

Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 09:48 am BST

PDB ID : 5LF9

Title: Crystal structure of human NUDT22

Authors: Tallant, C.; Siejka, P.; Mathea, S.; Shrestha, L.; Krojer, T.; Srikannathasan,

V.; Elkins, J.M.; Burgess-Brown, N.; von Delft, F.; Arrowsmith, C.H.; Ed-

wards, A.M.; Bountra, C.; Huber, K.; Structural Genomics Consortium (SGC)

Deposited on : 2016-06-30

Resolution : 1.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

with specific help available everywhere you see the (i) symbol.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp

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

MolProbity : 4.02b-467 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)

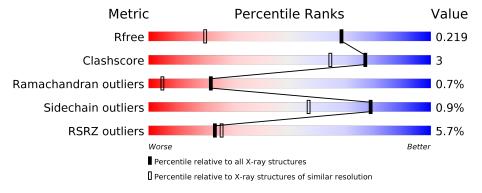
Validation Pipeline (wwPDB-VP) : 2.11

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 1.45 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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 chain	
			5%	
1	A	304	85%	7% • 7%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2287 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 Nucleoside diphosphate-linked moiety X motif 22.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	282	Total 2196	C 1388	N 385	O 417	S 6	0	5	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	_	expression tag	UNP Q9BRQ3
A	261	ARG	GLN	variant	UNP Q9BRQ3
A	264	PRO	LEU	variant	UNP Q9BRQ3

• Molecule 2 is water.

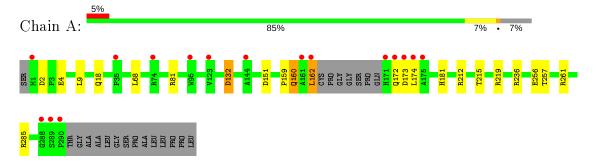
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	91	Total O 91 91	0	0



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.

• Molecule 1: Nucleoside diphosphate-linked moiety X motif 22





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	49.81Å 52.11Å 101.78Å	Danagitan
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.39 - 1.45	Depositor
Resolution (A)	29.39 - 1.45	EDS
% Data completeness	99.9 (29.39-1.45)	Depositor
(in resolution range)	99.9 (29.39-1.45)	EDS
R_{merge}	0.08	Depositor
R_{sym}	0.02	Depositor
$< I/\sigma(I) > 1$	1.82 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
D D.	0.171 , 0.207	Depositor
R, R_{free}	0.184 , 0.219	DCC
R_{free} test set	2378 reflections $(4.98%)$	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36 , 45.6	EDS
L-test for twinning ²	$< L >=0.46, < L^2>=0.29$	Xtriage
Estimated twinning fraction	0.036 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2287	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.30% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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).

Mol	Chain	Boı	nd lengths	Bo	nd angles
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	A	0.87	$1/2251 \ (0.0\%)$	0.88	8/3069 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	A	256	GLU	CD-OE1	7.30	1.33	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	A	236	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	236	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	81	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	212[A]	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	212[B]	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	285	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	151	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	285	ARG	NE-CZ-NH1	5.05	122.83	120.30

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	2196	0	2153	13	1

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Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
2	A	91	0	0	4	2
All	All	2287	0	2153	13	2

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 3.

All (13) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} \ (ext{\AA}) \end{array}$	Clash overlap (Å)
1:A:261:ARG:HB2	2:A:419:HOH:O	1.62	0.98
1:A:172:GLN:O	2:A:401:HOH:O	2.04	0.74
1:A:173:ASP:HB2	2:A:442:HOH:O	2.04	0.57
1:A:9:LEU:CD1	1:A:68:LEU:HD11	2.38	0.53
1:A:2:ASP:OD1	1:A:4:GLU:OE1	2.27	0.53
1:A:162:LEU:C	1:A:162:LEU:HD22	2.29	0.52
1:A:4:GLU:HB2	1:A:215:THR:HG23	1.92	0.52
1:A:18:GLN:HE22	1:A:181:HIS:HD2	1.60	0.49
1:A:132[B]:ASP:OD1	1:A:257:THR:OG1	2.27	0.45
1:A:9:LEU:HD12	1:A:68:LEU:HD11	1.99	0.45
1:A:18:GLN:HE22	1:A:181:HIS:CD2	2.38	0.41
1:A:172:GLN:HB3	2:A:481:HOH:O	2.20	0.40
1:A:159:PRO:O	1:A:160:GLN:HB3	2.21	0.40

All (2) 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	$egin{array}{l} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
2:A:482:HOH:O	2:A:491:HOH:O[4_565]	0.87	1.33
1:A:174:LEU:O	2:A:486:HOH:O[3_555]	2.15	0.05

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	283/304 (93%)	275 (97%)	5 (2%)	3 (1%)	14 2

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	A	132[A]	ASP
1	A	132[B]	ASP

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	232/244 (95%)	230 (99%)	2 (1%)	78 57

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	LEU
1	A	219	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	177	GLN
1	A	181	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)

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	$OWAB(m \AA^2)$	Q<0.9
1	A	282/304 (92%)	0.22	16 (5%) 23	26	15, 23, 42, 81	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	ALA	9.2
1	A	162	LEU	8.8
1	A	1	MET	6.4
1	A	171	HIS	5.8
1	A	172	GLN	5.1
1	A	290	PRO	4.6
1	A	173	ASP	4.0
1	A	95	TRP	3.9
1	A	289	SER	3.8
1	A	144	ALA	2.8
1	A	35	PRO	2.7
1	A	288	GLY	2.5
1	A	74	ARG	2.2
1	A	123	VAL	2.1
1	A	174	LEU	2.0
1	A	175	ALA	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.

