



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2017 – 04:11 PM EST

PDB ID : 5WLZ
Title : Crystal Structure of Amino Acids 1677-1758 of Human Beta Cardiac Myosin Fused to Xrcc4
Authors : Andreas, M.P.; Ajay, G.; Gellings, J.; Rayment, I.
Deposited on : 2017-07-28
Resolution : 3.50 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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030736

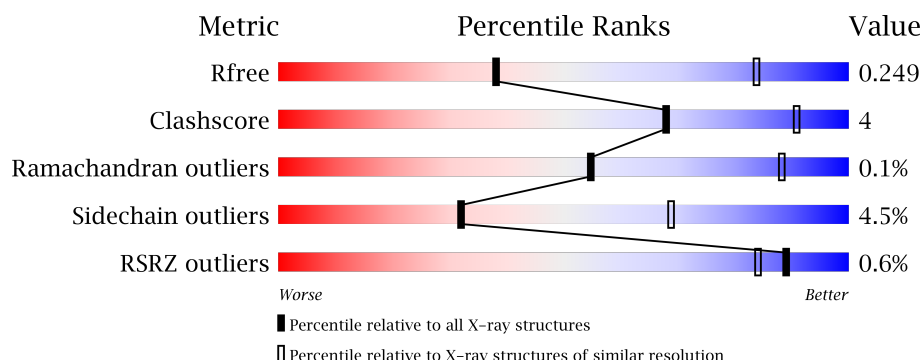
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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 $\leq 5\%$. 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	216	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 16%, yellow 16%, yellow 80%, green 80%, green 100%);"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; text-align: center;"> </div> </div> </div>
1	B	216	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, green 0%, green 76%, yellow 76%, yellow 89%, orange 89%, orange 100%);"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; text-align: center;"> </div> </div> </div>
1	C	216	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, green 0%, green 80%, yellow 80%, yellow 94%, orange 94%, orange 100%);"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; text-align: center;"> </div> </div> </div>
1	D	216	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, green 0%, green 80%, yellow 80%, yellow 93%, orange 93%, orange 100%);"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; text-align: center;"> </div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6360 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 DNA repair protein XRCC4,Myosin-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	206	Total	C	N	O	S	0	0	0
			1642	1029	285	324	4			
1	D	200	Total	C	N	O	S	0	0	0
			1601	1006	278	314	3			
1	A	193	Total	C	N	O	S	0	0	0
			1554	979	271	301	3			
1	B	195	Total	C	N	O	S	0	0	0
			1563	983	273	304	3			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP Q13426
C	0	SER	-	expression tag	UNP Q13426
C	1	GLY	-	expression tag	UNP Q13426
C	29	LYS	GLU	engineered mutation	UNP Q13426
C	51	LYS	GLU	engineered mutation	UNP Q13426
C	57	ALA	ASP	engineered mutation	UNP Q13426
C	58	THR	ASP	engineered mutation	UNP Q13426
C	62	ASN	GLU	engineered mutation	UNP Q13426
C	93	ARG	CYS	engineered mutation	UNP Q13426
C	98	LYS	GLU	engineered mutation	UNP Q13426
C	128	ASP	CYS	engineered mutation	UNP Q13426
C	130	ALA	CYS	engineered mutation	UNP Q13426
D	-1	GLY	-	expression tag	UNP Q13426
D	0	SER	-	expression tag	UNP Q13426
D	1	GLY	-	expression tag	UNP Q13426
D	29	LYS	GLU	engineered mutation	UNP Q13426
D	51	LYS	GLU	engineered mutation	UNP Q13426
D	57	ALA	ASP	engineered mutation	UNP Q13426
D	58	THR	ASP	engineered mutation	UNP Q13426
D	62	ASN	GLU	engineered mutation	UNP Q13426
D	93	ARG	CYS	engineered mutation	UNP Q13426

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Chain	Residue	Modelled	Actual	Comment	Reference
D	98	LYS	GLU	engineered mutation	UNP Q13426
D	128	ASP	CYS	engineered mutation	UNP Q13426
D	130	ALA	CYS	engineered mutation	UNP Q13426
A	-1	GLY	-	expression tag	UNP Q13426
A	0	SER	-	expression tag	UNP Q13426
A	1	GLY	-	expression tag	UNP Q13426
A	29	LYS	GLU	engineered mutation	UNP Q13426
A	51	LYS	GLU	engineered mutation	UNP Q13426
A	57	ALA	ASP	engineered mutation	UNP Q13426
A	58	THR	ASP	engineered mutation	UNP Q13426
A	62	ASN	GLU	engineered mutation	UNP Q13426
A	93	ARG	CYS	engineered mutation	UNP Q13426
A	98	LYS	GLU	engineered mutation	UNP Q13426
A	128	ASP	CYS	engineered mutation	UNP Q13426
A	130	ALA	CYS	engineered mutation	UNP Q13426
B	-1	GLY	-	expression tag	UNP Q13426
B	0	SER	-	expression tag	UNP Q13426
B	1	GLY	-	expression tag	UNP Q13426
B	29	LYS	GLU	engineered mutation	UNP Q13426
B	51	LYS	GLU	engineered mutation	UNP Q13426
B	57	ALA	ASP	engineered mutation	UNP Q13426
B	58	THR	ASP	engineered mutation	UNP Q13426
B	62	ASN	GLU	engineered mutation	UNP Q13426
B	93	ARG	CYS	engineered mutation	UNP Q13426
B	98	LYS	GLU	engineered mutation	UNP Q13426
B	128	ASP	CYS	engineered mutation	UNP Q13426
B	130	ALA	CYS	engineered mutation	UNP Q13426

GLU	VAL	GLU	GLU	ALA	VAL	GLN	GLU	CYS	ARG	ASN	ALA	GLU	GLU	LYS	ALA	LYS	LYS	ALA
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.29Å 102.94Å 136.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.07 – 3.50 44.07 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.07-3.50) 99.8 (44.07-3.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575)	Depositor
R, R_{free}	0.213 , 0.249 0.212 , 0.249	Depositor DCC
R_{free} test set	784 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6360	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% 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 [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	0.24	0/1576	0.39	0/2117
1	B	0.26	0/1585	0.41	0/2128
1	C	0.25	0/1665	0.41	0/2239
1	D	0.24	0/1622	0.39	0/2179
All	All	0.25	0/6448	0.40	0/8663

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 [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	1554	0	1570	21	0
1	B	1563	0	1579	16	0
1	C	1642	0	1647	15	0
1	D	1601	0	1612	12	0
All	All	6360	0	6408	56	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 4.

All (56) 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:1696:GLU:HG3	1:A:1699:ARG:HH12	1.54	0.72
1:A:69:GLU:HB3	1:A:108:LEU:HD21	1.74	0.70
1:B:90:LYS:O	1:B:92:SER:N	2.28	0.66
1:B:1721:THR:O	1:B:1725:ASN:ND2	2.28	0.65
1:A:37:THR:HG22	1:A:39:GLY:H	1.62	0.65
1:B:1716:LEU:HA	1:B:1719:GLN:HB3	1.78	0.64
1:B:71:ARG:HD3	1:B:75:LEU:HD12	1.81	0.63
1:C:3:ARG:NH1	1:C:125:GLU:OE2	2.30	0.62
1:A:128:ASP:OD2	1:B:7:ARG:NH1	2.33	0.60
1:A:71:ARG:HG3	1:A:75:LEU:HD22	1.84	0.60
1:C:47:VAL:HA	1:C:51:LYS:HD2	1.84	0.60
1:B:8:ILE:HD13	1:B:20:LEU:HB2	1.85	0.58
1:C:16:ILE:HD11	1:C:18:HIS:CE1	2.38	0.58
1:A:1699:ARG:HG3	1:B:1699:ARG:HA	1.86	0.58
1:D:130:ALA:O	1:D:1678:ASN:ND2	2.34	0.57
1:A:116:VAL:HG12	1:A:118:ASN:H	1.70	0.56
1:C:21:GLN:HB3	1:C:35:THR:HB	1.87	0.56
1:A:3:ARG:HH22	1:A:125:GLU:HG2	1.73	0.54
1:A:1723:LEU:HD22	1:B:1723:LEU:HB3	1.90	0.53
1:B:83:VAL:HG23	1:B:99:LYS:HG2	1.91	0.53
1:C:5:ILE:HG12	1:C:21:GLN:HG3	1.89	0.53
1:C:78:ALA:HB3	1:A:80:PRO:HA	1.91	0.53
1:C:86:PHE:HB2	1:C:94:TYR:HD1	1.74	0.52
1:A:4:LYS:HE3	1:A:5:ILE:H	1.74	0.51
1:D:8:ILE:HA	1:D:78:ALA:HB3	1.92	0.51
1:A:6:SER:HB3	1:A:77:GLY:HA2	1.91	0.51
1:C:11:VAL:HG22	1:C:85:THR:HG23	1.93	0.51
1:A:85:THR:OG1	1:A:100:ASN:OD1	2.25	0.50
1:D:54:GLN:O	1:D:58:THR:OG1	2.24	0.50
1:D:8:ILE:HD11	1:D:36:LEU:HD13	1.94	0.50
1:B:8:ILE:HD11	1:B:36:LEU:HD13	1.94	0.49
1:D:5:ILE:HG12	1:D:21:GLN:HG3	1.96	0.47
1:B:22:VAL:HG21	1:B:74:LEU:HB3	1.97	0.47
1:A:1720:ASN:HD21	1:B:1720:ASN:HB2	1.79	0.47
1:C:10:LEU:HD13	1:C:86:PHE:HB3	1.95	0.47
1:A:1688:LEU:HD21	1:B:1689:ARG:HG2	1.97	0.46
1:C:19:PHE:HE2	1:D:124:ARG:HG3	1.81	0.46
1:C:7:ARG:HH11	1:C:17:THR:HG21	1.81	0.45
1:A:1696:GLU:HG2	1:A:1700:LYS:HE2	1.98	0.45
1:A:98:LYS:HB3	1:A:107:ARG:HA	1.98	0.45
1:D:97:PHE:HE2	1:D:108:LEU:HD23	1.81	0.44
1:B:50:SER:O	1:B:54:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:LEU:HD11	1:B:34:ILE:HD11	2.00	0.43
1:A:37:THR:HG21	1:A:123:ILE:HG12	1.99	0.43
1:D:1720:ASN:O	1:D:1724:ILE:HG13	2.19	0.43
1:D:27:THR:HG22	1:D:29:LYS:H	1.84	0.43
1:B:100:ASN:HB2	1:B:102:LYS:HD3	2.00	0.43
1:D:24:TRP:HB3	1:D:32:PHE:HB3	2.01	0.43
1:D:35:THR:HG23	1:D:44:THR:HB	2.01	0.42
1:C:18:HIS:CD2	1:C:38:ASP:HB3	2.55	0.42
1:A:1687:GLU:O	1:A:1691:VAL:HG23	2.20	0.42
1:A:88:PHE:HB2	1:A:95:PHE:HD1	1.85	0.42
1:C:5:ILE:HD13	1:C:126:LEU:HG	2.02	0.41
1:C:1709:THR:HG22	1:D:1709:THR:HG22	2.02	0.41
1:A:98:LYS:HB3	1:A:98:LYS:HE2	1.87	0.41
1:C:1736:GLN:O	1:C:1740:GLU:HB2	2.19	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	189/216 (88%)	181 (96%)	8 (4%)	0	100	100
1	B	191/216 (88%)	178 (93%)	12 (6%)	1 (0%)	32	73
1	C	204/216 (94%)	196 (96%)	8 (4%)	0	100	100
1	D	196/216 (91%)	188 (96%)	8 (4%)	0	100	100
All	All	780/864 (90%)	743 (95%)	36 (5%)	1 (0%)	55	88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	91	GLU

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	173/189 (92%)	166 (96%)	7 (4%)	36	71
1	B	174/189 (92%)	167 (96%)	7 (4%)	36	71
1	C	182/189 (96%)	170 (93%)	12 (7%)	19	57
1	D	177/189 (94%)	171 (97%)	6 (3%)	42	75
All	All	706/756 (93%)	674 (96%)	32 (4%)	32	69

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	16	ILE
1	C	74	LEU
1	C	88	PHE
1	C	91	GLU
1	C	103	ASP
1	C	113	LEU
1	C	1715	LEU
1	C	1716	LEU
1	C	1734	LEU
1	C	1740	GLU
1	C	1743	GLU
1	C	1747	GLU
1	D	25	GLU
1	D	94	TYR
1	D	1699	ARG
1	D	1701	LEU
1	D	1703	GLU
1	D	1713	VAL
1	A	4	LYS
1	A	17	THR
1	A	27	THR
1	A	82	ASP
1	A	1706	LEU
1	A	1723	LEU

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Mol	Chain	Res	Type
1	A	1738	GLN
1	B	90	LYS
1	B	99	LYS
1	B	103	ASP
1	B	1715	LEU
1	B	1716	LEU
1	B	1727	LYS
1	B	1730	MET

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 [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	193/216 (89%)	-0.17	3 (1%) 72 64	11, 42, 106, 141	0
1	B	195/216 (90%)	-0.19	1 (0%) 90 86	14, 42, 98, 130	0
1	C	206/216 (95%)	-0.11	1 (0%) 90 86	20, 50, 89, 111	0
1	D	200/216 (92%)	-0.09	0 100 100	22, 44, 86, 110	0
All	All	794/864 (91%)	-0.14	5 (0%) 89 84	11, 46, 96, 141	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1731	ASP	2.4
1	C	89	SER	2.4
1	B	89	SER	2.1
1	A	1737	LEU	2.1
1	A	1736	GLN	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

There are no such residues in this entry.