wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2022 – 01:19 pm BST

PDB ID	:	7ZLX
Title	:	Crystal Structure of the TSG101-UEV domain:space group P21
Authors	:	Camara-Artigas, A.
Deposited on	:	2022-04-16
Resolution	:	2.25 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 (i) symbol.

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

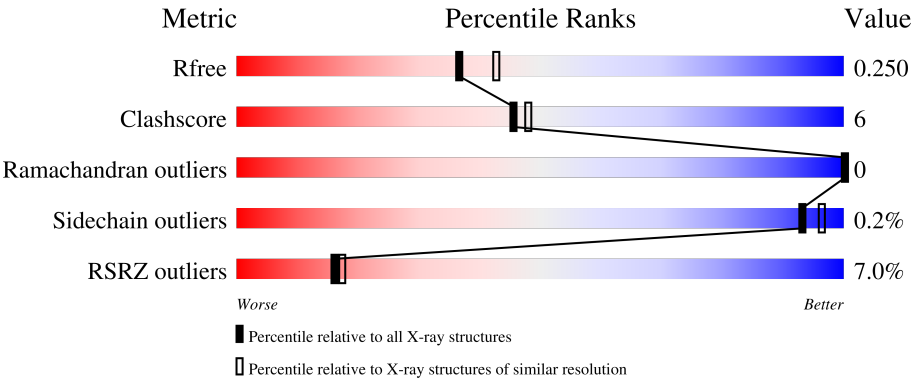
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	A	159	7% 84% 7% 9%
1	B	159	6% 80% 11% 9%
1	C	159	6% 83% 9% 8%
1	D	159	5% 73% 19% 8%
1	E	159	6% 80% 13% 8%

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Mol	Chain	Length	Quality of chain
1	F	159	3% 82% 11% 7%
1	G	159	8% 77% 11% 12%
1	H	159	4% 74% 13% 13%
1	I	159	9% 83% 10% 7%
1	J	159	8% 76% 14% 10%
1	K	159	6% 70% 15% 14%
1	L	159	8% 77% 11% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25404 atoms, of which 11976 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 Tumor susceptibility gene 101 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	144	Total	C	H	N	O	S	0	0	0
			2083	710	1002	165	200	6			
1	B	145	Total	C	H	N	O	S	0	0	0
			2104	712	1016	170	199	7			
1	C	146	Total	C	H	N	O	S	0	0	0
			2206	733	1083	177	206	7			
1	D	146	Total	C	H	N	O	S	0	0	0
			2164	726	1057	172	202	7			
1	E	147	Total	C	H	N	O	S	0	0	0
			2144	723	1041	169	204	7			
1	F	148	Total	C	H	N	O	S	0	0	0
			2145	723	1038	173	203	8			
1	G	140	Total	C	H	N	O	S	0	0	0
			1892	663	889	158	176	6			
1	H	138	Total	C	H	N	O	S	0	0	0
			1994	680	958	162	188	6			
1	I	148	Total	C	H	N	O	S	0	0	0
			2103	715	1013	168	199	8			
1	J	143	Total	C	H	N	O	S	0	0	0
			2018	694	963	161	193	7			
1	K	136	Total	C	H	N	O	S	0	0	0
			1965	672	947	156	184	6			
1	L	140	Total	C	H	N	O	S	0	0	0
			2013	689	969	165	184	6			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q99816
A	-12	ARG	-	expression tag	UNP Q99816
A	-11	GLY	-	expression tag	UNP Q99816
A	-10	SER	-	expression tag	UNP Q99816
A	-9	HIS	-	expression tag	UNP Q99816

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	expression tag	UNP Q99816
A	-7	HIS	-	expression tag	UNP Q99816
A	-6	HIS	-	expression tag	UNP Q99816
A	-5	HIS	-	expression tag	UNP Q99816
A	-4	HIS	-	expression tag	UNP Q99816
A	-3	GLY	-	expression tag	UNP Q99816
A	-2	MET	-	expression tag	UNP Q99816
A	-1	ALA	-	expression tag	UNP Q99816
A	0	SER	-	expression tag	UNP Q99816
B	-13	MET	-	initiating methionine	UNP Q99816
B	-12	ARG	-	expression tag	UNP Q99816
B	-11	GLY	-	expression tag	UNP Q99816
B	-10	SER	-	expression tag	UNP Q99816
B	-9	HIS	-	expression tag	UNP Q99816
B	-8	HIS	-	expression tag	UNP Q99816
B	-7	HIS	-	expression tag	UNP Q99816
B	-6	HIS	-	expression tag	UNP Q99816
B	-5	HIS	-	expression tag	UNP Q99816
B	-4	HIS	-	expression tag	UNP Q99816
B	-3	GLY	-	expression tag	UNP Q99816
B	-2	MET	-	expression tag	UNP Q99816
B	-1	ALA	-	expression tag	UNP Q99816
B	0	SER	-	expression tag	UNP Q99816
C	-13	MET	-	initiating methionine	UNP Q99816
C	-12	ARG	-	expression tag	UNP Q99816
C	-11	GLY	-	expression tag	UNP Q99816
C	-10	SER	-	expression tag	UNP Q99816
C	-9	HIS	-	expression tag	UNP Q99816
C	-8	HIS	-	expression tag	UNP Q99816
C	-7	HIS	-	expression tag	UNP Q99816
C	-6	HIS	-	expression tag	UNP Q99816
C	-5	HIS	-	expression tag	UNP Q99816
C	-4	HIS	-	expression tag	UNP Q99816
C	-3	GLY	-	expression tag	UNP Q99816
C	-2	MET	-	expression tag	UNP Q99816
C	-1	ALA	-	expression tag	UNP Q99816
C	0	SER	-	expression tag	UNP Q99816
D	-13	MET	-	initiating methionine	UNP Q99816
D	-12	ARG	-	expression tag	UNP Q99816
D	-11	GLY	-	expression tag	UNP Q99816
D	-10	SER	-	expression tag	UNP Q99816
D	-9	HIS	-	expression tag	UNP Q99816

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	HIS	-	expression tag	UNP Q99816
D	-7	HIS	-	expression tag	UNP Q99816
D	-6	HIS	-	expression tag	UNP Q99816
D	-5	HIS	-	expression tag	UNP Q99816
D	-4	HIS	-	expression tag	UNP Q99816
D	-3	GLY	-	expression tag	UNP Q99816
D	-2	MET	-	expression tag	UNP Q99816
D	-1	ALA	-	expression tag	UNP Q99816
D	0	SER	-	expression tag	UNP Q99816
E	-13	MET	-	initiating methionine	UNP Q99816
E	-12	ARG	-	expression tag	UNP Q99816
E	-11	GLY	-	expression tag	UNP Q99816
E	-10	SER	-	expression tag	UNP Q99816
E	-9	HIS	-	expression tag	UNP Q99816
E	-8	HIS	-	expression tag	UNP Q99816
E	-7	HIS	-	expression tag	UNP Q99816
E	-6	HIS	-	expression tag	UNP Q99816
E	-5	HIS	-	expression tag	UNP Q99816
E	-4	HIS	-	expression tag	UNP Q99816
E	-3	GLY	-	expression tag	UNP Q99816
E	-2	MET	-	expression tag	UNP Q99816
E	-1	ALA	-	expression tag	UNP Q99816
E	0	SER	-	expression tag	UNP Q99816
F	-13	MET	-	initiating methionine	UNP Q99816
F	-12	ARG	-	expression tag	UNP Q99816
F	-11	GLY	-	expression tag	UNP Q99816
F	-10	SER	-	expression tag	UNP Q99816
F	-9	HIS	-	expression tag	UNP Q99816
F	-8	HIS	-	expression tag	UNP Q99816
F	-7	HIS	-	expression tag	UNP Q99816
F	-6	HIS	-	expression tag	UNP Q99816
F	-5	HIS	-	expression tag	UNP Q99816
F	-4	HIS	-	expression tag	UNP Q99816
F	-3	GLY	-	expression tag	UNP Q99816
F	-2	MET	-	expression tag	UNP Q99816
F	-1	ALA	-	expression tag	UNP Q99816
F	0	SER	-	expression tag	UNP Q99816
G	-13	MET	-	initiating methionine	UNP Q99816
G	-12	ARG	-	expression tag	UNP Q99816
G	-11	GLY	-	expression tag	UNP Q99816
G	-10	SER	-	expression tag	UNP Q99816
G	-9	HIS	-	expression tag	UNP Q99816

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	HIS	-	expression tag	UNP Q99816
G	-7	HIS	-	expression tag	UNP Q99816
G	-6	HIS	-	expression tag	UNP Q99816
G	-5	HIS	-	expression tag	UNP Q99816
G	-4	HIS	-	expression tag	UNP Q99816
G	-3	GLY	-	expression tag	UNP Q99816
G	-2	MET	-	expression tag	UNP Q99816
G	-1	ALA	-	expression tag	UNP Q99816
G	0	SER	-	expression tag	UNP Q99816
H	-13	MET	-	initiating methionine	UNP Q99816
H	-12	ARG	-	expression tag	UNP Q99816
H	-11	GLY	-	expression tag	UNP Q99816
H	-10	SER	-	expression tag	UNP Q99816
H	-9	HIS	-	expression tag	UNP Q99816
H	-8	HIS	-	expression tag	UNP Q99816
H	-7	HIS	-	expression tag	UNP Q99816
H	-6	HIS	-	expression tag	UNP Q99816
H	-5	HIS	-	expression tag	UNP Q99816
H	-4	HIS	-	expression tag	UNP Q99816
H	-3	GLY	-	expression tag	UNP Q99816
H	-2	MET	-	expression tag	UNP Q99816
H	-1	ALA	-	expression tag	UNP Q99816
H	0	SER	-	expression tag	UNP Q99816
I	-13	MET	-	initiating methionine	UNP Q99816
I	-12	ARG	-	expression tag	UNP Q99816
I	-11	GLY	-	expression tag	UNP Q99816
I	-10	SER	-	expression tag	UNP Q99816
I	-9	HIS	-	expression tag	UNP Q99816
I	-8	HIS	-	expression tag	UNP Q99816
I	-7	HIS	-	expression tag	UNP Q99816
I	-6	HIS	-	expression tag	UNP Q99816
I	-5	HIS	-	expression tag	UNP Q99816
I	-4	HIS	-	expression tag	UNP Q99816
I	-3	GLY	-	expression tag	UNP Q99816
I	-2	MET	-	expression tag	UNP Q99816
I	-1	ALA	-	expression tag	UNP Q99816
I	0	SER	-	expression tag	UNP Q99816
J	-13	MET	-	initiating methionine	UNP Q99816
J	-12	ARG	-	expression tag	UNP Q99816
J	-11	GLY	-	expression tag	UNP Q99816
J	-10	SER	-	expression tag	UNP Q99816
J	-9	HIS	-	expression tag	UNP Q99816

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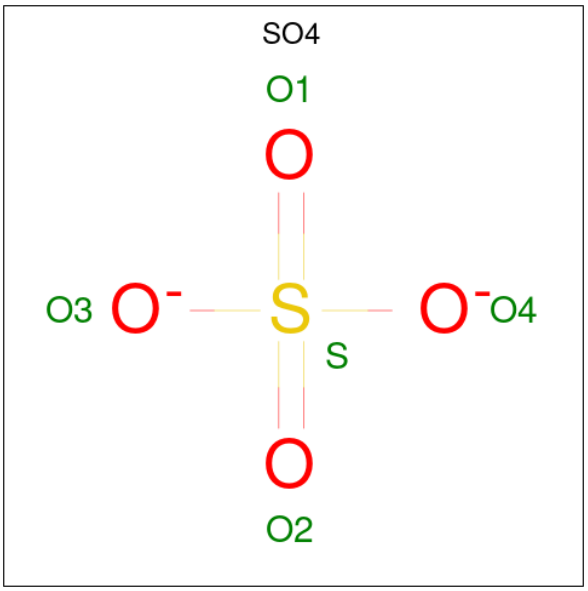
Chain	Residue	Modelled	Actual	Comment	Reference
J	-8	HIS	-	expression tag	UNP Q99816
J	-7	HIS	-	expression tag	UNP Q99816
J	-6	HIS	-	expression tag	UNP Q99816
J	-5	HIS	-	expression tag	UNP Q99816
J	-4	HIS	-	expression tag	UNP Q99816
J	-3	GLY	-	expression tag	UNP Q99816
J	-2	MET	-	expression tag	UNP Q99816
J	-1	ALA	-	expression tag	UNP Q99816
J	0	SER	-	expression tag	UNP Q99816
K	-13	MET	-	initiating methionine	UNP Q99816
K	-12	ARG	-	expression tag	UNP Q99816
K	-11	GLY	-	expression tag	UNP Q99816
K	-10	SER	-	expression tag	UNP Q99816
K	-9	HIS	-	expression tag	UNP Q99816
K	-8	HIS	-	expression tag	UNP Q99816
K	-7	HIS	-	expression tag	UNP Q99816
K	-6	HIS	-	expression tag	UNP Q99816
K	-5	HIS	-	expression tag	UNP Q99816
K	-4	HIS	-	expression tag	UNP Q99816
K	-3	GLY	-	expression tag	UNP Q99816
K	-2	MET	-	expression tag	UNP Q99816
K	-1	ALA	-	expression tag	UNP Q99816
K	0	SER	-	expression tag	UNP Q99816
L	-13	MET	-	initiating methionine	UNP Q99816
L	-12	ARG	-	expression tag	UNP Q99816
L	-11	GLY	-	expression tag	UNP Q99816
L	-10	SER	-	expression tag	UNP Q99816
L	-9	HIS	-	expression tag	UNP Q99816
L	-8	HIS	-	expression tag	UNP Q99816
L	-7	HIS	-	expression tag	UNP Q99816
L	-6	HIS	-	expression tag	UNP Q99816
L	-5	HIS	-	expression tag	UNP Q99816
L	-4	HIS	-	expression tag	UNP Q99816
L	-3	GLY	-	expression tag	UNP Q99816
L	-2	MET	-	expression tag	UNP Q99816
L	-1	ALA	-	expression tag	UNP Q99816
L	0	SER	-	expression tag	UNP Q99816

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	40	Total O 40 40	0	0
3	B	65	Total O 65 65	0	0

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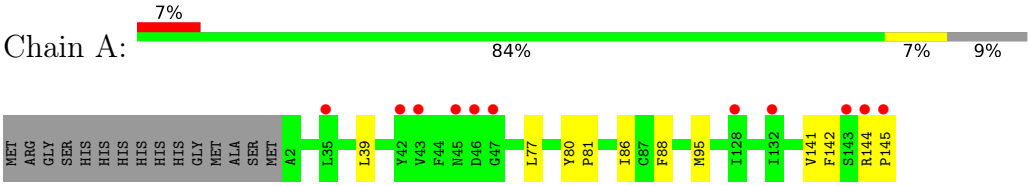
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	47	Total O 47 47	0	0
3	D	61	Total O 61 61	0	0
3	E	52	Total O 52 52	0	0
3	F	54	Total O 54 54	0	0
3	G	28	Total O 28 28	0	0
3	H	41	Total O 41 41	0	0
3	I	28	Total O 28 28	0	0
3	J	39	Total O 39 39	0	0
3	K	45	Total O 45 45	0	0
3	L	23	Total O 23 23	0	0

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.

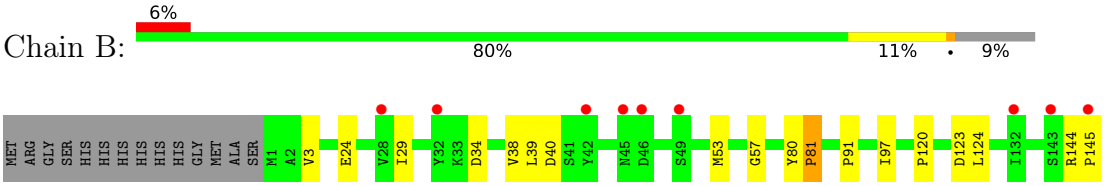
• Molecule 1: Tumor susceptibility gene 101 protein

Chain A:



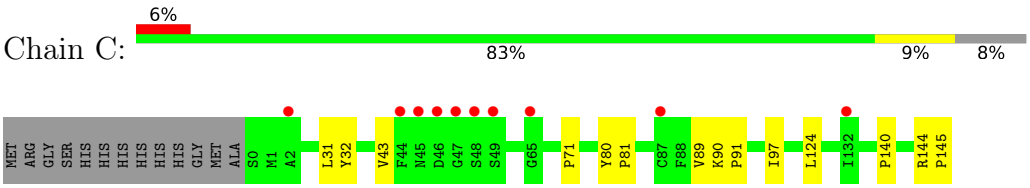
• Molecule 1: Tumor susceptibility gene 101 protein

Chain B:



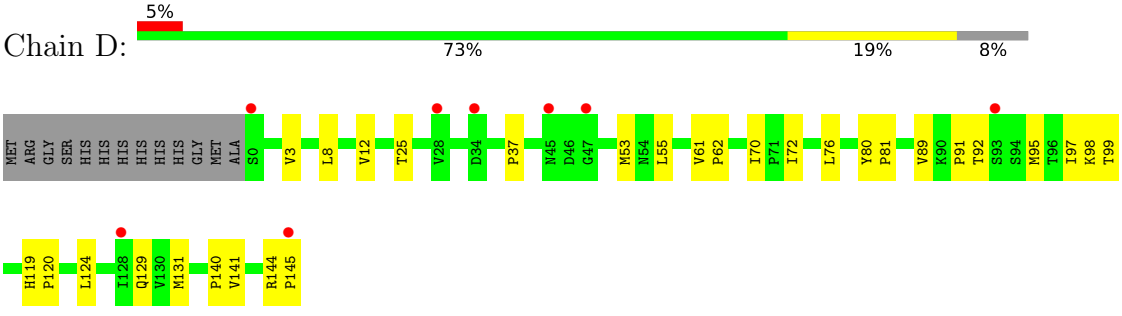
• Molecule 1: Tumor susceptibility gene 101 protein

Chain C:



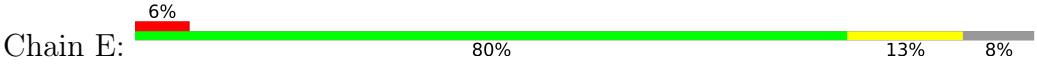
• Molecule 1: Tumor susceptibility gene 101 protein

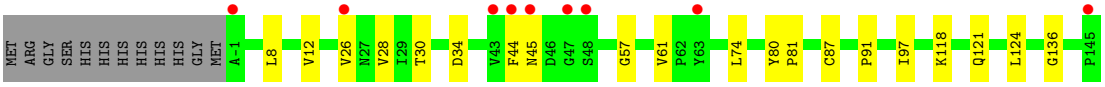
Chain D:



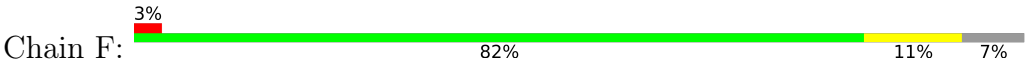
• Molecule 1: Tumor susceptibility gene 101 protein

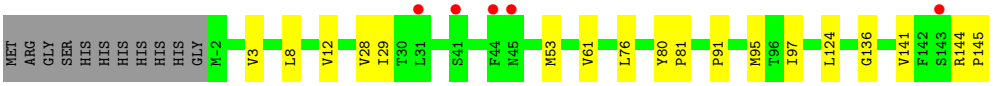
Chain E:



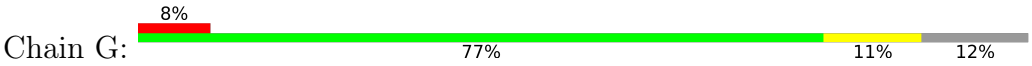


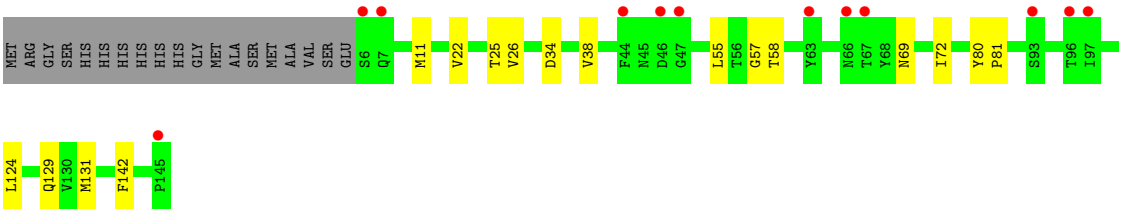
• Molecule 1: Tumor susceptibility gene 101 protein



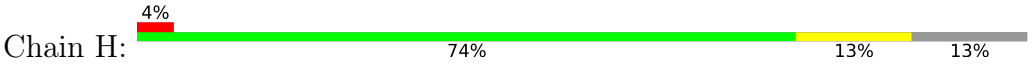


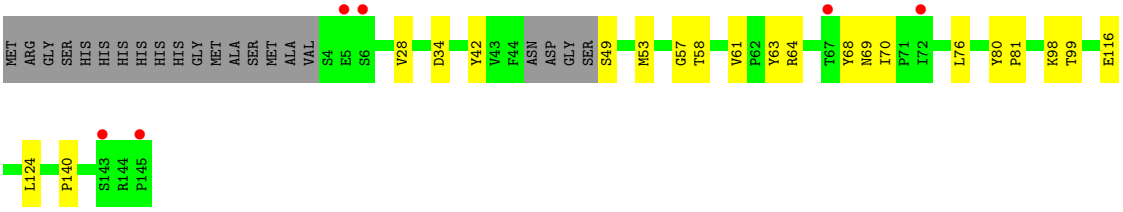
• Molecule 1: Tumor susceptibility gene 101 protein



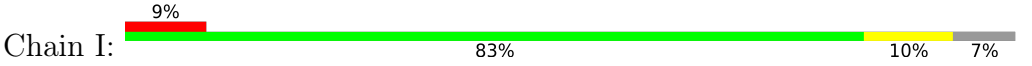


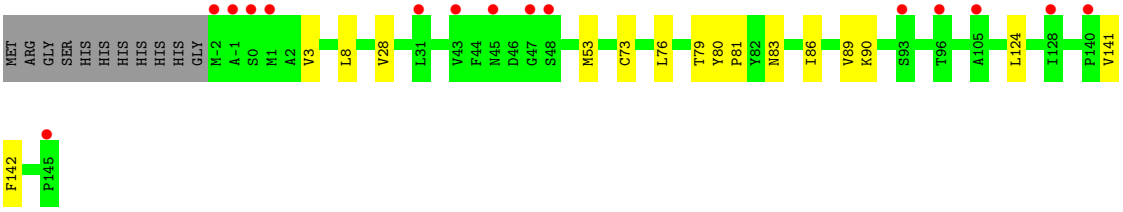
• Molecule 1: Tumor susceptibility gene 101 protein



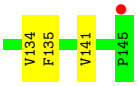


• Molecule 1: Tumor susceptibility gene 101 protein



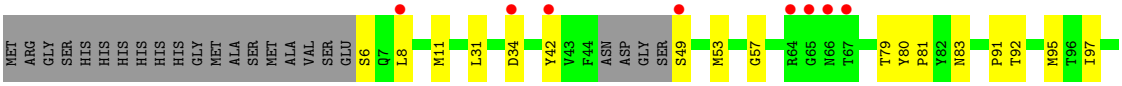


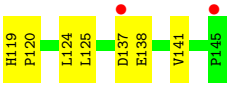
• Molecule 1: Tumor susceptibility gene 101 protein



• Molecule 1: Tumor susceptibility gene 101 protein

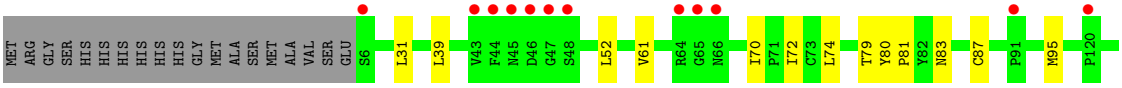
Chain K:

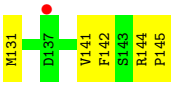




• Molecule 1: Tumor susceptibility gene 101 protein

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	38.92Å 168.22Å 195.55Å 90.00° 92.91° 90.00°	Depositor
Resolution (Å)	39.06 – 2.25 39.06 – 2.25	Depositor EDS
% Data completeness (in resolution range)	90.2 (39.06-2.25) 90.2 (39.06-2.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.20.4459	Depositor
R, R_{free}	0.226 , 0.244 0.233 , 0.250	Depositor DCC
R_{free} test set	5170 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	25404	wwPDB-VP
Average B, all atoms (Å^2)	48.0	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 19.83 % 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 9.9271e-03. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.66	0/1114	0.77	0/1537
1	B	0.61	0/1121	0.79	0/1546
1	C	0.66	0/1156	0.82	0/1587
1	D	0.67	0/1140	0.80	0/1569
1	E	0.64	0/1136	0.78	0/1564
1	F	0.67	0/1140	0.82	0/1569
1	G	0.55	0/1035	0.73	0/1432
1	H	0.67	0/1067	0.84	0/1470
1	I	0.60	0/1122	0.77	0/1548
1	J	0.61	0/1086	0.75	0/1500
1	K	0.67	0/1049	0.83	0/1447
1	L	0.62	0/1077	0.84	0/1484
All	All	0.64	0/13243	0.79	0/18253

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1081	1002	1002	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1088	1016	1018	9	0
1	C	1123	1083	1085	9	0
1	D	1107	1057	1059	20	0
1	E	1103	1041	1042	15	0
1	F	1107	1038	1040	13	0
1	G	1003	889	888	13	0
1	H	1036	958	957	18	0
1	I	1090	1013	1015	14	0
1	J	1055	963	964	17	0
1	K	1018	947	945	15	0
1	L	1044	969	968	16	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	L	5	0	0	0	0
3	A	40	0	0	0	0
3	B	65	0	0	0	0
3	C	47	0	0	0	0
3	D	61	0	0	0	0
3	E	52	0	0	0	0
3	F	54	0	0	0	0
3	G	28	0	0	0	0
3	H	41	0	0	0	0
3	I	28	0	0	0	0
3	J	39	0	0	0	0
3	K	45	0	0	0	0
3	L	23	0	0	0	0
All	All	13428	11976	11983	158	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 6.

The worst 5 of 158 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:L:61:VAL:HG21	1:L:70:ILE:HD12	1.43	1.01
1:D:61:VAL:HG21	1:D:70:ILE:HD12	1.58	0.82
1:L:61:VAL:CG2	1:L:70:ILE:HD12	2.19	0.68
1:K:31:LEU:HD23	1:K:125:LEU:HD11	1.77	0.67
1:D:92:THR:HG23	1:D:95:MET:HE3	1.78	0.66

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	142/159 (89%)	138 (97%)	4 (3%)	0	100	100
1	B	143/159 (90%)	140 (98%)	3 (2%)	0	100	100
1	C	144/159 (91%)	142 (99%)	2 (1%)	0	100	100
1	D	144/159 (91%)	141 (98%)	3 (2%)	0	100	100
1	E	145/159 (91%)	143 (99%)	2 (1%)	0	100	100
1	F	146/159 (92%)	143 (98%)	3 (2%)	0	100	100
1	G	138/159 (87%)	134 (97%)	4 (3%)	0	100	100
1	H	134/159 (84%)	132 (98%)	2 (2%)	0	100	100
1	I	146/159 (92%)	143 (98%)	3 (2%)	0	100	100
1	J	139/159 (87%)	137 (99%)	2 (1%)	0	100	100
1	K	132/159 (83%)	129 (98%)	3 (2%)	0	100	100
1	L	138/159 (87%)	136 (99%)	2 (1%)	0	100	100
All	All	1691/1908 (89%)	1658 (98%)	33 (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	A	112/147 (76%)	112 (100%)	0	100 100
1	B	114/147 (78%)	112 (98%)	2 (2%)	59 68
1	C	123/147 (84%)	123 (100%)	0	100 100
1	D	119/147 (81%)	119 (100%)	0	100 100
1	E	117/147 (80%)	117 (100%)	0	100 100
1	F	116/147 (79%)	116 (100%)	0	100 100
1	G	92/147 (63%)	92 (100%)	0	100 100
1	H	106/147 (72%)	106 (100%)	0	100 100
1	I	111/147 (76%)	111 (100%)	0	100 100
1	J	105/147 (71%)	105 (100%)	0	100 100
1	K	104/147 (71%)	104 (100%)	0	100 100
1	L	104/147 (71%)	104 (100%)	0	100 100
All	All	1323/1764 (75%)	1321 (100%)	2 (0%)	93 96

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

Mol	Chain	Res	Type
1	B	81	PRO
1	B	120	PRO

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)

10 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	$\#\|Z\| > 2$
2	SO4	B	201	-	4,4,4	0.21	0	6,6,6	0.42	0
2	SO4	D	201	-	4,4,4	0.16	0	6,6,6	0.27	0
2	SO4	A	201	-	4,4,4	0.26	0	6,6,6	0.65	0
2	SO4	F	201	-	4,4,4	0.52	0	6,6,6	0.07	0
2	SO4	G	201	-	4,4,4	0.15	0	6,6,6	0.29	0
2	SO4	L	201	-	4,4,4	0.30	0	6,6,6	0.31	0
2	SO4	C	201	-	4,4,4	0.22	0	6,6,6	0.18	0
2	SO4	J	201	-	4,4,4	0.21	0	6,6,6	0.33	0
2	SO4	H	201	-	4,4,4	0.14	0	6,6,6	0.54	0
2	SO4	I	201	-	4,4,4	0.36	0	6,6,6	0.44	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	A	144/159 (90%)	0.66	11 (7%) 13 15	24, 40, 68, 92	0
1	B	145/159 (91%)	0.57	9 (6%) 20 22	22, 37, 58, 85	0
1	C	146/159 (91%)	0.66	10 (6%) 17 18	24, 37, 68, 88	0
1	D	146/159 (91%)	0.65	8 (5%) 25 27	26, 39, 56, 83	0
1	E	147/159 (92%)	0.78	9 (6%) 21 23	28, 40, 67, 106	0
1	F	148/159 (93%)	0.72	5 (3%) 45 47	28, 41, 65, 101	0
1	G	140/159 (88%)	0.66	12 (8%) 10 11	37, 51, 73, 90	0
1	H	138/159 (86%)	0.54	6 (4%) 35 37	30, 43, 67, 72	0
1	I	148/159 (93%)	0.80	15 (10%) 7 7	29, 45, 75, 97	0
1	J	143/159 (89%)	0.77	12 (8%) 11 12	31, 46, 61, 81	0
1	K	136/159 (85%)	0.60	10 (7%) 14 15	31, 43, 69, 79	0
1	L	140/159 (88%)	0.70	13 (9%) 8 9	39, 51, 70, 91	0
All	All	1721/1908 (90%)	0.68	120 (6%) 16 17	22, 43, 69, 106	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	PRO	6.6
1	E	45	ASN	6.3
1	L	45	ASN	6.1
1	J	93	SER	5.9
1	F	44	PHE	5.8

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

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	L	201	5/5	0.84	0.22	61,68,82,85	0
2	SO4	I	201	5/5	0.91	0.15	38,42,61,64	0
2	SO4	F	201	5/5	0.92	0.23	54,55,57,61	0
2	SO4	A	201	5/5	0.93	0.13	41,46,49,56	0
2	SO4	J	201	5/5	0.94	0.12	47,50,60,63	0
2	SO4	H	201	5/5	0.95	0.20	56,58,68,68	0
2	SO4	G	201	5/5	0.95	0.13	43,54,59,60	0
2	SO4	D	201	5/5	0.96	0.11	47,48,60,61	0
2	SO4	B	201	5/5	0.97	0.20	43,43,49,52	0
2	SO4	C	201	5/5	0.98	0.21	51,51,61,69	0

6.5 Other polymers (i)

There are no such residues in this entry.