



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:03 PM GMT

PDB ID : 1NB7
Title : HC-J4 RNA polymerase complexed with short RNA template strand
Authors : O'Farrell, D.J.; Trowbridge, R.; Rowlands, D.J.; Jaeger, J.
Deposited on : 2002-12-02
Resolution : 2.90 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
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

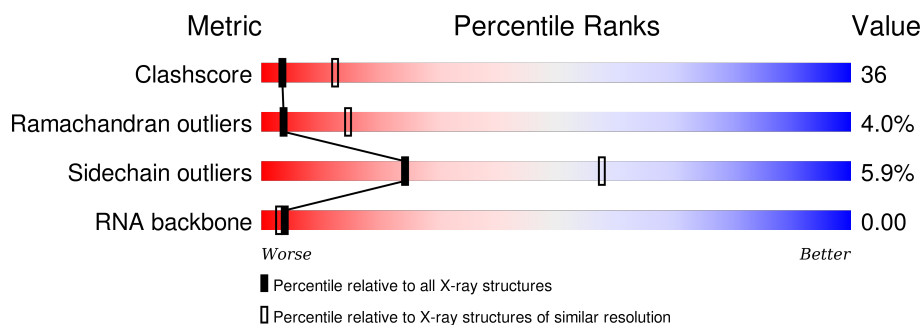
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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	E	4	<div> <div>75%</div> <div>25%</div> </div>
1	F	4	<div> <div>75%</div> <div>25%</div> </div>
2	A	570	<div> <div>44%</div> <div>51%</div> <div>5% •</div> </div>
2	B	570	<div> <div>44%</div> <div>50%</div> <div>5% •</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8927 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 5'-R(*UP*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			
1	F	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			

- Molecule 2 is a protein called polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	566	Total	C	N	O	S	0	0	0
			4388	2763	777	816	32			
2	B	565	Total	C	N	O	S	0	0	0
			4381	2758	776	815	32			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mn	0	0
			2	2		
3	A	2	Total	Mn	0	0
			2	2		

D546
L547
S548
G549
W550
F551
S556
G557
L560
Y561
H562
S563
L564
S565
R566
ALA
ARG
PRO
ARG

• Molecule 2: polypeptide

Chain B:  44% 50% 5%

K533	I462	P388	V315	T227	Q148	V78	S1
L463	L463	T389	N316	S231	P149	K79	M2
K535	E464	T390	G317	S231	E150	A80	S3
P540	L465	P391	D318	D232	K151	K81	Y4
	A541	L392	D319	L233	G152	L82	T5
A542	H467	A395	L320	R234	G153	L83	M6
S543	S476	R394	V321	V235	P156	E86	T7
Q544	P479	E398	V322	E237	A157	E87	L10
L545		R401	E325	S238	R158	A88	I11
D546	E480	H402	T329	I239	L159	C90	T12
L547	E481	T403	Q330	A249	I160	L91	P13
S548	L482	P404	E331	I253	V167	T92	C14
W550	R483	L405	D332		R168	P93	E18
Y555	V485	N406	A333	R254	V169	P94	L21
	A486	S407	A334	S255	G170	H95	P22
S556	S487	H408	A335	L256	E171	S96	T23
G557	C488	L409	L336	T257	K172	A97	P25
G558	L489	Y415	R337	E258	Y176	K98	R28
D559	R490	A416	A338	R259	D177	F101	S27
I560	V494	P417	F339	L260	V178	L26	L26
Y661	P495	L496	T340	Y261	V179	A104	S29
L564	P496		Y346	G263	L182	A105	G104
S565	L497	R422	S347	G264	L187	D107	V37
ALA	R498	N423	P350	T267	M187	V108	X38
ARG	T499	L424	G351	N268	Y191	R109	A39
ARC	W500	L425	P354	S269	G192	N110	S42
PRO	R501	L426	Q355	K270	L111	L111	
ARG	H502	T427	Q356	G271	F193	S112	S44
S506	V507	L432	E357	C274	Y195	R114	A45
							S196
V508	L433	L434	Y358	G275	S197	A115	L47
A509	A435	A436	D359	Y276	P197	V116	R48
K510	Q436	Q436	L360	R277	K198	N117	Q49
L511	E437	E437	L362	C278	Q199	H118	K50
L512	Q438	Q438	L363	R279	R200	I119	V51
S513	L439	L439	T364	A281	V201	V122	V52
Q514	E440	E440	S365	S282	E202	L26	D55
S515	G516	A442	C366	G283	L204	L130	R56
R517	R516	A442	S367	V284	N206	E131	L57
A518	L443	L443	S368	T287	K211	T132	O58
A519	C445	C445	R369	S288	K212	P133	V59
T520	Q446	Q446	V370	C289	I134	D135	L60
C521	L447	L447	S371	T292	G215	D81	Y64
G522	A450	A450	A373	Y296	I138	R65	R65
R523			H374	Y219	K141	L68	
Y524	L454	L454	G378	L308	D220	E142	L68
F526	E455	P456	Y382	Q309	T221	S142	K74
N527	L457	L457	X382	D310	R222	V144	A75
A529	D458	D458	L384	C311	C223	F145	S76
V530	L459	L459	T385	T312	F224	C146	T77
R531	R530	R530	R386	M313	D225	V416	S77
T532	Q461	Q461	D387	L314	C326	U412	

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	106.66Å 108.50Å 134.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (22.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8927	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	E	1.39	0/84	1.33	2/128 (1.6%)
1	F	1.23	0/84	1.44	1/128 (0.8%)
2	A	0.49	0/4484	0.74	1/6087 (0.0%)
2	B	0.52	1/4477 (0.0%)	0.73	0/6077
All	All	0.53	1/9129 (0.0%)	0.75	4/12420 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	142	SER	CB-OG	7.89	1.52	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	3	U	O4'-C1'-N1	7.28	114.03	108.20
1	E	4	U	C2'-C3'-O3'	5.29	122.17	113.70
2	A	351	GLY	N-CA-C	-5.12	100.29	113.10
1	E	4	U	N1-C1'-C2'	5.03	120.53	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	4	U	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	E	77	0	42	22	0
1	F	77	0	42	23	0
2	A	4388	0	4383	326	0
2	B	4381	0	4374	302	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
All	All	8927	0	8841	641	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 36.

The worst 5 of 641 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:B:515:GLY:HA2	2:B:519:ALA:HB2	1.33	1.06
2:B:144:VAL:HG22	2:B:394:ARG:HG2	1.35	1.03
2:B:160:ILE:HD12	2:B:282:SER:HG	1.27	1.00
1:F:1:U:HO5'	1:F:1:U:H6	1.03	1.00
2:A:195:TYR:HB3	2:A:199:GLN:HB2	1.43	1.00

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	564/570 (99%)	466 (83%)	74 (13%)	24 (4%)	3	13
2	B	563/570 (99%)	466 (83%)	76 (14%)	21 (4%)	4	17
All	All	1127/1140 (99%)	932 (83%)	150 (13%)	45 (4%)	4	15

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	23	ILE
2	A	505	ARG
2	A	565	SER
2	B	109	ARG
2	B	113	SER

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	475/485 (98%)	450 (95%)	25 (5%)	28	63
2	B	474/485 (98%)	443 (94%)	31 (6%)	21	52
All	All	949/970 (98%)	893 (94%)	56 (6%)	24	58

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	29	SER
2	B	98	LYS
2	B	513	SER
2	B	55	ASP
2	B	68	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	483	ASN
2	A	514	GLN
2	B	483	ASN
2	A	502	HIS
2	B	24	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	4/4 (100%)	3 (75%)	3 (75%)
1	F	4/4 (100%)	3 (75%)	3 (75%)
All	All	8/8 (100%)	6 (75%)	6 (75%)

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	2	U
1	E	3	U
1	E	4	U
1	F	2	U
1	F	3	U

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	E	3	U
1	F	3	U
1	F	1	U
1	E	2	U
1	F	2	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - 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

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 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.