



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:20 AM UTC

PDB ID : 1EG4 / pdb_00001eg4
Title : STRUCTURE OF A DYSTROPHIN WW DOMAIN FRAGMENT IN COM-
PLEX WITH A BETA-DYSTROGLYCAN PEPTIDE
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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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

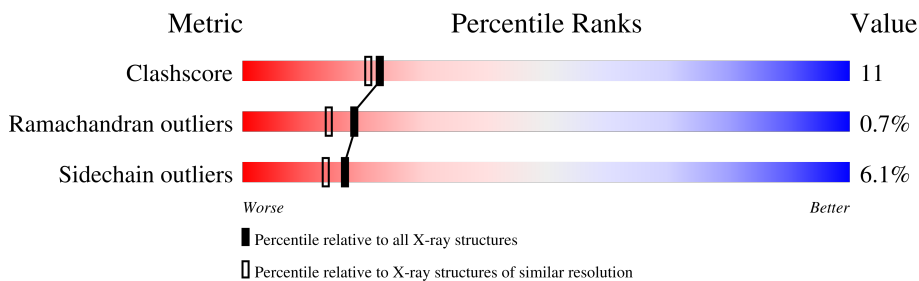
1 Overall quality at a glance

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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 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 $\leq 5\%$.

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.

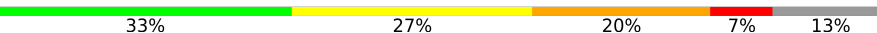
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	15	Total	O	0	0
			15	15		
3	A	268	Total	O	0	0
			268	268		

3 Residue-property plots

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. 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. 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.

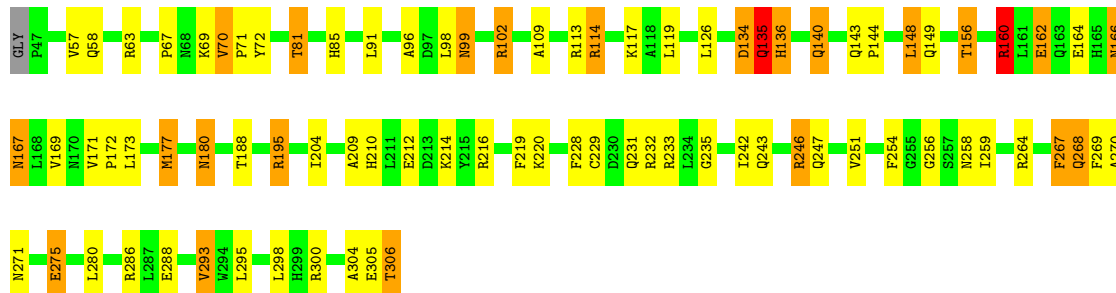
• Molecule 1: BETA-DYSTROGLYCAN

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 (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	P	1.10	1/112 (0.9%)	1.93	4/156 (2.6%)
2	A	1.05	2/2135 (0.1%)	2.18	69/2897 (2.4%)
All	All	1.05	3/2247 (0.1%)	2.17	73/3053 (2.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	160	ARG	CD-NE	-7.33	1.35	1.46
2	A	114	ARG	CD-NE	-6.04	1.37	1.46
1	P	14	PRO	N-CD	5.43	1.55	1.47

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	160	ARG	CD-NE-CZ	36.29	175.21	124.40
2	A	233	ARG	CD-NE-CZ	20.17	152.64	124.40
2	A	212	GLU	CB-CG-CD	11.87	132.78	112.60
2	A	246	ARG	CD-NE-CZ	11.44	140.41	124.40
2	A	113	ARG	CD-NE-CZ	10.99	139.78	124.40
2	A	195	ARG	NE-CZ-NH1	-10.95	110.55	121.50
2	A	160	ARG	CG-CD-NE	10.78	135.72	112.00
2	A	177	MET	CA-CB-CG	10.47	135.05	114.10
2	A	113	ARG	CG-CD-NE	10.24	134.53	112.00
2	A	114	ARG	CD-NE-CZ	10.07	138.50	124.40
2	A	300	ARG	NE-CZ-NH1	-9.43	112.07	121.50
2	A	135	GLN	CB-CG-CD	9.40	128.58	112.60
2	A	246	ARG	NE-CZ-NH2	8.76	127.09	119.20
2	A	136	HIS	CA-CB-CG	-8.63	105.17	113.80
2	A	195	ARG	NH1-CZ-NH2	8.62	130.51	119.30
2	A	114	ARG	NE-CZ-NH1	-8.54	112.96	121.50
2	A	135	GLN	OE1-CD-NE2	-8.46	114.14	122.60
1	P	13	VAL	CA-C-O	8.37	131.17	119.95
2	A	214	LYS	CG-CD-CE	8.36	130.53	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	246	ARG	NE-CZ-NH1	-8.28	113.22	121.50
2	A	267	PHE	CA-CB-CG	-8.22	105.58	113.80
2	A	304	ALA	CA-C-N	7.67	136.20	121.54
2	A	304	ALA	C-N-CA	7.67	136.20	121.54
2	A	271	ASN	CB-CG-ND2	7.66	127.88	116.40
2	A	134	ASP	CA-CB-CG	-7.49	105.11	112.60
2	A	166	ASN	N-CA-C	7.37	121.80	108.17
2	A	232	ARG	NH1-CZ-NH2	-7.27	109.85	119.30
2	A	70	VAL	CA-C-O	7.20	123.87	119.19
2	A	247	GLN	OE1-CD-NE2	-7.10	115.50	122.60
2	A	67	PRO	CA-C-N	6.92	134.90	122.38
2	A	67	PRO	C-N-CA	6.92	134.90	122.38
2	A	293	VAL	O-C-N	-6.78	114.33	122.06
2	A	271	ASN	OD1-CG-ND2	-6.75	115.85	122.60
2	A	177	MET	CB-CG-SD	6.68	132.75	112.70
2	A	268	GLN	OE1-CD-NE2	-6.67	115.93	122.60
2	A	63	ARG	NE-CZ-NH2	-6.64	113.23	119.20
2	A	254	PHE	CA-CB-CG	-6.56	107.24	113.80
2	A	113	ARG	NE-CZ-NH1	6.53	128.03	121.50
2	A	114	ARG	NE-CZ-NH2	6.53	125.07	119.20
2	A	232	ARG	NE-CZ-NH1	6.50	128.00	121.50
2	A	148	LEU	CA-C-O	-6.45	113.59	120.42
2	A	99	ASN	CA-C-N	6.44	131.63	120.68
2	A	99	ASN	C-N-CA	6.44	131.63	120.68
1	P	7	ARG	CA-C-O	-6.37	113.86	120.99
2	A	216	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	P	5	PRO	N-CA-C	-6.30	105.43	114.18
2	A	180	ASN	CA-CB-CG	6.24	118.83	112.60
1	P	14	PRO	CA-N-CD	-6.21	103.30	112.00
2	A	243	GLN	OE1-CD-NE2	-6.13	116.47	122.60
2	A	98	LEU	CA-C-O	6.07	126.45	119.35
2	A	269	PHE	CA-C-O	5.92	126.79	120.10
2	A	275	GLU	CA-CB-CG	5.80	125.71	114.10
2	A	91	LEU	O-C-N	-5.79	115.98	122.12
2	A	228	PHE	CA-CB-CG	-5.78	108.02	113.80
2	A	167	ASN	CA-CB-CG	-5.69	106.91	112.60
2	A	188	THR	CA-C-O	-5.54	114.65	120.63
2	A	169	VAL	N-CA-C	5.49	115.50	107.37
2	A	156	THR	N-CA-C	-5.48	105.22	111.14
2	A	177	MET	CB-CA-C	-5.43	102.32	110.90
2	A	140	GLN	OE1-CD-NE2	5.38	127.98	122.60
2	A	214	LYS	CB-CG-CD	5.33	123.56	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	102	ARG	NE-CZ-NH2	5.31	123.98	119.20
2	A	258	ASN	CB-CG-ND2	-5.29	108.46	116.40
2	A	293	VAL	CA-C-O	5.29	126.43	120.03
2	A	210	HIS	CA-CB-CG	-5.24	108.56	113.80
2	A	162	GLU	CA-CB-CG	-5.16	103.79	114.10
2	A	235	GLY	CA-C-N	5.10	127.43	120.54
2	A	235	GLY	C-N-CA	5.10	127.43	120.54
2	A	306	THR	CB-CA-C	5.06	120.24	109.10
2	A	216	ARG	NE-CZ-NH1	-5.03	116.47	121.50
2	A	256	GLY	CA-C-O	5.03	127.20	122.57
2	A	232	ARG	CB-CA-C	-5.02	102.99	110.88
2	A	149	GLN	OE1-CD-NE2	5.01	127.61	122.60

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	P	106	0	101	8	0
2	A	2089	0	2078	41	0
3	A	268	0	0	14	0
3	P	15	0	0	0	0
All	All	2478	0	2179	46	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 11.

All (46) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:72:TYR:CD1	2:A:81:THR:HG23	2.39	0.56
2:A:96:ALA:HA	2:A:99:ASN:ND2	2.20	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:166:ASN:C	3:A:573:HOH:O	2.55	0.49
2:A:148:LEU:HD13	3:A:562:HOH:O	2.13	0.48
1:P:13:VAL:O	1:P:14:PRO:C	2.54	0.48
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:70:VAL:HA	2:A:71:PRO:HD3	1.86	0.44
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:259:ILE:C	2:A:259:ILE:HD12	2.46	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
1:P:4:THR:H	1:P:5:PRO:HD3	1.86	0.40
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:3:MET:SD	1:P:4:THR:N	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	0	0
2	A	258/261 (99%)	254 (98%)	3 (1%)	1 (0%)	30	27
All	All	269/276 (98%)	263 (98%)	4 (2%)	2 (1%)	18	14

All (2) Ramachandran outliers are listed below:

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

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	P	13/15 (87%)	12 (92%)	1 (8%)	12	8
2	A	233/233 (100%)	219 (94%)	14 (6%)	17	14
All	All	246/248 (99%)	231 (94%)	15 (6%)	17	14

All (15) 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	81	THR
2	A	102	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	204	ILE
2	A	275	GLU
2	A	295	LEU
2	A	306	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	136	HIS
2	A	140	GLN
2	A	143	GLN
2	A	180	ASN
2	A	239	HIS
2	A	247	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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

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.