



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2020 – 12:04 am BST

PDB ID : 6HEK
Title : Structure of human USP28 bound to Ubiquitin-PA
Authors : Gersch, M.; Komander, D.
Deposited on : 2018-08-20
Resolution : 3.03 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 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 : 2.11
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

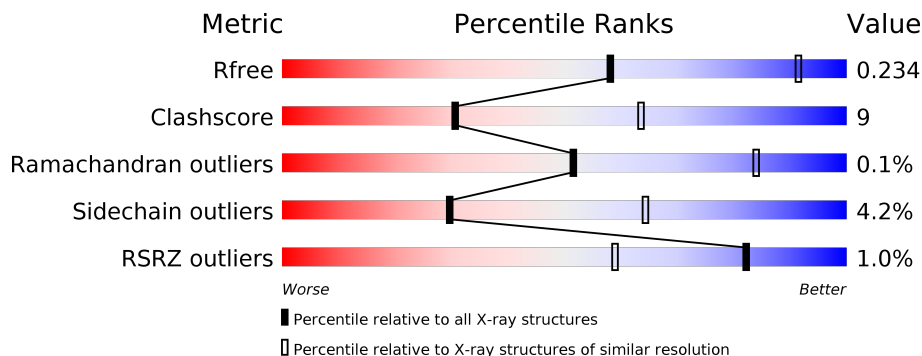
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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 $\leq 5\%$. 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	556	
1	C	556	
2	B	78	
2	D	78	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 8503 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 Ubiquitin carboxyl-terminal hydrolase 28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	453	3649	2331	611	687	20	0	0	0
1	C	459	3673	2337	623	694	19	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	GLY	-	expression tag	UNP Q96RU2
C	148	GLY	-	expression tag	UNP Q96RU2

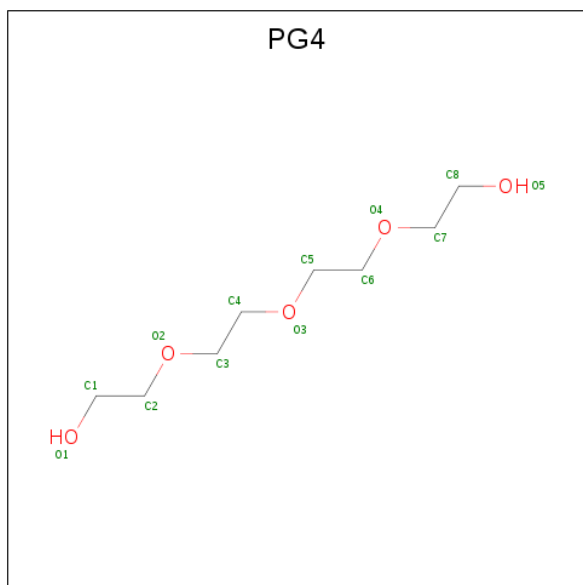
- Molecule 2 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	78	589	373	103	112	1	0	0	0
2	D	75	574	360	100	114		0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P0CG47
B	0	PRO	-	expression tag	UNP P0CG47
D	-1	GLY	-	expression tag	UNP P0CG47
D	0	PRO	-	expression tag	UNP P0CG47

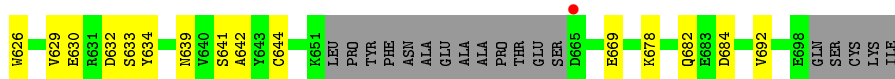
- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0
3	A	1	Total C O 7 5 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0



- Molecule 2: Polyubiquitin-B



- Molecule 2: Polyubiquitin-B



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	103.20Å 199.79Å 204.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	143.05 – 3.03 143.05 – 3.03	Depositor EDS
% Data completeness (in resolution range)	73.6 (143.05-3.03) 73.6 (143.05-3.03)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.13 _2998), REFMAC	Depositor
R, R_{free}	0.218 , 0.237 0.216 , 0.234	Depositor DCC
R_{free} test set	1518 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	93.6	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.029 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8503	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: AYE, PG4, CL

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	0.29	0/3737	0.44	0/5071
1	C	0.27	0/3760	0.42	0/5106
2	B	0.35	0/592	0.64	0/801
2	D	0.27	0/576	0.59	0/780
All	All	0.28	0/8665	0.46	0/11758

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	3649	0	3407	67	0
1	C	3673	0	3401	69	0
2	B	589	0	600	26	0
2	D	574	0	570	22	0
3	A	17	0	19	1	0
4	A	1	0	0	0	0
All	All	8503	0	7997	151	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 9.

The worst 5 of 151 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:C:151:PRO:HG3	1:C:692:VAL:HA	1.39	1.02
2:B:38:PRO:HA	2:B:41:GLN:NE2	1.75	1.01
1:A:539:ASN:O	1:A:543:THR:HG23	1.57	1.01
1:C:253:GLN:HB3	2:D:74:ARG:HB3	1.53	0.91
2:B:37:PRO:C	2:B:41:GLN:HE21	1.78	0.86

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	441/556 (79%)	427 (97%)	14 (3%)	0	100	100
1	C	447/556 (80%)	427 (96%)	20 (4%)	0	100	100
2	B	75/78 (96%)	73 (97%)	1 (1%)	1 (1%)	12	42
2	D	72/78 (92%)	71 (99%)	1 (1%)	0	100	100
All	All	1035/1268 (82%)	998 (96%)	36 (4%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	0	PRO

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	382/513 (74%)	369 (97%)	13 (3%)	37	70
1	C	381/513 (74%)	362 (95%)	19 (5%)	24	58
2	B	63/69 (91%)	60 (95%)	3 (5%)	25	60
2	D	62/69 (90%)	60 (97%)	2 (3%)	39	72
All	All	888/1164 (76%)	851 (96%)	37 (4%)	30	64

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	152	ASN
1	C	264	LEU
1	C	632	ASP
1	C	170	THR
1	C	215	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	595	GLN
2	B	41	GLN
1	C	182	GLN
1	C	216	GLN
1	C	315	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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$
2	AYE	D	76	1,2	3,3,3	2.27	1 (33%)	1,2,2	2.42	1 (100%)
2	AYE	B	76	1,2	3,3,3	2.21	1 (33%)	1,2,2	2.27	1 (100%)

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	AYE	D	76	1,2	-	0/1/1/1	-
2	AYE	B	76	1,2	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	76	AYE	C3-C2	3.79	1.54	1.28
2	B	76	AYE	C3-C2	3.68	1.53	1.28

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	76	AYE	C1-C2-C3	-2.42	114.87	125.74
2	B	76	AYE	C1-C2-C3	-2.27	115.57	125.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	76	AYE	1	0
2	B	76	AYE	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
3	PG4	A	801	-	9,9,12	0.81	0	8,8,11	0.56	0
3	PG4	A	802	-	6,6,12	0.94	0	5,5,11	0.30	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
3	PG4	A	801	-	-	5/7/7/10	-
3	PG4	A	802	-	-	3/4/4/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	PG4	O2-C3-C4-O3
3	A	802	PG4	C6-C5-O3-C4
3	A	801	PG4	C5-C6-O4-C7
3	A	801	PG4	C6-C5-O3-C4
3	A	801	PG4	C8-C7-O4-C6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	PG4	1	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 [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	453/556 (81%)	-0.14	0 100 100	40, 77, 129, 164	0
1	C	459/556 (82%)	-0.10	5 (1%) 80 56	41, 95, 150, 169	0
2	B	77/78 (98%)	-0.04	0 100 100	64, 98, 114, 132	0
2	D	74/78 (94%)	0.19	6 (8%) 12 3	87, 154, 180, 187	0
All	All	1063/1268 (83%)	-0.09	11 (1%) 82 59	40, 88, 154, 187	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	20	SER	4.3
2	D	16	GLU	3.6
2	D	2	GLN	3.3
1	C	242	LEU	3.0
1	C	665	ASP	2.9

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	AYE	D	76	4/4	0.96	0.18	118,118,121,125	0
2	AYE	B	76	4/4	0.96	0.22	72,78,81,86	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(Å ²)	Q<0.9
4	CL	A	803	1/1	0.67	0.32	112,112,112,112	1
3	PG4	A	801	10/13	0.86	0.22	53,65,78,81	0
3	PG4	A	802	7/13	0.91	0.23	69,76,88,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.