Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 09:36 PM EDT

PDB ID	:	3UEK
Title	:	Crystal structure of the catalytic domain of rat poly (ADP-ribose) glycohydrolase
Authors	:	Kim, I.K.; Kiefer, J.R.; Stegemann, R.A.; Classen, S.; Tainer, J.A.; Ellenberger, T.
Deposited on	:	2011-10-30
Resolution	:	1.95 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 (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:

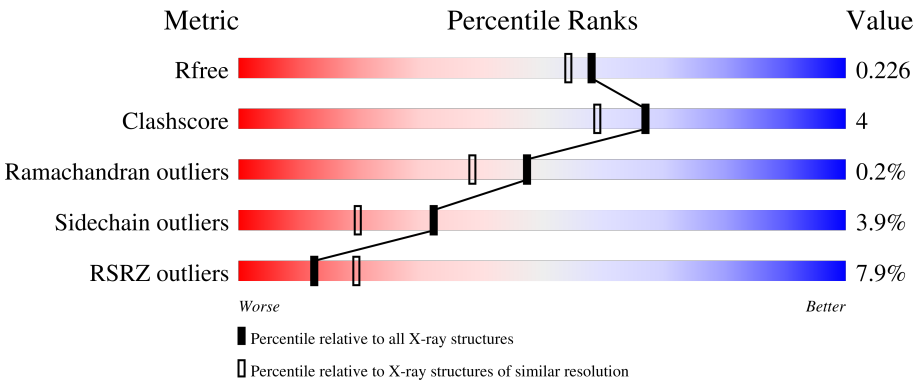
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	588	7% 80% 7% • 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4354 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 Poly(ADP-ribose) glycohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	521	4151	2653	714	761	23	0	0	0

- Molecule 2 is water.

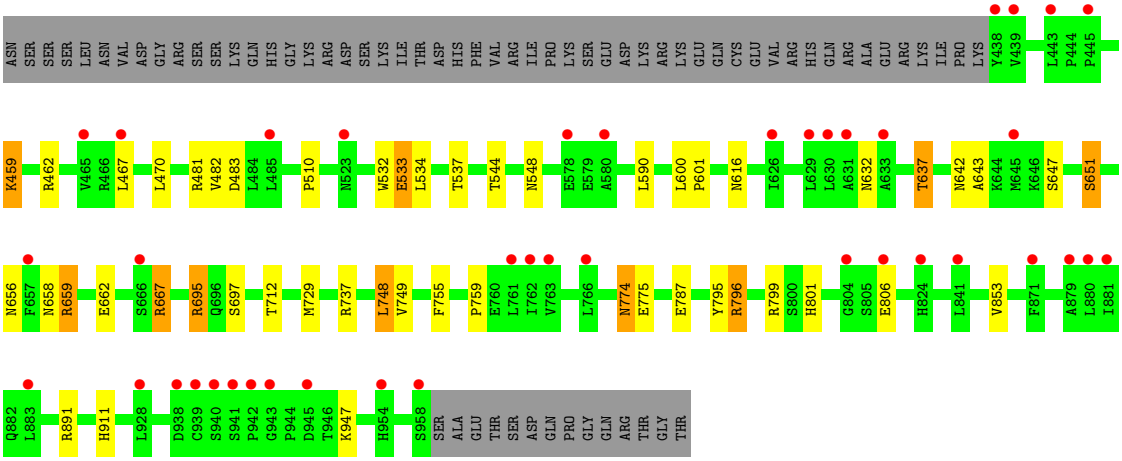
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	203	203	203	0	0

3 Residue-property plots (i)

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: Poly(ADP-ribose) glycohydrolase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	126.54Å 199.50Å 50.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95 29.43 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-1.95) 98.1 (29.43-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.180 , 0.217 0.188 , 0.226	Depositor DCC
R_{free} test set	2342 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	35.0	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4354	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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.

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	0.75	2/4259 (0.0%)	0.84	5/5787 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	532	TRP	CD2-CE2	5.57	1.48	1.41
1	A	651	SER	CB-OG	-5.19	1.35	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	695	ARG	NE-CZ-NH1	13.15	126.88	120.30
1	A	695	ARG	NE-CZ-NH2	-12.29	114.16	120.30
1	A	659	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	A	891	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	695	ARG	CD-NE-CZ	5.50	131.30	123.60

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	4151	0	4034	32	0
2	A	203	0	0	2	2
All	All	4354	0	4034	32	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 4.

All (32) 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:632:ASN:OD1	1:A:637:THR:HG21	1.65	0.96
1:A:642:ASN:HD21	1:A:656:ASN:HD22	1.24	0.83
1:A:774:ASN:HD22	1:A:774:ASN:H	1.36	0.71
1:A:642:ASN:ND2	1:A:656:ASN:HD22	1.98	0.59
1:A:544:THR:H	1:A:548:ASN:HD22	1.52	0.57
1:A:659:ARG:O	1:A:662:GLU:HG2	2.08	0.54
1:A:667:ARG:HG3	1:A:748:LEU:HD12	1.89	0.54
1:A:533:GLU:O	1:A:537:THR:HG23	2.08	0.53
1:A:616:ASN:HD21	1:A:697:SER:H	1.57	0.53
1:A:667:ARG:HD2	1:A:667:ARG:N	2.25	0.52
1:A:774:ASN:HD22	1:A:774:ASN:N	2.01	0.52
1:A:510:PRO:HB3	1:A:637:THR:HG23	1.92	0.51
1:A:616:ASN:ND2	1:A:697:SER:H	2.10	0.50
1:A:481:ARG:NH2	1:A:483:ASP:OD2	2.44	0.49
1:A:510:PRO:HG3	1:A:637:THR:CG2	2.44	0.47
1:A:642:ASN:ND2	2:A:17:HOH:O	2.36	0.47
1:A:658:ASN:ND2	2:A:17:HOH:O	2.34	0.46
1:A:695:ARG:HD3	1:A:775:GLU:OE2	2.15	0.46
1:A:470:LEU:O	1:A:482:VAL:HG11	2.16	0.45
1:A:510:PRO:CB	1:A:637:THR:HG23	2.46	0.45
1:A:544:THR:H	1:A:548:ASN:ND2	2.15	0.44
1:A:748:LEU:HD13	1:A:795:TYR:HB3	1.99	0.44
1:A:755:PHE:O	1:A:759:PRO:HA	2.18	0.44
1:A:667:ARG:NE	1:A:667:ARG:HA	2.35	0.42
1:A:510:PRO:HG3	1:A:637:THR:HG23	2.02	0.42
1:A:787:GLU:HG3	1:A:801:HIS:HB2	2.02	0.42
1:A:459:LYS:HE2	1:A:729:MET:HE3	2.03	0.41
1:A:643:ALA:HB3	1:A:647:SER:HB3	2.03	0.41
1:A:774:ASN:H	1:A:774:ASN:ND2	2.11	0.40
1:A:795:TYR:C	1:A:796:ARG:HG2	2.40	0.40
1:A:600:LEU:N	1:A:601:PRO:HD2	2.36	0.40
1:A:712:THR:O	1:A:911:HIS:HE1	2.05	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	Interatomic distance (Å)	Clash overlap (Å)
2:A:103:HOH:O	2:A:206:HOH:O[4_556]	1.48	0.72
2:A:195:HOH:O	2:A:200:HOH:O[4_556]	1.73	0.47

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	519/588 (88%)	499 (96%)	19 (4%)	1 (0%)	47 38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	749	VAL

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	441/520 (85%)	424 (96%)	17 (4%)	32 19

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	459	LYS
1	A	462	ARG
1	A	467	LEU
1	A	533	GLU

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Mol	Chain	Res	Type
1	A	534	LEU
1	A	590	LEU
1	A	637	THR
1	A	651	SER
1	A	667	ARG
1	A	737	ARG
1	A	748	LEU
1	A	774	ASN
1	A	796	ARG
1	A	799	ARG
1	A	806	GLU
1	A	853	VAL
1	A	947	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	504	ASN
1	A	536	GLN
1	A	548	ASN
1	A	557	ASN
1	A	616	ASN
1	A	642	ASN
1	A	658	ASN
1	A	774	ASN
1	A	911	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 monosaccharides 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	521/588 (88%)	0.30	41 (7%)	12	19	26, 44, 74, 99	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	942	PRO	5.9
1	A	465	VAL	4.9
1	A	439	VAL	4.8
1	A	438	TYR	4.3
1	A	940	SER	4.2
1	A	630	LEU	3.7
1	A	883	LEU	3.4
1	A	645	MET	3.4
1	A	763	VAL	3.4
1	A	943	GLY	3.3
1	A	881	ILE	3.2
1	A	666	SER	3.2
1	A	629	LEU	3.1
1	A	945	ASP	3.1
1	A	761	LEU	3.1
1	A	824	HIS	2.9
1	A	939	CYS	2.9
1	A	762	ILE	2.8
1	A	958	SER	2.7
1	A	445	PRO	2.7
1	A	578	GLU	2.6
1	A	580	ALA	2.6
1	A	879	ALA	2.5
1	A	941	SER	2.5
1	A	626	ILE	2.5
1	A	633	ALA	2.4
1	A	880	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	657	PHE	2.3
1	A	467	LEU	2.3
1	A	806	GLU	2.3
1	A	443	LEU	2.2
1	A	804	GLY	2.2
1	A	766	LEU	2.2
1	A	928	LEU	2.2
1	A	954	HIS	2.2
1	A	631	ALA	2.1
1	A	841	LEU	2.1
1	A	523	ASN	2.1
1	A	485	LEU	2.1
1	A	871	PHE	2.0
1	A	938	ASP	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 monosaccharides 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.