wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 13, 2024 – 04:20 am BST

PDB ID	:	5NVG
Title	:	Thr12 Phosphorylated Ubiquitin
Authors	:	Huguenin-Dezot, N.
Deposited on	:	2017-05-04
Resolution	:	1.07 Å(reported)

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

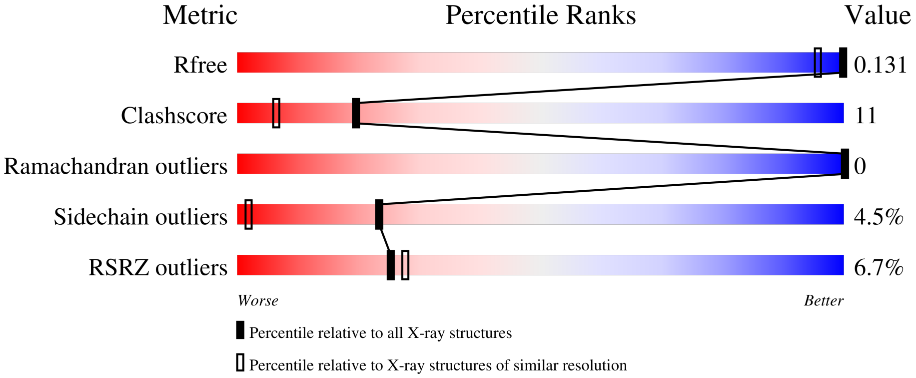
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.07 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	1502 (1.10-1.06)
Clashscore	180529	1658 (1.10-1.06)
Ramachandran outliers	177936	1614 (1.10-1.06)
Sidechain outliers	177891	1611 (1.10-1.06)
RSRZ outliers	164620	1502 (1.10-1.06)

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	76	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	101	-	X	-	-

2 Entry composition ⓘ

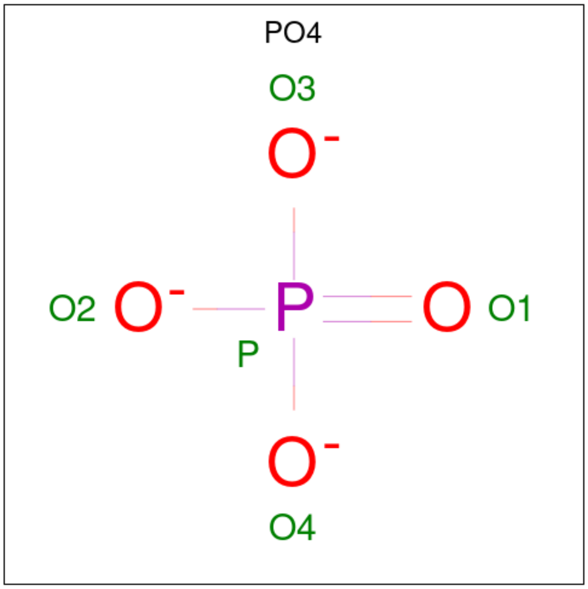
There are 4 unique types of molecules in this entry. The entry contains 825 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Polyubiquitin-B.

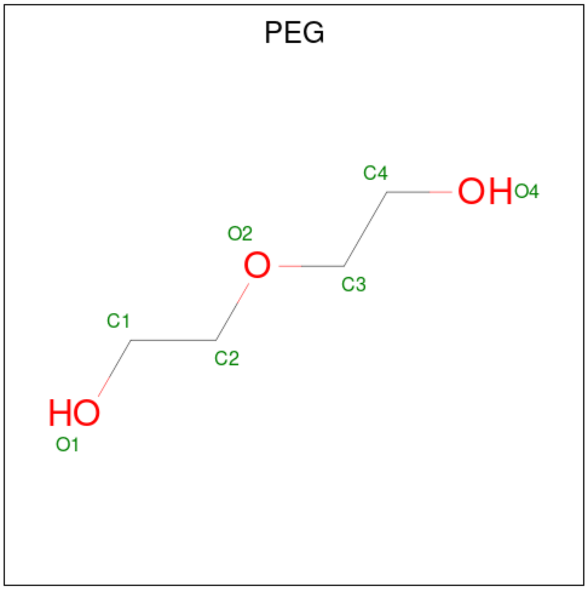
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	76	748	471	127	147	2	1	0	18	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0

- Molecule 4 is water.

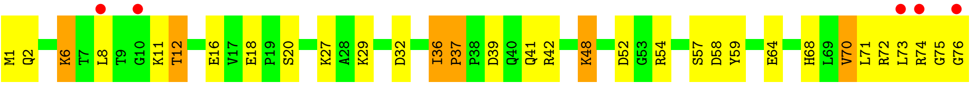
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	62	Total O 65 65	0	3

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: Polyubiquitin-B

Chain A:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	50.46Å 24.74Å 47.65Å 90.00° 113.17° 90.00°	Depositor
Resolution (Å)	43.81 – 1.07 43.81 – 1.07	Depositor EDS
% Data completeness (in resolution range)	95.1 (43.81-1.07) 95.1 (43.81-1.07)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 1.07Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.129 , 0.167 0.131 , 0.131	Depositor DCC
R_{free} test set	1227 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	10.4	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 50.5	EDS
L-test for twinning[2]	$< \|L\| >$ = 0.49, $< L^2 >$ = 0.32	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	825	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, PEG, PO4

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	1.76	14/749 (1.9%)	1.58	15/1005 (1.5%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	GLU	CD-OE2	14.13	1.41	1.25
1	A	39	ASP	CB-CG	-8.59	1.33	1.51
1	A	27	LYS	CD-CE	-6.66	1.34	1.51
1	A	37	PRO	C-O	6.28	1.35	1.23
1	A	54[A]	ARG	CZ-NH1	5.84	1.40	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	42	ARG	NE-CZ-NH1	12.36	126.48	120.30
1	A	72	ARG	NE-CZ-NH2	8.80	124.70	120.30
1	A	6[A]	LYS	CD-CE-NZ	6.93	127.64	111.70
1	A	6[B]	LYS	CD-CE-NZ	6.93	127.64	111.70
1	A	54[A]	ARG	NE-CZ-NH2	-6.70	116.95	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	748	0	787	18	3
2	A	5	0	0	0	1
3	A	7	0	10	2	0
4	A	65	0	0	8	7
All	All	825	0	797	18	8

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.

The worst 5 of 18 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:12[B]:TPO:O1P	4:A:201:HOH:O	1.69	1.08
1:A:20:SER:HA	3:A:102:PEG:H41	1.80	0.62
1:A:18[A]:GLU:HG3	4:A:202:HOH:O	2.01	0.59
1:A:8[B]:LEU:HB2	4:A:253[B]:HOH:O	2.02	0.58
1:A:11:LYS:NZ	4:A:206:HOH:O	2.38	0.55

The worst 5 of 8 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)
4:A:213:HOH:O	4:A:213:HOH:O[2_556]	0.89	1.31
4:A:209:HOH:O	4:A:225:HOH:O[3_455]	1.03	1.17
1:A:12[B]:TPO:O2P	1:A:52:ASP:OD2[1_545]	1.73	0.47
2:A:101:PO4:O3	4:A:217:HOH:O[3_545]	1.80	0.40
4:A:257:HOH:O	4:A:257:HOH:O[2_555]	1.99	0.21

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	92/76 (121%)	90 (98%)	2 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	84/67 (125%)	77 (92%)	7 (8%)	9 0

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48[B]	LYS
1	A	48[C]	LYS
1	A	74	ARG
1	A	48[D]	LYS
1	A	36[C]	ILE

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TPO	A	12[A]	1	8,10,11	2.77	3 (37%)	10,14,16	1.52	2 (20%)
1	TPO	A	12[B]	1	8,10,11	1.87	1 (12%)	10,14,16	2.76	4 (40%)

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**
1	TPO	A	12[A]	1	-	1/9/11/13	-
1	TPO	A	12[B]	1	-	1/9/11/13	-

All (4) bond length outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(Å)**	**Ideal(Å)**
1	A	12[A]	TPO	P-OG1	5.93	1.70	1.59
1	A	12[B]	TPO	P-OG1	4.27	1.67	1.59
1	A	12[A]	TPO	P-O1P	3.42	1.61	1.50
1	A	12[A]	TPO	CG2-CB	2.36	1.57	1.51

The worst 5 of 6 bond angle outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(^{o})**	**Ideal(^{o})**
1	A	12[B]	TPO	O3P-P-O2P	6.30	131.70	107.64
1	A	12[B]	TPO	OG1-P-O1P	-3.89	94.39	109.39
1	A	12[B]	TPO	O3P-P-O1P	-3.27	97.88	110.68
1	A	12[A]	TPO	O3P-P-O1P	2.97	122.31	110.68
1	A	12[B]	TPO	P-OG1-CB	-2.57	115.43	123.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**
1	A	12[A]	TPO	CB-OG1-P-O3P
1	A	12[B]	TPO	CB-OG1-P-O2P

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	12[A]	TPO	1	0
1	A	12[B]	TPO	2	1

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	PEG	A	102	-	6,6,6	0.97	0	5,5,5	1.89	2 (40%)
2	PO4	A	101	-	4,4,4	3.15	1 (25%)	6,6,6	2.46	3 (50%)

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
3	PEG	A	102	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	PO4	P-O2	-6.10	1.36	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	101	PO4	O4-P-O3	3.71	119.89	107.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	101	PO4	O4-P-O2	-3.13	97.93	107.97
3	A	102	PEG	O1-C1-C2	-3.06	94.09	111.81
2	A	101	PO4	O2-P-O1	2.76	121.01	110.89
3	A	102	PEG	C3-O2-C2	-2.63	101.91	113.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	102	PEG	O2-C3-C4-O4
3	A	102	PEG	O1-C1-C2-O2
3	A	102	PEG	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	102	PEG	2	0
2	A	101	PO4	0	1

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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(Å^2)	Q<0.9
1	A	75/76 (98%)	0.24	5 (6%)	25	28	4, 11, 35, 61	18 (24%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	LEU	3.1
1	A	76	GLY	2.5
1	A	10	GLY	2.4
1	A	8[A]	LEU	2.3
1	A	74	ARG	2.1

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

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, 95^{th} 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
1	TPO	A	12[A]	11/12	0.96	0.07	14,17,29,31	11
1	TPO	A	12[B]	11/12	0.96	0.07	14,17,25,26	11

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, 95^{th} 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	PEG	A	102	7/7	0.85	0.17	14,19,25,26	7
2	PO4	A	101	5/5	0.93	0.10	22,24,32,36	5

6.5 Other polymers ⓘ

There are no such residues in this entry.