12,12	1.01	0	17,17,17	1.65	4 (23%)
3	FLC	T	101	-	12,12,12	1.18	0	17,17,17	1.50	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FLC	S	101	-	12,12,12	1.15	0	17,17,17	1.60	3 (17%)
3	FLC	U	101	-	12,12,12	1.16	0	17,17,17	1.37	2 (11%)
3	FLC	P	101	-	12,12,12	1.12	0	17,17,17	1.62	4 (23%)
3	FLC	N	101	-	12,12,12	1.12	0	17,17,17	1.54	2 (11%)
3	FLC	Q	101	-	12,12,12	0.90	0	17,17,17	1.72	4 (23%)
3	FLC	O	101	-	12,12,12	1.00	0	17,17,17	1.62	4 (23%)
3	FLC	V	101	-	12,12,12	1.20	0	17,17,17	1.32	2 (11%)
3	FLC	W	101	-	12,12,12	1.08	0	17,17,17	1.54	3 (17%)
3	FLC	M	101	-	12,12,12	1.02	0	17,17,17	1.44	3 (17%)
3	FLC	R	101	-	12,12,12	1.21	0	17,17,17	1.14	1 (5%)

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
3	FLC	X	101	-	-	4/16/16/16	-
3	FLC	T	101	-	-	0/16/16/16	-
3	FLC	S	101	-	-	0/16/16/16	-
3	FLC	U	101	-	-	0/16/16/16	-
3	FLC	P	101	-	-	6/16/16/16	-
3	FLC	N	101	-	-	0/16/16/16	-
3	FLC	Q	101	-	-	8/16/16/16	-
3	FLC	O	101	-	-	5/16/16/16	-
3	FLC	V	101	-	-	0/16/16/16	-
3	FLC	W	101	-	-	8/16/16/16	-
3	FLC	M	101	-	-	8/16/16/16	-
3	FLC	R	101	-	-	0/16/16/16	-

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	101	FLC	OB2-CBC-CB	4.08	120.14	113.05
3	X	101	FLC	OB2-CBC-CB	4.02	120.02	113.05
3	Q	101	FLC	OB2-CBC-CB	3.95	119.92	113.05
3	W	101	FLC	OB2-CBC-CB	3.73	119.52	113.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	101	FLC	OB2-CBC-CB	3.64	119.38	113.05
3	S	101	FLC	OB2-CBC-CB	3.55	119.22	113.05
3	N	101	FLC	OB2-CBC-CB	3.51	119.14	113.05
3	P	101	FLC	OB2-CBC-CB	3.43	119.01	113.05
3	M	101	FLC	OB2-CBC-CB	3.23	118.65	113.05
3	O	101	FLC	OB2-CBC-CB	3.22	118.64	113.05
3	T	101	FLC	OB1-CBC-CB	-2.90	118.15	122.25
3	N	101	FLC	OB1-CBC-CB	-2.67	118.47	122.25
3	S	101	FLC	OB1-CBC-CB	-2.66	118.49	122.25
3	V	101	FLC	CA-CB-CBC	-2.59	104.53	110.11
3	X	101	FLC	OG2-CGC-CG	2.53	122.49	114.35
3	V	101	FLC	OB2-CBC-CB	2.47	117.35	113.05
3	U	101	FLC	OB1-CBC-CB	-2.44	118.80	122.25
3	Q	101	FLC	OB1-CBC-CB	-2.37	118.89	122.25
3	O	101	FLC	OG2-CGC-CG	2.35	121.90	114.35
3	R	101	FLC	OB2-CBC-CB	2.34	117.11	113.05
3	Q	101	FLC	OA2-CAC-CA	2.30	121.75	114.35
3	P	101	FLC	OA2-CAC-CA	2.23	121.52	114.35
3	X	101	FLC	OA2-CAC-CA	2.20	121.41	114.35
3	O	101	FLC	OB1-CBC-CB	-2.18	119.16	122.25
3	Q	101	FLC	OG2-CGC-CG	2.18	121.35	114.35
3	O	101	FLC	OA2-CAC-CA	2.15	121.25	114.35
3	W	101	FLC	OA2-CAC-CA	2.13	121.19	114.35
3	W	101	FLC	OG2-CGC-CG	2.10	121.09	114.35
3	P	101	FLC	OB1-CBC-CB	-2.09	119.29	122.25
3	P	101	FLC	CB-CG-CGC	-2.08	108.77	113.81
3	S	101	FLC	OA2-CAC-CA	2.08	121.02	114.35
3	X	101	FLC	OG2-CGC-OG1	-2.05	118.20	123.30
3	M	101	FLC	OG2-CGC-CG	2.04	120.90	114.35
3	M	101	FLC	OA2-CAC-CA	2.02	120.83	114.35

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	101	FLC	CA-CB-CBC-OB2
3	M	101	FLC	CG-CB-CBC-OB1
3	M	101	FLC	CG-CB-CBC-OB2
3	Q	101	FLC	CA-CB-CBC-OB1
3	Q	101	FLC	CG-CB-CBC-OB1
3	Q	101	FLC	CG-CB-CBC-OB2
3	W	101	FLC	CA-CB-CBC-OB1

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Mol	Chain	Res	Type	Atoms
3	W	101	FLC	CA-CB-CBC-OB2
3	W	101	FLC	CG-CB-CBC-OB1
3	W	101	FLC	CG-CB-CBC-OB2
3	M	101	FLC	CA-CB-CBC-OB1
3	P	101	FLC	CG-CB-CBC-OB1
3	Q	101	FLC	CA-CB-CBC-OB2
3	O	101	FLC	CA-CB-CBC-OB1
3	P	101	FLC	CA-CB-CBC-OB1
3	O	101	FLC	CB-CG-CGC-OG2
3	Q	101	FLC	CB-CA-CAC-OA2
3	P	101	FLC	CB-CG-CGC-OG2
3	O	101	FLC	CB-CG-CGC-OG1
3	P	101	FLC	CB-CA-CAC-OA1
3	P	101	FLC	CB-CG-CGC-OG1
3	Q	101	FLC	CB-CA-CAC-OA1
3	M	101	FLC	CB-CA-CAC-OA1
3	Q	101	FLC	CB-CG-CGC-OG1
3	P	101	FLC	CB-CA-CAC-OA2
3	W	101	FLC	CB-CG-CGC-OG1
3	X	101	FLC	CB-CG-CGC-OG1
3	M	101	FLC	CB-CA-CAC-OA2
3	M	101	FLC	CB-CG-CGC-OG1
3	M	101	FLC	CB-CG-CGC-OG2
3	O	101	FLC	CB-CA-CAC-OA1
3	Q	101	FLC	CB-CG-CGC-OG2
3	W	101	FLC	CB-CG-CGC-OG2
3	X	101	FLC	CB-CA-CAC-OA1
3	X	101	FLC	CB-CA-CAC-OA2
3	X	101	FLC	CB-CG-CGC-OG2
3	O	101	FLC	CB-CA-CAC-OA2
3	W	101	FLC	CB-CA-CAC-OA1
3	W	101	FLC	CB-CA-CAC-OA2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	101	FLC	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	M	75/78 (96%)	-0.68	0 100 100	9, 17, 28, 34	0
1	N	75/78 (96%)	-0.67	0 100 100	8, 15, 28, 33	0
1	O	75/78 (96%)	-0.60	0 100 100	10, 19, 33, 38	0
1	P	75/78 (96%)	-0.56	0 100 100	8, 18, 32, 39	0
1	Q	75/78 (96%)	-0.46	0 100 100	13, 22, 35, 40	0
1	R	75/78 (96%)	-0.71	0 100 100	10, 17, 28, 35	0
1	S	75/78 (96%)	-0.33	0 100 100	11, 25, 44, 47	0
1	T	75/78 (96%)	-0.48	0 100 100	9, 21, 37, 42	0
1	U	75/78 (96%)	0.04	3 (4%) 38 32	16, 35, 55, 57	0
1	V	75/78 (96%)	-0.48	0 100 100	11, 20, 31, 41	0
1	W	75/78 (96%)	0.22	4 (5%) 26 21	12, 38, 62, 68	0
1	X	75/78 (96%)	-0.34	1 (1%) 77 74	10, 25, 36, 54	0
2	A	162/168 (96%)	-0.38	1 (0%) 89 88	10, 18, 40, 57	0
2	B	163/168 (97%)	-0.43	0 100 100	8, 15, 32, 41	0
2	C	163/168 (97%)	-0.42	1 (0%) 89 88	9, 17, 36, 66	0
2	D	162/168 (96%)	-0.45	1 (0%) 89 88	9, 15, 35, 65	0
2	E	162/168 (96%)	-0.36	0 100 100	12, 20, 37, 53	0
2	F	161/168 (95%)	-0.42	1 (0%) 89 88	10, 18, 40, 58	0
2	G	163/168 (97%)	-0.30	1 (0%) 89 88	12, 22, 49, 59	0
2	H	162/168 (96%)	-0.41	1 (0%) 89 88	8, 17, 38, 56	0
2	I	161/168 (95%)	-0.20	0 100 100	14, 24, 43, 64	0
2	J	163/168 (97%)	-0.45	0 100 100	9, 16, 34, 47	0
2	K	161/168 (95%)	0.05	4 (2%) 57 52	15, 32, 55, 71	0
2	L	163/168 (97%)	-0.27	1 (0%) 89 88	12, 21, 40, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
All	All	2846/2952 (96%)	-0.36	19 (0%)	87 86	8, 20, 44, 71	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	38	GLY	5.3
2	K	171	TYR	3.8
1	W	57	SER	3.5
2	D	201	SER	3.5
2	L	171	TYR	3.3
2	K	177	ASP	3.2
2	H	171	TYR	2.8
2	K	199	ASN	2.7
1	W	62	GLN	2.4
2	F	49	GLY	2.3
2	K	169	GLY	2.2
1	U	19	PRO	2.2
1	X	62	GLN	2.2
1	U	57	SER	2.1
1	U	54	ARG	2.1
1	W	59	TYR	2.0
2	G	41	ASN	2.0
1	W	54	ARG	2.0
2	A	49	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

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
3	FLC	S	101	13/13	0.89	0.14	33,38,41,43	0
3	FLC	T	101	13/13	0.91	0.12	25,31,39,41	0
3	FLC	N	101	13/13	0.92	0.12	20,25,32,34	0
3	FLC	R	101	13/13	0.93	0.13	21,26,36,38	0
3	FLC	U	101	13/13	0.93	0.10	26,32,37,38	0
3	FLC	W	101	13/13	0.93	0.12	30,33,40,40	0
3	FLC	Q	101	13/13	0.94	0.09	22,26,33,34	0
3	FLC	X	101	13/13	0.94	0.10	24,28,35,35	0
3	FLC	P	101	13/13	0.95	0.10	20,24,29,30	0
3	FLC	V	101	13/13	0.96	0.07	17,22,29,29	0
3	FLC	M	101	13/13	0.96	0.09	19,25,35,35	0
3	FLC	O	101	13/13	0.96	0.10	20,25,29,33	0

6.5 Other polymers (i)

There are no such residues in this entry.