



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 14, 2023 – 10:59 PM EDT

PDB ID : 1R4N
Title : APPBP1-UBA3-NEDD8, an E1-ubiquitin-like protein complex with ATP
Authors : Walden, H.; Podgorski, M.S.; Holton, J.M.; Schulman, B.A.
Deposited on : 2003-10-07
Resolution : 3.60 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
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) : 2.35

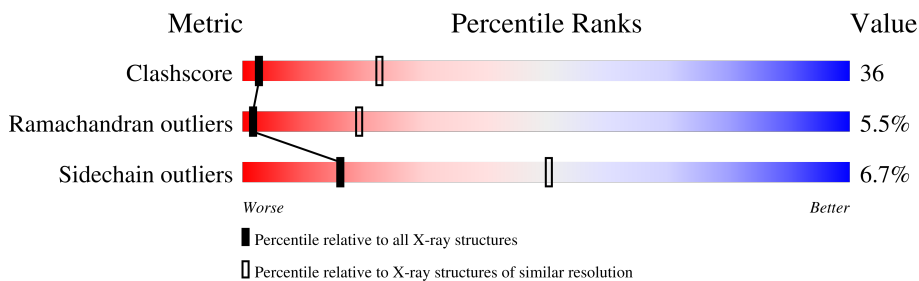
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)


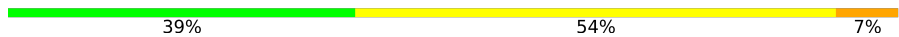


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	529	50% 41% 6% ..
1	C	529	49% 43% 5% ..
1	E	529	50% 41% 5% ..
1	G	529	52% 39% 6% ..
2	B	431	44% 42% 9% ..
2	D	431	45% 41% 9% ..
2	F	431	46% 40% 9% ..
2	H	431	45% 43% 8% ..

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Mol	Chain	Length	Quality of chain
3	I	76	 42% 54%
3	J	76	 39% 54% 7%
3	K	76	 39% 55% 5%
3	L	76	 42% 53% 5%

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
4	ATP	H	8	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 31744 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
			Total	C	N	O	S			
1	A	516	4105	2602	699	789	15	0	0	0
1	C	516	4105	2602	699	789	15	0	0	0
1	E	516	4105	2602	699	789	15	0	0	0
1	G	516	4105	2602	699	789	15	0	0	0

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
			Total	C	N	O	S			
2	B	418	Total 3199	C 2038	N 549	O 595	S 17	0	0	0
2	D	418	Total 3199	C 2038	N 549	O 595	S 17	0	0	0
2	F	418	Total 3199	C 2038	N 549	O 595	S 17	0	0	0
2	H	418	Total 3199	C 2038	N 549	O 595	S 17	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	150	ALA	CYS	engineered mutation	UNP Q8TBC4
D	150	ALA	CYS	engineered mutation	UNP Q8TBC4
F	150	ALA	CYS	engineered mutation	UNP Q8TBC4
H	150	ALA	CYS	engineered mutation	UNP Q8TBC4

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

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

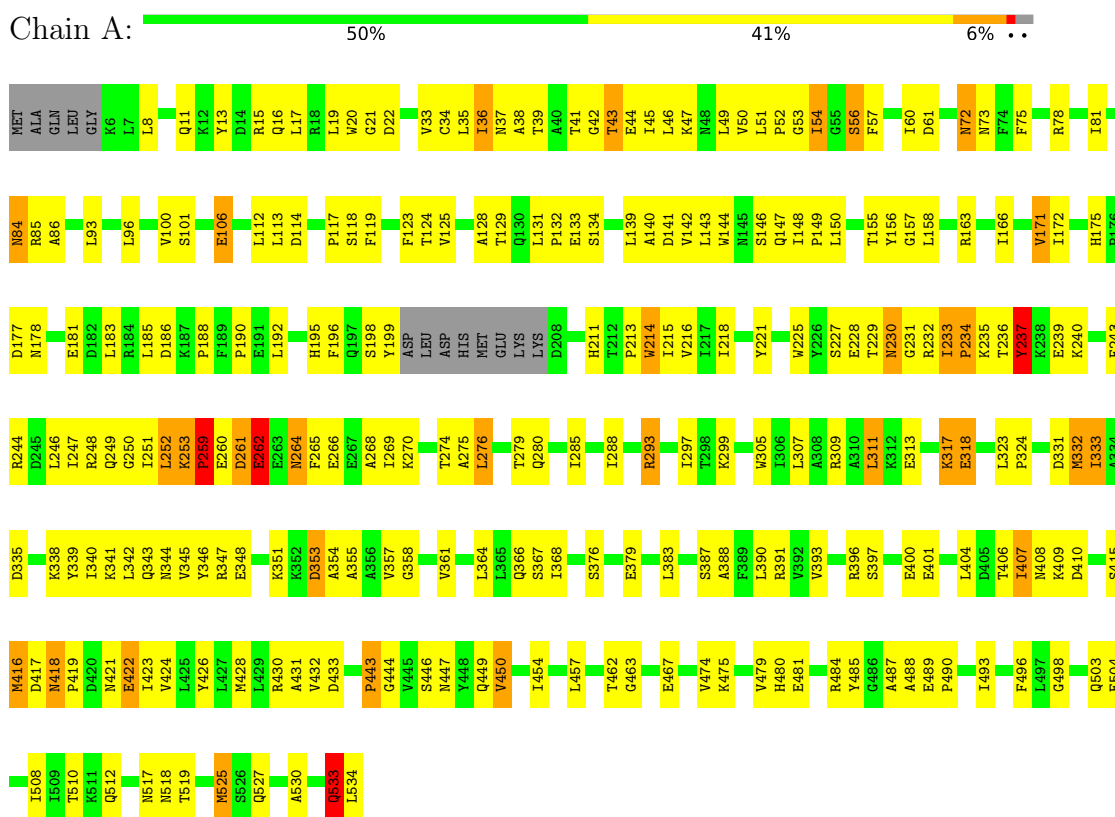
- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

3 Residue-property plots

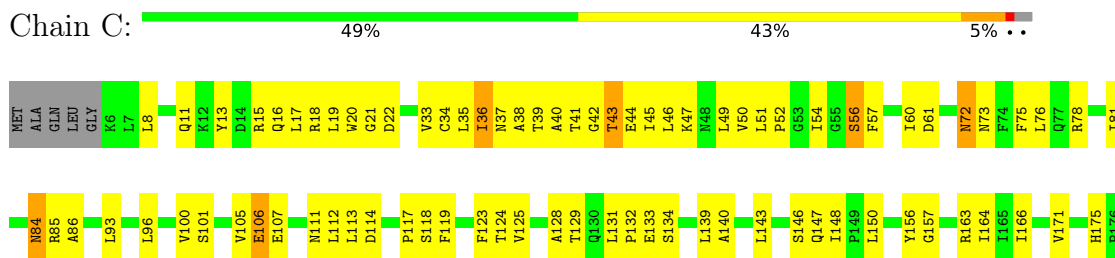
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

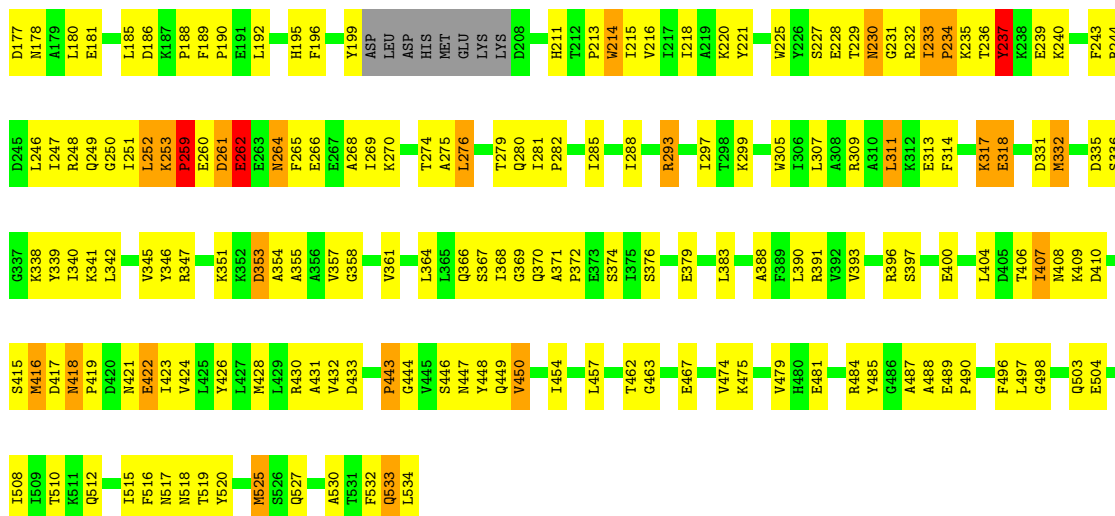
Note EDS was not executed.

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

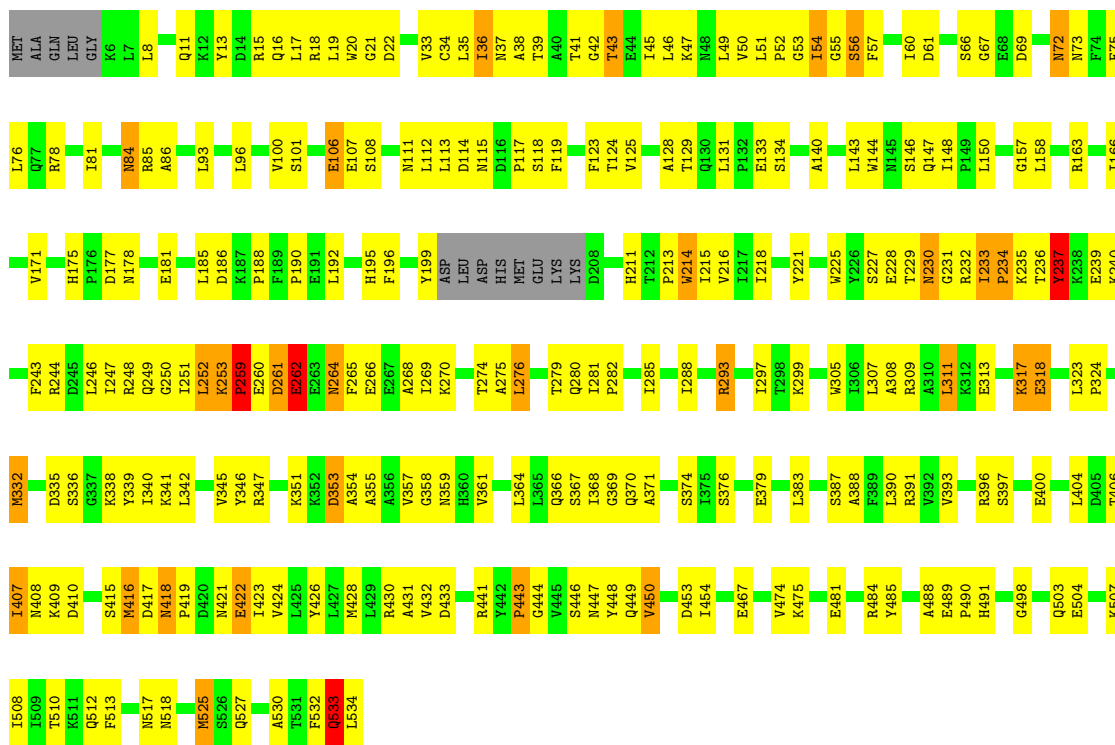


- Molecule 1: amyloid beta precursor protein-binding protein 1

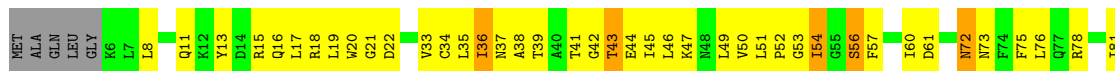


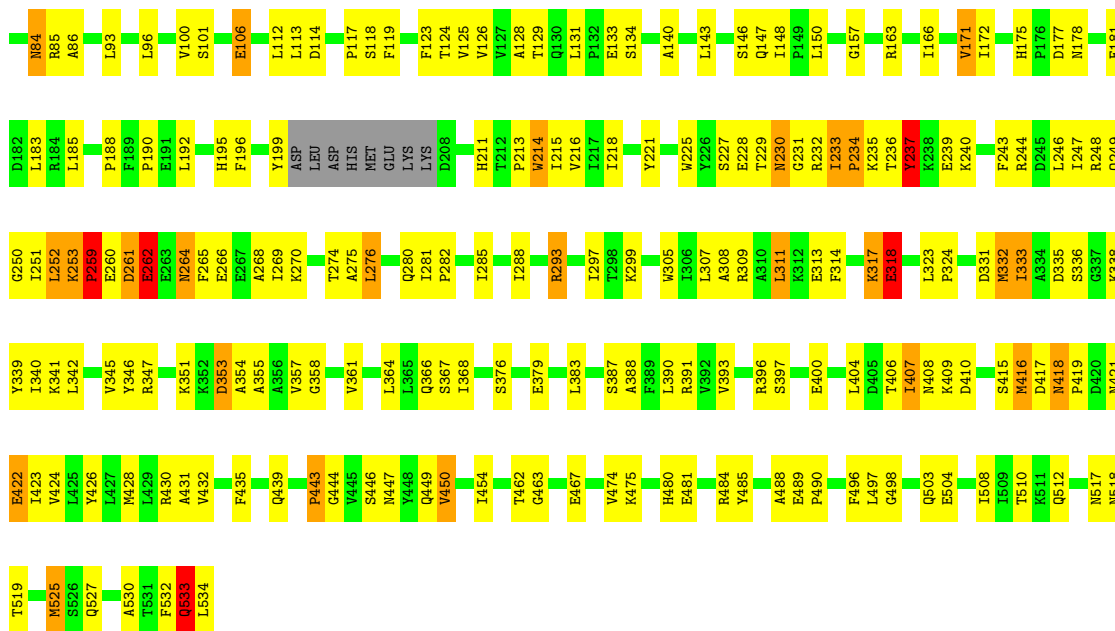


• Molecule 1: amyloid beta precursor protein-binding protein 1

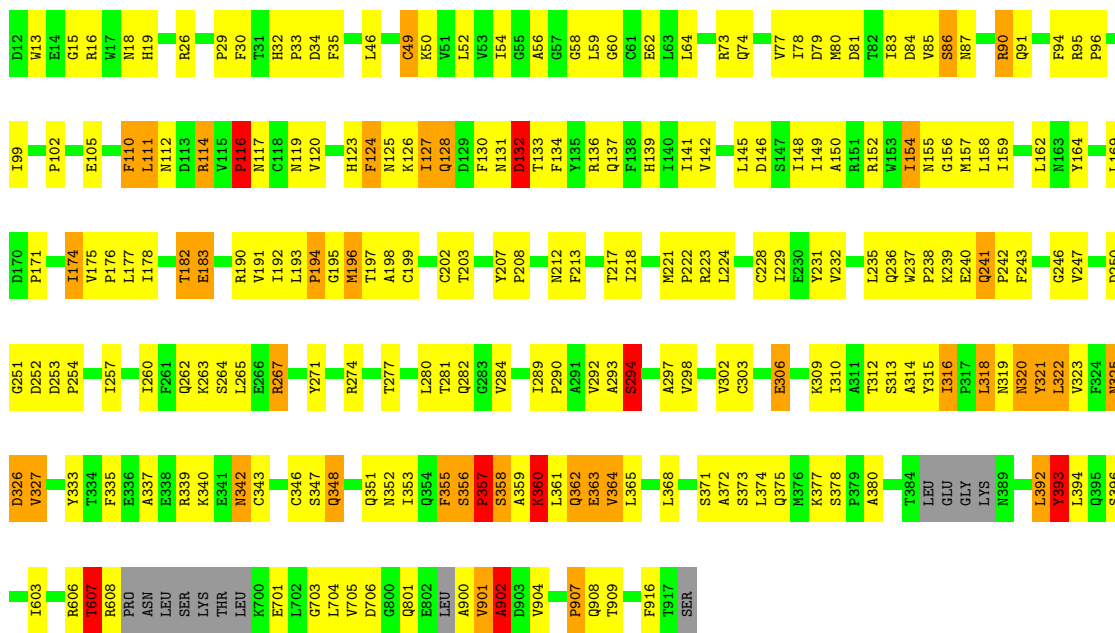


• Molecule 1: amyloid beta precursor protein-binding protein 1

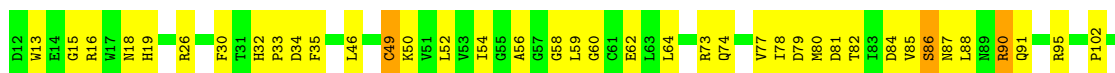


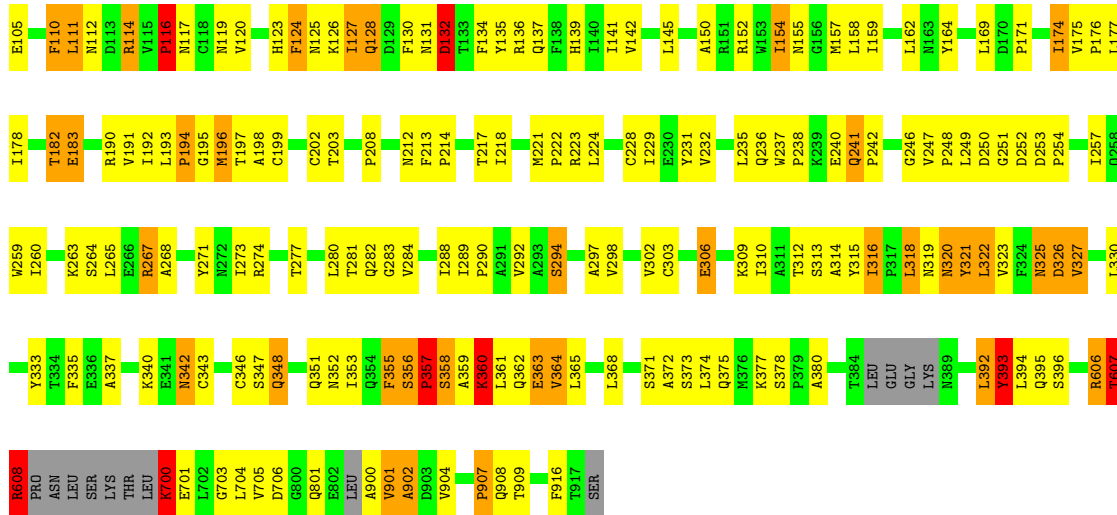


• Molecule 2: ubiquitin-activating enzyme E1C

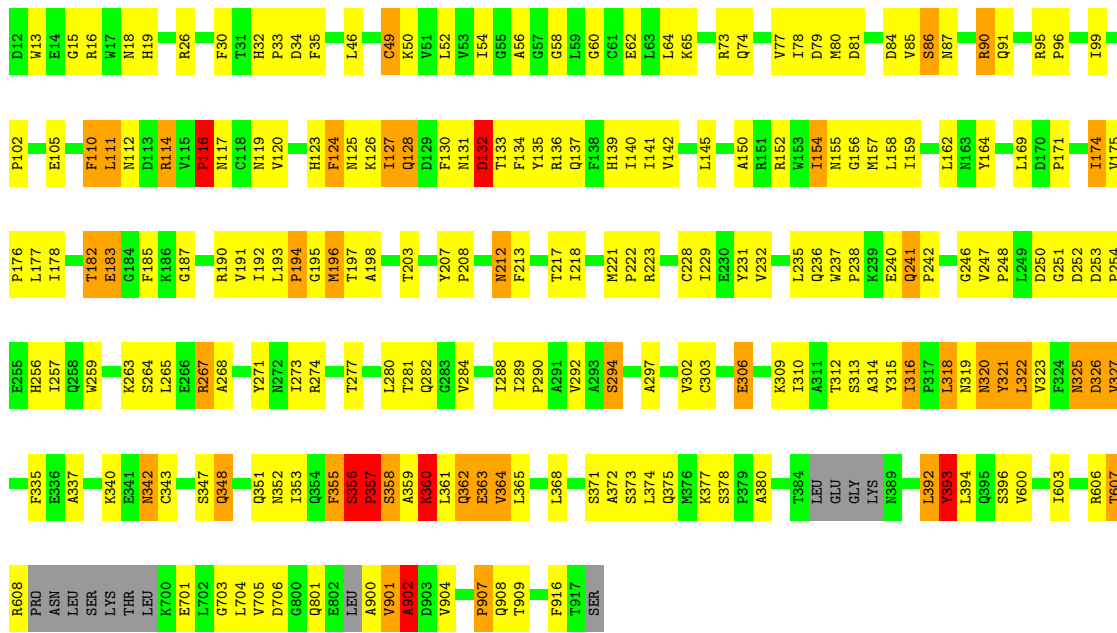


• Molecule 2: ubiquitin-activating enzyme E1C

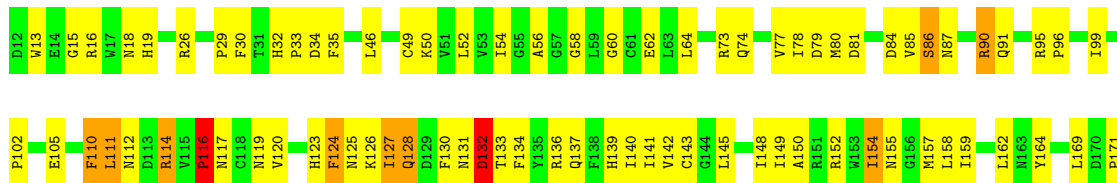
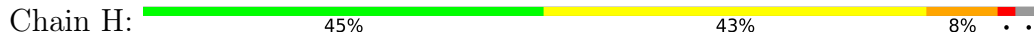


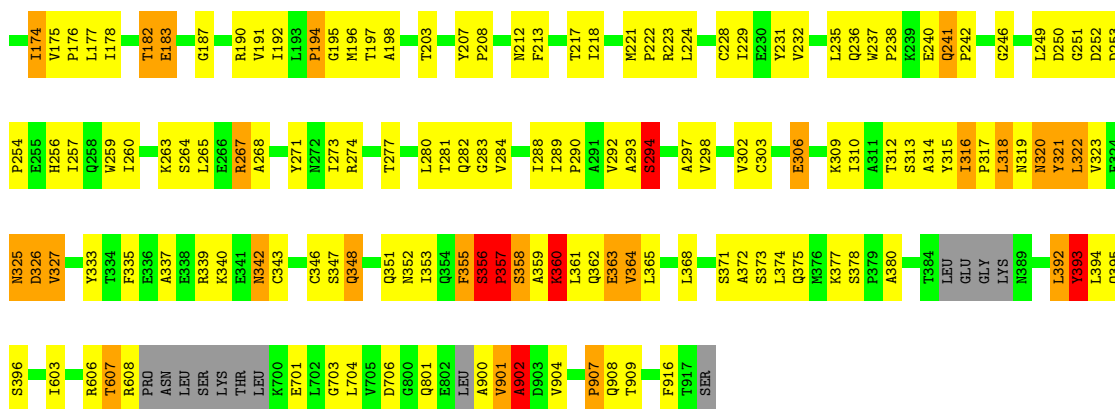


• Molecule 2: ubiquitin-activating enzyme E1C



• Molecule 2: ubiquitin-activating enzyme E1C





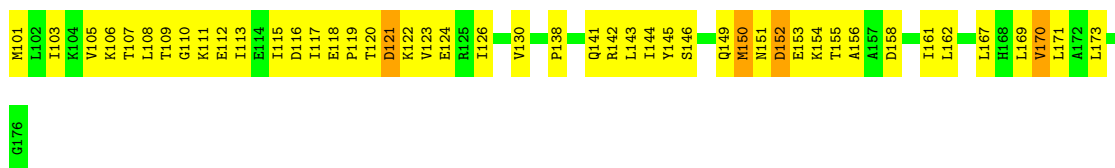
- Molecule 3: Ubiquitin-like protein NEDD8



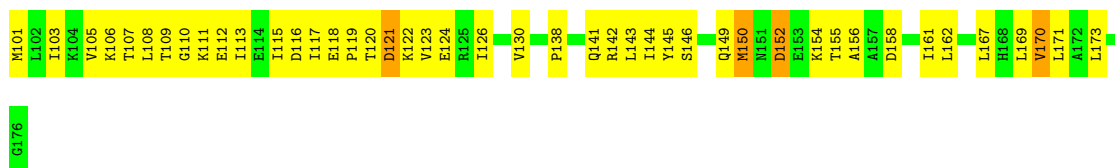
- Molecule 3: Ubiquitin-like protein NEDD8



- Molecule 3: Ubiquitin-like protein NEDD8



- Molecule 3: Ubiquitin-like protein NEDD8



4 Data and refinement statistics

Xtrriage (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	135.00Å 197.90Å 211.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-3.60)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.251 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	31744	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

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: ZN, ATP

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	0.54	5/4185 (0.1%)	0.72	9/5661 (0.2%)
1	C	0.52	6/4185 (0.1%)	0.75	9/5661 (0.2%)
1	E	0.56	3/4185 (0.1%)	0.74	9/5661 (0.2%)
1	G	0.54	6/4185 (0.1%)	0.74	11/5661 (0.2%)
2	B	0.53	1/3268 (0.0%)	0.93	8/4447 (0.2%)
2	D	0.75	9/3269 (0.3%)	0.82	12/4450 (0.3%)
2	F	0.50	1/3268 (0.0%)	0.77	8/4447 (0.2%)
2	H	0.49	2/3268 (0.1%)	0.76	7/4447 (0.2%)
3	I	0.36	0/605	0.67	0/808
3	J	0.32	0/605	0.66	0/808
3	K	0.35	0/605	0.66	0/808
3	L	0.34	0/605	0.66	0/808
All	All	0.54	33/32233 (0.1%)	0.77	73/43667 (0.2%)

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	A	0	1
1	C	0	1
1	G	0	1
2	B	0	1
2	D	0	2
2	F	0	1
2	H	0	1
All	All	0	8

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	700	LYS	N-CA	16.70	1.79	1.46
1	C	259	PRO	N-CA	14.05	1.71	1.47
1	A	259	PRO	N-CA	13.99	1.71	1.47
2	D	608	ARG	N-CA	13.42	1.73	1.46
2	B	392	LEU	CG-CD2	-13.03	1.03	1.51

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	392	LEU	CB-CG-CD2	-32.12	56.40	111.00
2	B	392	LEU	CB-CG-CD1	14.82	136.20	111.00
1	C	259	PRO	CA-N-CD	-14.32	91.45	111.50
1	E	259	PRO	CA-N-CD	-12.19	94.43	111.50
2	D	700	LYS	N-CA-C	11.93	143.21	111.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	259	PRO	Peptide
2	B	355	PHE	Sidechain
1	C	259	PRO	Peptide
2	D	355	PHE	Sidechain
2	D	393	TYR	Sidechain

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	4105	0	4063	272	0
1	C	4105	0	4063	266	0
1	E	4105	0	4063	278	0
1	G	4105	0	4063	264	0
2	B	3199	0	3066	265	0
2	D	3199	0	3067	263	0
2	F	3199	0	3062	255	0
2	H	3199	0	3062	261	0
3	I	600	0	635	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	600	0	635	60	0
3	K	600	0	635	64	0
3	L	600	0	635	61	0
4	B	31	0	12	3	0
4	D	31	0	12	4	0
4	F	31	0	11	6	0
4	H	31	0	12	10	0
5	F	1	0	0	0	0
5	H	2	0	0	0	0
5	J	1	0	0	0	0
All	All	31744	0	31096	2256	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 36.

The worst 5 of 2256 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:253:LYS:CA	1:A:253:LYS:C	1.76	1.54
1:C:253:LYS:CA	1:C:253:LYS:C	1.76	1.52
1:E:253:LYS:C	1:E:253:LYS:CA	1.77	1.50
2:D:700:LYS:CA	2:D:700:LYS:C	1.80	1.49
2:D:608:ARG:N	2:D:608:ARG:CA	1.73	1.47

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%)	418 (82%)	66 (13%)	28 (6%)	2	19
1	C	512/529 (97%)	418 (82%)	67 (13%)	27 (5%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	512/529 (97%)	416 (81%)	70 (14%)	26 (5%)	2	20
1	G	512/529 (97%)	412 (80%)	72 (14%)	28 (6%)	2	19
2	B	408/431 (95%)	310 (76%)	73 (18%)	25 (6%)	1	17
2	D	410/431 (95%)	307 (75%)	76 (18%)	27 (7%)	1	16
2	F	408/431 (95%)	309 (76%)	75 (18%)	24 (6%)	1	18
2	H	408/431 (95%)	308 (76%)	77 (19%)	23 (6%)	2	19
3	I	74/76 (97%)	65 (88%)	7 (10%)	2 (3%)	5	35
3	J	74/76 (97%)	65 (88%)	6 (8%)	3 (4%)	3	26
3	K	74/76 (97%)	66 (89%)	6 (8%)	2 (3%)	5	35
3	L	74/76 (97%)	66 (89%)	6 (8%)	2 (3%)	5	35
All	All	3978/4144 (96%)	3160 (79%)	601 (15%)	217 (6%)	2	19

5 of 217 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	ILE
1	A	259	PRO
1	A	262	GLU
1	A	275	ALA
1	A	533	GLN

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	450/461 (98%)	428 (95%)	22 (5%)	25	59
1	C	450/461 (98%)	428 (95%)	22 (5%)	25	59
1	E	450/461 (98%)	428 (95%)	22 (5%)	25	59
1	G	450/461 (98%)	427 (95%)	23 (5%)	24	58
2	B	334/379 (88%)	301 (90%)	33 (10%)	8	35
2	D	334/379 (88%)	302 (90%)	32 (10%)	8	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	334/379 (88%)	302 (90%)	32 (10%)	8	37
2	H	334/379 (88%)	304 (91%)	30 (9%)	9	39
3	I	66/66 (100%)	64 (97%)	2 (3%)	41	71
3	J	66/66 (100%)	63 (96%)	3 (4%)	27	62
3	K	66/66 (100%)	63 (96%)	3 (4%)	27	62
3	L	66/66 (100%)	63 (96%)	3 (4%)	27	62
All	All	3400/3624 (94%)	3173 (93%)	227 (7%)	16	50

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	43	THR
2	H	363	GLU
2	F	132	ASP
2	H	348	GLN
2	H	128	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	115	ASN
2	F	87	ASN
2	H	128	GLN
1	E	197	GLN
1	E	418	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 [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
4	ATP	H	8	-	26,33,33	1.42	4 (15%)	31,52,52	1.93	8 (25%)
4	ATP	B	5	-	26,33,33	1.60	5 (19%)	31,52,52	1.92	10 (32%)
4	ATP	F	7	-	26,33,33	1.46	5 (19%)	31,52,52	1.94	7 (22%)
4	ATP	D	6	-	26,33,33	1.31	4 (15%)	31,52,52	1.88	9 (29%)

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	ATP	H	8	-	-	10/18/38/38	0/3/3/3
4	ATP	B	5	-	-	9/18/38/38	0/3/3/3
4	ATP	F	7	-	-	7/18/38/38	0/3/3/3
4	ATP	D	6	-	-	9/18/38/38	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5	ATP	C2-N3	5.00	1.40	1.32
4	F	7	ATP	C2-N3	3.98	1.38	1.32
4	D	6	ATP	C2-N3	3.80	1.38	1.32
4	H	8	ATP	C2-N3	3.42	1.37	1.32
4	H	8	ATP	O4'-C1'	3.33	1.45	1.41

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	7	ATP	N3-C2-N1	-5.89	119.48	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	5	ATP	N3-C2-N1	-5.40	120.23	128.68
4	H	8	ATP	N3-C2-N1	-5.38	120.26	128.68
4	D	6	ATP	N3-C2-N1	-5.08	120.74	128.68
4	H	8	ATP	C5-C6-N6	4.51	127.20	120.35

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

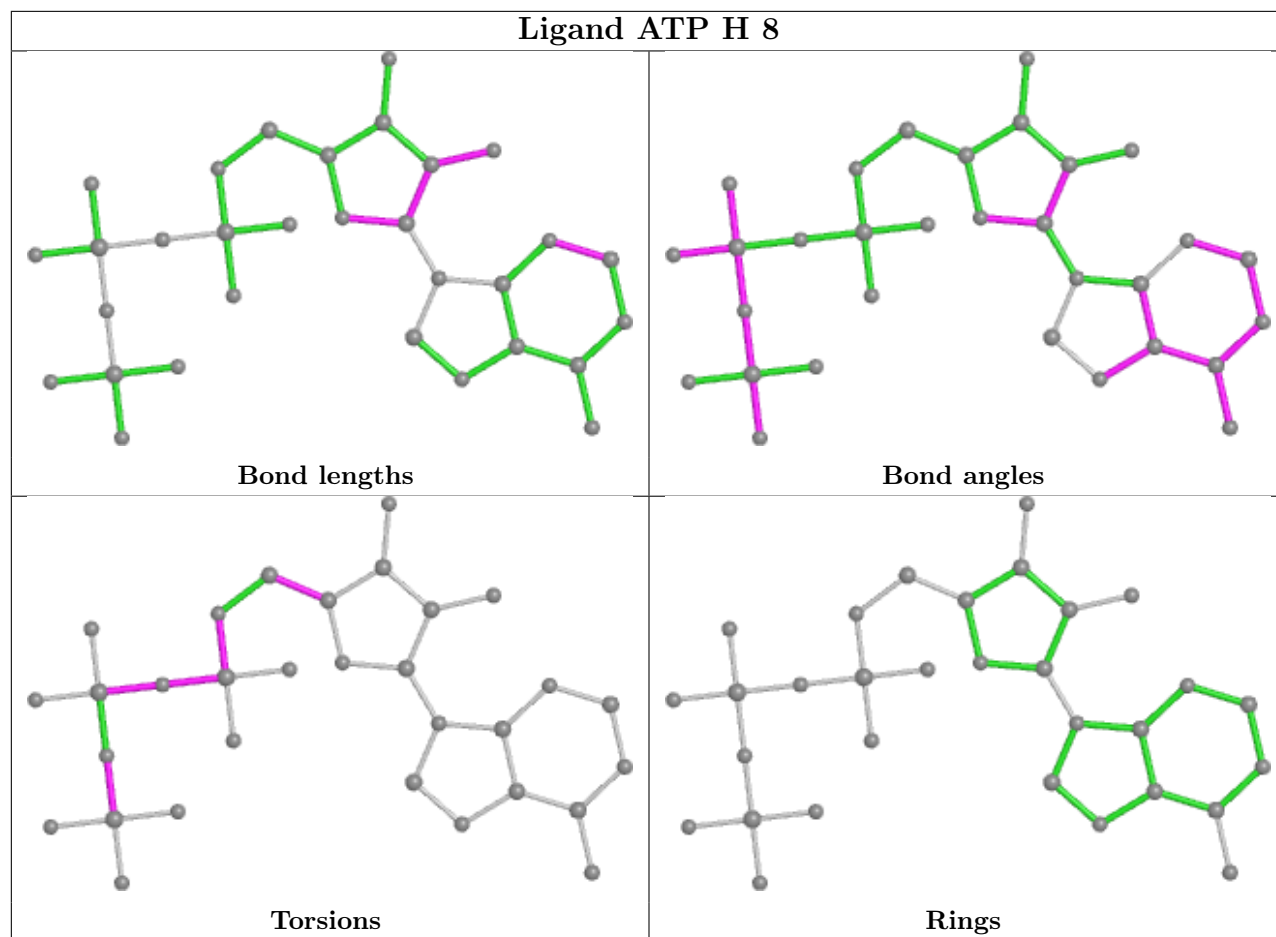
Mol	Chain	Res	Type	Atoms
4	B	5	ATP	C5'-O5'-PA-O3A
4	B	5	ATP	O4'-C4'-C5'-O5'
4	D	6	ATP	C5'-O5'-PA-O1A
4	D	6	ATP	C5'-O5'-PA-O2A
4	D	6	ATP	C5'-O5'-PA-O3A

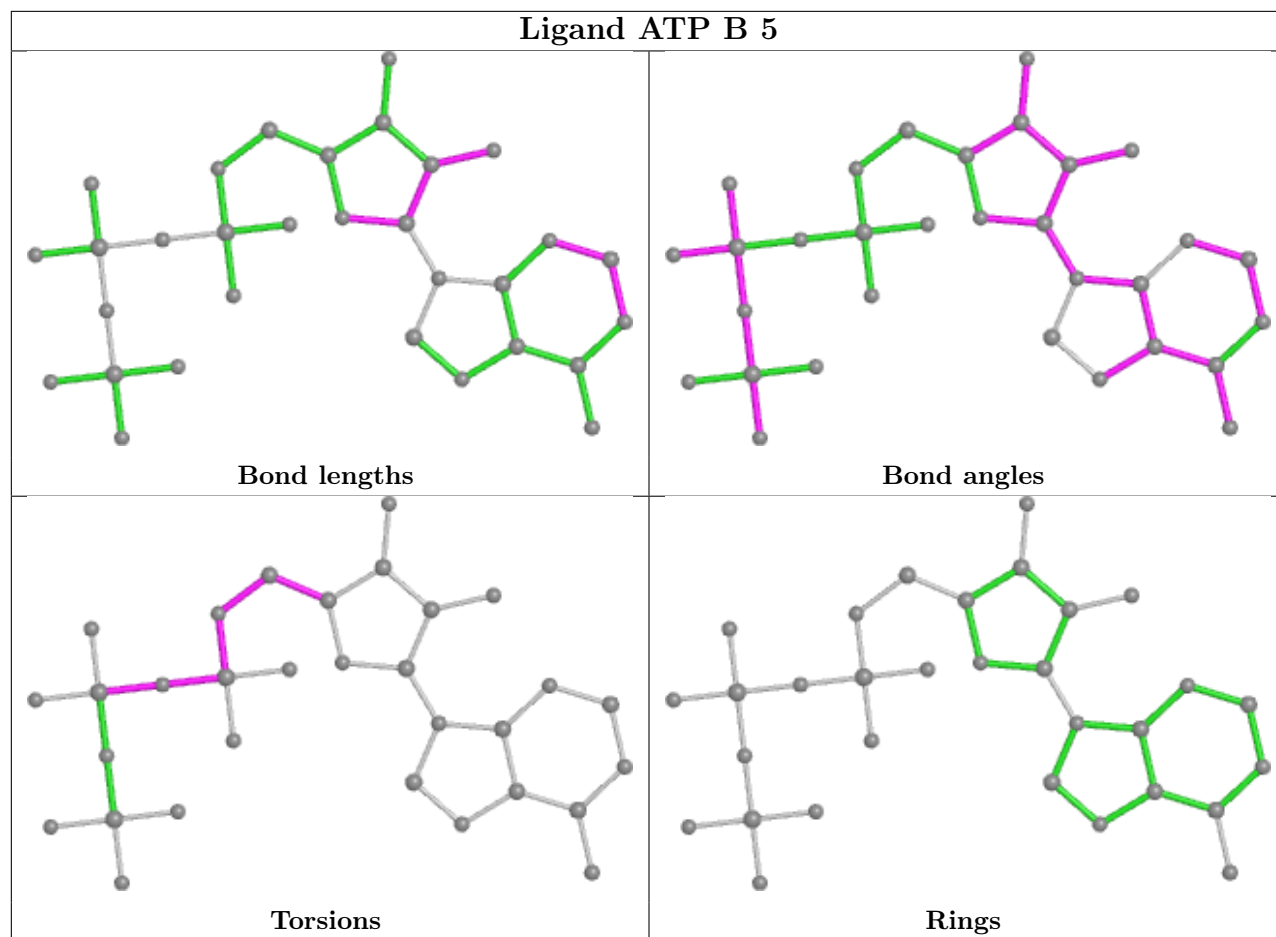
There are no ring outliers.

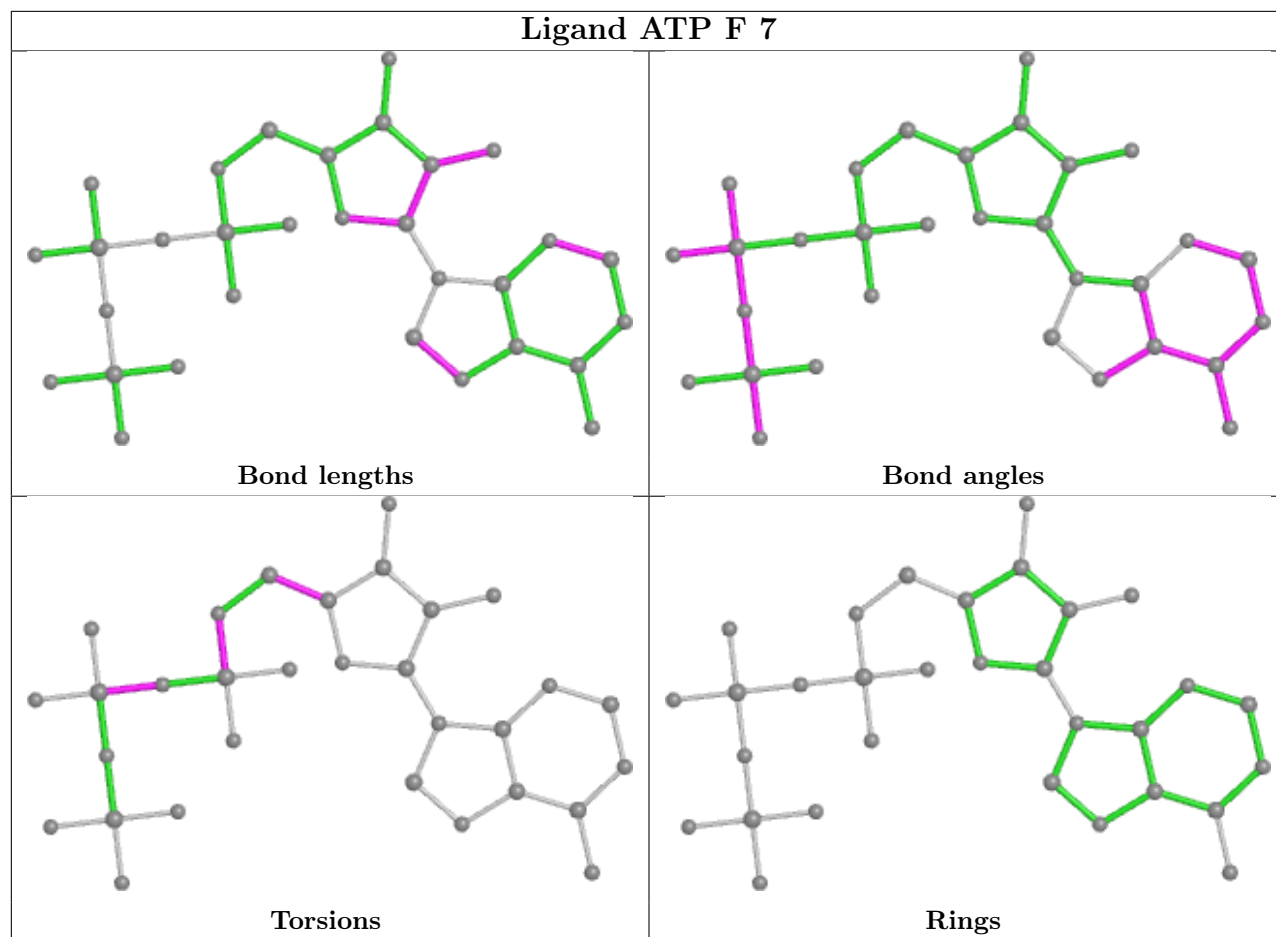
4 monomers are involved in 23 short contacts:

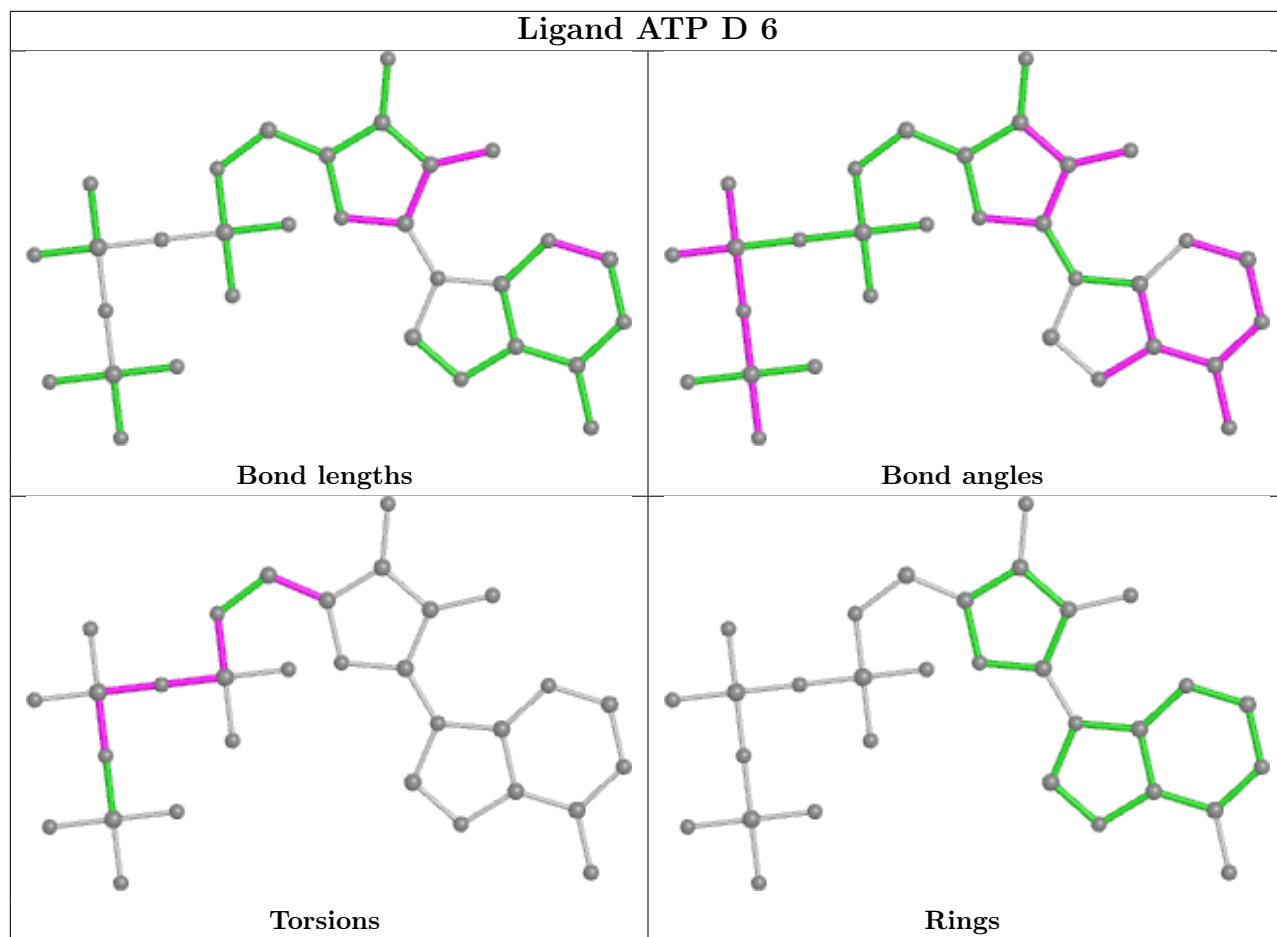
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	8	ATP	10	0
4	B	5	ATP	3	0
4	F	7	ATP	6	0
4	D	6	ATP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	D	2
2	B	1
2	H	1
2	F	1
1	C	1
1	A	1
1	G	1

The worst 5 of 8 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	2.96
1	D	396:SER	C	600:VAL	N	2.96
1	H	396:SER	C	600:VAL	N	2.96
1	F	396:SER	C	600:VAL	N	2.95
1	D	700:LYS	C	701:GLU	N	1.61

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.