Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:14 pm BST

PDB ID	:	6O0S
Title	:	Crystal structure of the tandem SAM domains from human SARM1
Authors	:	Horsefield, S.; Burdett, H.; Zhang, X.; Manik, M.K.; Shi, Y.; Chen, J.; Tiancong, Q.; Gilley, J.; Lai, J.; Gu, W.; Rank, M.; Deerain, N.; Casey, L.; Ericsson, D.J.; Foley, G.; Hughes, R.O.; Bosanac, T.; von Itzstein, M.; Rathjen, J.P.; Nanson, J.D.; Boden, M.; Dry, I.B.; Williams, S.J.; Staskawicz, B.J.; Coleman, M.P.; Ve, T.; Dodds, P.N.; Kobe, B.
Deposited on	:	2019-02-17
Resolution	:	2.70 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 following versions of software and data (see references ①) were used in the production of this report:

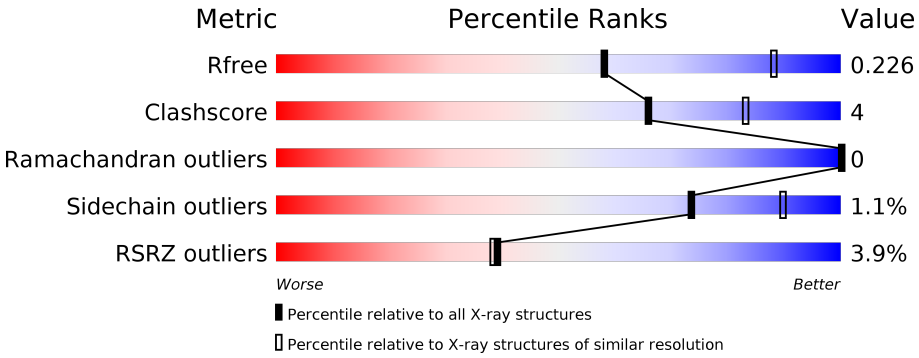
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	177	2% 69% 10% 21%
1	B	177	5% 68% 11% 21%
1	C	177	5% 73% 8% 19%
1	D	177	3% 66% 13% 21%
1	E	177	% 69% 10% 21%
1	F	177	5% 76% 5% 19%

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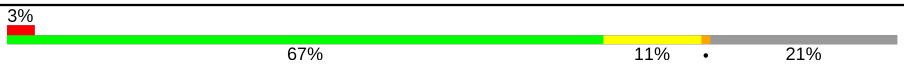
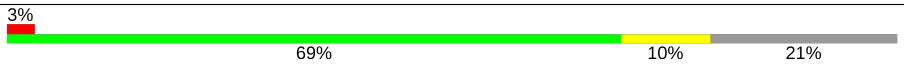
Mol	Chain	Length	Quality of chain
1	G	177	
1	H	177	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9202 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 Sterile alpha and TIR motif-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	0	0
			1142	715	205	216	6			
1	B	140	Total	C	N	O	S	0	0	0
			1142	715	205	216	6			
1	C	143	Total	C	N	O	S	0	0	0
			1174	738	209	221	6			
1	D	139	Total	C	N	O	S	0	0	0
			1136	712	204	214	6			
1	E	140	Total	C	N	O	S	0	0	0
			1142	715	205	216	6			
1	F	144	Total	C	N	O	S	0	0	0
			1182	744	210	222	6			
1	G	140	Total	C	N	O	S	0	0	0
			1142	715	205	216	6			
1	H	140	Total	C	N	O	S	0	0	0
			1142	715	205	216	6			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	385	MET	-	expression tag	UNP Q6SZW1
A	386	HIS	-	expression tag	UNP Q6SZW1
A	387	HIS	-	expression tag	UNP Q6SZW1
A	388	HIS	-	expression tag	UNP Q6SZW1
A	389	HIS	-	expression tag	UNP Q6SZW1
A	390	HIS	-	expression tag	UNP Q6SZW1
A	391	HIS	-	expression tag	UNP Q6SZW1
A	392	SER	-	expression tag	UNP Q6SZW1
A	393	SER	-	expression tag	UNP Q6SZW1
A	394	GLY	-	expression tag	UNP Q6SZW1
A	395	VAL	-	expression tag	UNP Q6SZW1
A	396	ASP	-	expression tag	UNP Q6SZW1
A	397	LEU	-	expression tag	UNP Q6SZW1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	398	GLY	-	expression tag	UNP Q6SZW1
A	399	THR	-	expression tag	UNP Q6SZW1
A	400	GLU	-	expression tag	UNP Q6SZW1
A	401	ASN	-	expression tag	UNP Q6SZW1
A	402	LEU	-	expression tag	UNP Q6SZW1
A	403	TYR	-	expression tag	UNP Q6SZW1
A	404	PHE	-	expression tag	UNP Q6SZW1
A	405	GLN	-	expression tag	UNP Q6SZW1
A	406	SER	-	expression tag	UNP Q6SZW1
A	407	ASN	-	expression tag	UNP Q6SZW1
A	408	ALA	-	expression tag	UNP Q6SZW1
A	473	PHE	LEU	engineered mutation	UNP Q6SZW1
B	385	MET	-	expression tag	UNP Q6SZW1
B	386	HIS	-	expression tag	UNP Q6SZW1
B	387	HIS	-	expression tag	UNP Q6SZW1
B	388	HIS	-	expression tag	UNP Q6SZW1
B	389	HIS	-	expression tag	UNP Q6SZW1
B	390	HIS	-	expression tag	UNP Q6SZW1
B	391	HIS	-	expression tag	UNP Q6SZW1
B	392	SER	-	expression tag	UNP Q6SZW1
B	393	SER	-	expression tag	UNP Q6SZW1
B	394	GLY	-	expression tag	UNP Q6SZW1
B	395	VAL	-	expression tag	UNP Q6SZW1
B	396	ASP	-	expression tag	UNP Q6SZW1
B	397	LEU	-	expression tag	UNP Q6SZW1
B	398	GLY	-	expression tag	UNP Q6SZW1
B	399	THR	-	expression tag	UNP Q6SZW1
B	400	GLU	-	expression tag	UNP Q6SZW1
B	401	ASN	-	expression tag	UNP Q6SZW1
B	402	LEU	-	expression tag	UNP Q6SZW1
B	403	TYR	-	expression tag	UNP Q6SZW1
B	404	PHE	-	expression tag	UNP Q6SZW1
B	405	GLN	-	expression tag	UNP Q6SZW1
B	406	SER	-	expression tag	UNP Q6SZW1
B	407	ASN	-	expression tag	UNP Q6SZW1
B	408	ALA	-	expression tag	UNP Q6SZW1
B	473	PHE	LEU	engineered mutation	UNP Q6SZW1
C	385	MET	-	expression tag	UNP Q6SZW1
C	386	HIS	-	expression tag	UNP Q6SZW1
C	387	HIS	-	expression tag	UNP Q6SZW1
C	388	HIS	-	expression tag	UNP Q6SZW1
C	389	HIS	-	expression tag	UNP Q6SZW1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	390	HIS	-	expression tag	UNP Q6SZW1
C	391	HIS	-	expression tag	UNP Q6SZW1
C	392	SER	-	expression tag	UNP Q6SZW1
C	393	SER	-	expression tag	UNP Q6SZW1
C	394	GLY	-	expression tag	UNP Q6SZW1
C	395	VAL	-	expression tag	UNP Q6SZW1
C	396	ASP	-	expression tag	UNP Q6SZW1
C	397	LEU	-	expression tag	UNP Q6SZW1
C	398	GLY	-	expression tag	UNP Q6SZW1
C	399	THR	-	expression tag	UNP Q6SZW1
C	400	GLU	-	expression tag	UNP Q6SZW1
C	401	ASN	-	expression tag	UNP Q6SZW1
C	402	LEU	-	expression tag	UNP Q6SZW1
C	403	TYR	-	expression tag	UNP Q6SZW1
C	404	PHE	-	expression tag	UNP Q6SZW1
C	405	GLN	-	expression tag	UNP Q6SZW1
C	406	SER	-	expression tag	UNP Q6SZW1
C	407	ASN	-	expression tag	UNP Q6SZW1
C	408	ALA	-	expression tag	UNP Q6SZW1
C	473	PHE	LEU	engineered mutation	UNP Q6SZW1
D	385	MET	-	expression tag	UNP Q6SZW1
D	386	HIS	-	expression tag	UNP Q6SZW1
D	387	HIS	-	expression tag	UNP Q6SZW1
D	388	HIS	-	expression tag	UNP Q6SZW1
D	389	HIS	-	expression tag	UNP Q6SZW1
D	390	HIS	-	expression tag	UNP Q6SZW1
D	391	HIS	-	expression tag	UNP Q6SZW1
D	392	SER	-	expression tag	UNP Q6SZW1
D	393	SER	-	expression tag	UNP Q6SZW1
D	394	GLY	-	expression tag	UNP Q6SZW1
D	395	VAL	-	expression tag	UNP Q6SZW1
D	396	ASP	-	expression tag	UNP Q6SZW1
D	397	LEU	-	expression tag	UNP Q6SZW1
D	398	GLY	-	expression tag	UNP Q6SZW1
D	399	THR	-	expression tag	UNP Q6SZW1
D	400	GLU	-	expression tag	UNP Q6SZW1
D	401	ASN	-	expression tag	UNP Q6SZW1
D	402	LEU	-	expression tag	UNP Q6SZW1
D	403	TYR	-	expression tag	UNP Q6SZW1
D	404	PHE	-	expression tag	UNP Q6SZW1
D	405	GLN	-	expression tag	UNP Q6SZW1
D	406	SER	-	expression tag	UNP Q6SZW1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	407	ASN	-	expression tag	UNP Q6SZW1
D	408	ALA	-	expression tag	UNP Q6SZW1
D	473	PHE	LEU	engineered mutation	UNP Q6SZW1
E	385	MET	-	expression tag	UNP Q6SZW1
E	386	HIS	-	expression tag	UNP Q6SZW1
E	387	HIS	-	expression tag	UNP Q6SZW1
E	388	HIS	-	expression tag	UNP Q6SZW1
E	389	HIS	-	expression tag	UNP Q6SZW1
E	390	HIS	-	expression tag	UNP Q6SZW1
E	391	HIS	-	expression tag	UNP Q6SZW1
E	392	SER	-	expression tag	UNP Q6SZW1
E	393	SER	-	expression tag	UNP Q6SZW1
E	394	GLY	-	expression tag	UNP Q6SZW1
E	395	VAL	-	expression tag	UNP Q6SZW1
E	396	ASP	-	expression tag	UNP Q6SZW1
E	397	LEU	-	expression tag	UNP Q6SZW1
E	398	GLY	-	expression tag	UNP Q6SZW1
E	399	THR	-	expression tag	UNP Q6SZW1
E	400	GLU	-	expression tag	UNP Q6SZW1
E	401	ASN	-	expression tag	UNP Q6SZW1
E	402	LEU	-	expression tag	UNP Q6SZW1
E	403	TYR	-	expression tag	UNP Q6SZW1
E	404	PHE	-	expression tag	UNP Q6SZW1
E	405	GLN	-	expression tag	UNP Q6SZW1
E	406	SER	-	expression tag	UNP Q6SZW1
E	407	ASN	-	expression tag	UNP Q6SZW1
E	408	ALA	-	expression tag	UNP Q6SZW1
E	473	PHE	LEU	engineered mutation	UNP Q6SZW1
F	385	MET	-	expression tag	UNP Q6SZW1
F	386	HIS	-	expression tag	UNP Q6SZW1
F	387	HIS	-	expression tag	UNP Q6SZW1
F	388	HIS	-	expression tag	UNP Q6SZW1
F	389	HIS	-	expression tag	UNP Q6SZW1
F	390	HIS	-	expression tag	UNP Q6SZW1
F	391	HIS	-	expression tag	UNP Q6SZW1
F	392	SER	-	expression tag	UNP Q6SZW1
F	393	SER	-	expression tag	UNP Q6SZW1
F	394	GLY	-	expression tag	UNP Q6SZW1
F	395	VAL	-	expression tag	UNP Q6SZW1
F	396	ASP	-	expression tag	UNP Q6SZW1
F	397	LEU	-	expression tag	UNP Q6SZW1
F	398	GLY	-	expression tag	UNP Q6SZW1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	399	THR	-	expression tag	UNP Q6SZW1
F	400	GLU	-	expression tag	UNP Q6SZW1
F	401	ASN	-	expression tag	UNP Q6SZW1
F	402	LEU	-	expression tag	UNP Q6SZW1
F	403	TYR	-	expression tag	UNP Q6SZW1
F	404	PHE	-	expression tag	UNP Q6SZW1
F	405	GLN	-	expression tag	UNP Q6SZW1
F	406	SER	-	expression tag	UNP Q6SZW1
F	407	ASN	-	expression tag	UNP Q6SZW1
F	408	ALA	-	expression tag	UNP Q6SZW1
F	473	PHE	LEU	engineered mutation	UNP Q6SZW1
G	385	MET	-	expression tag	UNP Q6SZW1
G	386	HIS	-	expression tag	UNP Q6SZW1
G	387	HIS	-	expression tag	UNP Q6SZW1
G	388	HIS	-	expression tag	UNP Q6SZW1
G	389	HIS	-	expression tag	UNP Q6SZW1
G	390	HIS	-	expression tag	UNP Q6SZW1
G	391	HIS	-	expression tag	UNP Q6SZW1
G	392	SER	-	expression tag	UNP Q6SZW1
G	393	SER	-	expression tag	UNP Q6SZW1
G	394	GLY	-	expression tag	UNP Q6SZW1
G	395	VAL	-	expression tag	UNP Q6SZW1
G	396	ASP	-	expression tag	UNP Q6SZW1
G	397	LEU	-	expression tag	UNP Q6SZW1
G	398	GLY	-	expression tag	UNP Q6SZW1
G	399	THR	-	expression tag	UNP Q6SZW1
G	400	GLU	-	expression tag	UNP Q6SZW1
G	401	ASN	-	expression tag	UNP Q6SZW1
G	402	LEU	-	expression tag	UNP Q6SZW1
G	403	TYR	-	expression tag	UNP Q6SZW1
G	404	PHE	-	expression tag	UNP Q6SZW1
G	405	GLN	-	expression tag	UNP Q6SZW1
G	406	SER	-	expression tag	UNP Q6SZW1
G	407	ASN	-	expression tag	UNP Q6SZW1
G	408	ALA	-	expression tag	UNP Q6SZW1
G	473	PHE	LEU	engineered mutation	UNP Q6SZW1
H	385	MET	-	expression tag	UNP Q6SZW1
H	386	HIS	-	expression tag	UNP Q6SZW1
H	387	HIS	-	expression tag	UNP Q6SZW1
H	388	HIS	-	expression tag	UNP Q6SZW1
H	389	HIS	-	expression tag	UNP Q6SZW1
H	390	HIS	-	expression tag	UNP Q6SZW1

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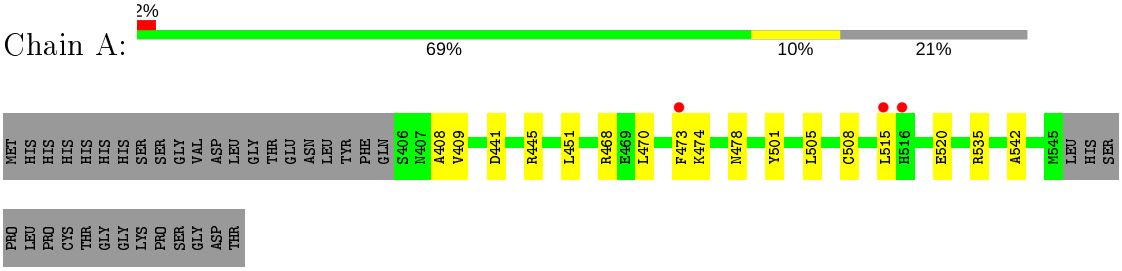
Chain	Residue	Modelled	Actual	Comment	Reference
H	391	HIS	-	expression tag	UNP Q6SZW1
H	392	SER	-	expression tag	UNP Q6SZW1
H	393	SER	-	expression tag	UNP Q6SZW1
H	394	GLY	-	expression tag	UNP Q6SZW1
H	395	VAL	-	expression tag	UNP Q6SZW1
H	396	ASP	-	expression tag	UNP Q6SZW1
H	397	LEU	-	expression tag	UNP Q6SZW1
H	398	GLY	-	expression tag	UNP Q6SZW1
H	399	THR	-	expression tag	UNP Q6SZW1
H	400	GLU	-	expression tag	UNP Q6SZW1
H	401	ASN	-	expression tag	UNP Q6SZW1
H	402	LEU	-	expression tag	UNP Q6SZW1
H	403	TYR	-	expression tag	UNP Q6SZW1
H	404	PHE	-	expression tag	UNP Q6SZW1
H	405	GLN	-	expression tag	UNP Q6SZW1
H	406	SER	-	expression tag	UNP Q6SZW1
H	407	ASN	-	expression tag	UNP Q6SZW1
H	408	ALA	-	expression tag	UNP Q6SZW1
H	473	PHE	LEU	engineered mutation	UNP Q6SZW1

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

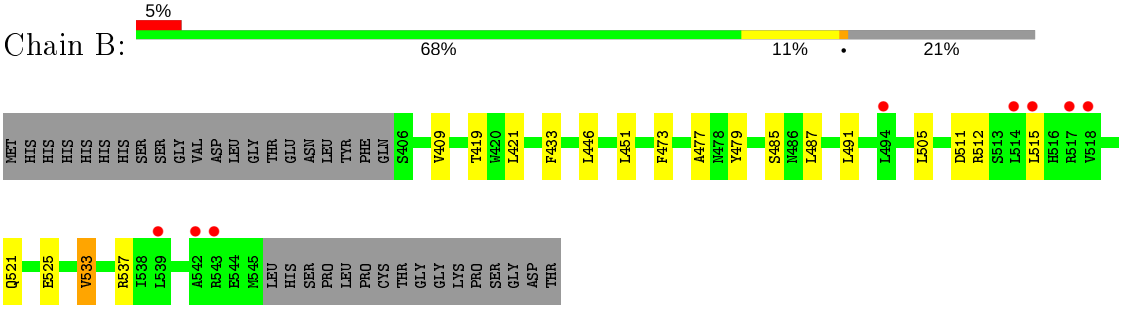
- Molecule 1: Sterile alpha and TIR motif-containing protein 1

Chain A:



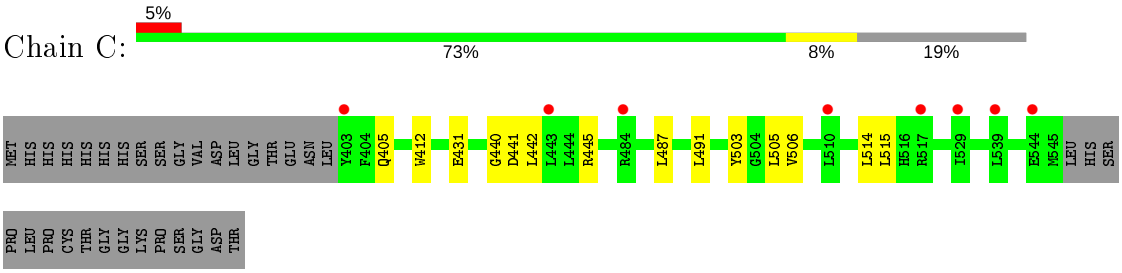
- Molecule 1: Sterile alpha and TIR motif-containing protein 1

Chain B:



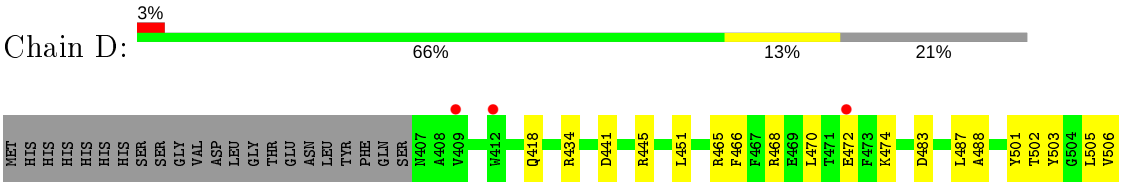
- Molecule 1: Sterile alpha and TIR motif-containing protein 1

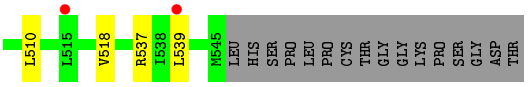
Chain C:



- Molecule 1: Sterile alpha and TIR motif-containing protein 1

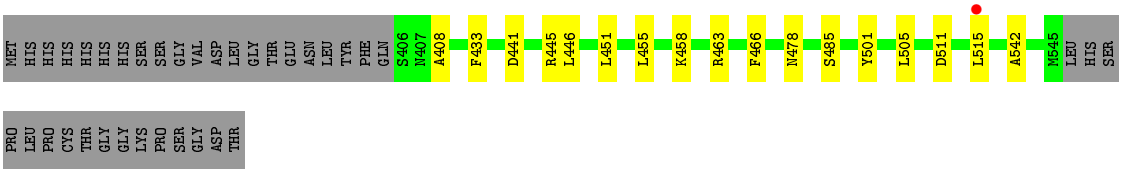
Chain D:





• Molecule 1: Sterile alpha and TIR motif-containing protein 1

Chain E:

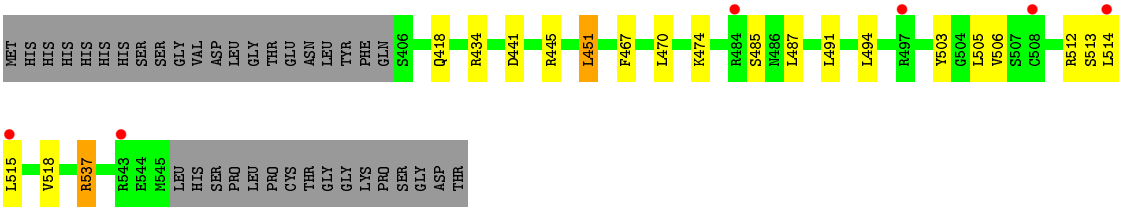


• Molecule 1: Sterile alpha and TIR motif-containing protein 1

Chain F:

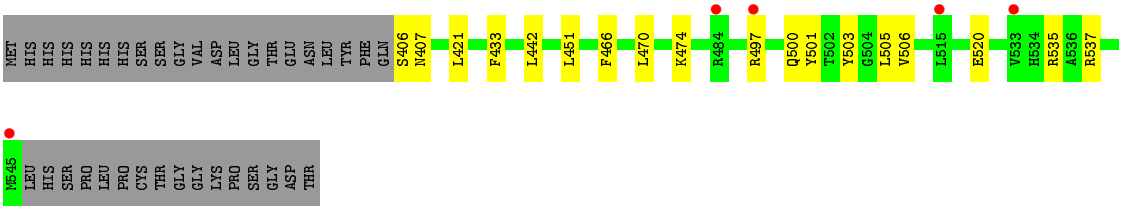
• Molecule 1: Sterile alpha and TIR motif-containing protein 1

Chain G:



• Molecule 1: Sterile alpha and TIR motif-containing protein 1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	94.61Å 154.46Å 121.88Å 90.00° 93.82° 90.00°	Depositor
Resolution (Å)	60.81 – 2.70 60.81 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (60.81-2.70) 99.4 (60.81-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.69Å)	Xtriage
Refinement program	PHENIX (DEV_3357: ???)	Depositor
R, R_{free}	0.205 , 0.226 0.204 , 0.226	Depositor DCC
R_{free} test set	2444 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	56.8	Xtriage
Anisotropy	0.763	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9202	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.25	0/1163	0.45	0/1566
1	B	0.27	0/1163	0.48	0/1566
1	C	0.25	0/1197	0.45	0/1612
1	D	0.24	0/1157	0.45	0/1558
1	E	0.24	0/1163	0.44	0/1566
1	F	0.25	0/1205	0.45	0/1623
1	G	0.25	0/1163	0.47	0/1566
1	H	0.24	0/1163	0.47	0/1566
All	All	0.25	0/9374	0.46	0/12623

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	1142	0	1116	10	0
1	B	1142	0	1116	12	0
1	C	1174	0	1142	7	0
1	D	1136	0	1111	13	0
1	E	1142	0	1116	9	0
1	F	1182	0	1153	5	0
1	G	1142	0	1116	11	0
1	H	1142	0	1116	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9202	0	8986	72	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 4.

All (72) 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:B:487:LEU:HD11	1:B:515:LEU:HD11	1.61	0.82
1:D:518:VAL:HG12	1:D:539:LEU:HD21	1.85	0.57
1:G:487:LEU:HD11	1:G:515:LEU:HD11	1.86	0.57
1:G:470:LEU:HG	1:G:474:LYS:HE3	1.88	0.55
1:B:521:GLN:NE2	1:B:525:GLU:OE2	2.35	0.55
1:G:491:LEU:HD11	1:G:505:LEU:HD12	1.88	0.54
1:G:494:LEU:O	1:G:537:ARG:NH2	2.41	0.54
1:G:485:SER:O	1:G:512:ARG:HD2	2.08	0.54
1:D:501:TYR:O	1:D:505:LEU:HD12	2.08	0.54
1:H:520:GLU:HG2	1:H:535:ARG:HE	1.73	0.53
1:A:409:VAL:HG22	1:A:473:PHE:HE2	1.74	0.52
1:H:501:TYR:O	1:H:505:LEU:HD12	2.09	0.52
1:D:470:LEU:HG	1:D:474:LYS:HE3	1.91	0.51
1:H:470:LEU:HG	1:H:474:LYS:HE3	1.91	0.51
1:C:514:LEU:HD13	1:D:537:ARG:HD2	1.91	0.51
1:F:521:GLN:HE21	1:F:525:GLU:CD	2.15	0.50
1:A:409:VAL:HG22	1:A:473:PHE:CE2	2.46	0.50
1:B:511:ASP:O	1:B:515:LEU:HG	2.13	0.48
1:E:441:ASP:OD2	1:E:445:ARG:NH1	2.47	0.48
1:B:521:GLN:HE21	1:B:525:GLU:CD	2.17	0.47
1:A:508:CYS:HB3	1:B:533:VAL:HG21	1.95	0.47
1:A:520:GLU:HG2	1:A:535:ARG:HE	1.79	0.47
1:D:441:ASP:OD2	1:D:445:ARG:NH1	2.47	0.47
1:A:468:ARG:NH1	1:H:442:LEU:HG	2.30	0.47
1:G:418:GLN:NE2	1:G:434:ARG:HB2	2.28	0.47
1:D:451:LEU:HD11	1:D:466:PHE:CD1	2.50	0.47
1:B:409:VAL:HG22	1:B:473:PHE:HE2	1.80	0.47
1:C:503:TYR:HA	1:C:506:VAL:HG22	1.96	0.47
1:F:421:LEU:HD11	1:F:433:PHE:CG	2.50	0.47
1:H:503:TYR:HA	1:H:506:VAL:HG22	1.96	0.46
1:F:491:LEU:HD11	1:F:505:LEU:HD12	1.97	0.46
1:A:408:ALA:HA	1:A:478:ASN:HB3	1.98	0.46
1:C:487:LEU:HD11	1:C:515:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:514:LEU:HD13	1:H:537:ARG:HD2	1.98	0.45
1:D:505:LEU:O	1:D:510:LEU:HB2	2.17	0.45
1:A:515:LEU:HB3	1:A:542:ALA:HB1	1.99	0.44
1:F:521:GLN:NE2	1:F:525:GLU:OE2	2.51	0.44
1:C:441:ASP:OD2	1:C:445:ARG:NH1	2.50	0.44
1:E:501:TYR:O	1:E:505:LEU:HD12	2.17	0.44
1:A:501:TYR:O	1:A:505:LEU:HD12	2.17	0.44
1:C:442:LEU:HD11	1:D:465:ARG:HG2	2.00	0.43
1:D:468:ARG:O	1:D:472:GLU:HG2	2.18	0.43
1:H:451:LEU:HD11	1:H:466:PHE:CD1	2.53	0.43
1:B:491:LEU:HD11	1:B:505:LEU:HD12	2.00	0.43
1:C:412:TRP:HB2	1:C:440:GLY:HA3	2.00	0.43
1:E:408:ALA:HA	1:E:478:ASN:HB3	2.00	0.43
1:E:485:SER:HB3	1:E:511:ASP:HB2	2.01	0.43
1:H:497:ARG:O	1:H:500:GLN:HG2	2.18	0.43
1:B:485:SER:HB2	1:B:512:ARG:HG3	2.00	0.43
1:F:451:LEU:HD12	1:F:467:PHE:CE2	2.54	0.43
1:B:421:LEU:HD11	1:B:433:PHE:CG	2.54	0.42
1:C:491:LEU:HD11	1:C:505:LEU:HD12	2.01	0.42
1:E:515:LEU:HB3	1:E:542:ALA:HB1	2.01	0.42
1:H:406:SER:OG	1:H:407:ASN:N	2.52	0.42
1:E:451:LEU:HD11	1:E:466:PHE:CD1	2.54	0.42
1:B:451:LEU:HD23	1:B:451:LEU:HA	1.88	0.42
1:E:446:LEU:HA	1:E:446:LEU:HD23	1.93	0.42
1:D:418:GLN:NE2	1:D:434:ARG:HB2	2.35	0.42
1:D:503:TYR:HA	1:D:506:VAL:HG22	2.01	0.42
1:E:458:LYS:O	1:E:463:ARG:NH1	2.53	0.41
1:D:483:ASP:OD2	1:D:487:LEU:N	2.52	0.41
1:B:446:LEU:HD23	1:B:446:LEU:HA	1.93	0.41
1:H:421:LEU:HD11	1:H:433:PHE:CG	2.55	0.41
1:A:470:LEU:O	1:A:474:LYS:HG3	2.20	0.41
1:G:503:TYR:HA	1:G:506:VAL:HG22	2.03	0.41
1:E:433:PHE:CZ	1:E:455:LEU:HD13	2.56	0.41
1:A:441:ASP:OD2	1:A:445:ARG:NH1	2.54	0.41
1:B:477:ALA:HB3	1:B:479:TYR:CZ	2.56	0.41
1:G:451:LEU:HD12	1:G:467:PHE:CE2	2.56	0.40
1:G:515:LEU:O	1:G:518:VAL:HG12	2.22	0.40
1:G:441:ASP:OD2	1:G:445:ARG:NH1	2.55	0.40
1:D:488:ALA:HB2	1:D:502:THR:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	138/177 (78%)	134 (97%)	4 (3%)	0	100	100
1	B	138/177 (78%)	134 (97%)	4 (3%)	0	100	100
1	C	141/177 (80%)	137 (97%)	4 (3%)	0	100	100
1	D	137/177 (77%)	133 (97%)	4 (3%)	0	100	100
1	E	138/177 (78%)	134 (97%)	4 (3%)	0	100	100
1	F	142/177 (80%)	137 (96%)	5 (4%)	0	100	100
1	G	138/177 (78%)	135 (98%)	3 (2%)	0	100	100
1	H	138/177 (78%)	134 (97%)	4 (3%)	0	100	100
All	All	1110/1416 (78%)	1078 (97%)	32 (3%)	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	124/156 (80%)	123 (99%)	1 (1%)	81	93
1	B	124/156 (80%)	121 (98%)	3 (2%)	49	77
1	C	127/156 (81%)	125 (98%)	2 (2%)	62	85
1	D	123/156 (79%)	123 (100%)	0	100	100
1	E	124/156 (80%)	124 (100%)	0	100	100
1	F	128/156 (82%)	126 (98%)	2 (2%)	62	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	124/156 (80%)	121 (98%)	3 (2%)	49 77
1	H	124/156 (80%)	124 (100%)	0	100 100
All	All	998/1248 (80%)	987 (99%)	11 (1%)	73 90

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	451	LEU
1	B	419	THR
1	B	533	VAL
1	B	537	ARG
1	C	405	GLN
1	C	431	GLU
1	F	402	LEU
1	F	451	LEU
1	G	451	LEU
1	G	513	SER
1	G	537	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	521	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	140/177 (79%)	0.60	3 (2%)	63	65	46, 61, 84, 110	0
1	B	140/177 (79%)	0.60	8 (5%)	23	22	49, 73, 99, 128	0
1	C	143/177 (80%)	0.73	8 (5%)	24	23	54, 79, 103, 128	0
1	D	139/177 (78%)	0.60	5 (3%)	42	42	52, 69, 93, 113	0
1	E	140/177 (79%)	0.54	1 (0%)	87	89	43, 60, 84, 112	0
1	F	144/177 (81%)	0.68	8 (5%)	24	23	49, 69, 100, 122	0
1	G	140/177 (79%)	0.75	6 (4%)	35	33	51, 74, 101, 116	0
1	H	140/177 (79%)	0.55	5 (3%)	42	42	45, 65, 96, 124	0
All	All	1126/1416 (79%)	0.63	44 (3%)	39	38	43, 69, 99, 128	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	484	ARG	5.5
1	F	517	ARG	3.6
1	A	473	PHE	3.5
1	C	484	ARG	3.3
1	B	543	ARG	3.2
1	B	539	LEU	3.2
1	D	515	LEU	3.1
1	B	515	LEU	2.8
1	C	517	ARG	2.7
1	F	514	LEU	2.7
1	H	497	ARG	2.6
1	F	494	LEU	2.6
1	G	497	ARG	2.6
1	F	515	LEU	2.6
1	G	543	ARG	2.5
1	A	516	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	484	ARG	2.5
1	F	545	MET	2.4
1	G	514	LEU	2.4
1	F	539	LEU	2.3
1	B	518	VAL	2.3
1	B	514	LEU	2.2
1	C	539	LEU	2.2
1	D	412	TRP	2.2
1	H	533	VAL	2.2
1	C	544	GLU	2.2
1	G	508	CYS	2.2
1	A	515	LEU	2.1
1	G	515	LEU	2.1
1	H	484	ARG	2.1
1	D	472	GLU	2.1
1	C	403	TYR	2.1
1	C	529	ILE	2.1
1	D	539	LEU	2.1
1	F	543	ARG	2.1
1	C	443	LEU	2.1
1	C	510	LEU	2.1
1	D	409	VAL	2.1
1	E	515	LEU	2.1
1	H	515	LEU	2.1
1	B	542	ALA	2.1
1	B	517	ARG	2.1
1	B	494	LEU	2.0
1	H	545	MET	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 carbohydrates 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.