



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:48 pm BST

PDB ID : 6IXQ
Title : Structure of Myo2-GTD in complex with Smy1
Authors : Tang, K.; Wei, Z.
Deposited on : 2018-12-11
Resolution : 3.06 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

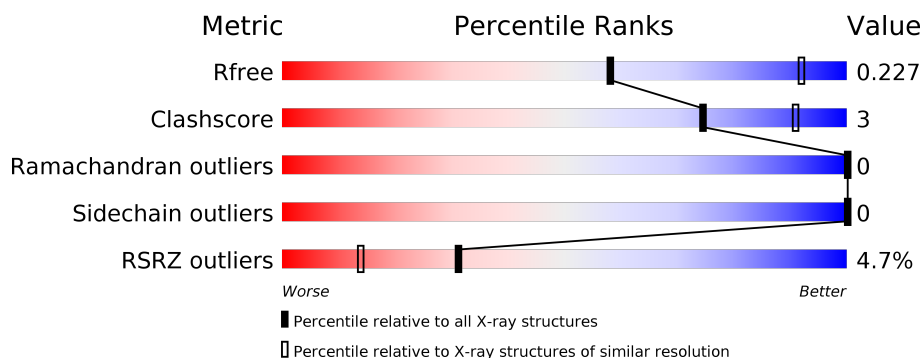
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 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 $\leq 5\%$. 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	430	<div> <div>4%</div> <div>82%</div> <div>9%</div> <div>9%</div> </div>
2	B	48	<div> <div>2%</div> <div>29%</div> <div>69%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3258 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 Myosin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3146	2039	502	595	10			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1139	SER	-	expression tag	UNP P19524
A	1140	GLY	-	expression tag	UNP P19524
A	1141	SER	-	expression tag	UNP P19524
A	1142	GLY	-	expression tag	UNP P19524
A	1143	SER	-	expression tag	UNP P19524
A	1144	GLY	-	expression tag	UNP P19524
A	1145	SER	-	expression tag	UNP P19524
A	1146	GLY	-	expression tag	UNP P19524
A	1147	SER	-	expression tag	UNP P19524
A	1148	GLY	-	expression tag	UNP P19524
A	1149	SER	-	expression tag	UNP P19524
A	1150	GLU	-	expression tag	UNP P19524
A	1151	PHE	-	expression tag	UNP P19524
A	?	-	PHE	deletion	UNP P19524
A	?	-	LEU	deletion	UNP P19524
A	?	-	ASN	deletion	UNP P19524
A	?	-	LYS	deletion	UNP P19524
A	?	-	ILE	deletion	UNP P19524
A	?	-	PHE	deletion	UNP P19524

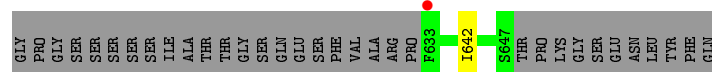
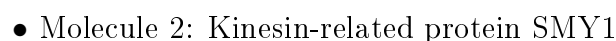
- Molecule 2 is a protein called Kinesin-related protein SMY1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	0	0	0
			112	72	20	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	611	GLY	-	expression tag	UNP P32364
B	612	PRO	-	expression tag	UNP P32364
B	613	GLY	-	expression tag	UNP P32364
B	614	SER	-	expression tag	UNP P32364
B	651	GLY	-	expression tag	UNP P32364
B	652	SER	-	expression tag	UNP P32364
B	653	GLU	-	expression tag	UNP P32364
B	654	ASN	-	expression tag	UNP P32364
B	655	LEU	-	expression tag	UNP P32364
B	656	TYR	-	expression tag	UNP P32364
B	657	PHE	-	expression tag	UNP P32364
B	658	GLN	-	expression tag	UNP P32364

- Molecule 1: Myosin-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.51Å 93.51Å 204.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.72 – 3.06 75.28 – 3.06	Depositor EDS
% Data completeness (in resolution range)	98.9 (39.72-3.06) 99.7 (75.28-3.06)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.203 , 0.223 0.210 , 0.227	Depositor DCC
R_{free} test set	985 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	126.3	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 149.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3258	wwPDB-VP
Average B, all atoms (Å ²)	172.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.25	0/3206	0.40	0/4357
2	B	0.35	0/113	0.40	0/150
All	All	0.25	0/3319	0.40	0/4507

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	3146	0	3147	21	0
2	B	112	0	116	1	0
All	All	3258	0	3263	21	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 3.

All (21) 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:1417:VAL:HG11	1:A:1440:ILE:HG12	1.78	0.65
1:A:1317:LEU:HD12	1:A:1386:LEU:HD22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1434:GLU:HA	1:A:1437:GLN:HG2	1.88	0.55
1:A:1565:VAL:HG11	2:B:642:ILE:HD13	1.89	0.54
1:A:1324:ALA:O	1:A:1328:SER:HB3	2.08	0.54
1:A:1229:LEU:HD23	1:A:1301:LEU:HD22	1.94	0.50
1:A:1401:LYS:O	1:A:1477:GLN:NE2	2.45	0.50
1:A:1175:THR:HG21	1:A:1227:GLN:HG2	1.96	0.48
1:A:1247:SER:O	1:A:1250:PHE:HB3	2.14	0.48
1:A:1200:TYR:CD2	1:A:1201:PRO:HD3	2.50	0.47
1:A:1165:GLU:HG3	1:A:1220:GLN:HE22	1.81	0.46
1:A:1200:TYR:CG	1:A:1201:PRO:HD3	2.49	0.46
1:A:1377:GLU:HB2	1:A:1537:ILE:HD11	1.98	0.46
1:A:1309:TRP:CZ2	1:A:1313:LEU:HD11	2.51	0.46
1:A:1177:GLY:HA3	1:A:1555:LEU:HD21	1.98	0.46
1:A:1255:VAL:HG21	1:A:1305:ILE:HD13	1.98	0.45
1:A:1488:PRO:HB2	1:A:1491:ILE:HG12	1.98	0.45
1:A:1218:THR:HG23	1:A:1290:LEU:HD22	1.98	0.45
1:A:1490:GLU:OE1	1:A:1493:ARG:NH2	2.52	0.43
1:A:1171:ASN:ND2	1:A:1227:GLN:OE1	2.53	0.41
1:A:1201:PRO:HD2	1:A:1254:ASN:OD1	2.21	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	383/430 (89%)	371 (97%)	12 (3%)	0	100	100
2	B	13/48 (27%)	11 (85%)	2 (15%)	0	100	100
All	All	396/478 (83%)	382 (96%)	14 (4%)	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	350/384 (91%)	350 (100%)	0	100	100
2	B	13/41 (32%)	13 (100%)	0	100	100
All	All	363/425 (85%)	363 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some 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 carbohydrates 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 ⓘ

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	391/430 (90%)	0.39	18 (4%)	32 15	121, 167, 232, 316	1 (0%)
2	B	15/48 (31%)	0.52	1 (6%)	17 7	165, 187, 267, 269	0
All	All	406/478 (84%)	0.39	19 (4%)	31 14	121, 168, 238, 316	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1450	LYS	3.1
1	A	1187	ALA	3.1
1	A	1474	LEU	2.9
1	A	1331	LEU	2.7
1	A	1459	LEU	2.7
1	A	1399	ILE	2.5
1	A	1189	VAL	2.4
1	A	1487	ILE	2.3
1	A	1252	LEU	2.2
1	A	1287	TYR	2.2
1	A	1164	LEU	2.2
1	A	1298	PHE	2.1
2	B	633	PHE	2.1
1	A	1475	ILE	2.1
1	A	1405	LEU	2.1
1	A	1207	ILE	2.1
1	A	1540	ARG	2.1
1	A	1446	LEU	2.1
1	A	1372	PHE	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.