

Full wwPDB X-ray Structure Validation Report (i)

Oct 25, 2023 – 02:30 AM EDT

PDB ID : 3G2V

Title: VHS Domain of human GGA1 complexed with Sotilin C-terminal Phospho-

peptide

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Deposited on : 2009-02-01

Resolution : 2.10 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 (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 (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

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)

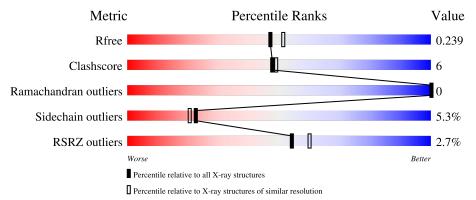
Validation Pipeline (wwPDB-VP) : 2.36

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 2.10 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	Q	uality of chain	
1	A	149	2%	0%	11% • 6%
1	В	149	3%	0%	13% • 6%
2	С	13	54%	15%	31%
2	D	13	46%	8%	46%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2548 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 ADP-ribosylation factor-binding protein GGA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	140	Total	С	N	О	S	0	0	0
1	1 A		1126	721	192	208	5	0		
1	D	140	Total	С	N	О	S	0	0	0
1		140	1126	721	192	208	5	0	U	U

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9UJY5
A	0	SER	-	expression tag	UNP Q9UJY5
В	-1	GLY	-	expression tag	UNP Q9UJY5
В	0	SER	-	expression tag	UNP Q9UJY5

• Molecule 2 is a protein called C-terminal fragment of Sortilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	С	N	О	Р	0	0	0
2			77	41	9	26	1	U		
9	D	7	Total	С	N	О	Р	0	0	0
2		1	61	33	7	20	1	U	0	U

• Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

\mathbf{M}	[ol	Chain	Residues	Atoms	ZeroOcc	AltConf
ę	3	A	3	Total I 3 3	0	0
	3	В	2	Total I 2 2	0	0

• Molecule 4 is water.



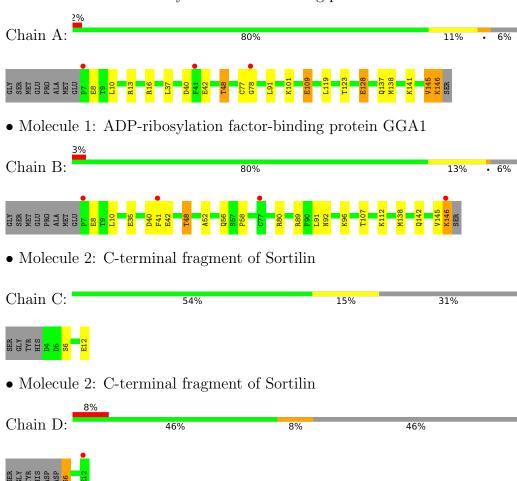
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	79	Total O 79 79	0	0
4	С	6	Total O 6 6	0	0
4	В	66	Total O 66 66	0	0
4	D	2	Total O 2 2	0	0



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: ADP-ribosylation factor-binding protein GGA1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	48.00Å 72.90Å 102.50Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.47 - 2.10	Depositor
Resolution (A)	43.47 - 2.10	EDS
% Data completeness	100.0 (43.47-2.10)	Depositor
(in resolution range)	100.0 (43.47-2.10)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.16 (at 2.10Å)	Xtriage
Refinement program	PHENIX	Depositor
D D.	0.204 , 0.244	Depositor
R, R_{free}	0.200 , 0.239	DCC
R_{free} test set	1082 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 47.9	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2548	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.51% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.51	0/1148	0.57	0/1548	
1	В	0.43	0/1148	0.49	0/1548	
2	С	0.40	0/65	0.50	0/84	
2	D	0.36	0/50	0.50	0/65	
All	All	0.47	0/2411	0.53	0/3245	

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 maintenain group or atoms of a sidechain that are expected to be planar.

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	VAL	Peptide
1	A	77	CYS	Peptide
1	A	78	GLY	Peptide

5.2 Too-close contacts (i)

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



4 1	, .	• 1	1	α	α_1 1	1	1	1 , 1	1 1
the ass	mmetric	nnit	whereas	7	vmm-Clashes	ligte	symmetry	v_related	Clashes
unc as		um,	wiicicas	\sim	y min Orabitos	11000	SYMMETICUL	y iciauca	Clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1126	0	1151	16	0
1	В	1126	0	1151	13	0
2	С	77	0	53	1	0
2	D	61	0	47	1	0
3	A	3	0	0	1	0
3	В	2	0	0	0	0
4	A	79	0	0	5	0
4	В	66	0	0	3	0
4	С	6	0	0	0	0
4	D	2	0	0	0	0
All	All	2548	0	2402	29	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.

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)
1:B:41:PHE:HA	1:B:80:ARG:HH12	1.14	1.06
1:B:41:PHE:HA	1:B:80:ARG:NH1	1.73	1.03
1:A:48:THR:HG23	4:A:208:HOH:O	1.79	0.81
1:B:48:THR:CG2	4:B:213:HOH:O	2.33	0.76
1:A:137:GLN:O	1:A:137:GLN:NE2	2.19	0.75
1:B:41:PHE:CA	1:B:80:ARG:HH12	1.96	0.75
1:A:48:THR:CG2	4:A:208:HOH:O	2.32	0.74
1:A:137:GLN:NE2	1:A:141:LYS:HB2	2.08	0.68
1:A:145:VAL:HG23	1:A:146:LYS:HA	1.77	0.67
1:A:137:GLN:HE21	1:A:141:LYS:HB2	1.64	0.61
1:A:42:GLU:HG3	4:A:185:HOH:O	2.01	0.61
1:A:138:MET:SD	2:C:12:GLU:HG2	2.43	0.59
1:B:8:GLU:HA	4:B:192:HOH:O	2.03	0.59
1:B:145:VAL:HG13	1:B:146:LYS:HG3	1.88	0.56
1:A:8:GLU:OE1	1:A:16:ARG:NH1	2.40	0.55
1:A:37:LEU:HD12	1:A:37:LEU:C	2.26	0.54
1:A:13:ARG:NH2	4:A:171:HOH:O	2.22	0.51
1:B:48:THR:HG22	4:B:213:HOH:O	2.05	0.49
1:A:109:GLU:HG2	4:A:206:HOH:O	2.13	0.49
1:A:137:GLN:NE2	1:A:141:LYS:CB	2.76	0.48
1:A:128:GLU:H	1:A:128:GLU:CD	2.17	0.47
1:B:89:ARG:NH2	2:D:6:SEP:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ASN:O	1:B:96:LYS:HG3	2.18	0.44
1:A:119:LEU:O	1:A:123:THR:HG23	2.18	0.43
3:A:148:IOD:I	1:B:58:PRO:HD2	2.89	0.42
1:B:107:THR:O	1:B:112:LYS:HE2	2.19	0.42
1:A:101:LYS:HB3	1:A:101:LYS:HE3	1.90	0.42
1:B:138:MET:O	1:B:142:GLN:HG3	2.21	0.41
1:B:52:ALA:O	1:B:56:GLN:HG3	2.21	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	138/149 (93%)	137 (99%)	1 (1%)	0	100 100
1	В	138/149 (93%)	137 (99%)	1 (1%)	0	100 100
2	C	6/13 (46%)	6 (100%)	0	0	100 100
2	D	5/13 (38%)	5 (100%)	0	0	100 100
All	All	287/324~(89%)	285 (99%)	2 (1%)	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	$124/131 \ (95\%)$	117 (94%)	7 (6%)	21 18
1	В	124/131 (95%)	117 (94%)	7 (6%)	21 18
2	\mathbf{C}	8/11 (73%)	8 (100%)	0	100 100
2	D	6/11 (54%)	6 (100%)	0	100 100
All	All	262/284~(92%)	248 (95%)	14 (5%)	22 20

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	40	ASP
1	A	48	THR
1	A	91	LEU
1	A	109	GLU
1	A	128	GLU
1	A	146	LYS
1	В	10	LEU
1	В	35	GLU
1	В	40	ASP
1	В	42	GLU
1	В	48	THR
1	В	91	LEU
1	В	146	LYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such side chains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	38	ASN
1	A	56	GLN
1	A	113	ASN
1	A	137	GLN
1	В	36	GLN
1	В	56	GLN
1	В	113	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

2 non-standard protein/DNA/RNA residues 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	Trino	Chain	Bond lengths		Bond angles					
MIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	SEP	D	6	2	8,9,10	1.64	1 (12%)	8,12,14	1.71	2 (25%)
2	SEP	С	6	2	8,9,10	1.58	1 (12%)	8,12,14	1.27	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

\mathbf{Mol}	\mathbf{Type}	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	D	6	2	-	1/5/8/10	-
2	SEP	С	6	2	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\mathring{\mathrm{A}})$	Ideal(Å)
2	D	6	SEP	P-O1P	3.52	1.61	1.50
2	С	6	SEP	P-O1P	3.40	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
2	D	6	SEP	OG-CB-CA	3.57	111.62	108.14
2	D	6	SEP	P-OG-CB	-2.50	111.41	118.30
2	С	6	SEP	P-OG-CB	-2.09	112.55	118.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	6	SEP	CA-CB-OG-P



There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	6	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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>	$\# \mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	140/149 (93%)	0.25	3 (2%) 63 68	20, 31, 57, 98	0
1	В	140/149 (93%)	0.19	4 (2%) 51 57	25, 39, 68, 104	0
2	С	8/13 (61%)	0.31	0 100 100	37, 44, 57, 71	0
2	D	6/13 (46%)	0.80	1 (16%) 1 2	47, 55, 62, 101	0
All	All	$294/324 \ (90\%)$	0.23	8 (2%) 54 60	20, 35, 67, 104	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	7	PRO	11.0
1	A	41	PHE	4.5
1	В	41	PHE	3.9
1	A	78	GLY	3.6
2	D	12	GLU	3.5
1	В	146	LYS	3.2
1	В	77	CYS	3.1
1	A	7	PRO	2.6

6.2 Non-standard residues in protein, DNA, RNA chains (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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	SEP	D	6	10/11	0.48	0.19	86,93,106,107	0
2	SEP	С	6	10/11	0.93	0.11	37,43,58,58	0



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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	IOD	A	150	1/1	0.85	0.21	74,74,74,74	1
3	IOD	В	149	1/1	0.90	0.13	84,84,84,84	1
3	IOD	A	149	1/1	0.99	0.20	27,27,27,27	1
3	IOD	В	148	1/1	1.00	0.09	38,38,38,38	1
3	IOD	A	148	1/1	1.00	0.14	32,32,32,32	1

6.5 Other polymers (i)

There are no such residues in this entry.

