



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 10:41 pm GMT

PDB ID : 1EG4
Title : STRUCTURE OF A DYSTROPHIN WW DOMAIN FRAGMENT IN COMPLEX WITH A BETA-DYSTROGLYCAN PEPTIDE
Authors : Huang, X.; Poy, F.; Zhang, R.; Joachimiak, A.; Sudol, M.; Eck, M.J.
Deposited on : 2000-02-11
Resolution : 2.00 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

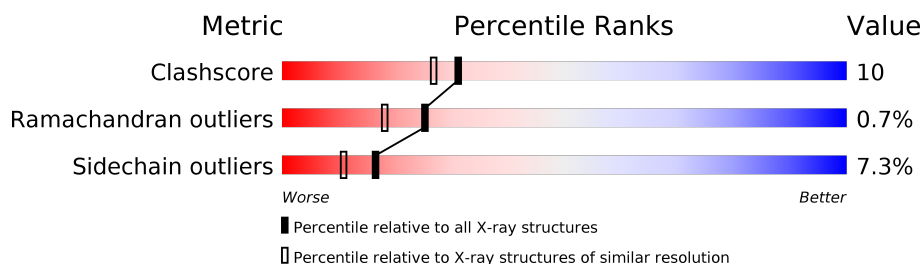
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	P	15	
2	A	261	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2478 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 BETA-DYSTROGLYCAN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	13	Total	C	N	O	S	0	0	0
			106	70	17	18	1			

- Molecule 2 is a protein called DYSTROPHIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	260	Total	C	N	O	S	0	0	0
			2089	1321	370	383	15			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	268	Total	O	0	0
			268	268		
3	P	15	Total	O	0	0
			15	15		

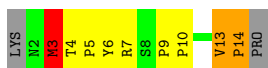
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

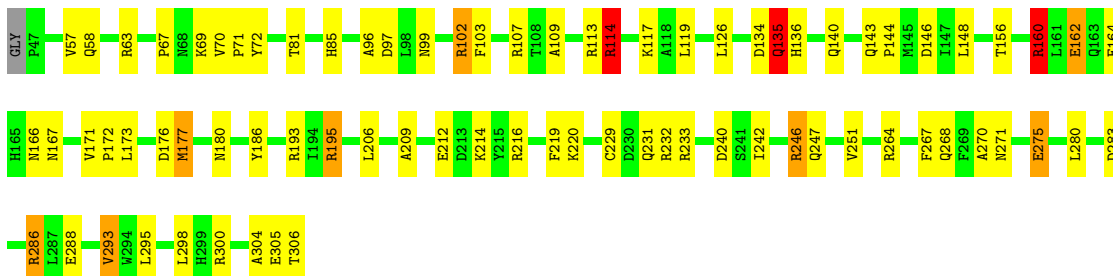
• Molecule 1: BETA-DYSTROGLYCAN

Chain P: 



• Molecule 2: DYSTROPHIN

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.68Å 67.05Å 83.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	98.3 (20.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.197 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2478	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

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	P	0.91	1/112 (0.9%)	1.76	6/156 (3.8%)
2	A	0.81	2/2135 (0.1%)	2.02	49/2897 (1.7%)
All	All	0.82	3/2247 (0.1%)	2.01	55/3053 (1.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	160	ARG	CD-NE	-6.16	1.35	1.46
1	P	14	PRO	N-CD	5.36	1.55	1.47
2	A	114	ARG	CD-NE	-5.09	1.37	1.46

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	160	ARG	CD-NE-CZ	36.86	175.21	123.60
2	A	233	ARG	CD-NE-CZ	20.74	152.64	123.60
2	A	195	ARG	NE-CZ-NH1	-19.50	110.55	120.30
2	A	300	ARG	NE-CZ-NH1	-16.46	112.07	120.30
2	A	113	ARG	NE-CZ-NH1	15.45	128.03	120.30
2	A	232	ARG	NE-CZ-NH1	15.40	128.00	120.30
2	A	114	ARG	NE-CZ-NH1	-14.69	112.96	120.30
2	A	246	ARG	NE-CZ-NH1	-14.16	113.22	120.30
2	A	63	ARG	NE-CZ-NH2	-14.14	113.23	120.30
2	A	246	ARG	NE-CZ-NH2	13.57	127.09	120.30
2	A	177	MET	CA-CB-CG	12.79	135.05	113.30
2	A	246	ARG	CD-NE-CZ	12.01	140.41	123.60
2	A	113	ARG	CD-NE-CZ	11.56	139.78	123.60
2	A	160	ARG	CG-CD-NE	11.39	135.72	111.80
2	A	113	ARG	CG-CD-NE	10.82	134.53	111.80
2	A	114	ARG	CD-NE-CZ	10.64	138.50	123.60
2	A	195	ARG	NH1-CZ-NH2	10.10	130.51	119.40
2	A	107	ARG	NE-CZ-NH1	9.80	125.20	120.30
2	A	240	ASP	CB-CG-OD2	9.67	127.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	114	ARG	NE-CZ-NH2	9.54	125.07	120.30
2	A	216	ARG	NE-CZ-NH2	9.15	124.87	120.30
2	A	232	ARG	NH1-CZ-NH2	-8.69	109.85	119.40
2	A	286	ARG	NE-CZ-NH2	-8.39	116.10	120.30
2	A	113	ARG	NE-CZ-NH2	-8.01	116.30	120.30
2	A	216	ARG	NE-CZ-NH1	-7.66	116.47	120.30
2	A	162	GLU	OE1-CD-OE2	7.65	132.48	123.30
2	A	102	ARG	NE-CZ-NH2	7.35	123.98	120.30
2	A	186	TYR	CB-CG-CD1	-7.06	116.76	121.00
2	A	212	GLU	CB-CG-CD	6.88	132.78	114.20
2	A	177	MET	CB-CG-SD	6.78	132.75	112.40
2	A	286	ARG	NE-CZ-NH1	6.62	123.61	120.30
2	A	135	GLN	CB-CG-CD	6.53	128.58	111.60
2	A	97	ASP	CB-CG-OD1	6.41	124.06	118.30
1	P	6	TYR	CB-CG-CD1	-6.24	117.25	121.00
2	A	63	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	A	214	LYS	CG-CD-CE	6.21	130.53	111.90
2	A	300	ARG	NE-CZ-NH2	5.92	123.26	120.30
2	A	233	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	P	14	PRO	CA-N-CD	-5.86	103.30	111.50
2	A	283	ASP	CB-CG-OD2	5.82	123.54	118.30
2	A	304	ALA	C-N-CA	5.80	136.20	121.70
2	A	146	ASP	CB-CG-OD1	5.72	123.45	118.30
2	A	275	GLU	CA-CB-CG	5.59	125.71	113.40
2	A	102	ARG	NE-CZ-NH1	-5.55	117.52	120.30
2	A	240	ASP	OD1-CG-OD2	-5.44	112.96	123.30
2	A	67	PRO	C-N-CA	5.28	134.90	121.70
1	P	13	VAL	CA-C-O	5.27	131.17	120.10
1	P	6	TYR	CB-CG-CD2	5.27	124.16	121.00
1	P	13	VAL	C-N-CD	5.23	139.38	128.40
2	A	293	VAL	O-C-N	-5.23	114.33	122.70
2	A	114	ARG	CG-CD-NE	5.15	122.61	111.80
2	A	103	PHE	CB-CG-CD1	-5.08	117.24	120.80
2	A	206	LEU	CB-CG-CD2	5.08	119.64	111.00
1	P	7	ARG	CD-NE-CZ	5.06	130.68	123.60
2	A	160	ARG	NE-CZ-NH2	5.01	122.80	120.30

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	P	106	0	101	8	0
2	A	2089	0	2078	40	0
3	A	268	0	0	14	0
3	P	15	0	0	0	0
All	All	2478	0	2179	45	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 10.

All (45) 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:P:9:PRO:HG2	2:A:81:THR:HG22	1.62	0.82
2:A:85:HIS:H	2:A:180:ASN:ND2	1.85	0.75
2:A:173:LEU:O	2:A:177:MET:HG2	1.92	0.70
1:P:10:PRO:O	2:A:81:THR:HG21	1.91	0.69
1:P:9:PRO:CG	2:A:81:THR:HG22	2.27	0.65
2:A:140:GLN:HE21	2:A:143:GLN:NE2	1.95	0.63
1:P:4:THR:N	1:P:5:PRO:HD3	2.15	0.61
2:A:286:ARG:NH2	3:A:482:HOH:O	2.35	0.58
2:A:242:ILE:HA	3:A:403:HOH:O	2.04	0.58
2:A:72:TYR:HD1	2:A:81:THR:HG23	1.70	0.57
2:A:96:ALA:HA	2:A:99:ASN:ND2	2.20	0.56
2:A:72:TYR:CD1	2:A:81:THR:HG23	2.39	0.56
2:A:166:ASN:N	3:A:573:HOH:O	2.38	0.56
2:A:166:ASN:CA	3:A:573:HOH:O	2.53	0.55
1:P:4:THR:N	1:P:5:PRO:CD	2.69	0.55
2:A:195:ARG:HD2	3:A:346:HOH:O	2.06	0.55
2:A:264:ARG:O	2:A:268:GLN:HG3	2.07	0.54
2:A:140:GLN:HE21	2:A:143:GLN:HE22	1.58	0.52
2:A:136:HIS:HE1	2:A:156:THR:OG1	1.93	0.51
2:A:140:GLN:NE2	2:A:143:GLN:HE22	2.09	0.51
2:A:69:LYS:HE2	3:A:537:HOH:O	2.10	0.50
2:A:219:PHE:CZ	2:A:229:CYS:HB2	2.48	0.49
2:A:148:LEU:HD13	3:A:562:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:220:LYS:HE3	3:A:531:HOH:O	2.14	0.48
2:A:246:ARG:HA	2:A:251:VAL:HB	1.96	0.47
2:A:109:ALA:HB1	2:A:298:LEU:HA	1.97	0.46
2:A:114:ARG:HD3	3:A:434:HOH:O	2.15	0.45
2:A:288:GLU:HB3	2:A:293:VAL:HG23	1.98	0.45
2:A:166:ASN:C	3:A:573:HOH:O	2.55	0.44
2:A:70:VAL:HA	2:A:71:PRO:HD3	1.86	0.44
1:P:13:VAL:O	1:P:14:PRO:C	2.54	0.43
2:A:126:LEU:HB2	2:A:209:ALA:HB2	2.00	0.42
2:A:148:LEU:HD12	2:A:148:LEU:O	2.19	0.42
2:A:160:ARG:HD3	2:A:164:GLU:OE2	2.19	0.42
2:A:171:VAL:HB	2:A:172:PRO:HD3	2.01	0.42
2:A:135:GLN:HG2	3:A:410:HOH:O	2.19	0.42
2:A:173:LEU:HD11	2:A:177:MET:SD	2.60	0.41
2:A:246:ARG:NH1	3:A:522:HOH:O	2.44	0.41
2:A:270:ALA:HB2	2:A:280:LEU:HD11	2.02	0.41
2:A:117:LYS:NZ	3:A:472:HOH:O	2.53	0.41
2:A:143:GLN:HA	2:A:144:PRO:HD3	1.96	0.40
2:A:231:GLN:HG2	2:A:267:PHE:CD1	2.56	0.40
1:P:4:THR:H	1:P:5:PRO:HD3	1.86	0.40
1:P:3:MET:SD	1:P:4:THR:N	2.94	0.40
2:A:268:GLN:NE2	3:A:411:HOH:O	2.54	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	P	11/15 (73%)	9 (82%)	1 (9%)	1 (9%)	1	0
2	A	258/261 (99%)	254 (98%)	3 (1%)	1 (0%)	38	33
All	All	269/276 (98%)	263 (98%)	4 (2%)	2 (1%)	25	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	305	GLU
1	P	3	MET

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	P	13/15 (87%)	12 (92%)	1 (8%)	15	9
2	A	233/233 (100%)	216 (93%)	17 (7%)	16	11
All	All	246/248 (99%)	228 (93%)	18 (7%)	16	11

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	3	MET
2	A	57	VAL
2	A	58	GLN
2	A	102	ARG
2	A	114	ARG
2	A	119	LEU
2	A	134	ASP
2	A	135	GLN
2	A	160	ARG
2	A	162	GLU
2	A	167	ASN
2	A	176	ASP
2	A	193	ARG
2	A	247	GLN
2	A	271	ASN
2	A	275	GLU
2	A	295	LEU
2	A	306	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	136	HIS
2	A	140	GLN
2	A	180	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](#)

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.