



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 16, 2018 – 07:34 pm GMT

PDB ID : 1R4M
Title : APPBP1-UBA3-NEDD8, an E1-ubiquitin-like protein complex
Authors : Walden, H.; Podgorski, M.S.; Holton, J.M.; Schulman, B.A.
Deposited on : 2003-10-07
Resolution : 3.00 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

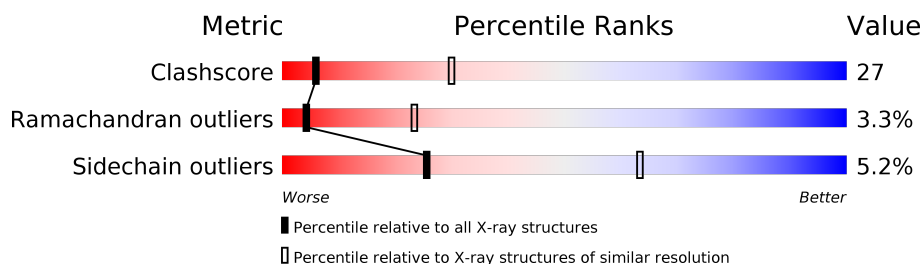
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	122078	2167 (3.00-3.00)
Ramachandran outliers	120005	2101 (3.00-3.00)
Sidechain outliers	119972	2104 (3.00-3.00)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	529	
1	C	529	
1	E	529	
1	G	529	
2	B	431	
2	D	431	
2	F	431	

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Mol	Chain	Length	Quality of chain
2	H	431	<div><div></div><div>52%39%5%••</div></div>
3	I	76	<div><div></div><div>53%42%5%</div></div>
3	J	76	<div><div></div><div>57%38%5%</div></div>
3	K	76	<div><div></div><div>57%37%7%</div></div>
3	L	76	<div><div></div><div>51%42%7%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31620 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 amyloid beta precursor protein-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4105	2602	699	789	15			
1	C	516	Total	C	N	O	S	0	0	0
			4105	2602	699	789	15			
1	E	516	Total	C	N	O	S	0	0	0
			4105	2602	699	789	15			
1	G	516	Total	C	N	O	S	0	0	0
			4105	2602	699	789	15			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	DELETION	UNP Q13564
A	?	-	GLU	DELETION	UNP Q13564
A	?	-	ASN	DELETION	UNP Q13564
A	?	-	GLY	DELETION	UNP Q13564
A	?	-	ALA	DELETION	UNP Q13564
C	?	-	ASN	DELETION	UNP Q13564
C	?	-	GLU	DELETION	UNP Q13564
C	?	-	ASN	DELETION	UNP Q13564
C	?	-	GLY	DELETION	UNP Q13564
C	?	-	ALA	DELETION	UNP Q13564
E	?	-	ASN	DELETION	UNP Q13564
E	?	-	GLU	DELETION	UNP Q13564
E	?	-	ASN	DELETION	UNP Q13564
E	?	-	GLY	DELETION	UNP Q13564
E	?	-	ALA	DELETION	UNP Q13564
G	?	-	ASN	DELETION	UNP Q13564
G	?	-	GLU	DELETION	UNP Q13564
G	?	-	ASN	DELETION	UNP Q13564
G	?	-	GLY	DELETION	UNP Q13564
G	?	-	ALA	DELETION	UNP Q13564

- Molecule 2 is a protein called ubiquitin-activating enzyme E1C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	418	Total	C	N	O	S	0	0	0
			3199	2038	549	595	17			
2	D	418	Total	C	N	O	S	0	0	0
			3199	2038	549	595	17			
2	F	418	Total	C	N	O	S	0	0	0
			3199	2038	549	595	17			
2	H	418	Total	C	N	O	S	0	0	0
			3199	2038	549	595	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	216	ALA	CYS	ENGINEERED	UNP Q8TBC4
D	216	ALA	CYS	ENGINEERED	UNP Q8TBC4
F	216	ALA	CYS	ENGINEERED	UNP Q8TBC4
H	216	ALA	CYS	ENGINEERED	UNP Q8TBC4

- Molecule 3 is a protein called Ubiquitin-like protein NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	76	Total	C	N	O	S	0	0	0
			600	378	104	116	2			
3	J	76	Total	C	N	O	S	0	0	0
			600	378	104	116	2			
3	K	76	Total	C	N	O	S	0	0	0
			600	378	104	116	2			
3	L	76	Total	C	N	O	S	0	0	0
			600	378	104	116	2			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

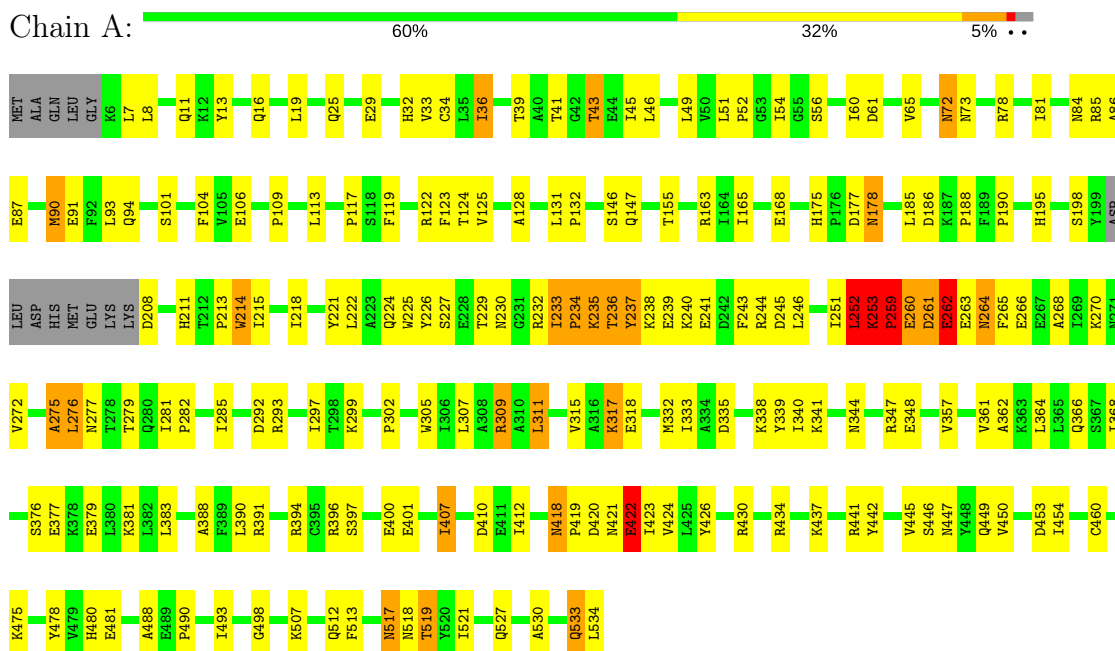
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	2	Total	Zn	0	0
			2	2		
4	J	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

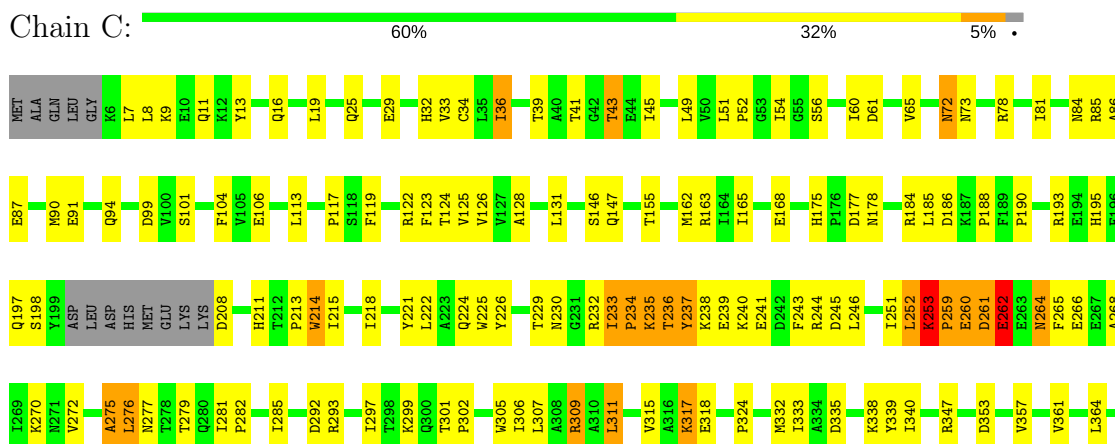
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

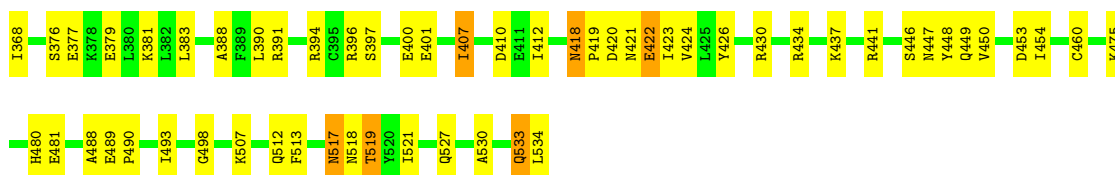
Note EDS was not executed.

- Molecule 1: amyloid beta precursor protein-binding protein 1

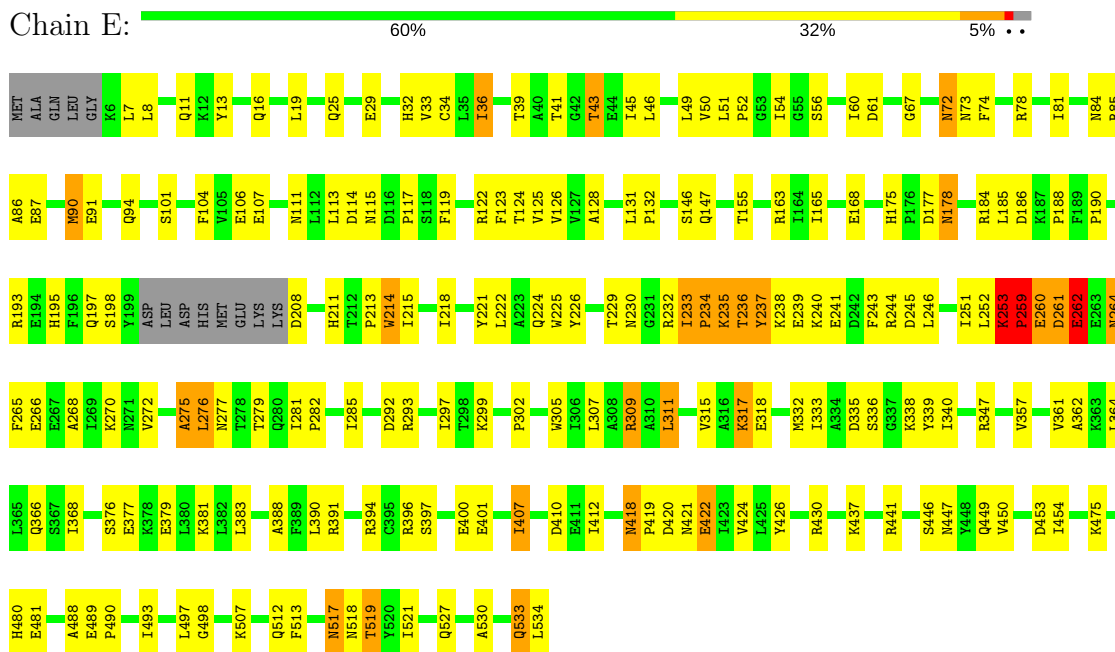


- Molecule 1: amyloid beta precursor protein-binding protein 1

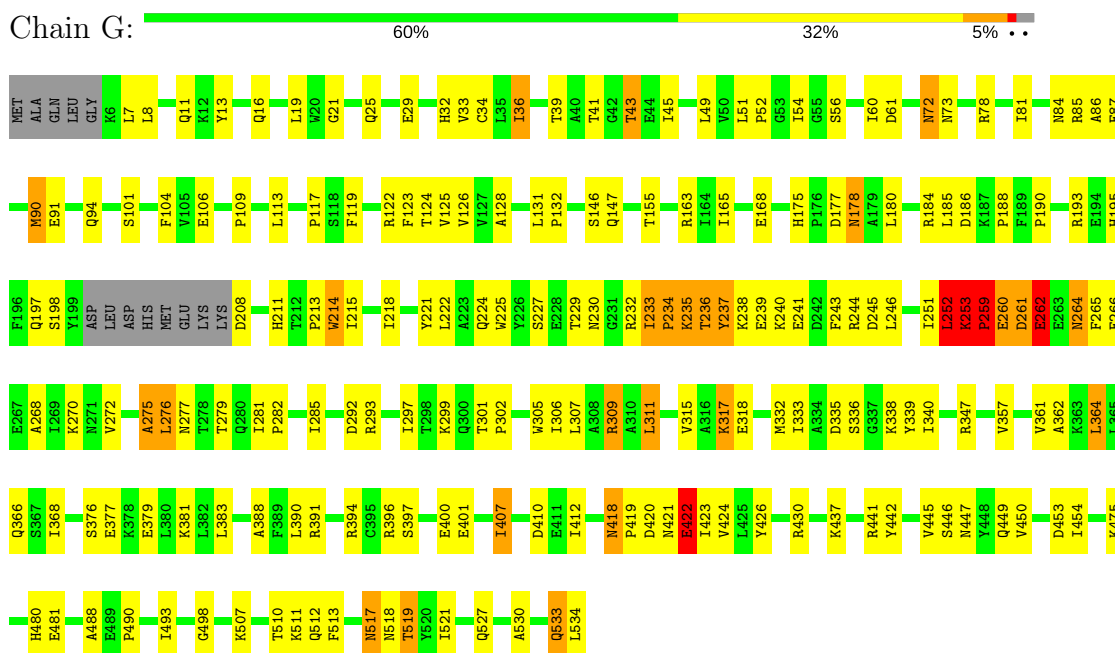




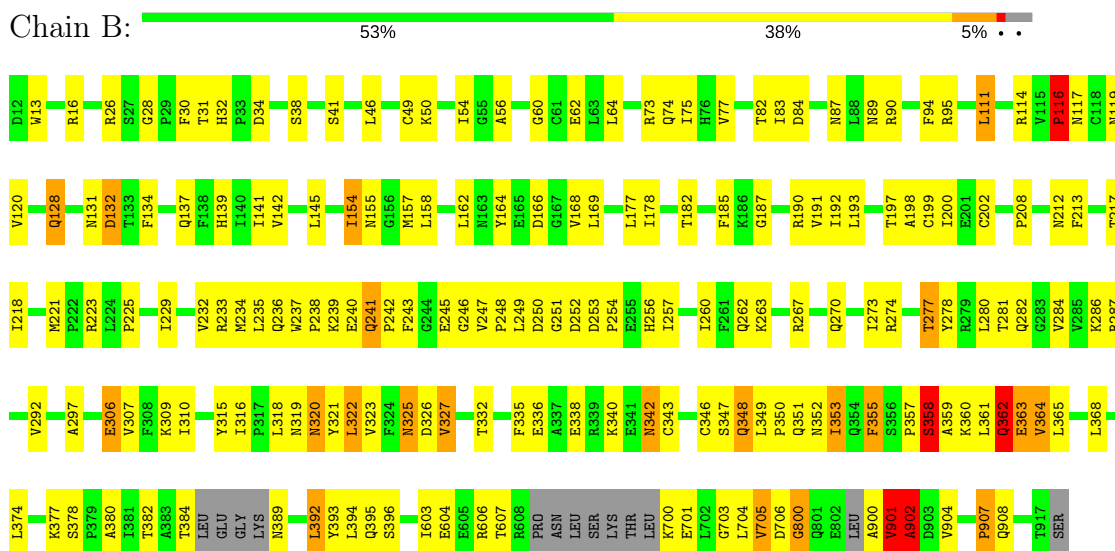
- Molecule 1: amyloid beta precursor protein-binding protein 1



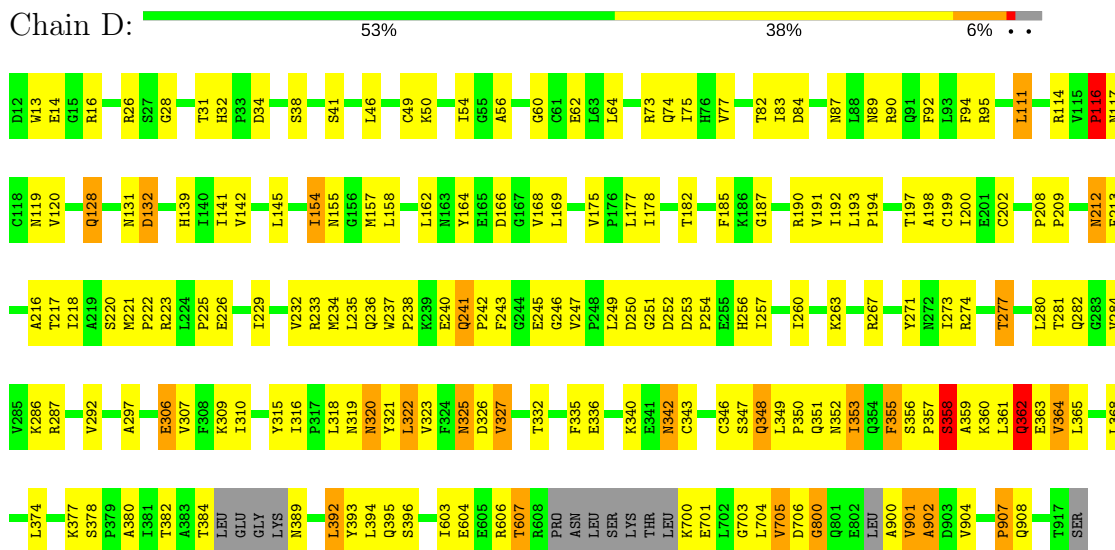
- Molecule 1: amyloid beta precursor protein-binding protein 1



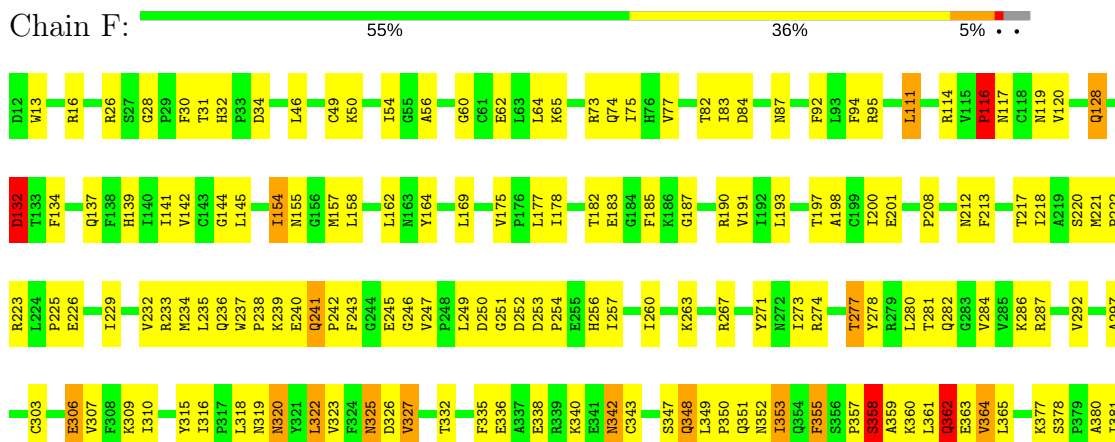
- Molecule 2: ubiquitin-activating enzyme E1C

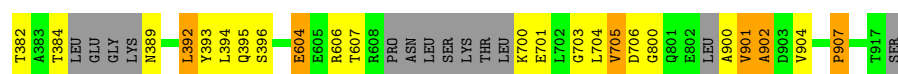


- Molecule 2: ubiquitin-activating enzyme E1C



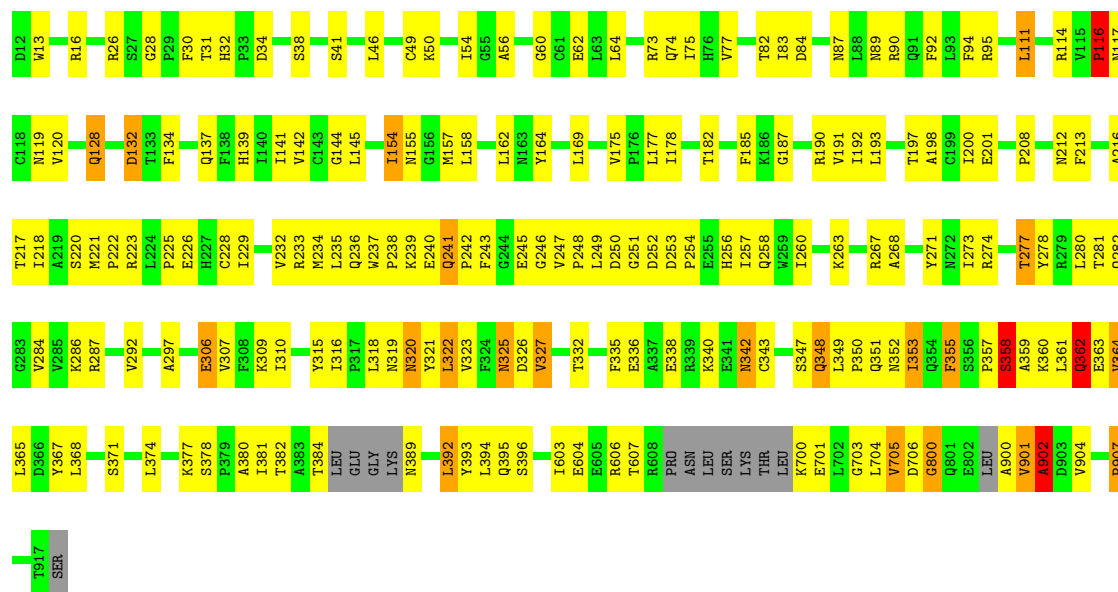
- Molecule 2: ubiquitin-activating enzyme E1C





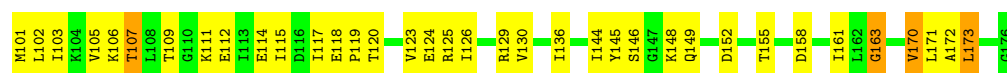
• Molecule 2: ubiquitin-activating enzyme E1C

Chain H: 52% 39% 5% ..



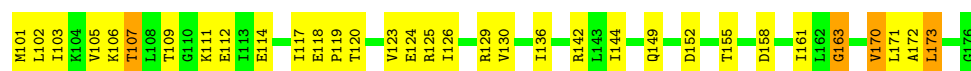
• Molecule 3: Ubiquitin-like protein NEDD8

Chain I: 53% 42% 5%



• Molecule 3: Ubiquitin-like protein NEDD8

Chain J: 57% 38% 5%



• Molecule 3: Ubiquitin-like protein NEDD8

Chain K: 57% 37% 7%



• Molecule 3: Ubiquitin-like protein NEDD8

Chain L: 51% 42% 7%

M101	L102	I103	K104	V105	K106	T107	L108	G110	K111	E112	T113	E114	I115	D116	I117	E118	P119	T120	V123	E124	R125	I126	R129	V130	G135	I136	Q141	I144	K148	Q149	D152	T155	A156	A157	D158	I161	L162	G163	V170	L171	A172	L173	G176
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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	135.40Å 198.90Å 209.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	99.9 (50.00-3.00)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31620	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.44	2/4185 (0.0%)	0.68	5/5661 (0.1%)
1	C	0.44	3/4185 (0.1%)	0.65	2/5661 (0.0%)
1	E	0.42	0/4185	0.66	1/5661 (0.0%)
1	G	0.45	2/4185 (0.0%)	0.69	5/5661 (0.1%)
2	B	0.44	0/3268	0.72	5/4447 (0.1%)
2	D	0.43	0/3268	0.71	4/4447 (0.1%)
2	F	0.45	0/3268	0.72	5/4447 (0.1%)
2	H	0.44	0/3268	0.73	6/4447 (0.1%)
3	I	0.38	0/605	0.72	1/808 (0.1%)
3	J	0.38	0/605	0.72	1/808 (0.1%)
3	K	0.38	0/605	0.73	1/808 (0.1%)
3	L	0.36	0/605	0.71	1/808 (0.1%)
All	All	0.43	7/32232 (0.0%)	0.70	37/43664 (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
2	B	0	1
2	D	0	1
2	F	0	1
All	All	0	3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	253	LYS	C-N	6.87	1.47	1.34
1	A	259	PRO	N-CA	6.64	1.58	1.47
1	C	259	PRO	N-CA	6.41	1.58	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	LYS	C-N	6.04	1.45	1.34
1	G	259	PRO	N-CA	5.93	1.57	1.47

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	259	PRO	CA-N-CD	-15.83	89.34	111.50
1	E	259	PRO	CA-N-CD	-14.39	91.35	111.50
1	A	259	PRO	CA-N-CD	-12.29	94.29	111.50
1	C	252	LEU	O-C-N	-8.30	109.42	122.70
2	B	800	GLY	N-CA-C	-8.16	92.69	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	355	PHE	Sidechain
2	D	355	PHE	Sidechain
2	F	355	PHE	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	4105	0	4063	201	0
1	C	4105	0	4063	203	0
1	E	4105	0	4063	218	0
1	G	4105	0	4063	204	0
2	B	3199	0	3066	199	0
2	D	3199	0	3066	197	0
2	F	3199	0	3062	189	0
2	H	3199	0	3062	194	0
3	I	600	0	635	44	0
3	J	600	0	635	42	0
3	K	600	0	635	46	0
3	L	600	0	635	46	0
4	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	2	0	0	0	0
4	J	1	0	0	0	0
All	All	31620	0	31048	1663	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 27.

The worst 5 of 1663 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)
3:K:123:VAL:HB	3:K:152:ASP:HA	1.31	1.11
1:A:252:LEU:O	1:A:253:LYS:C	1.90	1.09
3:J:123:VAL:HB	3:J:152:ASP:HA	1.33	1.08
3:I:123:VAL:HB	3:I:152:ASP:HA	1.30	1.08
2:B:274:ARG:HH22	1:E:107:GLU:HA	1.18	1.07

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	512/529 (97%)	459 (90%)	34 (7%)	19 (4%)	4	21
1	C	512/529 (97%)	458 (90%)	38 (7%)	16 (3%)	4	25
1	E	512/529 (97%)	459 (90%)	36 (7%)	17 (3%)	4	23
1	G	512/529 (97%)	460 (90%)	32 (6%)	20 (4%)	3	19
2	B	408/431 (95%)	342 (84%)	52 (13%)	14 (3%)	4	22
2	D	408/431 (95%)	341 (84%)	55 (14%)	12 (3%)	5	26
2	F	408/431 (95%)	342 (84%)	54 (13%)	12 (3%)	5	26
2	H	408/431 (95%)	345 (85%)	51 (12%)	12 (3%)	5	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	74/76 (97%)	63 (85%)	9 (12%)	2 (3%)	5	29
3	J	74/76 (97%)	64 (86%)	8 (11%)	2 (3%)	5	29
3	K	74/76 (97%)	64 (86%)	8 (11%)	2 (3%)	5	29
3	L	74/76 (97%)	64 (86%)	8 (11%)	2 (3%)	5	29
All	All	3976/4144 (96%)	3461 (87%)	385 (10%)	130 (3%)	4	23

5 of 130 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	PRO
1	A	235	LYS
1	A	236	THR
1	A	259	PRO
1	A	261	ASP

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	450/461 (98%)	430 (96%)	20 (4%)	31	69
1	C	450/461 (98%)	432 (96%)	18 (4%)	34	72
1	E	450/461 (98%)	430 (96%)	20 (4%)	31	69
1	G	450/461 (98%)	430 (96%)	20 (4%)	31	69
2	B	334/379 (88%)	311 (93%)	23 (7%)	17	51
2	D	334/379 (88%)	311 (93%)	23 (7%)	17	51
2	F	334/379 (88%)	311 (93%)	23 (7%)	17	51
2	H	334/379 (88%)	311 (93%)	23 (7%)	17	51
3	I	66/66 (100%)	64 (97%)	2 (3%)	44	79
3	J	66/66 (100%)	64 (97%)	2 (3%)	44	79
3	K	66/66 (100%)	64 (97%)	2 (3%)	44	79
3	L	66/66 (100%)	64 (97%)	2 (3%)	44	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3400/3624 (94%)	3222 (95%)	178 (5%)	25 63

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	348	GLN
1	E	292	ASP
2	H	306	GLU
2	D	358	SER
1	E	90	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	241	GLN
1	E	209	HIS
2	H	139	HIS
2	D	342	ASN
1	E	37	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	1
2	B	1
2	D	1
2	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	396:SER	C	600:VAL	N	3.82
1	H	396:SER	C	600:VAL	N	3.80
1	D	396:SER	C	600:VAL	N	3.78
1	F	396:SER	C	600:VAL	N	3.78

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.