



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:45 PM UTC

PDB ID : 1B3H / pdb_00001b3h
Title : OLIGO-PEPTIDE BINDING PROTEIN COMPLEXED WITH LYSYL-CYCLOHEXYLALANYL-LYSINE
Authors : Davies, T.G.; Tame, J.R.H.
Deposited on : 1998-11-16
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
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

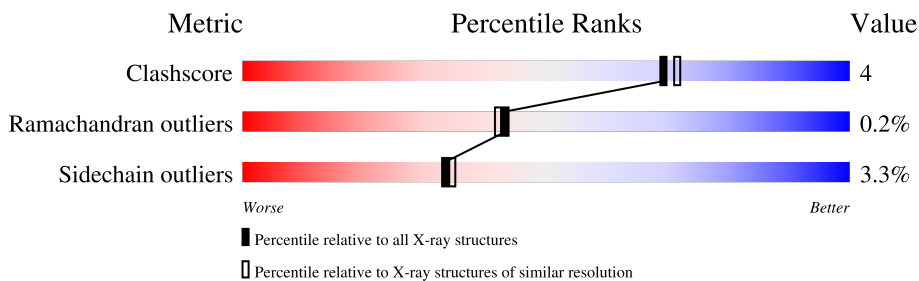
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	A	517	
2	B	3	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4455 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 OLIGOPEPTIDE-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	38	1	0
			4168	2667	700	796	5			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			30	21	5	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.

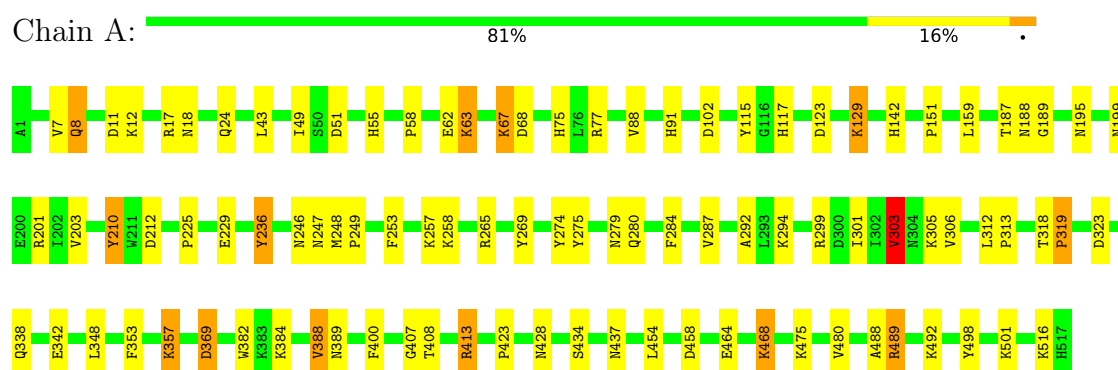
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	246	Total	O	0	0
			246	246		
4	B	3	Total	O	0	0
			3	3		

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 OLIGOPEPTIDE-BINDING PROTEIN



• Molecule 2: LYS-ALC-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	109.67Å 75.57Å 70.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	98.0 (20.00-2.00)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4455	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: ALC, U1

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	0.88	6/4284 (0.1%)	1.65	51/5841 (0.9%)
2	B	0.94	0/17	1.60	0/16
All	All	0.88	6/4301 (0.1%)	1.65	51/5857 (0.9%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	357	LYS	CG-CD	16.41	2.01	1.52
1	A	475	LYS	CD-CE	11.02	1.85	1.52
1	A	516	LYS	CG-CD	10.85	1.85	1.52
1	A	129	LYS	CG-CD	6.56	1.72	1.52
1	A	12	LYS	CE-NZ	-6.18	1.30	1.49
1	A	189	GLY	N-CA	5.17	1.50	1.45

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	LYS	CG-CD-CE	12.05	139.01	111.30
1	A	516	LYS	CB-CG-CD	-10.51	87.13	111.30
1	A	357	LYS	CB-CG-CD	-9.05	90.47	111.30
1	A	413	ARG	NE-CZ-NH2	-8.64	111.42	119.20
1	A	117	HIS	CA-CB-CG	-8.53	105.28	113.80
1	A	280	GLN	OE1-CD-NE2	8.34	130.94	122.60
1	A	468	LYS	CB-CG-CD	7.78	129.19	111.30
1	A	353	PHE	CA-CB-CG	-7.54	106.26	113.80
1	A	247	ASN	CA-CB-CG	7.23	119.83	112.60
1	A	389	ASN	CA-CB-CG	-7.08	105.52	112.60
1	A	188	ASN	CA-C-N	-7.05	115.29	122.27
1	A	188	ASN	C-N-CA	-7.05	115.29	122.27
1	A	246	ASN	CA-C-N	6.91	132.62	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ASN	C-N-CA	6.91	132.62	122.39
1	A	18	ASN	CA-CB-CG	-6.89	105.70	112.60
1	A	201	ARG	NE-CZ-NH2	6.84	125.36	119.20
1	A	142	HIS	CA-CB-CG	-6.53	107.27	113.80
1	A	489	ARG	CD-NE-CZ	6.53	133.54	124.40
1	A	407	GLY	N-CA-C	-6.28	105.41	115.08
1	A	88	VAL	CA-C-O	-6.27	113.62	120.71
1	A	284	PHE	CA-CB-CG	-6.19	107.61	113.80
1	A	319	PRO	CA-C-N	6.00	125.68	119.56
1	A	319	PRO	C-N-CA	6.00	125.68	119.56
1	A	91	HIS	CA-CB-CG	-5.92	107.88	113.80
1	A	75	HIS	CA-CB-CG	-5.90	107.90	113.80
1	A	275	TYR	CA-CB-CG	-5.86	103.35	113.90
1	A	24	GLN	CB-CA-C	-5.86	100.89	110.85
1	A	369	ASP	CA-CB-CG	-5.73	106.87	112.60
1	A	400	PHE	CA-CB-CG	5.71	119.50	113.80
1	A	303	VAL	N-CA-C	5.66	115.85	110.53
1	A	236	TYR	N-CA-C	-5.64	105.05	111.14
1	A	369	ASP	CB-CA-C	-5.51	102.23	110.88
1	A	199	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	A	159	LEU	N-CA-C	5.44	119.54	113.01
1	A	253	PHE	N-CA-C	5.43	117.63	111.11
1	A	8	GLN	CA-CB-CG	5.41	124.92	114.10
1	A	210	TYR	CA-C-O	-5.28	114.90	120.92
1	A	11	ASP	N-CA-C	-5.28	105.42	111.07
1	A	287	VAL	O-C-N	-5.25	116.57	121.87
1	A	49	ILE	CA-C-O	-5.19	116.22	121.67
1	A	292	ALA	CA-C-O	5.19	126.27	120.82
1	A	67	LYS	CG-CD-CE	5.19	123.23	111.30
1	A	279	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	A	102	ASP	CA-C-N	5.18	124.97	119.28
1	A	102	ASP	C-N-CA	5.18	124.97	119.28
1	A	17	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	A	275	TYR	N-CA-CB	5.08	118.69	110.42
1	A	77	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	A	274	TYR	CA-C-O	-5.01	116.09	121.45
1	A	413	ARG	NH1-CZ-NH2	5.01	125.81	119.30
1	A	458	ASP	CA-CB-CG	5.00	117.60	112.60

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	A	4168	0	4076	29	1
2	B	30	0	42	1	0
3	A	8	0	0	0	1
4	A	246	0	0	0	0
4	B	3	0	0	0	0
All	All	4455	0	4118	29	1

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 (29) 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:123:ASP:HB3	1:A:129:LYS:HG3	1.77	0.66
1:A:62:GLU:HG3	1:A:63:LYS:HD2	1.81	0.62
1:A:51:ASP:OD1	1:A:55:HIS:HD2	1.84	0.60
1:A:301:ILE:HA	1:A:305:LYS:HD2	1.85	0.58
1:A:115:TYR:CE1	1:A:428:ASN:HB3	2.39	0.57
1:A:382:TRP:HB3	1:A:388:VAL:HG22	1.87	0.56
1:A:269:TYR:OH	2:B:3:LYS:HE2	2.10	0.52
1:A:248:MET:HA	1:A:248:MET:HE2	1.95	0.49
1:A:299:ARG:O	1:A:303:VAL:HG23	2.12	0.49
1:A:229:GLU:HB3	1:A:249:PRO:HD3	1.95	0.48
1:A:210:TYR:CE2	1:A:212:ASP:HB3	2.49	0.48
1:A:489:ARG:NH1	1:A:498:TYR:OH	2.41	0.47
1:A:229:GLU:OE1	1:A:369:ASP:HB2	2.16	0.46
1:A:67:LYS:HD3	1:A:67:LYS:C	2.40	0.46
1:A:67:LYS:HD3	1:A:68:ASP:N	2.33	0.44
1:A:294:LYS:HA	1:A:480:VAL:HG13	1.99	0.43
1:A:236:TYR:CE2	1:A:492:LYS:HE3	2.54	0.43
1:A:151:PRO:O	1:A:454:LEU:HD22	2.19	0.43
1:A:434:SER:HB3	1:A:437:ASN:HB2	2.01	0.42
1:A:115:TYR:CD1	1:A:428:ASN:HB3	2.55	0.42
1:A:323:ASP:O	1:A:423:PRO:HD3	2.19	0.41
1:A:318:THR:HA	1:A:319:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:GLU:O	1:A:468:LYS:HG3	2.20	0.41
1:A:195:ASN:HD22	1:A:203:VAL:HB	1.87	0.40
1:A:51:ASP:OD1	1:A:55:HIS:CD2	2.71	0.40
1:A:265:ARG:O	1:A:488:ALA:HA	2.21	0.40
1:A:348:LEU:HD23	1:A:348:LEU:HA	1.91	0.40
1:A:43:LEU:O	1:A:187:THR:HB	2.21	0.40
1:A:312:LEU:HA	1:A:313:PRO:HD3	1.95	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:GLU:OE1	3:A:525:U1:U[1_556]	1.79	0.41

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	516/517 (100%)	502 (97%)	13 (2%)	1 (0%)	43	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	PRO

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	A	456/455 (100%)	441 (97%)	15 (3%)	33	34
2	B	2/2 (100%)	2 (100%)	0	100	100
All	All	458/457 (100%)	443 (97%)	15 (3%)	33	34

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	8	GLN
1	A	58	PRO
1	A	63	LYS
1	A	257	LYS
1	A	258	LYS
1	A	303	VAL
1	A	306	VAL
1	A	338	GLN
1	A	357	LYS
1	A	384	LYS
1	A	388	VAL
1	A	408	THR
1	A	413	ARG
1	A	501	LYS

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	55	HIS
1	A	117	HIS
1	A	195	ASN
1	A	199	ASN
1	A	279	ASN
1	A	304	ASN
1	A	436	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	ALC	B	2	2	9,11,12	1.43	1 (11%)	11,13,15	1.30	3 (27%)

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	ALC	B	2	2	-	1/5/14/16	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	ALC	CB-CG	3.36	1.58	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	ALC	CB-CA-C	-2.19	107.62	110.99
2	B	2	ALC	CB-CG-CD1	-2.15	106.70	111.71
2	B	2	ALC	CG-CB-CA	-2.14	111.64	114.52

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	ALC	CA-CB-CG-CD1

There are no ring outliers.

No monomer is involved in short contacts.

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.