



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:46 pm GMT

PDB ID : 1B40  
Title : OLIGO-PEPTIDE BINDING PROTEIN (OPPA) COMPLEXED WITH KFK  
Authors : Tame, J.R.H.; Wilkinson, A.J.  
Deposited on : 1998-11-23  
Resolution : 2.20 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](mailto: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.

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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

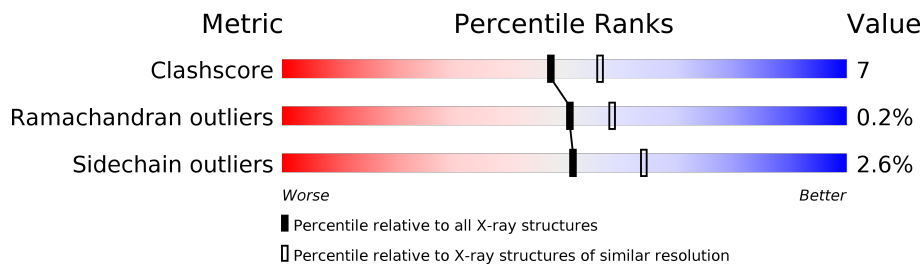
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)

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  $\geq 3$ , 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 [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4364 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.

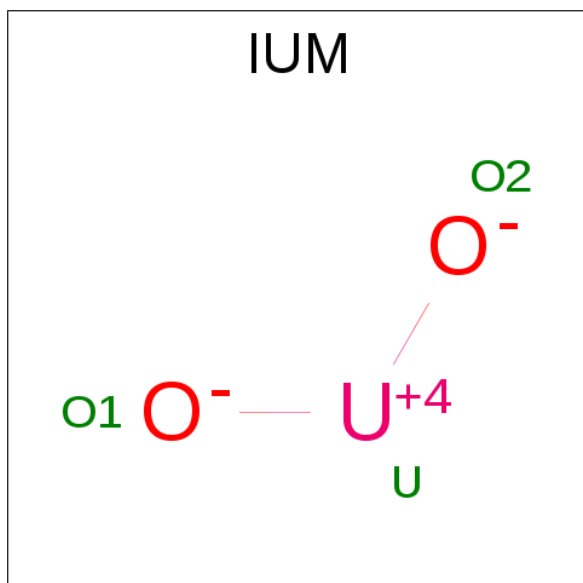
- Molecule 1 is a protein called PROTEIN (OLIGO-PEPTIDE BINDING PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			4164	2666	700	793	5			

- Molecule 2 is a protein called PROTEIN (LYS-PHE-LYS).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			29	21	5	3			

- Molecule 3 is URANYL (VI) ION (three-letter code: IUM) (formula: O<sub>2</sub>U).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	U	0	0
			1	1		
3	A	1	Total	U	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	U 1	0	0
3	A	1	Total 1	U 1	0	0
3	A	1	Total 1	U 1	0	0
3	A	1	Total 1	U 1	0	0
3	A	1	Total 1	U 1	0	0
3	A	1	Total 1	U 1	0	0

- Molecule 4 is water.

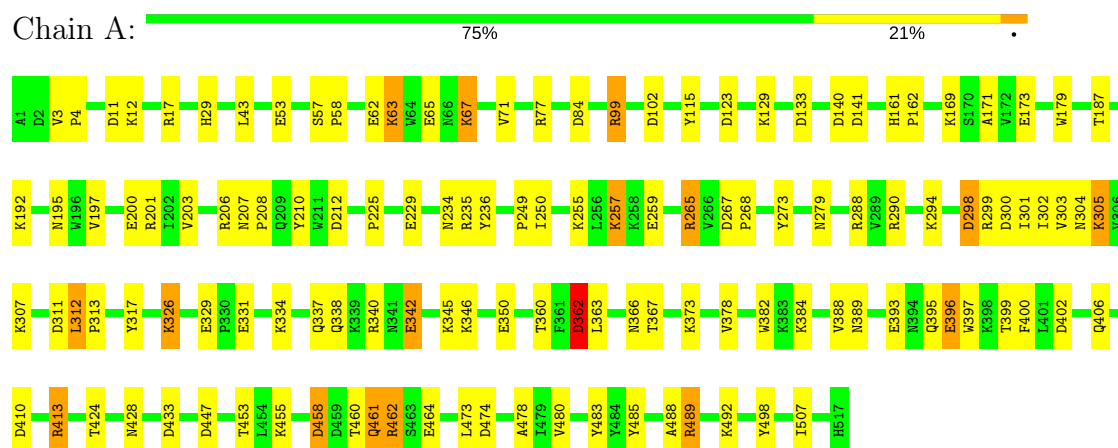
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	163	Total 163	O 163	0	0

### 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: PROTEIN (OLIGO-PEPTIDE BINDING PROTEIN)



#### • Molecule 2: PROTEIN (LYS-PHE-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, $\alpha$ , $\beta$ , $\gamma$	109.69Å 75.16Å 69.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20	Depositor
% Data completeness (in resolution range)	98.4 (15.00-2.20)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.199 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4364	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	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: IUM

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	0.63	1/4275 (0.0%)	1.48	50/5830 (0.9%)
2	B	0.80	0/29	0.93	0/35
All	All	0.63	1/4304 (0.0%)	1.47	50/5865 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	342	GLU	CD-OE2	6.51	1.32	1.25

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	489	ARG	NE-CZ-NH1	12.85	126.72	120.30
1	A	133	ASP	CB-CG-OD2	-10.62	108.74	118.30
1	A	17	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	A	99	ARG	NE-CZ-NH1	-9.37	115.62	120.30
1	A	410	ASP	CB-CG-OD1	9.16	126.54	118.30
1	A	396	GLU	CB-CG-CD	8.69	137.65	114.20
1	A	433	ASP	CB-CG-OD1	8.12	125.60	118.30
1	A	458	ASP	CB-CG-OD2	7.93	125.44	118.30
1	A	362	ASP	CB-CG-OD2	7.88	125.39	118.30
1	A	102	ASP	CB-CG-OD1	7.86	125.37	118.30
1	A	447	ASP	CB-CG-OD1	7.79	125.31	118.30
1	A	288	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	235	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	A	489	ARG	CD-NE-CZ	7.21	133.70	123.60
1	A	474	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	299	ARG	CD-NE-CZ	6.83	133.16	123.60
1	A	273	TYR	CB-CG-CD2	-6.73	116.96	121.00
1	A	485	TYR	CB-CG-CD2	6.70	125.02	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	485	TYR	CA-CB-CG	6.58	125.90	113.40
1	A	340	ARG	NE-CZ-NH2	6.53	123.56	120.30
1	A	206	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	A	265	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	317	TYR	CB-CG-CD2	-6.39	117.17	121.00
1	A	201	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	84	ASP	CB-CG-OD1	5.95	123.66	118.30
1	A	489	ARG	NH1-CZ-NH2	-5.82	113.00	119.40
1	A	77	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	265	ARG	CD-NE-CZ	5.65	131.51	123.60
1	A	11	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	53	GLU	OE1-CD-OE2	5.52	129.92	123.30
1	A	462	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	410	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	140	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	A	179	TRP	CA-CB-CG	5.28	123.73	113.70
1	A	234	ASN	N-CA-CB	5.27	120.08	110.60
1	A	473	LEU	CA-CB-CG	5.23	127.34	115.30
1	A	384	LYS	CA-CB-CG	5.21	124.87	113.40
1	A	141	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	340	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	A	273	TYR	CB-CG-CD1	5.19	124.11	121.00
1	A	192	LYS	CB-CA-C	-5.14	100.12	110.40
1	A	326	LYS	N-CA-CB	5.14	119.86	110.60
1	A	290	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	A	201	ARG	CD-NE-CZ	5.11	130.75	123.60
1	A	298	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	257	LYS	CA-CB-CG	5.10	124.62	113.40
1	A	65	GLU	CB-CA-C	-5.05	100.30	110.40
1	A	413	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	171	ALA	N-CA-CB	5.00	117.11	110.10

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	4164	0	4076	58	1
2	B	29	0	37	0	0
3	A	8	0	0	0	1
4	A	163	0	0	2	0
All	All	4364	0	4113	58	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 7.

All (58) 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:294:LYS:HA	1:A:480:VAL:HG13	1.69	0.73
1:A:169:LYS:HE2	1:A:173:GLU:OE2	1.92	0.69
1:A:460:THR:O	1:A:464:GLU:HG3	1.93	0.69
1:A:326:LYS:HD2	4:A:678:HOH:O	1.98	0.63
1:A:307:LYS:HE3	1:A:483:TYR:OH	1.99	0.62
1:A:257:LYS:HG2	4:A:683:HOH:O	2.03	0.58
1:A:458:ASP:HB3	1:A:461:GLN:HB2	1.87	0.56
1:A:402:ASP:O	1:A:406:GLN:HG3	2.07	0.54
1:A:453:THR:HB	1:A:462:ARG:HG3	1.88	0.54
1:A:396:GLU:HG2	1:A:397:TRP:N	2.21	0.54
1:A:195:ASN:HB2	1:A:203:VAL:HB	1.90	0.54
1:A:255:LYS:HD2	1:A:259:GLU:OE2	2.08	0.54
1:A:62:GLU:HG3	1:A:63:LYS:HD2	1.90	0.53
1:A:115:TYR:CE1	1:A:428:ASN:HB3	2.44	0.53
1:A:301:ILE:HA	1:A:305:LYS:HG3	1.90	0.52
1:A:301:ILE:HA	1:A:305:LYS:CG	2.40	0.52
1:A:250:ILE:HB	1:A:373:LYS:HD3	1.92	0.51
1:A:345:LYS:HB2	1:A:345:LYS:HZ2	1.75	0.51
1:A:300:ASP:OD1	1:A:304:ASN:ND2	2.40	0.51
1:A:345:LYS:HB2	1:A:345:LYS:NZ	2.26	0.51
1:A:43:LEU:O	1:A:187:THR:HB	2.11	0.50
1:A:382:TRP:HB3	1:A:388:VAL:CG2	2.41	0.50
1:A:265:ARG:O	1:A:488:ALA:HA	2.12	0.49
1:A:123:ASP:HB3	1:A:129:LYS:HG3	1.95	0.48
1:A:395:GLN:NE2	1:A:399:THR:HG22	2.29	0.48
1:A:489:ARG:NH1	1:A:498:TYR:OH	2.40	0.48
1:A:424:THR:HB	1:A:428:ASN:ND2	2.29	0.47
1:A:197:VAL:HB	1:A:200:GLU:HB3	1.96	0.47
1:A:346:LYS:O	1:A:350:GLU:HG3	2.15	0.47
1:A:210:TYR:CE2	1:A:212:ASP:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:TYR:CZ	1:A:492:LYS:HE3	2.50	0.46
1:A:115:TYR:CD1	1:A:428:ASN:HB3	2.51	0.46
1:A:279:ASN:HD21	1:A:478:ALA:HA	1.80	0.46
1:A:123:ASP:CB	1:A:129:LYS:HG3	2.46	0.46
1:A:402:ASP:OD2	1:A:406:GLN:NE2	2.49	0.46
1:A:302:ILE:HD11	1:A:378:VAL:HG22	1.97	0.45
1:A:29:HIS:ND1	1:A:99:ARG:NH1	2.65	0.45
1:A:329:GLU:OE2	1:A:334:LYS:HE3	2.17	0.45
1:A:298:ASP:OD2	1:A:337:GLN:HG2	2.18	0.44
1:A:302:ILE:CD1	1:A:378:VAL:HG22	2.48	0.44
1:A:267:ASP:HB3	1:A:268:PRO:CD	2.48	0.44
1:A:161:HIS:CD2	1:A:162:PRO:HD2	2.53	0.43
1:A:312:LEU:HA	1:A:313:PRO:HD3	1.92	0.43
1:A:207:ASN:HA	1:A:208:PRO:HD2	1.90	0.43
1:A:3:VAL:HA	1:A:4:PRO:HD3	1.87	0.43
1:A:229:GLU:HB3	1:A:249:PRO:HD3	2.01	0.43
1:A:303:VAL:HG13	1:A:311:ASP:HB2	2.01	0.42
1:A:57:SER:HB3	1:A:58:PRO:HD2	2.02	0.42
1:A:362:ASP:OD1	1:A:362:ASP:N	2.53	0.42
1:A:366:ASN:O	1:A:367:THR:C	2.55	0.42
1:A:267:ASP:HB3	1:A:268:PRO:HD2	2.01	0.41
1:A:67:LYS:HE2	1:A:71:VAL:HG21	2.03	0.41
1:A:342:GLU:CD	1:A:345:LYS:HZ1	2.23	0.41
1:A:331:GLU:OE2	1:A:334:LYS:NZ	2.44	0.41
1:A:360:THR:HA	1:A:389:ASN:O	2.21	0.41
1:A:366:ASN:HB3	1:A:400:PHE:CD2	2.56	0.41
1:A:236:TYR:CE1	1:A:492:LYS:HE3	2.56	0.40
1:A:362:ASP:OD2	1:A:393:GLU:OE2	2.40	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:OE2	3:A:525:IUM:U[1_556]	1.94	0.26

## 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	515/517 (100%)	496 (96%)	18 (4%)	1 (0%)	51	58
2	B	1/3 (33%)	1 (100%)	0	0	100	100
All	All	516/520 (99%)	497 (96%)	18 (4%)	1 (0%)	51	58

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	455/455 (100%)	443 (97%)	12 (3%)	51	64
2	B	3/3 (100%)	3 (100%)	0	100	100
All	All	458/458 (100%)	446 (97%)	12 (3%)	51	64

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

Mol	Chain	Res	Type
1	A	12	LYS
1	A	63	LYS
1	A	67	LYS
1	A	305	LYS
1	A	312	LEU

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Mol	Chain	Res	Type
1	A	338	GLN
1	A	362	ASP
1	A	363	LEU
1	A	413	ARG
1	A	455	LYS
1	A	461	GLN
1	A	507	ILE

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

Mol	Chain	Res	Type
1	A	104	ASN
1	A	195	ASN
1	A	199	ASN
1	A	209	GLN
1	A	279	ASN
1	A	395	GLN
1	A	428	ASN

### 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 modelled with single atom - 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.