



wwPDB X-ray Structure Validation Summary Report

Oct 11, 2023 – 02:01 PM EDT

PDB ID : 7RD5
Title : Crystal structure of Tspan15 large extracellular loop (Tspan15 LEL) in complex with 1C12 Fab
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 : 3.60 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

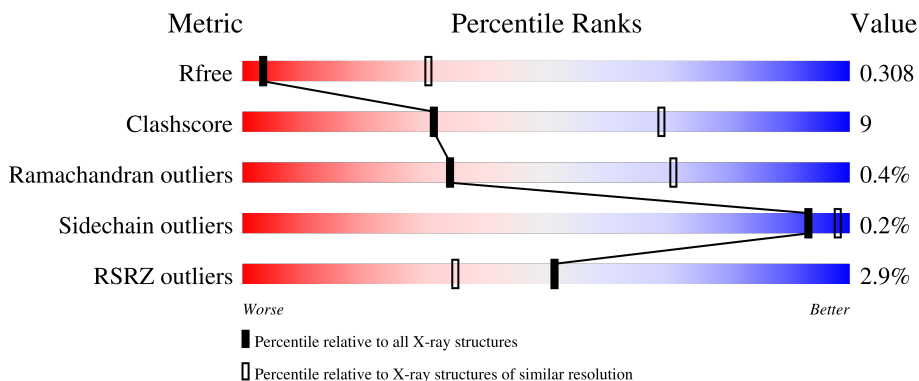
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	220	 7% 82% 18%
1	C	220	 3% 78% 21%
2	B	226	 % 77% 23%
2	D	226	 % 79% 21%
3	E	122	 2% 81% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	122	 <p>5% 83% 17%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8279 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 1C12 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	220	1593	996	262	328	7	0	0	0
1	C	220	1584	992	261	324	7	0	0	0

- Molecule 2 is a protein called 1C12 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	226	1614	1035	256	316	7	0	0	0
2	D	226	1621	1037	258	319	7	0	0	0

- Molecule 3 is a protein called Tetraspanin-15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	F	122	937	589	154	183	11	0	0	0
3	E	122	930	587	151	181	11	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

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

Continued on next page...

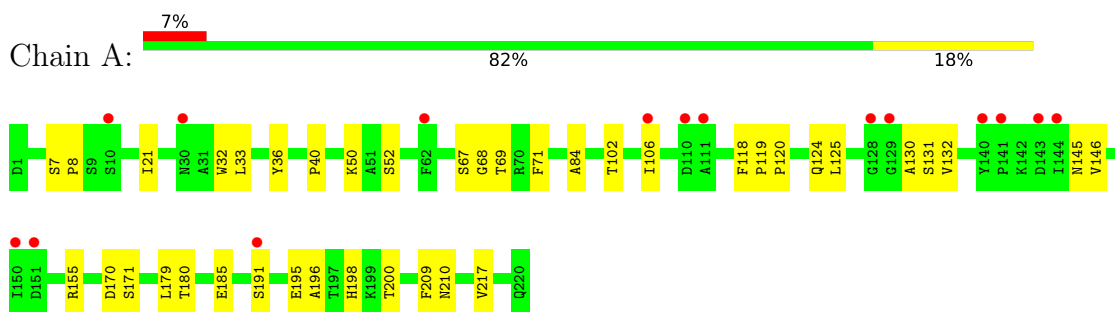
Continued from previous page...

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

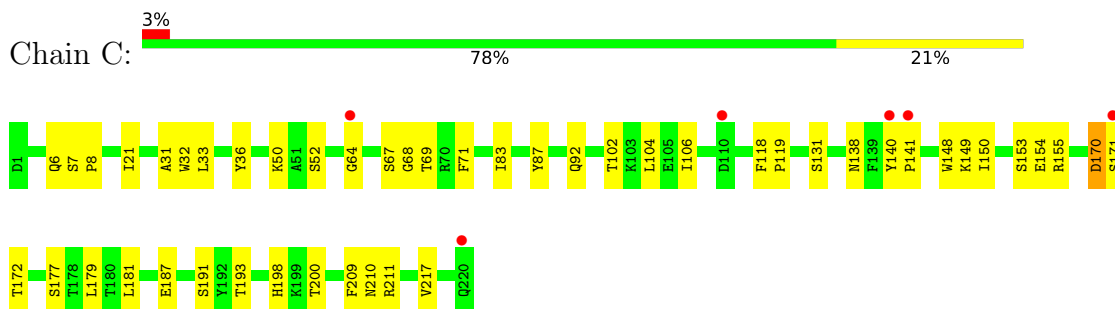
3 Residue-property plots [i](#)

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.

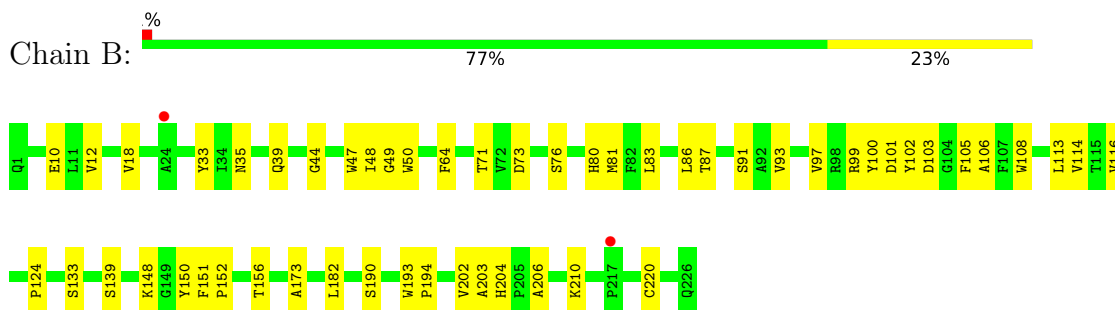
- Molecule 1: 1C12 Fab Light Chain



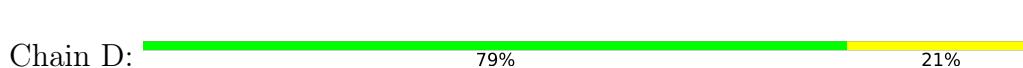
- Molecule 1: 1C12 Fab Light Chain

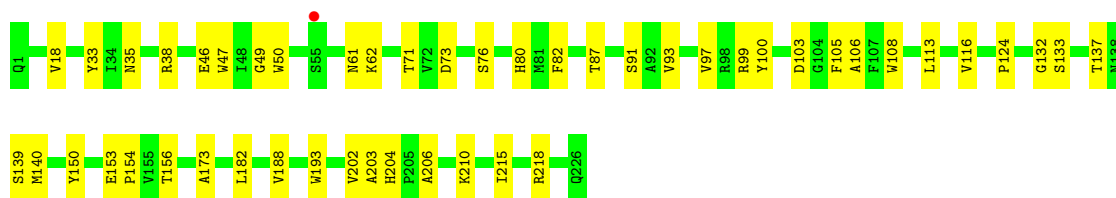


- Molecule 2: 1C12 Fab Heavy Chain

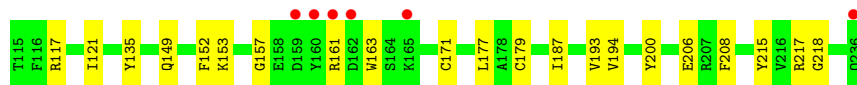
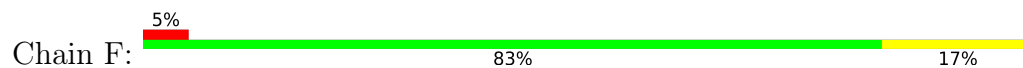


- Molecule 2: 1C12 Fab Heavy Chain

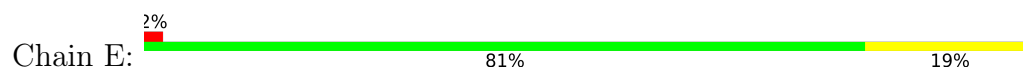




- Molecule 3: Tetraspanin-15



- Molecule 3: Tetraspanin-15



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	171.30Å 124.64Å 116.12Å 90.00° 98.17° 90.00°	Depositor
Resolution (Å)	47.50 – 3.60 47.50 – 3.60	Depositor EDS
% Data completeness (in resolution range)	95.6 (47.50-3.60) 95.6 (47.50-3.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.57Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122+SVN	Depositor
R, R_{free}	0.271 , 0.309 0.270 , 0.308	Depositor DCC
R_{free} test set	1983 reflections (7.34%)	wwPDB-VP
Wilson B-factor (Å ²)	121.6	Xtrriage
Anisotropy	0.256	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 83.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8279	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.52 % 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 8.5014e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.28	0/1630	0.53	0/2236
1	C	0.27	0/1621	0.53	0/2224
2	B	0.28	0/1663	0.52	0/2300
2	D	0.27	0/1669	0.52	0/2308
3	E	0.27	0/950	0.49	0/1294
3	F	0.27	0/957	0.50	0/1302
All	All	0.28	0/8490	0.52	0/11664

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	102	TYR	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	A	1593	0	1428	24	0
1	C	1584	0	1415	32	0
2	B	1614	0	1460	35	0
2	D	1621	0	1472	32	0
3	E	930	0	819	15	0
3	F	937	0	825	14	0
All	All	8279	0	7419	141	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 9.

The worst 5 of 141 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:D:132:GLY:HA2	2:D:218:ARG:HD2	1.56	0.87
1:C:149:LYS:HE2	1:C:154:GLU:HG3	1.60	0.84
1:C:106:ILE:HG21	1:C:171:SER:HB3	1.57	0.84
2:D:91:SER:HB2	2:D:116:VAL:HG22	1.61	0.83
1:C:155:ARG:HH12	1:C:181:LEU:HG	1.57	0.68

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	A	218/220 (99%)	203 (93%)	13 (6%)	2 (1%)	17	57
1	C	218/220 (99%)	202 (93%)	14 (6%)	2 (1%)	17	57
2	B	224/226 (99%)	219 (98%)	5 (2%)	0	100	100
2	D	224/226 (99%)	219 (98%)	5 (2%)	0	100	100
3	E	120/122 (98%)	111 (92%)	9 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
All	All	1124/1136 (99%)	1066 (95%)	54 (5%)	4 (0%)	34	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	GLY
1	C	68	GLY
1	A	170	ASP
1	C	170	ASP

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	168/196 (86%)	168 (100%)	0	100	100
1	C	165/196 (84%)	164 (99%)	1 (1%)	86	94
2	B	168/196 (86%)	167 (99%)	1 (1%)	86	94
2	D	170/196 (87%)	170 (100%)	0	100	100
3	E	96/112 (86%)	96 (100%)	0	100	100
3	F	97/112 (87%)	97 (100%)	0	100	100
All	All	864/1008 (86%)	862 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	220	CYS
1	C	153	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

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	220/220 (100%)	0.19	15 (6%) 17 10	103, 137, 180, 216	0
1	C	220/220 (100%)	0.07	6 (2%) 54 38	90, 119, 167, 213	0
2	B	226/226 (100%)	-0.03	2 (0%) 84 73	105, 135, 165, 231	0
2	D	226/226 (100%)	-0.13	1 (0%) 92 86	87, 121, 149, 201	0
3	E	122/122 (100%)	-0.08	3 (2%) 57 41	82, 105, 191, 263	0
3	F	122/122 (100%)	0.00	6 (4%) 29 18	95, 117, 154, 222	0
All	All	1136/1136 (100%)	0.01	33 (2%) 51 35	82, 125, 172, 263	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	236	GLN	5.1
1	C	110	ASP	4.6
1	C	171	SER	4.2
1	A	151	ASP	3.5
3	F	159	ASP	3.4

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.