Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID	:	5EI0
Title	:	Structure of RCL-cleaved vaspin (serpinA12)
Authors	:	Pippel, J.; Kuettner, B.E.; Ulbricht, D.; Daberger, J.; Schultz, S.; Heiker, J.T.; Strater, N.
Deposited on	:	2015-10-29
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

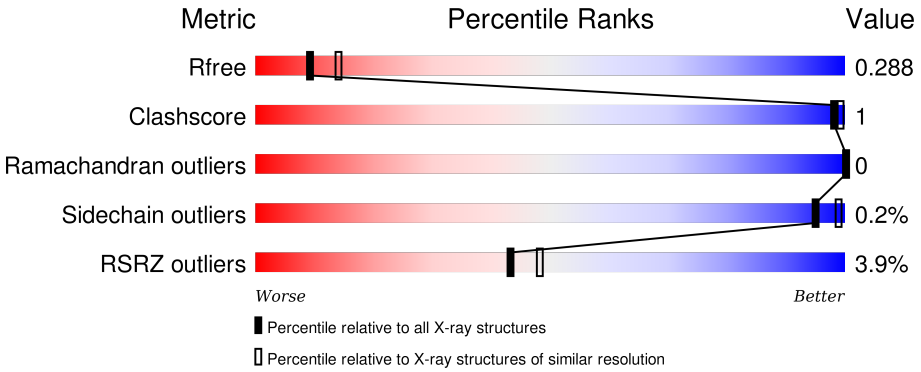
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	413	3% 87% • 10%
1	E	413	4% 88% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12246 atoms, of which 6176 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 A12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	372	Total	C	H	N	O	S	0	4	0
			6128	1949	3103	515	549	12			
1	E	371	Total	C	H	N	O	S	0	2	0
			6075	1936	3073	510	543	13			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	HIS	-	cloning artifact	UNP Q8IW75
A	3	HIS	-	cloning artifact	UNP Q8IW75
A	4	HIS	-	cloning artifact	UNP Q8IW75
A	5	HIS	-	cloning artifact	UNP Q8IW75
A	6	HIS	-	cloning artifact	UNP Q8IW75
A	7	HIS	-	cloning artifact	UNP Q8IW75
A	8	HIS	-	cloning artifact	UNP Q8IW75
A	9	HIS	-	cloning artifact	UNP Q8IW75
A	10	HIS	-	cloning artifact	UNP Q8IW75
A	11	HIS	-	cloning artifact	UNP Q8IW75
A	12	SER	-	cloning artifact	UNP Q8IW75
A	13	SER	-	cloning artifact	UNP Q8IW75
A	14	GLY	-	cloning artifact	UNP Q8IW75
A	15	HIS	-	cloning artifact	UNP Q8IW75
A	16	ILE	-	cloning artifact	UNP Q8IW75
A	17	GLU	-	cloning artifact	UNP Q8IW75
A	18	GLY	-	cloning artifact	UNP Q8IW75
A	19	ARG	-	cloning artifact	UNP Q8IW75
A	20	HIS	-	cloning artifact	UNP Q8IW75
A	21	MET	-	cloning artifact	UNP Q8IW75
E	2	HIS	-	cloning artifact	UNP Q8IW75
E	3	HIS	-	cloning artifact	UNP Q8IW75
E	4	HIS	-	cloning artifact	UNP Q8IW75
E	5	HIS	-	cloning artifact	UNP Q8IW75
E	6	HIS	-	cloning artifact	UNP Q8IW75

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Chain	Residue	Modelled	Actual	Comment	Reference
E	7	HIS	-	cloning artifact	UNP Q8IW75
E	8	HIS	-	cloning artifact	UNP Q8IW75
E	9	HIS	-	cloning artifact	UNP Q8IW75
E	10	HIS	-	cloning artifact	UNP Q8IW75
E	11	HIS	-	cloning artifact	UNP Q8IW75
E	12	SER	-	cloning artifact	UNP Q8IW75
E	13	SER	-	cloning artifact	UNP Q8IW75
E	14	GLY	-	cloning artifact	UNP Q8IW75
E	15	HIS	-	cloning artifact	UNP Q8IW75
E	16	ILE	-	cloning artifact	UNP Q8IW75
E	17	GLU	-	cloning artifact	UNP Q8IW75
E	18	GLY	-	cloning artifact	UNP Q8IW75
E	19	ARG	-	cloning artifact	UNP Q8IW75
E	20	HIS	-	cloning artifact	UNP Q8IW75
E	21	MET	-	cloning artifact	UNP Q8IW75

- Molecule 2 is water.

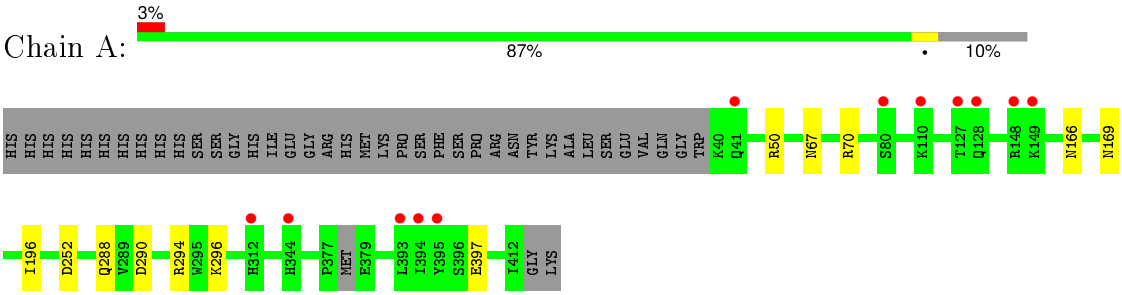
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	15	Total O 15 15	0	0
2	E	28	Total O 28 28	0	0

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 errors 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.

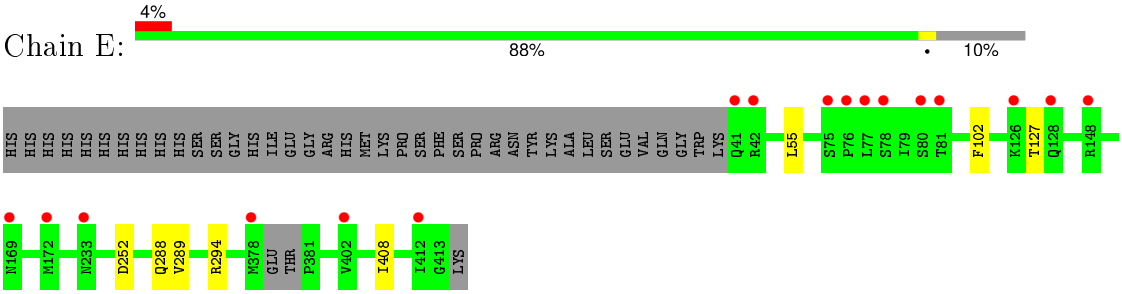
- Molecule 1: Serpin A12

Chain A:



- Molecule 1: Serpin A12

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.39Å 104.42Å 62.97Å 90.00° 96.90° 90.00°	Depositor
Resolution (Å)	29.19 – 2.50 29.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.3 (29.19-2.50) 88.4 (29.19-2.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.224 , 0.275 0.241 , 0.288	Depositor DCC
R_{free} test set	1205 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	50.2	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 21.8	EDS
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 23753 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12246	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.22	0/3099	0.36	0/4173
1	E	0.22	0/3070	0.36	0/4132
All	All	0.22	0/6169	0.36	0/8305

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	3025	3103	3103	8	0
1	E	3002	3073	3076	4	0
2	A	15	0	0	1	0
2	E	28	0	0	0	0
All	All	6070	6176	6179	12	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 1.

All (12) 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:A:50[B]:ARG:NH1	1:A:290:ASP:OD1	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASN:ND2	1:A:169:ASN:OD1	2.34	0.60
1:A:67[A]:ASN:OD1	1:A:70:ARG:NH2	2.37	0.58
1:A:67[B]:ASN:OD1	1:A:70:ARG:NH2	2.37	0.58
1:A:296:LYS:NZ	1:A:397:GLU:OE1	2.40	0.53
1:A:288[B]:GLN:NE2	2:A:503:HOH:O	2.41	0.53
1:E:252:ASP:OD1	1:E:294:ARG:NH2	2.42	0.51
1:A:196:ILE:N	1:A:196:ILE:HD12	2.33	0.44
1:A:252:ASP:OD1	1:A:294:ARG:NH2	2.48	0.44
1:E:408:ILE:N	1:E:408:ILE:HD12	2.35	0.42
1:E:55:LEU:HD21	1:E:102:PHE:CD2	2.55	0.41
1:E:288:GLN:HG2	1:E:289:VAL:H	1.86	0.41

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	372/413 (90%)	345 (93%)	27 (7%)	0	100	100
1	E	369/413 (89%)	349 (95%)	20 (5%)	0	100	100
All	All	741/826 (90%)	694 (94%)	47 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	337/369 (91%)	337 (100%)	0	100 100
1	E	333/369 (90%)	332 (100%)	1 (0%)	94 99
All	All	670/738 (91%)	669 (100%)	1 (0%)	95 99

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	127	THR

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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	372/413 (90%)	0.19	12 (3%) 51 56	37, 55, 81, 107	0
1	E	371/413 (89%)	0.21	17 (4%) 36 41	35, 51, 80, 101	0
All	All	743/826 (89%)	0.20	29 (3%) 43 48	35, 53, 80, 107	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	GLN	4.5
1	A	110	LYS	3.7
1	E	169	ASN	3.5
1	A	127	THR	3.3
1	E	172	MET	3.2
1	E	77	LEU	3.2
1	A	344	HIS	3.1
1	E	128	GLN	3.1
1	E	78	SER	2.6
1	E	148	ARG	2.6
1	E	81	THR	2.5
1	E	378	MET	2.5
1	E	402	VAL	2.4
1	E	233	ASN	2.3
1	E	76	PRO	2.3
1	A	148	ARG	2.3
1	E	75	SER	2.3
1	E	80	SER	2.2
1	A	393	LEU	2.2
1	A	394	ILE	2.2
1	A	312	HIS	2.2
1	E	126	LYS	2.2
1	E	41	GLN	2.2
1	A	395	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	149	LYS	2.1
1	A	80	SER	2.1
1	A	128	GLN	2.1
1	E	42	ARG	2.1
1	E	412	ILE	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.