

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	$5 \mathrm{WTJ}$
Title	:	Crystal structure of an endonuclease
Authors	:	Liu, L.; Wang, Y.
Deposited on	:	2016-12-13
Resolution	:	$3.50 \mathrm{\AA(reported)}$

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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 respectively. 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.

Mol	Chain	Length		Quality of ch	ain	
1	А	1397	% 	33%	9% •	27%
1	В	1397	3%	31%	9% •	28%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15952 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.

Mol	Chain	Residues			Atom	s			ZeroOcc	AltConf	Trace	
1	Δ	1010	Total	С	Ν	Ο	\mathbf{S}	Se	0	0	0	
	A	1019	8013	5109	1350	1538	5	11	0	0	0	
1	р	1019	Total	С	Ν	Ο	S	Se	0	0	0	
	1012	7938	5055	1326	1541	6	10	0	0	U		

• Molecule 1 is a protein called CRISPR-associated endoribonuclease C2c2.

Chain	Residue	Modelled	Actual	Comment	Reference
A	1390	LEU	-	expression tag	UNP P0DOC6
A	1391	GLU	-	expression tag	UNP P0DOC6
A	1392	HIS	-	expression tag	UNP P0DOC6
A	1393	HIS	-	expression tag	UNP P0DOC6
A	1394	HIS	-	expression tag	UNP P0DOC6
A	1395	HIS	-	expression tag	UNP P0DOC6
A	1396	HIS	-	expression tag	UNP P0DOC6
A	1397	HIS	-	expression tag	UNP P0DOC6
В	1390	LEU	-	expression tag	UNP P0DOC6
В	1391	GLU	-	expression tag	UNP P0DOC6
В	1392	HIS	-	expression tag	UNP P0DOC6
В	1393	HIS	-	expression tag	UNP P0DOC6
В	1394	HIS	-	expression tag	UNP P0DOC6
В	1395	HIS	-	expression tag	UNP P0DOC6
В	1396	HIS	-	expression tag	UNP P0DOC6
B	1397	HIS	_	expression tag	UNP P0DOC6

There are 16 discrepancies between the modelled and reference sequences:

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total O 1 1	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 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.







I431	Y432 B433	Y434	L435 KA26	G437	R438	I 439	I442	NAA9	VAL	ARG	LEU	TAS	MSE	GLU	I457	E458	K461	1462 - 400	L403 N464	E465	S466 1467	L468		1472 L473		V4/6 K477	0478 770	1718 T480	L481 E482	H483	1 40 4 M 485	Y486 L487	G488 7.480	L490	R491 H402	N493	1495	0 4 96	T499 V500
N501	T502 D503	D504	F505 CEA6	B507	1508	4510 A510	K511	E512 BF13	L514	D515		1519	T520	F521	S524	ME 07	E528		I532	F533	S534 B535	E536	N537	1538 N539	N540	D541 E542	CE 40	D550	R551 E552	K553	Y555	V556 1.557	D558 VEEO	K560	1561 1562	N563	S504 K565	I568	1569 R570
	F574 T575	D576	N577 VE70	N579		T582 N583		1586 B507	K588	F589	T590 KF01	1592	G593	T594 N595		1600 TEA1	H602		K606	E607	R608	L610	Q611	G612 T613	0614 2015	D615 D616	Y617 N619	K619	V620	1623	1024 Q625	N626 1.627	K628 1620	5630 S630	D631	V634	K636	A63/ L638	NG39 L640
D641	V642 V643	F644	K645 D646	K647	K648	N649 I650	1651	TGEA	N655	D656	I657 Kef8	I659		E662 N663	N664	N665	1667	K668	1669 L670	P671	S672 F673	S674	K675	V676 L677	P678	L681	N682 1603	1684	R685 N686		D SON	D694 T695	1696 1696	T698	E699 K700	1701	A705	1707 1707	N710
K711	E712	Y714	K715 K716		1718	L719 E720		L723 F774	E725	N726	E727	K729		F732 L733	Q734	E735 1736	K737	K738	1/39 L740	G741	N742 1743	D744	E745	I746 D747	E748	N/49 1750	I751 • E753	N753	Y754 Y755	K756 W757	A758	Q759	S761	N766	N767	A769	K771	K/72 Y773	<mark>Q774</mark> K775
K776	V777 1778		1782 7783	Y784		N788	L792	F793	F795	S796	D797 DHF	SAT	MSE .	ASN ILE	Q 803	E804 T805	K806	K807	1809 1809	K810	D811 1812		K816	T817 Y818		1821 T822	V823 V824	T825	5826 D827	K828 1000	1829 1830	V831 1832	N833	D835	F836 E837	7838	1842	F 843 A844	L845 L846
N8 47	5848 N840	A850	V851 T052	1002 N853	K854	1855 R856	2	T862	L866		S869	N873	1874	1875 D876	1877	F880	1881	M882	u883 1884	N885	T886 1887	R888	N8 89	E890 C891	1892	1893	W896 M907	1898 1898	1900 1900	E901	F903	1904	M907	00 EV	E911 K012	D913	1915 D915	1916 F917	K918 I919
<mark>0920</mark>	T921	E924	1925 	Y929	Y930	E931	K934	N935 N026	1937	L938	T939 F040	F941	K942	D943 D944	1945	N946	D949	V950	K953	K954	TQ58	VAL	ILE	PHE ASP	ASP	THR	DHF SYJ	E968	0260	1075	1976 1976	0 <mark>977 </mark>	0980 0980	K982	L983 S084	N985	1980 N987	D990	L991
V995	TOOD		D1003	11006		L1011	11015	1 1001	K1022	K1023	K100	E1027	11028	D1029 N1030	L1031	11032 F1033	D1034	M1035	E1036 S1037	E1038	N1039	N1041	K1042	F 1043 Q 1044	E1045	11046 Y1047	Y1048	K1050	E1051 R1052	K1053	N1034 E1055	L1056 Y1057	11058	K1060	K1061 N1062	L1063	11067	61068 N1069	P1070 N1071
F1072	T1075	Y1076	G1077	11079		11083 K1084		K1089	L1091	F1092	N1093 T1004	D1095	G 1096	11099		N1102 K1103	1110 4	S1105	00117	L111	K1112 N1113	L1114	N1115	D1116 K1117	L1118	G1119 G1120	Y1121 51122	X1123	E1124	E1127	Y1120 Y1129	I1130	L1133	E1135	N1136	D1138	F1140	K1142	N1143 I1144
Q1145	N1146 K1127	N1148	Y1149	F1152		D1155 Y1156		V1159	E1161	Y1162	K1163 K1164	11165	R1166	E1170	F1171	117 <u>4</u>	N1175	K1176	E1178		N1185	L1188		Q1191 M1192	A1193	K1194 F1195	E1196 B1107	D1198	M1199 H1200	Y1201	V1203	N1204	R1207	00717	11212	N1218	ATZTI	K1223 A1224	Y1241
K1242	F1243 F1244		Y1249 V1260	K1251	F1252	E1253 K1254	I1255	C1256	F1259	G1260	11261	L1263	S1264	E1265 N1266	S1267	E1268 11260	N1270	K1271	E1273	N1274	11077	R1278		N1289 P1290	F1291	A1292 D1293	Y1294	11 <mark>300</mark>	D1301 R1302	V1303	L1306	L1307 S1308	Y1309	V1321	F1322	V1329	D1332	K1341	L1342
N1345	N1346 D1347	11348 11348	L1349 F1360	R1351	L1352	M1353 K1354	P1355	K1356 K1356	V1358	S1359	V1360 11361	E1362	L1363	E1364 S1365	¥1366	N1367		11371	L1374		L1378	K1381	11382	E1383 ASN	THR	ASP	THR	TEU	GLU	SIH	SIH	SIH	1						



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	91.66\AA 94.23\AA 338.22\AA	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	48.38 - 3.50	Depositor
Resolution (A)	48.37 - 3.50	EDS
% Data completeness	81.0 (48.38-3.50)	Depositor
(in resolution range)	$75.3 \ (48.37 - 3.50)$	EDS
R _{merge}	0.09	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.71 (at 3.48 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
D D .	0.263 , 0.291	Depositor
Π, Π_{free}	0.263 , 0.291	DCC
R_{free} test set	1546 reflections $(5.05%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	18.6	Xtriage
Anisotropy	0.648	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.25 , -0.8	EDS
L-test for twinning ²	$< L >=0.44, < L^2>=0.26$	Xtriage
Estimated twinning fraction	0.053 for k,h,-l	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	15952	wwPDB-VP
Average B, all atoms $(Å^2)$	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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).

Mal	Chain	Bo	nd lengths	B	ond angles
	Cham	$ RMSZ \qquad \# Z > 5$		RMSZ	# Z > 5
1	А	0.48	2/8117~(0.0%)	0.67	16/10925~(0.1%)
1	В	0.42	2/8038~(0.0%)	0.66	11/10824~(0.1%)
All	All	0.45	4/16155~(0.0%)	0.66	27/21749~(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
1	А	0	2
1	В	0	7
All	All	0	9

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
1	А	671	PRO	N-CD	5.24	1.55	1.47
1	В	1038	GLU	CB-CG	-5.17	1.42	1.52
1	А	1272	PRO	N-CD	5.09	1.54	1.47
1	В	671	PRO	N-CD	5.09	1.54	1.47

All (4) bond length outliers are listed below:

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	634	VAL	CB-CA-C	-11.15	90.21	111.40
1	А	997	GLN	CB-CA-C	6.94	124.28	110.40
1	В	1021	LEU	CB-CG-CD1	-6.59	99.80	111.00
1	В	403	ILE	CB-CA-C	-6.57	98.46	111.60
1	А	758	ALA	CB-CA-C	-6.33	100.60	110.10

There are no chirality outliers.



Mol	Chain	Res	Type	Group
1	А	1051	GLU	Peptide
1	А	1356	LYS	Peptide
1	В	412	PHE	Peptide
1	В	605	SER	Peptide
1	В	644	PHE	Peptide

5 of 9 planarity outliers are listed below:

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	А	8013	0	7662	834	3
1	В	7938	0	7580	876	1
2	А	1	0	0	0	0
All	All	15952	0	15242	1710	4

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 1710 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic}\\ {\rm distance}~({\rm \AA}) \end{array}$	Clash overlap (Å)
1:B:976:LEU:HD23	1:B:977:GLN:N	1.22	1.45
1:A:696:ILE:CB	1:A:699:GLU:HB3	1.55	1.35
1:B:817:THR:CG2	1:B:818:TYR:HA	1.54	1.35
1:B:914:PHE:HA	1:B:915:ASP:CB	1.47	1.34
1:B:914:PHE:CA	1:B:915:ASP:HB2	1.54	1.32

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:GLU:OE1	1:B:1037:SER:OG[4_446]	1.51	0.69
1:A:776:LYS:CB	1:A:1348:ILE:CD1[3_655]	1.91	0.29
1:A:398:THR:CB	1:A:907:MSE:CE[3_655]	2.08	0.12

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Atom-1	Atom-2	${f Interatomic} \ {f distance} \ ({ m \AA})$	Clash overlap (Å)
1:A:776:LYS:CD	1:A:1348:ILE:CD1[3_655]	2.10	0.10

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	$ \mathbf{P} $	erc	entil	es
1	А	1013/1397~(72%)	908 (90%)	79 (8%)	26 (3%)		5	33	
1	В	1004/1397~(72%)	888 (88%)	84 (8%)	32 (3%)		4	29	
All	All	2017/2794 (72%)	1796 (89%)	163 (8%)	58 (3%)		4	31	

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	392	LYS
1	А	410	VAL
1	А	458	GLU
1	А	460	GLU
1	А	461	LYS

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	А	824/1316~(63%)	$681 \ (83\%)$	143~(17%)	2 11
1	В	822/1316~(62%)	693 (84%)	129 (16%)	2 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1646/2632~(62%)	1374 (84%)	272 (16%)	2 13

5 of 272 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	1185	ASN
1	В	438	ARG
1	В	1084	LYS
1	А	1244	PHE
1	А	1368	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	464	ASN
1	В	501	ASN
1	В	1175	ASN
1	В	492	HIS
1	В	539	ASN

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, 95^{th} 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	$\mathbf{OWAB}(\mathbf{\AA}^2)$	$Q{<}0.9$
1	А	1008/1397~(72%)	-0.36	14 (1%) 75 69	2, 42, 106, 153	0
1	В	1002/1397~(71%)	0.08	48 (4%) 30 27	12, 67, 134, 199	0
All	All	2010/2794~(71%)	-0.14	62 (3%) 49 43	2, 55, 128, 199	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	726	ASN	8.0
1	В	744	ASP	6.9
1	В	728	SER	6.7
1	В	743	ILE	6.7
1	В	727	GLU	6.0

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.

