



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:49 PM UTC

PDB ID : 1XXV / pdb_00001xxv
Title : Yersinia YopH (residues 163-468) binds phosphonodifluoromethyl-Phe containing hexapeptide at two sites
Authors : Ivanov, M.I.; Stuckey, J.A.; Schubert, H.L.; Saper, M.A.; Bliska, J.B.
Deposited on : 2004-11-08
Resolution : 2.50 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

<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
Mogul	:	2022.3.0, CSD as543be (2022)
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

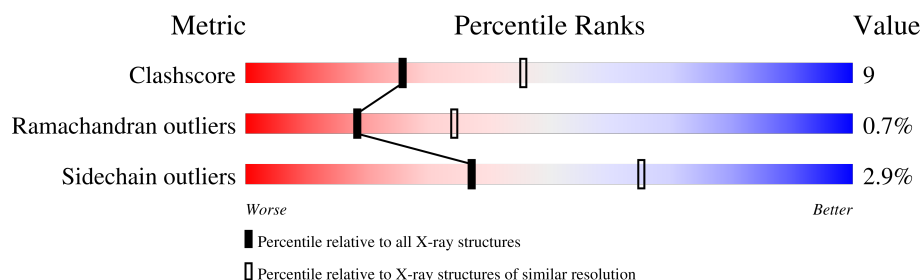
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	306	
1	B	306	
2	C	8	
2	D	8	
2	E	8	
2	F	8	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4831 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 Protein-tyrosine phosphatase yopH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2166	1323	402	425	16			
1	B	282	Total	C	N	O	S	0	0	0
			2166	1323	402	425	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	ARG	CYS	engineered mutation	UNP P15273
B	235	ARG	CYS	engineered mutation	UNP P15273

- Molecule 2 is a protein called Epidermal growth factor receptor derived peptide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	5	Total 44	C 25	F 2	N 5	O 11	P 1	0	0	1
2	D	7	Total 57	C 32	F 2	N 7	O 15	P 1	0	0	1
2	E	5	Total 44	C 25	F 2	N 5	O 11	P 1	4	0	1
2	F	7	Total 57	C 32	F 2	N 7	O 15	P 1	0	0	1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	154	Total	O	0	0
			154	154		
3	B	134	Total	O	0	0
			134	134		
3	C	1	Total	O	0	0
			1	1		

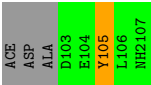
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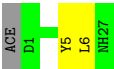
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	3	Total 3	O 3	0	0
3	E	1	Total 1	O 1	0	0
3	F	4	Total 4	O 4	0	0



- Molecule 2: Epidermal growth factor receptor derived peptide



- Molecule 2: Epidermal growth factor receptor derived peptide



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.13Å 47.17Å 71.82Å 104.45° 115.05° 89.97°	Depositor
Resolution (Å)	50.00 – 2.50	Depositor
% Data completeness (in resolution range)	85.5 (50.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.178 , 0.229	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4831	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, FTY

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	0.47	0/2193	0.86	0/2962
1	B	0.47	0/2193	0.86	0/2962
2	C	0.51	0/23	0.37	0/28
2	D	0.46	0/36	0.67	0/46
2	E	0.48	0/23	0.41	0/28
2	F	0.40	0/36	0.59	0/46
All	All	0.47	0/4504	0.86	0/6072

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	2166	0	2167	39	0
1	B	2166	0	2167	43	0
2	C	44	0	27	3	0
2	D	57	0	39	2	0
2	E	44	0	27	1	0
2	F	57	0	39	1	0
3	A	154	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	134	0	0	6	0
3	C	1	0	0	0	0
3	D	3	0	0	0	0
3	E	1	0	0	0	0
3	F	4	0	0	0	0
All	All	4831	0	4466	85	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 9.

All (85) 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:241:ARG:HD3	1:A:244:LEU:HD12	1.72	0.70
1:B:241:ARG:HD3	1:B:244:LEU:HD12	1.72	0.70
1:A:272:ARG:HG3	1:A:311:ILE:HD11	1.75	0.68
1:A:342:LYS:HD3	2:D:5:FTY:HE1	1.74	0.68
1:B:363:GLU:HB2	3:B:821:HOH:O	1.94	0.67
1:B:272:ARG:HG3	1:B:311:ILE:HD11	1.78	0.65
1:A:357:GLN:HB2	3:A:788:HOH:O	1.95	0.65
1:A:192:GLU:CD	1:A:192:GLU:H	2.04	0.65
1:B:227:ASN:HB2	3:B:806:HOH:O	1.97	0.64
1:A:245:ASN:HB3	1:A:260:GLN:HG2	1.79	0.64
1:B:192:GLU:H	1:B:192:GLU:CD	2.06	0.64
1:A:429:VAL:HA	1:A:432:MET:HE3	1.80	0.63
1:A:356:ASP:O	1:A:358:THR:HG23	1.98	0.63
1:A:272:ARG:HG2	3:A:626:HOH:O	1.99	0.63
1:B:429:VAL:HA	1:B:432:MET:HE3	1.81	0.62
1:A:384:GLU:HG2	1:A:391:VAL:HG11	1.81	0.61
1:B:228:ARG:HH21	1:B:298:MET:HG3	1.65	0.61
1:B:356:ASP:O	1:B:358:THR:HG23	2.00	0.60
1:B:384:GLU:HG2	1:B:391:VAL:HG11	1.82	0.60
1:B:245:ASN:HB3	1:B:260:GLN:HG2	1.84	0.59
1:B:447:LYS:HB2	1:B:450:GLN:HG3	1.84	0.59
1:A:228:ARG:HH21	1:A:298:MET:HG3	1.68	0.58
1:A:447:LYS:HB2	1:A:450:GLN:HG3	1.86	0.57
1:B:259:CYS:O	1:B:402:HIS:HB2	2.03	0.57
1:A:259:CYS:O	1:A:402:HIS:HB2	2.04	0.57
1:A:227:ASN:HB2	3:A:726:HOH:O	2.06	0.54
1:B:303:ARG:HG2	1:B:332:TYR:CZ	2.43	0.54
1:A:303:ARG:HG2	1:A:332:TYR:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:SER:O	1:A:391:VAL:HG22	2.08	0.53
1:B:388:SER:O	1:B:391:VAL:HG22	2.08	0.52
1:A:419:MET:HE2	1:A:432:MET:HE1	1.91	0.52
1:A:278:ARG:HD2	1:A:383:TYR:CE2	2.45	0.52
1:B:251:VAL:HG13	1:B:418:CYS:SG	2.50	0.51
1:B:321:VAL:HG23	1:B:331:MET:CE	2.39	0.51
1:B:278:ARG:HD2	1:B:383:TYR:CE2	2.46	0.51
1:B:467:ASN:O	1:B:468:SER:HB3	2.11	0.50
1:B:419:MET:HE2	1:B:432:MET:HE1	1.94	0.49
1:B:425:SER:O	1:B:426:GLN:HB2	2.11	0.49
1:A:425:SER:O	1:A:426:GLN:HB2	2.11	0.49
3:A:745:HOH:O	2:C:106:LEU:HD13	2.12	0.49
1:A:251:VAL:HG13	1:A:418:CYS:SG	2.52	0.49
1:B:211:ALA:O	1:B:214:ASP:HB2	2.13	0.49
1:B:334:LEU:O	1:B:345:SER:HA	2.13	0.49
1:B:222:GLY:HA3	3:B:584:HOH:O	2.11	0.48
1:B:313:VAL:CG1	1:B:334:LEU:HD22	2.43	0.48
1:A:313:VAL:CG1	1:A:334:LEU:HD22	2.43	0.48
1:A:321:VAL:HG23	1:A:331:MET:CE	2.42	0.48
1:A:334:LEU:O	1:A:345:SER:HA	2.14	0.48
1:B:205:ARG:NH1	3:B:710:HOH:O	2.46	0.48
1:B:323:LEU:HD11	1:B:329:ALA:HB2	1.95	0.48
1:A:211:ALA:O	1:A:214:ASP:HB2	2.14	0.48
1:A:228:ARG:NH2	1:A:297:GLY:O	2.47	0.47
1:A:323:LEU:HD11	1:A:329:ALA:HB2	1.96	0.47
1:A:421:ASP:HB3	1:A:424:ASN:ND2	2.29	0.47
1:B:343:THR:HG21	2:F:6:LEU:HD11	1.98	0.46
1:B:228:ARG:HH21	1:B:298:MET:CG	2.29	0.45
1:B:228:ARG:NH2	1:B:297:GLY:O	2.50	0.45
1:B:421:ASP:HB3	1:B:424:ASN:ND2	2.31	0.45
1:B:400:VAL:C	1:B:401:ILE:HG13	2.42	0.45
1:B:229:PHE:CG	2:E:105:FTY:HB3	2.52	0.44
2:C:106:LEU:HD23	2:C:106:LEU:O	2.16	0.44
1:B:188:PRO:HD2	3:B:801:HOH:O	2.18	0.44
1:A:390:ALA:HB1	1:A:397:LEU:HD13	1.98	0.43
1:A:400:VAL:C	1:A:401:ILE:HG13	2.43	0.43
1:B:321:VAL:HG23	1:B:331:MET:HE2	2.01	0.43
1:A:229:PHE:CG	2:C:105:FTY:HB3	2.53	0.43
1:B:251:VAL:CG1	1:B:418:CYS:SG	3.06	0.43
1:A:240:VAL:HG12	1:A:241:ARG:HG3	2.00	0.42
1:A:228:ARG:HH21	1:A:298:MET:CG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:PRO:HA	1:A:379:LYS:HG2	2.02	0.42
1:A:331:MET:HA	1:A:348:VAL:O	2.20	0.42
1:A:244:LEU:CD2	1:A:266:GLN:HB3	2.51	0.41
1:A:251:VAL:CG1	1:A:418:CYS:SG	3.08	0.41
1:B:316:LYS:CG	1:B:333:THR:HB	2.51	0.41
1:B:444:MET:O	1:B:445:VAL:HB	2.21	0.41
1:A:444:MET:O	1:A:445:VAL:HB	2.21	0.41
1:A:245:ASN:HB3	1:A:260:GLN:CG	2.49	0.41
1:B:240:VAL:HG12	1:B:241:ARG:HG3	2.02	0.41
1:B:250:GLN:HB2	3:B:656:HOH:O	2.21	0.41
1:B:244:LEU:CD2	1:B:266:GLN:HB3	2.51	0.41
1:B:420:ASN:HD22	1:B:420:ASN:HA	1.61	0.40
1:A:420:ASN:HD22	1:A:420:ASN:HA	1.60	0.40
1:B:280:PRO:HA	1:B:379:LYS:HG2	2.04	0.40
1:B:390:ALA:HB1	1:B:397:LEU:HD13	2.02	0.40
2:D:3:ASP:HB3	2:D:6:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	280/306 (92%)	263 (94%)	15 (5%)	2 (1%)	18	34
1	B	280/306 (92%)	266 (95%)	12 (4%)	2 (1%)	18	34
2	C	2/8 (25%)	1 (50%)	1 (50%)	0	100	100
2	D	4/8 (50%)	4 (100%)	0	0	100	100
2	E	2/8 (25%)	2 (100%)	0	0	100	100
2	F	4/8 (50%)	4 (100%)	0	0	100	100
All	All	572/644 (89%)	540 (94%)	28 (5%)	4 (1%)	18	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	442	GLY
1	A	445	VAL
1	B	445	VAL
1	B	442	GLY

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	238/255 (93%)	232 (98%)	6 (2%)	42	69
1	B	238/255 (93%)	230 (97%)	8 (3%)	32	60
2	C	3/4 (75%)	3 (100%)	0	100	100
2	D	4/4 (100%)	4 (100%)	0	100	100
2	E	3/4 (75%)	3 (100%)	0	100	100
2	F	4/4 (100%)	4 (100%)	0	100	100
All	All	490/526 (93%)	476 (97%)	14 (3%)	37	65

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	GLU
1	A	251	VAL
1	A	319	GLN
1	A	366	LYS
1	A	397	LEU
1	A	420	ASN
1	B	192	GLU
1	B	251	VAL
1	B	319	GLN
1	B	353	ASN
1	B	366	LYS
1	B	397	LEU
1	B	420	ASN

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Mol	Chain	Res	Type
1	B	425	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	A	264	GLN
1	A	294	GLN
1	A	420	ASN
1	A	435	GLN
1	B	233	GLN
1	B	294	GLN
1	B	420	ASN
1	B	435	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FTY	D	5	2	16,18,19	1.42	3 (18%)	17,27,29	1.54	2 (11%)
2	FTY	E	105	2	16,18,19	1.42	3 (18%)	17,27,29	1.50	2 (11%)
2	FTY	C	105	2	16,18,19	1.40	3 (18%)	17,27,29	1.50	2 (11%)
2	FTY	F	5	2	16,18,19	1.41	4 (25%)	17,27,29	1.54	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FTY	D	5	2	-	5/15/21/23	0/1/1/1
2	FTY	E	105	2	-	0/15/21/23	0/1/1/1
2	FTY	C	105	2	-	0/15/21/23	0/1/1/1
2	FTY	F	5	2	-	6/15/21/23	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5	FTY	F2-C1	3.45	1.42	1.37
2	F	5	FTY	F2-C1	3.23	1.41	1.37
2	E	105	FTY	F1-C1	2.87	1.41	1.37
2	E	105	FTY	F2-C1	2.84	1.41	1.37
2	C	105	FTY	F2-C1	2.67	1.41	1.37
2	C	105	FTY	F1-C1	2.64	1.41	1.37
2	E	105	FTY	P-O2P	-2.61	1.48	1.54
2	C	105	FTY	P-O2P	-2.44	1.48	1.54
2	D	5	FTY	P-O2P	-2.44	1.48	1.54
2	F	5	FTY	P-O2P	-2.39	1.48	1.54
2	F	5	FTY	F1-C1	2.32	1.40	1.37
2	D	5	FTY	F1-C1	2.29	1.40	1.37
2	F	5	FTY	P-O3P	-2.20	1.49	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	5	FTY	P-C1-CZ	4.54	122.59	108.95
2	D	5	FTY	P-C1-CZ	4.28	121.79	108.95
2	E	105	FTY	P-C1-CZ	4.17	121.48	108.95
2	C	105	FTY	P-C1-CZ	4.10	121.28	108.95
2	D	5	FTY	O1P-P-C1	-3.11	105.04	111.78
2	C	105	FTY	O1P-P-C1	-2.94	105.41	111.78
2	F	5	FTY	O1P-P-C1	-2.85	105.59	111.78
2	E	105	FTY	O1P-P-C1	-2.58	106.19	111.78

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	5	FTY	F2-C1-P-O1P

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Mol	Chain	Res	Type	Atoms
2	F	5	FTY	O-C-CA-CB
2	F	5	FTY	F1-C1-CZ-CE1
2	F	5	FTY	F1-C1-CZ-CE2
2	F	5	FTY	CA-CB-CG-CD1
2	F	5	FTY	CA-CB-CG-CD2
2	D	5	FTY	F1-C1-CZ-CE1
2	D	5	FTY	F2-C1-CZ-CE1
2	D	5	FTY	F1-C1-CZ-CE2
2	F	5	FTY	F2-C1-CZ-CE1
2	D	5	FTY	CA-CB-CG-CD1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	5	FTY	1	0
2	E	105	FTY	1	0
2	C	105	FTY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.