wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:07 PM GMT

PDB ID	:	1NKP
Title	:	Crystal structure of Myc-Max recognizing DNA
Authors	:	Nair, S.K.; Burley, S.K.
Deposited on	:	2003-01-03
Resolution	:	1.80 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:

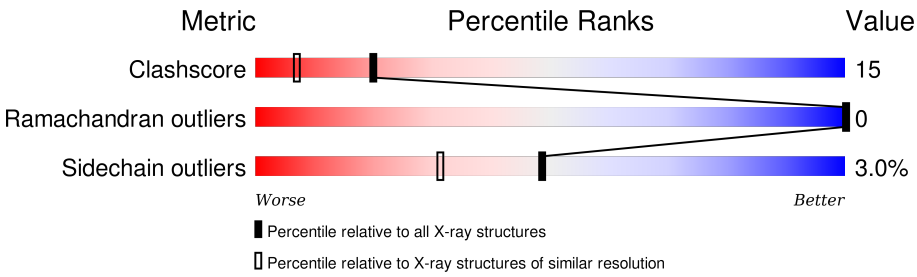
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.80 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	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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	F	19	74% 21% 5%
1	G	19	84% 16%
1	H	19	79% 21%
1	J	19	79% 21%
2	A	88	60% 39% •
2	D	88	63% 32% 6%
3	B	83	71% 27% •

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Mol	Chain	Length	Quality of chain
3	E	83	73% 24%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4906 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(*CP*GP*AP*GP*TP*AP*GP*CP*AP*CP*GP*TP*GP*CP*TP*AP*CP*TP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	F	19	385	184	71	112	18	0	0	0
1	G	19	385	184	71	112	18	0	0	0
1	H	19	385	184	71	112	18	0	0	0
1	J	19	385	184	71	112	18	0	0	0

- Molecule 2 is a protein called Myc proto-oncogene protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	88	733	455	145	131	2	0	0	0
2	D	83	705	440	138	126	1	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	897	GLY	-	CLONING ARTIFACT	UNP P01106
A	898	HIS	-	CLONING ARTIFACT	UNP P01106
A	899	MET	-	CLONING ARTIFACT	UNP P01106
A	982	GLY	-	INSERTION	UNP P01106
A	983	GLY	-	INSERTION	UNP P01106
A	984	CYS	-	INSERTION	UNP P01106
D	497	GLY	-	CLONING ARTIFACT	UNP P01106
D	498	HIS	-	CLONING ARTIFACT	UNP P01106
D	499	MET	-	CLONING ARTIFACT	UNP P01106
D	582	GLY	-	INSERTION	UNP P01106
D	583	GLY	-	INSERTION	UNP P01106

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Chain	Residue	Modelled	Actual	Comment	Reference
D	584	CYS	-	INSERTION	UNP P01106

- Molecule 3 is a protein called Max protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	83	686	414	143	127	2	0	0	0
			Total	C	N	O	S			
3	E	81	661	399	139	121	2	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	282	GLY	-	INSERTION	UNP P61244
B	283	GLY	-	INSERTION	UNP P61244
B	284	CYS	-	INSERTION	UNP P61244
E	782	GLY	-	INSERTION	UNP P61244
E	783	GLY	-	INSERTION	UNP P61244
E	784	CYS	-	INSERTION	UNP P61244

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	91	91	91	0	0
			Total	O		
4	B	75	75	75	0	0
			Total	O		
4	D	82	82	82	0	0
			Total	O		
4	E	79	79	79	0	0
			Total	O		
4	F	62	62	62	0	0
			Total	O		
4	G	67	67	67	0	0
			Total	O		
4	H	60	60	60	0	0
			Total	O		
4	J	65	65	65	0	0

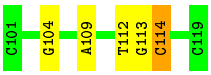
3 Residue-property plots (i)

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.

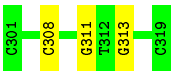
• Molecule 1: 5'-D(*CP*GP*AP*GP*TP*AP*GP*CP*AP*CP*GP*TP*GP*CP*TP*AP*CP*TP*C)-3'

Chain F: 74% 21% 5%



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

Chain G: 84% 16%



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

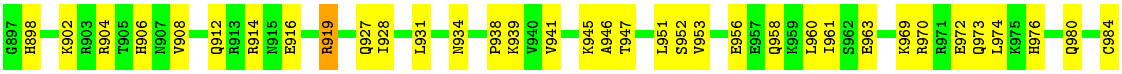
Chain H: 79% 21%

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

Chain J: 79% 21%

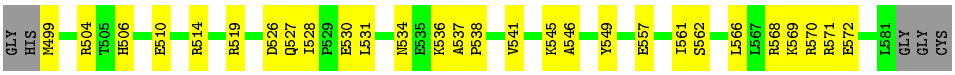
• Molecule 2: Myc proto-oncogene protein

Chain A: 60% 39%



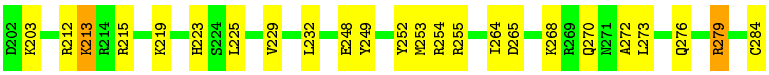
- Molecule 2: Myc proto-oncogene protein

Chain D:



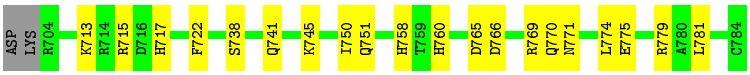
- Molecule 3: Max protein

Chain B:



- Molecule 3: Max protein

Chain E:



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 1	Depositor
Cell constants a, b, c, α, β, γ	39.24Å 45.13Å 86.48Å 87.91° 84.61° 71.50°	Depositor
Resolution (Å)	20.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4906	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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	F	0.41	0/431	0.77	0/663
1	G	0.37	0/431	0.75	0/663
1	H	0.37	0/431	0.74	0/663
1	J	0.38	0/431	0.72	0/663
2	A	0.31	0/740	0.48	0/985
2	D	0.31	0/711	0.48	0/947
3	B	0.30	0/695	0.49	0/927
3	E	0.30	0/670	0.47	0/896
All	All	0.34	0/4540	0.61	0/6407

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	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	114	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	F	385	0	215	5	0
1	G	385	0	215	3	0
1	H	385	0	215	5	0
1	J	385	0	215	3	0
2	A	733	0	771	39	0
2	D	705	0	750	33	0
3	B	686	0	681	31	0
3	E	661	0	649	20	0
4	A	91	0	0	6	0
4	B	75	0	0	6	0
4	D	82	0	0	12	0
4	E	79	0	0	6	0
4	F	62	0	0	2	0
4	G	67	0	0	0	0
4	H	60	0	0	3	0
4	J	65	0	0	0	0
All	All	4906	0	3711	119	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 15.

The worst 5 of 119 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:908:VAL:HB	4:A:287:HOH:O	1.51	1.08
2:A:927:GLN:HE21	3:B:254:ARG:NH2	1.52	1.06
2:A:927:GLN:HE21	3:B:254:ARG:HH22	1.09	0.93
2:D:534:ASN:ND2	2:D:537:ALA:HB2	1.89	0.88
3:B:229:VAL:HG21	3:B:232:LEU:HD12	1.61	0.82

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	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
2	D	81/88 (92%)	80 (99%)	1 (1%)	0	100	100
3	B	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
3	E	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
All	All	327/342 (96%)	317 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	80/80 (100%)	78 (98%)	2 (2%)	55	39
2	D	78/80 (98%)	76 (97%)	2 (3%)	54	37
3	B	73/73 (100%)	70 (96%)	3 (4%)	37	19
3	E	69/73 (94%)	67 (97%)	2 (3%)	50	34
All	All	300/306 (98%)	291 (97%)	9 (3%)	48	31

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	279	ARG
3	E	774	LEU
2	D	570	ARG
3	B	213	LYS
2	D	526	ASP

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

Mol	Chain	Res	Type
2	D	506	HIS
2	D	507	ASN
3	E	708	ASN
2	A	980	GLN
3	E	760	HIS

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.