



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 5, 2019 – 12:05 PM EST

PDB ID : 6MSG
EMDB ID: : EMD-9219
Title : Cryo-EM structures and dynamics of substrate-engaged human 26S proteasome
Authors : Mao, Y.D.
Deposited on : 2018-10-16
Resolution : 3.50 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

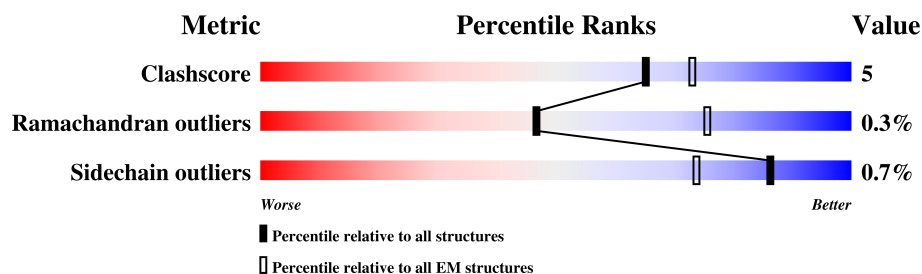
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.





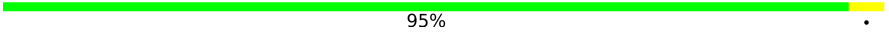






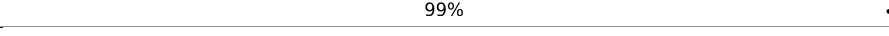
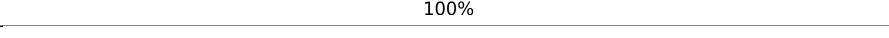

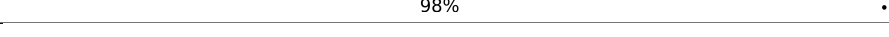

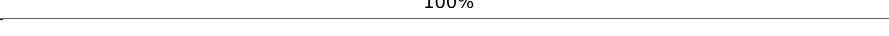
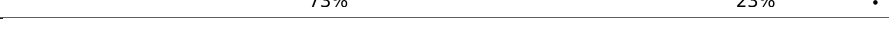
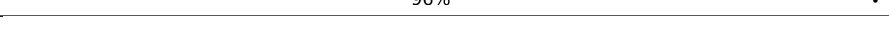

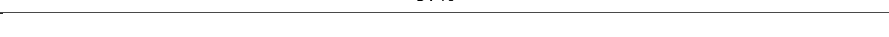



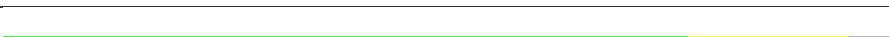


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	U	953	75% 11% 14%
2	V	533	76% 14% 10%
3	W	456	84% 16%
4	X	422	80% 10% 10%
5	Y	389	85% 13% .
6	Z	324	77% 10% 12%
7	a	376	98% ..
8	b	377	51% 49%
9	c	309	88% 5% 7%

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Mol	Chain	Length	Quality of chain
10	d	349	
11	e	70	
12	f	892	
13	A	433	
14	B	440	
15	C	398	
16	D	418	
17	E	403	
18	F	439	
19	u	76	
20	v	24	
21	G	245	
21	g	245	
22	H	233	
22	h	233	
23	I	260	
23	i	260	
24	J	247	
24	j	247	
25	K	240	
25	k	240	
26	L	268	
26	l	268	
27	M	254	
27	m	254	

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Mol	Chain	Length	Quality of chain
28	N	238	 76% 5% 20%
28	n	238	 80% 20%
29	O	276	 72% 8% 20%
29	o	276	 80% 20%
30	P	204	 88% 12%
30	p	204	 100%
31	Q	201	 88% 11% .
31	q	201	 99% .
32	R	262	 72% 5% 23%
32	r	262	 77% 23%
33	S	240	 79% 10% 11%
33	s	240	 89% 11%
34	T	263	 72% 10% 18%
34	t	263	 81% 18%

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 104399 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 proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	822	Total	C	N	O	S	0	0
			6414	4072	1088	1210	44		

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

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

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	380	Total	C	N	O	S	0	0
			3009	1918	509	570	12		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 11 is a protein called 26S proteasome complex subunit SEM1.

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

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	889	Total	C	N	O	S	0	0
			6866	4315	1174	1331	46		

- Molecule 13 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	356	Total	C	N	O	S	0	0
			2767	1741	488	521	17		

- Molecule 14 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	347	Total	C	N	O	S	0	0
			2691	1694	455	530	12		

- Molecule 15 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	396	Total	C	N	O	S	0	0
			3105	1954	558	576	17		

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

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

- Molecule 17 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	389	Total	C	N	O	S	0	0
			3097	1947	552	581	17		

- Molecule 18 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	395	Total	C	N	O	S	0	0
			3098	1951	533	596	18		

- Molecule 19 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	u	76	Total	C	N	O	S	0	0
			603	378	107	117	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	63	ARG	LYS	conflict	UNP P0CG47

- Molecule 20 is a protein called substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	v	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 21 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 22 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		
22	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 23 is a protein called Proteasome subunit alpha type-4.

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

- Molecule 24 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 25 is a protein called Proteasome subunit alpha type-5.

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

- Molecule 26 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 27 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 28 is a protein called Proteasome subunit beta type-6.

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

- Molecule 29 is a protein called Proteasome subunit beta type-7.

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

- Molecule 30 is a protein called Proteasome subunit beta type-3.

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

- Molecule 31 is a protein called Proteasome subunit beta type-2.

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

- Molecule 32 is a protein called Proteasome subunit beta type-5.

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

- Molecule 33 is a protein called Proteasome subunit beta type-1.

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

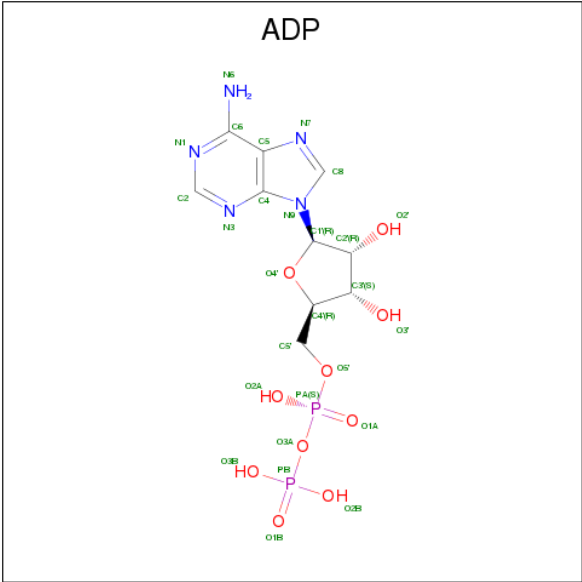
- Molecule 34 is a protein called Proteasome subunit beta type-4.

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

- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

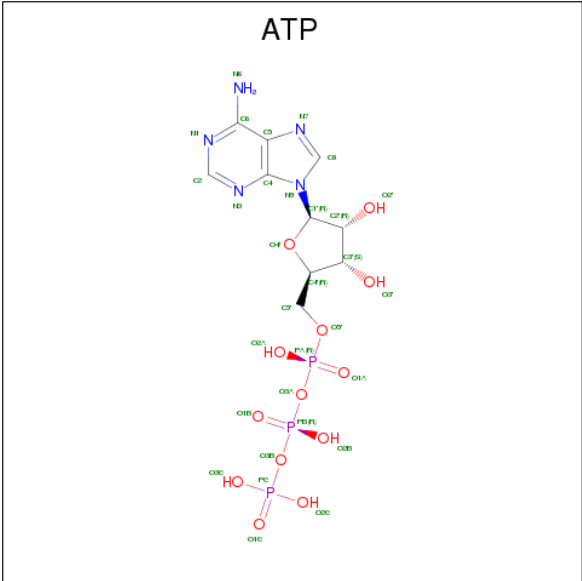
Mol	Chain	Residues	Atoms		AltConf
35	c	1	Total	Zn	0
			1	1	

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
36	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 37 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

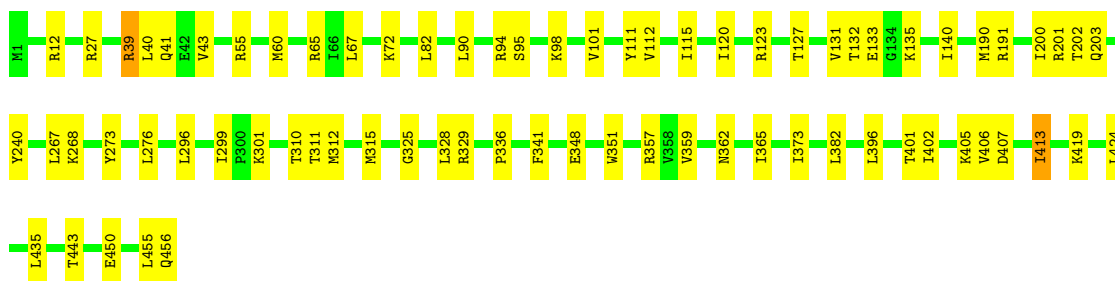
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Mol	Chain	Residues	Atoms					AltConf
37	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
37	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

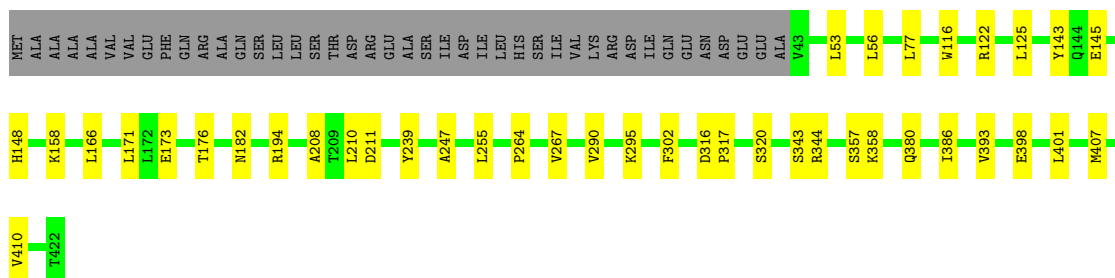
- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	D	1	Total	Mg	0
			1	1	
38	C	1	Total	Mg	0
			1	1	
38	E	1	Total	Mg	0
			1	1	



- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 80% 10% 10%



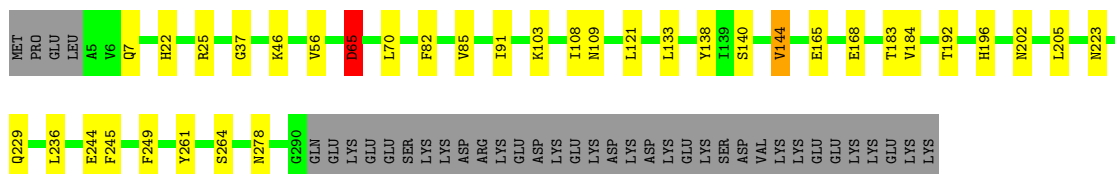
- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 85% 13% .



- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 77% 10% 12%



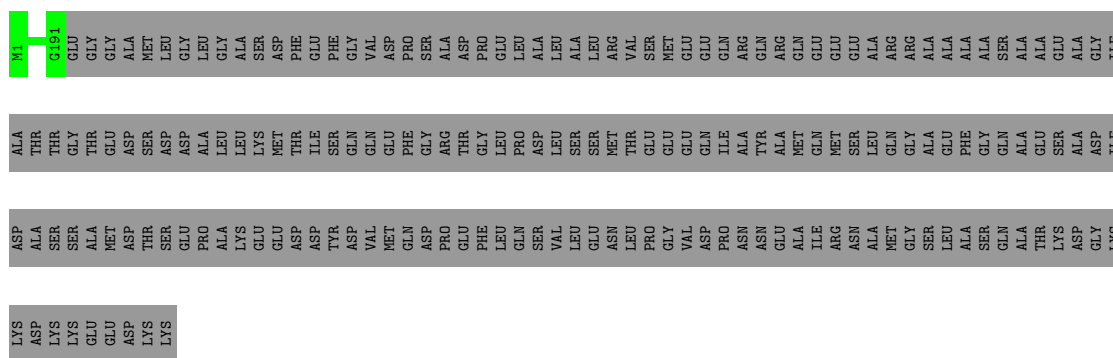
- Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

Chain a: 98% ..




- Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

Chain b: 51% 49%



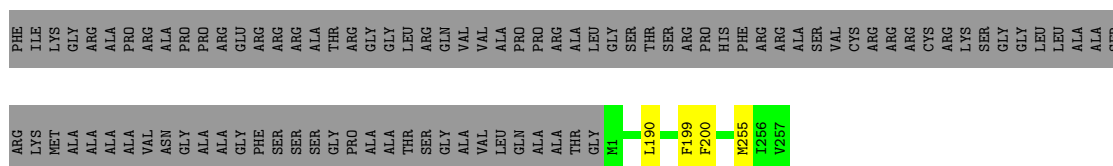
- Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

Chain c:  88% 5% 7%



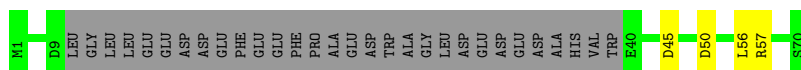
- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

Chain d:  72% . 26%



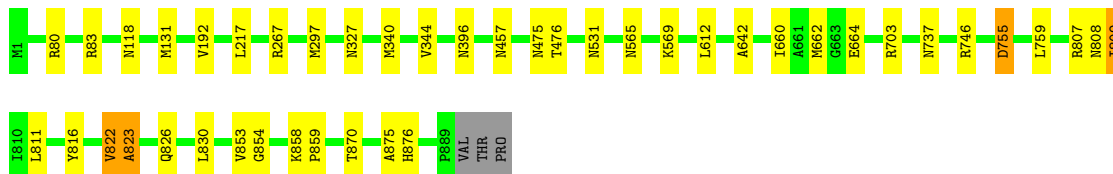
- Molecule 11: 26S proteasome complex subunit SEM1

Chain e: 51% 6% 43%



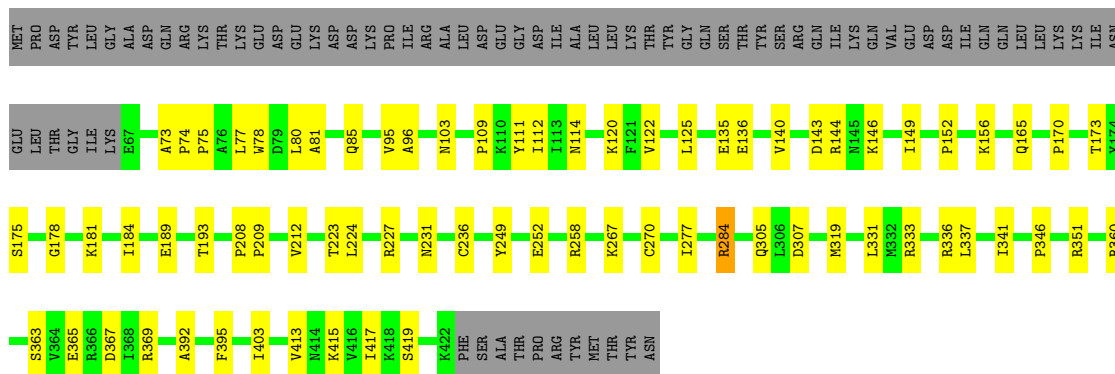
- Molecule 12: 26S proteasome non-ATPase regulatory subunit 2

Chain f: 95% .

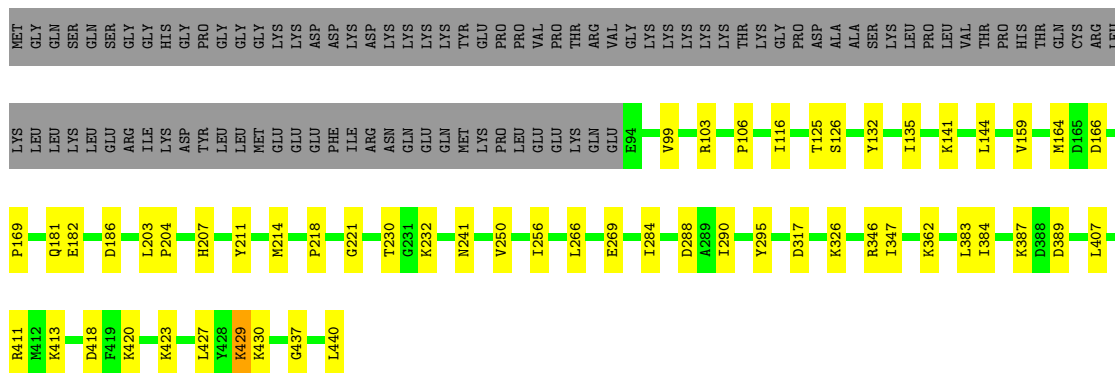


- Molecule 13: 26S proteasome regulatory subunit 7

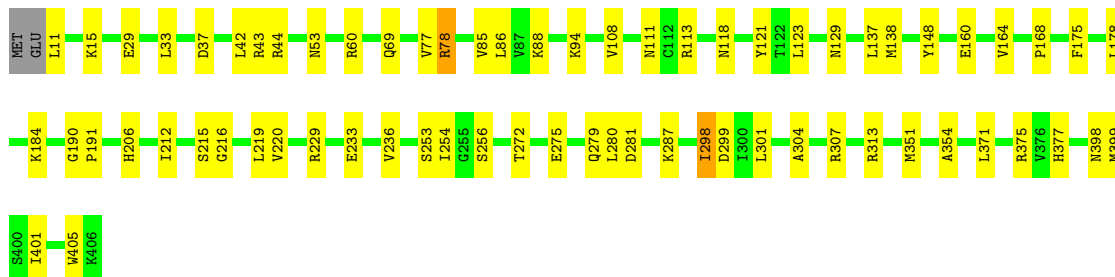
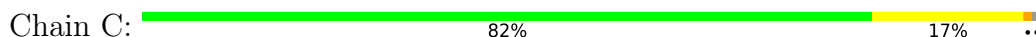
Chain A: 65% 17% 18%



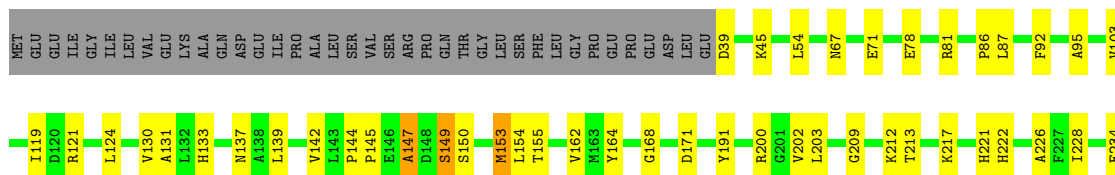
- Molecule 14: 26S proteasome regulatory subunit 4

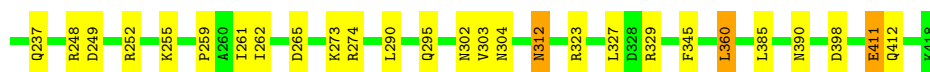


- Molecule 15: 26S proteasome regulatory subunit 8



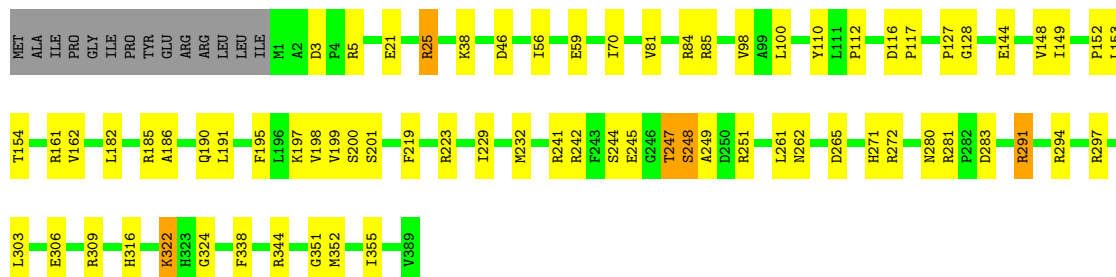
- Molecule 16: 26S proteasome regulatory subunit 6B





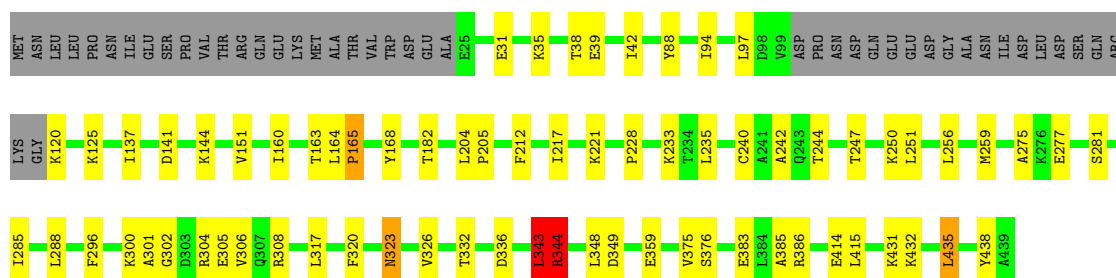
• Molecule 17: 26S proteasome regulatory subunit 10B

Chain E: 78% 17% ..



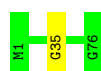
• Molecule 18: 26S proteasome regulatory subunit 6A

Chain F: 74% 15% • 10%



• Molecule 19: Ubiquitin

Chain u: 99% .



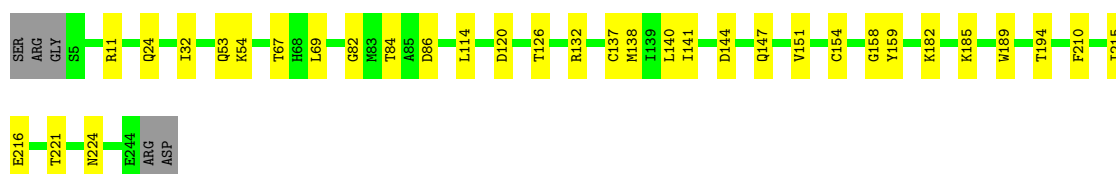
• Molecule 20: substrate

Chain v: 100%

There are no outlier residues recorded for this chain.

• Molecule 21: Proteasome subunit alpha type-6

Chain G: 84% 13% .



- Molecule 21: Proteasome subunit alpha type-6

Chain g:  98% .



- Molecule 22: Proteasome subunit alpha type-2

Chain H:  88% 12% .



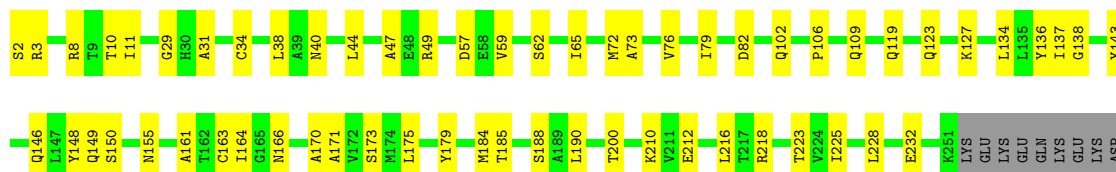
- Molecule 22: Proteasome subunit alpha type-2

Chain h:  100% .



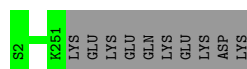
- Molecule 23: Proteasome subunit alpha type-4

Chain I:  73% 23% .




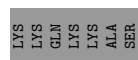
- Molecule 23: Proteasome subunit alpha type-4

Chain i:  96% .



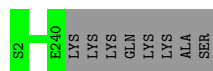
- Molecule 24: Proteasome subunit alpha type-7

Chain J:  85% 12% .




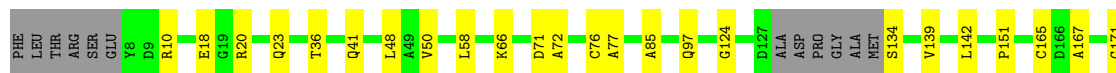
- Molecule 24: Proteasome subunit alpha type-7

Chain j:  97% .



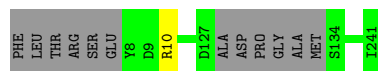
• Molecule 25: Proteasome subunit alpha type-5

Chain K:  80% 15% 5%



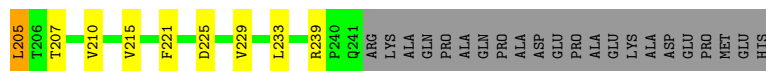
• Molecule 25: Proteasome subunit alpha type-5

Chain k:  95% 5%




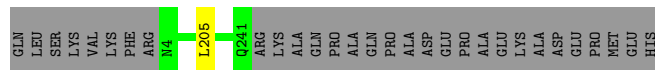
• Molecule 26: Proteasome subunit alpha type-1

Chain L:  75% 13% 11%




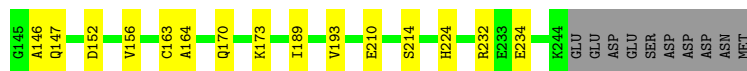
• Molecule 26: Proteasome subunit alpha type-1

Chain l:  88% 11%



• Molecule 27: Proteasome subunit alpha type-3

Chain M:  77% 18% 6%



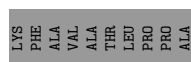
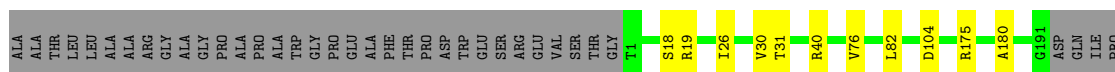
• Molecule 27: Proteasome subunit alpha type-3

Chain m:  94% 6%



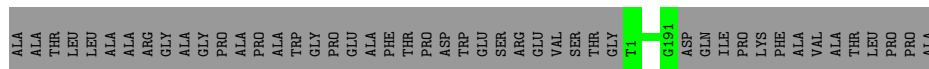
• Molecule 28: Proteasome subunit beta type-6

Chain N:  76% 5% 20%



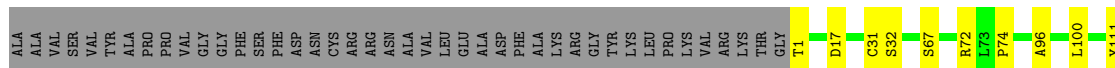
• Molecule 28: Proteasome subunit beta type-6

Chain n:  80% 20%




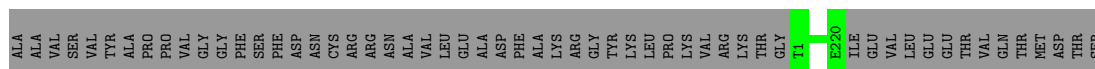
• Molecule 29: Proteasome subunit beta type-7

Chain O:  72% 8% 20%




• Molecule 29: Proteasome subunit beta type-7

Chain o:  80% 20%



• Molecule 30: Proteasome subunit beta type-3

Chain P:  88% 12%




• Molecule 30: Proteasome subunit beta type-3

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 31: Proteasome subunit beta type-2

Chain Q:  88% 11%



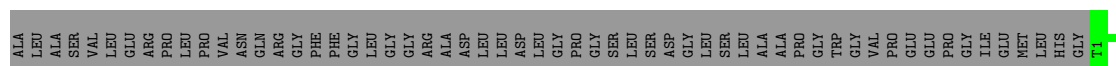
- Molecule 31: Proteasome subunit beta type-2

Chain q:  99%




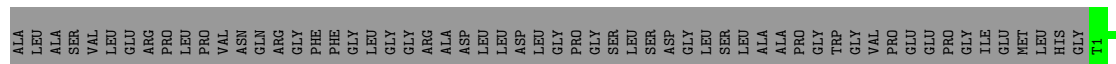
- Molecule 32: Proteasome subunit beta type-5

Chain R:  72% 5% 23%




- Molecule 32: Proteasome subunit beta type-5

Chain r:  77% 23%




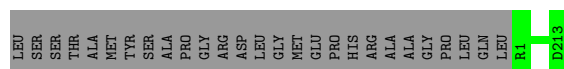
- Molecule 33: Proteasome subunit beta type-1

Chain S:  79% 10% 11%

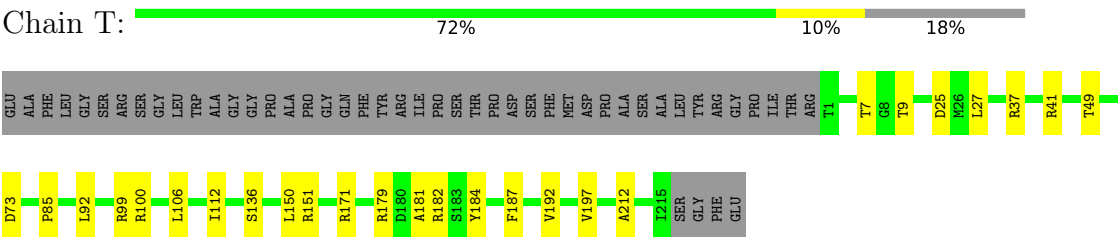


- Molecule 33: Proteasome subunit beta type-1

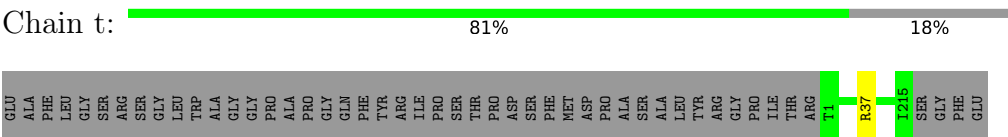
Chain s:  89% 11%



● Molecule 34: Proteasome subunit beta type-4



● Molecule 34: Proteasome subunit beta type-4



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	112776	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
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, MG, ADP

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	U	0.30	0/6530	0.54	1/8840 (0.0%)
10	d	0.30	0/2162	0.61	1/2919 (0.0%)
11	e	0.32	0/338	0.73	0/450
12	f	0.33	1/6980 (0.0%)	0.71	6/9433 (0.1%)
13	A	0.29	0/2814	0.53	0/3801
14	B	0.28	0/2730	0.53	0/3688
15	C	0.30	0/3146	0.54	0/4226
16	D	0.31	0/3090	0.61	0/4168
17	E	0.31	0/3145	0.59	1/4233 (0.0%)
18	F	0.30	0/3137	0.62	6/4223 (0.1%)
19	u	0.23	0/609	0.39	0/819
2	V	0.32	0/3929	0.59	0/5309
21	G	0.34	0/1859	0.55	1/2523 (0.0%)
21	g	0.34	0/1859	0.55	1/2523 (0.0%)
22	H	0.37	0/1743	0.53	0/2372
22	h	0.37	0/1743	0.53	0/2372
23	I	0.32	0/1942	0.53	0/2628
23	i	0.32	0/1942	0.53	0/2628
24	J	0.31	0/1728	0.51	0/2358
24	j	0.31	0/1728	0.51	0/2358
25	K	0.30	0/1747	0.53	0/2364
25	k	0.30	0/1747	0.53	0/2364
26	L	0.32	0/1885	0.54	0/2552
26	l	0.32	0/1885	0.54	0/2552
27	M	0.35	0/1891	0.53	0/2552
27	m	0.35	0/1891	0.53	0/2552
28	N	0.32	0/1454	0.49	0/1967
28	n	0.32	0/1454	0.49	0/1967
29	O	0.32	0/1670	0.51	0/2265
29	o	0.32	0/1670	0.51	0/2265
3	W	0.29	0/3751	0.56	0/5042
30	P	0.32	0/1614	0.50	0/2177

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
30	p	0.32	0/1614	0.50	0/2177
31	Q	0.34	0/1603	0.56	0/2174
31	q	0.34	0/1603	0.56	0/2174
32	R	0.35	0/1579	0.48	0/2134
32	r	0.35	0/1579	0.48	0/2134
33	S	0.32	0/1671	0.50	0/2253
33	s	0.32	0/1671	0.50	0/2253
34	T	0.33	0/1700	0.50	0/2305
34	t	0.33	0/1700	0.50	0/2305
4	X	0.28	0/3053	0.52	0/4115
5	Y	0.31	0/3173	0.57	0/4273
6	Z	0.32	0/2324	0.59	2/3150 (0.1%)
7	a	0.29	0/3053	0.57	1/4133 (0.0%)
8	b	0.28	0/1478	0.55	0/2001
9	c	0.34	0/2302	0.65	3/3110 (0.1%)
All	All	0.32	1/105916 (0.0%)	0.56	23/143181 (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
10	d	0	2
11	e	0	2
12	f	0	12
13	A	0	1
15	C	0	1
16	D	0	4
18	F	0	1
2	V	0	1
4	X	0	1
6	Z	0	2
7	a	0	1
9	c	0	2
All	All	0	30

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	f	192	VAL	C-N	5.94	1.45	1.34

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	g	210	PHE	C-N-CA	8.26	142.34	121.70
21	G	210	PHE	C-N-CA	8.25	142.34	121.70
12	f	830	LEU	CA-CB-CG	7.96	133.61	115.30
18	F	348	LEU	CA-CB-CG	7.24	131.94	115.30
12	f	759	LEU	CA-CB-CG	6.75	130.81	115.30

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	V	29	PRO	Peptide
4	X	393	VAL	Peptide
6	Z	144	VAL	Peptide
6	Z	183	THR	Peptide
7	a	214	GLY	Peptide

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	U	6414	0	6435	60	0
2	V	3852	0	3893	49	0
3	W	3703	0	3822	44	0
4	X	3009	0	3113	23	0
5	Y	3115	0	3120	29	0
6	Z	2281	0	2312	21	0
7	a	2995	0	3012	0	0
8	b	1458	0	1505	0	0
9	c	2260	0	2276	0	0
10	d	2116	0	2146	0	0
11	e	334	0	294	0	0
12	f	6866	0	6866	0	0
13	A	2767	0	2787	44	0
14	B	2691	0	2725	36	0
15	C	3105	0	3219	45	0
16	D	3040	0	3076	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	E	3097	0	3173	49	0
18	F	3098	0	3187	38	0
19	u	603	0	629	0	0
20	v	120	0	33	0	0
21	G	1826	0	1796	21	0
21	g	1826	0	1796	0	0
22	H	1708	0	1594	20	0
22	h	1708	0	1594	0	0
23	I	1912	0	1851	39	0
23	i	1912	0	1851	0	0
24	J	1704	0	1517	26	0
24	j	1704	0	1517	0	0
25	K	1722	0	1673	22	0
25	k	1722	0	1673	0	0
26	L	1850	0	1822	27	0
26	l	1850	0	1822	0	0
27	M	1856	0	1814	31	0
27	m	1856	0	1814	0	0
28	N	1430	0	1398	8	0
28	n	1430	0	1398	0	0
29	O	1643	0	1644	16	0
29	o	1643	0	1644	0	0
30	P	1585	0	1598	21	0
30	p	1585	0	1598	0	0
31	Q	1570	0	1547	14	0
31	q	1570	0	1547	0	0
32	R	1548	0	1499	8	0
32	r	1548	0	1499	0	0
33	S	1641	0	1616	18	0
33	s	1641	0	1616	0	0
34	T	1667	0	1628	19	0
34	t	1667	0	1628	0	0
35	c	1	0	0	0	0
36	A	27	0	12	2	0
36	F	27	0	12	1	0
37	C	31	0	12	0	0
37	D	31	0	12	5	0
37	E	31	0	12	2	0
38	C	1	0	0	0	0
38	D	1	0	0	0	0
38	E	1	0	0	0	0
All	All	104399	0	103677	666	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 5.

The worst 5 of 666 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)
30:P:56:LEU:HG	30:P:58:THR:HG22	5.00	0.77
1:U:792:ASN:HB3	1:U:914:LEU:H	1.53	0.72
3:W:435:LEU:HD23	6:Z:236:LEU:HB3	1.70	0.72
16:D:200:ARG:HH12	16:D:303:VAL:HA	1.57	0.69
5:Y:300:ARG:NH1	17:E:59:GLU:OE1	73.60	0.69

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 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	U	816/953 (86%)	753 (92%)	62 (8%)	1 (0%)	53	86
2	V	478/533 (90%)	426 (89%)	52 (11%)	0	100	100
3	W	454/456 (100%)	408 (90%)	46 (10%)	0	100	100
4	X	378/422 (90%)	357 (94%)	20 (5%)	1 (0%)	43	78
5	Y	376/389 (97%)	345 (92%)	31 (8%)	0	100	100
6	Z	284/324 (88%)	247 (87%)	34 (12%)	3 (1%)	16	56
7	a	371/376 (99%)	341 (92%)	28 (8%)	2 (0%)	31	71
8	b	189/377 (50%)	167 (88%)	22 (12%)	0	100	100
9	c	285/309 (92%)	238 (84%)	44 (15%)	3 (1%)	16	56
10	d	255/349 (73%)	212 (83%)	42 (16%)	1 (0%)	36	75
11	e	36/70 (51%)	24 (67%)	10 (28%)	2 (6%)	2	19
12	f	887/892 (99%)	712 (80%)	164 (18%)	11 (1%)	14	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	A	354/433 (82%)	306 (86%)	47 (13%)	1 (0%)	43	78
14	B	345/440 (78%)	305 (88%)	40 (12%)	0	100	100
15	C	394/398 (99%)	344 (87%)	50 (13%)	0	100	100
16	D	378/418 (90%)	326 (86%)	49 (13%)	3 (1%)	21	62
17	E	387/403 (96%)	340 (88%)	42 (11%)	5 (1%)	13	52
18	F	391/439 (89%)	358 (92%)	29 (7%)	4 (1%)	17	57
19	u	74/76 (97%)	67 (90%)	6 (8%)	1 (1%)	12	50
21	G	238/245 (97%)	227 (95%)	11 (5%)	0	100	100
21	g	238/245 (97%)	227 (95%)	11 (5%)	0	100	100
22	H	230/233 (99%)	216 (94%)	14 (6%)	0	100	100
22	h	230/233 (99%)	217 (94%)	13 (6%)	0	100	100
23	I	248/260 (95%)	229 (92%)	19 (8%)	0	100	100
23	i	248/260 (95%)	229 (92%)	19 (8%)	0	100	100
24	J	237/247 (96%)	223 (94%)	14 (6%)	0	100	100
24	j	237/247 (96%)	223 (94%)	14 (6%)	0	100	100
25	K	224/240 (93%)	208 (93%)	16 (7%)	0	100	100
25	k	224/240 (93%)	208 (93%)	16 (7%)	0	100	100
26	L	236/268 (88%)	225 (95%)	11 (5%)	0	100	100
26	l	236/268 (88%)	225 (95%)	11 (5%)	0	100	100
27	M	238/254 (94%)	219 (92%)	19 (8%)	0	100	100
27	m	238/254 (94%)	219 (92%)	19 (8%)	0	100	100
28	N	189/238 (79%)	184 (97%)	5 (3%)	0	100	100
28	n	189/238 (79%)	184 (97%)	5 (3%)	0	100	100
29	O	218/276 (79%)	211 (97%)	7 (3%)	0	100	100
29	o	218/276 (79%)	211 (97%)	7 (3%)	0	100	100
30	P	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
30	p	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
31	Q	197/201 (98%)	184 (93%)	13 (7%)	0	100	100
31	q	197/201 (98%)	184 (93%)	13 (7%)	0	100	100
32	R	199/262 (76%)	194 (98%)	5 (2%)	0	100	100
32	r	199/262 (76%)	194 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	S	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
33	s	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
34	T	213/263 (81%)	202 (95%)	11 (5%)	0	100	100
34	t	213/263 (81%)	202 (95%)	11 (5%)	0	100	100
All	All	13292/14919 (89%)	12109 (91%)	1145 (9%)	38 (0%)	47	78

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	c	271	ALA
9	c	272	ILE
10	d	200	PHE
12	f	808	ASN
12	f	853	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	U	702/816 (86%)	699 (100%)	3 (0%)	92	96
2	V	414/459 (90%)	412 (100%)	2 (0%)	90	95
3	W	416/416 (100%)	411 (99%)	5 (1%)	74	88
4	X	327/362 (90%)	327 (100%)	0	100	100
5	Y	334/344 (97%)	331 (99%)	3 (1%)	81	91
6	Z	257/295 (87%)	257 (100%)	0	100	100
7	a	333/336 (99%)	331 (99%)	2 (1%)	87	95
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	252/267 (94%)	241 (96%)	11 (4%)	31	66
10	d	231/293 (79%)	231 (100%)	0	100	100
11	e	38/63 (60%)	38 (100%)	0	100	100
12	f	745/748 (100%)	727 (98%)	18 (2%)	52	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	A	297/372 (80%)	293 (99%)	4 (1%)	71	88
14	B	300/385 (78%)	297 (99%)	3 (1%)	78	90
15	C	340/346 (98%)	336 (99%)	4 (1%)	74	88
16	D	333/366 (91%)	325 (98%)	8 (2%)	52	79
17	E	341/353 (97%)	335 (98%)	6 (2%)	62	83
18	F	340/379 (90%)	337 (99%)	3 (1%)	81	91
19	u	68/68 (100%)	68 (100%)	0	100	100
21	G	193/209 (92%)	193 (100%)	0	100	100
21	g	193/209 (92%)	193 (100%)	0	100	100
22	H	164/190 (86%)	164 (100%)	0	100	100
22	h	164/190 (86%)	164 (100%)	0	100	100
23	I	193/220 (88%)	193 (100%)	0	100	100
23	i	193/220 (88%)	193 (100%)	0	100	100
24	J	152/210 (72%)	152 (100%)	0	100	100
24	j	152/210 (72%)	152 (100%)	0	100	100
25	K	186/202 (92%)	185 (100%)	1 (0%)	90	95
25	k	186/202 (92%)	185 (100%)	1 (0%)	90	95
26	L	198/229 (86%)	197 (100%)	1 (0%)	90	95
26	l	198/229 (86%)	197 (100%)	1 (0%)	90	95
27	M	192/211 (91%)	192 (100%)	0	100	100
27	m	192/211 (91%)	192 (100%)	0	100	100
28	N	148/180 (82%)	148 (100%)	0	100	100
28	n	148/180 (82%)	148 (100%)	0	100	100
29	O	177/227 (78%)	177 (100%)	0	100	100
29	o	177/227 (78%)	177 (100%)	0	100	100
30	P	172/173 (99%)	172 (100%)	0	100	100
30	p	172/173 (99%)	172 (100%)	0	100	100
31	Q	164/171 (96%)	163 (99%)	1 (1%)	87	95
31	q	164/171 (96%)	163 (99%)	1 (1%)	87	95
32	R	153/201 (76%)	153 (100%)	0	100	100
32	r	153/201 (76%)	153 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	S	174/198 (88%)	174 (100%)	0	100	100
33	s	174/198 (88%)	174 (100%)	0	100	100
34	T	175/214 (82%)	174 (99%)	1 (1%)	87	95
34	t	175/214 (82%)	174 (99%)	1 (1%)	87	95
All	All	11117/12650 (88%)	11037 (99%)	80 (1%)	86	94

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	f	565	ASN
13	A	284	ARG
26	L	205	LEU
12	f	569	LYS
12	f	703	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

Mol	Chain	Res	Type
12	f	396	ASN
14	B	277	HIS
25	k	155	HIS
12	f	531	ASN
12	f	737	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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
36	ADP	A	501	-	25,29,29	1.02	1 (4%)	25,45,45	1.76	3 (12%)
37	ATP	C	501	38	27,33,33	0.99	1 (3%)	27,52,52	1.85	4 (14%)
37	ATP	D	501	38	27,33,33	1.00	1 (3%)	27,52,52	1.94	4 (14%)
37	ATP	E	401	38	27,33,33	1.00	2 (7%)	27,52,52	1.96	4 (14%)
36	ADP	F	501	-	25,29,29	1.03	2 (8%)	25,45,45	1.83	3 (12%)

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
36	ADP	A	501	-	-	0/12/32/32	0/3/3/3
37	ATP	C	501	38	-	0/18/38/38	0/3/3/3
37	ATP	D	501	38	-	0/18/38/38	0/3/3/3
37	ATP	E	401	38	-	0/18/38/38	0/3/3/3
36	ADP	F	501	-	-	0/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	F	501	ADP	C8-N9	-2.08	1.34	1.36
37	E	401	ATP	C8-N9	-2.00	1.34	1.36
37	D	501	ATP	C5-C4	3.00	1.47	1.40
36	F	501	ADP	C5-C4	3.02	1.47	1.40
37	E	401	ATP	C5-C4	3.03	1.47	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
37	C	501	ATP	N3-C2-N1	-6.65	123.17	128.86
36	A	501	ADP	N3-C2-N1	-6.24	123.52	128.86
36	F	501	ADP	N3-C2-N1	-6.01	123.72	128.86
37	E	401	ATP	N3-C2-N1	-6.00	123.72	128.86
37	D	501	ATP	N3-C2-N1	-5.89	123.82	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	A	501	ADP	2	0
37	D	501	ATP	5	0
37	E	401	ATP	2	0
36	F	501	ADP	1	0

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.