



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:22 AM UTC

PDB ID : 1B4H / pdb_00001b4h
Title : OLIGO-PEPTIDE BINDING PROTEIN COMPLEXED WITH LYSYL-DIAMINO BUTYRIC ACID-LYSINE
Authors : Davies, T.G.; Tame, J.R.H.
Deposited on : 1998-11-11
Resolution : 1.90 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

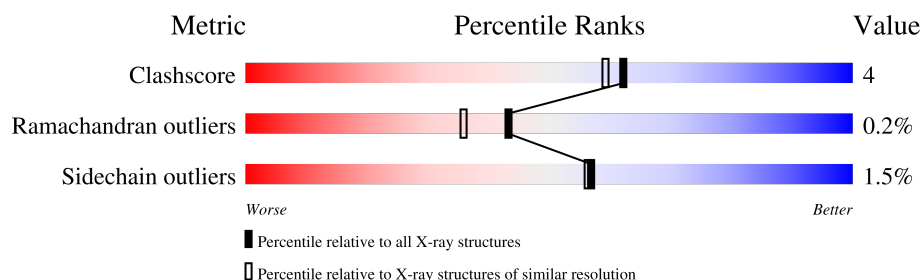
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	517	 85% 14% .
2	B	3	 33% 67%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4579 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 PERIPLASMIC OLIGO-PEPTIDE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	7	2	0
			4171	2670	700	796	5			

- Molecule 2 is a protein called LYS-DAB-LYS PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	1	0
			27	16	7	4			

- Molecule 3 is URANIUM ATOM (CCD ID: U1) (formula: U).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	U	0	0
			8	8		

- Molecule 4 is water.

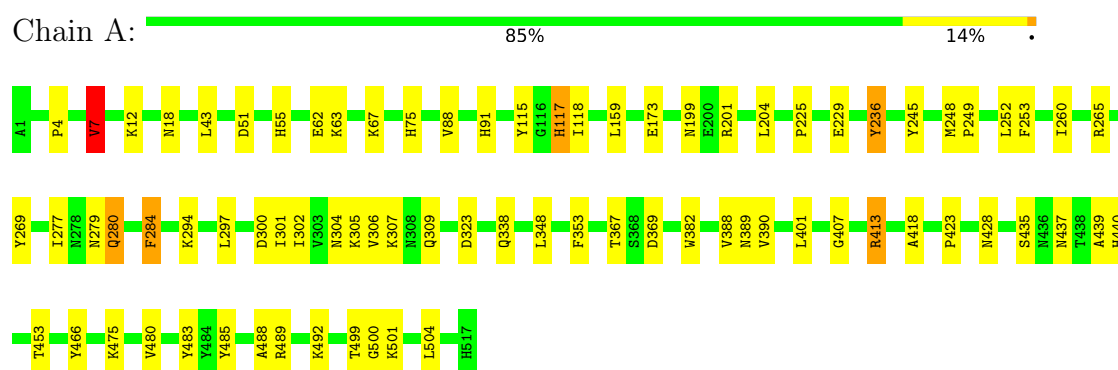
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	369	Total	O	0	0
			369	369		
4	B	4	Total	O	0	0
			4	4		

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: PERIPLASMIC OLIGO-PEPTIDE BINDING PROTEIN



• Molecule 2: LYS-DAB-LYS PEPTIDE



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	109.72Å 75.95Å 70.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90	Depositor
% Data completeness (in resolution range)	99.8 (20.00-1.90)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.230	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4579	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: U1, DAB

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	0.77	0/4292	1.52	35/5852 (0.6%)
2	B	0.95	0/17	1.47	0/16
All	All	0.77	0/4309	1.52	35/5868 (0.6%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	HIS	CA-CB-CG	-8.85	104.95	113.80
1	A	437	ASN	OD1-CG-ND2	-8.38	114.22	122.60
1	A	284	PHE	CA-CB-CG	-7.13	106.67	113.80
1	A	413	ARG	NE-CZ-NH2	-7.06	112.85	119.20
1	A	437	ASN	CA-CB-CG	6.98	119.58	112.60
1	A	7	VAL	N-CA-CB	6.76	119.53	110.26
1	A	413	ARG	CD-NE-CZ	6.28	133.19	124.40
1	A	485	TYR	CA-CB-CG	6.17	125.01	113.90
1	A	500	GLY	N-CA-C	-6.15	106.75	115.43
1	A	279	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	A	159	LEU	N-CA-C	5.95	120.27	113.19
1	A	12	LYS	CG-CD-CE	5.87	124.81	111.30
1	A	252	LEU	N-CA-C	5.79	121.38	113.97
1	A	91	HIS	CA-CB-CG	-5.69	108.11	113.80
1	A	18	ASN	CA-CB-CG	-5.62	106.98	112.60
1	A	439	ALA	N-CA-C	-5.55	106.01	112.89
1	A	413	ARG	CG-CD-NE	-5.55	99.80	112.00
1	A	173	GLU	CA-CB-CG	-5.52	103.05	114.10
1	A	389	ASN	CA-CB-CG	-5.49	107.11	112.60
1	A	338	GLN	CB-CG-CD	5.47	121.90	112.60
1	A	260	ILE	CA-C-N	5.42	125.50	119.32
1	A	260	ILE	C-N-CA	5.42	125.50	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	367	THR	CA-CB-OG1	-5.39	101.51	109.60
1	A	280	GLN	CA-CB-CG	5.38	124.86	114.10
1	A	201	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	A	88	VAL	CA-C-O	-5.21	114.59	120.74
1	A	353	PHE	CA-CB-CG	-5.17	108.63	113.80
1	A	245	TYR	N-CA-C	-5.16	103.87	110.53
1	A	236	TYR	N-CA-C	-5.13	105.14	111.40
1	A	199	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	407	GLY	N-CA-C	-5.09	107.24	115.08
1	A	435	SER	O-C-N	-5.07	115.80	122.39
1	A	75	HIS	CA-CB-CG	-5.07	108.73	113.80
1	A	252	LEU	N-CA-CB	-5.05	103.65	110.67
1	A	489	ARG	CD-NE-CZ	5.02	131.43	124.40

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	4171	0	4083	34	0
2	B	27	0	36	3	0
3	A	8	0	0	0	0
4	A	369	0	0	1	0
4	B	4	0	0	0	0
All	All	4579	0	4119	34	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 (34) 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:301:ILE:HA	1:A:305:LYS:HD2	1.72	0.71
1:A:401:LEU:HD22	2:B:2[B]:DAB:HD1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ALA:HB3	1:A:504:LEU:HD22	1.87	0.57
1:A:229:GLU:OE1	1:A:369:ASP:HB2	2.05	0.55
1:A:294:LYS:HA	1:A:480:VAL:HG13	1.89	0.55
1:A:253:PHE:CD2	1:A:309:GLN:HG2	2.42	0.55
1:A:4:PRO:O	1:A:7:VAL:HG13	2.07	0.54
1:A:115:TYR:CE1	1:A:428:ASN:HB3	2.42	0.54
1:A:43:LEU:HD21	1:A:204:LEU:HD22	1.91	0.53
1:A:300:ASP:OD2	1:A:305:LYS:NZ	2.43	0.52
1:A:301:ILE:HG12	1:A:305:LYS:HD2	1.93	0.51
1:A:297:LEU:HD21	1:A:302:ILE:HD12	1.93	0.50
1:A:382:TRP:HB3	1:A:388:VAL:CG2	2.42	0.48
1:A:62:GLU:HG3	1:A:63:LYS:HD3	1.96	0.48
1:A:117:HIS:HE1	4:A:1179:HOH:O	1.97	0.47
1:A:67:LYS:HA	1:A:67:LYS:HE3	1.96	0.47
1:A:248:MET:HA	1:A:248:MET:HE2	1.98	0.46
1:A:323:ASP:O	1:A:423:PRO:HD3	2.15	0.46
1:A:265:ARG:O	1:A:488:ALA:HA	2.17	0.45
1:A:475:LYS:HB2	1:A:475:LYS:HE3	1.77	0.43
1:A:269:TYR:HE2	2:B:3:LYS:HE3	1.83	0.43
1:A:307:LYS:HE3	1:A:483:TYR:OH	2.19	0.43
1:A:280:GLN:HG3	1:A:440:HIS:HB3	2.01	0.42
1:A:453:THR:HG21	1:A:466:TYR:CE2	2.54	0.42
1:A:499:THR:OG1	1:A:501:LYS:HB2	2.20	0.42
1:A:229:GLU:HB3	1:A:249:PRO:HD3	2.01	0.42
1:A:300:ASP:OD1	1:A:304:ASN:OD1	2.37	0.42
1:A:236:TYR:CE1	1:A:492:LYS:HE3	2.56	0.41
1:A:269:TYR:CE2	2:B:3:LYS:HE3	2.56	0.41
1:A:277:ILE:CG2	1:A:284:PHE:HB3	2.51	0.41
1:A:51:ASP:OD1	1:A:55:HIS:HD2	2.04	0.41
1:A:118:ILE:HD12	1:A:118:ILE:N	2.35	0.41
1:A:418:ALA:HB3	1:A:504:LEU:CD2	2.50	0.41
1:A:62:GLU:HG3	1:A:63:LYS:CD	2.52	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	517/517 (100%)	503 (97%)	13 (2%)	1 (0%)	43 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	PRO

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	324/455 (71%)	319 (98%)	5 (2%)	57 56
2	B	2/2 (100%)	2 (100%)	0	100 100
All	All	326/457 (71%)	321 (98%)	5 (2%)	57 56

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	306	VAL
1	A	348	LEU
1	A	390	VAL
1	A	413	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	117	HIS
1	A	209	GLN

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Mol	Chain	Res	Type
1	A	279	ASN
1	A	304	ASN
1	A	395	GLN
1	A	472	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	DAB	B	2[A]	-	5,6,7	0.66	0	1,6,8	0.67	0
2	DAB	B	2[B]	-	5,6,7	0.62	0	1,6,8	0.01	0

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	DAB	B	2[A]	-	-	0/4/5/7	-
2	DAB	B	2[B]	-	-	0/4/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2[B]	DAB	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.