wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2023 – 11:42 AM EDT

PDB ID	:	1OOA
Title	:	CRYSTAL STRUCTURE OF NF-kB(p50)2 COMPLEXED TO A HIGH-AFFINITY RNA APTAMER
Authors	:	Huang, D.B.; Vu, D.; Cassiday, L.A.; Zimmerman, J.M.; Maher III, L.J.; Ghosh, G.
Deposited on	:	2003-03-03
Resolution	:	2.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

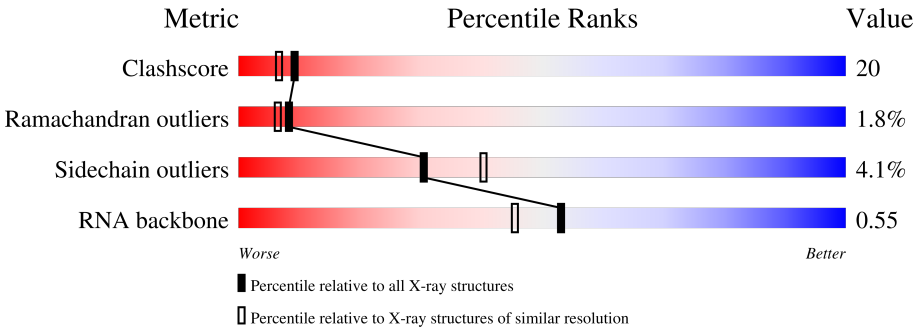
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.45 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	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RNA backbone	3102	1001 (2.80-2.12)

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	C	29	31% 31% 28% 10%
1	D	29	38% 34% 24% .
2	A	326	70% 25% . .
2	B	326	64% 30% . .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6442 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 RNA chain called RNA aptamer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	29	Total	C	N	O	P	0	0	0
			617	277	110	202	28			
1	D	29	Total	C	N	O	P	0	0	0
			617	277	110	202	28			

- Molecule 2 is a protein called Nuclear factor NF-kappa-B p105 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	313	Total	C	N	O	S	0	0	0
			2457	1556	429	460	12			
2	B	313	Total	C	N	O	S	0	0	0
			2457	1556	429	460	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLY	-	cloning artifact	UNP P25799
B	38	GLY	-	cloning artifact	UNP P25799

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	33	Total	O	0	0
			33	33		
3	D	11	Total	O	0	0
			11	11		
3	A	157	Total	O	0	0
			157	157		
3	B	93	Total	O	0	0
			93	93		

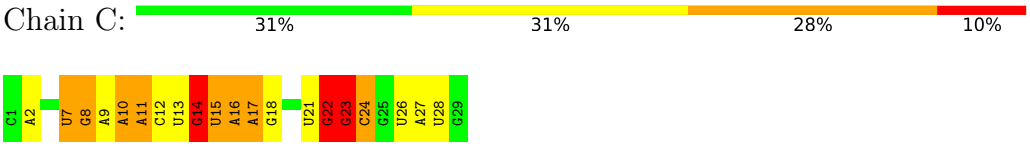
3 Residue-property plots (i)

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: RNA aptamer

Chain C:

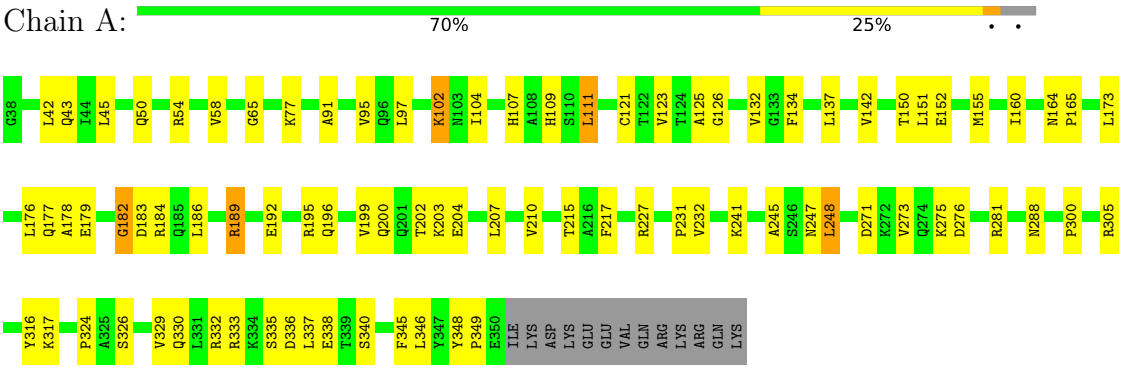


• Molecule 1: RNA aptamer

Chain D:

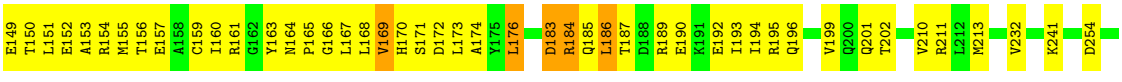
• Molecule 2: Nuclear factor NF-kappa-B p105 subunit

Chain A:



• Molecule 2: Nuclear factor NF-kappa-B p105 subunit

Chain B:




V260
Y267
L268
D271
K272
V273
Q279
E285
N288
G289
G290
F295
F307
P314
K315
Y316
K317
D318
V319
N320
I321
T322
K323
V329
R332
R333
D336
F345
E350
ILE
LYS
ASP
LYS
GLU
GLU
VAL
GLN
ARG
LYS
ARG
GLN
LYS

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	76.75Å 151.06Å 95.63Å 90.00° 105.95° 90.00°	Depositor
Resolution (Å)	28.99 – 2.45	Depositor
% Data completeness (in resolution range)	86.7 (28.99-2.45)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.208 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6442	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	C	0.43	0/690	0.84	2/1074 (0.2%)
1	D	0.32	0/690	0.70	0/1074
2	A	0.40	0/2509	0.65	0/3389
2	B	0.37	0/2509	0.61	0/3389
All	All	0.38	0/6398	0.67	2/8926 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	22	G	N9-C1'-C2'	6.34	122.25	114.00
1	C	14	G	N9-C1'-C2'	5.13	120.67	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	23	G	Sidechain
1	D	23	G	Sidechain

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	C	617	0	312	30	0
1	D	617	0	312	49	0
2	A	2457	0	2454	68	0
2	B	2457	0	2454	93	0
3	A	157	0	0	7	0
3	B	93	0	0	1	0
3	C	33	0	0	0	0
3	D	11	0	0	1	0
All	All	6442	0	5532	231	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 20.

The worst 5 of 231 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:C:23:G:H4'	1:C:24:C:OP1	1.62	0.98
2:A:107:HIS:HD2	2:A:109:HIS:H	1.15	0.94
1:C:17:A:H2'	1:C:18:G:O4'	1.71	0.91
2:B:107:HIS:HD2	2:B:109:HIS:H	1.19	0.90
1:D:15:U:H3	2:B:63:SER:HB2	1.36	0.90

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
2	A	311/326 (95%)	288 (93%)	17 (6%)	6 (2%)	8 6
2	B	311/326 (95%)	278 (89%)	28 (9%)	5 (2%)	9 8
All	All	622/652 (95%)	566 (91%)	45 (7%)	11 (2%)	8 6

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	178	ALA
2	A	335	SER
2	B	172	ASP
2	A	126	GLY
2	A	288	ASN

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
2	A	268/281 (95%)	258 (96%)	10 (4%)	34 45
2	B	268/281 (95%)	256 (96%)	12 (4%)	27 36
All	All	536/562 (95%)	514 (96%)	22 (4%)	30 40

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	136	ASN
2	B	176	LEU
2	B	167	LEU
2	B	183	ASP
2	A	248	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	136	ASN

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Mol	Chain	Res	Type
2	B	279	GLN
2	A	247	ASN
2	B	86	ASN
2	B	100	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	28/29 (96%)	7 (25%)	5 (17%)
1	D	28/29 (96%)	5 (17%)	4 (14%)
All	All	56/58 (96%)	12 (21%)	9 (16%)

5 of 12 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	8	G
1	C	11	A
1	C	14	G
1	C	16	A
1	C	17	A

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	15	U
1	D	23	G
1	C	22	G
1	C	23	G
1	D	7	U

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.