Full wwPDB EM Validation Report ⓘ

Feb 20, 2025 – 03:48 PM EST

PDB ID	:	8K0G
EMDB ID	:	EMD-36764
Title	:	Cryo-EM structure of human 26S RP (Ed state) bound to K11/K48-branched ubiquitin (Ub) chain composed of four Ub.
Authors	:	Hsu, S.T.D.; Draczkowski, P.; Wang, Y.S.
Deposited on	:	2023-07-09
Resolution	:	3.80 Å(reported)
Based on initial model	:	6MSK

This is a Full wwPDB EM Validation 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/EMValidationReportHelp
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:

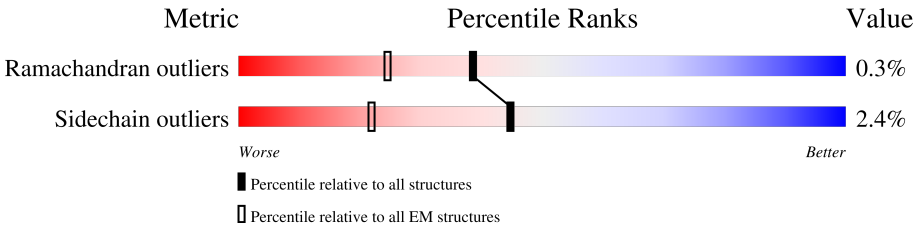
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	433	92% • 5%
2	B	440	91% • 8%
3	D	418	90% 9%
4	F	439	87% • 12%
5	C	406	95% • •
6	G	246	96% • •
7	H	234	97% • •
8	I	261	94% • 5%
9	J	248	96% •
10	K	241	94% • 5%

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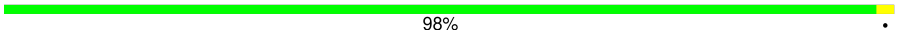
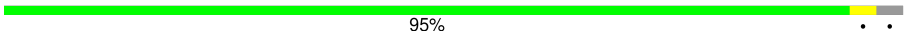
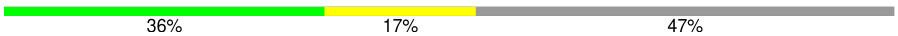
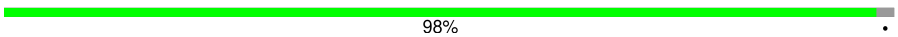
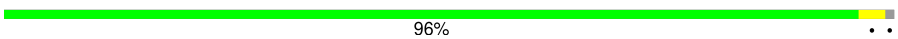
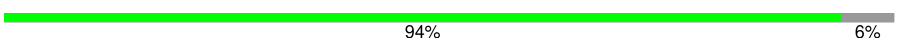
Mol	Chain	Length	Quality of chain
11	L	263	
12	M	255	
13	V	534	
14	W	456	
15	X	422	
16	Y	389	
17	d	350	
18	e	70	
19	f	908	
20	y	69	
21	E	389	
22	U	953	
23	Z	324	
24	a	376	
25	b	377	
26	c	310	
27	u	81	
27	v	81	
27	w	81	
27	x	81	

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 68848 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	413	3228	2032	567	611	18	0	0

- Molecule 2 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	404	3103	1953	532	604	14	0	0

- Molecule 3 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	380	3040	1923	524	580	13	0	0

- Molecule 4 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	387	2981	1879	518	567	17	0	0

- Molecule 5 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	391	3080	1937	552	573	18	0	0

- Molecule 6 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	239	1865	1186	309	357	13	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	230	Total	C	N	O	S	0	0
			1793	1147	302	338	6		

- Molecule 8 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	248	Total	C	N	O	S	0	0
			1954	1236	334	374	10		

- Molecule 9 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	239	Total	C	N	O	S	0	0
			1887	1183	334	365	5		

- Molecule 10 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	228	Total	C	N	O	S	0	0
			1753	1103	289	351	10		

- Molecule 11 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	238	Total	C	N	O	S	0	0
			1873	1172	337	353	11		

- Molecule 12 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

- Molecule 13 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	480	Total	C	N	O	S	0	0
			3197	1991	604	596	6		

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	380	Total	C	N	O	S	0	0
			2815	1779	490	537	9		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	d	257	Total	C	N	O	S	0	0
			1682	1057	304	316	5		

- Molecule 18 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	e	37	Total	C	N	O	S	0	0
			282	170	48	63	1		

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	f	889	Total	C	N	O	0	0
			4380	2602	889	889		

- Molecule 20 is a protein called Protein SIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	y	26	Total	C	N	O	S	0	0
			188	111	37	39	1		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	-9	MET	-	initiating methionine	UNP P38634
y	-8	GLU	-	expression tag	UNP P38634
y	-7	PHE	-	expression tag	UNP P38634
y	-2	PRO	-	insertion	UNP P38634
y	-1	PRO	-	insertion	UNP P38634
y	2	TYR	ARG	conflict	UNP P38634
y	26	ARG	LYS	conflict	UNP P38634
y	27	ALA	THR	conflict	UNP P38634
y	39	CYS	THR	conflict	UNP P38634
y	43	GLY	-	expression tag	UNP P38634
y	44	GLY	-	expression tag	UNP P38634
y	45	GLY	-	expression tag	UNP P38634
y	46	GLY	-	expression tag	UNP P38634
y	47	SER	-	expression tag	UNP P38634
y	48	LEU	-	expression tag	UNP P38634
y	49	PRO	-	expression tag	UNP P38634
y	50	GLU	-	expression tag	UNP P38634
y	51	THR	-	expression tag	UNP P38634
y	52	GLY	-	expression tag	UNP P38634
y	53	GLY	-	expression tag	UNP P38634
y	54	HIS	-	expression tag	UNP P38634
y	55	HIS	-	expression tag	UNP P38634
y	56	HIS	-	expression tag	UNP P38634
y	57	HIS	-	expression tag	UNP P38634
y	58	HIS	-	expression tag	UNP P38634
y	59	HIS	-	expression tag	UNP P38634

- Molecule 21 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	E	367	Total	C	N	O	S	0	0
			2900	1827	515	542	16		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	872	Total	C	N	O	S	0	0
			6590	4170	1136	1240	44		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 26 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 27 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	u	76	Total	C	N	O	S	0	0
			604	378	107	118	1		
27	v	76	Total	C	N	O	S	0	0
			603	378	107	117	1		
27	w	76	Total	C	N	O	S	0	0
			603	378	107	117	1		
27	x	76	Total	C	N	O	S	0	0
			603	378	107	117	1		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	-4	GLY	-	linker	UNP P0CG47
u	-3	SER	-	linker	UNP P0CG47
u	-2	GLY	-	linker	UNP P0CG47
u	-1	GLY	-	linker	UNP P0CG47
u	0	SER	-	linker	UNP P0CG47
u	63	ARG	LYS	engineered mutation	UNP P0CG47

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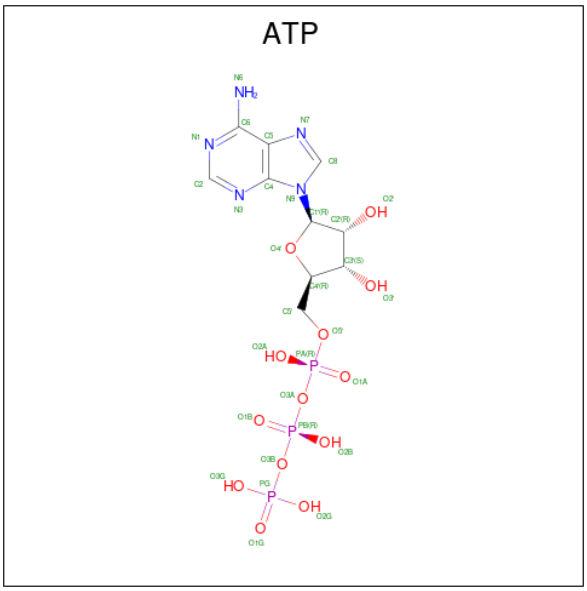
Chain	Residue	Modelled	Actual	Comment	Reference
v	-4	GLY	-	linker	UNP P0CG47
v	-3	SER	-	linker	UNP P0CG47
v	-2	GLY	-	linker	UNP P0CG47
v	-1	GLY	-	linker	UNP P0CG47
v	0	SER	-	linker	UNP P0CG47
v	63	ARG	LYS	engineered mutation	UNP P0CG47
w	-4	GLY	-	linker	UNP P0CG47
w	-3	SER	-	linker	UNP P0CG47
w	-2	GLY	-	linker	UNP P0CG47
w	-1	GLY	-	linker	UNP P0CG47
w	0	SER	-	linker	UNP P0CG47
w	63	ARG	LYS	engineered mutation	UNP P0CG47
x	-4	GLY	-	linker	UNP P0CG47
x	-3	SER	-	linker	UNP P0CG47
x	-2	GLY	-	linker	UNP P0CG47
x	-1	GLY	-	linker	UNP P0CG47
x	0	SER	-	linker	UNP P0CG47
x	63	ARG	LYS	engineered mutation	UNP P0CG47

- Molecule 28 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
28	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

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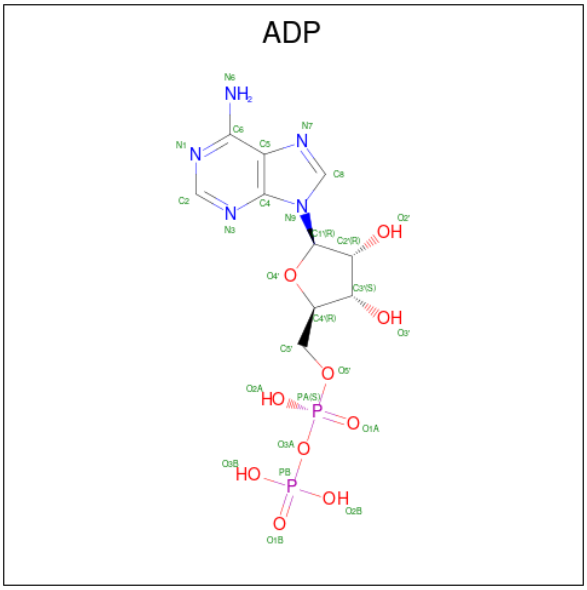
Mol	Chain	Residues	Atoms					AltConf
28	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 29 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
29	A	1	Total	Mg	0
			1	1	
29	B	1	Total	Mg	0
			1	1	
29	D	1	Total	Mg	0
			1	1	
29	C	1	Total	Mg	0
			1	1	

- Molecule 30 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



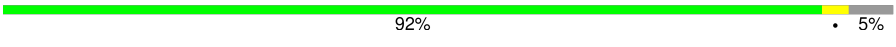
Mol	Chain	Residues	Atoms					AltConf
30	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
30	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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.

• Molecule 1: 26S protease regulatory subunit 7

Chain A:



• Molecule 2: 26S protease regulatory subunit 4

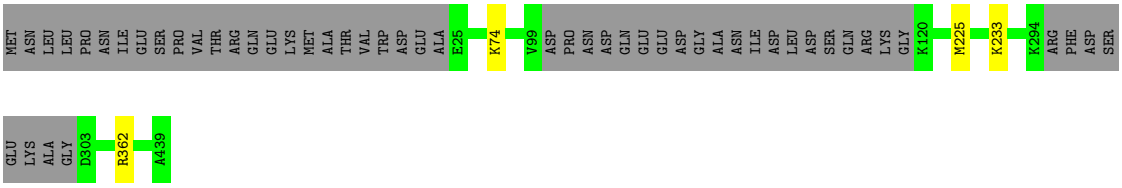
Chain B:

• Molecule 3: 26S protease regulatory subunit 6B

Chain D:

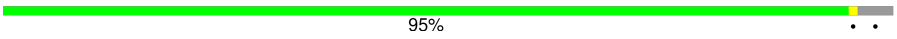
• Molecule 4: 26S protease regulatory subunit 6A

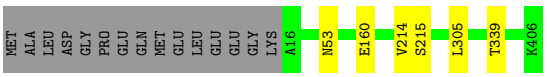
Chain F:



• Molecule 5: 26S protease regulatory subunit 8

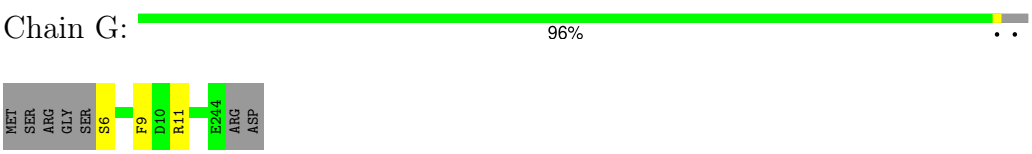
Chain C:





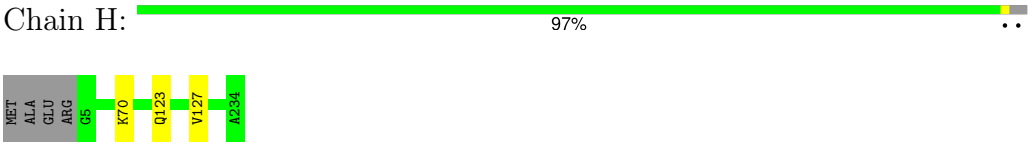
• Molecule 6: Proteasome subunit alpha type-6

Chain G:



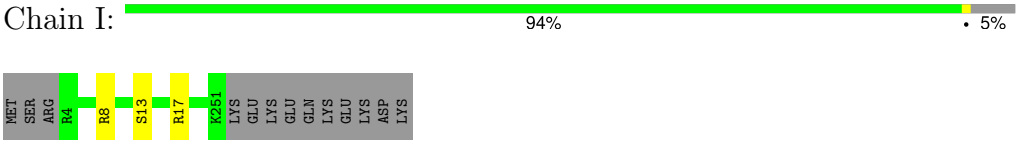
• Molecule 7: Proteasome subunit alpha type-2

Chain H:



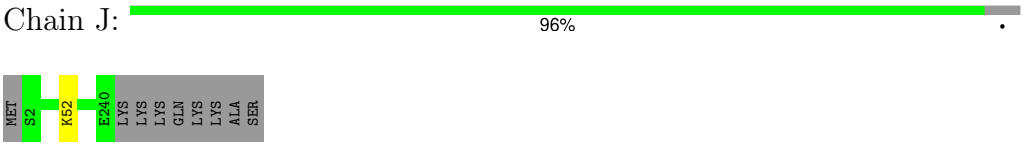
• Molecule 8: Proteasome subunit alpha type-4

Chain I:



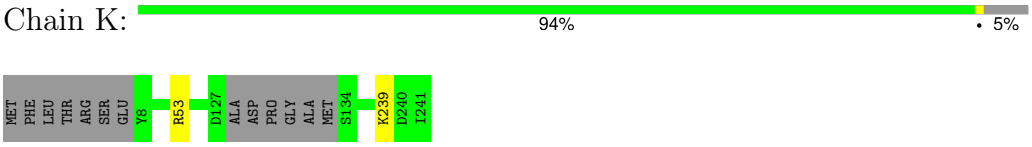
• Molecule 9: Proteasome subunit alpha type-7

Chain J:



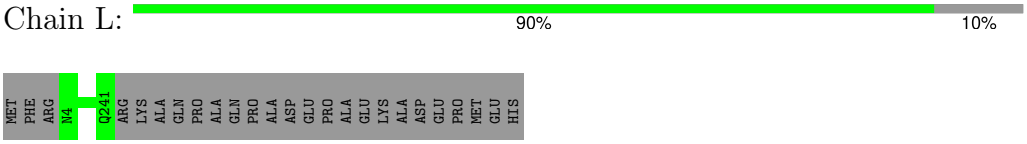
• Molecule 10: Proteasome subunit alpha type-5

Chain K:



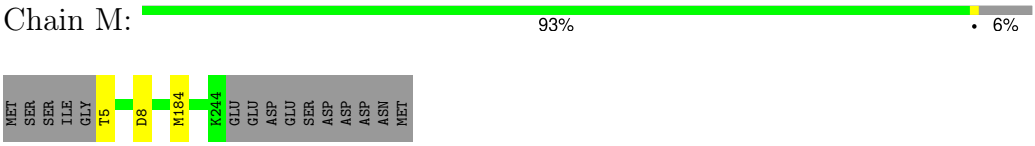
• Molecule 11: Proteasome subunit alpha type-1

Chain L:



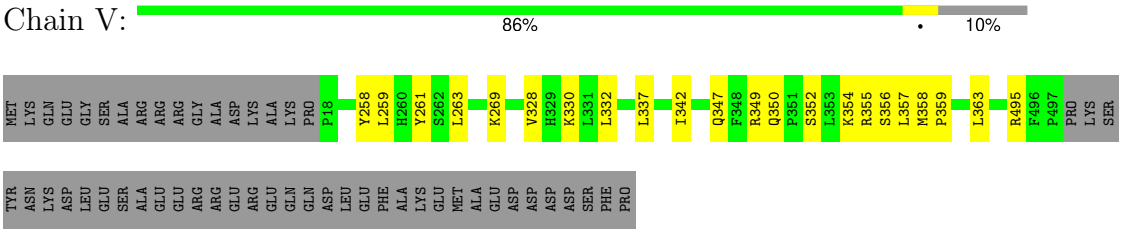
• Molecule 12: Proteasome subunit alpha type-3

Chain M:



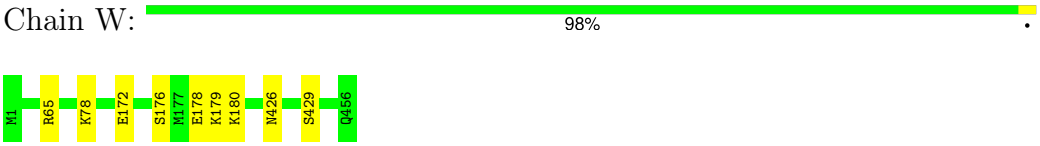
• Molecule 13: 26S proteasome non-ATPase regulatory subunit 3

Chain V:



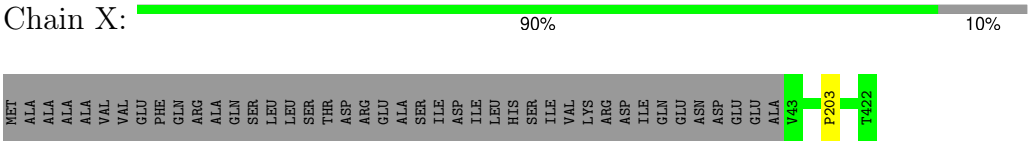
• Molecule 14: 26S proteasome non-ATPase regulatory subunit 12

Chain W:



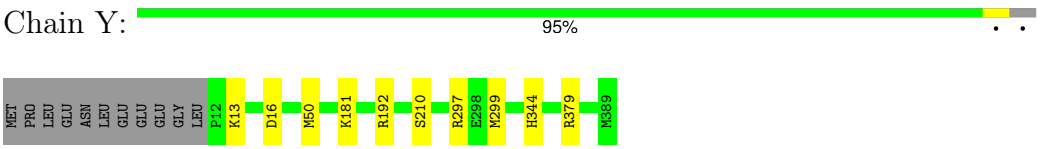
• Molecule 15: 26S proteasome non-ATPase regulatory subunit 11

Chain X:



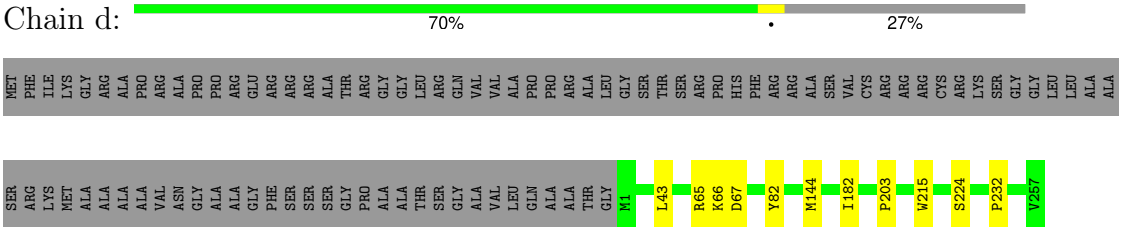
• Molecule 16: 26S proteasome non-ATPase regulatory subunit 6

Chain Y:



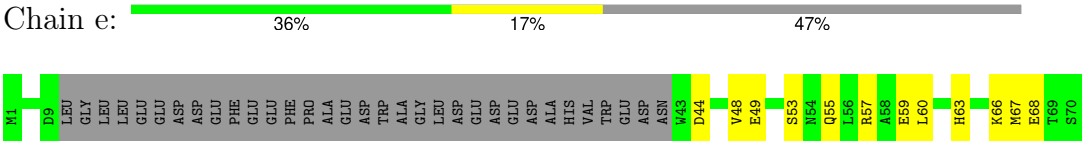
• Molecule 17: 26S proteasome non-ATPase regulatory subunit 8

Chain d:



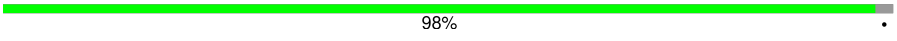
• Molecule 18: 26S proteasome complex subunit DSS1

Chain e:



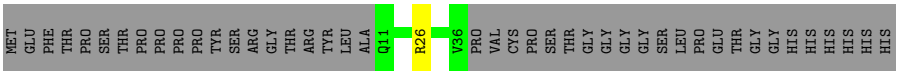
• Molecule 19: 26S proteasome non-ATPase regulatory subunit 2

Chain f:



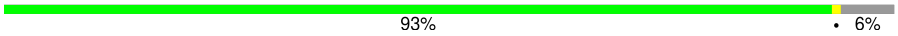
• Molecule 20: Protein SIC1

Chain y:



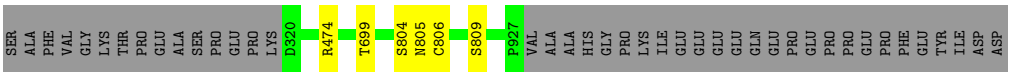
• Molecule 21: 26S protease regulatory subunit 10B

Chain E:



• Molecule 22: 26S proteasome non-ATPase regulatory subunit 1

Chain U:

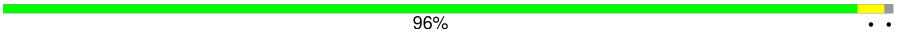


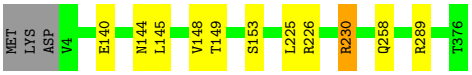
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 7

Chain Z:

• Molecule 24: 26S proteasome non-ATPase regulatory subunit 13

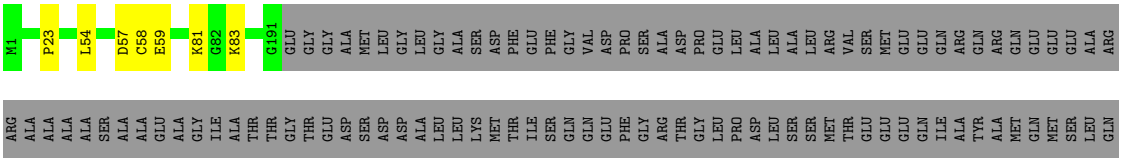
Chain a:

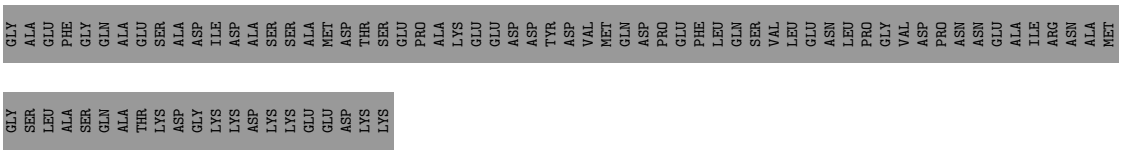




• Molecule 25: 26S proteasome non-ATPase regulatory subunit 4

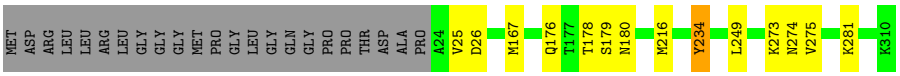
Chain b:





• Molecule 26: 26S proteasome non-ATPase regulatory subunit 14

Chain c:

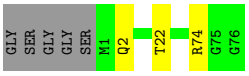


• Molecule 27: Polyubiquitin-B

Chain u:

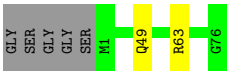
• Molecule 27: Polyubiquitin-B

Chain v:



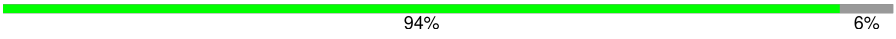
• Molecule 27: Polyubiquitin-B

Chain w:



• Molecule 27: Polyubiquitin-B

Chain x:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	84476	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	70000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP, MG

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	0.46	0/3281	0.62	0/4431
2	B	0.50	0/3148	0.66	0/4257
3	D	0.49	0/3090	0.61	0/4168
4	F	0.32	0/3018	0.55	0/4069
5	C	0.54	0/3121	0.67	1/4194 (0.0%)
6	G	0.38	0/1899	0.56	0/2568
7	H	0.40	0/1832	0.58	0/2481
8	I	0.36	0/1984	0.57	0/2672
9	J	0.38	0/1913	0.59	0/2581
10	K	0.41	0/1779	0.55	0/2400
11	L	0.36	0/1908	0.57	0/2579
12	M	0.37	0/1916	0.57	0/2580
13	V	0.36	0/3237	0.58	0/4419
14	W	0.35	0/3751	0.58	0/5042
15	X	0.37	0/2855	0.53	0/3865
16	Y	0.47	0/3173	0.64	0/4273
17	d	0.33	0/1702	0.54	0/2325
18	e	0.40	0/285	0.60	0/382
19	f	0.25	0/4379	0.44	0/6090
20	y	0.27	0/190	0.57	0/256
21	E	0.31	0/2943	0.58	0/3963
22	U	0.45	0/6700	0.58	0/9082
23	Z	0.52	0/2324	0.63	0/3150
24	a	0.38	0/3053	0.56	0/4133
25	b	0.38	0/1478	0.59	0/2001
26	c	0.50	0/2302	0.66	0/3110
27	u	0.40	0/610	0.63	0/819
27	v	0.25	0/609	0.54	0/819
27	w	0.32	0/609	0.57	0/819
27	x	0.28	0/609	0.60	0/819
All	All	0.41	0/69698	0.58	1/94347 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	305	LEU	CA-CB-CG	5.71	128.44	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 PDB entries followed by that with respect to all EM entries.

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	411/433 (95%)	369 (90%)	42 (10%)	0	100	100
2	B	402/440 (91%)	343 (85%)	57 (14%)	2 (0%)	25	58
3	D	378/418 (90%)	341 (90%)	35 (9%)	2 (0%)	25	58
4	F	381/439 (87%)	352 (92%)	29 (8%)	0	100	100
5	C	389/406 (96%)	355 (91%)	33 (8%)	1 (0%)	37	69
6	G	237/246 (96%)	230 (97%)	7 (3%)	0	100	100
7	H	228/234 (97%)	214 (94%)	14 (6%)	0	100	100
8	I	246/261 (94%)	222 (90%)	24 (10%)	0	100	100
9	J	237/248 (96%)	213 (90%)	24 (10%)	0	100	100
10	K	224/241 (93%)	208 (93%)	16 (7%)	0	100	100
11	L	236/263 (90%)	224 (95%)	12 (5%)	0	100	100
12	M	238/255 (93%)	229 (96%)	9 (4%)	0	100	100
13	V	478/534 (90%)	419 (88%)	56 (12%)	3 (1%)	22	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	W	454/456 (100%)	423 (93%)	31 (7%)	0	100	100
15	X	378/422 (90%)	353 (93%)	24 (6%)	1 (0%)	37	69
16	Y	376/389 (97%)	336 (89%)	38 (10%)	2 (0%)	25	58
17	d	255/350 (73%)	224 (88%)	26 (10%)	5 (2%)	6	32
18	e	33/70 (47%)	29 (88%)	4 (12%)	0	100	100
19	f	887/908 (98%)	749 (84%)	135 (15%)	3 (0%)	37	69
20	y	24/69 (35%)	21 (88%)	3 (12%)	0	100	100
21	E	363/389 (93%)	337 (93%)	23 (6%)	3 (1%)	16	49
22	U	868/953 (91%)	799 (92%)	69 (8%)	0	100	100
23	Z	284/324 (88%)	258 (91%)	26 (9%)	0	100	100
24	a	371/376 (99%)	335 (90%)	34 (9%)	2 (0%)	25	58
25	b	189/377 (50%)	171 (90%)	17 (9%)	1 (0%)	25	58
26	c	285/310 (92%)	245 (86%)	38 (13%)	2 (1%)	19	52
27	u	74/81 (91%)	68 (92%)	6 (8%)	0	100	100
27	v	74/81 (91%)	70 (95%)	4 (5%)	0	100	100
27	w	74/81 (91%)	72 (97%)	2 (3%)	0	100	100
27	x	74/81 (91%)	72 (97%)	2 (3%)	0	100	100
All	All	9148/10135 (90%)	8281 (90%)	840 (9%)	27 (0%)	38	69

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	V	269	LYS
17	d	203	PRO
17	d	232	PRO
19	f	756	PRO
21	E	175	PRO
13	V	359	PRO
16	Y	210	SER
19	f	762	VAL
25	b	23	PRO
2	B	40	THR
5	C	339	THR
21	E	122	MET
21	E	137	GLY
24	a	230	ARG

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Mol	Chain	Res	Type
13	V	495	ARG
17	d	224	SER
17	d	182	ILE
17	d	215	TRP
24	a	289	ARG
26	c	234	TYR
3	D	126	PRO
15	X	203	PRO
16	Y	344	HIS
19	f	345	PRO
26	c	216	MET
2	B	252	GLY
3	D	197	ASP

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 PDB entries followed by that with respect to all EM entries.

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	349/372 (94%)	335 (96%)	14 (4%)	27 50
2	B	334/385 (87%)	333 (100%)	1 (0%)	91 92
3	D	333/366 (91%)	333 (100%)	0	100 100
4	F	317/379 (84%)	313 (99%)	4 (1%)	65 76
5	C	340/352 (97%)	336 (99%)	4 (1%)	67 77
6	G	204/210 (97%)	201 (98%)	3 (2%)	60 74
7	H	188/191 (98%)	185 (98%)	3 (2%)	58 73
8	I	208/221 (94%)	205 (99%)	3 (1%)	62 75
9	J	203/211 (96%)	202 (100%)	1 (0%)	86 90
10	K	193/203 (95%)	191 (99%)	2 (1%)	73 80
11	L	204/224 (91%)	204 (100%)	0	100 100
12	M	198/212 (93%)	195 (98%)	3 (2%)	60 74
13	V	226/460 (49%)	207 (92%)	19 (8%)	9 32
14	W	416/416 (100%)	407 (98%)	9 (2%)	47 64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	X	267/362 (74%)	267 (100%)	0	100 100
16	Y	334/344 (97%)	326 (98%)	8 (2%)	44 62
17	d	111/294 (38%)	105 (95%)	6 (5%)	18 43
18	e	26/63 (41%)	14 (54%)	12 (46%)	0 0
20	y	22/57 (39%)	21 (96%)	1 (4%)	23 47
21	E	316/341 (93%)	313 (99%)	3 (1%)	75 82
22	U	677/816 (83%)	662 (98%)	15 (2%)	47 64
23	Z	257/295 (87%)	245 (95%)	12 (5%)	22 46
24	a	333/336 (99%)	323 (97%)	10 (3%)	36 58
25	b	167/312 (54%)	161 (96%)	6 (4%)	30 54
26	c	252/268 (94%)	239 (95%)	13 (5%)	19 44
27	u	68/70 (97%)	65 (96%)	3 (4%)	24 48
27	v	68/70 (97%)	65 (96%)	3 (4%)	24 48
27	w	68/70 (97%)	66 (97%)	2 (3%)	37 58
27	x	68/70 (97%)	68 (100%)	0	100 100
All	All	6747/7970 (85%)	6587 (98%)	160 (2%)	45 62

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	63	THR
1	A	66	LYS
1	A	70	THR
1	A	72	LEU
1	A	94	GLN
1	A	95	VAL
1	A	222	LYS
1	A	268	LYS
1	A	332	MET
1	A	369	ARG
1	A	428	ARG
1	A	430	MET
1	A	431	THR
2	B	116	ILE
4	F	74	LYS
4	F	225	MET

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Mol	Chain	Res	Type
4	F	233	LYS
4	F	362	ARG
5	C	53	ASN
5	C	160	GLU
5	C	214	VAL
5	C	215	SER
6	G	6	SER
6	G	9	PHE
6	G	11	ARG
7	H	70	LYS
7	H	123	GLN
7	H	127	VAL
8	I	8	ARG
8	I	13	SER
8	I	17	ARG
9	J	52	LYS
10	K	53	ARG
10	K	239	LYS
12	M	5	THR
12	M	8	ASP
12	M	184	MET
13	V	258	TYR
13	V	259	LEU
13	V	261	TYR
13	V	263	LEU
13	V	328	VAL
13	V	330	LYS
13	V	332	LEU
13	V	337	LEU
13	V	342	ILE
13	V	347	GLN
13	V	349	ARG
13	V	350	GLN
13	V	352	SER
13	V	354	LYS
13	V	355	ARG
13	V	356	SER
13	V	357	LEU
13	V	358	MET
13	V	363	LEU
14	W	65	ARG
14	W	78	LYS

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Mol	Chain	Res	Type
14	W	172	GLU
14	W	176	SER
14	W	178	GLU
14	W	179	LYS
14	W	180	LYS
14	W	426	ASN
14	W	429	SER
16	Y	13	LYS
16	Y	16	ASP
16	Y	50	MET
16	Y	181	LYS
16	Y	192	ARG
16	Y	297	ARG
16	Y	299	MET
16	Y	379	ARG
17	d	43	LEU
17	d	65	ARG
17	d	66	LYS
17	d	67	ASP
17	d	82	TYR
17	d	144	MET
18	e	44	ASP
18	e	48	VAL
18	e	49	GLU
18	e	53	SER
18	e	55	GLN
18	e	57	ARG
18	e	59	GLU
18	e	60	LEU
18	e	63	HIS
18	e	66	LYS
18	e	67	MET
18	e	68	GLU
20	y	26	ARG
21	E	122	MET
21	E	124	HIS
21	E	182	LEU
22	U	19	LEU
22	U	26	LYS
22	U	35	TRP
22	U	55	ARG
22	U	133	ILE

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Mol	Chain	Res	Type
22	U	136	LYS
22	U	139	GLN
22	U	140	ARG
22	U	149	GLN
22	U	474	ARG
22	U	699	THR
22	U	804	SER
22	U	805	ASN
22	U	806	CYS
22	U	809	SER
23	Z	15	VAL
23	Z	152	SER
23	Z	153	LYS
23	Z	154	THR
23	Z	175	LEU
23	Z	176	LEU
23	Z	178	ASP
23	Z	179	ILE
23	Z	180	LYS
23	Z	183	THR
23	Z	188	SER
23	Z	191	ILE
24	a	140	GLU
24	a	144	ASN
24	a	145	LEU
24	a	148	VAL
24	a	149	THR
24	a	153	SER
24	a	225	LEU
24	a	226	ARG
24	a	230	ARG
24	a	258	GLN
25	b	54	LEU
25	b	57	ASP
25	b	58	CYS
25	b	59	GLU
25	b	81	LYS
25	b	83	LYS
26	c	25	VAL
26	c	26	ASP
26	c	167	MET
26	c	176	GLN

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Mol	Chain	Res	Type
26	c	178	THR
26	c	179	SER
26	c	180	ASN
26	c	234	TYR
26	c	249	LEU
26	c	273	LYS
26	c	274	ASN
26	c	275	VAL
26	c	281	LYS
27	u	13	ILE
27	u	43	LEU
27	u	63	ARG
27	v	2	GLN
27	v	22	THR
27	v	74	ARG
27	w	49	GLN
27	w	63	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	305	GLN
7	H	21	GLN
14	W	86	ASN
14	W	444	HIS
21	E	280	ASN
21	E	339	ASN
23	Z	157	HIS
26	c	176	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)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
28	ATP	B	501	29	28,33,33	1.51	2 (7%)	34,52,52	0.75	1 (2%)
28	ATP	A	501	29	28,33,33	1.96	2 (7%)	34,52,52	0.84	1 (2%)
30	ADP	C	501	29	24,29,29	0.93	0	29,45,45	1.35	3 (10%)
30	ADP	D	501	29	24,29,29	0.82	0	29,45,45	1.29	4 (13%)
28	ATP	F	501	-	28,33,33	0.88	1 (3%)	34,52,52	0.62	1 (2%)

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
28	ATP	B	501	29	-	4/18/38/38	0/3/3/3
28	ATP	A	501	29	-	6/18/38/38	0/3/3/3
30	ADP	C	501	29	-	3/12/32/32	0/3/3/3
30	ADP	D	501	29	-	5/12/32/32	0/3/3/3
28	ATP	F	501	-	-	7/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	501	ATP	PB-O3B	-7.95	1.50	1.59
28	B	501	ATP	PA-O3A	-5.40	1.53	1.59
28	A	501	ATP	PA-O3A	-4.94	1.54	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	501	ATP	PB-O3B	-4.23	1.54	1.59
28	F	501	ATP	PB-O3B	-2.32	1.57	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	501	ADP	N3-C2-N1	-3.92	123.35	128.67
30	D	501	ADP	N3-C2-N1	-3.55	123.86	128.67
30	C	501	ADP	O3B-PB-O2B	2.54	117.34	107.80
28	F	501	ATP	C5-C6-N6	2.32	123.84	120.31
28	A	501	ATP	C5-C6-N6	2.29	123.81	120.31
28	B	501	ATP	C5-C6-N6	2.25	123.74	120.31
30	C	501	ADP	C5'-C4'-C3'	-2.14	107.52	115.21
30	D	501	ADP	C4-C5-N7	-2.11	107.11	109.34
30	D	501	ADP	O2A-PA-O1A	2.09	122.15	112.44
30	D	501	ADP	O3B-PB-O2B	2.06	115.52	107.80

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	501	ATP	C5'-O5'-PA-O1A
28	A	501	ATP	C5'-O5'-PA-O3A
28	A	501	ATP	O4'-C4'-C5'-O5'
28	F	501	ATP	PB-O3B-PG-O2G
28	F	501	ATP	PB-O3B-PG-O3G
30	D	501	ADP	C5'-O5'-PA-O2A
30	D	501	ADP	C5'-O5'-PA-O3A
30	D	501	ADP	O4'-C4'-C5'-O5'
28	B	501	ATP	C3'-C4'-C5'-O5'
30	C	501	ADP	C3'-C4'-C5'-O5'
30	D	501	ADP	C3'-C4'-C5'-O5'
30	C	501	ADP	O4'-C4'-C5'-O5'
28	A	501	ATP	C3'-C4'-C5'-O5'
28	B	501	ATP	O4'-C4'-C5'-O5'
28	F	501	ATP	PB-O3A-PA-O2A
28	A	501	ATP	C5'-O5'-PA-O2A
30	D	501	ADP	C5'-O5'-PA-O1A
30	C	501	ADP	C5'-O5'-PA-O3A
28	F	501	ATP	C4'-C5'-O5'-PA
28	B	501	ATP	PG-O3B-PB-O2B
28	F	501	ATP	C3'-C4'-C5'-O5'

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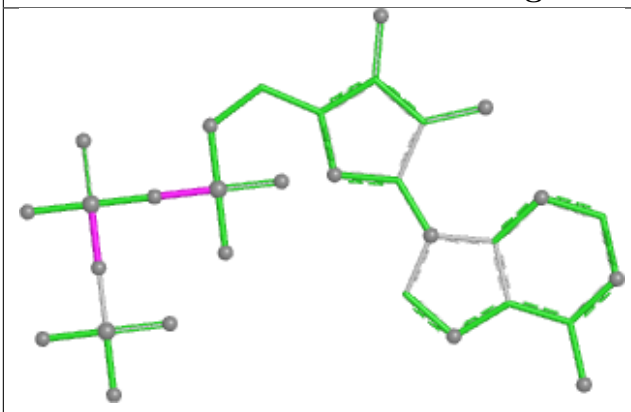
Mol	Chain	Res	Type	Atoms
28	A	501	ATP	PA-O3A-PB-O2B
28	B	501	ATP	PG-O3B-PB-O1B
28	F	501	ATP	PB-O3A-PA-O1A
28	F	501	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

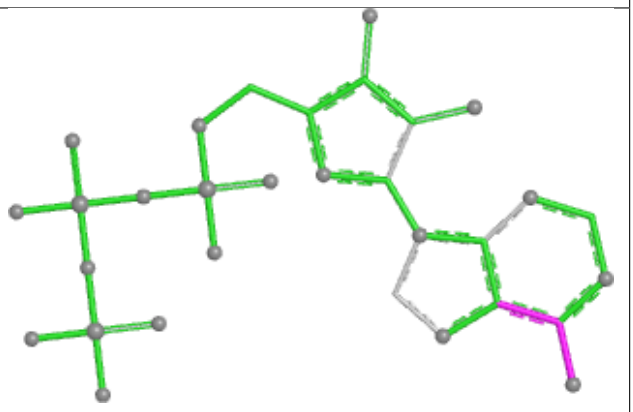
No monomer is involved in short contacts.

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 then 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.

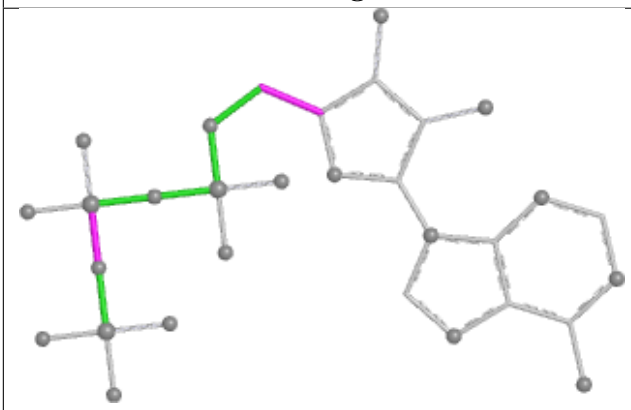
Ligand ATP B 501



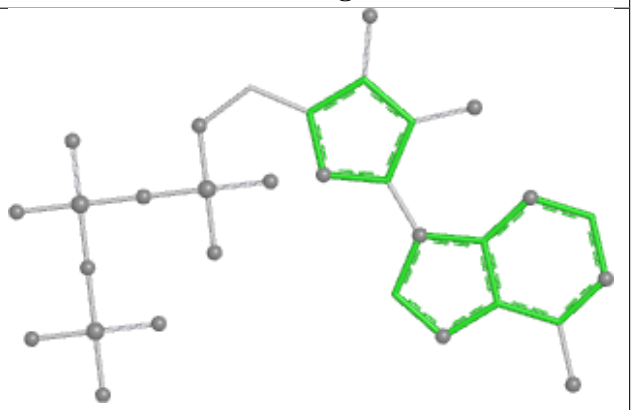
Bond lengths



Bond angles

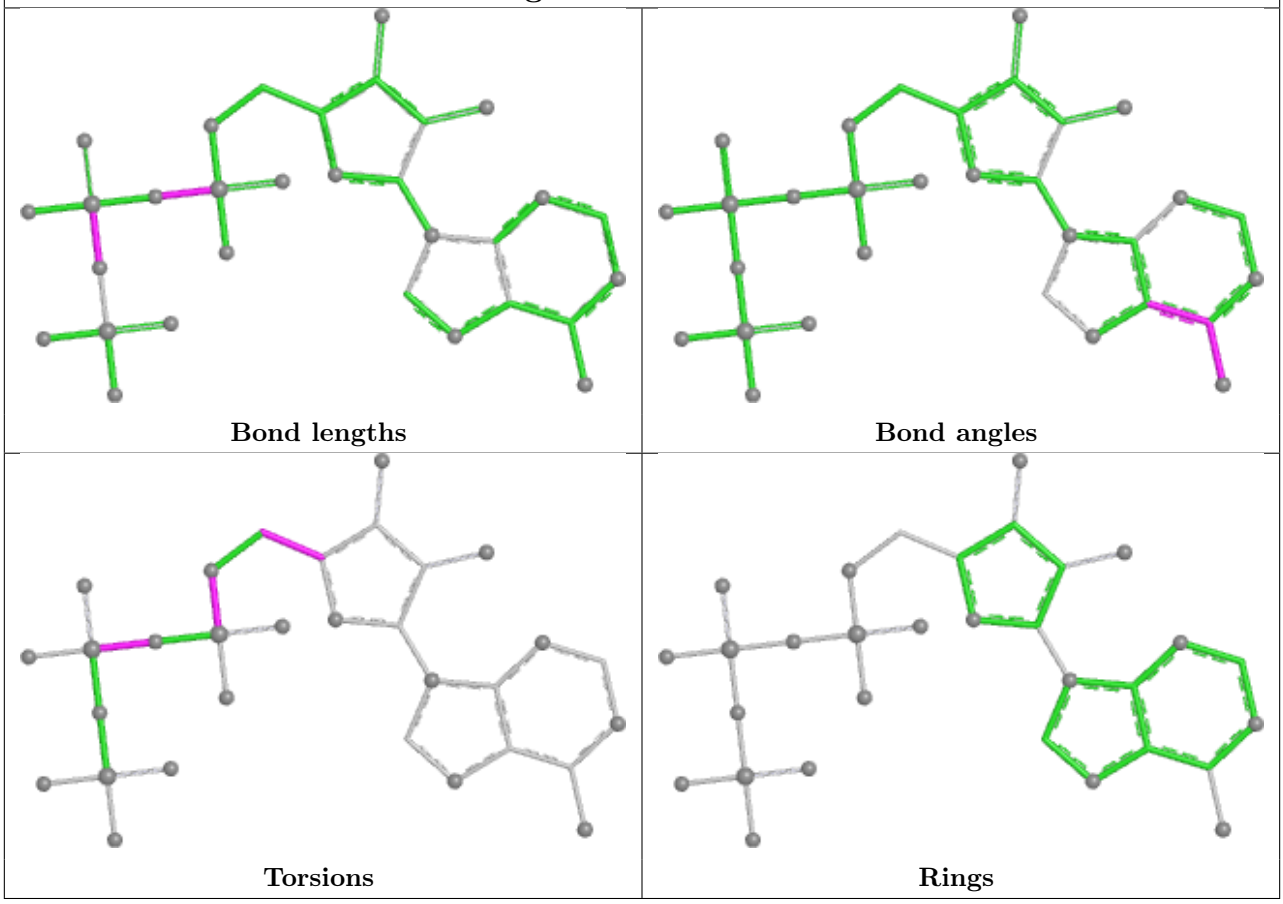


Torsions

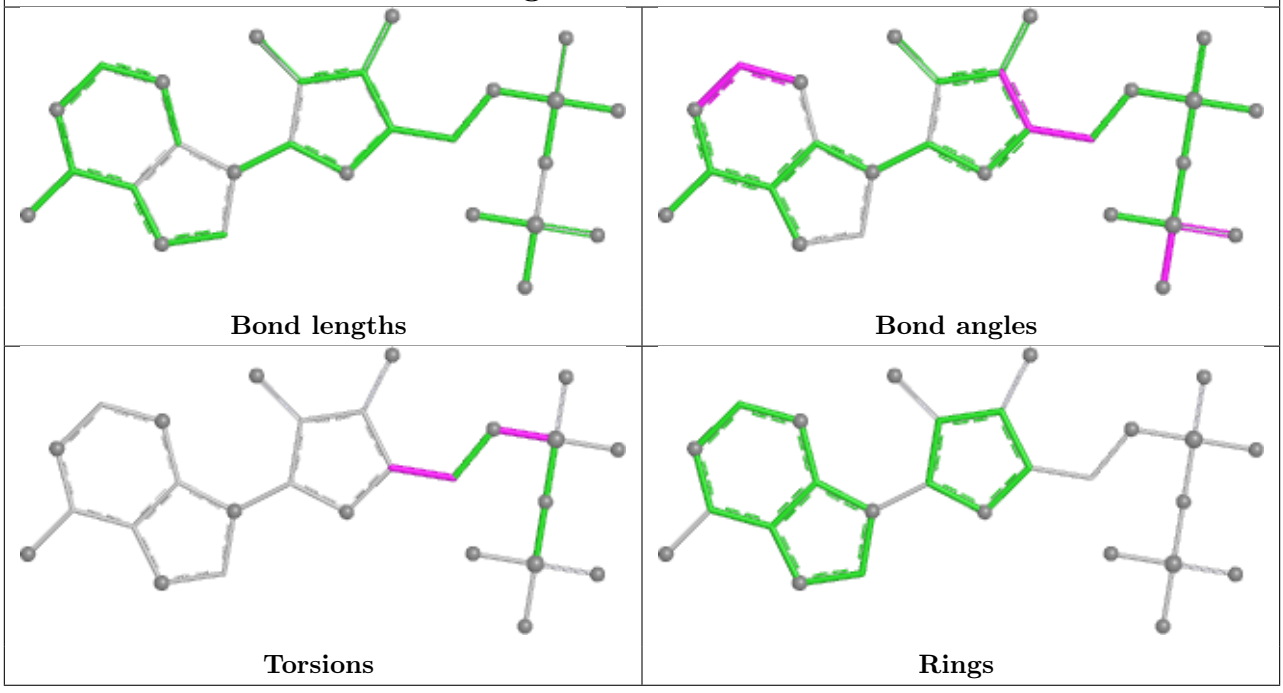


Rings

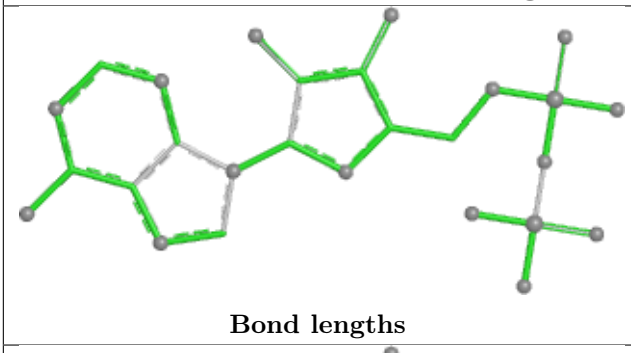
Ligand ATP A 501



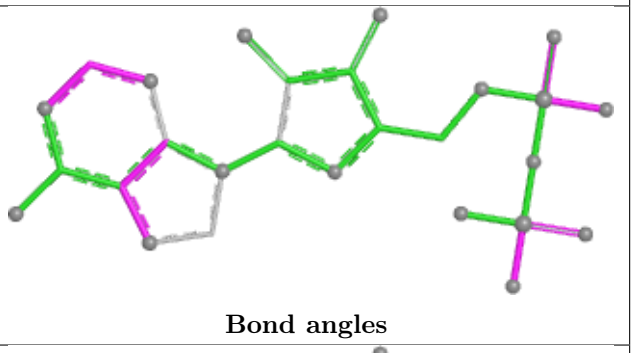
Ligand ADP C 501



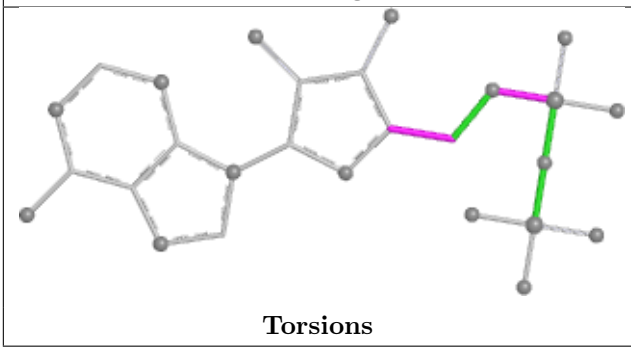
Ligand ADP D 501



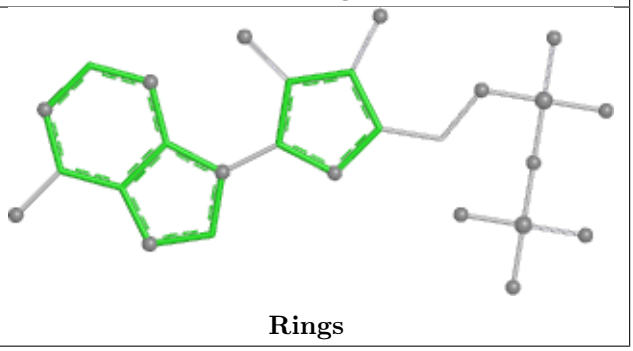
Bond lengths



Bond angles

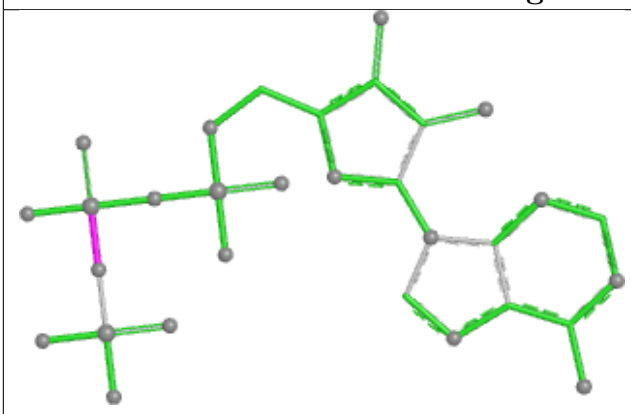


Torsions

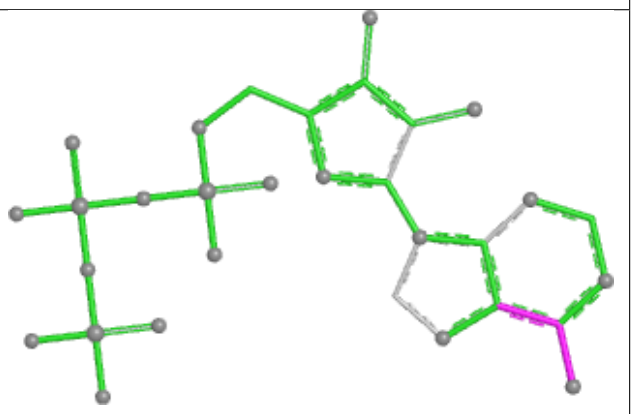


Rings

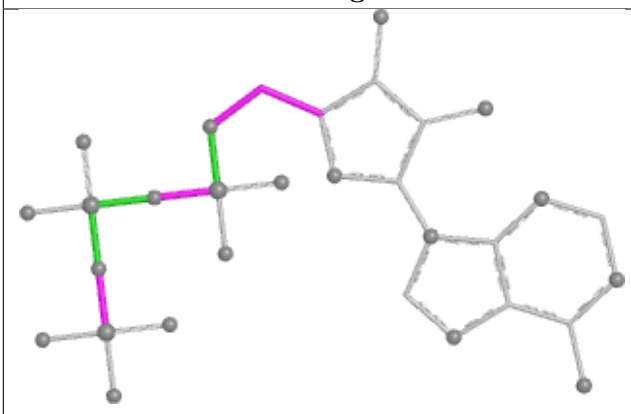
Ligand ATP F 501



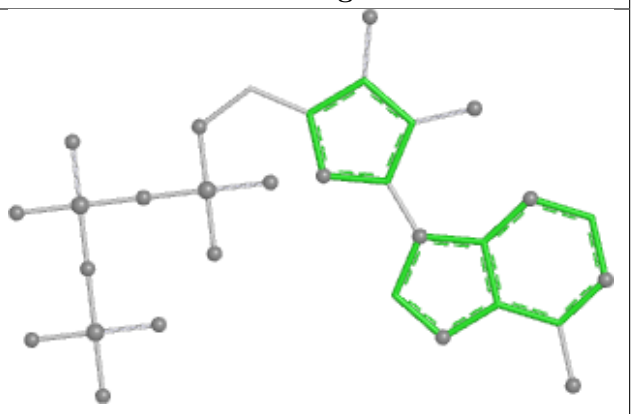
Bond lengths



Bond angles



Torsions



Rings

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 Map visualisation

This section contains visualisations of the EMDB entry EMD-36764. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.