wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	2XXZ
Title	:	Crystal structure of the human JMJD3 jumonji domain
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Deposited on	:	2010-11-12
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

PERCENTILES INFOmissingINFO

1 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5082 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 LYSINE-SPECIFIC DEMETHYLASE 6B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	292	2400	1530	415	444	11	0	11	0
1	B	286	2311	1479	400	422	10	0	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1171	SER	-	expression tag	UNP O15054
A	1172	MET	-	expression tag	UNP O15054
B	1171	SER	-	expression tag	UNP O15054
B	1172	MET	-	expression tag	UNP O15054

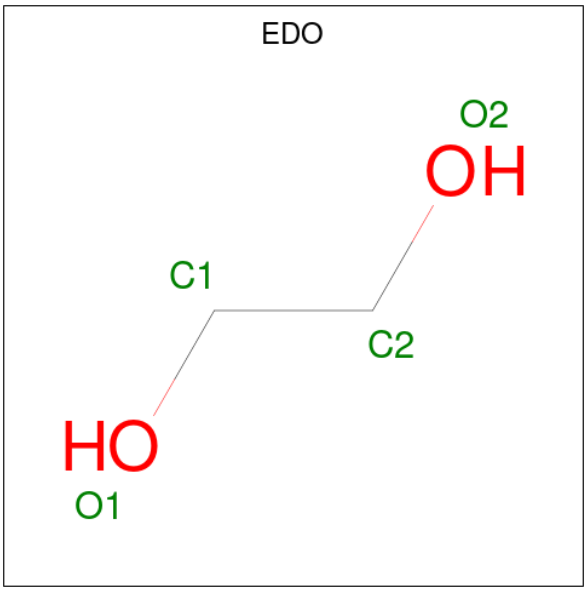
- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
2	A	2	2	2	0	0
2	B	1	1	1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

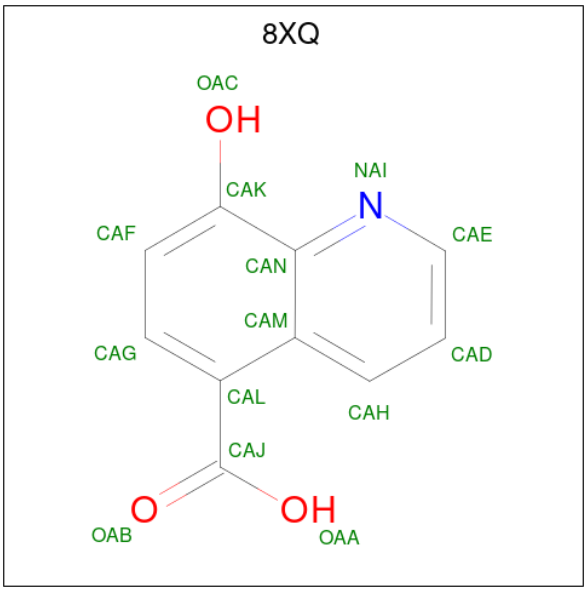
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	1	1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0
			Total	C	O		
4	A	1	4	2	2	0	0
			Total	C	O		
4	A	1	4	2	2	0	0
			Total	C	O		
4	A	1	4	2	2	0	0
			Total	C	O		
4	B	1	4	2	2	0	0

- Molecule 5 is 8-hydroxyquinoline-5-carboxylic acid (three-letter code: 8XQ) (formula: $C_{10}H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	10	1	3	0	0
			Total	C	N	O		
5	B	1	14	10	1	3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	164	164	164	0	0
			Total	O		
6	B	155	155	155	0	0

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.76Å 71.43Å 159.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.16 – 1.80 29.16 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.16-1.80) 99.7 (29.16-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.183 , 0.216 0.213 , 0.245	Depositor DCC
R_{free} test set	3058 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5082	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

3 Model quality (i)

3.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, NI, 8XQ, NA

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	0.66	0/2480	0.72	1/3386 (0.0%)
1	B	0.64	0/2390	0.68	0/3264
All	All	0.65	0/4870	0.70	1/6650 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1204	ASP	CB-CG-OD2	-5.21	113.61	118.30

There are no chirality outliers.

There are no planarity outliers.

3.2 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	2400	0	2313	24	0
1	B	2311	0	2222	32	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
4	A	16	0	24	0	0
4	B	4	0	6	3	0
5	A	14	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	14	0	5	0	0
6	A	164	0	0	3	0
6	B	155	0	0	4	1
All	All	5082	0	4575	56	1

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 6.

The worst 5 of 56 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:B:1251:ASP:OD1	1:B:1438:LEU:HD12	1.73	0.89
1:B:1191:ARG:HH11	4:B:2501:EDO:H12	1.40	0.87
1:B:1251:ASP:OD1	1:B:1438:LEU:CD1	2.26	0.82
1:A:1241:GLU:OE1	6:A:2034:HOH:O	2.10	0.70
1:A:1243[B]:ARG:HD3	1:A:1269:ARG:HG2	1.74	0.70

All (1) 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)
6:B:2058:HOH:O	6:B:2100:HOH:O[3_754]	2.13	0.07

3.3 Torsion angles (i)

3.3.1 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	299/332 (90%)	293 (98%)	6 (2%)	0	100	100
1	B	284/332 (86%)	279 (98%)	5 (2%)	0	100	100
All	All	583/664 (88%)	572 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

3.3.2 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	264/295 (90%)	261 (99%)	3 (1%)	73	68
1	B	250/295 (85%)	248 (99%)	2 (1%)	81	78
All	All	514/590 (87%)	509 (99%)	5 (1%)	76	71

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1209	ILE
1	A	1229	LYS
1	A	1325	PHE
1	B	1209	ILE
1	B	1251	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

3.3.3 RNA (i)

There are no RNA molecules in this entry.

3.4 Non-standard residues in protein, DNA, RNA chains (i)

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

3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

3.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	B	2501	-	3,3,3	0.31	0	2,2,2	0.59	0
5	8XQ	A	3001	2	15,15,15	1.19	1 (6%)	20,21,21	1.46	2 (10%)
4	EDO	A	2498	-	3,3,3	0.52	0	2,2,2	0.18	0
4	EDO	A	2499	-	3,3,3	0.34	0	2,2,2	0.09	0
5	8XQ	B	3001	2	15,15,15	1.20	1 (6%)	20,21,21	1.11	2 (10%)
4	EDO	A	2497	-	3,3,3	0.38	0	2,2,2	0.36	0
4	EDO	A	2496	-	3,3,3	0.53	0	2,2,2	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	2501	-	-	1/1/1/1	-
5	8XQ	A	3001	2	-	0/4/4/4	0/2/2/2
4	EDO	A	2498	-	-	1/1/1/1	-
4	EDO	A	2499	-	-	0/1/1/1	-
5	8XQ	B	3001	2	-	0/4/4/4	0/2/2/2
4	EDO	A	2497	-	-	0/1/1/1	-
4	EDO	A	2496	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3001	8XQ	CAN-NAI	-2.47	1.33	1.37
5	B	3001	8XQ	CAN-NAI	-2.24	1.34	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	3001	8XQ	CAE-NAI-CAN	4.19	122.52	117.30
5	B	3001	8XQ	CAE-NAI-CAN	2.97	121.00	117.30
5	B	3001	8XQ	OAB-CAJ-CAL	-2.33	116.00	122.23
5	A	3001	8XQ	OAB-CAJ-CAL	-2.20	116.35	122.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2501	EDO	O1-C1-C2-O2
4	A	2498	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2501	EDO	3	0

3.7 Other polymers (i)

There are no such residues in this entry.

3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

4 Fit of model and data (i)

4.1 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	292/332 (87%)	0.05	8 (2%)	54	49	14, 25, 51, 69	0
1	B	286/332 (86%)	0.27	11 (3%)	40	35	15, 31, 59, 74	0
All	All	578/664 (87%)	0.16	19 (3%)	46	40	14, 28, 58, 74	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1368	LEU	5.1
1	B	1356	THR	4.4
1	A	1292	GLU	4.2
1	B	1269	ARG	3.7
1	B	1289	LEU	3.4

4.2 Non-standard residues in protein, DNA, RNA chains (i)

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

4.3 Carbohydrates (i)

There are no monosaccharides in this entry.

4.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	A	2495	1/1	0.76	0.27	37,37,37,37	0
4	EDO	A	2498	4/4	0.87	0.24	29,45,50,53	0
4	EDO	A	2496	4/4	0.89	0.13	29,31,33,34	0
2	NI	A	2500	1/1	0.90	0.06	33,33,33,33	1
4	EDO	B	2501	4/4	0.92	0.28	25,26,29,30	0
4	EDO	A	2499	4/4	0.94	0.16	21,22,27,28	0
5	8XQ	B	3001	14/14	0.95	0.11	18,21,26,28	0
4	EDO	A	2497	4/4	0.96	0.10	25,26,27,28	0
5	8XQ	A	3001	14/14	0.98	0.06	12,18,20,21	0
2	NI	A	2494	1/1	0.98	0.09	20,20,20,20	0
2	NI	B	2500	1/1	0.99	0.10	22,22,22,22	0

4.5 Other polymers (i)

There are no such residues in this entry.