wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 06:18 PM GMT

PDB ID	:	1A3Q
Title	:	HUMAN NF-KAPPA-B P52 BOUND TO DNA
Authors	:	Cramer, P.; Larson, C.J.; Verdine, G.L.; Muller, C.W.
Deposited on	:	1998-01-23
Resolution	:	2.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

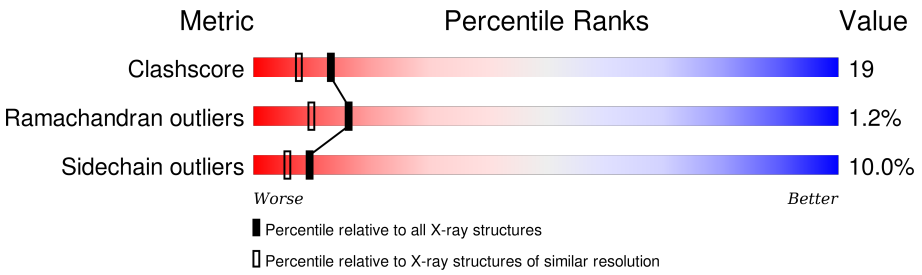
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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 <=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	C	11	91% 9%
2	D	11	45% 55%
3	A	285	60% 36% .
3	B	285	57% 37% . .

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5748 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 DNA chain called DNA (5'-D(*GP*GP*GP*GP*AP*AP*TP*CP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	11	223	106	44	63	10	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*GP*GP*GP*AP*TP*TP*CP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	11	222	106	41	65	10	0	0	0

- Molecule 3 is a protein called PROTEIN (NUCLEAR FACTOR KAPPA-B P52).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	285	2259	1423	409	415	12	0	0	0
3	B	285	2259	1423	409	415	12	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	ILE	THR	CONFLICT	UNP Q00653
B	213	ILE	THR	CONFLICT	UNP Q00653

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	377	377	377	0	0
4	B	335	335	335	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	32	Total O 32 32	0	0
4	D	41	Total O 41 41	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.

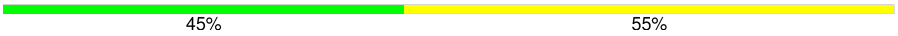
Note EDS was not executed.

- Molecule 1: DNA (5'-D(*GP*GP*GP*GP*AP*AP*TP*CP*CP*CP*C)-3')

Chain C:

- Molecule 2: DNA (5'-D(*GP*GP*GP*GP*AP*TP*TP*CP*CP*CP*C)-3')

Chain D:

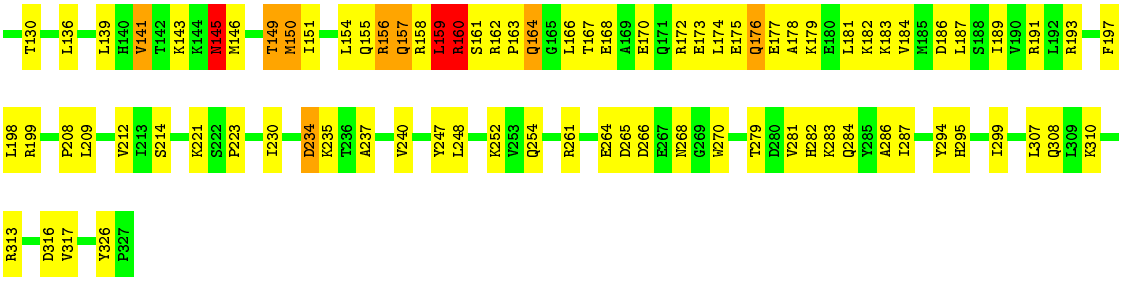


- Molecule 3: PROTEIN (NUCLEAR FACTOR KAPPA-B P52)

Chain A:

- Molecule 3: PROTEIN (NUCLEAR FACTOR KAPPA-B P52)

Chain B:


T130
L136
L139
H140
V141
T142
K143
K144
M145
M146
T149
M150
I151
L154
Q155
R156
Q157
R158
L159
R160
S161
R162
P163
Q164
G165
L166
T167
E168
A169
E170
Q171
R172
E173
L174
E175
Q176
E177
A178
K179
E180
L181
K182
K183
V184
M185
D186
L187
S188
I189
V190
R191
L192
R193
F197
L198
R199
P208
L209
V212
I213
S214
K221
S222
P223
I230
D234
K235
T236
A237
V240
Y247
L248
K252
V253
Q254
R261
E264
D265
D266
E267
N268
G269
W270
T279
D280
V281
H282
K283
Q284
Y285
A286
I287
Y294
H295
I299
L307
Q308
L309
K310
R313
D316
V317
Y326
P327

4 Data and refinement statistics (i)

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	44.20Å 121.00Å 134.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10	Depositor
% Data completeness (in resolution range)	91.8 (10.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	6.10	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.219 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5748	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	0.86	0/250	1.04	0/384
2	D	0.89	0/248	1.13	2/381 (0.5%)
3	A	0.60	0/2307	0.89	2/3104 (0.1%)
3	B	0.63	0/2307	0.91	6/3104 (0.2%)
All	All	0.65	0/5112	0.92	10/6973 (0.1%)

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
2	D	0	1
3	A	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	164	GLN	N-CA-C	7.45	131.12	111.00
3	B	117	LEU	CB-CG-CD1	-7.38	98.46	111.00
3	B	164	GLN	N-CA-C	6.82	129.42	111.00
3	A	117	LEU	CB-CG-CD1	-6.44	100.05	111.00
2	D	605	DG	O5'-C5'-C4'	5.79	125.47	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	263	TYR	Sidechain
2	D	614	DC	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	223	0	124	2	0
2	D	222	0	125	3	0
3	A	2259	0	2279	87	0
3	B	2259	0	2279	95	0
4	A	377	0	0	12	0
4	B	335	0	0	8	0
4	C	32	0	0	0	0
4	D	41	0	0	2	0
All	All	5748	0	4807	185	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 19.

The worst 5 of 185 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)
3:B:117:LEU:HD11	3:B:156:ARG:HD2	1.14	1.14
3:B:117:LEU:CD1	3:B:156:ARG:HD2	2.04	0.84
3:A:102:PRO:HG3	3:A:213:ILE:HD11	1.62	0.82
3:A:218:HIS:HB3	3:A:225:ALA:HB1	1.60	0.82
3:A:162:ARG:HB3	3:A:163:PRO:HD2	1.63	0.80

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
3	A	281/285 (99%)	250 (89%)	29 (10%)	2 (1%)	26 21
3	B	281/285 (99%)	252 (90%)	24 (8%)	5 (2%)	11 5
All	All	562/570 (99%)	502 (89%)	53 (9%)	7 (1%)	16 10

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	87	GLY
3	B	125	GLY
3	A	125	GLY
3	B	116	GLU
3	B	145	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
3	A	249/249 (100%)	226 (91%)	23 (9%)	11 7
3	B	249/249 (100%)	222 (89%)	27 (11%)	8 4
All	All	498/498 (100%)	448 (90%)	50 (10%)	9 6

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	313	ARG
3	B	103	ARG
3	B	268	ASN
3	B	72	LYS
3	B	79	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	322	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	84	ASN
3	B	157	GLN
3	A	295	HIS
3	B	176	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)

There are no ligands in this entry.

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 will therefore be empty.

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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