



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2024 – 05:04 AM EDT

PDB ID : 1Q33
Title : Crystal structure of human ADP-ribose pyrophosphatase NUDT9
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Deposited on : 2003-07-28
Resolution : 1.81 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

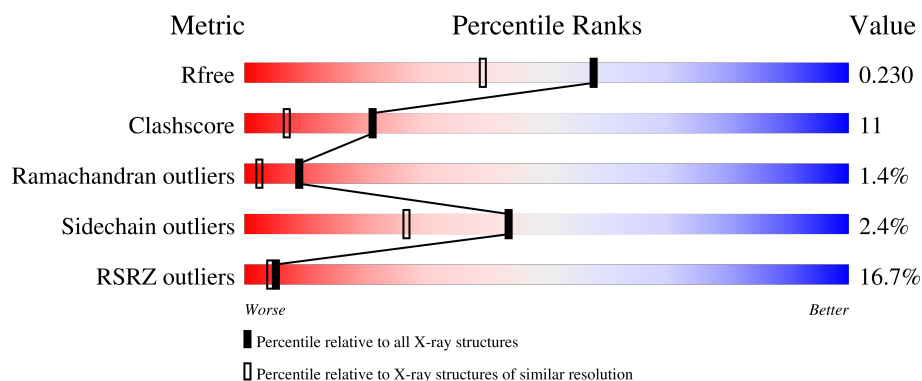
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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}	164625	9242 (1.84-1.80)
Clashscore	180529	1080 (1.82-1.82)
Ramachandran outliers	177936	1073 (1.82-1.82)
Sidechain outliers	177891	1073 (1.82-1.82)
RSRZ outliers	164620	9241 (1.84-1.80)

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 of 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 $\leq 5\%$. 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	292	<div> <div>16%</div> <div>82%</div> <div>17%</div> </div>

2 Entry composition [i](#)

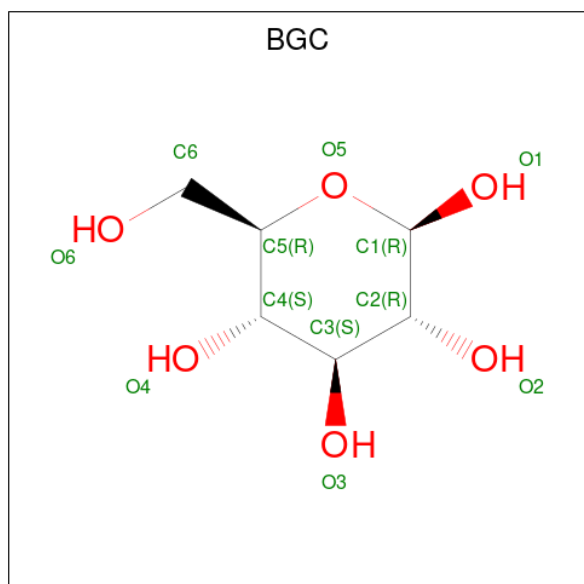
There are 4 unique types of molecules in this entry. The entry contains 2639 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ADP-ribose pyrophosphatase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	292	2362	1476	424	455	2	5	0	4	0

- Molecule 2 is beta-D-glucopyranose (three-letter code: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

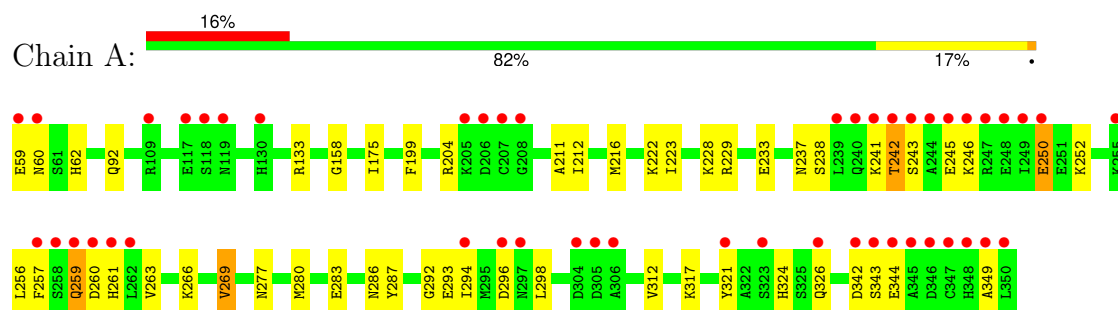
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	235	Total	O	0	0
			235	235		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: ADP-ribose pyrophosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	79.84Å 87.50Å 119.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.54 – 1.81 36.54 – 1.81	Depositor EDS
% Data completeness (in resolution range)	94.0 (36.54-1.81) 93.0 (36.54-1.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.64 (at 1.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.231 0.197 , 0.230	Depositor DCC
R_{free} test set	3601 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2639	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 4.76% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, BGC

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	0.41	0/2414	0.68	0/3253

There are no bond length outliers.

There are no bond angle outliers.

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	2362	0	2280	51	0
2	A	12	0	12	2	0
3	A	30	0	0	0	0
4	A	235	0	0	4	0
All	All	2639	0	2292	51	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 11.

All (51) 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:212:ILE:HD12	1:A:324:HIS:CG	1.82	1.14
1:A:256:LEU:HD12	1:A:259:GLN:HE22	1.46	0.80
1:A:212:ILE:HD12	1:A:324:HIS:ND1	2.06	0.69
1:A:266:LYS:HG2	1:A:283:GLU:HG3	1.74	0.68
1:A:256:LEU:HA	1:A:259:GLN:NE2	2.09	0.68
1:A:212:ILE:HD12	1:A:324:HIS:CB	2.25	0.67
1:A:269[B]:VAL:HG21	2:A:400:BGC:H6C2	1.76	0.65
1:A:158:GLY:H	1:A:277:ASN:HD22	1.43	0.63
1:A:292:GLY:O	1:A:296:ASP:HB3	1.99	0.62
1:A:238:SER:O	1:A:246:LYS:HE2	2.01	0.60
1:A:269[B]:VAL:HG21	2:A:400:BGC:C6	2.32	0.60
1:A:242:THR:HG22	1:A:245:GLU:HG3	1.84	0.58
1:A:212:ILE:CD1	1:A:324:HIS:CG	2.74	0.58
1:A:263:VAL:HG11	1:A:266:LYS:HE3	1.85	0.58
1:A:256:LEU:HD12	1:A:259:GLN:NE2	2.18	0.57
1:A:211:ALA:HB2	1:A:321:TYR:HB3	1.86	0.57
1:A:252:LYS:HD2	1:A:298:LEU:HD13	1.86	0.56
1:A:212:ILE:CD1	1:A:324:HIS:HB3	2.35	0.56
1:A:229:ARG:O	1:A:233:GLU:HG3	2.06	0.55
1:A:242:THR:O	1:A:243:SER:HB3	2.06	0.54
1:A:259:GLN:OE1	1:A:260:ASP:N	2.40	0.54
1:A:59:GLU:O	1:A:59:GLU:HG3	2.08	0.53
1:A:241:LYS:O	1:A:246:LYS:HE3	2.08	0.53
1:A:242:THR:HG22	1:A:245:GLU:OE2	2.10	0.52
1:A:259:GLN:HE21	1:A:294:ILE:CD1	2.22	0.52
1:A:293:GLU:O	1:A:296:ASP:OD1	2.27	0.52
1:A:212:ILE:CD1	1:A:324:HIS:CB	2.88	0.51
1:A:223:ILE:HG22	4:A:844:HOH:O	2.10	0.50
1:A:158:GLY:H	1:A:277:ASN:ND2	2.07	0.49
1:A:261:HIS:HA	1:A:286:ASN:O	2.12	0.49
1:A:133:ARG:HG2	4:A:625:HOH:O	2.11	0.49
1:A:204:ARG:HH11	1:A:204:ARG:HG2	1.77	0.49
1:A:263:VAL:HG11	1:A:266:LYS:CE	2.43	0.48
1:A:222:LYS:HB3	4:A:844:HOH:O	2.15	0.46
1:A:317:LYS:HE3	1:A:342:ASP:OD2	2.16	0.46
1:A:199:PHE:CE2	1:A:312[B]:VAL:CG1	2.99	0.45
1:A:256:LEU:HA	1:A:259:GLN:HE22	1.80	0.45
1:A:238:SER:HA	1:A:241:LYS:HG2	1.99	0.45
1:A:261:HIS:HB3	1:A:287:TYR:CD2	2.52	0.45
1:A:343:SER:O	1:A:344:GLU:HB2	2.18	0.43
1:A:175:ILE:HD12	1:A:175:ILE:N	2.33	0.43
1:A:216:MSE:SE	1:A:280:MSE:HE1	2.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLN:NE2	4:A:762:HOH:O	2.51	0.43
1:A:228:LYS:HD3	1:A:250:GLU:OE1	2.17	0.43
1:A:266:LYS:HE2	1:A:283:GLU:OE2	2.19	0.43
1:A:212:ILE:HD11	1:A:324:HIS:HB3	2.01	0.42
1:A:212:ILE:HD12	1:A:324:HIS:HB3	1.95	0.41
1:A:243:SER:HA	1:A:246:LYS:HD2	2.01	0.41
1:A:242:THR:CG2	1:A:245:GLU:HG3	2.49	0.41
1:A:256:LEU:HB2	1:A:294:ILE:HG21	2.02	0.41
1:A:199:PHE:CE2	1:A:312[B]:VAL:HG13	2.56	0.41

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	294/292 (101%)	281 (96%)	9 (3%)	4 (1%)	9 2

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	242	THR
1	A	349	ALA
1	A	257	PHE

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	252/243 (104%)	245 (97%)	7 (3%)	38 21

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	237	ASN
1	A	250	GLU
1	A	259	GLN
1	A	269[A]	VAL
1	A	269[B]	VAL
1	A	326	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	ASN
1	A	277	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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	$\# Z > 2$
3	SO4	A	504	-	4,4,4	0.36	0	6,6,6	0.08	0
3	SO4	A	503	-	4,4,4	0.37	0	6,6,6	0.06	0
3	SO4	A	501	-	4,4,4	0.39	0	6,6,6	0.11	0
3	SO4	A	505	-	4,4,4	0.36	0	6,6,6	0.10	0
3	SO4	A	502	-	4,4,4	0.36	0	6,6,6	0.12	0
3	SO4	A	500	-	4,4,4	0.43	0	6,6,6	0.26	0
2	BGC	A	400	-	12,12,12	0.38	0	17,17,17	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
2	BGC	A	400	-	-	0/2/22/22	0/1/1/1

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	BGC	2	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	287/292 (98%)	0.73	48 (16%) 5 4	8, 24, 61, 74	4 (1%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	THR	7.8
1	A	350	LEU	7.7
1	A	349	ALA	7.5
1	A	207	CYS	7.1
1	A	243	SER	5.6
1	A	345	ALA	5.2
1	A	304	ASP	4.9
1	A	346	ASP	4.7
1	A	261	HIS	4.2
1	A	208	GLY	4.1
1	A	259	GLN	4.1
1	A	348	HIS	3.9
1	A	342	ASP	3.7
1	A	241	LYS	3.7
1	A	205	LYS	3.7
1	A	347	CYS	3.6
1	A	244	ALA	3.6
1	A	294	ILE	3.6
1	A	247	ARG	3.5
1	A	60	ASN	3.5
1	A	248	GLU	3.5
1	A	130	HIS	3.5
1	A	258	SER	3.5
1	A	296	ASP	3.5
1	A	59	GLU	3.4
1	A	257	PHE	3.3
1	A	260	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	239	LEU	3.1
1	A	240	GLN	3.1
1	A	306	ALA	3.1
1	A	249	ILE	2.9
1	A	305	ASP	2.8
1	A	119	ASN	2.7
1	A	118	SER	2.6
1	A	206	ASP	2.6
1	A	245	GLU	2.6
1	A	246	LYS	2.4
1	A	344	GLU	2.4
1	A	250	GLU	2.4
1	A	297	ASN	2.3
1	A	255	LYS	2.2
1	A	262	LEU	2.2
1	A	117	GLU	2.2
1	A	321	TYR	2.2
1	A	323	SER	2.1
1	A	326	GLN	2.1
1	A	109	ARG	2.1
1	A	343	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	SO4	A	504	5/5	0.66	0.17	89,89,89,89	0
3	SO4	A	505	5/5	0.77	0.21	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	501	5/5	0.79	0.16	74,74,74,75	0
3	SO4	A	503	5/5	0.83	0.14	94,94,94,94	0
3	SO4	A	500	5/5	0.84	0.20	38,39,43,44	0
3	SO4	A	502	5/5	0.86	0.14	51,51,52,53	0
2	BGC	A	400	12/12	0.89	0.11	34,38,39,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.