wwPDB X-ray Structure Validation Summary Report (i)

Jun 11, 2024 – 07:58 PM EDT

PDB ID	:	1C4Z
Title	:	STRUCTURE OF AN E6AP-UBCH7 COMPLEX: INSIGHTS INTO THE UBIQUITINATION PATHWAY
Authors	:	Huang, L.; Kinnucan, E.; Wang, G.; Beaudenon, S.; Howley, P.M.; Huibregtse, J.M.; Pavletich, N.P.
Deposited on	:	1999-10-14
Resolution	:	2.60 Å(reported)

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

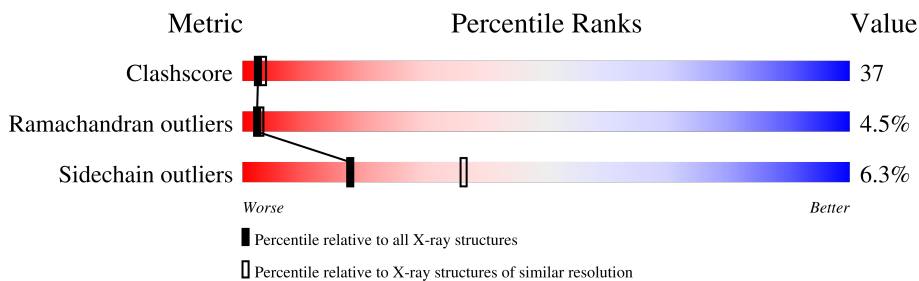|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	Percentile Ranks	Value
Clashscore		37
Ramachandran outliers		4.5%
Sidechain outliers		6.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	358	49% 43% 5% • •
1	B	358	49% 42% 7% •
1	C	358	53% 39% 6% •
2	D	154	27% 53% 12% • 6%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 10040 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-PROTEIN LIGASE E3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2861	1839	467	541	14			
1	B	350	Total	C	N	O	S	0	0	0
			2861	1839	467	541	14			
1	C	350	Total	C	N	O	S	0	0	0
			2861	1839	467	541	14			

- Molecule 2 is a protein called UBIQUITIN CONJUGATING ENZYME E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	144	Total	C	N	O	S	0	0	0
			1098	715	189	190	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	117	Total	O	0	0
			117	117		
3	B	99	Total	O	0	0
			99	99		
3	C	113	Total	O	0	0
			113	113		
3	D	30	Total	O	0	0
			30	30		

3 Residue-property plots ⓘ

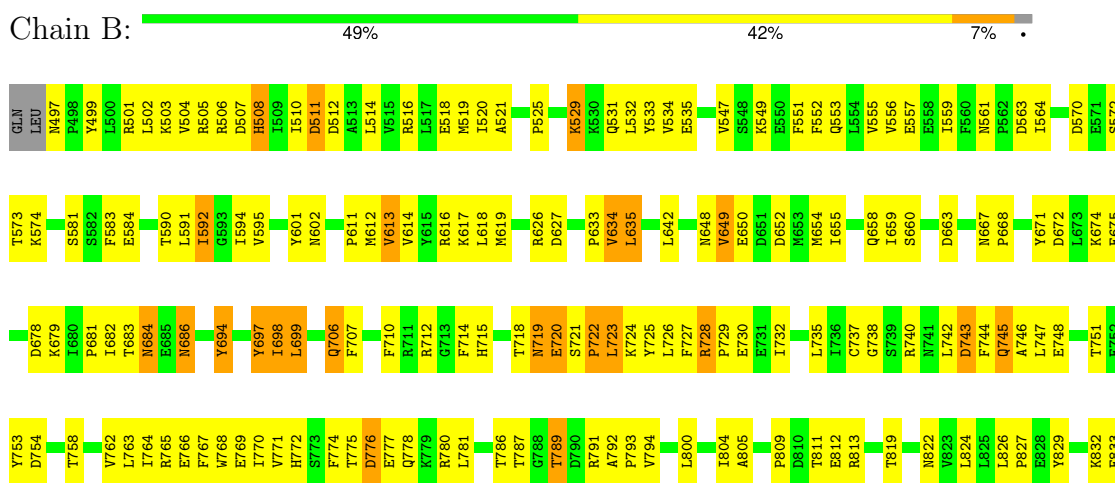These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.
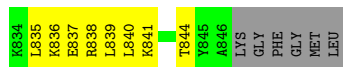
Note EDS was not executed.
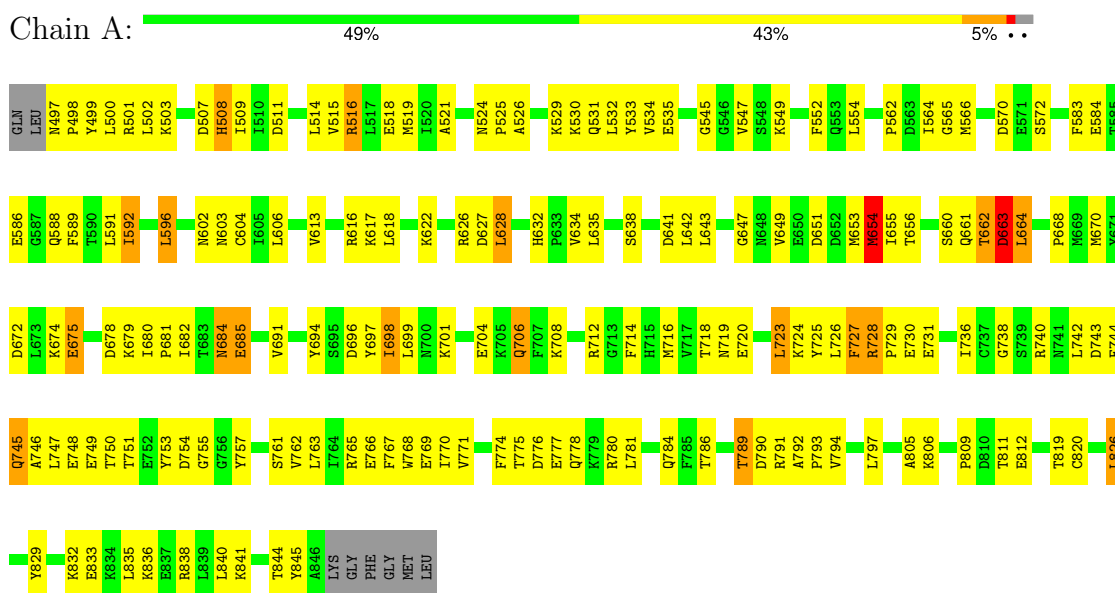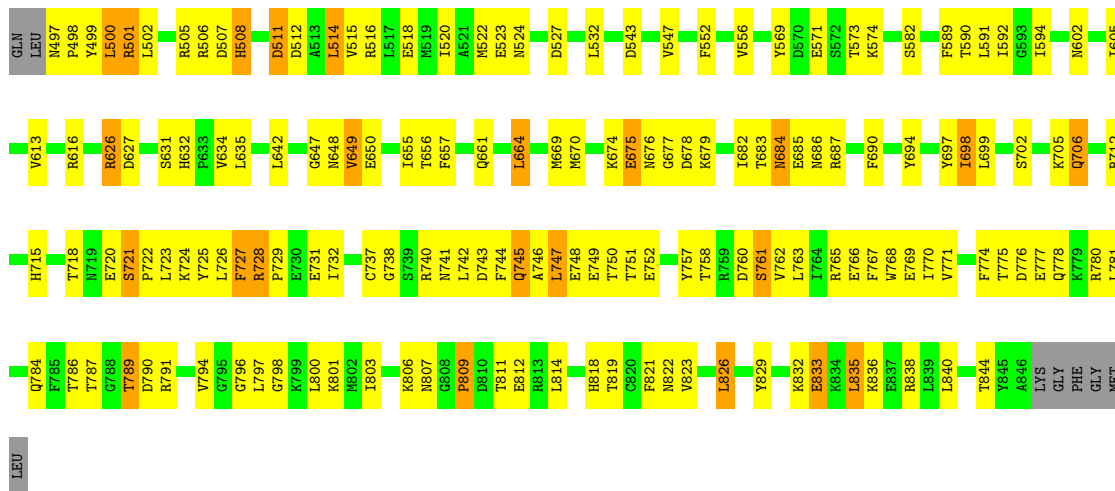
• Molecule 1: UBIQUITIN-PROTEIN LIGASE E3A

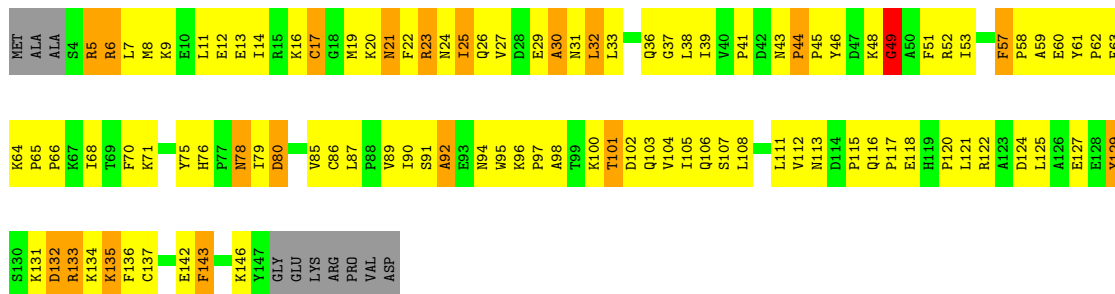• Molecule 1: UBIQUITIN-PROTEIN LIGASE E3A

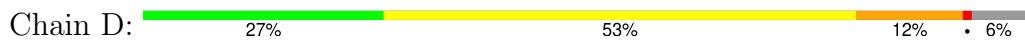K834 L835 K836 E837 R838 L839 L840 K841 T844 Y845 A846 LYS GLY PHE MET LEU

- Molecule 1: UBIQUITIN-PROTEIN LIGASE E3A

Chain C:

53%　　　　39%　　　　6%　•

GLN LEU N497 P498 Y499 L500 R501 L502 R505 R506 D507 H508 D511 D512 A513 L514 V515 R516 L517 E518 M519 I520 A521 M522 E523 N524 D527 L532 D543 V547 F552 V556 Y569 D570 E571 S572 T573 K574 S582 F589 T590 L591 I592 G593 I594 N602 I605

V613 R616 R626 D627 S631 H632 P633 V634 L635 L642 G647 N648 V649 E650 I655 T656 F657 Q661 L664 M669 M670 K674 E675 N676 G677 D678 K679 I682 T683 N684 E685 N686 R687 F690 Y694 Y697 I698 L699 S702 K705 Q706 R712

H715 T718 N719 E720 S721 P722 L723 K724 Y725 L726 F727 R728 P729 E730 E731 I732 C737 G738 S739 R740 N741 L742 D743 F744 Q745 A746 L747 E748 E749 T750 T751 E752 Y757 T758 R759 D760 S761 V762 L763 I764 R765 E766 F767 W768 E769 I770 V771 F774 T775 D776 E777 Q778 K779 R780 L781

Q784 F785 T786 T787 G788 T789 D790 R791 V794 G795 L797 G798 K799 L800 K801 M802 I803 K806 N807 G808 P809 D810 T811 E812 R813 L814 H818 T819 C820 F821 N822 V823 L826 Y829 K832 E833 K834 L835 K836 E837 R838 L839 L840 T844 Y845 A846 LYS GLY PHE MET

LEU

- Molecule 2: UBIQUITIN CONJUGATING ENZYME E2

Chain D:

27%　　　　53%　　　　12%　•　6%

MET ALA ALA S4 R5 R6 L7 M8 K9 E10 L11 E12 E13 I14 R15 K16 C17 G18 M19 K20 N21 F22 R23 N24 I25 Q26 V27 D28 E29 A30 N31 L32 L33 Q36 G37 L38 I39 V40 P41 D42 N43 P44 P45 Y46 D47 K48 G49 A50 F51 R52 I53 F57 P58 A59 E60 Y61 P62 F63

K64 P65 P66 K67 I68 T69 F70 K71 Y75 H76 P77 N78 I79 D80 V85 C86 L87 P88 V89 I90 S91 A92 E93 N94 W95 K96 P97 A98 T99 K100 T101 D102 Q103 V104 I105 Q106 S107 L108 L111 V112 N113 D114 P115 Q116 P117 E118 H119 P120 L121 R122 A123 D124 L125 A126 E127 E128 Y129

S130 K131 D132 R133 K134 K135 F136 C137 E142 F143 K146 Y147 GLY GLU LYS ARG PRO VAL ASP

4   Data and refinement statistics ⓘ

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.40Å 112.70Å 123.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60	Depositor
% Data completeness (in resolution range)	90.0 (15.00-2.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10040	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

5　Model quality ⓘ

5.1　Standard geometry ⓘ

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	0.53	0/2923	0.81	5/3943 (0.1%)
1	B	0.52	0/2923	0.80	2/3943 (0.1%)
1	C	0.56	1/2923 (0.0%)	0.83	2/3943 (0.1%)
2	D	0.44	0/1127	0.81	2/1536 (0.1%)
All	All	0.53	1/9896 (0.0%)	0.81	11/13365 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	626	ARG	CD-NE	-5.69	1.36	1.46

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	745	GLN	N-CA-C	-8.83	87.16	111.00
1	B	745	GLN	N-CA-C	-8.48	88.10	111.00
1	A	745	GLN	N-CA-C	-8.19	88.88	111.00
1	C	626	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	663	ASP	CA-C-N	-7.18	101.40	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	671	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	2861	0	2827	224	9
1	B	2861	0	2827	206	22
1	C	2861	0	2827	179	30
2	D	1098	0	1063	155	0
3	A	117	0	0	28	0
3	B	99	0	0	18	0
3	C	113	0	0	19	1
3	D	30	0	0	7	0
All	All	10040	0	9544	712	31

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 37.

The worst 5 of 712 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:626:ARG:HD2	3:A:60:HOH:O	1.38	1.19
2:D:80:ASP:OD1	2:D:121:LEU:HG	1.44	1.14
1:A:531:GLN:NE2	1:B:626:ARG:NE	1.99	1.09
1:A:531:GLN:NE2	1:B:626:ARG:CZ	2.16	1.09
1:A:531:GLN:NE2	1:B:626:ARG:CD	2.17	1.06

The worst 5 of 31 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)
1:B:813:ARG:NH1	1:C:762:VAL:CG1[3_656]	0.85	1.35
1:B:660:SER:OG	1:C:523:GLU:OE1[4_456]	0.89	1.31
1:B:813:ARG:NH2	1:C:762:VAL:CG2[3_656]	0.98	1.22
1:B:813:ARG:NH1	1:C:762:VAL:CB[3_656]	1.10	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:813:ARG:CZ	1:C:762:VAL:CB[3_656]	1.15	1.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	348/358 (97%)	306 (88%)	32 (9%)	10 (3%)	4	7
1	B	348/358 (97%)	305 (88%)	32 (9%)	11 (3%)	4	6
1	C	348/358 (97%)	309 (89%)	26 (8%)	13 (4%)	3	4
2	D	142/154 (92%)	91 (64%)	32 (22%)	19 (13%)	0	0
All	All	1186/1228 (97%)	1011 (85%)	122 (10%)	53 (4%)	2	3

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	508	HIS
1	A	698	ILE
1	A	776	ASP
1	B	508	HIS
1	B	675	GLU

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	317/323 (98%)	299 (94%)	18 (6%)	20	41
1	B	317/323 (98%)	295 (93%)	22 (7%)	15	31
1	C	317/323 (98%)	296 (93%)	21 (7%)	16	33
2	D	108/138 (78%)	102 (94%)	6 (6%)	21	42
All	All	1059/1107 (96%)	992 (94%)	67 (6%)	18	36

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	812	GLU
1	C	833	GLU
2	D	133	ARG
1	B	633	PRO
1	B	613	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	818	HIS
2	D	36	GLN
2	D	78	ASN
2	D	76	HIS
1	B	686	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.