



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2023 – 02:25 PM EDT

PDB ID : 7RDB
Title : Crystal structure of Tspan15 large extracellular loop (Tspan15 LEL)
Authors : Lipper, C.H.; Gabriel, K.H.; Seegar, T.C.M.; Durr, K.L.; Tomlinson, M.G.; Blacklow, S.C.
Deposited on : 2021-07-09
Resolution : 2.52 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
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

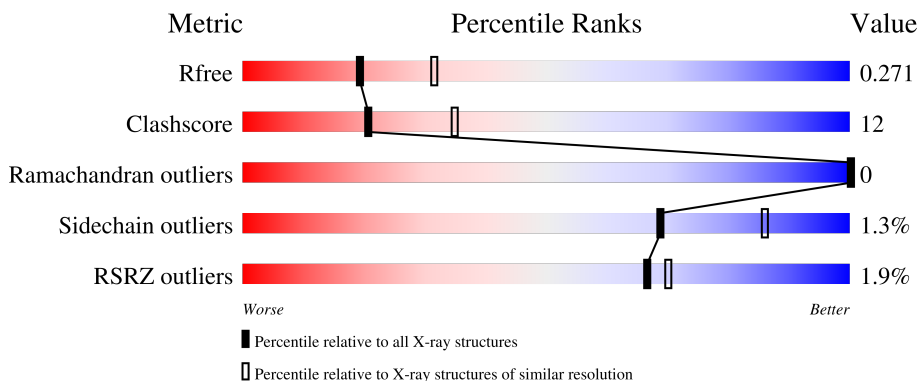
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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.



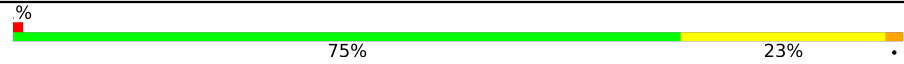

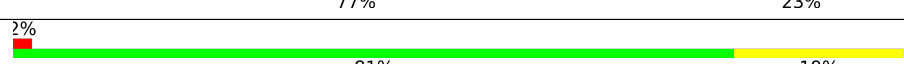
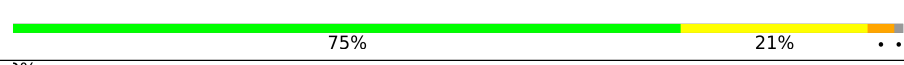
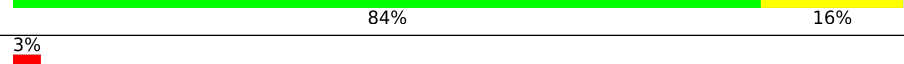
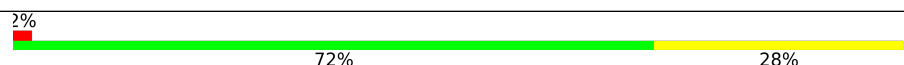

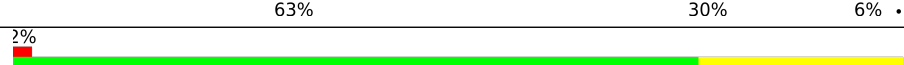
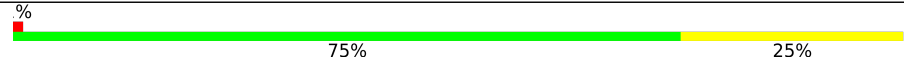

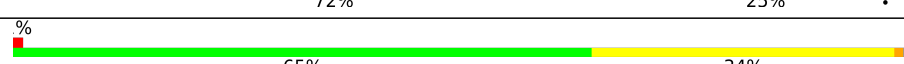


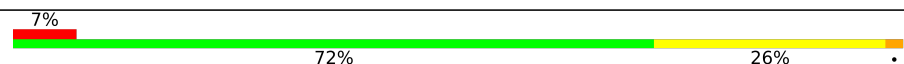





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	122	 75% 22%
1	B	122	 75% 25%
1	C	122	 79% 20%
1	D	122	 82% 17%
1	E	122	 84% 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	122	 75% 23% .
1	G	122	 74% 25% .
1	H	122	 77% 23%
1	I	122	 81% 19%
1	J	122	 75% 21% ..
1	K	122	 84% 16%
1	L	122	 82% 16% .
1	M	122	 72% 28%
1	N	122	 68% 31% .
1	O	122	 63% 30% 6% .
1	P	122	 77% 23%
1	Q	122	 75% 25%
1	R	122	 70% 27% .
1	S	122	 72% 25% .
1	T	122	 65% 34% ..
1	U	122	 77% 20% ..
1	V	122	 68% 26% ..
1	W	122	 69% 29% ..
1	X	122	 72% 26% .

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 22771 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 Tetraspanin-15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	122	Total 956	C 606	N 156	O 183	S 11	0	0	0
1	A	122	Total 973	C 610	N 162	O 190	S 11	0	0	0
1	C	122	Total 950	C 596	N 158	O 185	S 11	0	0	0
1	D	121	Total 949	C 599	N 159	O 180	S 11	0	0	0
1	E	122	Total 950	C 597	N 160	O 182	S 11	0	0	0
1	F	122	Total 972	C 615	N 160	O 186	S 11	0	0	0
1	G	122	Total 970	C 610	N 163	O 186	S 11	0	0	0
1	H	122	Total 948	C 592	N 159	O 186	S 11	0	0	0
1	I	122	Total 958	C 602	N 164	O 181	S 11	0	0	0
1	J	121	Total 934	C 585	N 156	O 182	S 11	0	0	0
1	K	122	Total 954	C 599	N 159	O 185	S 11	0	0	0
1	L	122	Total 948	C 596	N 156	O 185	S 11	0	0	0
1	M	122	Total 966	C 615	N 160	O 180	S 11	0	0	0
1	N	122	Total 954	C 602	N 160	O 181	S 11	0	0	0
1	O	121	Total 950	C 598	N 162	O 179	S 11	0	0	0
1	P	122	Total 950	C 599	N 158	O 182	S 11	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	122	939	591	156	181	11	0	0	0
1	R	122	958	605	160	182	11	0	0	0
1	S	122	943	593	158	181	11	0	0	0
1	T	121	950	601	156	182	11	0	0	0
1	U	121	931	589	153	178	11	0	0	0
1	V	119	908	570	151	176	11	0	0	0
1	W	121	917	578	152	176	11	0	0	0
1	X	122	902	568	147	177	10	0	0	0

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	118	GLN	ASN	engineered mutation	UNP O95858
B	189	ASP	ASN	engineered mutation	UNP O95858
B	231	LEU	-	expression tag	UNP O95858
B	232	GLU	-	expression tag	UNP O95858
B	233	VAL	-	expression tag	UNP O95858
B	234	LEU	-	expression tag	UNP O95858
B	235	PHE	-	expression tag	UNP O95858
B	236	GLN	-	expression tag	UNP O95858
A	118	GLN	ASN	engineered mutation	UNP O95858
A	189	ASP	ASN	engineered mutation	UNP O95858
A	231	LEU	-	expression tag	UNP O95858
A	232	GLU	-	expression tag	UNP O95858
A	233	VAL	-	expression tag	UNP O95858
A	234	LEU	-	expression tag	UNP O95858
A	235	PHE	-	expression tag	UNP O95858
A	236	GLN	-	expression tag	UNP O95858
C	118	GLN	ASN	engineered mutation	UNP O95858
C	189	ASP	ASN	engineered mutation	UNP O95858
C	231	LEU	-	expression tag	UNP O95858
C	232	GLU	-	expression tag	UNP O95858
C	233	VAL	-	expression tag	UNP O95858
C	234	LEU	-	expression tag	UNP O95858
C	235	PHE	-	expression tag	UNP O95858

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	236	GLN	-	expression tag	UNP 095858
D	118	GLN	ASN	engineered mutation	UNP 095858
D	189	ASP	ASN	engineered mutation	UNP 095858
D	231	LEU	-	expression tag	UNP 095858
D	232	GLU	-	expression tag	UNP 095858
D	233	VAL	-	expression tag	UNP 095858
D	234	LEU	-	expression tag	UNP 095858
D	235	PHE	-	expression tag	UNP 095858
D	236	GLN	-	expression tag	UNP 095858
E	118	GLN	ASN	engineered mutation	UNP 095858
E	189	ASP	ASN	engineered mutation	UNP 095858
E	231	LEU	-	expression tag	UNP 095858
E	232	GLU	-	expression tag	UNP 095858
E	233	VAL	-	expression tag	UNP 095858
E	234	LEU	-	expression tag	UNP 095858
E	235	PHE	-	expression tag	UNP 095858
E	236	GLN	-	expression tag	UNP 095858
F	118	GLN	ASN	engineered mutation	UNP 095858
F	189	ASP	ASN	engineered mutation	UNP 095858
F	231	LEU	-	expression tag	UNP 095858
F	232	GLU	-	expression tag	UNP 095858
F	233	VAL	-	expression tag	UNP 095858
F	234	LEU	-	expression tag	UNP 095858
F	235	PHE	-	expression tag	UNP 095858
F	236	GLN	-	expression tag	UNP 095858
G	118	GLN	ASN	engineered mutation	UNP 095858
G	189	ASP	ASN	engineered mutation	UNP 095858
G	231	LEU	-	expression tag	UNP 095858
G	232	GLU	-	expression tag	UNP 095858
G	233	VAL	-	expression tag	UNP 095858
G	234	LEU	-	expression tag	UNP 095858
G	235	PHE	-	expression tag	UNP 095858
G	236	GLN	-	expression tag	UNP 095858
H	118	GLN	ASN	engineered mutation	UNP 095858
H	189	ASP	ASN	engineered mutation	UNP 095858
H	231	LEU	-	expression tag	UNP 095858
H	232	GLU	-	expression tag	UNP 095858
H	233	VAL	-	expression tag	UNP 095858
H	234	LEU	-	expression tag	UNP 095858
H	235	PHE	-	expression tag	UNP 095858
H	236	GLN	-	expression tag	UNP 095858
I	118	GLN	ASN	engineered mutation	UNP 095858

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	189	ASP	ASN	engineered mutation	UNP 095858
I	231	LEU	-	expression tag	UNP 095858
I	232	GLU	-	expression tag	UNP 095858
I	233	VAL	-	expression tag	UNP 095858
I	234	LEU	-	expression tag	UNP 095858
I	235	PHE	-	expression tag	UNP 095858
I	236	GLN	-	expression tag	UNP 095858
J	118	GLN	ASN	engineered mutation	UNP 095858
J	189	ASP	ASN	engineered mutation	UNP 095858
J	231	LEU	-	expression tag	UNP 095858
J	232	GLU	-	expression tag	UNP 095858
J	233	VAL	-	expression tag	UNP 095858
J	234	LEU	-	expression tag	UNP 095858
J	235	PHE	-	expression tag	UNP 095858
J	236	GLN	-	expression tag	UNP 095858
K	118	GLN	ASN	engineered mutation	UNP 095858
K	189	ASP	ASN	engineered mutation	UNP 095858
K	231	LEU	-	expression tag	UNP 095858
K	232	GLU	-	expression tag	UNP 095858
K	233	VAL	-	expression tag	UNP 095858
K	234	LEU	-	expression tag	UNP 095858
K	235	PHE	-	expression tag	UNP 095858
K	236	GLN	-	expression tag	UNP 095858
L	118	GLN	ASN	engineered mutation	UNP 095858
L	189	ASP	ASN	engineered mutation	UNP 095858
L	231	LEU	-	expression tag	UNP 095858
L	232	GLU	-	expression tag	UNP 095858
L	233	VAL	-	expression tag	UNP 095858
L	234	LEU	-	expression tag	UNP 095858
L	235	PHE	-	expression tag	UNP 095858
L	236	GLN	-	expression tag	UNP 095858
M	118	GLN	ASN	engineered mutation	UNP 095858
M	189	ASP	ASN	engineered mutation	UNP 095858
M	231	LEU	-	expression tag	UNP 095858
M	232	GLU	-	expression tag	UNP 095858
M	233	VAL	-	expression tag	UNP 095858
M	234	LEU	-	expression tag	UNP 095858
M	235	PHE	-	expression tag	UNP 095858
M	236	GLN	-	expression tag	UNP 095858
N	118	GLN	ASN	engineered mutation	UNP 095858
N	189	ASP	ASN	engineered mutation	UNP 095858
N	231	LEU	-	expression tag	UNP 095858

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
N	232	GLU	-	expression tag	UNP 095858
N	233	VAL	-	expression tag	UNP 095858
N	234	LEU	-	expression tag	UNP 095858
N	235	PHE	-	expression tag	UNP 095858
N	236	GLN	-	expression tag	UNP 095858
O	118	GLN	ASN	engineered mutation	UNP 095858
O	189	ASP	ASN	engineered mutation	UNP 095858
O	231	LEU	-	expression tag	UNP 095858
O	232	GLU	-	expression tag	UNP 095858
O	233	VAL	-	expression tag	UNP 095858
O	234	LEU	-	expression tag	UNP 095858
O	235	PHE	-	expression tag	UNP 095858
O	236	GLN	-	expression tag	UNP 095858
P	118	GLN	ASN	engineered mutation	UNP 095858
P	189	ASP	ASN	engineered mutation	UNP 095858
P	231	LEU	-	expression tag	UNP 095858
P	232	GLU	-	expression tag	UNP 095858
P	233	VAL	-	expression tag	UNP 095858
P	234	LEU	-	expression tag	UNP 095858
P	235	PHE	-	expression tag	UNP 095858
P	236	GLN	-	expression tag	UNP 095858
Q	118	GLN	ASN	engineered mutation	UNP 095858
Q	189	ASP	ASN	engineered mutation	UNP 095858
Q	231	LEU	-	expression tag	UNP 095858
Q	232	GLU	-	expression tag	UNP 095858
Q	233	VAL	-	expression tag	UNP 095858
Q	234	LEU	-	expression tag	UNP 095858
Q	235	PHE	-	expression tag	UNP 095858
Q	236	GLN	-	expression tag	UNP 095858
R	118	GLN	ASN	engineered mutation	UNP 095858
R	189	ASP	ASN	engineered mutation	UNP 095858
R	231	LEU	-	expression tag	UNP 095858
R	232	GLU	-	expression tag	UNP 095858
R	233	VAL	-	expression tag	UNP 095858
R	234	LEU	-	expression tag	UNP 095858
R	235	PHE	-	expression tag	UNP 095858
R	236	GLN	-	expression tag	UNP 095858
S	118	GLN	ASN	engineered mutation	UNP 095858
S	189	ASP	ASN	engineered mutation	UNP 095858
S	231	LEU	-	expression tag	UNP 095858
S	232	GLU	-	expression tag	UNP 095858
S	233	VAL	-	expression tag	UNP 095858

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
S	234	LEU	-	expression tag	UNP 095858
S	235	PHE	-	expression tag	UNP 095858
S	236	GLN	-	expression tag	UNP 095858
T	118	GLN	ASN	engineered mutation	UNP 095858
T	189	ASP	ASN	engineered mutation	UNP 095858
T	231	LEU	-	expression tag	UNP 095858
T	232	GLU	-	expression tag	UNP 095858
T	233	VAL	-	expression tag	UNP 095858
T	234	LEU	-	expression tag	UNP 095858
T	235	PHE	-	expression tag	UNP 095858
T	236	GLN	-	expression tag	UNP 095858
U	118	GLN	ASN	engineered mutation	UNP 095858
U	189	ASP	ASN	engineered mutation	UNP 095858
U	231	LEU	-	expression tag	UNP 095858
U	232	GLU	-	expression tag	UNP 095858
U	233	VAL	-	expression tag	UNP 095858
U	234	LEU	-	expression tag	UNP 095858
U	235	PHE	-	expression tag	UNP 095858
U	236	GLN	-	expression tag	UNP 095858
V	118	GLN	ASN	engineered mutation	UNP 095858
V	189	ASP	ASN	engineered mutation	UNP 095858
V	231	LEU	-	expression tag	UNP 095858
V	232	GLU	-	expression tag	UNP 095858
V	233	VAL	-	expression tag	UNP 095858
V	234	LEU	-	expression tag	UNP 095858
V	235	PHE	-	expression tag	UNP 095858
V	236	GLN	-	expression tag	UNP 095858
W	118	GLN	ASN	engineered mutation	UNP 095858
W	189	ASP	ASN	engineered mutation	UNP 095858
W	231	LEU	-	expression tag	UNP 095858
W	232	GLU	-	expression tag	UNP 095858
W	233	VAL	-	expression tag	UNP 095858
W	234	LEU	-	expression tag	UNP 095858
W	235	PHE	-	expression tag	UNP 095858
W	236	GLN	-	expression tag	UNP 095858
X	118	GLN	ASN	engineered mutation	UNP 095858
X	189	ASP	ASN	engineered mutation	UNP 095858
X	231	LEU	-	expression tag	UNP 095858
X	232	GLU	-	expression tag	UNP 095858
X	233	VAL	-	expression tag	UNP 095858
X	234	LEU	-	expression tag	UNP 095858
X	235	PHE	-	expression tag	UNP 095858

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
X	236	GLN	-	expression tag	UNP O95858

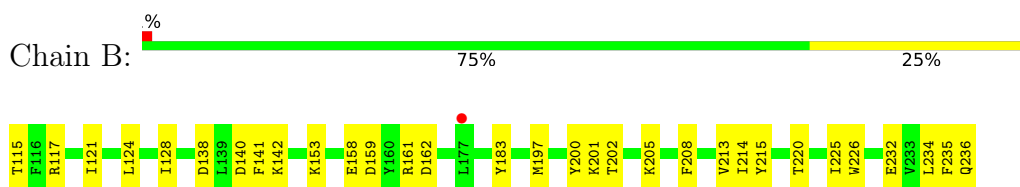
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	5	Total O 5 5	0	0
2	A	4	Total O 4 4	0	0
2	C	6	Total O 6 6	0	0
2	D	1	Total O 1 1	0	0
2	E	4	Total O 4 4	0	0
2	F	6	Total O 6 6	0	0
2	G	3	Total O 3 3	0	0
2	H	4	Total O 4 4	0	0
2	I	3	Total O 3 3	0	0
2	J	1	Total O 1 1	0	0
2	L	2	Total O 2 2	0	0
2	M	1	Total O 1 1	0	0
2	V	1	Total O 1 1	0	0

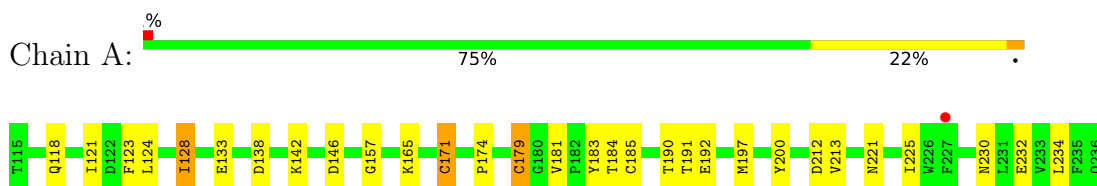
3 Residue-property plots [i](#)

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.

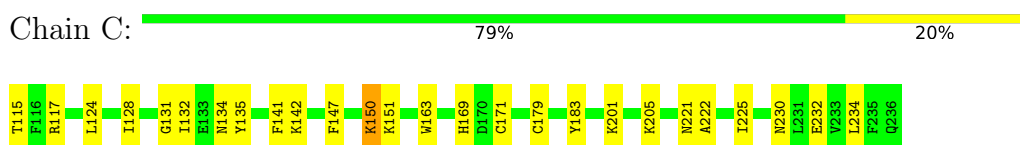
- Molecule 1: Tetraspanin-15



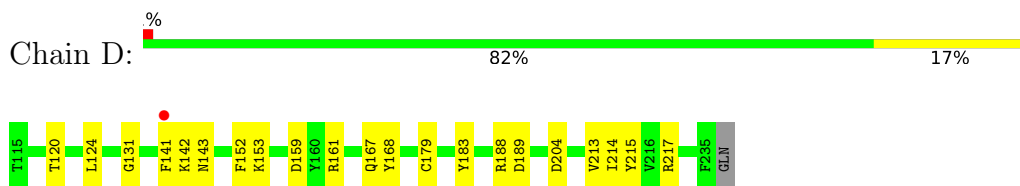
- Molecule 1: Tetraspanin-15



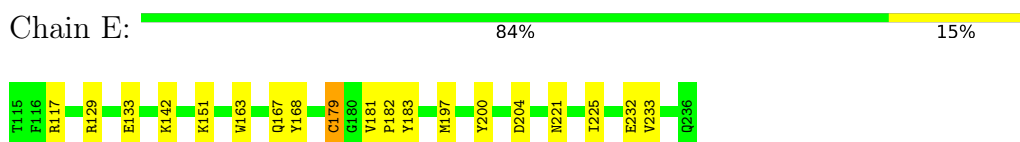
- Molecule 1: Tetraspanin-15



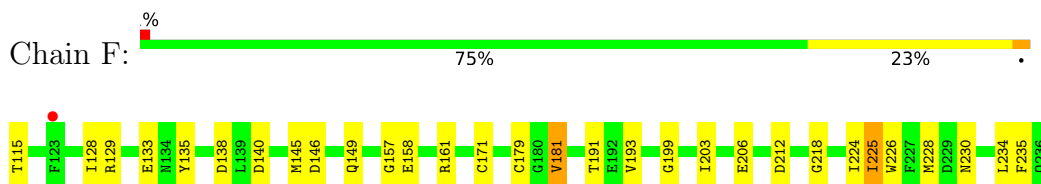
- Molecule 1: Tetraspanin-15



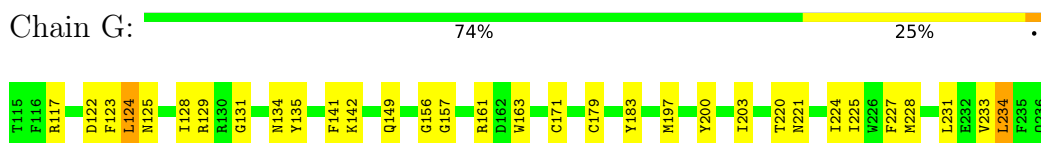
- Molecule 1: Tetraspanin-15



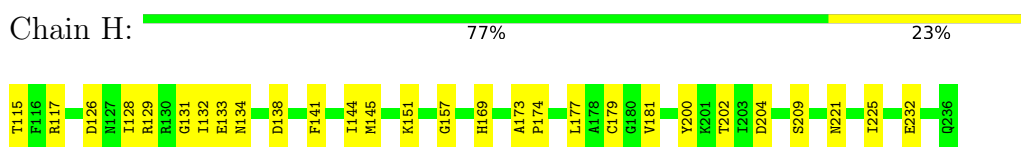
- Molecule 1: Tetraspanin-15



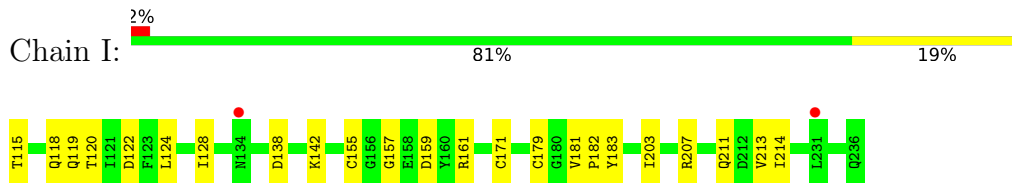
- Molecule 1: Tetraspanin-15



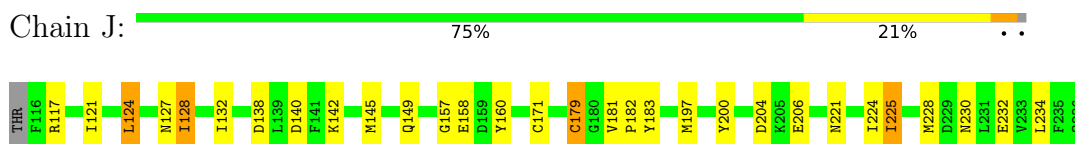
- Molecule 1: Tetraspanin-15



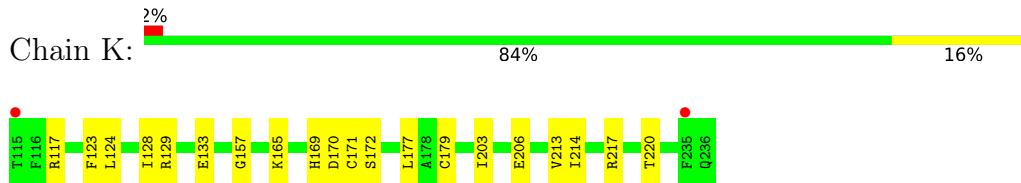
- Molecule 1: Tetraspanin-15



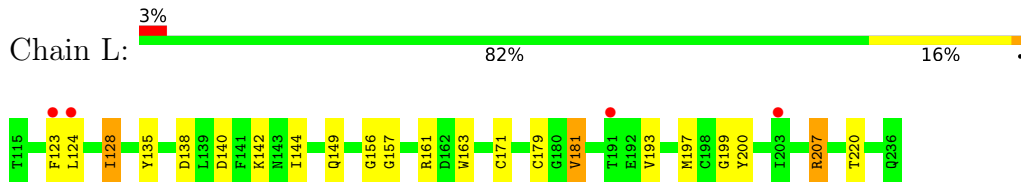
- Molecule 1: Tetraspanin-15



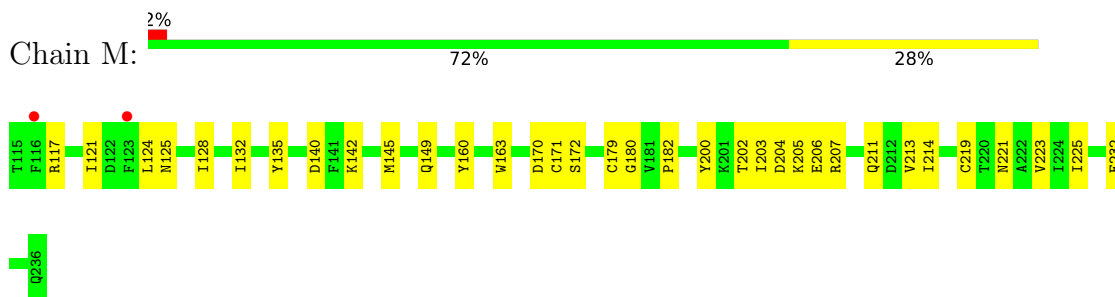
- Molecule 1: Tetraspanin-15



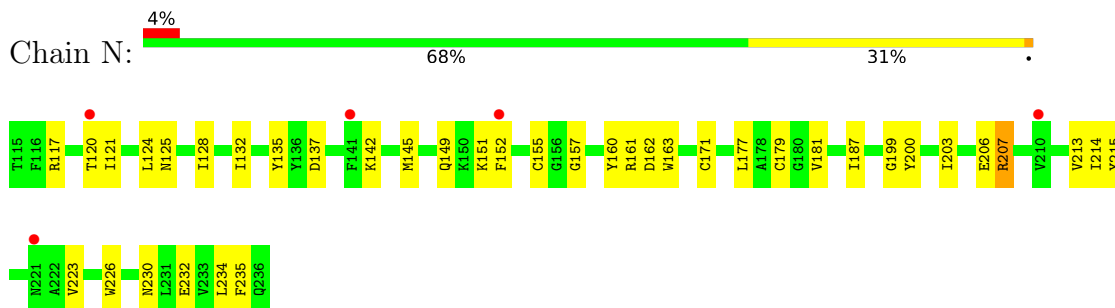
- Molecule 1: Tetraspanin-15



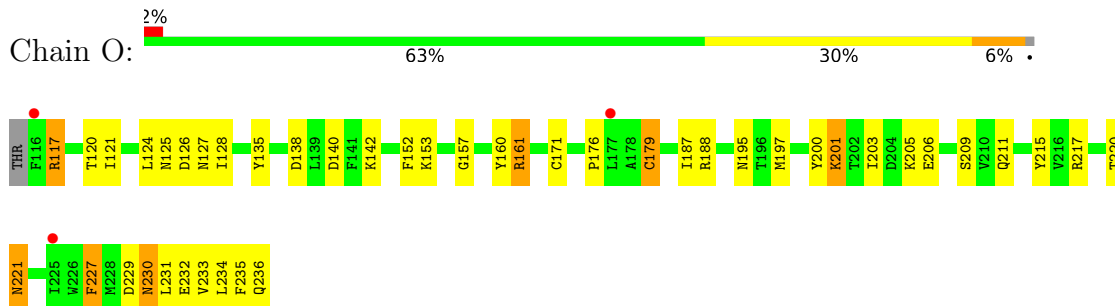
- Molecule 1: Tetraspanin-15



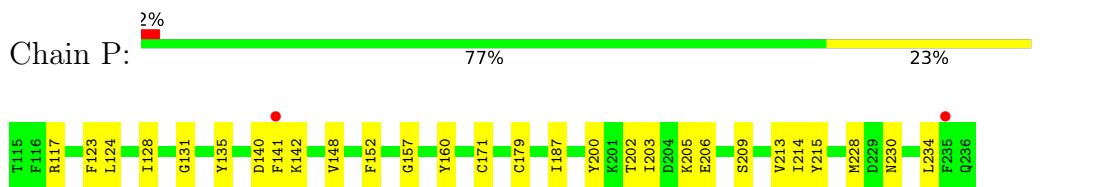
- Molecule 1: Tetraspanin-15



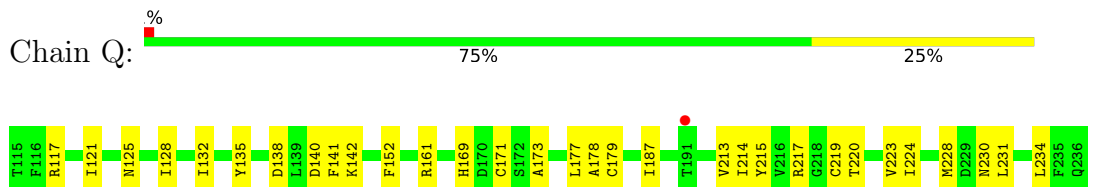
- Molecule 1: Tetraspanin-15



- Molecule 1: Tetraspanin-15

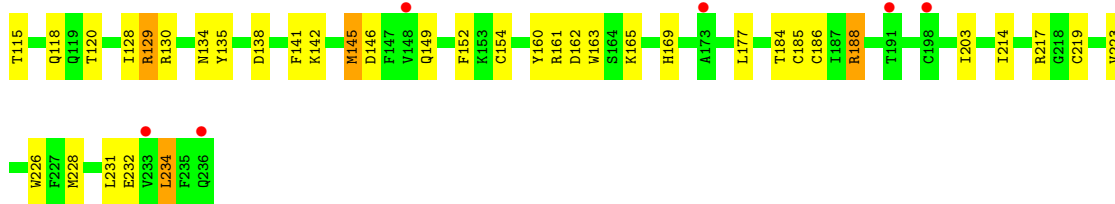


- Molecule 1: Tetraspanin-15

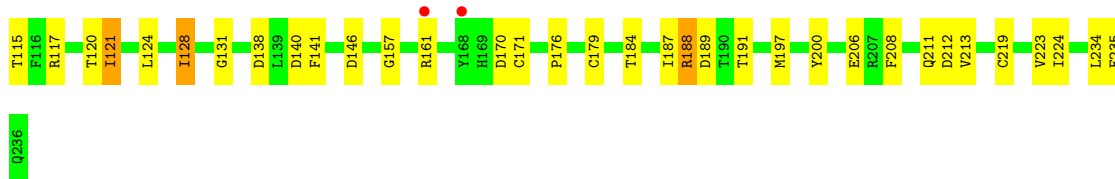


- Molecule 1: Tetraspanin-15

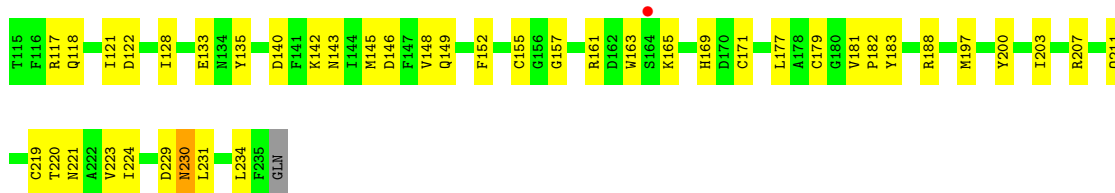




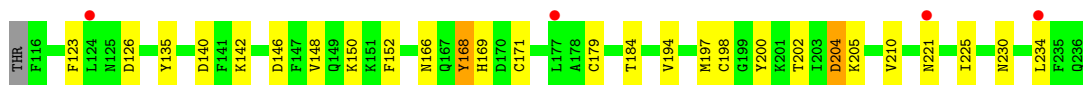
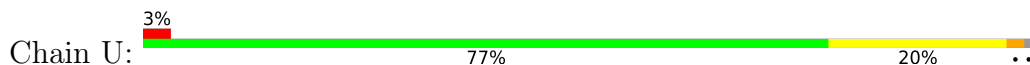
• Molecule 1: Tetraspanin-15



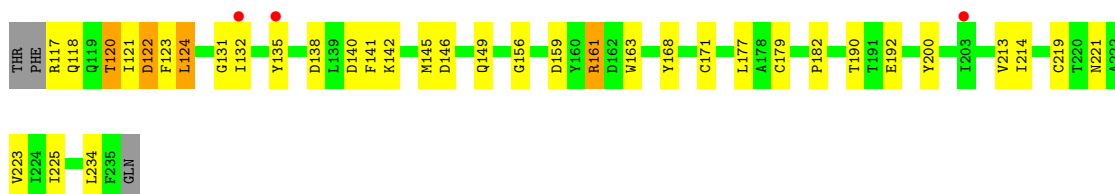
• Molecule 1: Tetraspanin-15



• Molecule 1: Tetraspanin-15

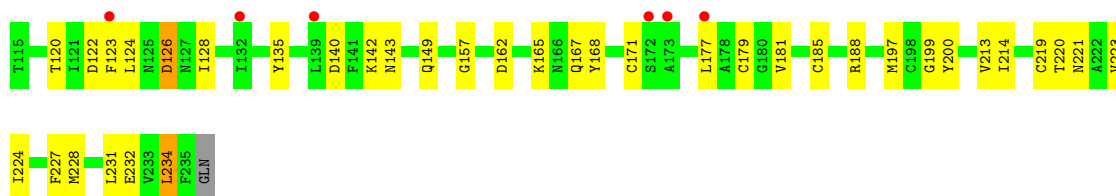


• Molecule 1: Tetraspanin-15

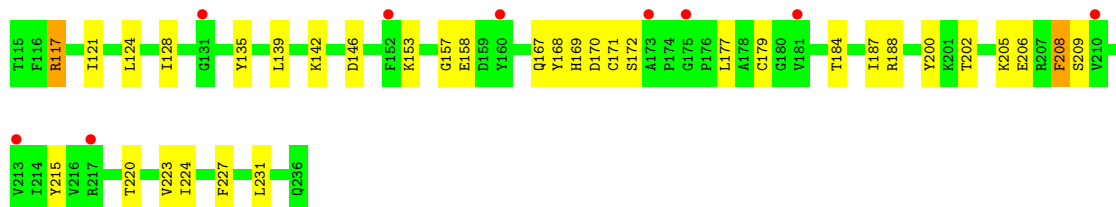
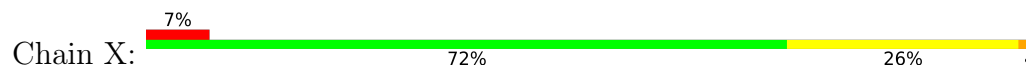


• Molecule 1: Tetraspanin-15





• Molecule 1: Tetraspanin-15



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	83.57Å 91.95Å 112.38Å 87.55° 86.52° 86.24°	Depositor
Resolution (Å)	48.67 – 2.52 48.67 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.67-2.52) 99.4 (48.67-2.52)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122+SVN	Depositor
R, R_{free}	0.235 , 0.273 0.232 , 0.271	Depositor DCC
R_{free} test set	1971 reflections (1.76%)	wwPDB-VP
Wilson B-factor (Å ²)	76.7	Xtrriage
Anisotropy	0.113	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22771	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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	A	0.70	3/993 (0.3%)	0.87	3/1346 (0.2%)
1	B	0.62	0/977	0.75	0/1326
1	C	0.59	1/969 (0.1%)	0.75	0/1317
1	D	0.69	0/969	0.70	0/1314
1	E	0.60	0/969	0.75	0/1315
1	F	0.62	0/993	0.82	1/1346 (0.1%)
1	G	0.65	0/990	0.87	3/1341 (0.2%)
1	H	0.62	0/966	0.83	1/1310 (0.1%)
1	I	0.56	0/977	0.79	0/1323
1	J	0.71	4/952 (0.4%)	0.79	3/1293 (0.2%)
1	K	0.62	1/973 (0.1%)	0.77	1/1320 (0.1%)
1	L	0.55	0/967	0.91	4/1313 (0.3%)
1	M	0.49	0/988	0.75	0/1338
1	N	0.52	0/974	0.79	3/1321 (0.2%)
1	O	0.71	2/969 (0.2%)	0.85	2/1312 (0.2%)
1	P	0.56	0/970	0.70	0/1317
1	Q	0.47	0/958	0.64	0/1300
1	R	0.70	4/978 (0.4%)	0.81	1/1325 (0.1%)
1	S	0.61	0/962	0.79	3/1307 (0.2%)
1	T	0.54	0/970	0.76	0/1316
1	U	0.51	0/951	0.73	1/1293 (0.1%)
1	V	0.48	0/927	0.67	0/1263
1	W	0.60	0/935	0.82	2/1273 (0.2%)
1	X	1.04	8/921 (0.9%)	0.82	1/1260 (0.1%)
All	All	0.63	23/23198 (0.1%)	0.78	29/31489 (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

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	158	GLU	CD-OE2	13.05	1.40	1.25
1	X	206	GLU	CD-OE1	10.50	1.37	1.25
1	X	158	GLU	CD-OE1	10.32	1.37	1.25
1	X	206	GLU	CD-OE2	10.32	1.37	1.25
1	X	206	GLU	CB-CG	9.33	1.69	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	207	ARG	NE-CZ-NH2	-17.80	111.40	120.30
1	L	207	ARG	CD-NE-CZ	11.42	139.59	123.60
1	N	207	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	N	207	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	A	171	CYS	CA-CB-SG	7.41	127.33	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	207	ARG	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	A	973	0	890	21	0
1	B	956	0	870	23	1
1	C	950	0	857	21	0
1	D	949	0	869	20	0
1	E	950	0	869	13	1
1	F	972	0	898	24	4
1	G	970	0	895	22	0
1	H	948	0	862	23	0
1	I	958	0	886	15	0
1	J	934	0	842	20	1
1	K	954	0	871	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	948	0	860	21	0
1	M	966	0	890	23	1
1	N	954	0	871	35	0
1	O	950	0	880	45	2
1	P	950	0	858	19	4
1	Q	939	0	847	23	1
1	R	958	0	880	26	1
1	S	943	0	854	31	3
1	T	950	0	871	36	0
1	U	931	0	835	16	3
1	V	908	0	801	31	1
1	W	917	0	825	24	2
1	X	902	0	763	30	1
2	A	4	0	0	0	0
2	B	5	0	0	0	0
2	C	6	0	0	0	0
2	D	1	0	0	0	0
2	E	4	0	0	0	0
2	F	6	0	0	0	0
2	G	3	0	0	0	0
2	H	4	0	0	0	0
2	I	3	0	0	0	0
2	J	1	0	0	0	0
2	L	2	0	0	0	0
2	M	1	0	0	0	0
2	V	1	0	0	1	0
All	All	22771	0	20644	535	13

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 12.

The worst 5 of 535 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)
1:S:187:ILE:CD1	1:S:213:VAL:O	1.86	1.23
1:S:187:ILE:HD12	1:S:213:VAL:O	0.97	1.11
1:S:187:ILE:HD12	1:S:213:VAL:C	1.77	1.04
1:O:195:ASN:ND2	1:O:197:MET:HB2	1.70	1.04
1:O:171:CYS:HA	1:O:179:CYS:HB2	1.47	0.96

The worst 5 of 13 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)
1:F:140:ASP:OD2	1:S:117:ARG:NH2[1_564]	1.90	0.30
1:S:188:ARG:NH2	1:W:143:ASN:OD1[1_556]	1.91	0.29
1:U:150:LYS:NZ	1:W:232:GLU:OE2[1_465]	1.93	0.27
1:U:140:ASP:OD1	1:X:188:ARG:NH2[1_554]	1.97	0.23
1:Q:161:ARG:NH1	1:S:170:ASP:OD2[1_554]	1.99	0.21

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	A	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	B	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	C	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	D	119/122 (98%)	112 (94%)	7 (6%)	0	100	100
1	E	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
1	F	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	G	120/122 (98%)	104 (87%)	16 (13%)	0	100	100
1	H	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
1	I	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
1	J	119/122 (98%)	109 (92%)	10 (8%)	0	100	100
1	K	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	L	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
1	M	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	N	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	O	119/122 (98%)	113 (95%)	6 (5%)	0	100	100
1	P	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
1	Q	120/122 (98%)	115 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
1	S	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
1	T	119/122 (98%)	114 (96%)	5 (4%)	0	100	100
1	U	119/122 (98%)	114 (96%)	5 (4%)	0	100	100
1	V	117/122 (96%)	113 (97%)	4 (3%)	0	100	100
1	W	119/122 (98%)	113 (95%)	6 (5%)	0	100	100
1	X	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
All	All	2871/2928 (98%)	2698 (94%)	173 (6%)	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	A	106/112 (95%)	106 (100%)	0	100	100
1	B	102/112 (91%)	102 (100%)	0	100	100
1	C	101/112 (90%)	101 (100%)	0	100	100
1	D	101/112 (90%)	100 (99%)	1 (1%)	76	89
1	E	101/112 (90%)	100 (99%)	1 (1%)	76	89
1	F	106/112 (95%)	105 (99%)	1 (1%)	78	91
1	G	105/112 (94%)	105 (100%)	0	100	100
1	H	101/112 (90%)	100 (99%)	1 (1%)	76	89
1	I	102/112 (91%)	100 (98%)	2 (2%)	55	78
1	J	98/112 (88%)	98 (100%)	0	100	100
1	K	102/112 (91%)	102 (100%)	0	100	100
1	L	101/112 (90%)	101 (100%)	0	100	100
1	M	103/112 (92%)	103 (100%)	0	100	100
1	N	101/112 (90%)	100 (99%)	1 (1%)	76	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	101/112 (90%)	96 (95%)	5 (5%)	24	44
1	P	100/112 (89%)	100 (100%)	0	100	100
1	Q	98/112 (88%)	98 (100%)	0	100	100
1	R	102/112 (91%)	98 (96%)	4 (4%)	32	55
1	S	99/112 (88%)	94 (95%)	5 (5%)	24	43
1	T	102/112 (91%)	100 (98%)	2 (2%)	55	78
1	U	97/112 (87%)	96 (99%)	1 (1%)	76	89
1	V	94/112 (84%)	89 (95%)	5 (5%)	22	40
1	W	95/112 (85%)	93 (98%)	2 (2%)	53	76
1	X	88/112 (79%)	88 (100%)	0	100	100
All	All	2406/2688 (90%)	2375 (99%)	31 (1%)	69	86

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	231	LEU
1	V	124	LEU
1	S	120	THR
1	W	126	ASP
1	V	120	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	V	221	ASN
1	V	149	GLN
1	P	118	GLN
1	U	143	ASN
1	O	221	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	122/122 (100%)	0.24	1 (0%) 86 88	52, 71, 101, 115	0
1	B	122/122 (100%)	0.03	1 (0%) 86 88	57, 76, 107, 117	0
1	C	122/122 (100%)	-0.19	0 100 100	54, 74, 115, 134	0
1	D	121/122 (99%)	-0.03	1 (0%) 86 88	60, 79, 114, 144	0
1	E	122/122 (100%)	-0.07	0 100 100	59, 78, 117, 138	0
1	F	122/122 (100%)	0.14	1 (0%) 86 88	57, 76, 108, 128	0
1	G	122/122 (100%)	0.15	0 100 100	59, 83, 111, 140	0
1	H	122/122 (100%)	-0.06	0 100 100	58, 78, 119, 135	0
1	I	122/122 (100%)	0.09	2 (1%) 72 74	63, 87, 115, 126	0
1	J	121/122 (99%)	0.08	0 100 100	64, 83, 136, 146	0
1	K	122/122 (100%)	-0.11	2 (1%) 72 74	61, 92, 122, 143	0
1	L	122/122 (100%)	0.09	4 (3%) 46 50	68, 88, 130, 148	0
1	M	122/122 (100%)	0.10	2 (1%) 72 74	69, 91, 126, 154	0
1	N	122/122 (100%)	0.35	5 (4%) 37 41	73, 102, 129, 137	0
1	O	121/122 (99%)	0.15	3 (2%) 57 61	74, 110, 153, 167	0
1	P	122/122 (100%)	0.08	2 (1%) 72 74	72, 101, 132, 151	0
1	Q	122/122 (100%)	0.08	1 (0%) 86 88	74, 98, 125, 155	0
1	R	122/122 (100%)	0.28	6 (4%) 29 32	81, 104, 133, 151	0
1	S	122/122 (100%)	0.06	2 (1%) 72 74	74, 105, 138, 162	0
1	T	121/122 (99%)	0.13	1 (0%) 86 88	77, 110, 129, 134	0
1	U	121/122 (99%)	0.29	4 (3%) 46 50	87, 104, 149, 167	0
1	V	119/122 (97%)	0.30	3 (2%) 57 61	85, 111, 151, 163	0
1	W	121/122 (99%)	0.23	6 (4%) 28 31	83, 115, 147, 156	0
1	X	122/122 (100%)	0.24	9 (7%) 14 15	96, 129, 156, 171	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	2919/2928 (99%)	0.11	56 (1%) 66 70	52, 94, 138, 171	0

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	132	ILE	4.9
1	W	173	ALA	4.7
1	V	203	ILE	4.4
1	V	135	TYR	4.1
1	P	235	PHE	3.9

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.