wwPDB EM Validation Summary Report ⓘ

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PDB ID	:	5T0I
EMDB ID	:	EMD-8336
Title	:	Structural basis for dynamic regulation of the human 26S proteasome
Authors	:	Chen, S.; Wu, J.; Lu, Y.; Ma, Y.B.; Lee, B.H.; Yu, Z.; Ouyang, Q.; Finley, D.; Kirschner, M.W.; Mao, Y.
Deposited on	:	2016-08-16
Resolution	:	8.00 Å(reported)

This is a wwPDB EM 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/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:

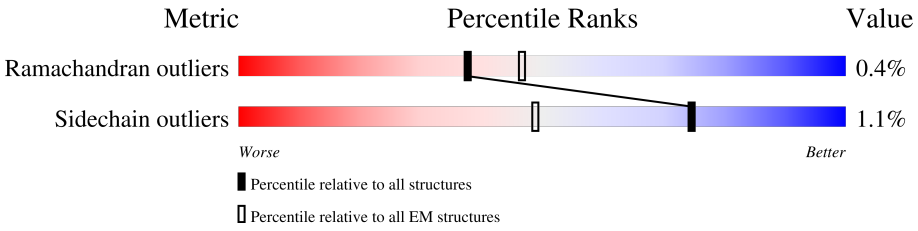
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 8.00 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)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	81% · 17%
2	B	440	77% · 21%
3	C	398	93% · ·
4	D	418	90% · 9%
5	E	403	87% · 12%
6	F	439	82% · 17%
7	G	245	96% · ·
8	H	233	100%
9	I	260	95% · ·
10	J	247	95% · ·

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Mol	Chain	Length	Quality of chain
11	K	240	93% 5%
12	L	268	88% 11%
13	M	254	94% 6%
14	N	238	80% 20%
15	O	276	79% 20%
16	P	204	100%
17	Q	201	99%
18	R	262	77% 23%
19	S	240	88% 11%
20	T	263	82% 18%
21	U	953	84% 15%
22	V	533	88% 10%
23	W	456	98%
24	X	422	57% 43%
25	Y	389	96%
26	Z	324	86% 12%
27	a	376	98%
28	b	377	50% 49%
29	c	309	87% 10%
30	d	349	72% 26%
31	e	70	56% 43%
32	f	749	90% 7%

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 76616 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	361	2835	1788	501	528	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	348	2717	1708	460	537	12	0	0

- Molecule 3 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	384	3015	1894	540	564	17	0	0

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

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

- Molecule 5 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	353	2790	1755	494	525	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	366	2863	1802	496	549	16	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	233	Total	C	N	O	S	0	0
			1713	1084	290	334	5		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 15 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 16 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 17 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 18 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 19 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

- Molecule 20 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	806	Total	C	N	O	S	0	0
			6287	3990	1075	1178	44		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	241	Total	C	N	O	S	0	0
			1905	1212	320	365	8		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	278	Total	C	N	O	S	0	0
			2187	1389	374	406	18		

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

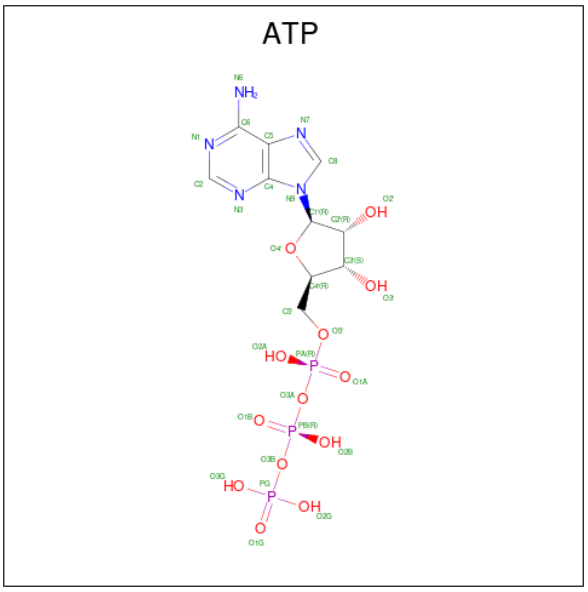
- Molecule 31 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	694	Total	C	N	O	S	0	0
			5331	3364	899	1027	41		

- Molecule 33 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
33	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
33	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
33	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

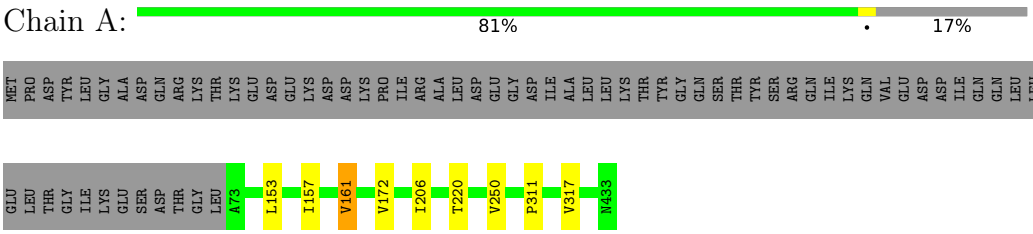
Mol	Chain	Residues	Atoms		AltConf
34	c	1	Total	Zn	0
			1	1	

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.

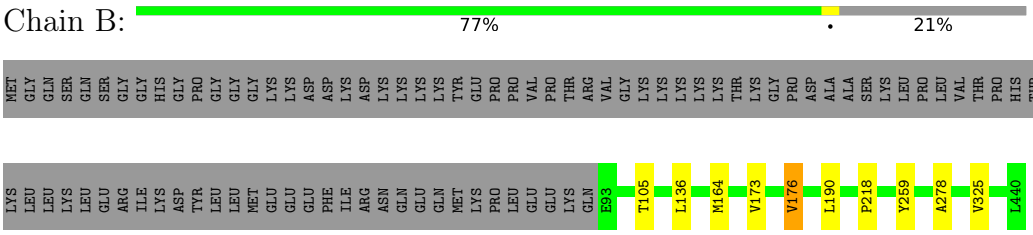
- Molecule 1: 26S protease regulatory subunit 7

Chain A:



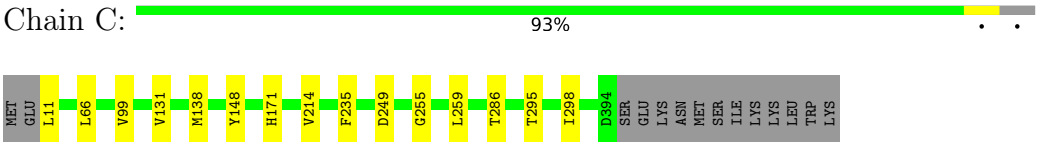
- Molecule 2: 26S protease regulatory subunit 4

Chain B:



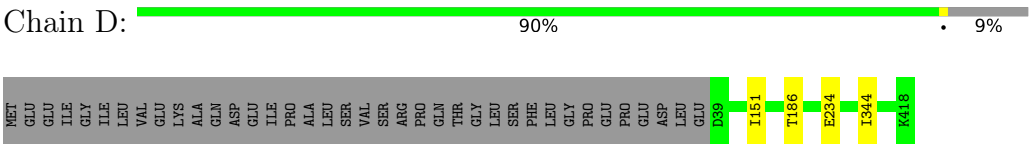
- Molecule 3: 26S protease regulatory subunit 8

Chain C:



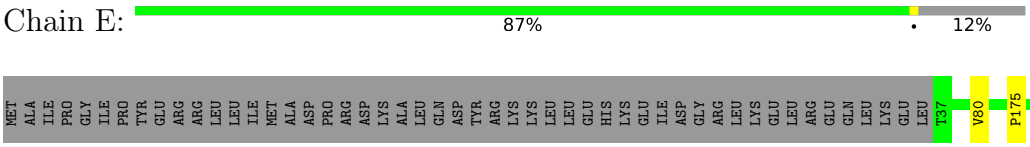
- Molecule 4: 26S protease regulatory subunit 6B

Chain D:



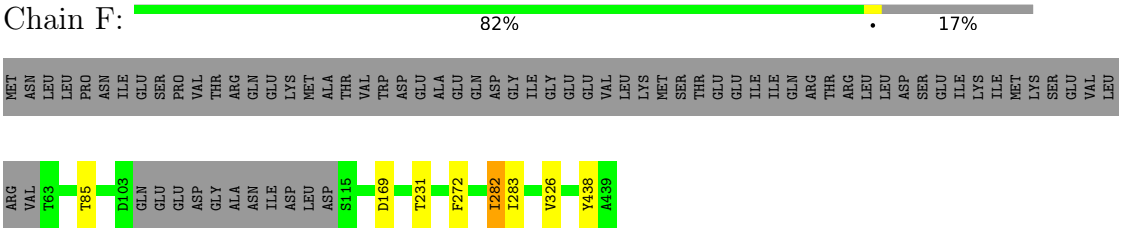
- Molecule 5: 26S protease regulatory subunit 10B

Chain E:



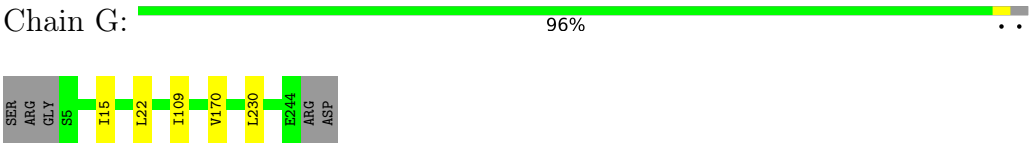
• Molecule 6: 26S protease regulatory subunit 6A

Chain F:



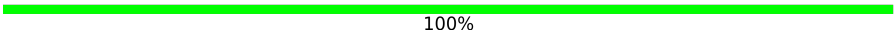
• Molecule 7: Proteasome subunit alpha type-6

Chain G:



• Molecule 8: Proteasome subunit alpha type-2

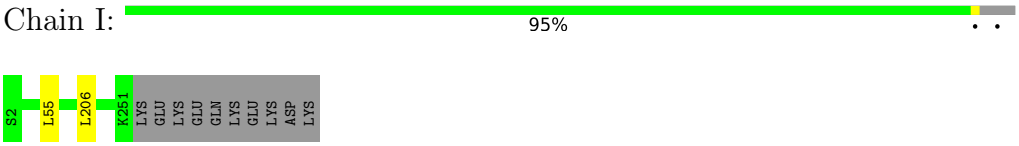
Chain H:



There are no outlier residues recorded for this chain.

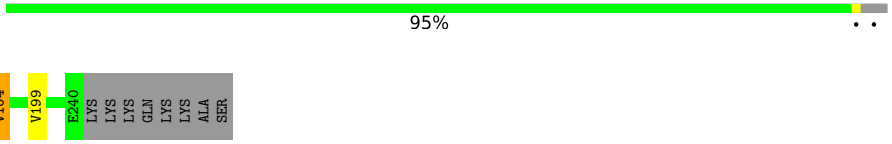
• Molecule 9: Proteasome subunit alpha type-4

Chain I:



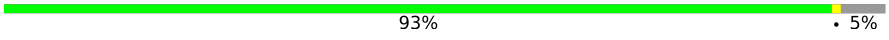
• Molecule 10: Proteasome subunit alpha type-7

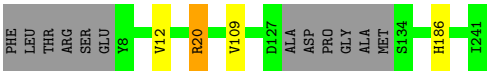
Chain J:



• Molecule 11: Proteasome subunit alpha type-5

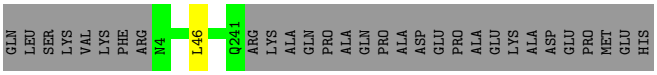
Chain K:





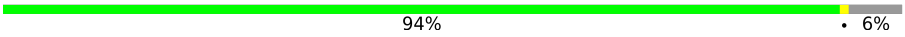
• Molecule 12: Proteasome subunit alpha type-1

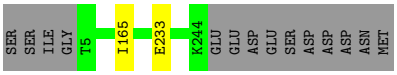
Chain L:



• Molecule 13: Proteasome subunit alpha type-3

Chain M:



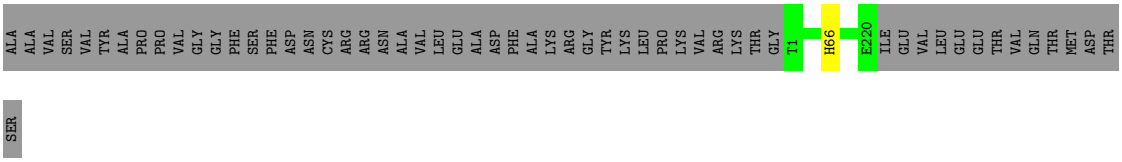


• Molecule 14: Proteasome subunit beta type-6

Chain N:

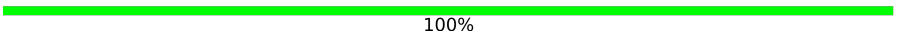
• Molecule 15: Proteasome subunit beta type-7

Chain O:



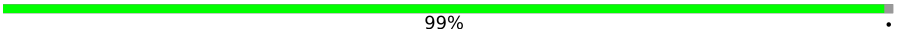
• Molecule 16: Proteasome subunit beta type-3

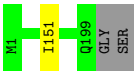
Chain P:



• Molecule 17: Proteasome subunit beta type-2

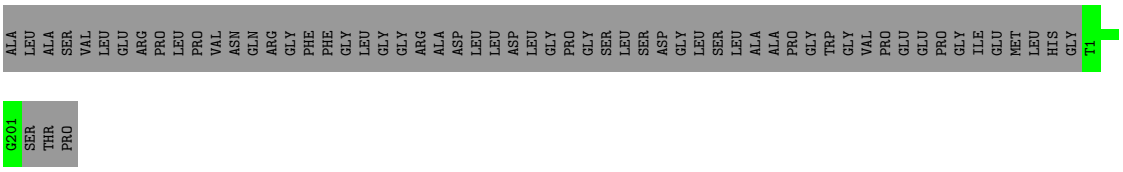
Chain Q:





• Molecule 18: Proteasome subunit beta type-5

Chain R:



• Molecule 19: Proteasome subunit beta type-1

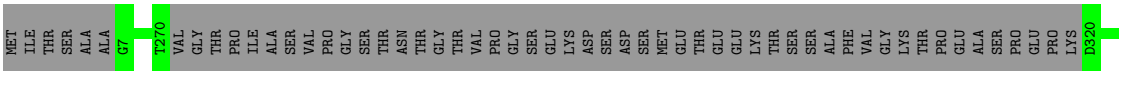
Chain S:

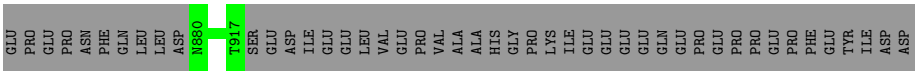
• Molecule 20: Proteasome subunit beta type-4

Chain T:

• Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

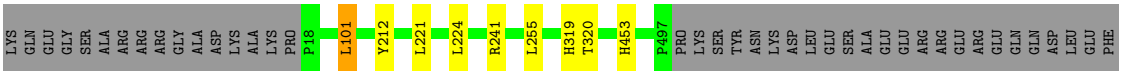
Chain U:





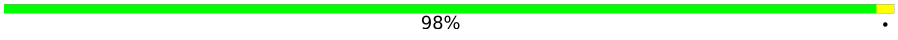
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

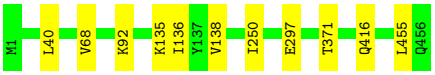
Chain V:



• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

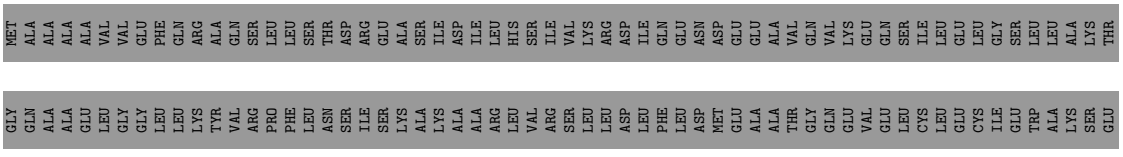
Chain W:

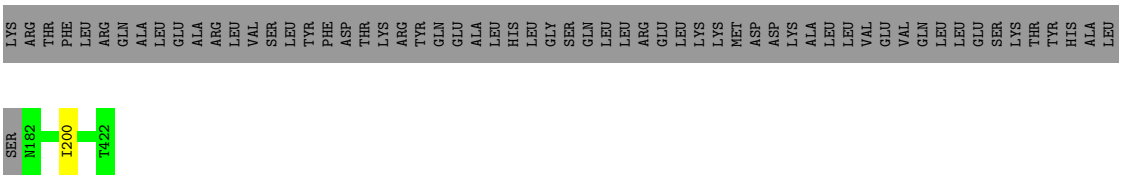




• Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

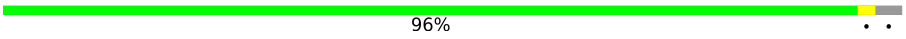
Chain X:

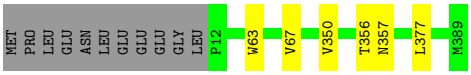




• Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

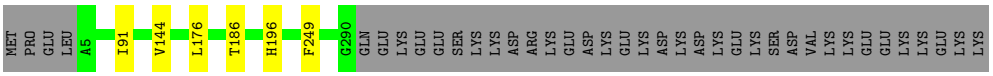
Chain Y:





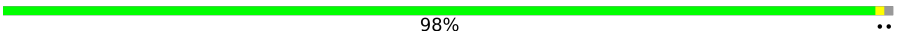
• Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

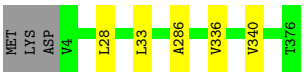
Chain Z:



• Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

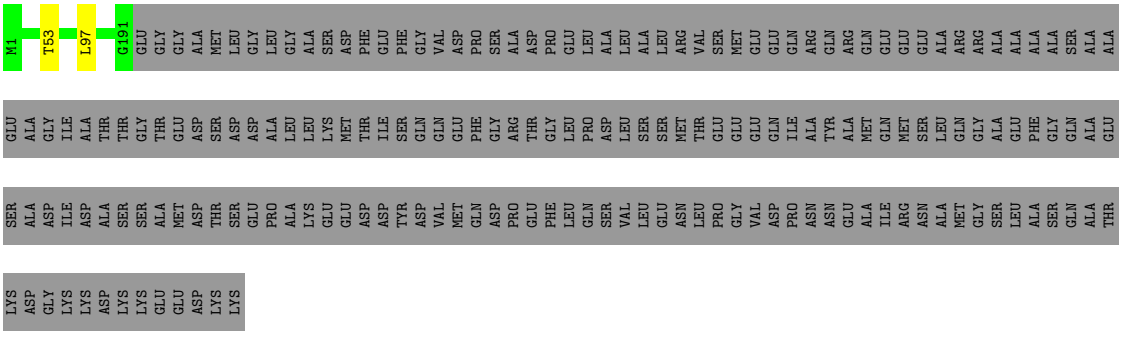
Chain a:





• Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

Chain b:

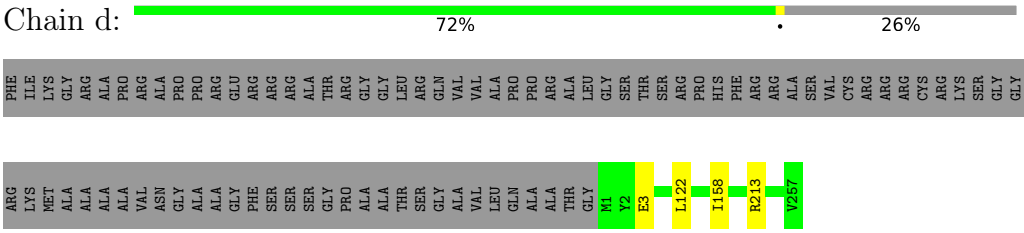


• Molecule 29: 26S proteasome non-ATPase regulatory subunit 14

Chain c:

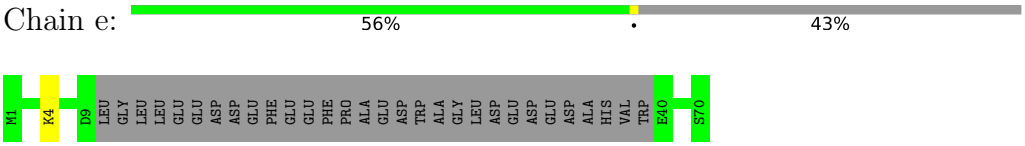
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 8

Chain d:



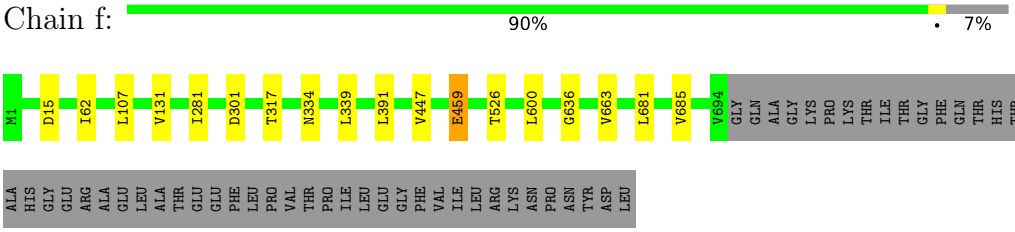
• Molecule 31: 26S proteasome complex subunit DSS1

Chain e:



• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2

Chain f:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10622	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k 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, 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	0.25	0/2886	0.48	0/3899
2	B	0.26	0/2757	0.57	0/3724
3	C	0.26	0/3054	0.48	0/4107
4	D	0.24	0/3090	0.46	0/4168
5	E	0.24	0/2835	0.44	0/3821
6	F	1.42	6/2903 (0.2%)	0.49	0/3912
7	G	0.24	0/1859	0.44	0/2523
8	H	0.24	0/1747	0.44	0/2376
9	I	0.24	0/1942	0.45	0/2628
10	J	0.25	0/1728	0.45	0/2358
11	K	1.56	1/1747 (0.1%)	0.53	2/2364 (0.1%)
12	L	0.24	0/1885	0.44	0/2552
13	M	0.25	0/1891	0.44	0/2552
14	N	0.24	0/1454	0.41	0/1967
15	O	0.24	0/1669	0.46	0/2262
16	P	0.24	0/1613	0.41	0/2174
17	Q	0.24	0/1603	0.42	0/2174
18	R	0.23	0/1579	0.39	0/2134
19	S	0.24	0/1671	0.41	0/2253
20	T	0.23	0/1700	0.41	0/2305
21	U	0.23	0/6396	0.41	0/8646
22	V	1.26	6/3929 (0.2%)	0.51	0/5309
23	W	0.24	0/3751	0.48	3/5042 (0.1%)
24	X	0.23	0/1936	0.43	0/2614
25	Y	0.24	0/3173	0.49	1/4273 (0.0%)
26	Z	0.24	0/2324	0.49	0/3150
27	a	0.23	0/3053	0.43	0/4133
28	b	0.25	0/1478	0.44	0/2001
29	c	0.27	1/2226 (0.0%)	0.48	0/3007
30	d	0.25	0/2162	0.50	0/2919
31	e	3.67	1/338 (0.3%)	0.74	2/450 (0.4%)
32	f	0.35	1/5413 (0.0%)	0.52	2/7317 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.57	16/77792 (0.0%)	0.47	10/105114 (0.0%)

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
2	B	0	2
3	C	0	2
22	V	0	2
23	W	0	1
25	Y	0	1
27	a	0	1
30	d	0	1
32	f	0	1
All	All	0	12

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	e	4	LYS	CD-CE	67.35	3.19	1.51
11	K	20	ARG	CB-CG	64.16	3.25	1.52
22	V	212	TYR	CD2-CE2	40.36	1.99	1.39
22	V	212	TYR	CD1-CE1	40.15	1.99	1.39
6	F	438	TYR	CD2-CE2	39.43	1.98	1.39

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	20	ARG	CA-CB-CG	10.22	135.88	113.40
11	K	20	ARG	CB-CG-CD	8.29	133.16	111.60
31	e	4	LYS	CD-CE-NZ	8.20	130.57	111.70
31	e	4	LYS	CG-CD-CE	7.33	133.88	111.90
32	f	459	GLU	N-CA-C	6.21	127.77	111.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	311	PRO	Peptide
2	B	176	VAL	Peptide
2	B	278	ALA	Peptide
3	C	171	HIS	Peptide
3	C	255	GLY	Peptide

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	359/433 (83%)	311 (87%)	44 (12%)	4 (1%)	14 52
2	B	346/440 (79%)	297 (86%)	46 (13%)	3 (1%)	17 57
3	C	382/398 (96%)	339 (89%)	41 (11%)	2 (0%)	29 69
4	D	378/418 (90%)	333 (88%)	44 (12%)	1 (0%)	41 77
5	E	351/403 (87%)	322 (92%)	28 (8%)	1 (0%)	41 77
6	F	362/439 (82%)	322 (89%)	38 (10%)	2 (1%)	25 66
7	G	238/245 (97%)	213 (90%)	23 (10%)	2 (1%)	19 60
8	H	229/233 (98%)	211 (92%)	18 (8%)	0	100 100
9	I	248/260 (95%)	220 (89%)	28 (11%)	0	100 100
10	J	237/247 (96%)	214 (90%)	20 (8%)	3 (1%)	12 48
11	K	224/240 (93%)	204 (91%)	18 (8%)	2 (1%)	17 57
12	L	236/268 (88%)	222 (94%)	14 (6%)	0	100 100
13	M	238/254 (94%)	216 (91%)	22 (9%)	0	100 100
14	N	189/238 (79%)	180 (95%)	9 (5%)	0	100 100
15	O	216/276 (78%)	197 (91%)	19 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	200/204 (98%)	185 (92%)	15 (8%)	0	100	100
17	Q	197/201 (98%)	180 (91%)	17 (9%)	0	100	100
18	R	199/262 (76%)	184 (92%)	15 (8%)	0	100	100
19	S	211/240 (88%)	200 (95%)	11 (5%)	0	100	100
20	T	213/263 (81%)	208 (98%)	5 (2%)	0	100	100
21	U	798/953 (84%)	735 (92%)	62 (8%)	1 (0%)	51	86
22	V	478/533 (90%)	413 (86%)	63 (13%)	2 (0%)	34	72
23	W	454/456 (100%)	407 (90%)	44 (10%)	3 (1%)	22	63
24	X	239/422 (57%)	213 (89%)	26 (11%)	0	100	100
25	Y	376/389 (97%)	335 (89%)	39 (10%)	2 (0%)	29	69
26	Z	284/324 (88%)	253 (89%)	30 (11%)	1 (0%)	34	72
27	a	371/376 (99%)	331 (89%)	38 (10%)	2 (0%)	29	69
28	b	189/377 (50%)	174 (92%)	15 (8%)	0	100	100
29	c	274/309 (89%)	242 (88%)	28 (10%)	4 (2%)	10	46
30	d	255/349 (73%)	227 (89%)	27 (11%)	1 (0%)	34	72
31	e	36/70 (51%)	31 (86%)	5 (14%)	0	100	100
32	f	686/749 (92%)	573 (84%)	109 (16%)	4 (1%)	25	66
All	All	9693/11269 (86%)	8692 (90%)	961 (10%)	40 (0%)	38	72

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	VAL
10	J	104	VAL
11	K	12	VAL
11	K	109	VAL
21	U	364	VAL

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	308/372 (83%)	303 (98%)	5 (2%)	62	79
2	B	304/385 (79%)	298 (98%)	6 (2%)	55	74
3	C	332/346 (96%)	321 (97%)	11 (3%)	38	61
4	D	333/366 (91%)	330 (99%)	3 (1%)	78	87
5	E	308/353 (87%)	306 (99%)	2 (1%)	86	92
6	F	312/379 (82%)	306 (98%)	6 (2%)	57	75
7	G	193/209 (92%)	190 (98%)	3 (2%)	62	79
8	H	164/190 (86%)	164 (100%)	0	100	100
9	I	193/220 (88%)	191 (99%)	2 (1%)	76	86
10	J	152/210 (72%)	150 (99%)	2 (1%)	69	81
11	K	186/202 (92%)	184 (99%)	2 (1%)	73	84
12	L	198/229 (86%)	197 (100%)	1 (0%)	88	93
13	M	192/211 (91%)	190 (99%)	2 (1%)	76	86
14	N	148/180 (82%)	147 (99%)	1 (1%)	84	90
15	O	177/227 (78%)	176 (99%)	1 (1%)	86	92
16	P	172/173 (99%)	171 (99%)	1 (1%)	86	92
17	Q	164/171 (96%)	163 (99%)	1 (1%)	86	92
18	R	153/201 (76%)	153 (100%)	0	100	100
19	S	174/198 (88%)	173 (99%)	1 (1%)	86	92
20	T	175/214 (82%)	175 (100%)	0	100	100
21	U	685/816 (84%)	681 (99%)	4 (1%)	86	92
22	V	414/459 (90%)	409 (99%)	5 (1%)	71	83
23	W	416/416 (100%)	412 (99%)	4 (1%)	76	86
24	X	208/362 (58%)	207 (100%)	1 (0%)	88	93
25	Y	334/344 (97%)	332 (99%)	2 (1%)	86	92
26	Z	257/295 (87%)	252 (98%)	5 (2%)	57	75
27	a	333/336 (99%)	331 (99%)	2 (1%)	86	92
28	b	167/312 (54%)	165 (99%)	2 (1%)	71	83
29	c	243/267 (91%)	240 (99%)	3 (1%)	71	83
30	d	231/293 (79%)	229 (99%)	2 (1%)	78	87
31	e	38/63 (60%)	38 (100%)	0	100	100
32	f	582/628 (93%)	571 (98%)	11 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	8246/9627 (86%)	8155 (99%)	91 (1%)	74 84

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	V	320	THR
27	a	28	LEU
23	W	250	ILE
25	Y	377	LEU
29	c	69	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
22	V	281	ASN
25	Y	365	GLN
22	V	459	GLN
23	W	444	HIS
26	Z	224	HIS

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 5 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
33	ATP	D	501	-	26,33,33	0.94	1 (3%)	31,52,52	1.52	5 (16%)
33	ATP	F	501	-	26,33,33	0.94	1 (3%)	31,52,52	1.64	5 (16%)
33	ATP	A	501	-	26,33,33	0.93	1 (3%)	31,52,52	1.62	5 (16%)
33	ATP	E	401	-	26,33,33	0.93	1 (3%)	31,52,52	1.61	5 (16%)

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
33	ATP	D	501	-	-	4/18/38/38	0/3/3/3
33	ATP	F	501	-	-	4/18/38/38	0/3/3/3
33	ATP	A	501	-	-	3/18/38/38	0/3/3/3
33	ATP	E	401	-	-	3/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	F	501	ATP	C5-C4	2.50	1.47	1.40
33	E	401	ATP	C5-C4	2.49	1.47	1.40
33	D	501	ATP	C5-C4	2.49	1.47	1.40
33	A	501	ATP	C5-C4	2.46	1.47	1.40

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	F	501	ATP	PA-O3A-PB	-4.31	118.02	132.83
33	A	501	ATP	PA-O3A-PB	-3.98	119.18	132.83
33	E	401	ATP	PB-O3B-PG	-3.76	119.92	132.83
33	D	501	ATP	PB-O3B-PG	-3.71	120.11	132.83
33	D	501	ATP	PA-O3A-PB	-3.63	120.36	132.83

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

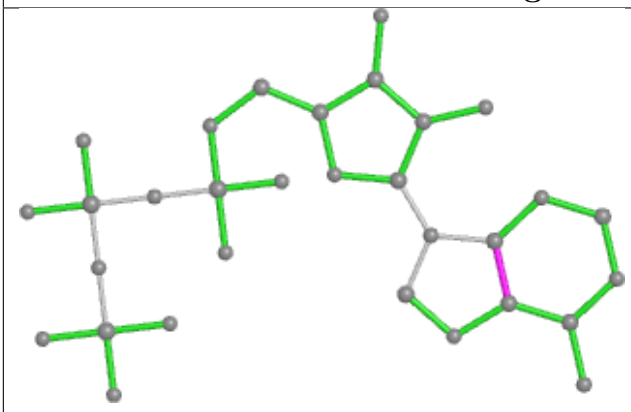
Mol	Chain	Res	Type	Atoms
33	D	501	ATP	C5'-O5'-PA-O1A
33	F	501	ATP	C5'-O5'-PA-O3A
33	F	501	ATP	O4'-C4'-C5'-O5'
33	F	501	ATP	C3'-C4'-C5'-O5'
33	D	501	ATP	PB-O3A-PA-O5'

There are no ring outliers.

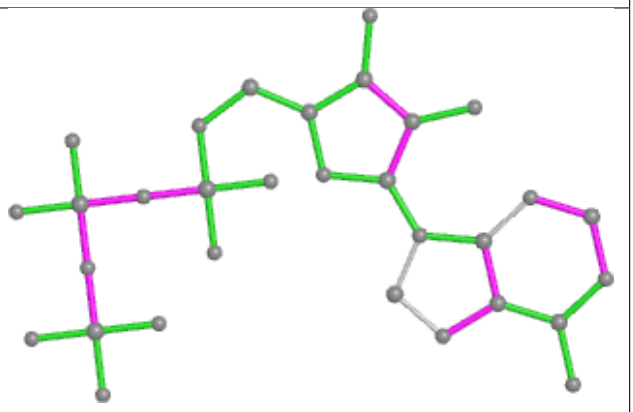
No monomer is involved in short contacts.

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.

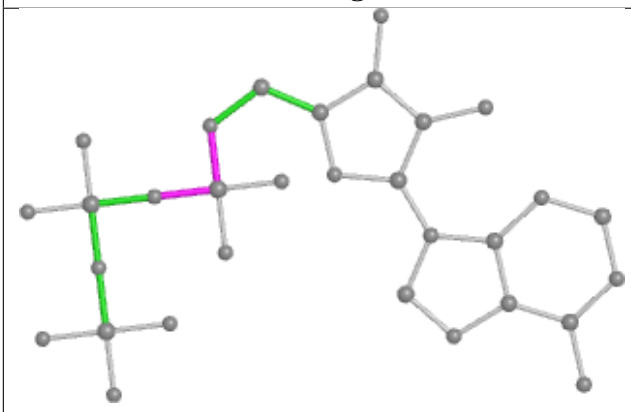
Ligand ATP D 501



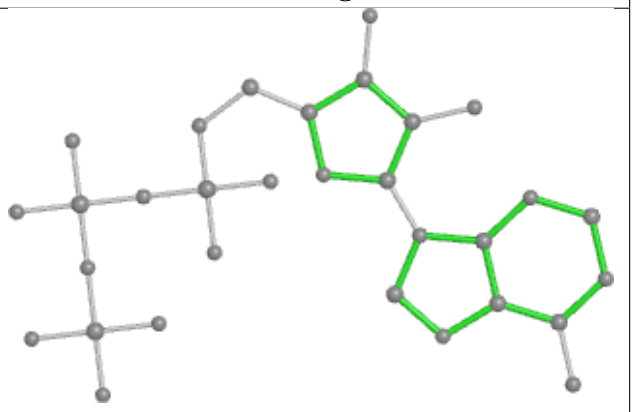
Bond lengths



Bond angles

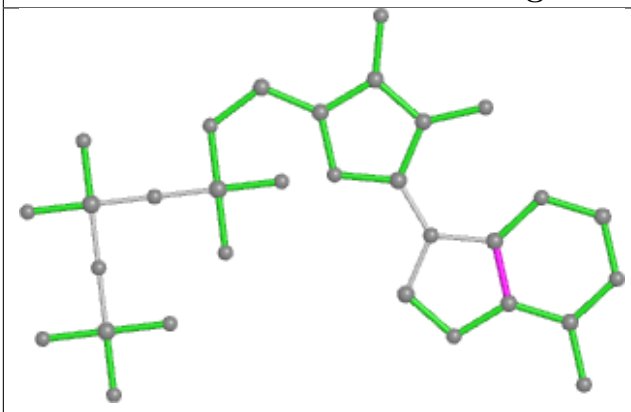


Torsions

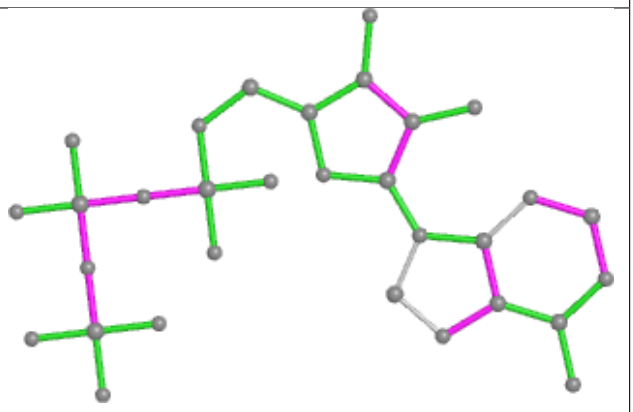


Rings

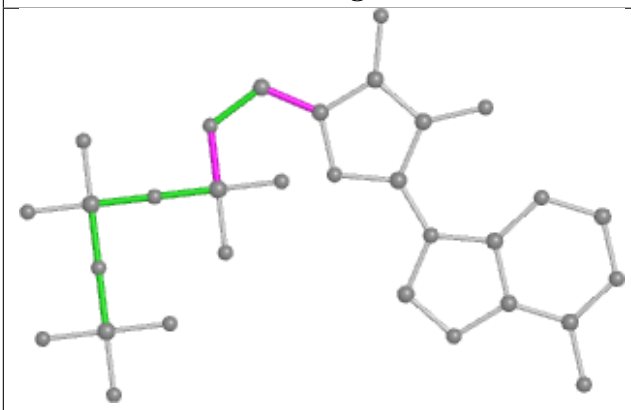
Ligand ATP F 501



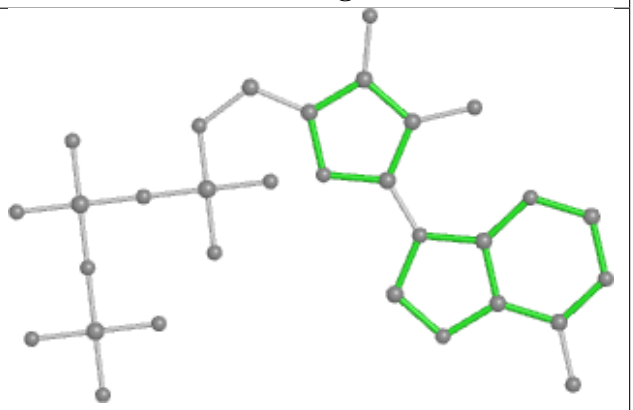
Bond lengths



Bond angles

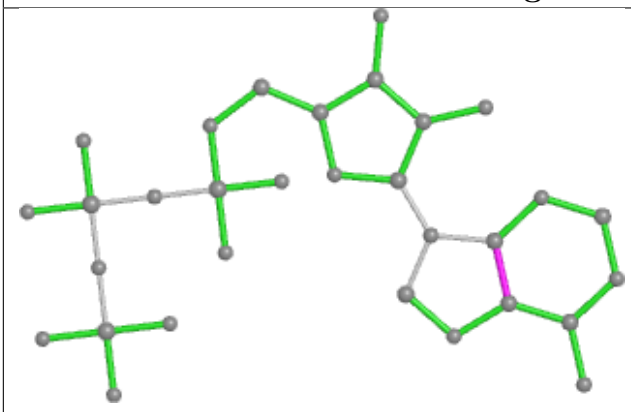


Torsions

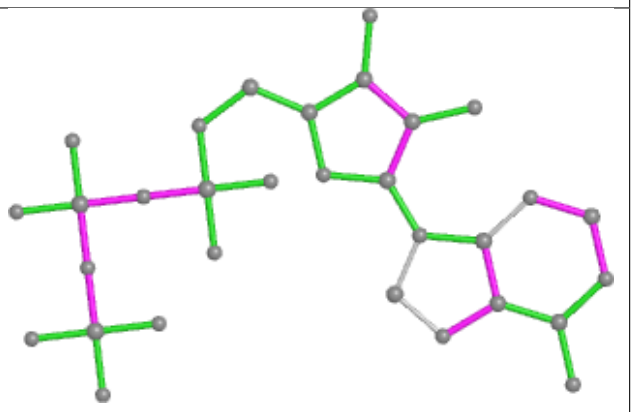


Rings

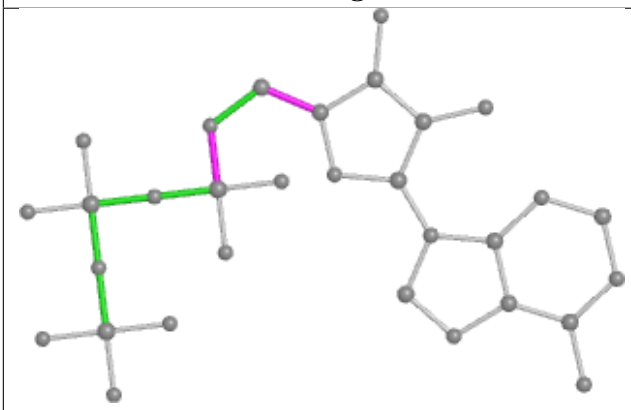
Ligand ATP A 501



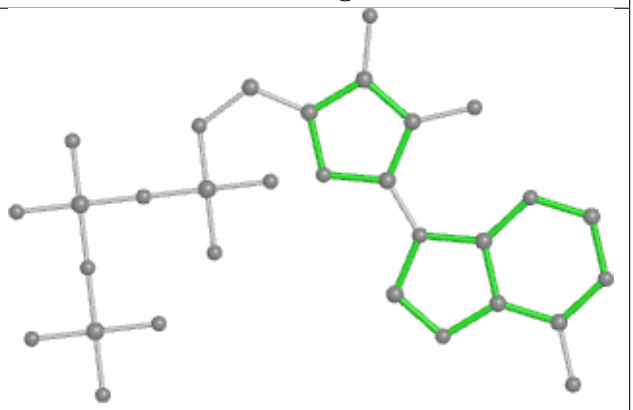
Bond lengths



Bond angles

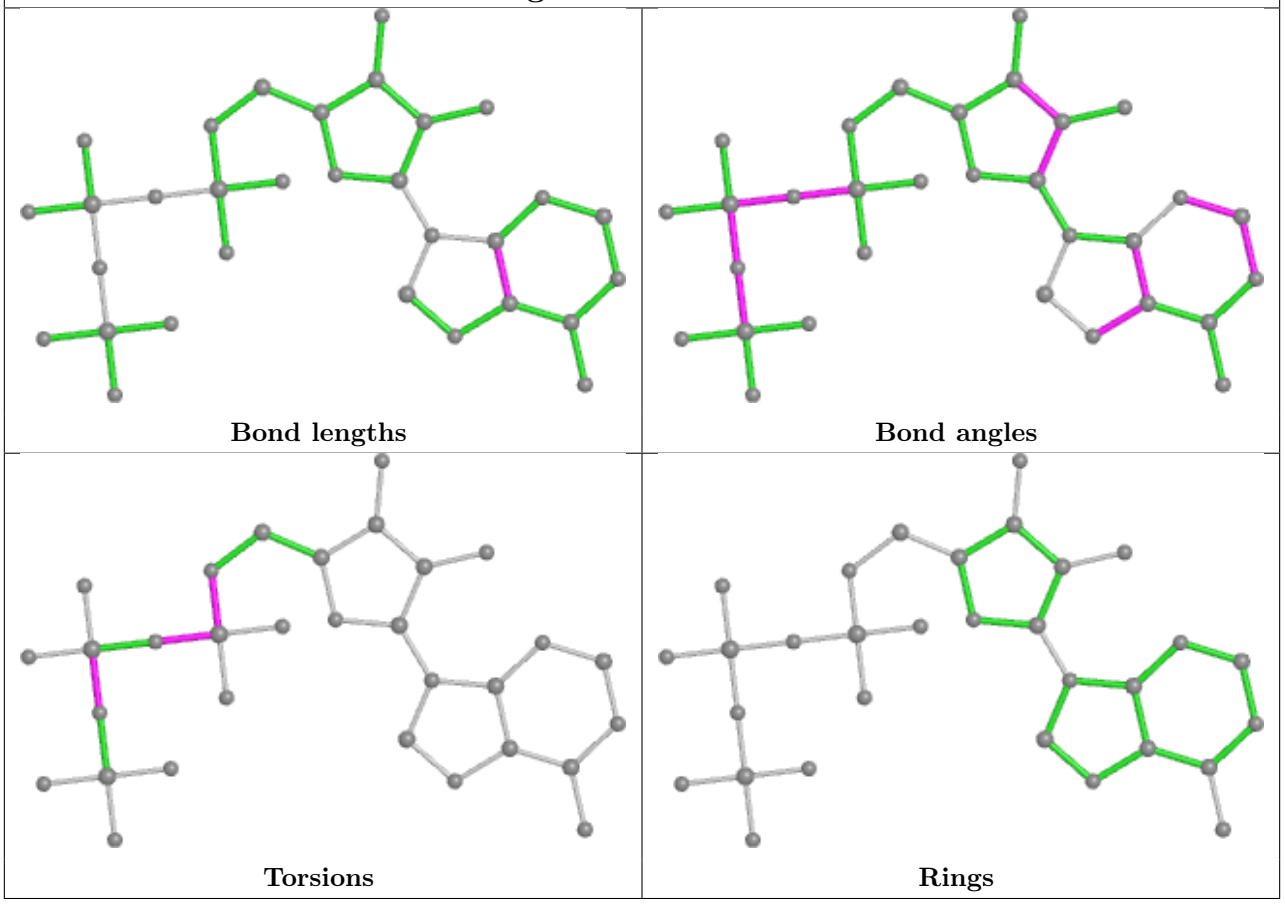


Torsions



Rings

Ligand ATP E 401



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
32	f	4
16	P	1
15	O	1
8	H	1

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	f	110:ALA	C	111:LEU	N	9.37
1	f	79:ASN	C	80:TYR	N	8.13

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	f	348:ASP	C	349:SER	N	6.07
1	P	81:GLN	C	82:ILE	N	4.19
1	O	74:PRO	C	75:ARG	N	3.14

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8336. 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 surface views

This section was not generated.

6.5 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

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

9 Map-model fit

This section was not generated.