



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2023 – 05:34 PM EDT

PDB ID : 3HKV
Title : Human poly(ADP-ribose) polymerase 10, catalytic fragment in complex with an inhibitor 3-aminobenzamide
Authors : Karlberg, T.; Moche, M.; Arrowsmith, C.H.; Berglund, H.; Bountra, C.; Collins, R.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Johansson, A.; Johansson, I.; Kotenyova, T.; Kotzsch, A.; Nielsen, T.K.; Nordlund, P.; Nyman, T.; Persson, C.; Roos, A.K.; Sagemark, J.; Schutz, P.; Siponen, M.I.; Thorsell, A.G.; Tresaugues, L.; Van Den Berg, S.; Weigelt, J.; Welin, M.; Wisniewska, M.; Schuler, H.; Structural Genomics Consortium (SGC)
Deposited on : 2009-05-26
Resolution : 2.10 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 ⓘ 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158

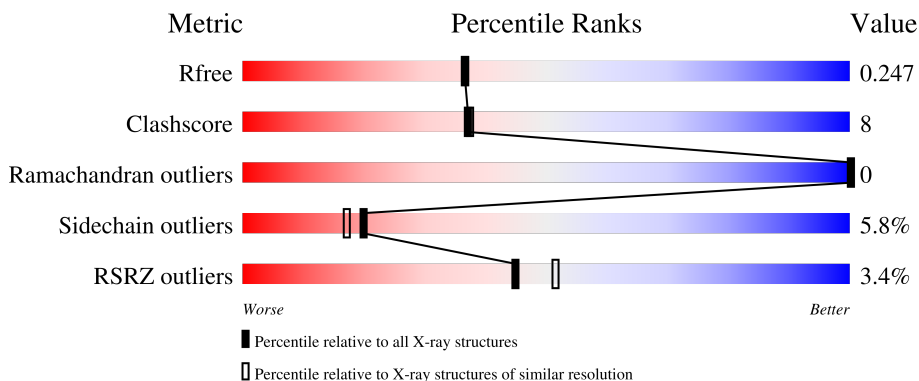
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	217	 2% 71% 14% 12%
1	B	217	 4% 79% 9% 12%

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 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3306 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] polymerase 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	192	1559	979	300	273	7	0	3	0
1	B	191	1527	957	290	273	7	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	808	MET	-	expression tag	UNP Q53GL7
A	922	LYS	ARG	engineered mutation	UNP Q53GL7
A	979	MET	VAL	engineered mutation	UNP Q53GL7
A	1018	ALA	-	expression tag	UNP Q53GL7
A	1019	HIS	-	expression tag	UNP Q53GL7
A	1020	HIS	-	expression tag	UNP Q53GL7
A	1021	HIS	-	expression tag	UNP Q53GL7
A	1022	HIS	-	expression tag	UNP Q53GL7
A	1023	HIS	-	expression tag	UNP Q53GL7
A	1024	HIS	-	expression tag	UNP Q53GL7
B	808	MET	-	expression tag	UNP Q53GL7
B	922	LYS	ARG	engineered mutation	UNP Q53GL7
B	979	MET	VAL	engineered mutation	UNP Q53GL7
B	1018	ALA	-	expression tag	UNP Q53GL7
B	1019	HIS	-	expression tag	UNP Q53GL7
B	1020	HIS	-	expression tag	UNP Q53GL7
B	1021	HIS	-	expression tag	UNP Q53GL7
B	1022	HIS	-	expression tag	UNP Q53GL7
B	1023	HIS	-	expression tag	UNP Q53GL7
B	1024	HIS	-	expression tag	UNP Q53GL7

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

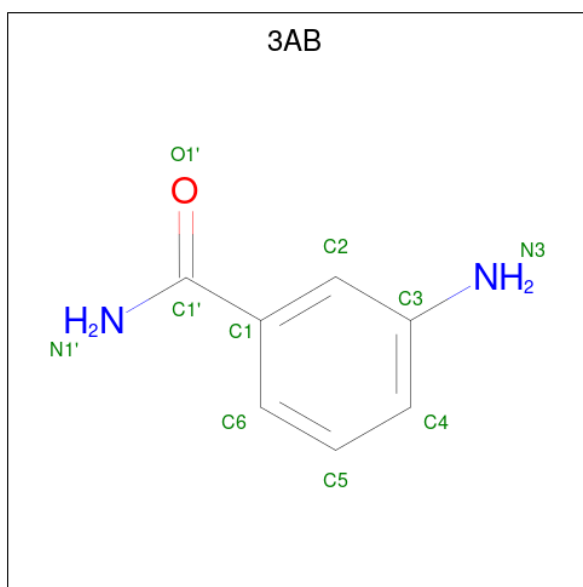


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0

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

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

- Molecule 4 is 3-aminobenzamide (three-letter code: 3AB) (formula: C₇H₈N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	7	2	1		
4	B	1	Total	C	N	O	0	0
			10	7	2	1		

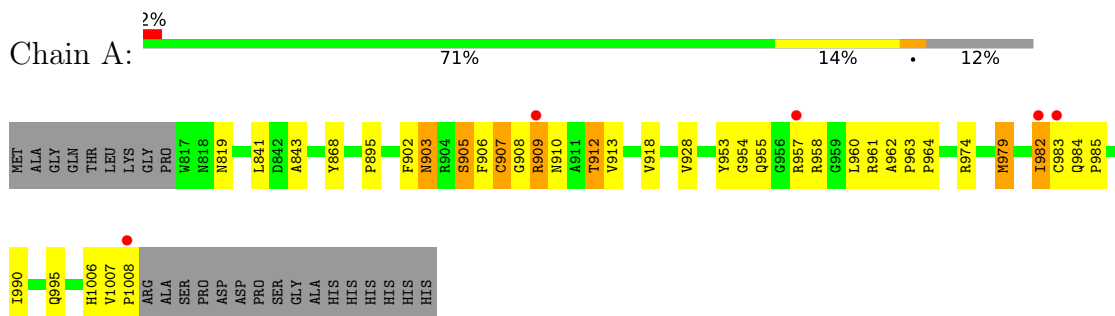
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	97	Total	O	0	0
			97	97		
5	B	86	Total	O	0	0
			86	86		

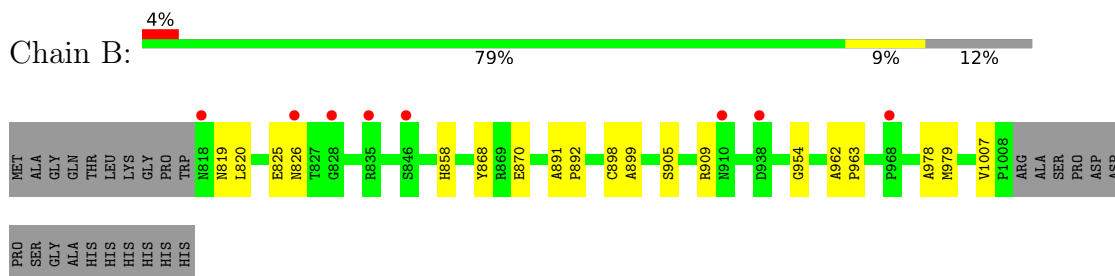
3 Residue-property plots [i](#)

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] polymerase 10



- Molecule 1: Poly [ADP-ribose] polymerase 10



4 Data and refinement statistics i

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.38Å 97.38Å 121.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 2.10 29.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.84-2.10) 99.7 (29.85-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.5.0035	Depositor
R, R_{free}	0.196 , 0.242 0.203 , 0.247	Depositor DCC
R_{free} test set	1728 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtrriage
Anisotropy	0.401	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3306	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: PO4, NA, 3AB

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	0.81	0/1606	0.83	0/2178
1	B	0.74	1/1566 (0.1%)	0.77	0/2125
All	All	0.78	1/3172 (0.0%)	0.80	0/4303

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	870	GLU	CB-CG	5.18	1.61	1.52

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	1559	0	1546	41	0
1	B	1527	0	1505	8	0
2	A	15	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	8	0	0
4	B	10	0	8	0	0
5	A	97	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	86	0	0	2	1
All	All	3306	0	3067	48	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 8.

The worst 5 of 48 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:903:ASN:O	1:A:907:CYS:HB2	1.60	1.02
1:A:953:TYR:HB2	1:A:979:MET:HE2	1.61	0.80
1:A:953:TYR:HB2	1:A:979:MET:CE	2.23	0.68
1:A:953:TYR:CD1	1:A:979:MET:HE2	2.28	0.68
1:B:891:ALA:HB3	1:B:892:PRO:HD3	1.77	0.65

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)
5:A:52:HOH:O	5:B:130: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	193/217 (89%)	190 (98%)	3 (2%)	0	100	100
1	B	190/217 (88%)	187 (98%)	3 (2%)	0	100	100
All	All	383/434 (88%)	377 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	166/182 (91%)	152 (92%)	14 (8%)	11	7
1	B	163/182 (90%)	158 (97%)	5 (3%)	40	43
All	All	329/364 (90%)	310 (94%)	19 (6%)	20	17

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	819	ASN
1	B	868	TYR
1	B	979	MET
1	B	826	ASN
1	A	928	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	819	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
2	PO4	A	1	-	4,4,4	0.84	0	6,6,6	0.73	0
2	PO4	A	2	-	4,4,4	0.93	0	6,6,6	0.49	0
4	3AB	A	1025	-	10,10,10	0.82	0	13,13,13	1.00	1 (7%)
4	3AB	B	1	-	10,10,10	0.89	1 (10%)	13,13,13	1.07	1 (7%)
2	PO4	A	3	-	4,4,4	0.39	0	6,6,6	0.56	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	3AB	A	1025	-	-	0/4/4/4	0/1/1/1
4	3AB	B	1	-	-	0/4/4/4	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	3AB	C1-C1'	2.30	1.54	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	3AB	O1'-C1'-N1'	2.16	125.65	122.58
4	A	1025	3AB	C4-C3-C2	2.13	121.39	118.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	192/217 (88%)	0.10	5 (2%) 56 61	22, 33, 52, 61	0
1	B	191/217 (88%)	0.08	8 (4%) 36 42	23, 37, 56, 66	0
All	All	383/434 (88%)	0.09	13 (3%) 45 51	22, 35, 54, 66	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1008	PRO	7.0
1	B	846	SER	3.9
1	A	982	ILE	3.9
1	A	983	CYS	3.7
1	B	818	ASN	3.5

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](#)

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(\AA^2)	Q<0.9
2	PO4	A	2	5/5	0.88	0.18	59,59,59,60	5
4	3AB	A	1025	10/10	0.89	0.18	30,41,43,48	0
2	PO4	A	1	5/5	0.93	0.12	78,78,79,79	0
4	3AB	B	1	10/10	0.95	0.11	28,29,31,34	0
3	NA	B	4	1/1	0.97	0.07	28,28,28,28	0
3	NA	A	5	1/1	0.98	0.07	38,38,38,38	0
2	PO4	A	3	5/5	0.98	0.07	36,36,39,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.