



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 06:23 pm GMT

PDB ID : 3DO7
Title : X-ray structure of a NF-kB p52/RelB/DNA complex
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Deposited on : 2008-07-03
Resolution : 3.05 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

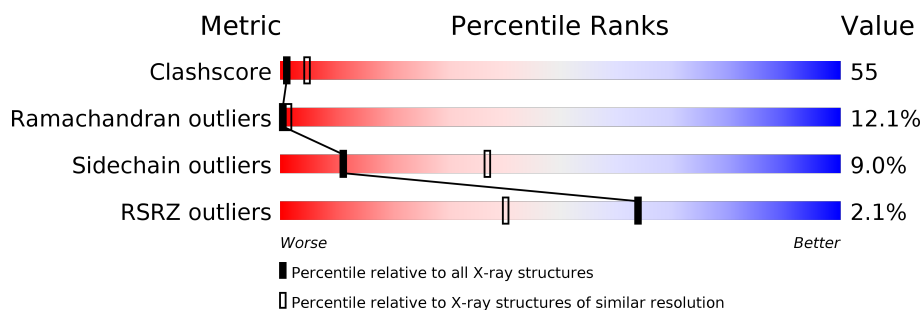
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	1462 (3.10-3.02)
Ramachandran outliers	110173	1410 (3.10-3.02)
Sidechain outliers	110143	1410 (3.10-3.02)
RSRZ outliers	101464	1355 (3.10-3.02)

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.

Mol	Chain	Length	Quality of chain
1	C	11	
1	D	11	
1	E	11	
2	A	296	
3	B	293	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5288 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 5'-D(*DCP*DGP*DGP*DGP*DAP*DAP*DTP*DTP*DCP*DCP*DC)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	10	Total	C	N	O	P	0	0	0
			202	97	38	58	9			
1	D	11	Total	C	N	O	P	0	0	0
			221	106	41	64	10			
1	E	11	Total	C	N	O	P	0	0	0
			221	106	41	64	10			

- Molecule 2 is a protein called Avian reticuloendotheliosis viral (V-rel) oncogene related B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	296	Total	C	N	O	S	0	0	0
			2327	1449	420	442	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	GLN	LEU	CONFLICT	UNP Q8VE46

- Molecule 3 is a protein called Nuclear factor NF-kappa-B p100 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	293	Total	C	N	O	S	0	0	0
			2268	1424	406	426	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	200	ASP	ALA	CONFLICT	UNP Q00653

- Molecule 4 is water.

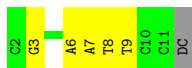
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total 18	O 18	0	0
4	B	23	Total 23	O 23	0	0
4	C	1	Total 1	O 1	0	0
4	D	3	Total 3	O 3	0	0
4	E	4	Total 4	O 4	0	0

3 Residue-property plots

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.

- Molecule 1: 5'-D(*DCP*DGP*DGP*DGP*DAP*DAP*DTP*DTP*DCP*DCP*DC)-3'

Chain C: 




- Molecule 1: 5'-D(*DCP*DGP*DGP*DGP*DAP*DAP*DTP*DTP*DCP*DCP*DC)-3'

Chain D: 



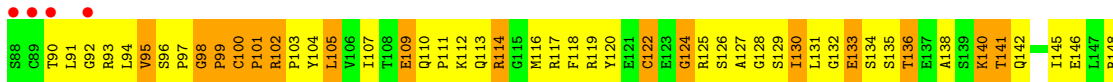
- Molecule 1: 5'-D(*DCP*DGP*DGP*DGP*DAP*DAP*DTP*DTP*DCP*DCP*DC)-3'

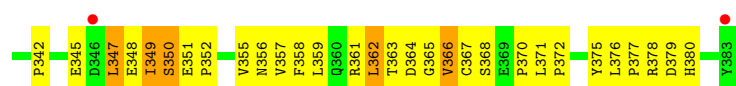
Chain E: 



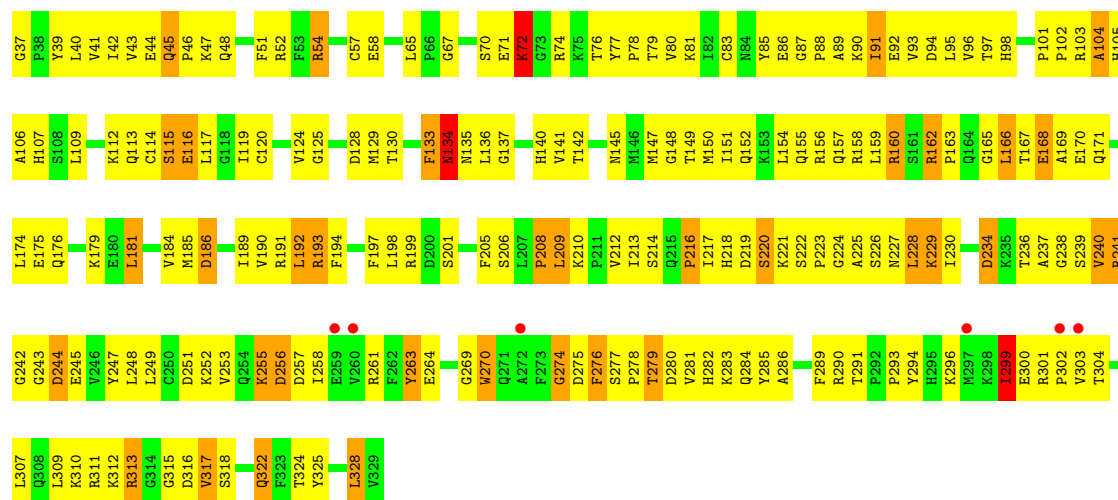
- Molecule 2: Avian reticuloendotheliosis viral (V-rel) oncogene related B

Chain A: 





● Molecule 3: Nuclear factor NF-kappa-B p100 subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	77.64Å 124.13Å 189.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.19 – 3.05 34.07 – 3.05	Depositor EDS
% Data completeness (in resolution range)	81.4 (29.19-3.05) 87.7 (34.07-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 3.06Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.273 0.242 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	80.9	Xtriage
Anisotropy	0.751	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 68.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5288	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0/226	0.78	0/347
1	D	0.44	0/247	0.72	0/379
1	E	0.51	0/247	1.02	1/379 (0.3%)
2	A	0.30	0/2378	0.55	0/3224
3	B	0.31	0/2315	0.58	0/3124
All	All	0.33	0/5413	0.61	1/7453 (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	E	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3	DG	O4'-C1'-N9	5.13	111.59	108.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	10	DC	Sidechain
1	E	3	DG	Sidechain
1	E	7	DA	Sidechain
1	E	8	DT	Sidechain
1	E	9	DT	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	202	0	114	12	0
1	D	221	0	125	13	0
1	E	221	0	125	15	0
2	A	2327	0	2282	292	0
3	B	2268	0	2248	245	0
4	A	18	0	0	2	0
4	B	23	0	0	0	0
4	C	1	0	0	0	0
4	D	3	0	0	2	0
4	E	4	0	0	0	0
All	All	5288	0	4894	561	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 55.

The worst 5 of 561 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)
2:A:127:ALA:HB1	2:A:202:ASN:HB3	1.41	1.01
2:A:361:ARG:HG2	2:A:363:THR:HG22	1.40	1.00
3:B:93:VAL:HG12	3:B:194:PHE:HA	1.42	0.99
2:A:292:PRO:HB2	2:A:294:THR:HG22	1.45	0.97
3:B:299:ILE:HD13	3:B:299:ILE:H	1.27	0.96

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	294/296 (99%)	187 (64%)	71 (24%)	36 (12%)	0	1
3	B	291/293 (99%)	187 (64%)	69 (24%)	35 (12%)	0	1
All	All	585/589 (99%)	374 (64%)	140 (24%)	71 (12%)	0	1

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	99	PRO
2	A	133	GLU
2	A	164	TRP
2	A	193	HIS
2	A	194	VAL

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	
2	A	262/265 (99%)	237 (90%)	25 (10%)	10	34
3	B	247/256 (96%)	226 (92%)	21 (8%)	12	41
All	All	509/521 (98%)	463 (91%)	46 (9%)	11	37

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	309	GLU
3	B	45	GLN
3	B	299	ILE
2	A	311	ILE
2	A	326	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	45	GLN
3	B	113	GLN
3	B	271	GLN
3	B	48	GLN
2	A	206	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](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	C	10/11 (90%)	-0.21	0	100	100	38, 49, 78, 80	0
1	D	11/11 (100%)	-0.46	0	100	100	38, 56, 68, 75	0
1	E	11/11 (100%)	-0.51	0	100	100	54, 66, 90, 133	0
2	A	296/296 (100%)	-0.19	7 (2%)	59	34	42, 105, 137, 141	0
3	B	293/293 (100%)	-0.33	6 (2%)	65	42	45, 103, 137, 141	0
All	All	621/622 (99%)	-0.27	13 (2%)	64	40	38, 102, 137, 141	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	89	CYS	4.7
2	A	250	ALA	4.1
3	B	272	ALA	3.4
2	A	88	SER	3.3
2	A	92	GLY	3.3

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.