



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:30 PM GMT

PDB ID : 1B3G
Title : OLIGO-PEPTIDE BINDING PROTEIN (OPPA) COMPLEXED WITH KIK
Authors : Tame, J.R.H.; Wilkinson, A.J.
Deposited on : 1998-12-10
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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

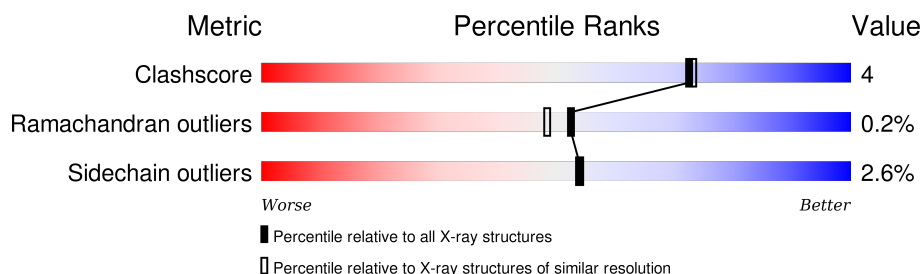
1 Overall quality at a glance

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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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	 81% 17% •
2	B	3	 67% 33%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4557 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.

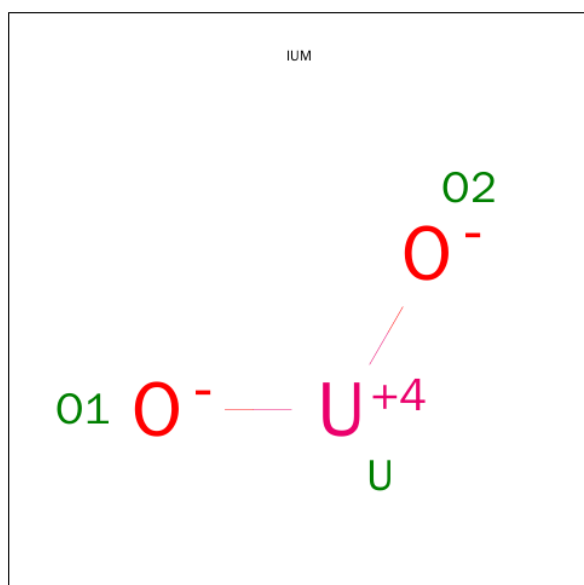
- Molecule 1 is a protein called PROTEIN (OLIGO-PEPTIDE BINDING PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	45	1	0
			4166	2666	700	795	5			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			27	18	5	4			

- Molecule 3 is URANYL (VI) ION (three-letter code: IUM) (formula: O₂U).



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.

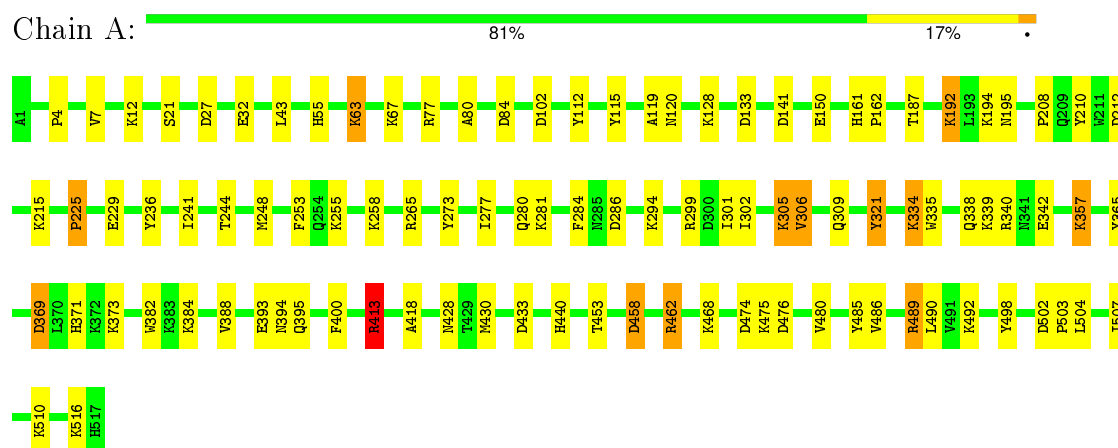
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	347	Total 354	O 354	0	7
4	B	2	Total 2	O 2	0	0

3 Residue-property plots [i](#)

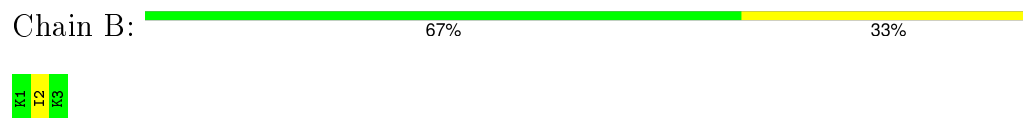
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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-ILE-LYS)



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.69Å 76.11Å 70.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00	Depositor
% Data completeness (in resolution range)	98.3 (15.00-2.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.189 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4557	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: 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	0.95	10/4282 (0.2%)	1.52	52/5839 (0.9%)
2	B	1.03	0/26	1.48	0/30
All	All	0.95	10/4308 (0.2%)	1.52	52/5869 (0.9%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	LYS	CD-CE	18.72	1.98	1.51
1	A	475	LYS	CG-CD	18.16	2.14	1.52
1	A	384	LYS	CD-CE	17.88	1.96	1.51
1	A	63	LYS	CD-CE	-14.57	1.14	1.51
1	A	128	LYS	CD-CE	-9.08	1.28	1.51
1	A	12	LYS	CD-CE	-8.13	1.30	1.51
1	A	357	LYS	CB-CG	-7.84	1.31	1.52
1	A	373	LYS	CB-CG	-7.03	1.33	1.52
1	A	255	LYS	CG-CD	-6.70	1.29	1.52
1	A	334	LYS	CB-CG	5.21	1.66	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	ARG	NE-CZ-NH2	-21.09	109.76	120.30
1	A	77	ARG	NE-CZ-NH1	15.43	128.02	120.30
1	A	413	ARG	NE-CZ-NH1	14.28	127.44	120.30
1	A	63	LYS	CG-CD-CE	13.95	153.76	111.90
1	A	462	ARG	NE-CZ-NH2	-11.75	114.42	120.30
1	A	102	ASP	CB-CG-OD1	11.28	128.45	118.30
1	A	133	ASP	CB-CG-OD2	-10.67	108.69	118.30
1	A	475	LYS	CB-CG-CD	-10.47	84.38	111.60
1	A	413	ARG	CD-NE-CZ	9.76	137.26	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	A	194	LYS	CG-CD-CE	9.04	139.00	111.90
1	A	468	LYS	CB-CG-CD	8.90	134.75	111.60
1	A	255	LYS	CB-CG-CD	8.82	134.54	111.60
1	A	273	TYR	CB-CG-CD2	-8.62	115.83	121.00
1	A	27	ASP	CB-CG-OD2	-8.06	111.04	118.30
1	A	12	LYS	CD-CE-NZ	-7.89	93.55	111.70
1	A	462	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	A	84	ASP	CB-CG-OD1	7.21	124.78	118.30
1	A	273	TYR	CB-CG-CD1	7.11	125.27	121.00
1	A	77	ARG	CD-NE-CZ	7.03	133.45	123.60
1	A	393	GLU	OE1-CD-OE2	-6.91	115.01	123.30
1	A	102	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	384	LYS	CG-CD-CE	-6.81	91.48	111.90
1	A	194	LYS	CD-CE-NZ	6.71	127.13	111.70
1	A	112	TYR	CB-CG-CD1	-6.19	117.29	121.00
1	A	141	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	485	TYR	CA-CB-CG	6.07	124.94	113.40
1	A	433	ASP	CB-CG-OD1	6.03	123.72	118.30
1	A	474	ASP	CB-CG-OD1	6.00	123.69	118.30
1	A	458	ASP	CB-CG-OD1	5.93	123.63	118.30
1	A	150	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	A	286	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	357	LYS	CA-CB-CG	5.73	126.00	113.40
1	A	112	TYR	CB-CG-CD2	5.73	124.44	121.00
1	A	12	LYS	CG-CD-CE	5.41	128.13	111.90
1	A	265	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	A	192	LYS	CA-CB-CG	5.33	125.13	113.40
1	A	195	ASN	CA-CB-CG	5.33	125.12	113.40
1	A	369	ASP	CB-CG-OD2	-5.33	113.51	118.30
1	A	299	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	21	SER	O-C-N	5.32	131.22	122.70
1	A	510	LYS	O-C-N	-5.31	114.21	122.70
1	A	299	ARG	CD-NE-CZ	5.28	130.99	123.60
1	A	55	HIS	CA-CB-CG	5.22	122.47	113.60
1	A	340	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	A	430	MET	CA-CB-CG	-5.19	104.47	113.30
1	A	486	VAL	N-CA-CB	5.16	122.86	111.50
1	A	489	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	476	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	458	ASP	CA-CB-CG	5.08	124.58	113.40
1	A	80	ALA	N-CA-CB	5.06	117.18	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	MET	CG-SD-CE	5.06	108.30	100.20

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	4166	0	4077	34	1
2	B	27	0	39	1	0
3	A	8	0	0	0	1
4	A	354	0	0	1	0
4	B	2	0	0	0	0
All	All	4557	0	4116	34	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 (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:HG3	1.56	0.85
1:A:489:ARG:NH1	1:A:498:TYR:OH	2.26	0.69
1:A:302:ILE:HA	1:A:306:VAL:HG13	1.74	0.68
1:A:371:HIS:CG	1:A:413:ARG:HD2	2.32	0.64
1:A:418:ALA:HB3	1:A:504:LEU:HD22	1.85	0.58
1:A:229:GLU:OE1	1:A:369:ASP:HB2	2.03	0.57
1:A:301:ILE:HA	1:A:305:LYS:CG	2.32	0.56
1:A:253:PHE:CD2	1:A:309:GLN:HG2	2.40	0.56
1:A:192:LYS:HE2	1:A:208:PRO:HD2	1.86	0.56
1:A:115:TYR:CE1	1:A:428:ASN:HB3	2.43	0.54
1:A:4:PRO:O	1:A:7:VAL:HG13	2.07	0.54
1:A:453:THR:HB	1:A:462:ARG:HG2	1.90	0.53
1:A:498:TYR:HE1	1:A:507:ILE:HD11	1.75	0.52
1:A:43:LEU:O	1:A:187:THR:HB	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ALA:O	1:A:120:ASN:HB2	2.14	0.47
1:A:32:GLU:HG3	2:B:2:ILE:HD12	1.96	0.47
1:A:335:TRP:CG	1:A:339:LYS:HD3	2.49	0.47
1:A:277:ILE:CG2	1:A:284:PHE:HB3	2.46	0.46
1:A:382:TRP:HB3	1:A:388:VAL:CG2	2.46	0.45
1:A:294:LYS:HA	1:A:480:VAL:HG13	1.98	0.45
1:A:236:TYR:CE2	1:A:492:LYS:HE3	2.53	0.44
1:A:210:TYR:CE2	1:A:212:ASP:HB3	2.52	0.44
1:A:244:THR:HG23	1:A:490:LEU:HB2	2.00	0.43
1:A:236:TYR:HA	1:A:241:ILE:HB	2.00	0.43
1:A:280:GLN:HG3	1:A:440:HIS:HB3	2.01	0.43
1:A:215:LYS:HD2	4:A:779:HOH:O	2.19	0.43
1:A:321:TYR:N	1:A:321:TYR:CD1	2.87	0.42
1:A:115:TYR:CD1	1:A:428:ASN:HB3	2.54	0.42
1:A:258:LYS:HA	1:A:258:LYS:HD3	1.64	0.42
1:A:498:TYR:CE1	1:A:507:ILE:HD11	2.54	0.41
1:A:395:GLN:HE21	1:A:400:PHE:HA	1.84	0.41
1:A:502:ASP:HA	1:A:503:PRO:HD2	1.98	0.41
1:A:161:HIS:HA	1:A:162:PRO:HD3	1.96	0.41
1:A:365:TYR:CZ	1:A:394:ASN:HB3	2.56	0.41

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:IUM:U[1_556]	1.91	0.29

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	516/517 (100%)	499 (97%)	16 (3%)	1 (0%)	52 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1/3 (33%)	1 (100%)	0	0	100	100
All	All	517/520 (99%)	500 (97%)	16 (3%)	1 (0%)	52	48

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	456/455 (100%)	444 (97%)	12 (3%)	54	54
2	B	3/3 (100%)	3 (100%)	0	100	100
All	All	459/458 (100%)	447 (97%)	12 (3%)	54	54

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

Mol	Chain	Res	Type
1	A	63	LYS
1	A	67	LYS
1	A	225	PRO
1	A	281	LYS
1	A	305	LYS
1	A	306	VAL
1	A	321	TYR
1	A	334	LYS
1	A	338	GLN
1	A	357	LYS
1	A	413	ARG
1	A	458	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	199	ASN
1	A	304	ASN
1	A	395	GLN
1	A	406	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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 [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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.