



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2018 – 11:05 PM EST

PDB ID : 5Y7Q
Title : Crystal structure of Nuclease
Authors : Jin, H.; Cho, Y.
Deposited on : 2017-08-17
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : rb-20030736
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) : rb-20030736

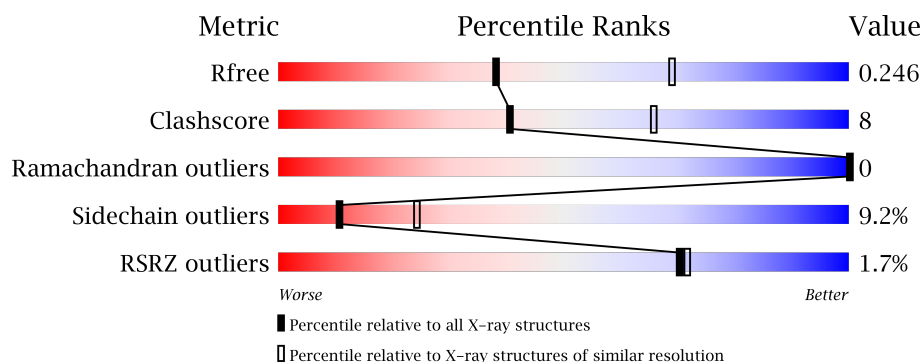
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
R_{free}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	A	580	<div> <div>2%</div> <div>75%</div> <div>17%</div> <div>6%</div> </div>
2	D	10	<div> <div>10%</div> <div>60%</div> <div>40%</div> </div>
3	B	13	<div> <div>8%</div> <div>46%</div> <div>46%</div> </div>
4	C	24	<div> <div>50%</div> <div>29%</div> <div>21%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5187 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 protein called Fanconi-associated nuclease 1 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	546	Total	C	N	O	S	0	0	0
			4444	2841	803	780	20			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q9I2N0
A	-19	GLY	-	expression tag	UNP Q9I2N0
A	-18	SER	-	expression tag	UNP Q9I2N0
A	-17	SER	-	expression tag	UNP Q9I2N0
A	-16	HIS	-	expression tag	UNP Q9I2N0
A	-15	HIS	-	expression tag	UNP Q9I2N0
A	-14	HIS	-	expression tag	UNP Q9I2N0
A	-13	HIS	-	expression tag	UNP Q9I2N0
A	-12	HIS	-	expression tag	UNP Q9I2N0
A	-11	HIS	-	expression tag	UNP Q9I2N0
A	-10	SER	-	expression tag	UNP Q9I2N0
A	-9	SER	-	expression tag	UNP Q9I2N0
A	-8	GLY	-	expression tag	UNP Q9I2N0
A	-7	LEU	-	expression tag	UNP Q9I2N0
A	-6	VAL	-	expression tag	UNP Q9I2N0
A	-5	PRO	-	expression tag	UNP Q9I2N0
A	-4	ARG	-	expression tag	UNP Q9I2N0
A	-3	GLY	-	expression tag	UNP Q9I2N0
A	-2	SER	-	expression tag	UNP Q9I2N0
A	-1	HIS	-	expression tag	UNP Q9I2N0
A	0	MET	-	expression tag	UNP Q9I2N0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	10	Total	C	N	O	P	0	0	0
			211	100	38	63	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	7	Total	C	N	O	P	0	0	0
			141	68	25	41	7			

- Molecule 4 is a DNA chain called DNA (5'-D(P*GP*AP*AP*TP*GP*TP*GP*TP*GP*TP*CP*TP*CP*AP*AP*TP*CP*CP*CP*AP*AP*CP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	19	Total	C	N	O	P	0	0	0
			382	182	68	113	19			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		
5	D	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.84Å 104.56Å 105.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.71 – 2.70 40.42 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.1 (33.71-2.70) 98.8 (40.42-2.49)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.10.1-2155_1069: ???)	Depositor
R, R_{free}	0.193 , 0.243 0.195 , 0.246	Depositor DCC
R_{free} test set	1246 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	77.3	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5187	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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 [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	A	0.47	0/4562	0.63	2/6180 (0.0%)
2	D	0.93	0/236	1.03	0/364
3	B	0.75	0/157	1.14	0/239
4	C	0.91	0/426	1.07	0/650
All	All	0.55	0/5381	0.73	2/7433 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	LEU	CB-CG-CD2	-5.92	100.94	111.00
1	A	166	LEU	CA-CB-CG	5.23	127.33	115.30

There are no chirality outliers.

There are no planarity outliers.

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	A	4444	0	4340	67	0
2	D	211	0	115	3	0
3	B	141	0	80	6	0
4	C	382	0	210	8	0
5	A	8	0	0	0	0
5	D	1	0	0	0	0
All	All	5187	0	4745	81	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 8.

All (81) 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:A:510:GLN:HE22	1:A:519:ARG:HH21	1.22	0.87
3:B:12:DC:H2''	3:B:13:DA:H5'	1.68	0.75
4:C:20:DA:H2''	4:C:21:DA:H5''	1.69	0.75
1:A:291:ARG:HD3	1:A:314:ALA:HB2	1.74	0.69
1:A:443:ASP:N	1:A:443:ASP:OD1	2.25	0.68
1:A:390:ILE:HD12	1:A:505:LEU:HD23	1.76	0.68
1:A:279:GLN:HG3	1:A:298:LEU:HG	1.77	0.67
1:A:116:LYS:HB2	1:A:119:GLU:HG3	1.77	0.65
1:A:73:LEU:HD11	1:A:110:GLN:HE21	1.62	0.65
1:A:39:ASP:OD2	1:A:210:ARG:NH2	2.30	0.65
1:A:510:GLN:NE2	1:A:519:ARG:HH21	1.95	0.65
1:A:363:GLU:HB3	1:A:364:PRO:HD2	1.79	0.64
1:A:174:ARG:NH2	1:A:219:ASP:OD1	2.21	0.64
1:A:220:ALA:HB3	1:A:254:LEU:HD21	1.79	0.62
1:A:387:ASN:HA	1:A:505:LEU:HD22	1.82	0.62
1:A:390:ILE:HD11	1:A:520:MET:HE1	1.84	0.59
1:A:438:LEU:HB3	1:A:488:ARG:HH11	1.68	0.58
1:A:382:VAL:HG22	1:A:510:GLN:HB3	1.86	0.58
1:A:427:ARG:NH2	1:A:492:GLU:OE2	2.36	0.57
1:A:510:GLN:HE21	1:A:519:ARG:HE	1.54	0.56
1:A:259:VAL:HG13	1:A:287:HIS:HB2	1.87	0.54
1:A:364:PRO:HA	1:A:365:CYS:HB3	1.90	0.54
1:A:468:GLU:H	1:A:468:GLU:CD	2.11	0.53
1:A:43:ASP:OD1	1:A:43:ASP:N	2.41	0.53
1:A:39:ASP:OD1	1:A:39:ASP:N	2.29	0.53
2:D:3:DT:H2''	2:D:4:DG:C8	2.44	0.53
4:C:17:DC:H1'	4:C:18:DC:H5'	1.91	0.52
1:A:189:GLU:OE1	1:A:200:TYR:OH	2.20	0.52
1:A:291:ARG:NH1	1:A:323:GLU:OE2	2.43	0.52
4:C:20:DA:C8	4:C:20:DA:H5'	2.44	0.52
1:A:510:GLN:NE2	1:A:519:ARG:HE	2.07	0.51
4:C:20:DA:H8	4:C:20:DA:H5'	1.75	0.51
3:B:12:DC:H2''	3:B:13:DA:H8	1.77	0.50
1:A:271:LYS:NZ	4:C:4:DT:H5'	2.27	0.49
1:A:385:VAL:HG23	1:A:386:GLU:H	1.77	0.49
1:A:27:ARG:NH1	1:A:60:GLN:OE1	2.45	0.49
1:A:255:GLU:O	1:A:259:VAL:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LEU:HD23	1:A:240:LEU:HD12	1.95	0.49
1:A:390:ILE:HD11	1:A:520:MET:CE	2.43	0.48
1:A:387:ASN:HB3	1:A:505:LEU:HB2	1.95	0.48
1:A:235:GLU:HG3	1:A:236:PRO:HD2	1.95	0.47
1:A:279:GLN:HG3	1:A:298:LEU:CG	2.45	0.47
1:A:156:GLN:CD	1:A:159:PHE:HB2	2.35	0.47
1:A:287:HIS:CG	1:A:288:PRO:HD2	2.49	0.47
1:A:210:ARG:HH11	1:A:213:ARG:HA	1.79	0.47
1:A:75:ARG:HD2	1:A:114:LEU:O	2.15	0.46
1:A:75:ARG:CZ	1:A:159:PHE:HZ	2.29	0.46
1:A:329:ARG:O	1:A:332:PRO:HD2	2.15	0.45
1:A:88:ARG:O	1:A:91:VAL:HG12	2.15	0.45
1:A:237:LEU:HA	1:A:240:LEU:HB2	1.96	0.45
1:A:515:GLN:HE21	1:A:515:GLN:HB3	1.63	0.45
3:B:13:DA:H2''	3:B:14:DA:H5''	1.98	0.45
2:D:1:DG:C8	2:D:2:DT:H72	2.50	0.45
1:A:115:LEU:HA	1:A:115:LEU:HD23	1.78	0.45
3:B:10:DT:H2'	3:B:11:DT:H71	1.99	0.45
2:D:1:DG:H2''	2:D:2:DT:OP2	2.17	0.45
1:A:122:GLN:HG3	1:A:125:ARG:HH21	1.81	0.44
1:A:150:ARG:HB3	1:A:154:GLU:HB2	1.98	0.44
1:A:184:TRP:CZ3	1:A:185:GLN:HG2	2.53	0.44
4:C:12:DT:H2'	4:C:12:DT:O2	2.18	0.43
1:A:210:ARG:NH1	1:A:213:ARG:HA	2.33	0.43
1:A:438:LEU:CB	1:A:488:ARG:HH11	2.30	0.43
1:A:191:VAL:HG13	1:A:192:LEU:HD13	1.99	0.43
1:A:63:LEU:HD12	1:A:63:LEU:HA	1.72	0.43
3:B:12:DC:C2	3:B:13:DA:N7	2.86	0.43
1:A:487:LEU:HD23	1:A:487:LEU:HA	1.82	0.42
1:A:171:LEU:O	1:A:171:LEU:HD12	2.20	0.42
1:A:174:ARG:O	1:A:178:MET:HE2	2.20	0.42
1:A:148:GLU:HG2	1:A:148:GLU:O	2.18	0.42
1:A:264:GLN:HE21	1:A:264:GLN:HB3	1.61	0.42
1:A:332:PRO:HA	1:A:335:GLN:HE21	1.85	0.42
4:C:4:DT:H2''	4:C:5:DG:N7	2.34	0.42
1:A:184:TRP:CE3	1:A:185:GLN:HG2	2.56	0.41
1:A:531:GLN:OE1	3:B:8:DC:H2'	2.21	0.41
1:A:23:LEU:HD11	1:A:60:GLN:HB3	2.02	0.41
1:A:32:TRP:O	1:A:36:ARG:HG2	2.21	0.41
1:A:34:GLY:O	1:A:38:ALA:HB2	2.21	0.41
1:A:262:LEU:HA	1:A:262:LEU:HD23	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLN:NE2	4:C:12:DT:O4	2.55	0.40
1:A:107:GLU:HB2	1:A:110:GLN:HG3	2.03	0.40
1:A:289:GLY:O	1:A:293:ARG:HG2	2.22	0.40

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	
1	A	544/580 (94%)	525 (96%)	19 (4%)	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	
1	A	446/478 (93%)	405 (91%)	41 (9%)	11	24

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	39	ASP
1	A	40	LEU

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Mol	Chain	Res	Type
1	A	42	ASP
1	A	43	ASP
1	A	70	LYS
1	A	72	THR
1	A	83	GLU
1	A	121	SER
1	A	125	ARG
1	A	128	LEU
1	A	136	ASP
1	A	140	GLU
1	A	141	ARG
1	A	148	GLU
1	A	167	ARG
1	A	177	LEU
1	A	188	SER
1	A	192	LEU
1	A	202	SER
1	A	208	ASP
1	A	210	ARG
1	A	253	TRP
1	A	259	VAL
1	A	264	GLN
1	A	271	LYS
1	A	279	GLN
1	A	280	ARG
1	A	300	ARG
1	A	331	LEU
1	A	384	TYR
1	A	400	GLU
1	A	427	ARG
1	A	443	ASP
1	A	453	ARG
1	A	476	GLU
1	A	492	GLU
1	A	510	GLN
1	A	515	GLN
1	A	528	ASP
1	A	558	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	272	GLN
1	A	335	GLN
1	A	343	GLN
1	A	510	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(Å ²)	Q<0.9
1	A	546/580 (94%)	-0.15	9 (1%) 72 73	46, 79, 129, 180	0
2	D	10/10 (100%)	-0.47	1 (10%) 8 6	67, 90, 170, 217	0
3	B	7/13 (53%)	-0.00	0 100 100	159, 167, 175, 187	0
4	C	19/24 (79%)	-0.47	0 100 100	95, 111, 179, 194	0
All	All	582/627 (92%)	-0.16	10 (1%) 70 72	46, 81, 142, 217	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	559	ASP	4.9
1	A	365	CYS	4.0
1	A	14	PRO	2.9
1	A	130	ARG	2.5
1	A	239	GLU	2.3
1	A	159	PHE	2.3
1	A	129	GLY	2.3
1	A	364	PRO	2.2
2	D	1	DG	2.0
1	A	345	ARG	2.0

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.