wwPDB X-ray Structure Validation Summary Report (i)

Sep 14, 2023 – 01:00 AM EDT

PDB ID	:	4RSQ
Title	:	2.9A resolution structure of SRPN2 (K198C/E359C) from Anopheles gambiae
Authors	:	Lovell, S.; Battaile, K.P.; Zhang, X.; Meekins, D.A.; An, C.; Michel, K.
Deposited on	:	2014-11-10
Resolution	:	2.90 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

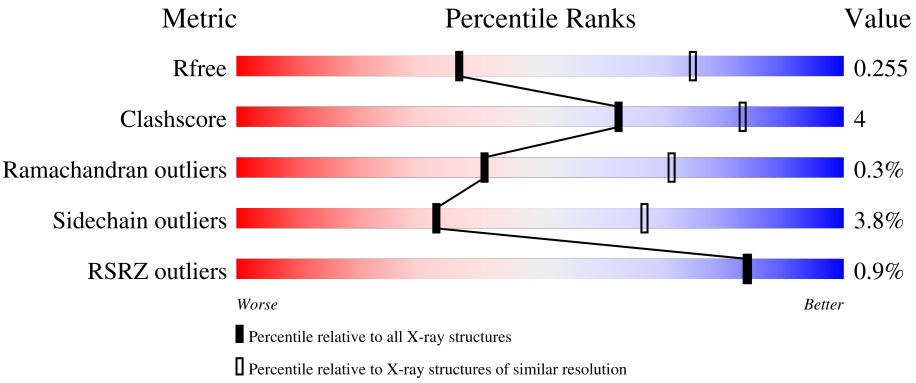
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	397	76% 13% • 10%
1	B	397	82% 7% • 11%
1	C	397	76% 13% 11%
1	D	397	76% 13% 11%
1	E	397	80% 9% 10%

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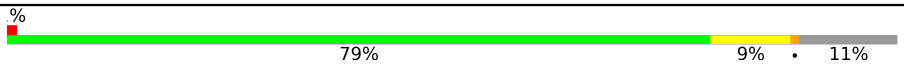
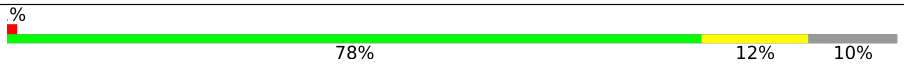
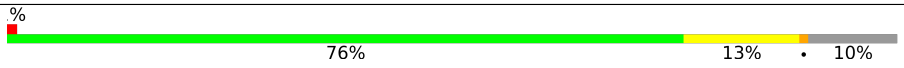
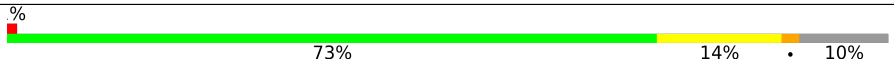
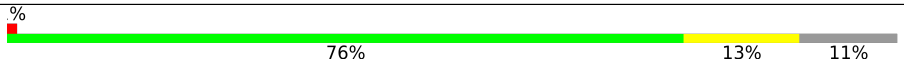
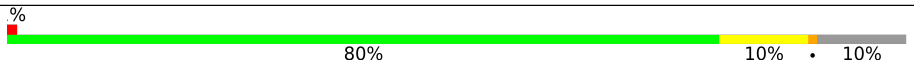
Mol	Chain	Length	Quality of chain
1	F	397	
1	G	397	
1	H	397	
1	I	397	
1	J	397	
1	K	397	
1	L	397	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 33765 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 Serpin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2827	1813	468	538	8			
1	B	355	Total	C	N	O	S	0	0	0
			2800	1800	460	532	8			
1	C	354	Total	C	N	O	S	0	0	0
			2816	1806	464	538	8			
1	D	355	Total	C	N	O	S	0	0	0
			2801	1797	463	533	8			
1	E	356	Total	C	N	O	S	0	0	0
			2816	1808	467	533	8			
1	F	353	Total	C	N	O	S	0	0	0
			2804	1802	461	533	8			
1	G	357	Total	C	N	O	S	0	0	0
			2829	1815	468	538	8			
1	H	357	Total	C	N	O	S	0	0	0
			2814	1807	465	534	8			
1	I	356	Total	C	N	O	S	0	0	0
			2814	1808	466	532	8			
1	J	355	Total	C	N	O	S	0	0	0
			2817	1808	465	536	8			
1	K	356	Total	C	N	O	S	0	0	0
			2807	1803	463	533	8			
1	L	356	Total	C	N	O	S	0	0	0
			2820	1807	468	537	8			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	MET	-	expression tag	UNP Q005N3
A	14	GLY	-	expression tag	UNP Q005N3
A	15	HIS	-	expression tag	UNP Q005N3
A	16	HIS	-	expression tag	UNP Q005N3
A	17	HIS	-	expression tag	UNP Q005N3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	18	HIS	-	expression tag	UNP Q005N3
A	19	HIS	-	expression tag	UNP Q005N3
A	20	HIS	-	expression tag	UNP Q005N3
A	21	GLY	-	expression tag	UNP Q005N3
A	198	CYS	LYS	engineered mutation	UNP Q005N3
A	359	CYS	GLU	engineered mutation	UNP Q005N3
B	13	MET	-	expression tag	UNP Q005N3
B	14	GLY	-	expression tag	UNP Q005N3
B	15	HIS	-	expression tag	UNP Q005N3
B	16	HIS	-	expression tag	UNP Q005N3
B	17	HIS	-	expression tag	UNP Q005N3
B	18	HIS	-	expression tag	UNP Q005N3
B	19	HIS	-	expression tag	UNP Q005N3
B	20	HIS	-	expression tag	UNP Q005N3
B	21	GLY	-	expression tag	UNP Q005N3
B	198	CYS	LYS	engineered mutation	UNP Q005N3
B	359	CYS	GLU	engineered mutation	UNP Q005N3
C	13	MET	-	expression tag	UNP Q005N3
C	14	GLY	-	expression tag	UNP Q005N3
C	15	HIS	-	expression tag	UNP Q005N3
C	16	HIS	-	expression tag	UNP Q005N3
C	17	HIS	-	expression tag	UNP Q005N3
C	18	HIS	-	expression tag	UNP Q005N3
C	19	HIS	-	expression tag	UNP Q005N3
C	20	HIS	-	expression tag	UNP Q005N3
C	21	GLY	-	expression tag	UNP Q005N3
C	198	CYS	LYS	engineered mutation	UNP Q005N3
C	359	CYS	GLU	engineered mutation	UNP Q005N3
D	13	MET	-	expression tag	UNP Q005N3
D	14	GLY	-	expression tag	UNP Q005N3
D	15	HIS	-	expression tag	UNP Q005N3
D	16	HIS	-	expression tag	UNP Q005N3
D	17	HIS	-	expression tag	UNP Q005N3
D	18	HIS	-	expression tag	UNP Q005N3
D	19	HIS	-	expression tag	UNP Q005N3
D	20	HIS	-	expression tag	UNP Q005N3
D	21	GLY	-	expression tag	UNP Q005N3
D	198	CYS	LYS	engineered mutation	UNP Q005N3
D	359	CYS	GLU	engineered mutation	UNP Q005N3
E	13	MET	-	expression tag	UNP Q005N3
E	14	GLY	-	expression tag	UNP Q005N3
E	15	HIS	-	expression tag	UNP Q005N3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	16	HIS	-	expression tag	UNP Q005N3
E	17	HIS	-	expression tag	UNP Q005N3
E	18	HIS	-	expression tag	UNP Q005N3
E	19	HIS	-	expression tag	UNP Q005N3
E	20	HIS	-	expression tag	UNP Q005N3
E	21	GLY	-	expression tag	UNP Q005N3
E	198	CYS	LYS	engineered mutation	UNP Q005N3
E	359	CYS	GLU	engineered mutation	UNP Q005N3
F	13	MET	-	expression tag	UNP Q005N3
F	14	GLY	-	expression tag	UNP Q005N3
F	15	HIS	-	expression tag	UNP Q005N3
F	16	HIS	-	expression tag	UNP Q005N3
F	17	HIS	-	expression tag	UNP Q005N3
F	18	HIS	-	expression tag	UNP Q005N3
F	19	HIS	-	expression tag	UNP Q005N3
F	20	HIS	-	expression tag	UNP Q005N3
F	21	GLY	-	expression tag	UNP Q005N3
F	198	CYS	LYS	engineered mutation	UNP Q005N3
F	359	CYS	GLU	engineered mutation	UNP Q005N3
G	13	MET	-	expression tag	UNP Q005N3
G	14	GLY	-	expression tag	UNP Q005N3
G	15	HIS	-	expression tag	UNP Q005N3
G	16	HIS	-	expression tag	UNP Q005N3
G	17	HIS	-	expression tag	UNP Q005N3
G	18	HIS	-	expression tag	UNP Q005N3
G	19	HIS	-	expression tag	UNP Q005N3
G	20	HIS	-	expression tag	UNP Q005N3
G	21	GLY	-	expression tag	UNP Q005N3
G	198	CYS	LYS	engineered mutation	UNP Q005N3
G	359	CYS	GLU	engineered mutation	UNP Q005N3
H	13	MET	-	expression tag	UNP Q005N3
H	14	GLY	-	expression tag	UNP Q005N3
H	15	HIS	-	expression tag	UNP Q005N3
H	16	HIS	-	expression tag	UNP Q005N3
H	17	HIS	-	expression tag	UNP Q005N3
H	18	HIS	-	expression tag	UNP Q005N3
H	19	HIS	-	expression tag	UNP Q005N3
H	20	HIS	-	expression tag	UNP Q005N3
H	21	GLY	-	expression tag	UNP Q005N3
H	198	CYS	LYS	engineered mutation	UNP Q005N3
H	359	CYS	GLU	engineered mutation	UNP Q005N3
I	13	MET	-	expression tag	UNP Q005N3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	14	GLY	-	expression tag	UNP Q005N3
I	15	HIS	-	expression tag	UNP Q005N3
I	16	HIS	-	expression tag	UNP Q005N3
I	17	HIS	-	expression tag	UNP Q005N3
I	18	HIS	-	expression tag	UNP Q005N3
I	19	HIS	-	expression tag	UNP Q005N3
I	20	HIS	-	expression tag	UNP Q005N3
I	21	GLY	-	expression tag	UNP Q005N3
I	198	CYS	LYS	engineered mutation	UNP Q005N3
I	359	CYS	GLU	engineered mutation	UNP Q005N3
J	13	MET	-	expression tag	UNP Q005N3
J	14	GLY	-	expression tag	UNP Q005N3
J	15	HIS	-	expression tag	UNP Q005N3
J	16	HIS	-	expression tag	UNP Q005N3
J	17	HIS	-	expression tag	UNP Q005N3
J	18	HIS	-	expression tag	UNP Q005N3
J	19	HIS	-	expression tag	UNP Q005N3
J	20	HIS	-	expression tag	UNP Q005N3
J	21	GLY	-	expression tag	UNP Q005N3
J	198	CYS	LYS	engineered mutation	UNP Q005N3
J	359	CYS	GLU	engineered mutation	UNP Q005N3
K	13	MET	-	expression tag	UNP Q005N3
K	14	GLY	-	expression tag	UNP Q005N3
K	15	HIS	-	expression tag	UNP Q005N3
K	16	HIS	-	expression tag	UNP Q005N3
K	17	HIS	-	expression tag	UNP Q005N3
K	18	HIS	-	expression tag	UNP Q005N3
K	19	HIS	-	expression tag	UNP Q005N3
K	20	HIS	-	expression tag	UNP Q005N3
K	21	GLY	-	expression tag	UNP Q005N3
K	198	CYS	LYS	engineered mutation	UNP Q005N3
K	359	CYS	GLU	engineered mutation	UNP Q005N3
L	13	MET	-	expression tag	UNP Q005N3
L	14	GLY	-	expression tag	UNP Q005N3
L	15	HIS	-	expression tag	UNP Q005N3
L	16	HIS	-	expression tag	UNP Q005N3
L	17	HIS	-	expression tag	UNP Q005N3
L	18	HIS	-	expression tag	UNP Q005N3
L	19	HIS	-	expression tag	UNP Q005N3
L	20	HIS	-	expression tag	UNP Q005N3
L	21	GLY	-	expression tag	UNP Q005N3
L	198	CYS	LYS	engineered mutation	UNP Q005N3

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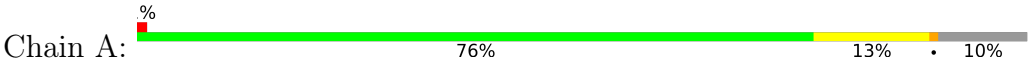
Chain	Residue	Modelled	Actual	Comment	Reference
L	359	CYS	GLU	engineered mutation	UNP Q005N3

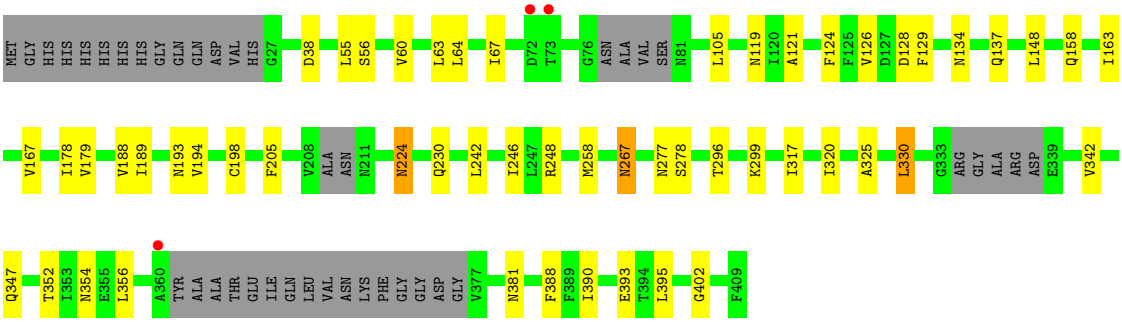
3 Residue-property plots (i)

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: Serpin 2

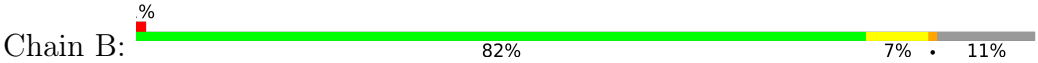
Chain A:

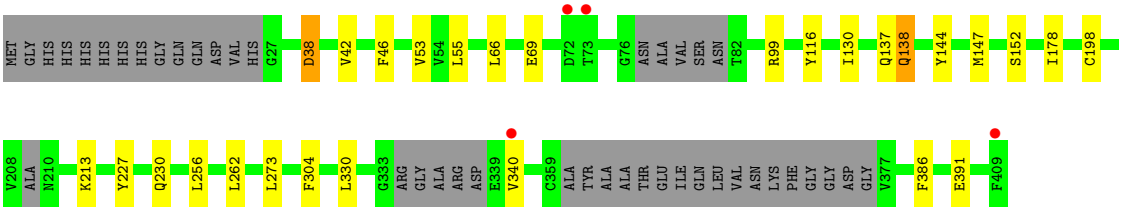




• Molecule 1: Serpin 2

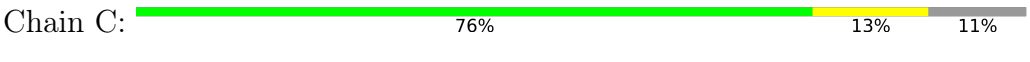
Chain B:

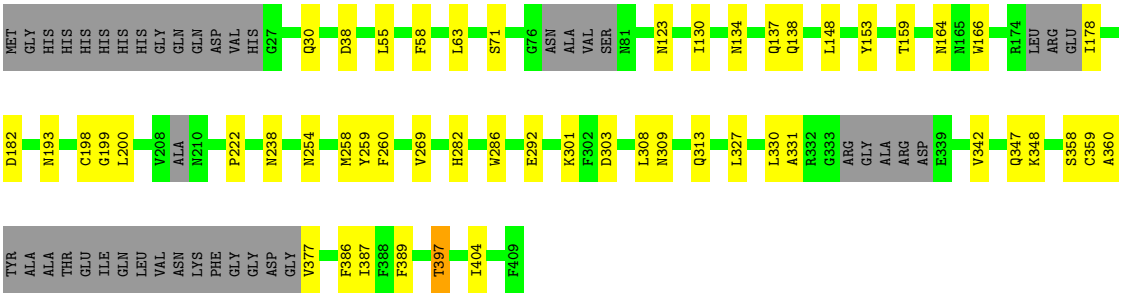




• Molecule 1: Serpin 2

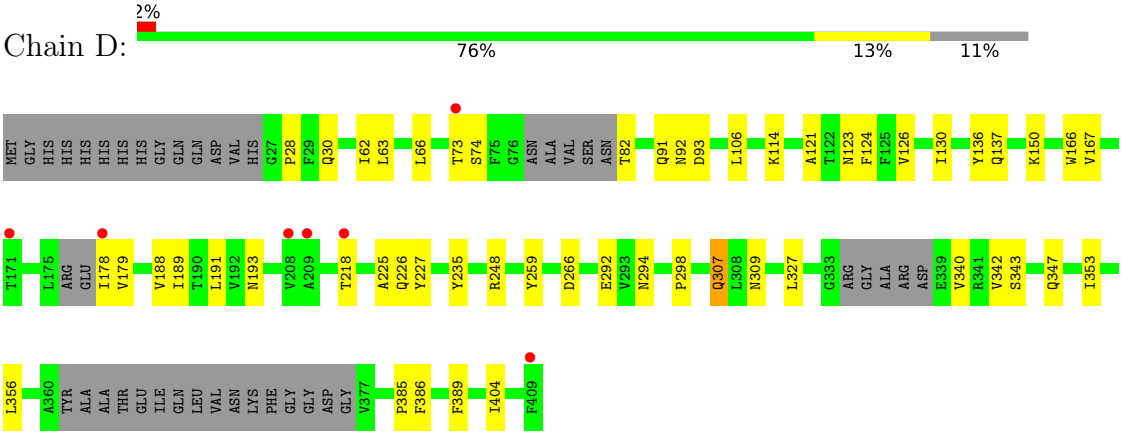
Chain C:





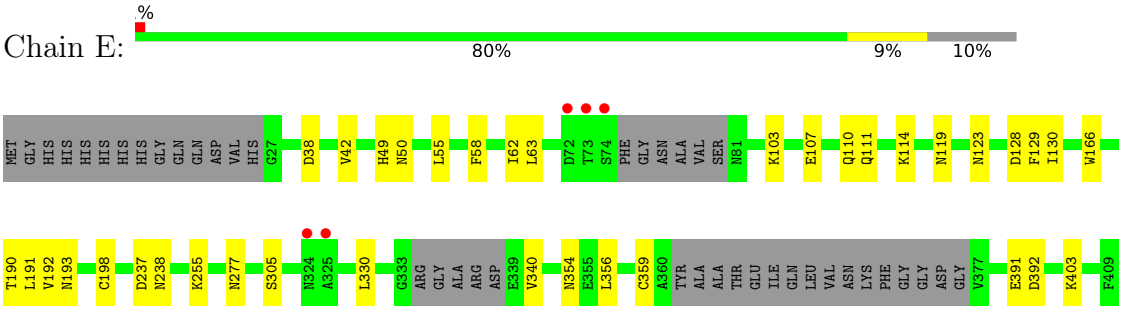
• Molecule 1: Serpin 2

Chain D:



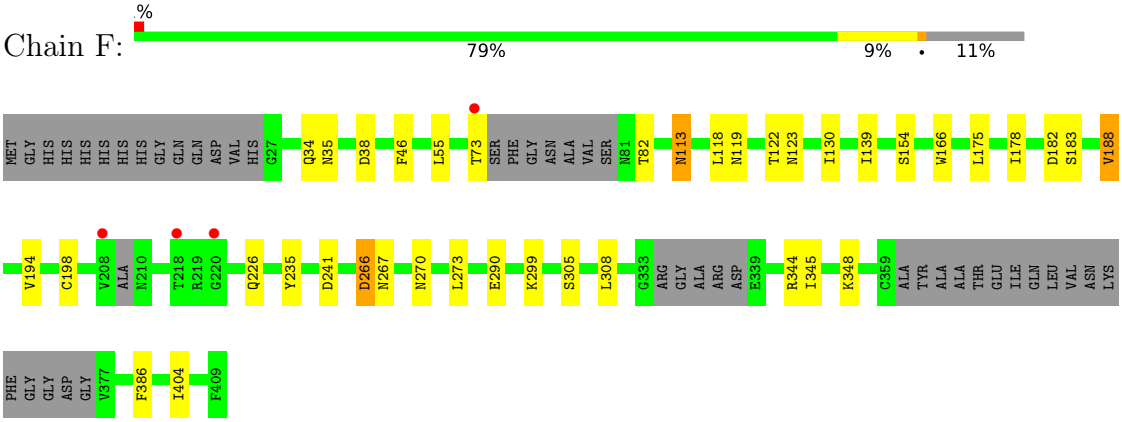
• Molecule 1: Serpin 2

Chain E:



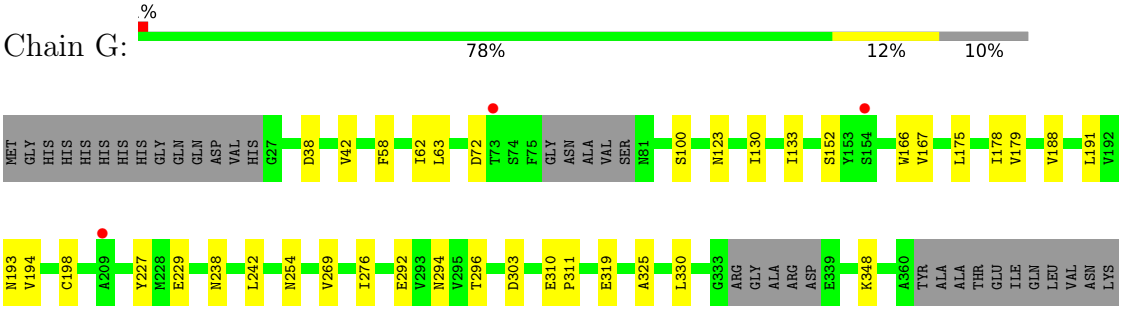
• Molecule 1: Serpin 2

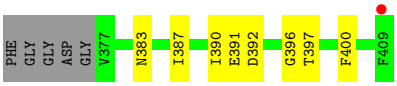
Chain F:



• Molecule 1: Serpin 2

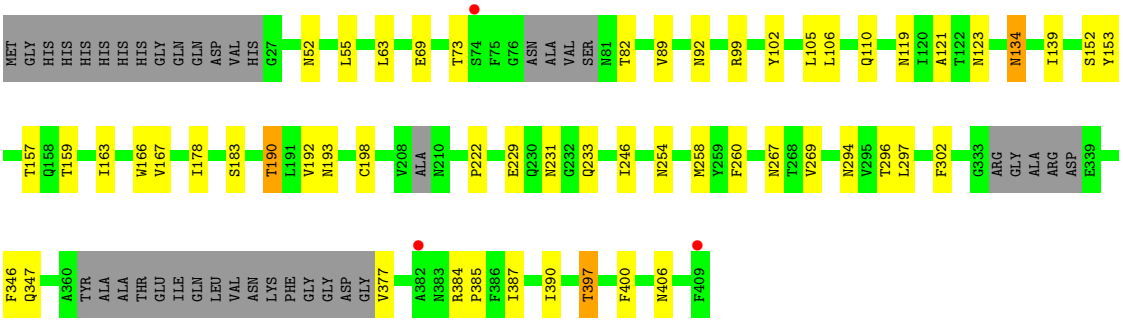
Chain G:





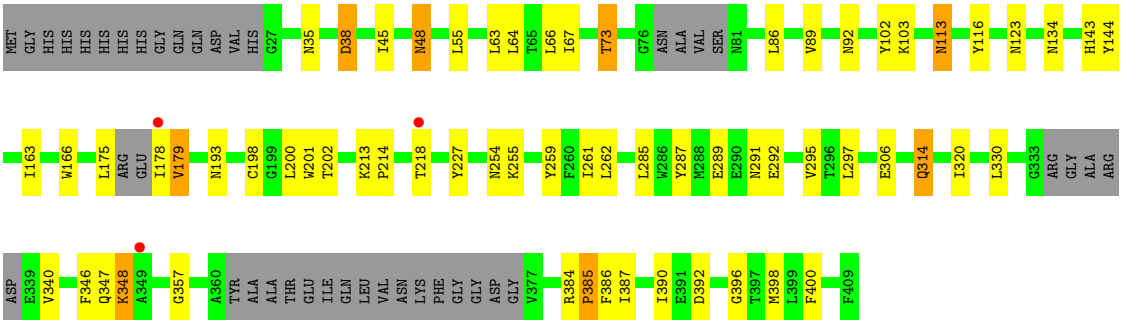
• Molecule 1: Serpin 2

Chain H:



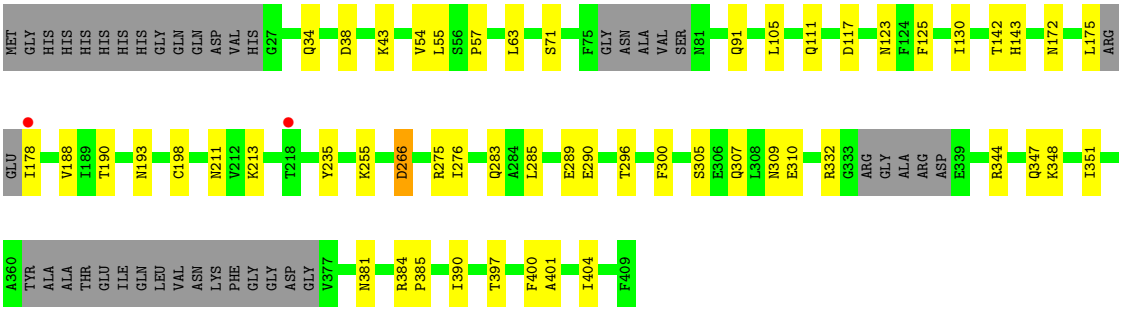
• Molecule 1: Serpin 2

Chain I:



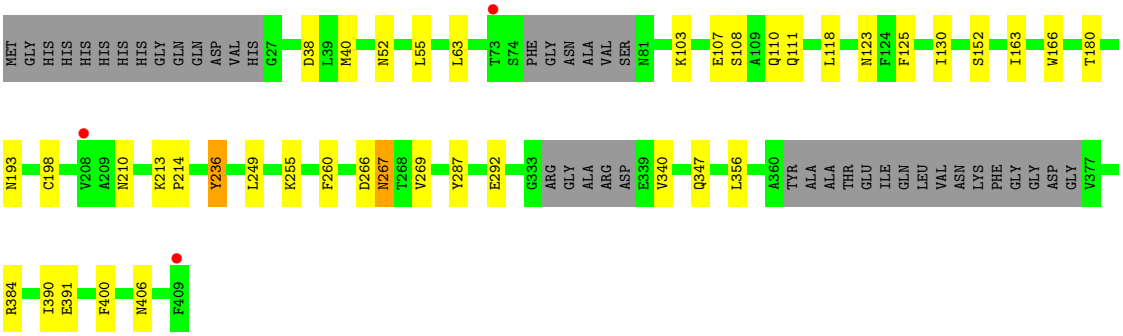
• Molecule 1: Serpin 2

Chain J:



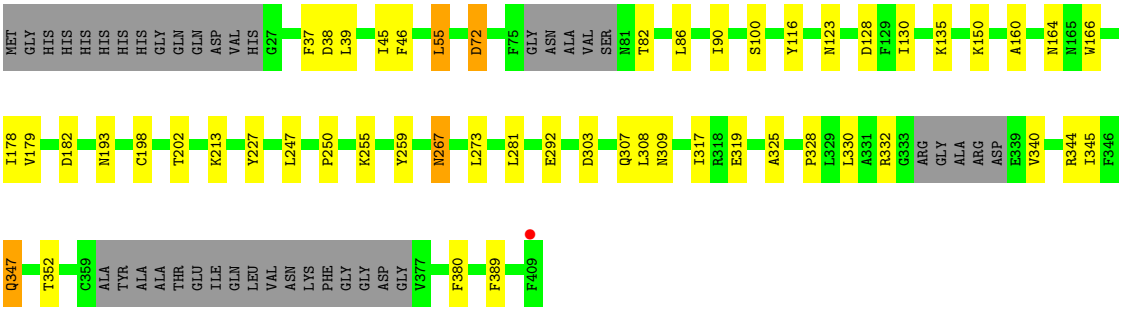
• Molecule 1: Serpin 2

Chain K:



• Molecule 1: Serpin 2

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	97.92Å 164.39Å 186.18Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	47.82 – 2.90 47.82 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.82-2.90) 99.3 (47.82-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.194 , 0.255 0.197 , 0.255	Depositor DCC
R_{free} test set	6286 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	40.3	Xtriage
Anisotropy	0.863	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 8.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.427 for h,-k,-l	Xtriage
Reported twinning fraction	0.445 for H, K, L 0.555 for h,-k,-l	Depositor
Outliers	0 of 129620 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	33765	wwPDB-VP
Average B, all atoms (Å^2)	43.0	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 30.85 % 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 1.2202e-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

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	0.37	0/2890	0.54	0/3928
1	B	0.35	0/2863	0.54	0/3894
1	C	0.37	0/2878	0.56	0/3909
1	D	0.37	0/2863	0.55	0/3892
1	E	0.38	0/2880	0.56	0/3918
1	F	0.34	0/2867	0.52	0/3898
1	G	0.34	0/2893	0.52	0/3935
1	H	0.35	0/2877	0.55	0/3913
1	I	0.37	0/2877	0.54	0/3911
1	J	0.37	0/2880	0.55	0/3916
1	K	0.36	0/2871	0.55	0/3908
1	L	0.36	0/2883	0.55	0/3923
All	All	0.36	0/34522	0.54	0/46945

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	2827	0	2699	30	0
1	B	2800	0	2658	14	0
1	C	2816	0	2689	24	0
1	D	2801	0	2672	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2816	0	2688	17	0
1	F	2804	0	2673	18	0
1	G	2829	0	2698	20	0
1	H	2814	0	2676	30	0
1	I	2814	0	2692	34	0
1	J	2817	0	2690	28	0
1	K	2807	0	2668	16	0
1	L	2820	0	2690	30	0
All	All	33765	0	32193	282	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.

The worst 5 of 282 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:E:63:LEU:HD21	1:E:193:ASN:HB2	1.65	0.77
1:A:63:LEU:HD21	1:A:193:ASN:HB2	1.65	0.77
1:G:130:ILE:HD11	1:G:188:VAL:HG12	1.69	0.74
1:G:178:ILE:HG23	1:G:179:VAL:HG13	1.70	0.73
1:K:130:ILE:HD11	1:K:340:VAL:HG11	1.72	0.71

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	346/397 (87%)	335 (97%)	10 (3%)	1 (0%)	41 71
1	B	345/397 (87%)	325 (94%)	19 (6%)	1 (0%)	41 71
1	C	342/397 (86%)	327 (96%)	14 (4%)	1 (0%)	41 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	345/397 (87%)	326 (94%)	17 (5%)	2 (1%)	25 58
1	E	348/397 (88%)	326 (94%)	22 (6%)	0	100 100
1	F	343/397 (86%)	329 (96%)	13 (4%)	1 (0%)	41 71
1	G	349/397 (88%)	335 (96%)	14 (4%)	0	100 100
1	H	347/397 (87%)	334 (96%)	10 (3%)	3 (1%)	17 48
1	I	346/397 (87%)	324 (94%)	19 (6%)	3 (1%)	17 48
1	J	345/397 (87%)	325 (94%)	20 (6%)	0	100 100
1	K	348/397 (88%)	333 (96%)	15 (4%)	0	100 100
1	L	348/397 (88%)	340 (98%)	8 (2%)	0	100 100
All	All	4152/4764 (87%)	3959 (95%)	181 (4%)	12 (0%)	41 71

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	92	ASN
1	H	92	ASN
1	D	74	SER
1	H	222	PRO
1	I	92	ASN

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	305/349 (87%)	295 (97%)	10 (3%)	38 72
1	B	299/349 (86%)	292 (98%)	7 (2%)	50 80
1	C	305/349 (87%)	294 (96%)	11 (4%)	35 69
1	D	300/349 (86%)	290 (97%)	10 (3%)	38 72
1	E	302/349 (86%)	292 (97%)	10 (3%)	38 72
1	F	302/349 (86%)	289 (96%)	13 (4%)	29 62
1	G	304/349 (87%)	293 (96%)	11 (4%)	35 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	301/349 (86%)	291 (97%)	10 (3%)	38 72
1	I	302/349 (86%)	284 (94%)	18 (6%)	19 49
1	J	304/349 (87%)	293 (96%)	11 (4%)	35 69
1	K	300/349 (86%)	285 (95%)	15 (5%)	24 57
1	L	304/349 (87%)	291 (96%)	13 (4%)	29 62
All	All	3628/4188 (87%)	3489 (96%)	139 (4%)	33 67

5 of 139 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	180	THR
1	K	266	ASP
1	L	128	ASP
1	F	34	GLN
1	E	391	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	313	GLN
1	L	91	GLN
1	E	277	ASN
1	E	270	ASN
1	L	137	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 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

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	356/397 (89%)	0.05	3 (0%)	86	86	24, 38, 62, 90	0
1	B	355/397 (89%)	0.10	4 (1%)	80	80	27, 43, 65, 90	0
1	C	354/397 (89%)	-0.00	0	100	100	18, 36, 58, 98	0
1	D	355/397 (89%)	0.13	7 (1%)	65	63	21, 41, 66, 94	0
1	E	356/397 (89%)	0.07	5 (1%)	75	75	23, 40, 65, 87	0
1	F	353/397 (88%)	0.09	4 (1%)	80	80	32, 45, 65, 89	0
1	G	357/397 (89%)	0.06	4 (1%)	80	80	24, 43, 63, 85	0
1	H	357/397 (89%)	0.14	3 (0%)	86	86	24, 46, 69, 95	0
1	I	356/397 (89%)	0.10	3 (0%)	86	86	24, 43, 69, 84	0
1	J	355/397 (89%)	0.07	2 (0%)	89	89	23, 42, 66, 88	0
1	K	356/397 (89%)	0.13	3 (0%)	86	86	26, 43, 75, 96	0
1	L	356/397 (89%)	0.01	1 (0%)	94	94	24, 40, 56, 83	0
All	All	4266/4764 (89%)	0.08	39 (0%)	84	84	18, 42, 66, 98	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	THR	4.2
1	B	73	THR	4.2
1	G	73	THR	3.5
1	B	72	ASP	3.4
1	D	409	PHE	3.2

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.