wwPDB X-ray Structure Validation Summary Report (i)

Jun 18, 2024 – 01:38 AM EDT

PDB ID	:	5V6H
Title	:	Crystal structure of Myosin VI in complex with GH2 domain of GIPC2
Authors	:	Shang, G.; Zhang, X.
Deposited on	:	2017-03-16
Resolution	:	3.60 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 (1)) were used in the production of this report:

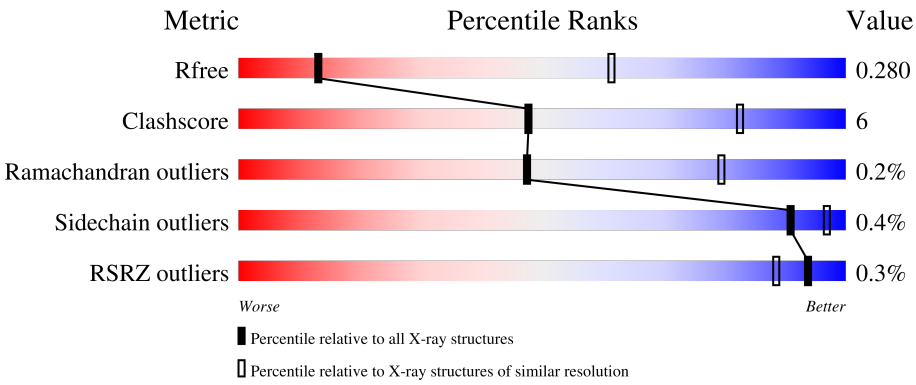
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 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	79	87% 8% 5%
1	C	79	77% 15% 8%
1	E	79	80% 15% • •
1	G	79	71% 22% 8%
1	I	79	82% 10% 8%

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Mol	Chain	Length	Quality of chain
2	B	49	76% 14% 10%
2	D	49	71% 18% 10%
2	F	49	4% 78% 12% 10%
2	H	49	80% 12% 8%
2	J	49	78% 12% 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4590 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 PDZ domain-containing protein GIPC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	75	557	356	83	115	3	0	0	0
1	C	73	546	350	81	112	3	0	0	0
1	E	76	582	372	88	118	4	0	0	0
1	G	73	547	350	81	113	3	0	0	0
1	I	73	542	348	81	110	3	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	236	GLY	-	expression tag	UNP Q9Z2H7
A	237	PRO	-	expression tag	UNP Q9Z2H7
A	238	HIS	-	expression tag	UNP Q9Z2H7
A	239	MET	-	expression tag	UNP Q9Z2H7
C	236	GLY	-	expression tag	UNP Q9Z2H7
C	237	PRO	-	expression tag	UNP Q9Z2H7
C	238	HIS	-	expression tag	UNP Q9Z2H7
C	239	MET	-	expression tag	UNP Q9Z2H7
E	236	GLY	-	expression tag	UNP Q9Z2H7
E	237	PRO	-	expression tag	UNP Q9Z2H7
E	238	HIS	-	expression tag	UNP Q9Z2H7
E	239	MET	-	expression tag	UNP Q9Z2H7
G	236	GLY	-	expression tag	UNP Q9Z2H7
G	237	PRO	-	expression tag	UNP Q9Z2H7
G	238	HIS	-	expression tag	UNP Q9Z2H7
G	239	MET	-	expression tag	UNP Q9Z2H7
I	236	GLY	-	expression tag	UNP Q9Z2H7
I	237	PRO	-	expression tag	UNP Q9Z2H7
I	238	HIS	-	expression tag	UNP Q9Z2H7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	239	MET	-	expression tag	UNP Q9Z2H7

- Molecule 2 is a protein called Unconventional myosin-VI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	44	372	236	69	65	2	0	0	0
2	D	44	356	227	65	63	1	0	0	0
2	F	44	361	228	64	67	2	0	0	0
2	H	45	374	236	69	67	2	0	0	0
2	J	44	353	222	66	63	2	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1048	GLY	-	expression tag	UNP Q64331
B	1049	PRO	-	expression tag	UNP Q64331
B	1050	GLY	-	expression tag	UNP Q64331
B	1051	SER	-	expression tag	UNP Q64331
D	1048	GLY	-	expression tag	UNP Q64331
D	1049	PRO	-	expression tag	UNP Q64331
D	1050	GLY	-	expression tag	UNP Q64331
D	1051	SER	-	expression tag	UNP Q64331
F	1048	GLY	-	expression tag	UNP Q64331
F	1049	PRO	-	expression tag	UNP Q64331
F	1050	GLY	-	expression tag	UNP Q64331
F	1051	SER	-	expression tag	UNP Q64331
H	1048	GLY	-	expression tag	UNP Q64331
H	1049	PRO	-	expression tag	UNP Q64331
H	1050	GLY	-	expression tag	UNP Q64331
H	1051	SER	-	expression tag	UNP Q64331
J	1048	GLY	-	expression tag	UNP Q64331
J	1049	PRO	-	expression tag	UNP Q64331
J	1050	GLY	-	expression tag	UNP Q64331
J	1051	SER	-	expression tag	UNP Q64331

3 Residue-property plots (i)

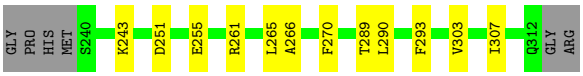
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PDZ domain-containing protein GIPC2

Chain A:

• Molecule 1: PDZ domain-containing protein GIPC2

Chain C:

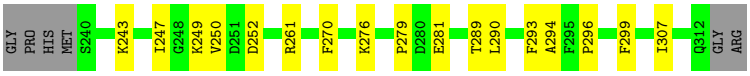


• Molecule 1: PDZ domain-containing protein GIPC2

Chain E:

• Molecule 1: PDZ domain-containing protein GIPC2

Chain G:

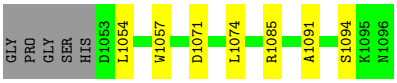


• Molecule 1: PDZ domain-containing protein GIPC2

Chain I:

• Molecule 2: Unconventional myosin-VI

Chain B:

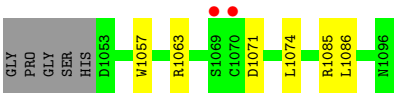


• Molecule 2: Unconventional myosin-VI

Chain D:

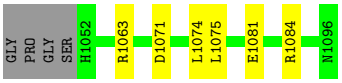
• Molecule 2: Unconventional myosin-VI

Chain F:



• Molecule 2: Unconventional myosin-VI

Chain H:



• Molecule 2: Unconventional myosin-VI

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	171.85Å 53.24Å 122.76Å 90.00° 108.23° 90.00°	Depositor
Resolution (Å)	42.93 – 3.60 42.93 – 3.60	Depositor EDS
% Data completeness (in resolution range)	77.8 (42.93-3.60) 77.8 (42.93-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.07 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.213 , 0.278 0.218 , 0.280	Depositor DCC
R_{free} test set	976 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.938	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 14.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4590	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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 (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	0.26	0/567	0.40	0/769
1	C	0.24	0/556	0.37	0/754
1	E	0.26	0/593	0.44	1/800 (0.1%)
1	G	0.25	0/557	0.38	0/755
1	I	0.24	0/552	0.36	0/749
2	B	0.25	0/380	0.37	0/510
2	D	0.23	0/364	0.38	0/492
2	F	0.23	0/369	0.37	0/499
2	H	0.23	0/383	0.40	0/517
2	J	0.24	0/361	0.35	0/489
All	All	0.24	0/4682	0.38	1/6334 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	237	PRO	N-CA-CB	6.05	110.56	103.30

There are no chirality outliers.

There are no planarity outliers.

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 the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	557	0	503	3	0
1	C	546	0	496	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	582	0	543	7	0
1	G	547	0	499	13	0
1	I	542	0	492	4	0
2	B	372	0	368	4	0
2	D	356	0	337	6	0
2	F	361	0	337	4	0
2	H	374	0	351	7	0
2	J	353	0	322	6	0
All	All	4590	0	4248	54	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.

The worst 5 of 54 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:G:279:PRO:HG3	2:J:1086:LEU:HD23	1.70	0.74
2:J:1079:ARG:O	2:J:1083:HIS:ND1	2.25	0.69
1:E:260:ILE:HD11	2:F:1086:LEU:HD22	1.76	0.66
1:G:293:PHE:O	2:H:1084:ARG:NH1	2.29	0.66
2:B:1071:ASP:HB3	2:B:1074:LEU:HB3	1.82	0.60

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	73/79 (92%)	69 (94%)	3 (4%)	1 (1%)	11 48
1	C	71/79 (90%)	67 (94%)	4 (6%)	0	100 100
1	E	74/79 (94%)	72 (97%)	2 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	71/79 (90%)	68 (96%)	3 (4%)	0	100	100
1	I	71/79 (90%)	69 (97%)	2 (3%)	0	100	100
2	B	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
2	D	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
2	F	42/49 (86%)	41 (98%)	1 (2%)	0	100	100
2	H	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
2	J	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
All	All	571/640 (89%)	549 (96%)	21 (4%)	1 (0%)	47	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	LYS

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	54/63 (86%)	54 (100%)	0	100	100
1	C	53/63 (84%)	53 (100%)	0	100	100
1	E	59/63 (94%)	58 (98%)	1 (2%)	60	82
1	G	54/63 (86%)	54 (100%)	0	100	100
1	I	52/63 (82%)	51 (98%)	1 (2%)	57	80
2	B	39/43 (91%)	39 (100%)	0	100	100
2	D	35/43 (81%)	35 (100%)	0	100	100
2	F	37/43 (86%)	37 (100%)	0	100	100
2	H	38/43 (88%)	38 (100%)	0	100	100
2	J	34/43 (79%)	34 (100%)	0	100	100
All	All	455/530 (86%)	453 (100%)	2 (0%)	91	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	251	ASP
1	I	300	LEU

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

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 (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, 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	75/79 (94%)	-0.49	0	100	100	24, 35, 54, 64	0
1	C	73/79 (92%)	-0.36	0	100	100	38, 58, 75, 94	0
1	E	76/79 (96%)	-0.39	0	100	100	36, 52, 86, 96	0
1	G	73/79 (92%)	-0.23	0	100	100	36, 63, 81, 87	0
1	I	73/79 (92%)	-0.20	0	100	100	37, 72, 98, 114	0
2	B	44/49 (89%)	-0.54	0	100	100	30, 43, 67, 76	0
2	D	44/49 (89%)	-0.23	0	100	100	61, 68, 81, 89	0
2	F	44/49 (89%)	-0.26	2 (4%)	33	21	55, 67, 82, 101	0
2	H	45/49 (91%)	-0.51	0	100	100	23, 29, 46, 62	0
2	J	44/49 (89%)	-0.41	0	100	100	55, 87, 109, 116	0
All	All	591/640 (92%)	-0.35	2 (0%)	94	88	23, 59, 90, 116	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1069	SER	2.8
2	F	1070	CYS	2.3

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 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.