Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 09:09 AM EST

PDB ID	:	1B3H
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 (i) 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 (i)) were used in the production of this report:

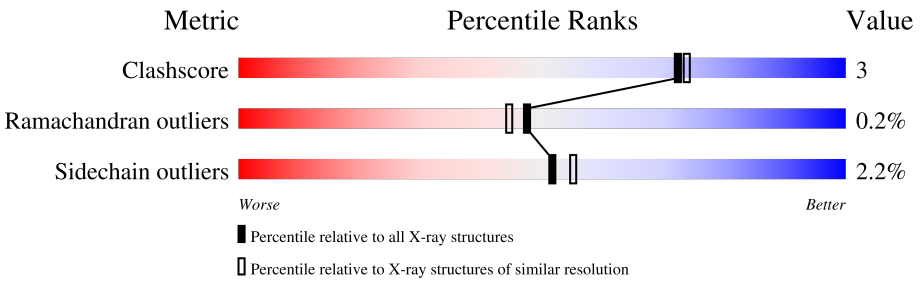
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	517	84% 14% •
2	B	3	33% 67%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	517	4168	2667	700	796	5	38	1	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	30	21	5	4	0	0	0

- Molecule 3 is URANIUM ATOM (three-letter code: U1) (formula: U).

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

- Molecule 4 is water.

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

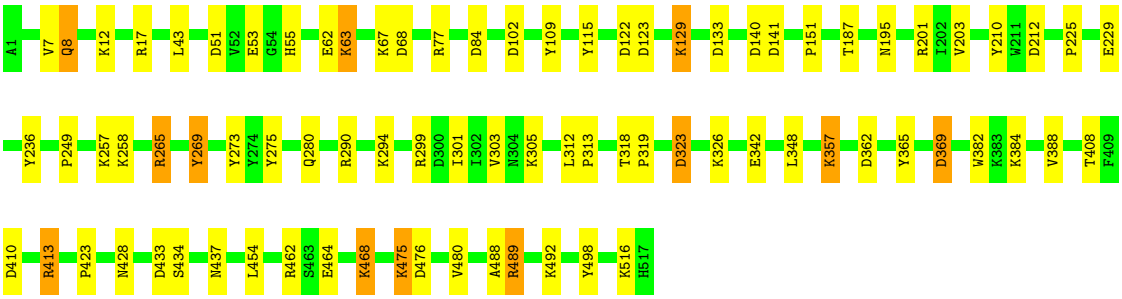
3 Residue-property plots (i)

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

Chain A: 84% 14%



• Molecule 2: LYS-ALC-LYS PEPTIDE

Chain B: 33% 67%

4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	0.75	5/4284 (0.1%)	1.35	40/5841 (0.7%)
2	B	0.90	0/17	1.48	0/16
All	All	0.75	5/4301 (0.1%)	1.35	40/5857 (0.7%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	357	LYS	CG-CD	14.48	2.01	1.52
1	A	475	LYS	CD-CE	13.70	1.85	1.51
1	A	516	LYS	CG-CD	9.58	1.85	1.52
1	A	12	LYS	CE-NZ	-7.29	1.30	1.49
1	A	129	LYS	CG-CD	5.79	1.72	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	413	ARG	NE-CZ-NH2	-17.76	111.42	120.30
1	A	201	ARG	NE-CZ-NH2	10.11	125.36	120.30
1	A	516	LYS	CB-CG-CD	-9.41	87.13	111.60
1	A	273	TYR	CB-CG-CD1	-9.10	115.54	121.00
1	A	357	LYS	CG-CD-CE	9.04	139.01	111.90
1	A	273	TYR	CB-CG-CD2	8.91	126.35	121.00
1	A	53	GLU	OE1-CD-OE2	8.91	133.99	123.30
1	A	109	TYR	CB-CG-CD2	-8.88	115.67	121.00
1	A	476	ASP	CB-CG-OD1	8.54	125.98	118.30
1	A	357	LYS	CB-CG-CD	-8.12	90.47	111.60
1	A	77	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	A	133	ASP	CB-CG-OD2	-7.65	111.41	118.30
1	A	109	TYR	CB-CG-CD1	7.46	125.48	121.00
1	A	489	ARG	CD-NE-CZ	7.10	133.54	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	ARG	NE-CZ-NH2	7.04	123.82	120.30
1	A	362	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	A	468	LYS	CB-CG-CD	6.77	129.19	111.60
1	A	102	ASP	CB-CG-OD1	-6.75	112.22	118.30
1	A	102	ASP	CB-CG-OD2	6.74	124.36	118.30
1	A	462	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	475	LYS	CD-CE-NZ	6.55	126.76	111.70
1	A	84	ASP	CB-CG-OD1	6.45	124.10	118.30
1	A	323	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	413	ARG	NH1-CZ-NH2	5.83	125.81	119.40
1	A	122	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	269	TYR	CB-CG-CD2	-5.74	117.55	121.00
1	A	365	TYR	CB-CG-CD2	5.70	124.42	121.00
1	A	433	ASP	CB-CG-OD1	5.66	123.40	118.30
1	A	141	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	290	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	369	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	265	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	280	GLN	CG-CD-OE1	-5.36	110.89	121.60
1	A	275	TYR	CA-CB-CG	-5.29	103.35	113.40
1	A	17	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	A	201	ARG	CD-NE-CZ	5.26	130.97	123.60
1	A	8	GLN	CA-CB-CG	5.24	124.92	113.40
1	A	140	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	410	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	326	LYS	N-CA-CB	5.02	119.64	110.60

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	A	4168	0	4076	28	1
2	B	30	0	42	1	0
3	A	8	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	246	0	0	0	0
4	B	3	0	0	0	0
All	All	4455	0	4118	28	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 3.

All (28) 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: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: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:67:LYS:HD3	1:A:67:LYS:C	2.40	0.41
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
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%)	47 44

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%)	446 (98%)	10 (2%)	52 55
2	B	2/2 (100%)	2 (100%)	0	100 100
All	All	458/457 (100%)	448 (98%)	10 (2%)	52 55

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	8	GLN

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Mol	Chain	Res	Type
1	A	63	LYS
1	A	257	LYS
1	A	258	LYS
1	A	357	LYS
1	A	384	LYS
1	A	408	THR
1	A	413	ARG
1	A	475	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) 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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	1.49	1 (11%)	10,13,15	1.23	2 (20%)

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	-	2/5/14/16	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	3.63	1.58	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	ALC	CB-CG-CD1	-2.31	106.70	111.73
2	B	2	ALC	CG-CB-CA	-2.14	111.64	114.52

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	ALC	C-CA-CB-CG
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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.