



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 02:13 PM GMT

PDB ID : 3RSE
Title : Structural and biochemical characterization of two binding sites for nucleation promoting factor WASp-VCA on Arp2/3 complex
Authors : Pollard, T.D.; Jurgenson, C.T.; Ti, S.; Nolen, B.J.
Deposited on : 2011-05-02
Resolution : 2.65 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

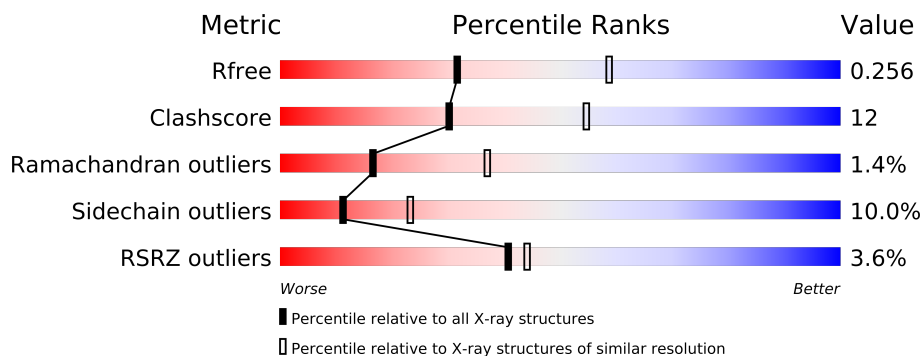
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.65 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}	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	418	
2	B	394	
3	C	372	
4	D	300	
5	E	178	
6	F	168	
7	G	151	
8	Z	3	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13807 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Actin-related protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3166	2033	531	588	14			

- Molecule 2 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	196	Total	C	N	O	S	0	0	0
			1566	1005	268	289	4			

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	354	Total	C	N	O	S	0	0	0
			2759	1748	487	505	19			

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	280	Total	C	N	O	S	0	0	0
			2262	1437	392	425	8			

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	173	Total	C	N	O	S	0	0	0
			1411	906	235	261	9			

- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	167	Total	C	N	O	S	0	0	0
			1371	875	239	248	9			

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	136	Total	C	N	O	S	0	0	0
			1031	647	179	202	3			

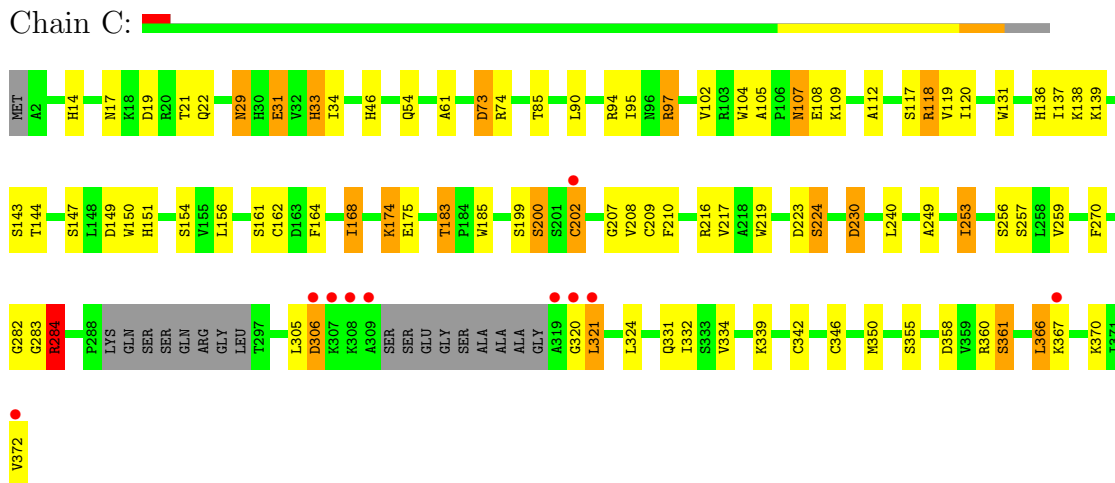
- Molecule 8 is a protein called CA fragment of Bos taurus N-WASP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	Z	3	Total	C	N	O	0	0	0
			33	21	4	8			

- Molecule 9 is water.

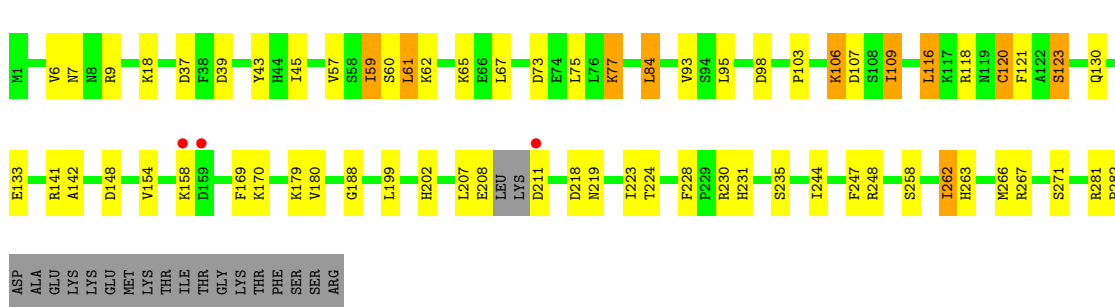
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	51	Total	O	0	0
			51	51		
9	B	13	Total	O	0	0
			13	13		
9	C	52	Total	O	0	0
			52	52		
9	D	47	Total	O	0	0
			47	47		
9	E	1	Total	O	0	0
			1	1		
9	F	35	Total	O	0	0
			35	35		
9	G	9	Total	O	0	0
			9	9		

Chain C:



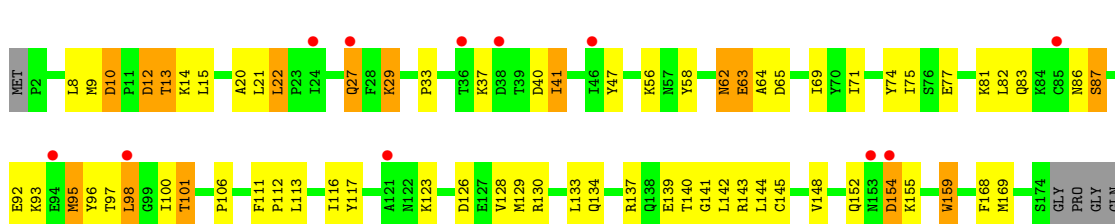
- Molecule 4: Actin-related protein 2/3 complex subunit 2

Chain D:



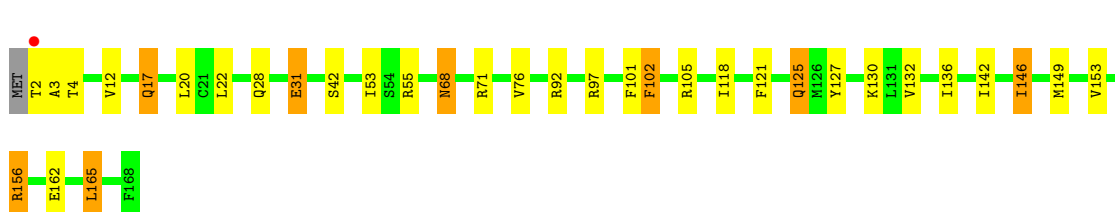
- Molecule 5: Actin-related protein 2/3 complex subunit 3

Chain E:



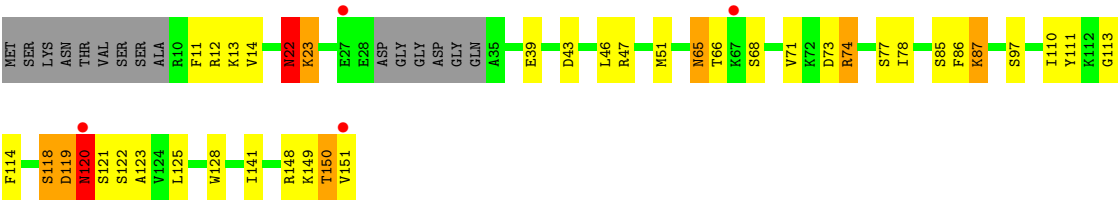
- Molecule 6: Actin-related protein 2/3 complex subunit 4

Chain F:



- Molecule 7: Actin-related protein 2/3 complex subunit 5

Chain G:



● Molecule 8: CA fragment of Bos taurus N-WASP

Chain Z: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.44Å 129.34Å 204.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 49.64 – 2.64	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.65) 99.1 (49.64-2.64)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.65Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.213 , 0.259 0.214 , 0.256	Depositor DCC
R_{free} test set	4317 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 86740 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13807	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.00	1/3247 (0.0%)	0.91	2/4406 (0.0%)
2	B	0.90	1/1596 (0.1%)	0.89	0/2157
3	C	1.04	2/2828 (0.1%)	1.03	12/3833 (0.3%)
4	D	1.04	3/2310 (0.1%)	0.96	4/3118 (0.1%)
5	E	0.84	0/1445	0.87	1/1949 (0.1%)
6	F	1.14	2/1393 (0.1%)	1.06	7/1868 (0.4%)
7	G	0.91	1/1043 (0.1%)	0.88	0/1403
8	Z	1.44	0/34	0.93	0/44
All	All	1.00	10/13896 (0.1%)	0.95	26/18778 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	202	CYS	CB-SG	7.64	1.95	1.82
4	D	120	CYS	CB-SG	-6.96	1.70	1.82
4	D	208	GLU	CG-CD	6.25	1.61	1.51
4	D	39	ASP	CB-CG	5.97	1.64	1.51
6	F	102	PHE	CE1-CZ	5.90	1.48	1.37

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	284	ARG	NE-CZ-NH1	7.73	124.17	120.30
5	E	98	LEU	CA-CB-CG	7.61	132.81	115.30
3	C	321	LEU	CA-CB-CG	7.54	132.65	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	ILE	CG1-CB-CG2	-6.77	96.50	111.40
4	D	73	ASP	CB-CG-OD1	6.77	124.39	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	282	GLY	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3166	0	3108	66	0
2	B	1566	0	1596	52	0
3	C	2759	0	2716	57	0
4	D	2262	0	2223	54	0
5	E	1411	0	1413	52	0
6	F	1371	0	1410	32	0
7	G	1031	0	1041	26	0
8	Z	33	0	21	1	0
9	A	51	0	0	3	0
9	B	13	0	0	2	0
9	C	52	0	0	0	0
9	D	47	0	0	3	0
9	E	1	0	0	0	0
9	F	35	0	0	2	0
9	G	9	0	0	0	0
All	All	13807	0	13528	326	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

The worst 5 of 326 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:183:THR:HG22	3:C:185:TRP:H	1.11	1.05
5:E:29:LYS:H	5:E:29:LYS:HD2	1.23	1.02
4:D:77:LYS:NZ	9:D:316:HOH:O	2.01	0.92
4:D:109:ILE:HD13	4:D:109:ILE:H	1.35	0.92
1:A:313:ARG:HD3	1:A:361:LYS:NZ	1.84	0.91

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	390/418 (93%)	360 (92%)	23 (6%)	7 (2%)	13	28
2	B	194/394 (49%)	173 (89%)	17 (9%)	4 (2%)	11	24
3	C	348/372 (94%)	322 (92%)	24 (7%)	2 (1%)	33	63
4	D	276/300 (92%)	267 (97%)	9 (3%)	0	100	100
5	E	171/178 (96%)	142 (83%)	23 (14%)	6 (4%)	6	11
6	F	165/168 (98%)	158 (96%)	7 (4%)	0	100	100
7	G	132/151 (87%)	119 (90%)	9 (7%)	4 (3%)	7	14
8	Z	1/3 (33%)	0	1 (100%)	0	100	100
All	All	1677/1984 (84%)	1541 (92%)	113 (7%)	23 (1%)	16	37

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	THR
1	A	263	SER
1	A	264	LYS
1	A	349	LEU
2	B	291	ILE

5.3.2 Protein sidechains ⓘ

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	344/363 (95%)	313 (91%)	31 (9%)	14	28
2	B	171/345 (50%)	146 (85%)	25 (15%)	5	10
3	C	301/313 (96%)	274 (91%)	27 (9%)	14	28
4	D	246/264 (93%)	226 (92%)	20 (8%)	17	34
5	E	156/159 (98%)	136 (87%)	20 (13%)	6	14
6	F	154/155 (99%)	148 (96%)	6 (4%)	43	74
7	G	110/123 (89%)	91 (83%)	19 (17%)	3	6
8	Z	3/3 (100%)	3 (100%)	0	100	100
All	All	1485/1725 (86%)	1337 (90%)	148 (10%)	11	23

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	154	SER
3	C	370	LYS
7	G	73	ASP
3	C	174	LYS
3	C	321	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	65	ASN
3	C	303	GLN
7	G	65	ASN
3	C	129	ASN
3	C	331	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	396/418 (94%)	-0.04	9 (2%) 57 61	25, 48, 95, 106	0
2	B	196/394 (49%)	0.41	22 (11%) 6 5	30, 60, 104, 110	0
3	C	354/372 (95%)	-0.15	10 (2%) 50 54	26, 42, 81, 116	0
4	D	280/300 (93%)	-0.22	3 (1%) 77 81	25, 42, 66, 89	0
5	E	173/178 (97%)	0.41	11 (6%) 19 20	47, 70, 100, 112	0
6	F	167/168 (99%)	-0.18	1 (0%) 86 90	26, 36, 52, 78	0
7	G	136/151 (90%)	0.01	4 (2%) 49 53	30, 59, 82, 87	0
8	Z	3/3 (100%)	1.07	1 (33%) 1 1	73, 73, 83, 84	0
All	All	1705/1984 (85%)	-0.00	61 (3%) 41 44	25, 48, 94, 116	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	173	PHE	6.7
2	B	183	ASP	4.4
2	B	182	LEU	4.1
4	D	159	ASP	3.6
3	C	319	ALA	3.5

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.