



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:48 pm GMT

PDB ID : 1B05
Title : Structure of oligo-peptide binding protein complexed with LYS-CYS-LYS
Authors : Tame, J.R.H.; Wilkinson, A.J.
Deposited on : 1998-11-17
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

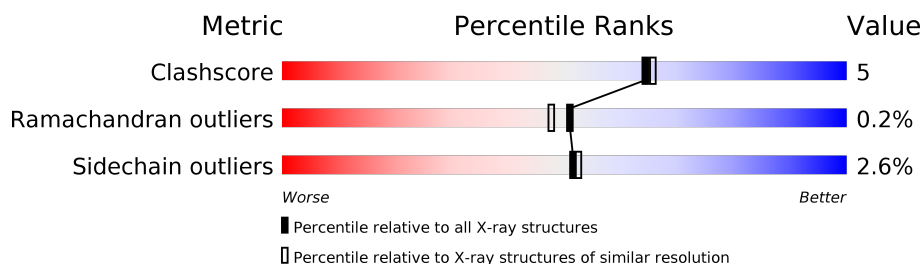
1 Overall quality at a glance

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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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 4377 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	0	0	0
			4156	2660	699	792	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	S	0	0	0
			25	15	5	4	1			

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

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

- Molecule 4 is water.

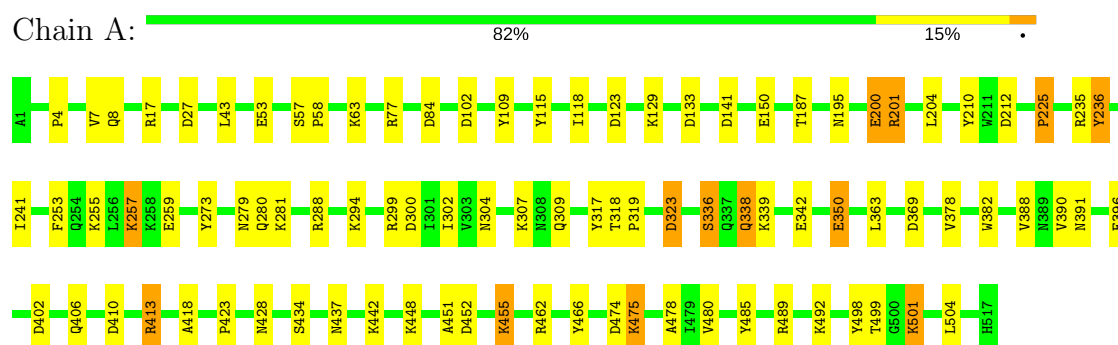
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	184	Total	O	0	0
			184	184		
4	B	4	Total	O	0	0
			4	4		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: PEPTIDE LYS-CYS-LYS



There are no outlier residues recorded for this chain.

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	109.55Å 76.12Å 70.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00	Depositor
% Data completeness (in resolution range)	96.2 (15.00-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4377	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

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	0.67	0/4267	1.43	41/5818 (0.7%)
2	B	1.09	0/24	1.53	0/27
All	All	0.67	0/4291	1.43	41/5845 (0.7%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ARG	NE-CZ-NH1	16.47	128.54	120.30
1	A	235	ARG	CD-NE-CZ	14.65	144.12	123.60
1	A	273	TYR	CB-CG-CD2	-10.49	114.71	121.00
1	A	235	ARG	NE-CZ-NH2	-10.12	115.24	120.30
1	A	84	ASP	CB-CG-OD1	9.73	127.06	118.30
1	A	150	GLU	CA-CB-CG	9.36	133.99	113.40
1	A	133	ASP	CB-CG-OD2	-8.95	110.25	118.30
1	A	17	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	A	413	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	77	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	273	TYR	CB-CG-CD1	7.71	125.63	121.00
1	A	350	GLU	OE1-CD-OE2	7.59	132.41	123.30
1	A	235	ARG	CG-CD-NE	7.00	126.50	111.80
1	A	141	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	102	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	A	27	ASP	CB-CG-OD1	6.60	124.24	118.30
1	A	323	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	A	77	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	A	410	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	27	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	485	TYR	CA-CB-CG	6.17	125.12	113.40
1	A	201	ARG	NE-CZ-NH2	6.08	123.34	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	GLU	CA-CB-CG	5.96	126.52	113.40
1	A	317	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	A	235	ARG	CA-CB-CG	-5.86	100.51	113.40
1	A	77	ARG	CD-NE-CZ	5.82	131.75	123.60
1	A	102	ASP	CB-CG-OD1	5.77	123.50	118.30
1	A	369	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	A	53	GLU	OE1-CD-OE2	5.69	130.13	123.30
1	A	342	GLU	OE1-CD-OE2	-5.61	116.57	123.30
1	A	475	LYS	CA-CB-CG	5.40	125.27	113.40
1	A	413	ARG	NH1-CZ-NH2	5.39	125.33	119.40
1	A	474	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	236	TYR	CB-CG-CD2	5.28	124.17	121.00
1	A	413	ARG	CG-CD-NE	-5.24	100.80	111.80
1	A	109	TYR	CB-CG-CD2	5.23	124.14	121.00
1	A	236	TYR	CB-CG-CD1	-5.16	117.91	121.00
1	A	200	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	A	410	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	A	336	SER	N-CA-CB	-5.04	102.94	110.50
1	A	299	ARG	NE-CZ-NH1	5.03	122.81	120.30

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	4156	0	4061	40	0
2	B	25	0	33	0	0
3	A	8	0	0	0	0
4	A	184	0	0	1	0
4	B	4	0	0	0	0
All	All	4377	0	4094	40	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 5.

All (40) 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:363:LEU:HB2	1:A:390:VAL:HG11	1.55	0.86
1:A:288:ARG:HD2	1:A:350:GLU:HG2	1.63	0.79
1:A:123:ASP:OD2	1:A:129:LYS:NZ	2.27	0.66
1:A:255:LYS:HG3	1:A:259:GLU:OE1	2.01	0.60
1:A:280:GLN:NE2	1:A:442:LYS:HE2	2.17	0.60
1:A:280:GLN:HE22	1:A:442:LYS:HE2	1.73	0.54
1:A:57:SER:HB3	1:A:58:PRO:HD2	1.89	0.54
1:A:451:ALA:O	1:A:455:LYS:HD3	2.08	0.54
1:A:253:PHE:CD2	1:A:309:GLN:HG2	2.43	0.53
1:A:382:TRP:HB3	1:A:388:VAL:CG2	2.38	0.53
1:A:336:SER:HB3	1:A:339:LYS:H	1.72	0.53
1:A:489:ARG:NH1	1:A:498:TYR:OH	2.42	0.52
1:A:300:ASP:O	1:A:304:ASN:HB2	2.11	0.51
1:A:115:TYR:CE1	1:A:428:ASN:HB3	2.45	0.51
1:A:4:PRO:O	1:A:7:VAL:HG13	2.11	0.51
1:A:294:LYS:HA	1:A:480:VAL:HG13	1.93	0.49
1:A:200:GLU:CD	1:A:201:ARG:HE	2.16	0.49
1:A:280:GLN:HG2	4:A:673:HOH:O	2.12	0.49
1:A:338:GLN:HG3	1:A:339:LYS:N	2.27	0.49
1:A:402:ASP:OD2	1:A:406:GLN:NE2	2.44	0.46
1:A:475:LYS:HB2	1:A:475:LYS:HE3	1.78	0.45
1:A:210:TYR:CE2	1:A:212:ASP:HB3	2.52	0.44
1:A:43:LEU:O	1:A:187:THR:HB	2.18	0.44
1:A:257:LYS:HD3	1:A:257:LYS:HA	1.89	0.44
1:A:418:ALA:HB3	1:A:504:LEU:CD2	2.48	0.43
1:A:434:SER:HB3	1:A:437:ASN:HB2	2.00	0.43
1:A:115:TYR:CD1	1:A:428:ASN:HB3	2.53	0.43
1:A:118:ILE:HD12	1:A:118:ILE:N	2.33	0.43
1:A:363:LEU:HB2	1:A:390:VAL:CG1	2.37	0.43
1:A:462:ARG:HG2	1:A:466:TYR:CZ	2.53	0.43
1:A:390:VAL:HG12	1:A:391:ASN:N	2.34	0.42
1:A:323:ASP:O	1:A:423:PRO:HD3	2.20	0.42
1:A:279:ASN:HD21	1:A:478:ALA:HA	1.85	0.42
1:A:318:THR:HA	1:A:319:PRO:HD3	1.95	0.42
1:A:236:TYR:HA	1:A:241:ILE:HB	2.02	0.42
1:A:499:THR:OG1	1:A:501:LYS:HB2	2.20	0.42
1:A:302:ILE:HD13	1:A:378:VAL:HG22	2.02	0.41
1:A:448:LYS:HE2	1:A:452:ASP:OD2	2.20	0.41
1:A:236:TYR:CE2	1:A:492:LYS:HE3	2.56	0.41
1:A:43:LEU:HD21	1:A:204:LEU:HD22	2.03	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	A	515/517 (100%)	497 (96%)	17 (3%)	1 (0%)	51	48
2	B	1/3 (33%)	1 (100%)	0	0	100	100
All	All	516/520 (99%)	498 (96%)	17 (3%)	1 (0%)	51	48

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	453/455 (100%)	441 (97%)	12 (3%)	51	52
2	B	3/3 (100%)	3 (100%)	0	100	100
All	All	456/458 (100%)	444 (97%)	12 (3%)	51	52

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	63	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	195	ASN
1	A	225	PRO
1	A	257	LYS
1	A	281	LYS
1	A	307	LYS
1	A	338	GLN
1	A	396	GLU
1	A	413	ARG
1	A	455	LYS
1	A	501	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
1	A	184	ASN
1	A	199	ASN
1	A	209	GLN
1	A	279	ASN
1	A	280	GLN
1	A	308	ASN
1	A	338	GLN
1	A	395	GLN
1	A	440	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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.