



# Full wwPDB EM Validation Report ⓘ

Dec 30, 2024 – 02:06 PM EST

PDB ID : 8CVT  
EMDB ID : EMD-27018  
Title : Human 19S-20S proteasome, state SD2  
Authors : Zhao, J.  
Deposited on : 2022-05-18  
Resolution : 3.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

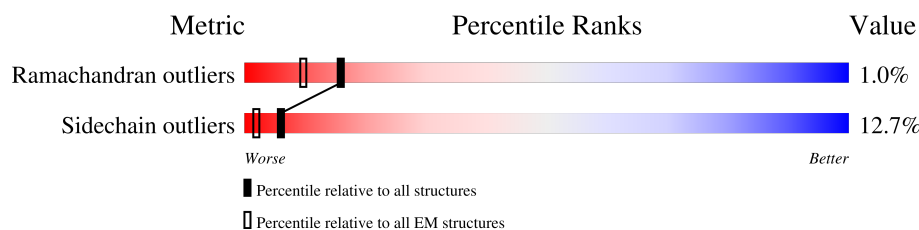
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

# 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 3.00 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.



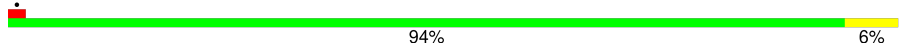

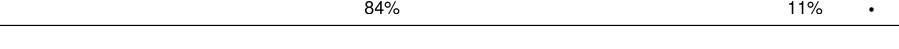
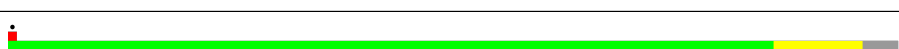



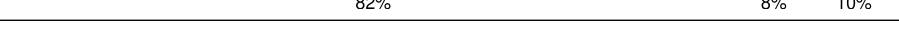



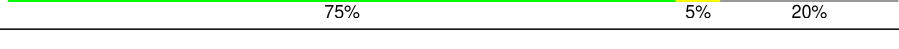

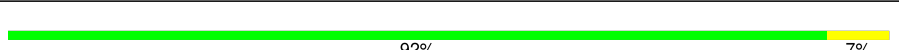
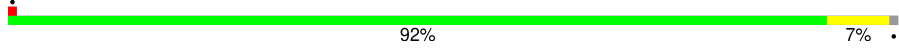

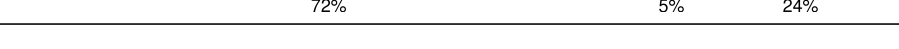







Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	 6% 76% 11% 12%
2	B	440	 5% 74% 10% 16%
3	C	406	 1% 79% 11% 11%
4	D	418	 6% 79% 12% 9%
5	E	389	 24% 87% 9% .
6	F	439	 12% 77% 8% 14%
7	G	246	 88% 9% .
7	g	246	 87% 10% .
8	H	234	 87% 11% .

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Mol	Chain	Length	Quality of chain
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	263	
12	l	263	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	Q	201	
17	q	201	
18	R	263	
18	r	263	
19	S	241	
19	s	241	
20	T	264	
20	t	264	

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Mol	Chain	Length	Quality of chain
21	U	953	
22	V	534	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	310	
30	d	350	
31	e	70	
32	f	908	

## 2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 101640 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 regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	380	Total	C	N	O	S	0	0
			2893	1817	515	543	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	370	Total	C	N	O	S	0	0
			2806	1763	478	553	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	363	Total	C	N	O	S	0	0
			2859	1804	513	525	17		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	375	Total	C	N	O	S	0	0
			2860	1796	512	536	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	376	Total	C	N	O	S	0	0
			2855	1799	495	546	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1820	1157	304	346	13		
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	230	Total	C	N	O	S	0	0
			1702	1082	285	330	5		
8	h	234	Total	C	N	O	S	0	0
			1721	1089	291	335	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	248	Total	C	N	O	S	0	0
			1895	1195	324	368	8		
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
			1708	1059	309	335	5		
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	237	Total	C	N	O	S	0	0
			1792	1122	296	363	11		
11	k	234	Total	C	N	O	S	0	0
			1759	1102	290	356	11		

- 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		
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		
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	195	Total	C	N	O	S	0	0
			1462	913	250	287	12		
14	n	205	Total	C	N	O	S	0	0
			1533	962	261	298	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	222	Total	C	N	O	S	0	0
			1660	1044	282	322	12		
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	205	Total	C	N	O	S	0	0
			1593	1015	263	295	20		
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		

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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		
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
			1644	1039	282	313	10		
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
			1673	1055	288	318	12		
20	t	215	Total	C	N	O	S	0	0
			1673	1055	288	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	447	Total	C	N	O	S	0	0
			3600	2287	639	660	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	380	Total	C	N	O	S	0	0
			3009	1918	509	570	12		

- 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		

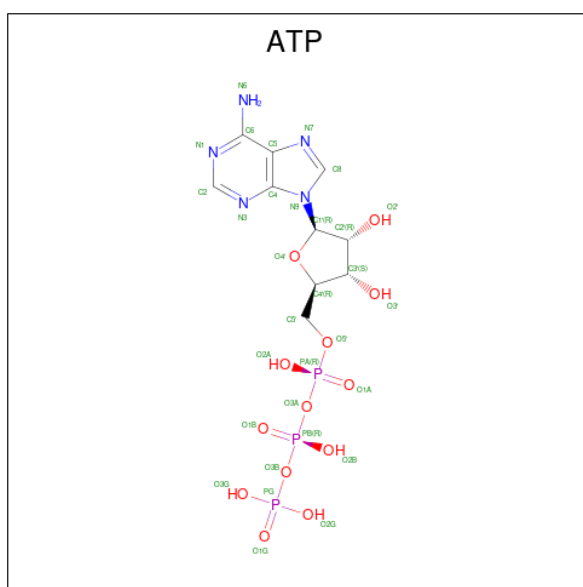
- Molecule 31 is a protein called 26S proteasome complex subunit SEM1.

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.

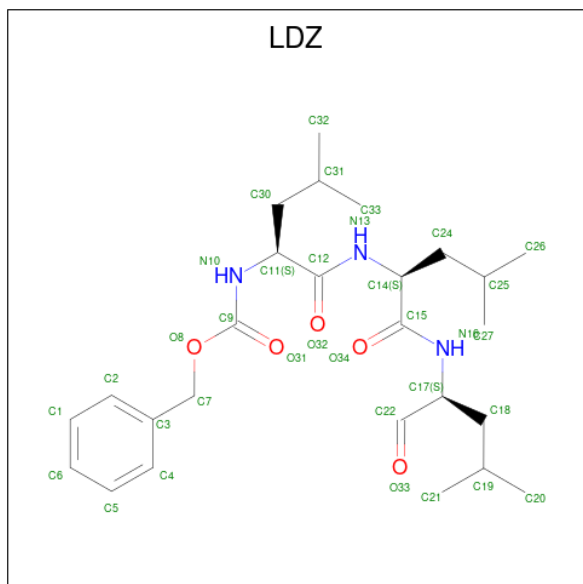
Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	689	Total	C	N	O	S	0	0
			5319	3343	904	1037	35		

- 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	C	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	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 34 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S)-4-methyl-1-oxopentan-2-yl]-L-leucine amide (three-letter code: LDZ) (formula:  $C_{26}H_{41}N_3O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
34	N	1	Total	C	N	O	0
			34	26	3	5	
34	O	1	Total	C	N	O	0
			34	26	3	5	
34	R	1	Total	C	N	O	0
			34	26	3	5	
34	n	1	Total	C	N	O	0
			34	26	3	5	
34	o	1	Total	C	N	O	0
			34	26	3	5	
34	r	1	Total	C	N	O	0
			34	26	3	5	

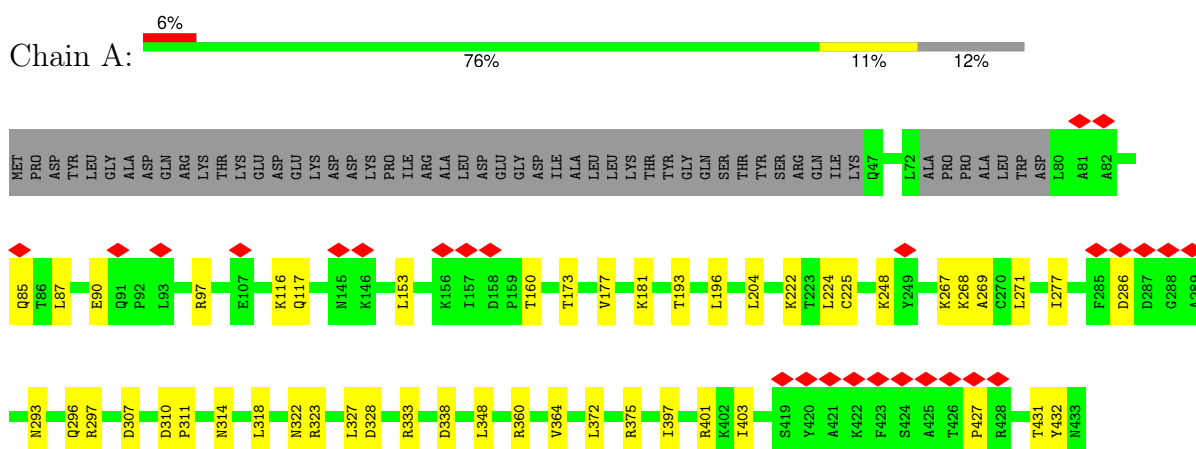
- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

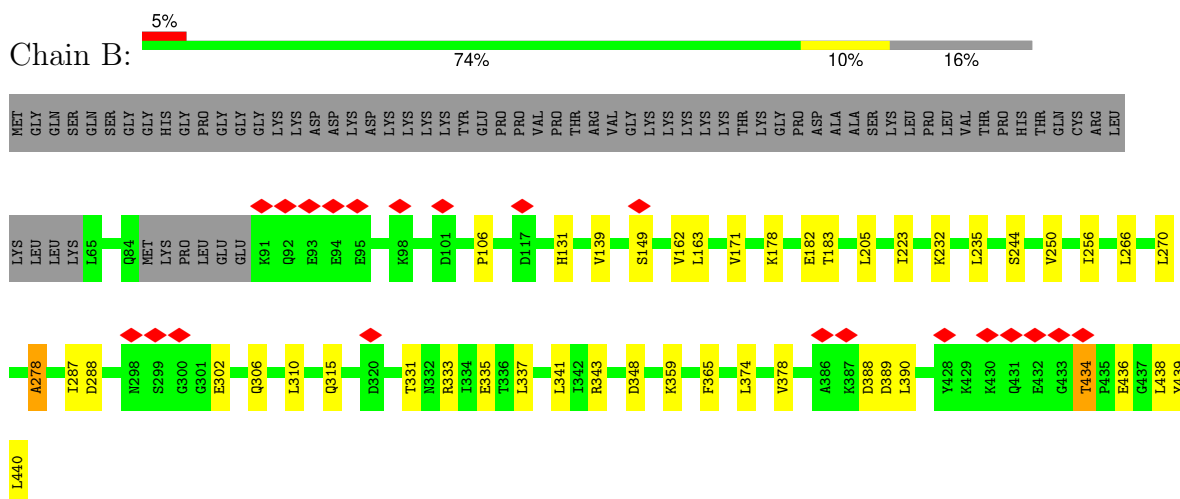
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 proteasome regulatory subunit 7

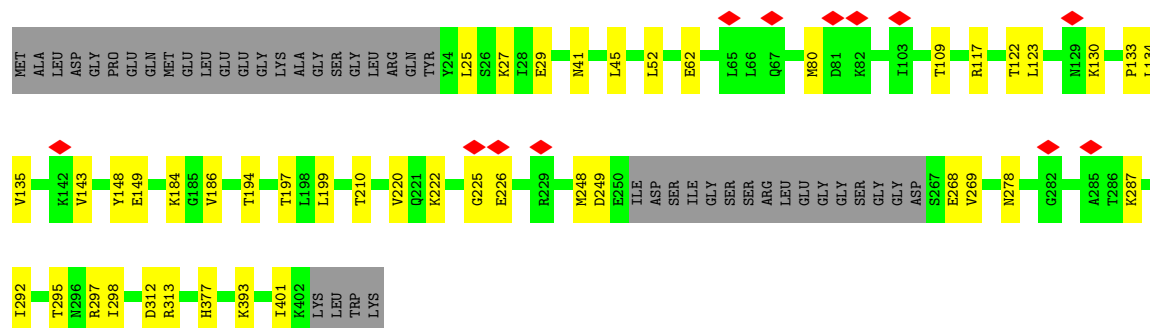


- Molecule 2: 26S proteasome regulatory subunit 4

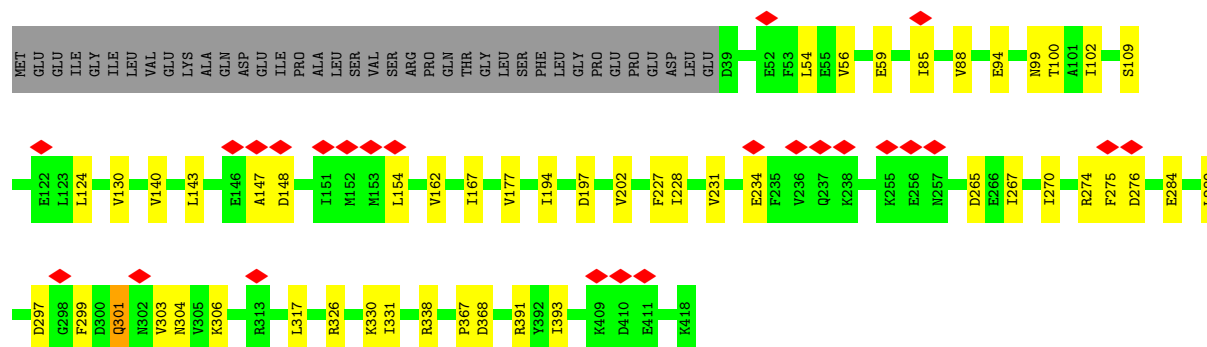
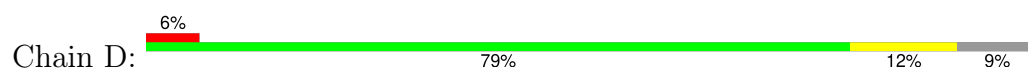


- Molecule 3: 26S protease regulatory subunit 8

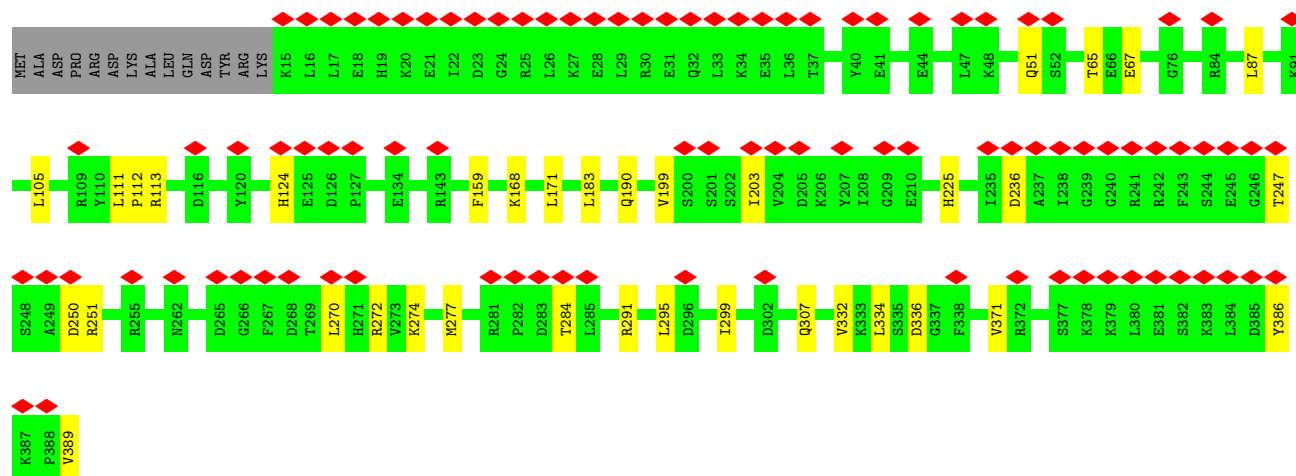
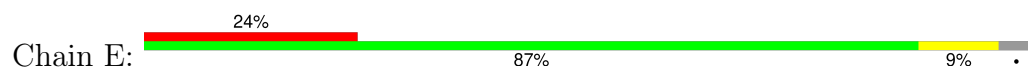




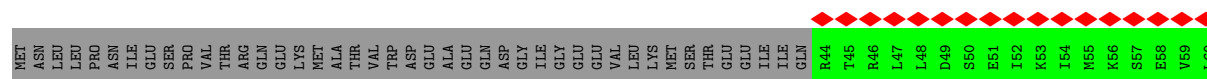
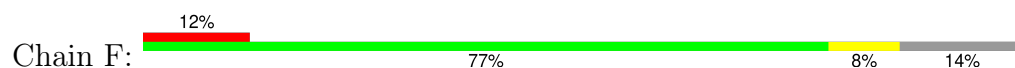
• Molecule 4: 26S proteasome regulatory subunit 6B

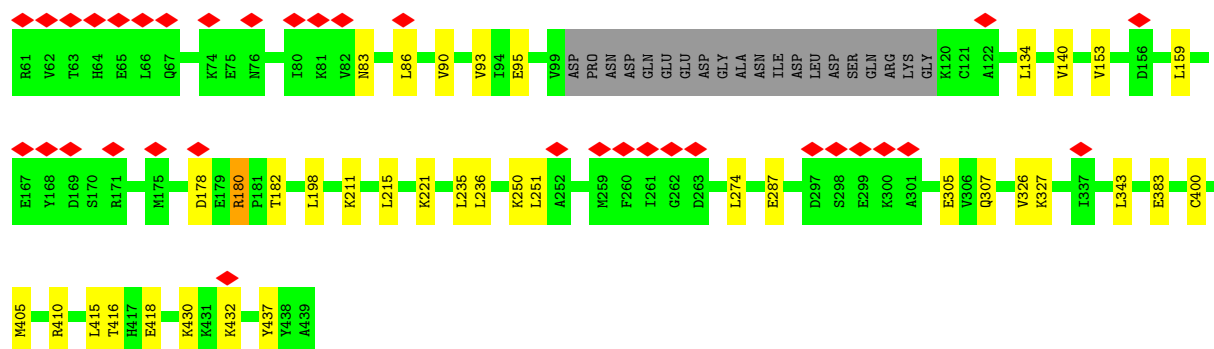


• Molecule 5: 26S protease regulatory subunit 10B



• Molecule 6: 26S proteasome regulatory subunit 6A





• Molecule 7: Proteasome subunit alpha type-6

Chain G: 88% 9% •



• Molecule 7: Proteasome subunit alpha type-6

Chain g: 87% 10% •



• Molecule 8: Proteasome subunit alpha type-2

Chain H: 87% 11% •



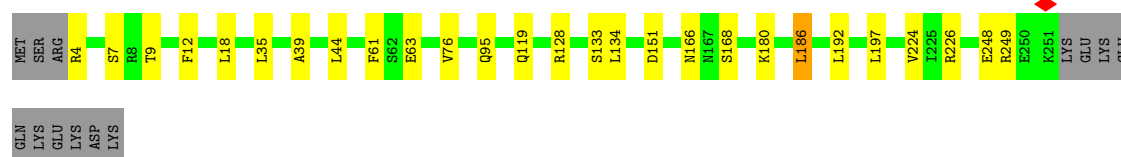
• Molecule 8: Proteasome subunit alpha type-2

Chain h: 94% 6% •

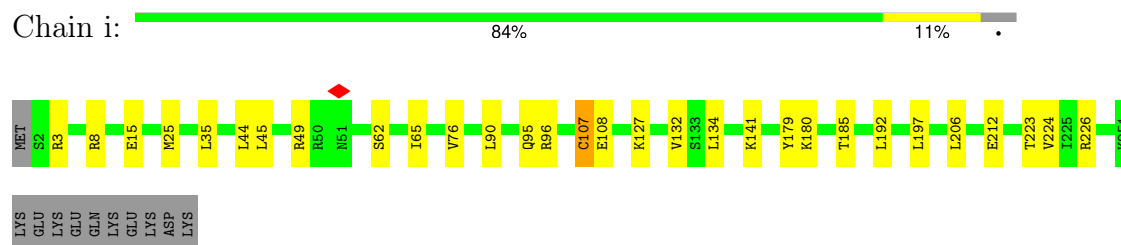


• Molecule 9: Proteasome subunit alpha type-4

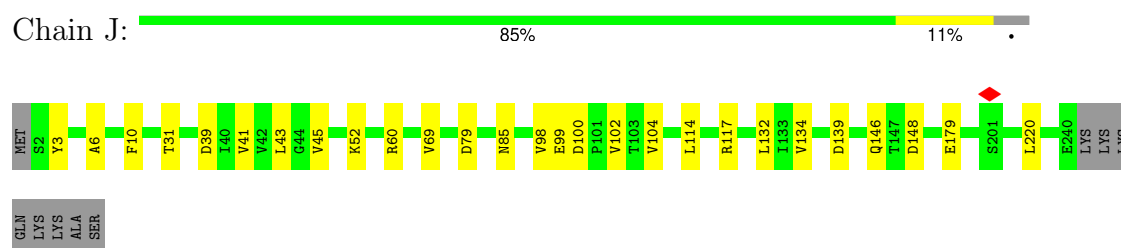
Chain I: 85% 10% 5%



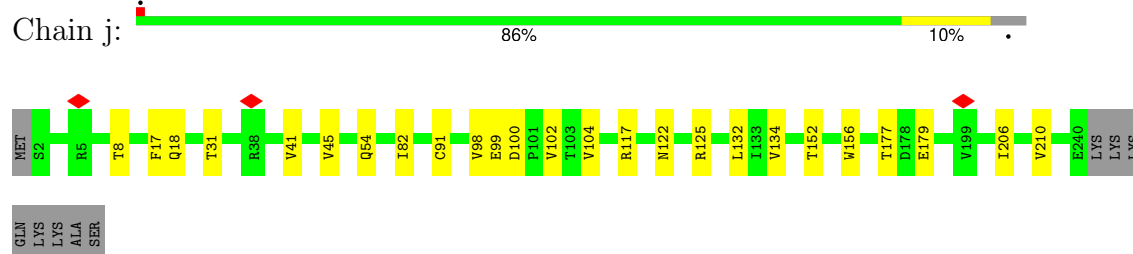
- Molecule 9: Proteasome subunit alpha type-4



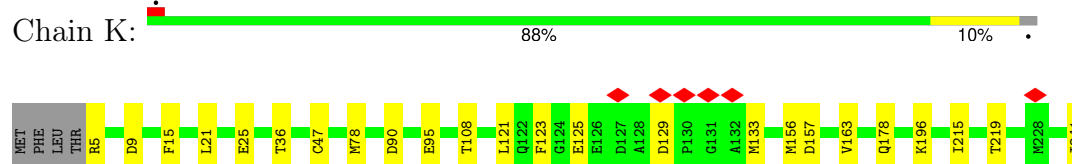
- Molecule 10: Proteasome subunit alpha type-7



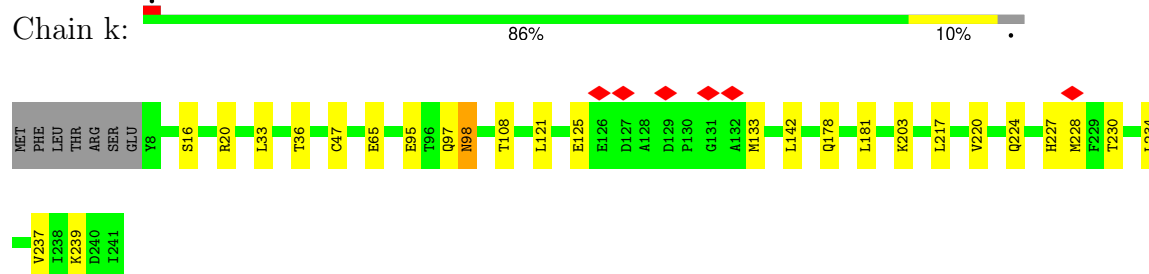
- Molecule 10: Proteasome subunit alpha type-7




- Molecule 11: Proteasome subunit alpha type-5

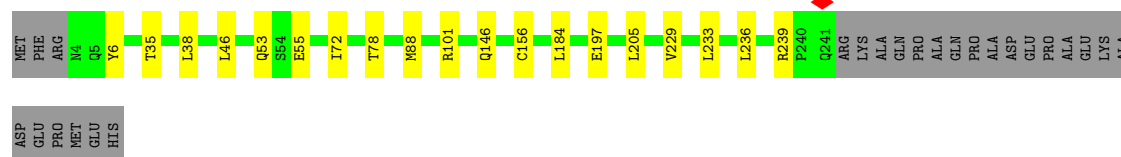


- Molecule 11: Proteasome subunit alpha type-5




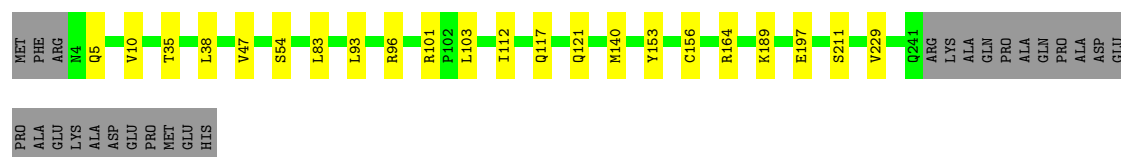
- Molecule 12: Proteasome subunit alpha type-1

Chain L:  83% 7% 10%




- Molecule 12: Proteasome subunit alpha type-1

Chain l:  82% 8% 10%




- Molecule 13: Proteasome subunit alpha type-3

Chain M:  86% 8% 6%



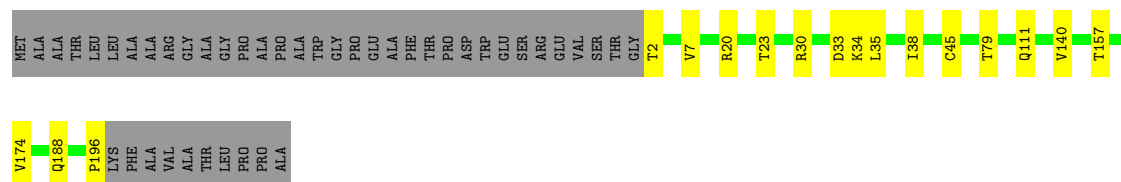
- Molecule 13: Proteasome subunit alpha type-3

Chain m:  86% 8% 6%




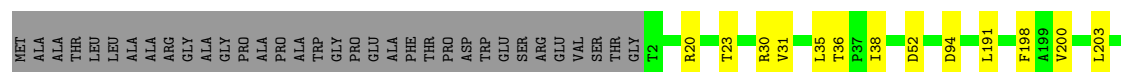
- Molecule 14: Proteasome subunit beta type-6

Chain N:  74% 7% 18%



- Molecule 14: Proteasome subunit beta type-6

Chain n:  80% 5% 14%

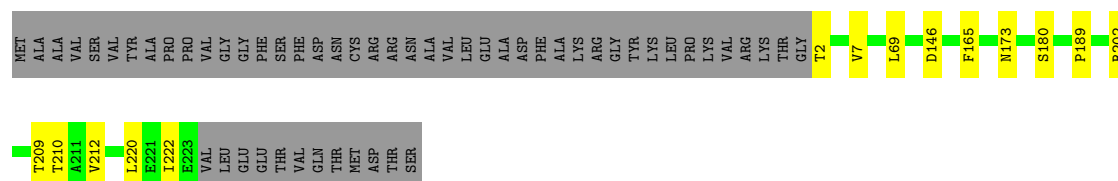






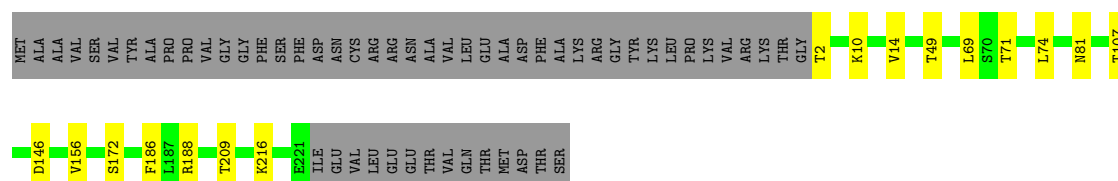
• Molecule 15: Proteasome subunit beta type-7

Chain O: 75% 5% 20%



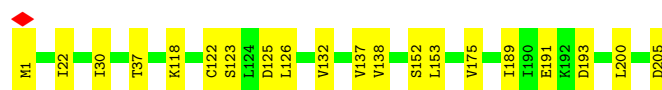
• Molecule 15: Proteasome subunit beta type-7

Chain o: 74% 6% 21%



• Molecule 16: Proteasome subunit beta type-3

Chain P: 90% 10%



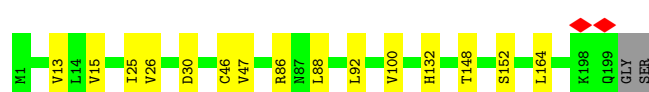
• Molecule 16: Proteasome subunit beta type-3

Chain p: 92% 7%



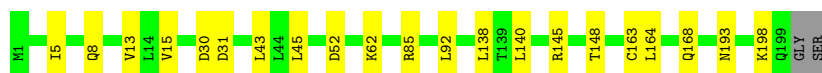
• Molecule 17: Proteasome subunit beta type-2

Chain Q: 92% 7%



• Molecule 17: Proteasome subunit beta type-2

Chain q: 89% 10%



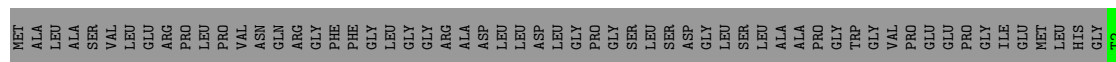
- Molecule 18: Proteasome subunit beta type-5

Chain R: 72% 5% 24%



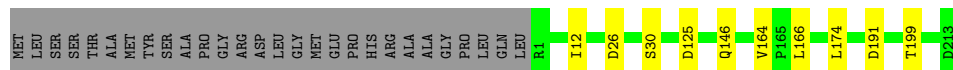
- Molecule 18: Proteasome subunit beta type-5

Chain r: 71% 6% 24%



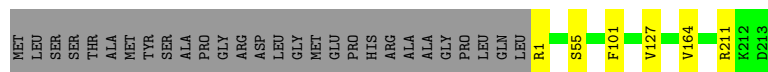
- Molecule 19: Proteasome subunit beta type-1

Chain S: 84% 12%



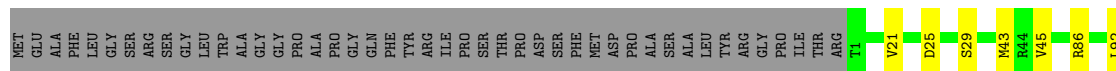
- Molecule 19: Proteasome subunit beta type-1

Chain s: 86% 12%



- Molecule 20: Proteasome subunit beta type-4

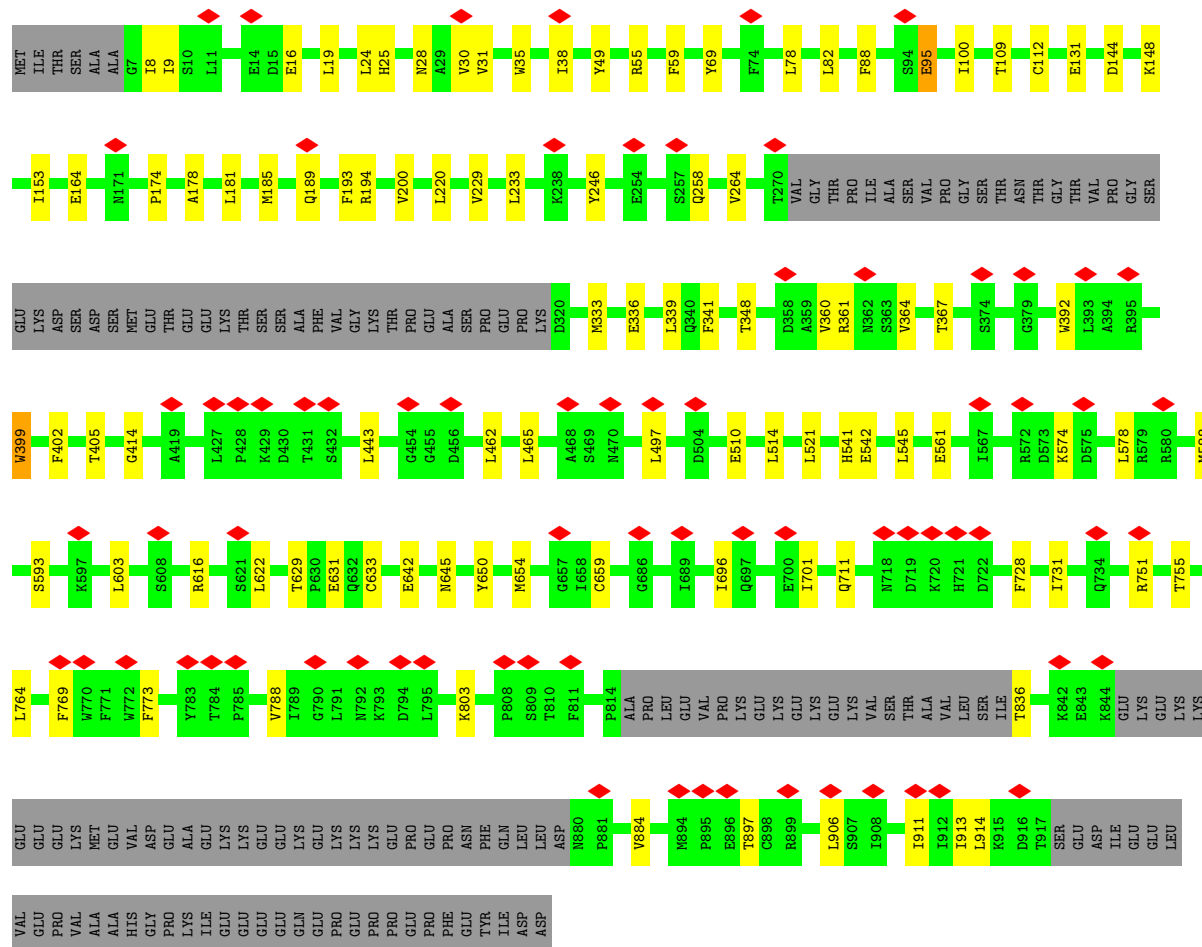
Chain T: 74% 8% 19%



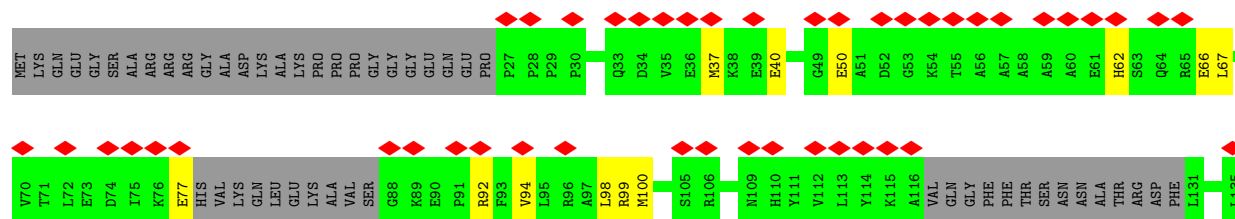
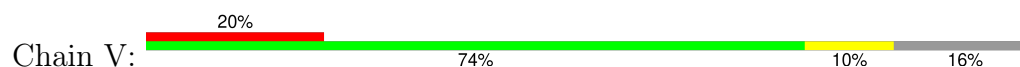
- Molecule 20: Proteasome subunit beta type-4

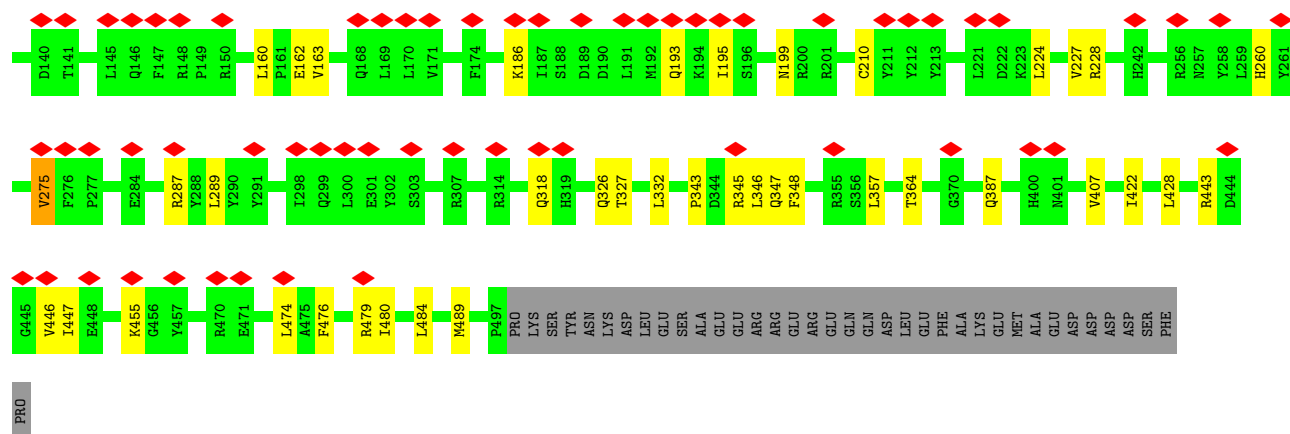
Chain t: 77% 5% 19%

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

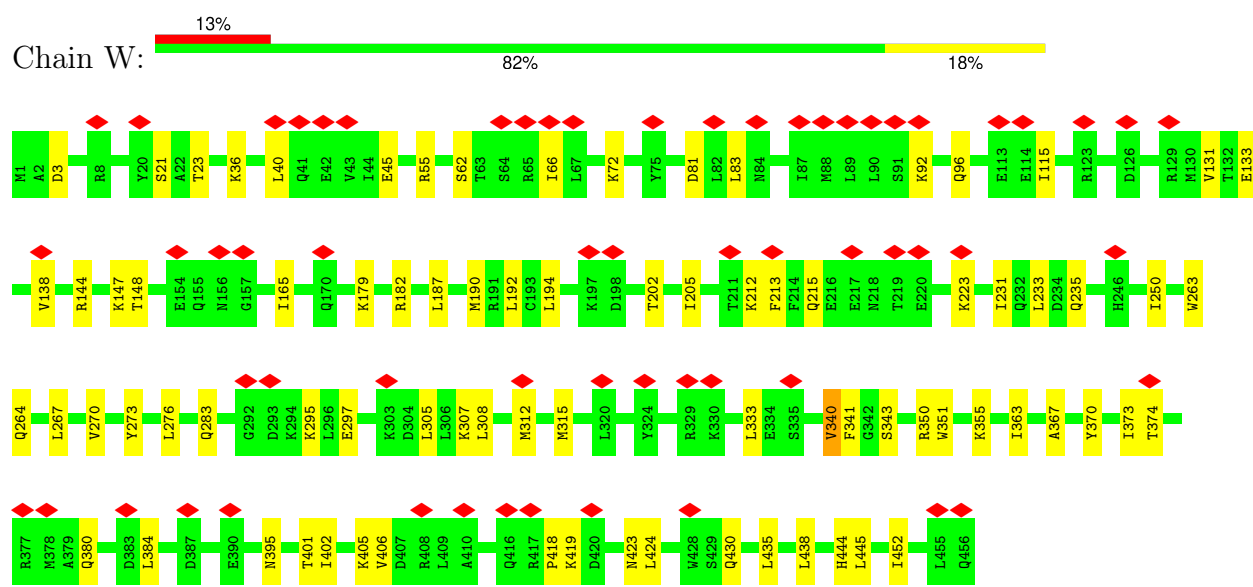


- Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

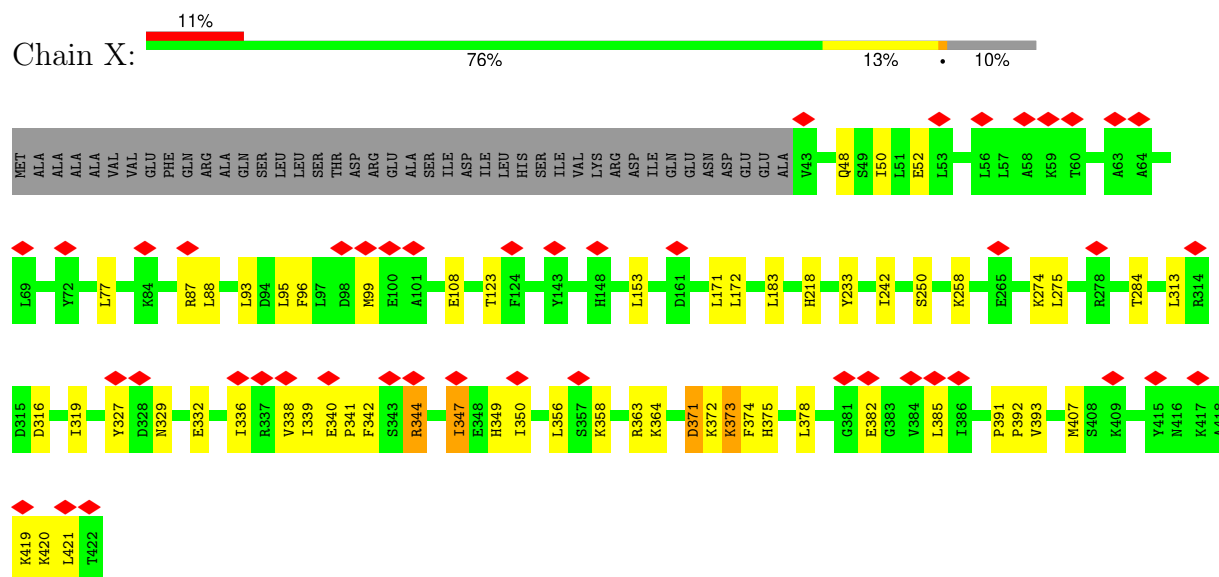





- Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

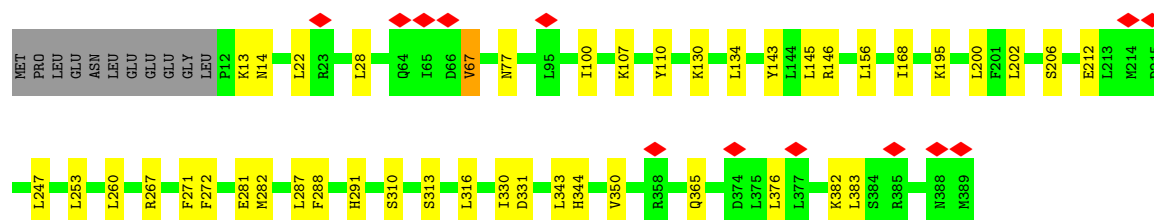


- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11



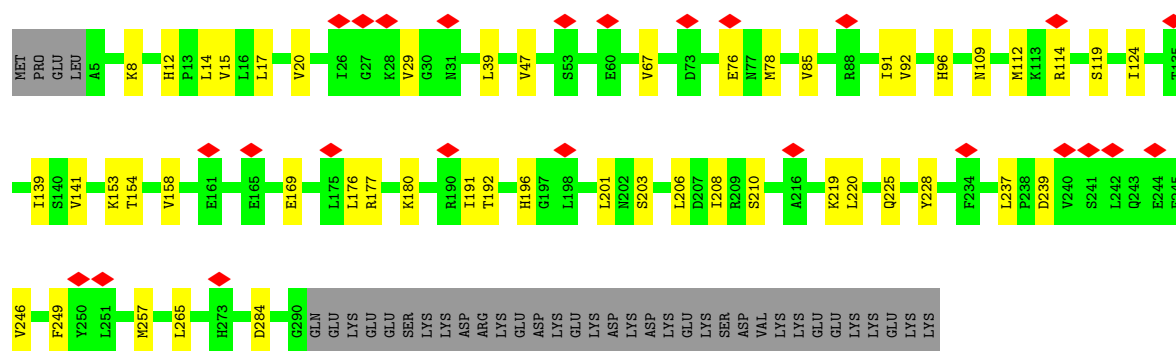
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 




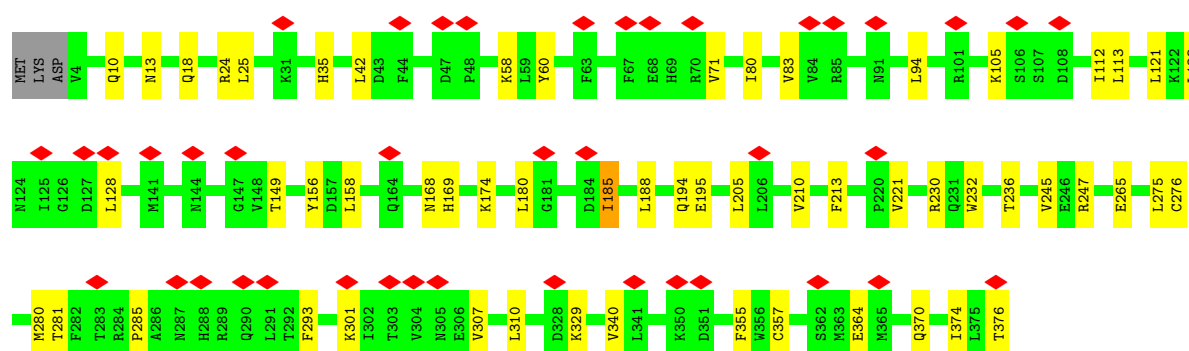
- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 

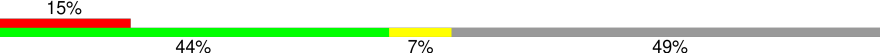


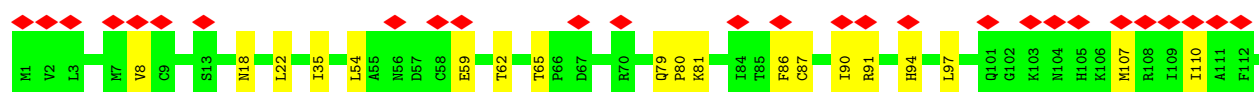
- Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

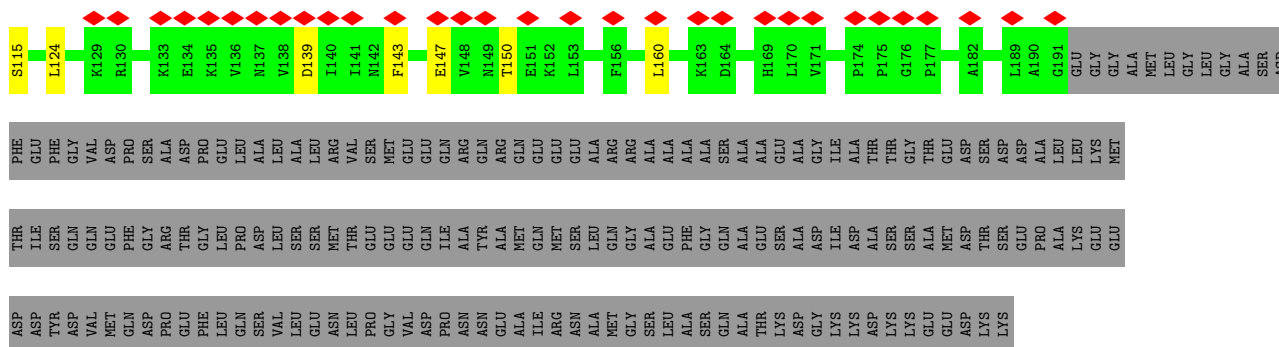
Chain a: 



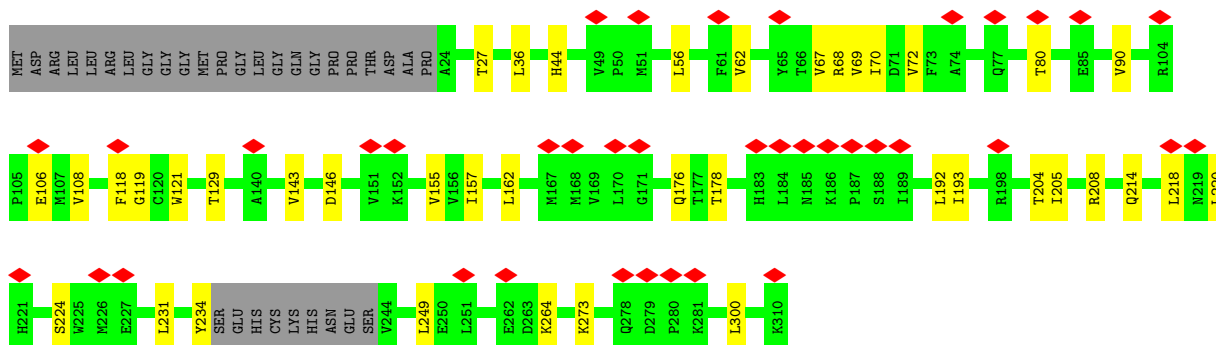
- Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

Chain b: 

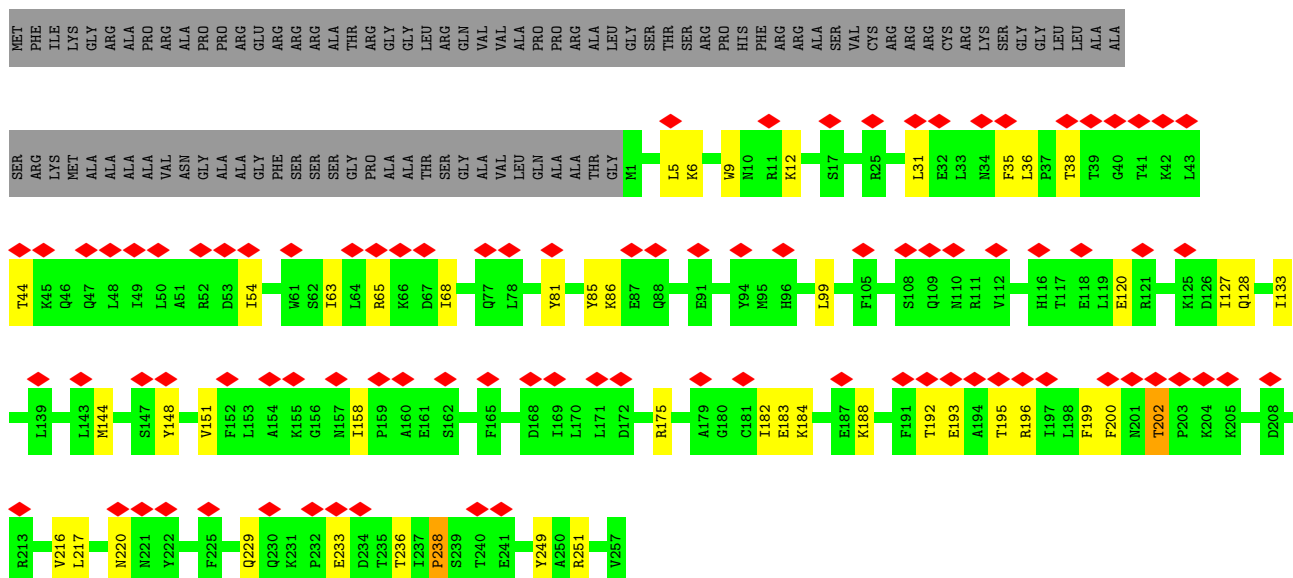




- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14

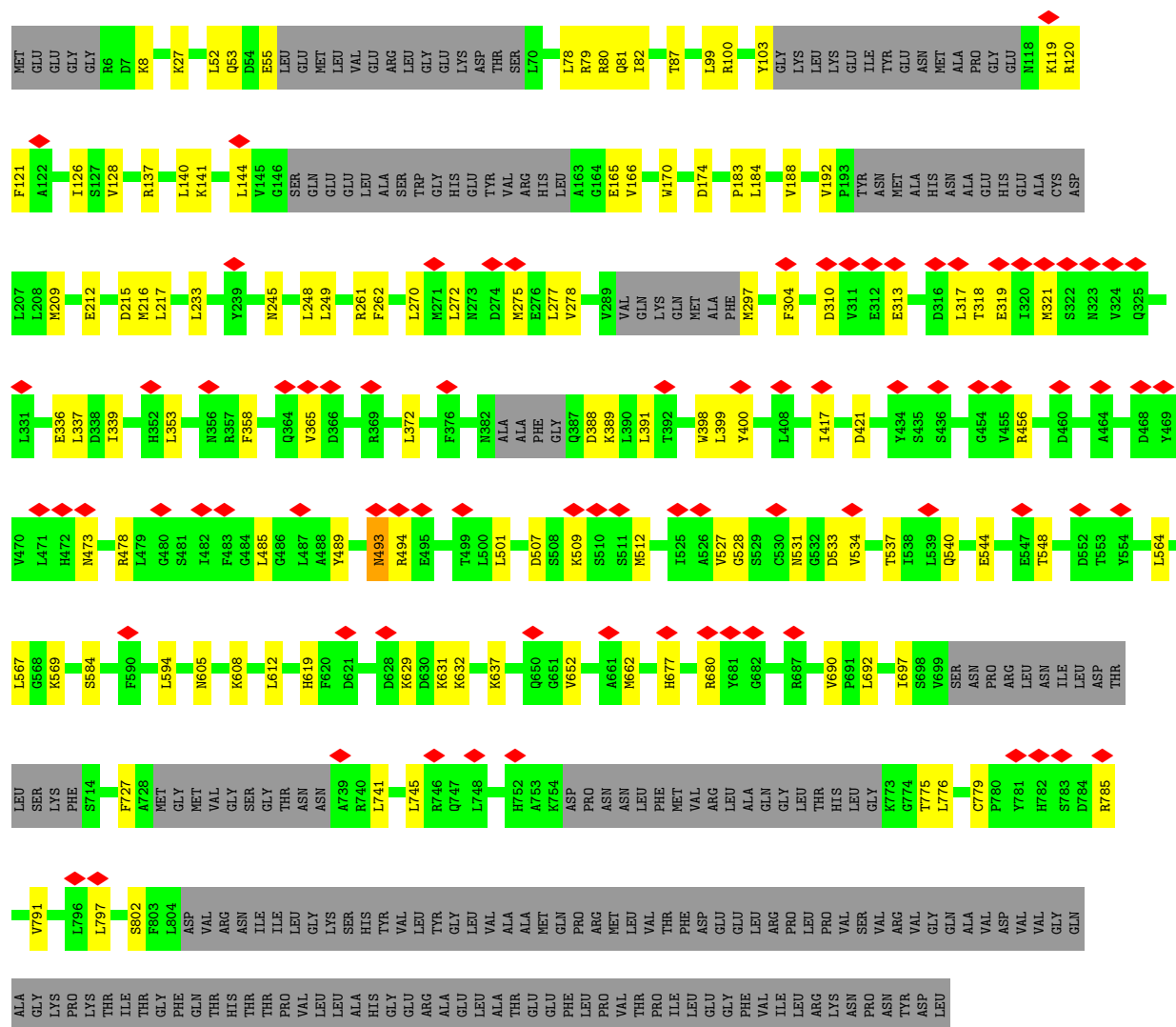


- Molecule 30: 26S proteasome non-ATPase regulatory subunit 8



- Molecule 31: 26S proteasome complex subunit SEM1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	147696	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 ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.235	Depositor
Minimum map value	-0.680	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.1	Depositor
Map size ( $\text{\AA}$ )	360.4, 360.4, 360.4	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.60	0/2939	0.72	0/3970
2	B	0.61	0/2844	0.73	1/3846 (0.0%)
3	C	0.60	0/2896	0.70	0/3895
4	D	0.59	0/3090	0.74	0/4168
5	E	0.62	0/2904	0.68	0/3924
6	F	0.61	0/2893	0.68	0/3908
7	G	0.58	0/1853	0.73	0/2515
7	g	0.59	0/1859	0.73	0/2523
8	H	0.59	0/1738	0.73	0/2365
8	h	0.60	0/1756	0.70	0/2389
9	I	0.59	0/1925	0.72	0/2606
9	i	0.60	0/1942	0.71	0/2628
10	J	0.61	0/1732	0.74	0/2362
10	j	0.62	0/1728	0.71	0/2358
11	K	0.60	0/1820	0.72	0/2464
11	k	0.59	0/1786	0.72	1/2419 (0.0%)
12	L	0.59	0/1885	0.73	0/2552
12	l	0.59	0/1885	0.71	0/2552
13	M	0.60	0/1891	0.73	0/2552
13	m	0.60	0/1891	0.72	0/2552
14	N	0.59	0/1487	0.75	0/2013
14	n	0.59	0/1561	0.77	0/2116
15	O	0.60	0/1687	0.78	1/2288 (0.0%)
15	o	0.59	0/1670	0.74	0/2265
16	P	0.57	0/1622	0.77	0/2187
16	p	0.56	0/1614	0.75	0/2177
17	Q	0.57	0/1603	0.75	0/2174
17	q	0.55	0/1603	0.73	0/2174
18	R	0.58	0/1579	0.74	0/2134
18	r	0.59	0/1579	0.74	0/2134
19	S	0.59	0/1674	0.77	0/2257
19	s	0.58	0/1671	0.76	1/2253 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
20	T	0.57	0/1706	0.76	0/2312
20	t	0.58	0/1706	0.74	0/2312
21	U	0.61	0/6396	0.68	0/8646
22	V	0.60	0/3668	0.71	1/4952 (0.0%)
23	W	0.60	0/3751	0.70	0/5042
24	X	0.60	0/3053	0.75	4/4115 (0.1%)
25	Y	0.57	0/3173	0.71	0/4273
26	Z	0.61	0/2324	0.73	0/3150
27	a	0.60	0/3053	0.71	0/4133
28	b	0.62	0/1478	0.69	0/2001
29	c	0.61	0/2226	0.71	0/3007
30	d	0.61	0/2162	0.72	0/2919
31	e	0.60	0/338	0.71	0/450
32	f	0.63	0/5393	0.75	0/7271
All	All	0.60	0/103034	0.72	9/139303 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	344	ARG	NE-CZ-NH1	7.94	124.27	120.30
22	V	345	ARG	CG-CD-NE	-7.94	95.13	111.80
24	X	344	ARG	CD-NE-CZ	6.84	133.18	123.60
19	s	101	PHE	CB-CA-C	6.51	123.43	110.40
15	O	165	PHE	CB-CA-C	6.49	123.37	110.40
24	X	344	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	B	278	ALA	CB-CA-C	6.13	119.30	110.10
11	k	98	ASN	CB-CA-C	5.63	121.66	110.40
24	X	375	HIS	CB-CA-C	5.24	120.87	110.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	376/433 (87%)	355 (94%)	14 (4%)	7 (2%)	6	31
2	B	366/440 (83%)	335 (92%)	25 (7%)	6 (2%)	8	34
3	C	359/406 (88%)	341 (95%)	14 (4%)	4 (1%)	12	44
4	D	378/418 (90%)	343 (91%)	26 (7%)	9 (2%)	5	25
5	E	373/389 (96%)	354 (95%)	18 (5%)	1 (0%)	37	70
6	F	372/439 (85%)	356 (96%)	14 (4%)	2 (0%)	25	61
7	G	237/246 (96%)	233 (98%)	3 (1%)	1 (0%)	30	66
7	g	238/246 (97%)	233 (98%)	3 (1%)	2 (1%)	16	51
8	H	228/234 (97%)	219 (96%)	5 (2%)	4 (2%)	7	32
8	h	232/234 (99%)	225 (97%)	7 (3%)	0	100	100
9	I	246/261 (94%)	236 (96%)	6 (2%)	4 (2%)	8	34
9	i	248/261 (95%)	238 (96%)	6 (2%)	4 (2%)	8	34
10	J	237/248 (96%)	225 (95%)	10 (4%)	2 (1%)	16	51
10	j	237/248 (96%)	225 (95%)	10 (4%)	2 (1%)	16	51
11	K	235/241 (98%)	226 (96%)	9 (4%)	0	100	100
11	k	232/241 (96%)	225 (97%)	7 (3%)	0	100	100
12	L	236/263 (90%)	232 (98%)	4 (2%)	0	100	100
12	l	236/263 (90%)	228 (97%)	7 (3%)	1 (0%)	30	66
13	M	238/255 (93%)	233 (98%)	4 (2%)	1 (0%)	30	66
13	m	238/255 (93%)	231 (97%)	6 (2%)	1 (0%)	30	66
14	N	193/239 (81%)	187 (97%)	6 (3%)	0	100	100
14	n	203/239 (85%)	193 (95%)	9 (4%)	1 (0%)	25	61
15	O	220/277 (79%)	210 (96%)	8 (4%)	2 (1%)	14	49
15	o	218/277 (79%)	210 (96%)	5 (2%)	3 (1%)	9	37
16	P	203/205 (99%)	189 (93%)	13 (6%)	1 (0%)	25	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	p	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
17	Q	197/201 (98%)	191 (97%)	6 (3%)	0	100	100
17	q	197/201 (98%)	192 (98%)	4 (2%)	1 (0%)	25	61
18	R	199/263 (76%)	199 (100%)	0	0	100	100
18	r	199/263 (76%)	197 (99%)	2 (1%)	0	100	100
19	S	211/241 (88%)	206 (98%)	4 (2%)	1 (0%)	25	61
19	s	211/241 (88%)	207 (98%)	4 (2%)	0	100	100
20	T	213/264 (81%)	207 (97%)	6 (3%)	0	100	100
20	t	213/264 (81%)	209 (98%)	4 (2%)	0	100	100
21	U	798/953 (84%)	769 (96%)	21 (3%)	8 (1%)	13	46
22	V	441/534 (83%)	414 (94%)	24 (5%)	3 (1%)	19	54
23	W	454/456 (100%)	426 (94%)	17 (4%)	11 (2%)	5	25
24	X	378/422 (90%)	355 (94%)	14 (4%)	9 (2%)	5	25
25	Y	376/389 (97%)	351 (93%)	21 (6%)	4 (1%)	12	44
26	Z	284/324 (88%)	256 (90%)	24 (8%)	4 (1%)	9	37
27	a	371/376 (99%)	345 (93%)	23 (6%)	3 (1%)	16	51
28	b	189/377 (50%)	179 (95%)	6 (3%)	4 (2%)	5	28
29	c	274/310 (88%)	256 (93%)	17 (6%)	1 (0%)	30	66
30	d	255/350 (73%)	232 (91%)	13 (5%)	10 (4%)	2	14
31	e	36/70 (51%)	29 (81%)	6 (17%)	1 (3%)	4	21
32	f	669/908 (74%)	612 (92%)	46 (7%)	11 (2%)	8	34
All	All	12946/14870 (87%)	12308 (95%)	509 (4%)	129 (1%)	16	46

All (129) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	LYS
1	A	117	GLN
1	A	431	THR
2	B	278	ALA
2	B	389	ASP
2	B	434	THR
4	D	276	ASP
4	D	297	ASP
4	D	301	GLN

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Mol	Chain	Res	Type
8	H	16	SER
8	H	233	ILE
9	I	186	LEU
10	J	6	ALA
21	U	95	GLU
21	U	174	PRO
21	U	258	GLN
21	U	399	TRP
21	U	728	PHE
23	W	367	ALA
23	W	402	ILE
24	X	382	GLU
26	Z	225	GLN
27	a	185	ILE
29	c	119	GLY
30	d	12	LYS
30	d	127	ILE
32	f	100	ARG
32	f	183	PRO
32	f	365	VAL
32	f	493	ASN
32	f	584	SER
32	f	802	SER
9	i	107	CYS
10	j	98	VAL
12	l	121	GLN
15	o	10	LYS
17	q	198	LYS
3	C	133	PRO
3	C	225	GLY
6	F	437	TYR
7	G	134	LEU
13	M	230	ASP
16	P	30	ILE
19	S	191	ASP
21	U	561	GLU
22	V	100	MET
23	W	340	VAL
23	W	405	LYS
24	X	363	ARG
24	X	373	LYS
24	X	378	LEU

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Mol	Chain	Res	Type
25	Y	67	VAL
25	Y	344	HIS
27	a	168	ASN
28	b	22	LEU
30	d	86	LYS
30	d	202	THR
32	f	421	ASP
14	n	20	ARG
1	A	269	ALA
1	A	311	PRO
2	B	436	GLU
4	D	234	GLU
4	D	270	ILE
4	D	367	PRO
8	H	180	GLU
9	I	39	ALA
9	I	63	GLU
10	J	52	LYS
21	U	178	ALA
23	W	235	GLN
23	W	343	SER
23	W	419	LYS
24	X	347	ILE
24	X	385	LEU
26	Z	239	ASP
26	Z	249	PHE
28	b	81	LYS
30	d	238	PRO
32	f	126	ILE
7	g	134	LEU
9	i	62	SER
9	i	185	THR
9	i	223	THR
1	A	310	ASP
2	B	302	GLU
3	C	220	VAL
4	D	197	ASP
4	D	368	ASP
8	H	216	ALA
9	I	7	SER
15	O	146	ASP
21	U	414	GLY

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Mol	Chain	Res	Type
22	V	275	VAL
23	W	21	SER
23	W	92	LYS
24	X	371	ASP
28	b	79	GLN
30	d	184	LYS
30	d	200	PHE
30	d	216	VAL
30	d	220	ASN
32	f	388	ASP
32	f	637	LYS
7	g	188	ASP
15	o	146	ASP
15	o	172	SER
4	D	147	ALA
5	E	112	PRO
25	Y	14	ASN
25	Y	28	LEU
26	Z	177	ARG
30	d	68	ILE
10	j	100	ASP
13	m	60	GLU
1	A	427	PRO
15	O	189	PRO
24	X	392	PRO
31	e	6	GLN
32	f	528	GLY
6	F	180	ARG
27	a	285	PRO
23	W	138	VAL
2	B	106	PRO
3	C	401	ILE
23	W	418	PRO
22	V	343	PRO
24	X	391	PRO
28	b	80	PRO

### 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	297/372 (80%)	255 (86%)	42 (14%)	3	13
2	B	300/385 (78%)	260 (87%)	40 (13%)	3	15
3	C	315/352 (90%)	275 (87%)	40 (13%)	3	17
4	D	333/366 (91%)	291 (87%)	42 (13%)	3	17
5	E	298/341 (87%)	263 (88%)	35 (12%)	4	19
6	F	295/379 (78%)	259 (88%)	36 (12%)	4	18
7	G	192/210 (91%)	171 (89%)	21 (11%)	5	22
7	g	193/210 (92%)	170 (88%)	23 (12%)	4	19
8	H	165/191 (86%)	143 (87%)	22 (13%)	3	15
8	h	165/191 (86%)	151 (92%)	14 (8%)	8	33
9	I	191/221 (86%)	167 (87%)	24 (13%)	3	17
9	i	193/221 (87%)	166 (86%)	27 (14%)	3	13
10	J	153/211 (72%)	128 (84%)	25 (16%)	2	9
10	j	152/211 (72%)	129 (85%)	23 (15%)	2	12
11	K	193/203 (95%)	169 (88%)	24 (12%)	4	17
11	k	189/203 (93%)	163 (86%)	26 (14%)	3	14
12	L	198/224 (88%)	179 (90%)	19 (10%)	7	27
12	l	198/224 (88%)	177 (89%)	21 (11%)	5	23
13	M	192/212 (91%)	172 (90%)	20 (10%)	5	23
13	m	192/212 (91%)	173 (90%)	19 (10%)	6	26
14	N	152/181 (84%)	135 (89%)	17 (11%)	5	21
14	n	159/181 (88%)	147 (92%)	12 (8%)	11	38
15	O	179/228 (78%)	168 (94%)	11 (6%)	15	46
15	o	177/228 (78%)	164 (93%)	13 (7%)	11	39
16	P	173/174 (99%)	154 (89%)	19 (11%)	5	22
16	p	172/174 (99%)	157 (91%)	15 (9%)	8	32
17	Q	164/171 (96%)	149 (91%)	15 (9%)	7	30
17	q	164/171 (96%)	144 (88%)	20 (12%)	4	18
18	R	153/202 (76%)	141 (92%)	12 (8%)	10	36
18	r	153/202 (76%)	138 (90%)	15 (10%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	S	175/199 (88%)	166 (95%)	9 (5%)	20	53
19	s	174/199 (87%)	169 (97%)	5 (3%)	37	70
20	T	176/215 (82%)	156 (89%)	20 (11%)	4	20
20	t	176/215 (82%)	163 (93%)	13 (7%)	11	38
21	U	685/816 (84%)	591 (86%)	94 (14%)	3	14
22	V	387/460 (84%)	338 (87%)	49 (13%)	3	17
23	W	416/416 (100%)	345 (83%)	71 (17%)	1	8
24	X	327/362 (90%)	275 (84%)	52 (16%)	2	10
25	Y	334/344 (97%)	293 (88%)	41 (12%)	4	18
26	Z	257/295 (87%)	212 (82%)	45 (18%)	1	8
27	a	333/336 (99%)	278 (84%)	55 (16%)	2	9
28	b	167/312 (54%)	145 (87%)	22 (13%)	3	15
29	c	243/268 (91%)	204 (84%)	39 (16%)	2	10
30	d	231/294 (79%)	193 (84%)	38 (16%)	2	9
31	e	38/63 (60%)	33 (87%)	5 (13%)	3	15
32	f	580/763 (76%)	470 (81%)	110 (19%)	1	7
All	All	10749/12608 (85%)	9389 (87%)	1360 (13%)	6	17

All (1360) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	87	LEU
1	A	90	GLU
1	A	97	ARG
1	A	153	LEU
1	A	160	THR
1	A	173	THR
1	A	177	VAL
1	A	181	LYS
1	A	193	THR
1	A	196	LEU
1	A	204	LEU
1	A	222	LYS
1	A	224	LEU
1	A	225	CYS

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Mol	Chain	Res	Type
1	A	248	LYS
1	A	267	LYS
1	A	268	LYS
1	A	271	LEU
1	A	277	ILE
1	A	286	ASP
1	A	293	ASN
1	A	296	GLN
1	A	297	ARG
1	A	307	ASP
1	A	314	ASN
1	A	318	LEU
1	A	322	ASN
1	A	323	ARG
1	A	327	LEU
1	A	328	ASP
1	A	333	ARG
1	A	338	ASP
1	A	348	LEU
1	A	360	ARG
1	A	364	VAL
1	A	372	LEU
1	A	375	ARG
1	A	397	ILE
1	A	401	ARG
1	A	403	ILE
1	A	432	TYR
2	B	131	HIS
2	B	139	VAL
2	B	149	SER
2	B	162	VAL
2	B	163	LEU
2	B	171	VAL
2	B	178	LYS
2	B	182	GLU
2	B	183	THR
2	B	205	LEU
2	B	223	ILE
2	B	232	LYS
2	B	235	LEU
2	B	244	SER
2	B	250	VAL

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Mol	Chain	Res	Type
2	B	256	ILE
2	B	266	LEU
2	B	270	LEU
2	B	287	ILE
2	B	288	ASP
2	B	306	GLN
2	B	310	LEU
2	B	315	GLN
2	B	331	THR
2	B	333	ARG
2	B	335	GLU
2	B	337	LEU
2	B	341	LEU
2	B	343	ARG
2	B	348	ASP
2	B	359	LYS
2	B	365	PHE
2	B	374	LEU
2	B	378	VAL
2	B	388	ASP
2	B	390	LEU
2	B	434	THR
2	B	438	LEU
2	B	439	TYR
2	B	440	LEU
3	C	25	LEU
3	C	27	LYS
3	C	29	GLU
3	C	41	ASN
3	C	45	LEU
3	C	52	LEU
3	C	62	GLU
3	C	80	MET
3	C	109	THR
3	C	117	ARG
3	C	122	THR
3	C	123	LEU
3	C	130	LYS
3	C	134	LEU
3	C	135	VAL
3	C	143	VAL
3	C	148	TYR

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Mol	Chain	Res	Type
3	C	149	GLU
3	C	184	LYS
3	C	186	VAL
3	C	194	THR
3	C	197	THR
3	C	199	LEU
3	C	210	THR
3	C	222	LYS
3	C	226	GLU
3	C	248	MET
3	C	249	ASP
3	C	268	GLU
3	C	269	VAL
3	C	278	ASN
3	C	287	LYS
3	C	292	ILE
3	C	295	THR
3	C	297	ARG
3	C	298	ILE
3	C	312	ASP
3	C	313	ARG
3	C	377	HIS
3	C	393	LYS
4	D	54	LEU
4	D	56	VAL
4	D	59	GLU
4	D	85	ILE
4	D	88	VAL
4	D	94	GLU
4	D	99	ASN
4	D	100	THR
4	D	102	ILE
4	D	109	SER
4	D	124	LEU
4	D	130	VAL
4	D	140	VAL
4	D	143	LEU
4	D	148	ASP
4	D	154	LEU
4	D	162	VAL
4	D	167	ILE
4	D	177	VAL

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Mol	Chain	Res	Type
4	D	194	ILE
4	D	202	VAL
4	D	227	PHE
4	D	228	ILE
4	D	231	VAL
4	D	265	ASP
4	D	267	ILE
4	D	274	ARG
4	D	275	PHE
4	D	284	GLU
4	D	289	LEU
4	D	299	PHE
4	D	301	GLN
4	D	303	VAL
4	D	304	ASN
4	D	306	LYS
4	D	317	LEU
4	D	326	ARG
4	D	330	LYS
4	D	331	ILE
4	D	338	ARG
4	D	391	ARG
4	D	393	ILE
5	E	51	GLN
5	E	65	THR
5	E	67	GLU
5	E	87	LEU
5	E	105	LEU
5	E	111	LEU
5	E	113	ARG
5	E	124	HIS
5	E	159	PHE
5	E	168	LYS
5	E	171	LEU
5	E	183	LEU
5	E	190	GLN
5	E	199	VAL
5	E	203	ILE
5	E	225	HIS
5	E	236	ASP
5	E	247	THR
5	E	250	ASP

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Mol	Chain	Res	Type
5	E	251	ARG
5	E	270	LEU
5	E	272	ARG
5	E	274	LYS
5	E	277	MET
5	E	284	THR
5	E	291	ARG
5	E	295	LEU
5	E	299	ILE
5	E	307	GLN
5	E	332	VAL
5	E	334	LEU
5	E	336	ASP
5	E	371	VAL
5	E	386	TYR
5	E	389	VAL
6	F	83	ASN
6	F	86	LEU
6	F	90	VAL
6	F	93	VAL
6	F	95	GLU
6	F	134	LEU
6	F	140	VAL
6	F	153	VAL
6	F	159	LEU
6	F	178	ASP
6	F	180	ARG
6	F	182	THR
6	F	198	LEU
6	F	211	LYS
6	F	215	LEU
6	F	221	LYS
6	F	235	LEU
6	F	236	LEU
6	F	250	LYS
6	F	251	LEU
6	F	274	LEU
6	F	287	GLU
6	F	305	GLU
6	F	307	GLN
6	F	326	VAL
6	F	327	LYS

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Mol	Chain	Res	Type
6	F	343	LEU
6	F	383	GLU
6	F	400	CYS
6	F	405	MET
6	F	410	ARG
6	F	415	LEU
6	F	416	THR
6	F	418	GLU
6	F	430	LYS
6	F	432	LYS
7	G	13	ILE
7	G	14	THR
7	G	16	PHE
7	G	25	VAL
7	G	34	GLN
7	G	37	LEU
7	G	47	CYS
7	G	61	LEU
7	G	81	THR
7	G	86	ASP
7	G	111	VAL
7	G	114	LEU
7	G	153	LYS
7	G	154	CYS
7	G	160	TYR
7	G	166	THR
7	G	210	PHE
7	G	211	LYS
7	G	215	ILE
7	G	230	LEU
7	G	231	THR
8	H	11	THR
8	H	13	PHE
8	H	14	SER
8	H	19	LEU
8	H	20	VAL
8	H	65	VAL
8	H	74	LEU
8	H	75	VAL
8	H	82	ASP
8	H	87	VAL
8	H	107	THR

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Mol	Chain	Res	Type
8	H	119	GLN
8	H	127	VAL
8	H	132	VAL
8	H	156	PHE
8	H	159	LYS
8	H	168	VAL
8	H	171	LYS
8	H	175	GLU
8	H	194	THR
8	H	208	ILE
8	H	213	CYS
9	I	4	ARG
9	I	9	THR
9	I	12	PHE
9	I	18	LEU
9	I	35	LEU
9	I	44	LEU
9	I	61	PHE
9	I	76	VAL
9	I	95	GLN
9	I	119	GLN
9	I	128	ARG
9	I	133	SER
9	I	134	LEU
9	I	151	ASP
9	I	166	ASN
9	I	168	SER
9	I	180	LYS
9	I	186	LEU
9	I	192	LEU
9	I	197	LEU
9	I	224	VAL
9	I	226	ARG
9	I	248	GLU
9	I	249	ARG
10	J	3	TYR
10	J	10	PHE
10	J	31	THR
10	J	39	ASP
10	J	41	VAL
10	J	43	LEU
10	J	45	VAL

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Mol	Chain	Res	Type
10	J	60	ARG
10	J	69	VAL
10	J	79	ASP
10	J	85	ASN
10	J	98	VAL
10	J	99	GLU
10	J	100	ASP
10	J	102	VAL
10	J	104	VAL
10	J	114	LEU
10	J	117	ARG
10	J	132	LEU
10	J	134	VAL
10	J	139	ASP
10	J	146	GLN
10	J	148	ASP
10	J	179	GLU
10	J	220	LEU
11	K	5	ARG
11	K	9	ASP
11	K	15	PHE
11	K	21	LEU
11	K	25	GLU
11	K	36	THR
11	K	47	CYS
11	K	78	MET
11	K	90	ASP
11	K	95	GLU
11	K	108	THR
11	K	121	LEU
11	K	123	PHE
11	K	125	GLU
11	K	129	ASP
11	K	133	MET
11	K	156	MET
11	K	157	ASP
11	K	163	VAL
11	K	178	GLN
11	K	196	LYS
11	K	215	ILE
11	K	219	THR
11	K	241	ILE

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Mol	Chain	Res	Type
12	L	6	TYR
12	L	35	THR
12	L	38	LEU
12	L	46	LEU
12	L	53	GLN
12	L	55	GLU
12	L	72	ILE
12	L	78	THR
12	L	88	MET
12	L	101	ARG
12	L	146	GLN
12	L	156	CYS
12	L	184	LEU
12	L	197	GLU
12	L	205	LEU
12	L	229	VAL
12	L	233	LEU
12	L	236	LEU
12	L	239	ARG
13	M	7	TYR
13	M	27	MET
13	M	41	CYS
13	M	54	LEU
13	M	56	LYS
13	M	87	LEU
13	M	100	SER
13	M	128	VAL
13	M	136	MET
13	M	142	VAL
13	M	158	TYR
13	M	185	THR
13	M	189	ILE
13	M	201	HIS
13	M	204	VAL
13	M	209	PHE
13	M	212	GLU
13	M	229	LYS
13	M	232	ARG
13	M	236	GLU
14	N	2	THR
14	N	7	VAL
14	N	20	ARG

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Mol	Chain	Res	Type
14	N	23	THR
14	N	30	ARG
14	N	33	ASP
14	N	34	LYS
14	N	35	LEU
14	N	38	ILE
14	N	45	CYS
14	N	79	THR
14	N	111	GLN
14	N	140	VAL
14	N	157	THR
14	N	174	VAL
14	N	188	GLN
14	N	196	PRO
15	O	2	THR
15	O	7	VAL
15	O	69	LEU
15	O	173	ASN
15	O	180	SER
15	O	202	ARG
15	O	209	THR
15	O	210	THR
15	O	212	VAL
15	O	220	LEU
15	O	222	ILE
16	P	1	MET
16	P	22	ILE
16	P	37	THR
16	P	118	LYS
16	P	122	CYS
16	P	123	SER
16	P	125	ASP
16	P	126	LEU
16	P	132	VAL
16	P	137	VAL
16	P	138	VAL
16	P	152	SER
16	P	153	LEU
16	P	175	VAL
16	P	189	ILE
16	P	191	GLU
16	P	193	ASP

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Mol	Chain	Res	Type
16	P	200	LEU
16	P	205	ASP
17	Q	13	VAL
17	Q	15	VAL
17	Q	25	ILE
17	Q	26	VAL
17	Q	30	ASP
17	Q	46	CYS
17	Q	47	VAL
17	Q	86	ARG
17	Q	88	LEU
17	Q	92	LEU
17	Q	100	VAL
17	Q	132	HIS
17	Q	148	THR
17	Q	152	SER
17	Q	164	LEU
18	R	15	VAL
18	R	33	LYS
18	R	36	ILE
18	R	63	GLN
18	R	74	ARG
18	R	76	SER
18	R	100	THR
18	R	137	TYR
18	R	139	VAL
18	R	142	ARG
18	R	167	ARG
18	R	183	ASP
19	S	12	ILE
19	S	26	ASP
19	S	30	SER
19	S	125	ASP
19	S	146	GLN
19	S	164	VAL
19	S	166	LEU
19	S	174	LEU
19	S	199	THR
20	T	21	VAL
20	T	25	ASP
20	T	29	SER
20	T	43	MET

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Mol	Chain	Res	Type
20	T	45	VAL
20	T	86	ARG
20	T	92	LEU
20	T	99	ARG
20	T	112	ILE
20	T	144	TYR
20	T	145	LEU
20	T	151	ARG
20	T	159	VAL
20	T	168	LEU
20	T	169	VAL
20	T	179	ARG
20	T	192	VAL
20	T	193	THR
20	T	205	THR
20	T	214	MET
21	U	8	ILE
21	U	9	ILE
21	U	16	GLU
21	U	19	LEU
21	U	24	LEU
21	U	25	HIS
21	U	28	ASN
21	U	30	VAL
21	U	31	VAL
21	U	35	TRP
21	U	38	ILE
21	U	49	TYR
21	U	55	ARG
21	U	59	PHE
21	U	69	TYR
21	U	78	LEU
21	U	82	LEU
21	U	88	PHE
21	U	95	GLU
21	U	100	ILE
21	U	109	THR
21	U	112	CYS
21	U	131	GLU
21	U	144	ASP
21	U	148	LYS
21	U	153	ILE

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Mol	Chain	Res	Type
21	U	164	GLU
21	U	181	LEU
21	U	185	MET
21	U	189	GLN
21	U	193	PHE
21	U	194	ARG
21	U	200	VAL
21	U	220	LEU
21	U	229	VAL
21	U	233	LEU
21	U	246	TYR
21	U	264	VAL
21	U	333	MET
21	U	336	GLU
21	U	339	LEU
21	U	341	PHE
21	U	348	THR
21	U	360	VAL
21	U	361	ARG
21	U	364	VAL
21	U	367	THR
21	U	392	TRP
21	U	399	TRP
21	U	402	PHE
21	U	405	THR
21	U	443	LEU
21	U	462	LEU
21	U	465	LEU
21	U	497	LEU
21	U	510	GLU
21	U	514	LEU
21	U	521	LEU
21	U	541	HIS
21	U	542	GLU
21	U	545	LEU
21	U	574	LYS
21	U	578	LEU
21	U	588	MET
21	U	593	SER
21	U	603	LEU
21	U	616	ARG
21	U	622	LEU

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Mol	Chain	Res	Type
21	U	629	THR
21	U	631	GLU
21	U	633	CYS
21	U	642	GLU
21	U	645	ASN
21	U	650	TYR
21	U	654	MET
21	U	659	CYS
21	U	696	ILE
21	U	701	ILE
21	U	711	GLN
21	U	731	ILE
21	U	751	ARG
21	U	755	THR
21	U	764	LEU
21	U	769	PHE
21	U	773	PHE
21	U	788	VAL
21	U	803	LYS
21	U	836	THR
21	U	884	VAL
21	U	897	THR
21	U	906	LEU
21	U	911	ILE
21	U	913	ILE
21	U	914	LEU
22	V	37	MET
22	V	40	GLU
22	V	50	GLU
22	V	62	HIS
22	V	66	GLU
22	V	67	LEU
22	V	77	GLU
22	V	92	ARG
22	V	94	VAL
22	V	98	LEU
22	V	99	ARG
22	V	160	LEU
22	V	162	GLU
22	V	163	VAL
22	V	186	LYS
22	V	193	GLN

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Mol	Chain	Res	Type
22	V	195	ILE
22	V	199	ASN
22	V	210	CYS
22	V	224	LEU
22	V	227	VAL
22	V	228	ARG
22	V	260	HIS
22	V	275	VAL
22	V	287	ARG
22	V	289	LEU
22	V	318	GLN
22	V	326	GLN
22	V	327	THR
22	V	332	LEU
22	V	346	LEU
22	V	347	GLN
22	V	348	PHE
22	V	357	LEU
22	V	364	THR
22	V	387	GLN
22	V	407	VAL
22	V	422	ILE
22	V	428	LEU
22	V	443	ARG
22	V	446	VAL
22	V	447	ILE
22	V	455	LYS
22	V	474	LEU
22	V	476	PHE
22	V	479	ARG
22	V	480	ILE
22	V	484	LEU
22	V	489	MET
23	W	3	ASP
23	W	23	THR
23	W	36	LYS
23	W	40	LEU
23	W	45	GLU
23	W	55	ARG
23	W	62	SER
23	W	66	ILE
23	W	72	LYS

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Mol	Chain	Res	Type
23	W	81	ASP
23	W	83	LEU
23	W	96	GLN
23	W	115	ILE
23	W	131	VAL
23	W	133	GLU
23	W	144	ARG
23	W	147	LYS
23	W	148	THR
23	W	165	ILE
23	W	179	LYS
23	W	182	ARG
23	W	187	LEU
23	W	190	MET
23	W	192	LEU
23	W	194	LEU
23	W	202	THR
23	W	205	ILE
23	W	212	LYS
23	W	213	PHE
23	W	215	GLN
23	W	223	LYS
23	W	231	ILE
23	W	233	LEU
23	W	250	ILE
23	W	263	TRP
23	W	264	GLN
23	W	267	LEU
23	W	270	VAL
23	W	273	TYR
23	W	276	LEU
23	W	283	GLN
23	W	295	LYS
23	W	297	GLU
23	W	305	LEU
23	W	307	LYS
23	W	308	LEU
23	W	312	MET
23	W	315	MET
23	W	333	LEU
23	W	340	VAL
23	W	341	PHE

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Mol	Chain	Res	Type
23	W	350	ARG
23	W	351	TRP
23	W	355	LYS
23	W	363	ILE
23	W	370	TYR
23	W	373	ILE
23	W	374	THR
23	W	380	GLN
23	W	384	LEU
23	W	395	ASN
23	W	401	THR
23	W	406	VAL
23	W	423	ASN
23	W	424	LEU
23	W	430	GLN
23	W	435	LEU
23	W	438	LEU
23	W	444	HIS
23	W	445	LEU
23	W	452	ILE
24	X	48	GLN
24	X	50	ILE
24	X	52	GLU
24	X	77	LEU
24	X	87	ARG
24	X	88	LEU
24	X	93	LEU
24	X	95	LEU
24	X	96	PHE
24	X	99	MET
24	X	108	GLU
24	X	123	THR
24	X	153	LEU
24	X	171	LEU
24	X	172	LEU
24	X	183	LEU
24	X	218	HIS
24	X	233	TYR
24	X	242	ILE
24	X	250	SER
24	X	258	LYS
24	X	274	LYS

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Mol	Chain	Res	Type
24	X	275	LEU
24	X	284	THR
24	X	313	LEU
24	X	316	ASP
24	X	319	ILE
24	X	327	TYR
24	X	329	ASN
24	X	332	GLU
24	X	336	ILE
24	X	338	VAL
24	X	339	ILE
24	X	340	GLU
24	X	341	PRO
24	X	342	PHE
24	X	344	ARG
24	X	347	ILE
24	X	349	HIS
24	X	350	ILE
24	X	356	LEU
24	X	358	LYS
24	X	364	LYS
24	X	371	ASP
24	X	372	LYS
24	X	373	LYS
24	X	374	PHE
24	X	393	VAL
24	X	407	MET
24	X	419	LYS
24	X	420	LYS
24	X	421	LEU
25	Y	13	LYS
25	Y	22	LEU
25	Y	67	VAL
25	Y	77	ASN
25	Y	100	ILE
25	Y	107	LYS
25	Y	110	TYR
25	Y	130	LYS
25	Y	134	LEU
25	Y	143	TYR
25	Y	145	LEU
25	Y	146	ARG

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Mol	Chain	Res	Type
25	Y	156	LEU
25	Y	168	ILE
25	Y	195	LYS
25	Y	200	LEU
25	Y	202	LEU
25	Y	206	SER
25	Y	212	GLU
25	Y	247	LEU
25	Y	253	LEU
25	Y	260	LEU
25	Y	267	ARG
25	Y	271	PHE
25	Y	272	PHE
25	Y	281	GLU
25	Y	282	MET
25	Y	287	LEU
25	Y	288	PHE
25	Y	291	HIS
25	Y	310	SER
25	Y	313	SER
25	Y	316	LEU
25	Y	330	ILE
25	Y	331	ASP
25	Y	343	LEU
25	Y	350	VAL
25	Y	365	GLN
25	Y	376	LEU
25	Y	382	LYS
25	Y	383	LEU
26	Z	8	LYS
26	Z	12	HIS
26	Z	14	LEU
26	Z	15	VAL
26	Z	17	LEU
26	Z	20	VAL
26	Z	29	VAL
26	Z	39	LEU
26	Z	47	VAL
26	Z	67	VAL
26	Z	76	GLU
26	Z	78	MET
26	Z	85	VAL

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Mol	Chain	Res	Type
26	Z	91	ILE
26	Z	92	VAL
26	Z	96	HIS
26	Z	109	ASN
26	Z	112	MET
26	Z	114	ARG
26	Z	119	SER
26	Z	124	ILE
26	Z	139	ILE
26	Z	141	VAL
26	Z	153	LYS
26	Z	154	THR
26	Z	158	VAL
26	Z	169	GLU
26	Z	176	LEU
26	Z	180	LYS
26	Z	191	ILE
26	Z	192	THR
26	Z	196	HIS
26	Z	201	LEU
26	Z	203	SER
26	Z	206	LEU
26	Z	208	ILE
26	Z	210	SER
26	Z	219	LYS
26	Z	220	LEU
26	Z	228	TYR
26	Z	237	LEU
26	Z	246	VAL
26	Z	257	MET
26	Z	265	LEU
26	Z	284	ASP
27	a	10	GLN
27	a	13	ASN
27	a	18	GLN
27	a	24	ARG
27	a	25	LEU
27	a	35	HIS
27	a	42	LEU
27	a	58	LYS
27	a	60	TYR
27	a	71	VAL

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Mol	Chain	Res	Type
27	a	80	ILE
27	a	83	VAL
27	a	94	LEU
27	a	105	LYS
27	a	112	ILE
27	a	113	LEU
27	a	121	LEU
27	a	123	LEU
27	a	128	LEU
27	a	149	THR
27	a	156	TYR
27	a	158	LEU
27	a	169	HIS
27	a	174	LYS
27	a	180	LEU
27	a	185	ILE
27	a	188	LEU
27	a	194	GLN
27	a	195	GLU
27	a	205	LEU
27	a	210	VAL
27	a	213	PHE
27	a	221	VAL
27	a	230	ARG
27	a	232	TRP
27	a	236	THR
27	a	245	VAL
27	a	247	ARG
27	a	265	GLU
27	a	275	LEU
27	a	276	CYS
27	a	280	MET
27	a	281	THR
27	a	293	PHE
27	a	301	LYS
27	a	307	VAL
27	a	310	LEU
27	a	329	LYS
27	a	340	VAL
27	a	355	PHE
27	a	357	CYS
27	a	364	GLU

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Mol	Chain	Res	Type
27	a	370	GLN
27	a	374	ILE
27	a	376	THR
28	b	8	VAL
28	b	18	ASN
28	b	35	ILE
28	b	54	LEU
28	b	59	GLU
28	b	62	THR
28	b	65	THR
28	b	86	PHE
28	b	87	CYS
28	b	90	ILE
28	b	91	ARG
28	b	94	HIS
28	b	97	LEU
28	b	107	MET
28	b	110	ILE
28	b	115	SER
28	b	124	LEU
28	b	139	ASP
28	b	143	PHE
28	b	147	GLU
28	b	150	THR
28	b	160	LEU
29	c	27	THR
29	c	36	LEU
29	c	44	HIS
29	c	56	LEU
29	c	62	VAL
29	c	67	VAL
29	c	68	ARG
29	c	69	VAL
29	c	70	ILE
29	c	72	VAL
29	c	80	THR
29	c	90	VAL
29	c	106	GLU
29	c	108	VAL
29	c	118	PHE
29	c	121	TRP
29	c	129	THR

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Mol	Chain	Res	Type
29	c	143	VAL
29	c	146	ASP
29	c	155	VAL
29	c	157	ILE
29	c	162	LEU
29	c	176	GLN
29	c	178	THR
29	c	192	LEU
29	c	193	ILE
29	c	204	THR
29	c	205	ILE
29	c	208	ARG
29	c	214	GLN
29	c	218	LEU
29	c	220	LEU
29	c	224	SER
29	c	231	LEU
29	c	234	TYR
29	c	249	LEU
29	c	264	LYS
29	c	273	LYS
29	c	300	LEU
30	d	5	LEU
30	d	6	LYS
30	d	9	TRP
30	d	31	LEU
30	d	35	PHE
30	d	36	LEU
30	d	38	THR
30	d	44	THR
30	d	54	ILE
30	d	63	ILE
30	d	65	ARG
30	d	81	TYR
30	d	85	TYR
30	d	99	LEU
30	d	120	GLU
30	d	128	GLN
30	d	133	ILE
30	d	144	MET
30	d	148	TYR
30	d	151	VAL

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Mol	Chain	Res	Type
30	d	158	ILE
30	d	175	ARG
30	d	182	ILE
30	d	183	GLU
30	d	188	LYS
30	d	192	THR
30	d	193	GLU
30	d	195	THR
30	d	196	ARG
30	d	199	PHE
30	d	202	THR
30	d	217	LEU
30	d	229	GLN
30	d	233	GLU
30	d	236	THR
30	d	238	PRO
30	d	249	TYR
30	d	251	ARG
31	e	43	TRP
31	e	56	LEU
31	e	57	ARG
31	e	60	LEU
31	e	61	GLU
32	f	8	LYS
32	f	27	LYS
32	f	52	LEU
32	f	53	GLN
32	f	55	GLU
32	f	78	LEU
32	f	79	ARG
32	f	80	ARG
32	f	81	GLN
32	f	82	ILE
32	f	87	THR
32	f	99	LEU
32	f	103	TYR
32	f	119	LYS
32	f	120	ARG
32	f	121	PHE
32	f	128	VAL
32	f	137	ARG
32	f	140	LEU

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Mol	Chain	Res	Type
32	f	141	LYS
32	f	144	LEU
32	f	165	GLU
32	f	166	VAL
32	f	170	TRP
32	f	174	ASP
32	f	184	LEU
32	f	188	VAL
32	f	192	VAL
32	f	209	MET
32	f	212	GLU
32	f	215	ASP
32	f	216	MET
32	f	217	LEU
32	f	233	LEU
32	f	245	ASN
32	f	248	LEU
32	f	249	LEU
32	f	261	ARG
32	f	262	PHE
32	f	270	LEU
32	f	272	LEU
32	f	275	MET
32	f	277	LEU
32	f	278	VAL
32	f	297	MET
32	f	304	PHE
32	f	310	ASP
32	f	313	GLU
32	f	317	LEU
32	f	318	THR
32	f	319	GLU
32	f	321	MET
32	f	336	GLU
32	f	337	LEU
32	f	339	ILE
32	f	353	LEU
32	f	358	PHE
32	f	372	LEU
32	f	389	LYS
32	f	391	LEU
32	f	398	TRP

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Mol	Chain	Res	Type
32	f	399	LEU
32	f	400	TYR
32	f	417	ILE
32	f	456	ARG
32	f	473	ASN
32	f	478	ARG
32	f	485	LEU
32	f	489	TYR
32	f	493	ASN
32	f	494	ARG
32	f	501	LEU
32	f	507	ASP
32	f	509	LYS
32	f	512	MET
32	f	527	VAL
32	f	531	ASN
32	f	533	ASP
32	f	534	VAL
32	f	537	THR
32	f	540	GLN
32	f	544	GLU
32	f	548	THR
32	f	564	LEU
32	f	567	LEU
32	f	569	LYS
32	f	594	LEU
32	f	605	ASN
32	f	608	LYS
32	f	612	LEU
32	f	619	HIS
32	f	629	LYS
32	f	631	LYS
32	f	632	LYS
32	f	652	VAL
32	f	662	MET
32	f	677	HIS
32	f	680	ARG
32	f	690	VAL
32	f	692	LEU
32	f	697	ILE
32	f	727	PHE
32	f	741	LEU

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Mol	Chain	Res	Type
32	f	745	LEU
32	f	775	THR
32	f	776	LEU
32	f	779	CYS
32	f	785	ARG
32	f	791	VAL
32	f	797	LEU
7	g	37	LEU
7	g	50	ILE
7	g	52	THR
7	g	53	GLN
7	g	54	LYS
7	g	69	LEU
7	g	73	THR
7	g	81	THR
7	g	83	MET
7	g	100	ASN
7	g	117	ARG
7	g	123	GLN
7	g	127	GLN
7	g	154	CYS
7	g	160	TYR
7	g	184	LYS
7	g	185	LYS
7	g	189	TRP
7	g	210	PHE
7	g	219	VAL
7	g	230	LEU
7	g	239	LEU
7	g	242	LEU
8	h	4	ARG
8	h	8	PHE
8	h	12	THR
8	h	20	VAL
8	h	69	THR
8	h	75	VAL
8	h	83	TYR
8	h	109	GLN
8	h	110	LEU
8	h	119	GLN
8	h	128	ARG
8	h	156	PHE

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Mol	Chain	Res	Type
8	h	168	VAL
8	h	189	HIS
9	i	3	ARG
9	i	8	ARG
9	i	15	GLU
9	i	25	MET
9	i	35	LEU
9	i	44	LEU
9	i	45	LEU
9	i	49	ARG
9	i	65	ILE
9	i	76	VAL
9	i	90	LEU
9	i	95	GLN
9	i	96	ARG
9	i	107	CYS
9	i	108	GLU
9	i	127	LYS
9	i	132	VAL
9	i	134	LEU
9	i	141	LYS
9	i	179	TYR
9	i	180	LYS
9	i	192	LEU
9	i	197	LEU
9	i	206	LEU
9	i	212	GLU
9	i	224	VAL
9	i	226	ARG
10	j	8	THR
10	j	17	PHE
10	j	18	GLN
10	j	31	THR
10	j	41	VAL
10	j	45	VAL
10	j	54	GLN
10	j	82	ILE
10	j	91	CYS
10	j	99	GLU
10	j	102	VAL
10	j	104	VAL
10	j	117	ARG

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Mol	Chain	Res	Type
10	j	122	ASN
10	j	125	ARG
10	j	132	LEU
10	j	134	VAL
10	j	152	THR
10	j	156	TRP
10	j	177	THR
10	j	179	GLU
10	j	206	ILE
10	j	210	VAL
11	k	16	SER
11	k	20	ARG
11	k	33	LEU
11	k	36	THR
11	k	47	CYS
11	k	65	GLU
11	k	95	GLU
11	k	97	GLN
11	k	98	ASN
11	k	108	THR
11	k	121	LEU
11	k	125	GLU
11	k	133	MET
11	k	142	LEU
11	k	178	GLN
11	k	181	LEU
11	k	203	LYS
11	k	217	LEU
11	k	220	VAL
11	k	224	GLN
11	k	227	HIS
11	k	228	MET
11	k	230	THR
11	k	234	LEU
11	k	237	VAL
11	k	239	LYS
12	l	5	GLN
12	l	10	VAL
12	l	35	THR
12	l	38	LEU
12	l	47	VAL
12	l	54	SER

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Mol	Chain	Res	Type
12	l	83	LEU
12	l	93	LEU
12	l	96	ARG
12	l	101	ARG
12	l	103	LEU
12	l	112	ILE
12	l	117	GLN
12	l	140	MET
12	l	153	TYR
12	l	156	CYS
12	l	164	ARG
12	l	189	LYS
12	l	197	GLU
12	l	211	SER
12	l	229	VAL
13	m	8	ASP
13	m	35	THR
13	m	41	CYS
13	m	42	LYS
13	m	52	LEU
13	m	57	LEU
13	m	71	ARG
13	m	81	LEU
13	m	87	LEU
13	m	93	GLU
13	m	133	CYS
13	m	142	VAL
13	m	178	LYS
13	m	185	THR
13	m	189	ILE
13	m	215	TRP
13	m	229	LYS
13	m	236	GLU
13	m	243	LEU
14	n	23	THR
14	n	30	ARG
14	n	31	VAL
14	n	35	LEU
14	n	36	THR
14	n	38	ILE
14	n	52	ASP
14	n	94	ASP

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Mol	Chain	Res	Type
14	n	191	LEU
14	n	198	PHE
14	n	200	VAL
14	n	203	LEU
15	o	2	THR
15	o	14	VAL
15	o	49	THR
15	o	69	LEU
15	o	71	THR
15	o	74	LEU
15	o	81	ASN
15	o	107	THR
15	o	156	VAL
15	o	186	PHE
15	o	188	ARG
15	o	209	THR
15	o	216	LYS
16	p	34	MET
16	p	49	LEU
16	p	53	LEU
16	p	71	LEU
16	p	94	LEU
16	p	99	ARG
16	p	116	THR
16	p	125	ASP
16	p	126	LEU
16	p	137	VAL
16	p	138	VAL
16	p	175	VAL
16	p	177	ARG
16	p	189	ILE
16	p	194	LYS
17	q	5	ILE
17	q	8	GLN
17	q	13	VAL
17	q	15	VAL
17	q	30	ASP
17	q	31	ASP
17	q	43	LEU
17	q	45	LEU
17	q	52	ASP
17	q	62	LYS

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Mol	Chain	Res	Type
17	q	85	ARG
17	q	92	LEU
17	q	138	LEU
17	q	140	LEU
17	q	145	ARG
17	q	148	THR
17	q	163	CYS
17	q	164	LEU
17	q	168	GLN
17	q	193	ASN
18	r	39	ASN
18	r	46	MET
18	r	52	ASP
18	r	63	GLN
18	r	76	SER
18	r	98	MET
18	r	103	CYS
18	r	118	GLU
18	r	137	TYR
18	r	139	VAL
18	r	142	ARG
18	r	147	ASP
18	r	150	VAL
18	r	179	HIS
18	r	187	ARG
19	s	1	ARG
19	s	55	SER
19	s	127	VAL
19	s	164	VAL
19	s	211	ARG
20	t	21	VAL
20	t	43	MET
20	t	49	THR
20	t	94	ARG
20	t	100	ARG
20	t	137	LEU
20	t	159	VAL
20	t	168	LEU
20	t	169	VAL
20	t	179	ARG
20	t	193	THR
20	t	205	THR

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Mol	Chain	Res	Type
20	t	211	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (204) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	293	ASN
1	A	314	ASN
1	A	322	ASN
1	A	353	HIS
1	A	379	ASN
1	A	414	ASN
2	B	120	HIS
2	B	131	HIS
2	B	193	GLN
2	B	195	GLN
3	C	46	GLN
3	C	69	GLN
3	C	205	HIS
3	C	221	GLN
3	C	332	HIS
3	C	337	ASN
4	D	48	GLN
4	D	74	HIS
4	D	76	GLN
4	D	83	GLN
4	D	135	HIS
4	D	278	GLN
4	D	340	GLN
5	E	364	GLN
6	F	214	ASN
6	F	321	GLN
6	F	434	ASN
7	G	34	GLN
7	G	92	GLN
7	G	147	GLN
7	G	172	GLN
7	G	193	GLN
8	H	63	HIS
8	H	71	HIS
8	H	109	GLN
8	H	112	GLN

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Mol	Chain	Res	Type
8	H	123	GLN
8	H	169	ASN
8	H	207	ASN
9	I	84	ASN
9	I	109	GLN
9	I	119	GLN
9	I	123	GLN
9	I	166	ASN
10	J	85	ASN
10	J	116	GLN
11	K	99	HIS
11	K	114	GLN
11	K	118	ASN
11	K	182	GLN
12	L	68	ASN
12	L	69	HIS
12	L	90	GLN
12	L	203	GLN
13	M	32	ASN
13	M	72	HIS
13	M	120	HIS
13	M	201	HIS
14	N	111	GLN
14	N	155	GLN
14	N	159	ASN
14	N	194	GLN
15	O	173	ASN
15	O	194	ASN
16	P	33	GLN
16	P	72	ASN
16	P	169	GLN
16	P	188	HIS
17	Q	71	ASN
17	Q	101	ASN
17	Q	168	GLN
17	Q	193	ASN
18	R	63	GLN
18	R	86	ASN
18	R	179	HIS
19	S	131	GLN
19	S	151	ASN
19	S	159	GLN

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Mol	Chain	Res	Type
20	T	2	GLN
20	T	147	GLN
20	T	188	GLN
21	U	25	HIS
21	U	28	ASN
21	U	149	GLN
21	U	267	ASN
21	U	355	ASN
21	U	384	GLN
21	U	415	HIS
21	U	463	ASN
21	U	491	GLN
21	U	596	ASN
21	U	647	HIS
21	U	718	ASN
21	U	805	ASN
22	V	64	GLN
22	V	266	GLN
22	V	318	GLN
22	V	350	GLN
22	V	400	HIS
22	V	452	ASN
22	V	453	HIS
22	V	487	HIS
22	V	488	ASN
23	W	156	ASN
23	W	235	GLN
23	W	362	ASN
23	W	426	ASN
23	W	430	GLN
23	W	456	GLN
24	X	322	HIS
24	X	329	ASN
24	X	334	ASN
24	X	375	HIS
25	Y	178	ASN
25	Y	184	GLN
25	Y	273	GLN
25	Y	351	ASN
25	Y	357	ASN
25	Y	365	GLN
25	Y	367	GLN

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Mol	Chain	Res	Type
26	Z	102	HIS
26	Z	104	ASN
26	Z	225	GLN
26	Z	256	GLN
26	Z	278	ASN
27	a	164	GLN
27	a	169	HIS
27	a	227	ASN
27	a	290	GLN
28	b	94	HIS
28	b	137	ASN
28	b	149	ASN
29	c	30	GLN
29	c	101	GLN
29	c	128	ASN
29	c	166	ASN
29	c	172	HIS
29	c	176	GLN
29	c	214	GLN
29	c	219	ASN
29	c	269	GLN
29	c	283	HIS
30	d	109	GLN
30	d	128	GLN
30	d	135	HIS
30	d	252	GLN
32	f	43	GLN
32	f	53	GLN
32	f	102	HIS
32	f	364	GLN
32	f	382	ASN
32	f	473	ASN
32	f	493	ASN
32	f	565	ASN
32	f	592	ASN
32	f	790	GLN
7	g	53	GLN
7	g	90	GLN
7	g	100	ASN
7	g	127	GLN
7	g	193	GLN
8	h	102	GLN

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Mol	Chain	Res	Type
8	h	109	GLN
8	h	112	GLN
8	h	166	ASN
8	h	169	ASN
8	h	207	ASN
9	i	40	ASN
9	i	84	ASN
9	i	102	GLN
9	i	149	GLN
10	j	85	ASN
10	j	200	GLN
11	k	73	HIS
11	k	98	ASN
11	k	99	HIS
11	k	114	GLN
11	k	221	GLN
11	k	224	GLN
12	l	5	GLN
12	l	43	HIS
12	l	53	GLN
12	l	65	HIS
12	l	68	ASN
12	l	69	HIS
12	l	90	GLN
12	l	117	GLN
12	l	146	GLN
12	l	203	GLN
13	m	32	ASN
13	m	72	HIS
14	n	78	HIS
14	n	155	GLN
14	n	159	ASN
15	o	194	ASN
16	p	72	ASN
17	q	63	ASN
17	q	71	ASN
17	q	168	GLN
18	r	39	ASN
20	t	46	ASN
20	t	147	GLN
20	t	188	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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$
34	LDZ	o	301	-	33,34,34	1.79	7 (21%)	42,44,44	1.36	6 (14%)
34	LDZ	r	301	-	33,34,34	1.86	7 (21%)	42,44,44	1.60	9 (21%)
33	ATP	F	501	-	28,33,33	0.75	0	34,52,52	0.79	1 (2%)
34	LDZ	n	301	-	33,34,34	1.84	7 (21%)	42,44,44	1.63	6 (14%)
34	LDZ	N	301	-	33,34,34	1.76	7 (21%)	42,44,44	1.30	5 (11%)
33	ATP	A	501	-	28,33,33	0.75	0	34,52,52	0.88	1 (2%)
34	LDZ	R	301	-	33,34,34	1.81	7 (21%)	42,44,44	1.68	7 (16%)
33	ATP	D	501	-	28,33,33	0.76	0	34,52,52	0.76	1 (2%)
33	ATP	C	501	-	28,33,33	0.74	0	34,52,52	0.74	1 (2%)
34	LDZ	O	301	-	33,34,34	1.82	7 (21%)	42,44,44	1.55	7 (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
34	LDZ	o	301	-	-	9/38/39/39	0/1/1/1
34	LDZ	r	301	-	-	12/38/39/39	0/1/1/1
33	ATP	F	501	-	-	6/18/38/38	0/3/3/3
34	LDZ	n	301	-	-	14/38/39/39	0/1/1/1
34	LDZ	N	301	-	-	17/38/39/39	0/1/1/1
33	ATP	A	501	-	-	2/18/38/38	0/3/3/3
34	LDZ	R	301	-	-	15/38/39/39	0/1/1/1
33	ATP	D	501	-	-	4/18/38/38	0/3/3/3
33	ATP	C	501	-	-	5/18/38/38	0/3/3/3
34	LDZ	O	301	-	-	16/38/39/39	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	r	301	LDZ	C12-N13	5.75	1.46	1.34
34	O	301	LDZ	C12-N13	5.65	1.46	1.34
34	n	301	LDZ	C15-N16	5.64	1.46	1.34
34	R	301	LDZ	C15-N16	5.52	1.45	1.34
34	R	301	LDZ	C12-N13	5.33	1.45	1.34
34	o	301	LDZ	C12-N13	5.25	1.45	1.34
34	N	301	LDZ	C12-N13	5.21	1.45	1.34
34	r	301	LDZ	C15-N16	5.20	1.45	1.34
34	n	301	LDZ	C12-N13	5.18	1.45	1.34
34	o	301	LDZ	C15-N16	4.87	1.44	1.34
34	O	301	LDZ	C15-N16	4.78	1.44	1.34
34	N	301	LDZ	C15-N16	4.67	1.44	1.34
34	N	301	LDZ	C9-N10	4.55	1.46	1.34
34	r	301	LDZ	C9-N10	4.50	1.45	1.34
34	O	301	LDZ	C9-N10	4.46	1.45	1.34
34	o	301	LDZ	C9-N10	4.36	1.45	1.34
34	n	301	LDZ	C9-N10	4.27	1.45	1.34
34	R	301	LDZ	C9-N10	4.26	1.45	1.34
34	n	301	LDZ	O34-C15	-2.81	1.18	1.23
34	N	301	LDZ	O34-C15	-2.74	1.18	1.23
34	R	301	LDZ	O34-C15	-2.74	1.18	1.23
34	n	301	LDZ	O32-C12	-2.72	1.18	1.23
34	r	301	LDZ	O32-C12	-2.71	1.18	1.23
34	O	301	LDZ	O34-C15	-2.67	1.18	1.23
34	n	301	LDZ	O8-C7	-2.65	1.40	1.45
34	N	301	LDZ	O8-C9	2.62	1.40	1.35
34	R	301	LDZ	O8-C7	-2.62	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	o	301	LDZ	O32-C12	-2.61	1.18	1.23
34	O	301	LDZ	O8-C7	-2.60	1.40	1.45
34	o	301	LDZ	O8-C9	2.60	1.40	1.35
34	r	301	LDZ	O8-C9	2.56	1.40	1.35
34	o	301	LDZ	O8-C7	-2.50	1.40	1.45
34	R	301	LDZ	O32-C12	-2.49	1.18	1.23
34	r	301	LDZ	O34-C15	-2.49	1.18	1.23
34	n	301	LDZ	O8-C9	2.47	1.40	1.35
34	O	301	LDZ	O8-C9	2.46	1.40	1.35
34	o	301	LDZ	O34-C15	-2.46	1.18	1.23
34	r	301	LDZ	O8-C7	-2.45	1.40	1.45
34	N	301	LDZ	O8-C7	-2.45	1.40	1.45
34	O	301	LDZ	O32-C12	-2.40	1.18	1.23
34	R	301	LDZ	O8-C9	2.38	1.39	1.35
34	N	301	LDZ	O32-C12	-2.33	1.18	1.23

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	O	301	LDZ	O8-C9-N10	5.17	121.51	110.45
34	n	301	LDZ	C14-C15-N16	4.99	127.27	116.63
34	r	301	LDZ	O8-C9-N10	4.92	120.97	110.45
34	r	301	LDZ	C11-C12-N13	4.65	126.56	116.63
34	R	301	LDZ	O8-C9-N10	4.57	120.23	110.45
34	R	301	LDZ	C14-C15-N16	4.48	126.18	116.63
34	o	301	LDZ	O8-C9-N10	4.46	119.98	110.45
34	R	301	LDZ	C18-C17-N16	4.36	117.27	110.69
34	n	301	LDZ	O8-C9-N10	4.17	119.37	110.45
34	N	301	LDZ	O8-C9-N10	3.84	118.67	110.45
34	n	301	LDZ	O34-C15-N16	-3.82	116.12	122.96
34	R	301	LDZ	O34-C15-N16	-3.65	116.42	122.96
34	O	301	LDZ	C11-C12-N13	3.57	124.25	116.63
34	r	301	LDZ	O32-C12-N13	-3.18	117.27	122.96
34	n	301	LDZ	C18-C17-N16	3.06	115.31	110.69
34	O	301	LDZ	O8-C9-O31	-3.05	118.42	124.26
34	o	301	LDZ	O31-C9-N10	-3.02	119.92	124.86
34	r	301	LDZ	O8-C9-O31	-3.01	118.49	124.26
34	O	301	LDZ	O32-C12-N13	-3.00	117.59	122.96
34	R	301	LDZ	O31-C9-N10	-2.96	120.01	124.86
34	O	301	LDZ	O31-C9-N10	-2.92	120.07	124.86
34	n	301	LDZ	O31-C9-N10	-2.90	120.10	124.86
34	N	301	LDZ	O34-C15-N16	-2.77	118.00	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	O	301	LDZ	C14-N13-C12	2.69	127.44	121.65
34	o	301	LDZ	O33-C22-C17	-2.67	117.91	124.77
34	R	301	LDZ	C18-C17-C22	2.64	115.05	110.99
34	r	301	LDZ	O31-C9-N10	-2.64	120.54	124.86
34	N	301	LDZ	C22-C17-N16	-2.60	104.47	109.50
34	N	301	LDZ	O8-C9-O31	-2.50	119.46	124.26
34	R	301	LDZ	O8-C9-O31	-2.35	119.76	124.26
33	D	501	ATP	C5-C6-N6	2.25	123.73	120.31
34	r	301	LDZ	C14-N13-C12	2.23	126.44	121.65
34	n	301	LDZ	O33-C22-C17	-2.21	119.08	124.77
34	o	301	LDZ	O8-C9-O31	-2.17	120.09	124.26
34	O	301	LDZ	C24-C14-N13	2.17	115.48	110.58
33	A	501	ATP	C5-C6-N6	2.17	123.62	120.31
34	o	301	LDZ	C18-C17-N16	-2.14	107.45	110.69
34	N	301	LDZ	C24-C14-N13	-2.09	105.86	110.58
33	F	501	ATP	C5-C6-N6	2.07	123.46	120.31
33	C	501	ATP	C5-C6-N6	2.06	123.44	120.31
34	r	301	LDZ	O32-C12-C11	-2.06	116.17	120.48
34	o	301	LDZ	C22-C17-N16	-2.04	105.57	109.50
34	r	301	LDZ	C21-C19-C18	2.01	118.30	111.08
34	r	301	LDZ	C18-C17-N16	2.00	113.71	110.69

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	C	501	ATP	C5'-O5'-PA-O2A
33	C	501	ATP	C5'-O5'-PA-O3A
33	F	501	ATP	C3'-C4'-C5'-O5'
34	N	301	LDZ	O31-C9-O8-C7
34	N	301	LDZ	N10-C9-O8-C7
34	O	301	LDZ	O8-C9-N10-C11
34	R	301	LDZ	O31-C9-O8-C7
34	R	301	LDZ	N10-C9-O8-C7
34	R	301	LDZ	N13-C14-C24-C25
34	R	301	LDZ	C18-C17-N16-C15
34	R	301	LDZ	C18-C17-C22-O33
34	n	301	LDZ	C18-C17-N16-C15
34	n	301	LDZ	C18-C17-C22-O33
34	o	301	LDZ	O8-C9-N10-C11
34	r	301	LDZ	O8-C9-N10-C11
34	r	301	LDZ	O31-C9-N10-C11

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Mol	Chain	Res	Type	Atoms
34	O	301	LDZ	O31-C9-N10-C11
34	n	301	LDZ	O31-C9-O8-C7
34	n	301	LDZ	N10-C9-O8-C7
34	o	301	LDZ	O31-C9-N10-C11
34	r	301	LDZ	O31-C9-O8-C7
34	r	301	LDZ	N10-C9-O8-C7
34	O	301	LDZ	C15-C14-C24-C25
34	r	301	LDZ	C12-C11-C30-C31
34	O	301	LDZ	N10-C9-O8-C7
34	o	301	LDZ	C12-C11-C30-C31
34	O	301	LDZ	O31-C9-O8-C7
34	O	301	LDZ	N13-C14-C24-C25
34	r	301	LDZ	N10-C11-C30-C31
34	O	301	LDZ	N10-C11-C30-C31
34	N	301	LDZ	N10-C11-C30-C31
34	n	301	LDZ	N10-C11-C30-C31
34	n	301	LDZ	C12-C11-C30-C31
34	o	301	LDZ	N10-C11-C30-C31
34	O	301	LDZ	C12-C11-C30-C31
34	R	301	LDZ	C15-C14-C24-C25
33	F	501	ATP	O4'-C4'-C5'-O5'
34	N	301	LDZ	C3-C7-O8-C9
34	n	301	LDZ	C14-C24-C25-C26
34	n	301	LDZ	C14-C24-C25-C27
34	r	301	LDZ	C11-C12-N13-C14
34	N	301	LDZ	C15-C14-C24-C25
34	N	301	LDZ	N16-C17-C18-C19
34	n	301	LDZ	O34-C15-N16-C17
34	n	301	LDZ	C17-C18-C19-C20
34	O	301	LDZ	O32-C12-N13-C14
34	R	301	LDZ	O34-C15-N16-C17
34	r	301	LDZ	O32-C12-N13-C14
34	n	301	LDZ	C17-C18-C19-C21
34	O	301	LDZ	C11-C12-N13-C14
34	n	301	LDZ	C14-C15-N16-C17
34	R	301	LDZ	C14-C24-C25-C27
34	N	301	LDZ	C17-C18-C19-C21
34	R	301	LDZ	C14-C15-N16-C17
34	r	301	LDZ	C14-C24-C25-C26
34	o	301	LDZ	C11-C30-C31-C33
34	N	301	LDZ	C12-C11-C30-C31
34	R	301	LDZ	C12-C11-C30-C31

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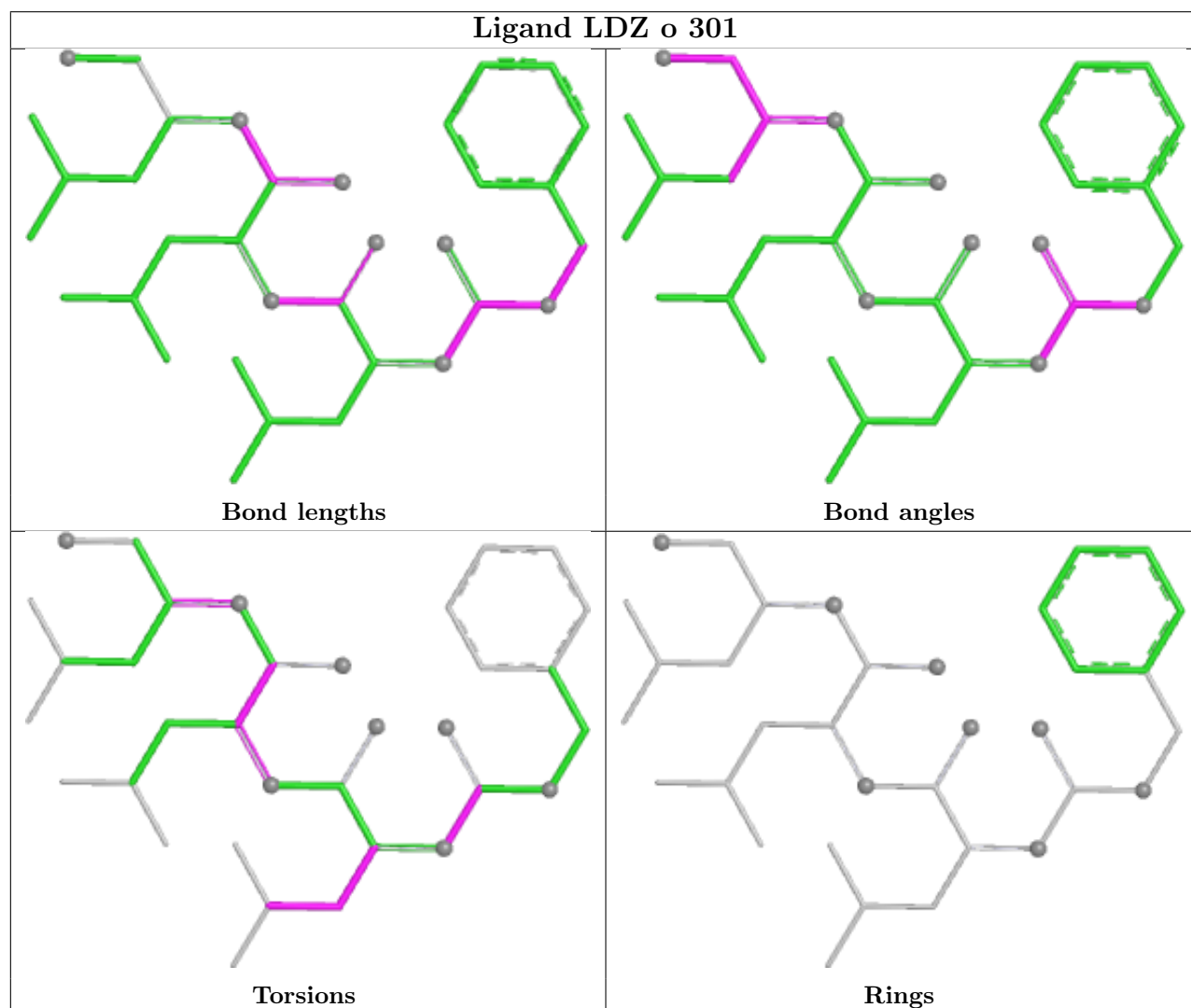
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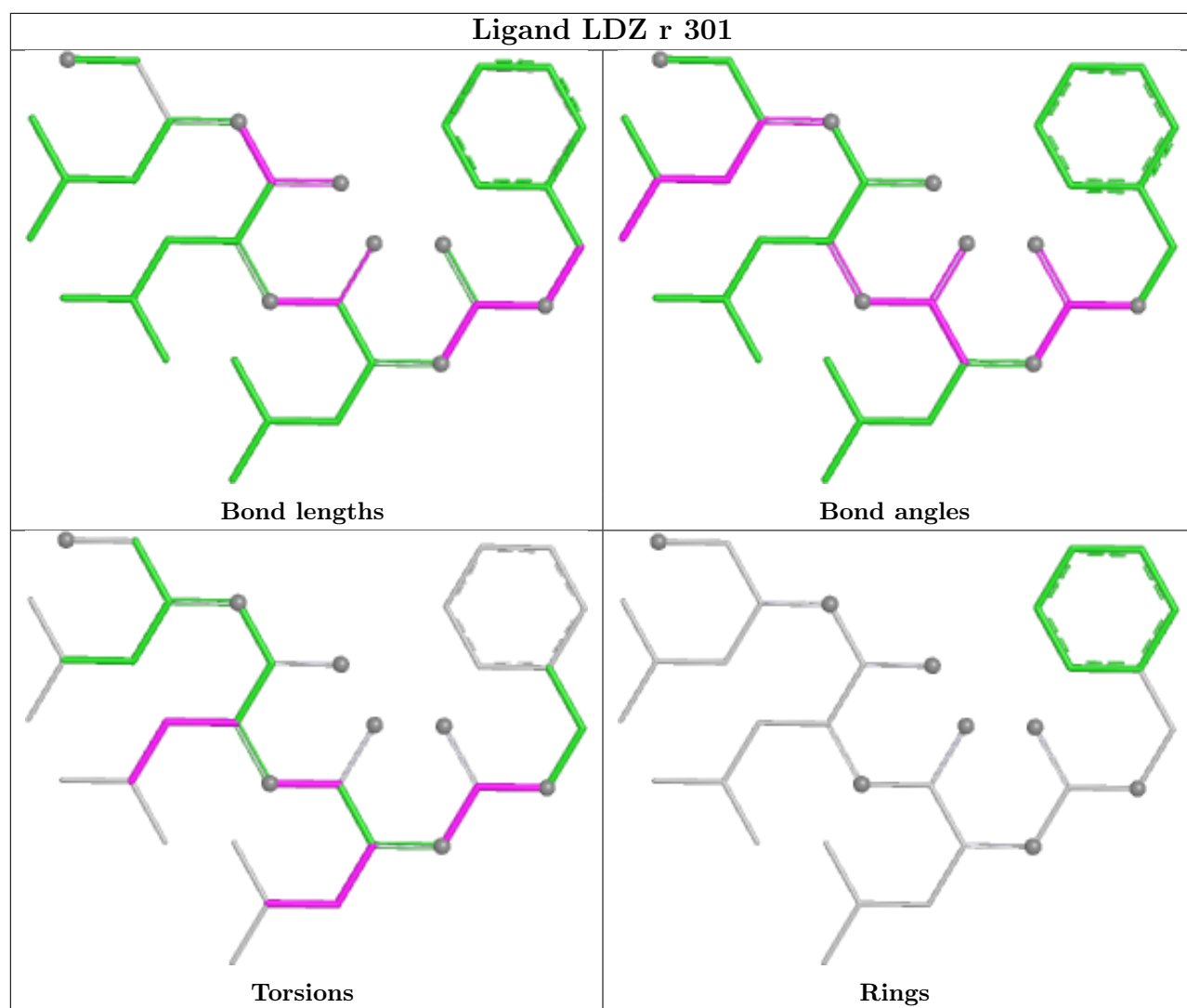
Mol	Chain	Res	Type	Atoms
34	O	301	LDZ	C30-C11-N10-C9
34	r	301	LDZ	C14-C24-C25-C27
33	C	501	ATP	O4'-C4'-C5'-O5'
34	N	301	LDZ	C17-C18-C19-C20
34	R	301	LDZ	C14-C24-C25-C26
34	n	301	LDZ	N16-C17-C18-C19
34	N	301	LDZ	N13-C14-C24-C25
34	R	301	LDZ	C17-C18-C19-C20
34	o	301	LDZ	C24-C14-N13-C12
34	R	301	LDZ	C17-C18-C19-C21
34	n	301	LDZ	N13-C14-C24-C25
33	A	501	ATP	C3'-C4'-C5'-O5'
34	N	301	LDZ	N10-C11-C12-O32
34	N	301	LDZ	N10-C11-C12-N13
33	A	501	ATP	O4'-C4'-C5'-O5'
34	N	301	LDZ	C22-C17-C18-C19
33	D	501	ATP	O4'-C4'-C5'-O5'
34	O	301	LDZ	N13-C14-C15-O34
34	N	301	LDZ	N13-C14-C15-O34
33	C	501	ATP	C3'-C4'-C5'-O5'
33	D	501	ATP	C3'-C4'-C5'-O5'
33	D	501	ATP	PG-O3B-PB-O1B
34	o	301	LDZ	C11-C30-C31-C32
34	O	301	LDZ	N13-C14-C15-N16
34	N	301	LDZ	N13-C14-C15-N16
33	C	501	ATP	C5'-O5'-PA-O1A
33	F	501	ATP	C5'-O5'-PA-O1A
34	r	301	LDZ	N13-C14-C24-C25
33	F	501	ATP	C4'-C5'-O5'-PA
33	D	501	ATP	PG-O3B-PB-O2B
34	N	301	LDZ	C30-C11-N10-C9
34	R	301	LDZ	N10-C11-C30-C31
34	R	301	LDZ	N16-C17-C18-C19
34	o	301	LDZ	C18-C17-N16-C15
33	F	501	ATP	PA-O3A-PB-O1B
34	O	301	LDZ	N10-C11-C12-O32
34	O	301	LDZ	N10-C11-C12-N13
34	O	301	LDZ	C24-C14-N13-C12
33	F	501	ATP	PA-O3A-PB-O3B
34	N	301	LDZ	C11-C30-C31-C33
34	o	301	LDZ	N13-C14-C15-N16
34	r	301	LDZ	C11-C30-C31-C33

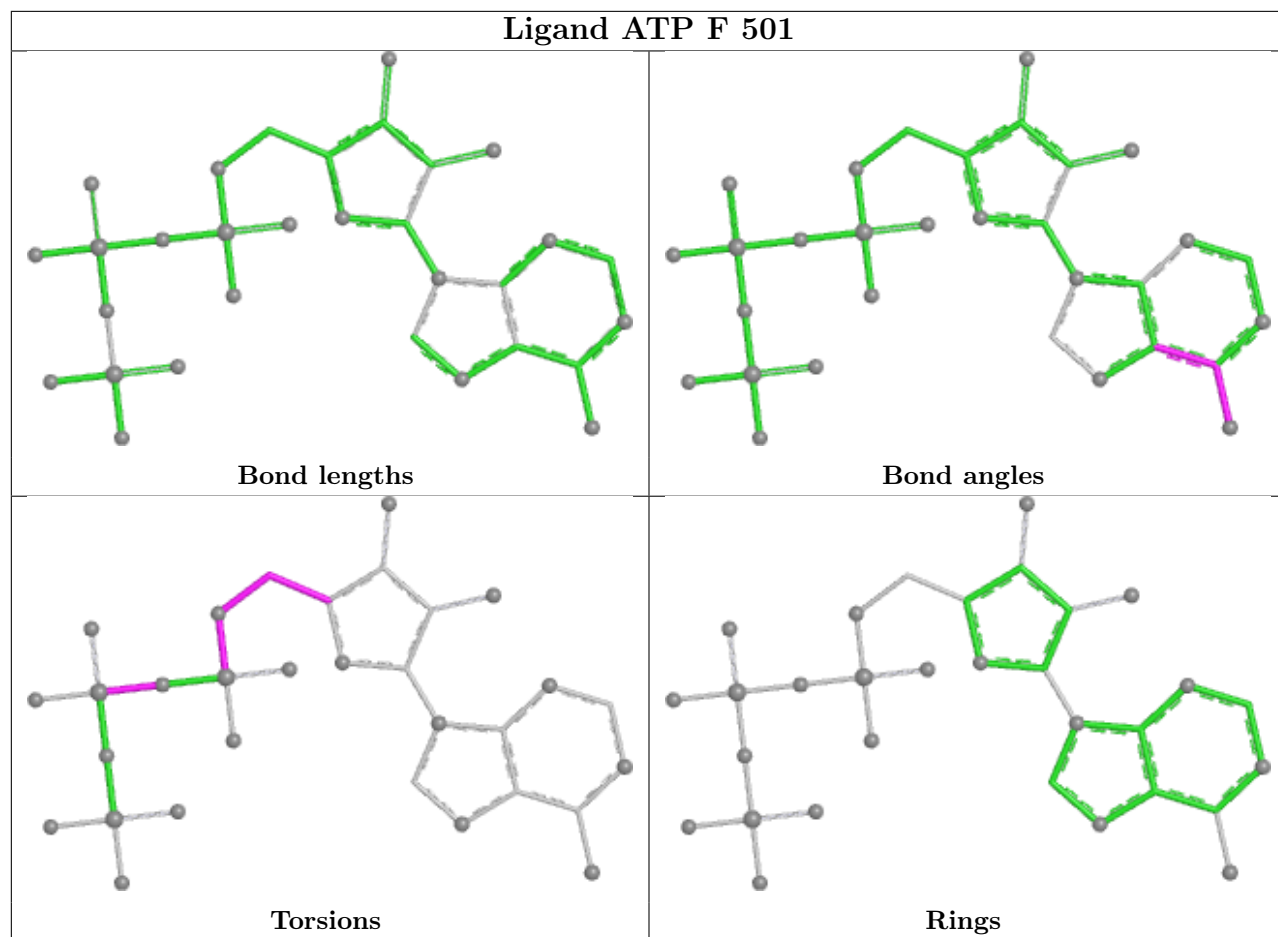
There are no ring outliers.

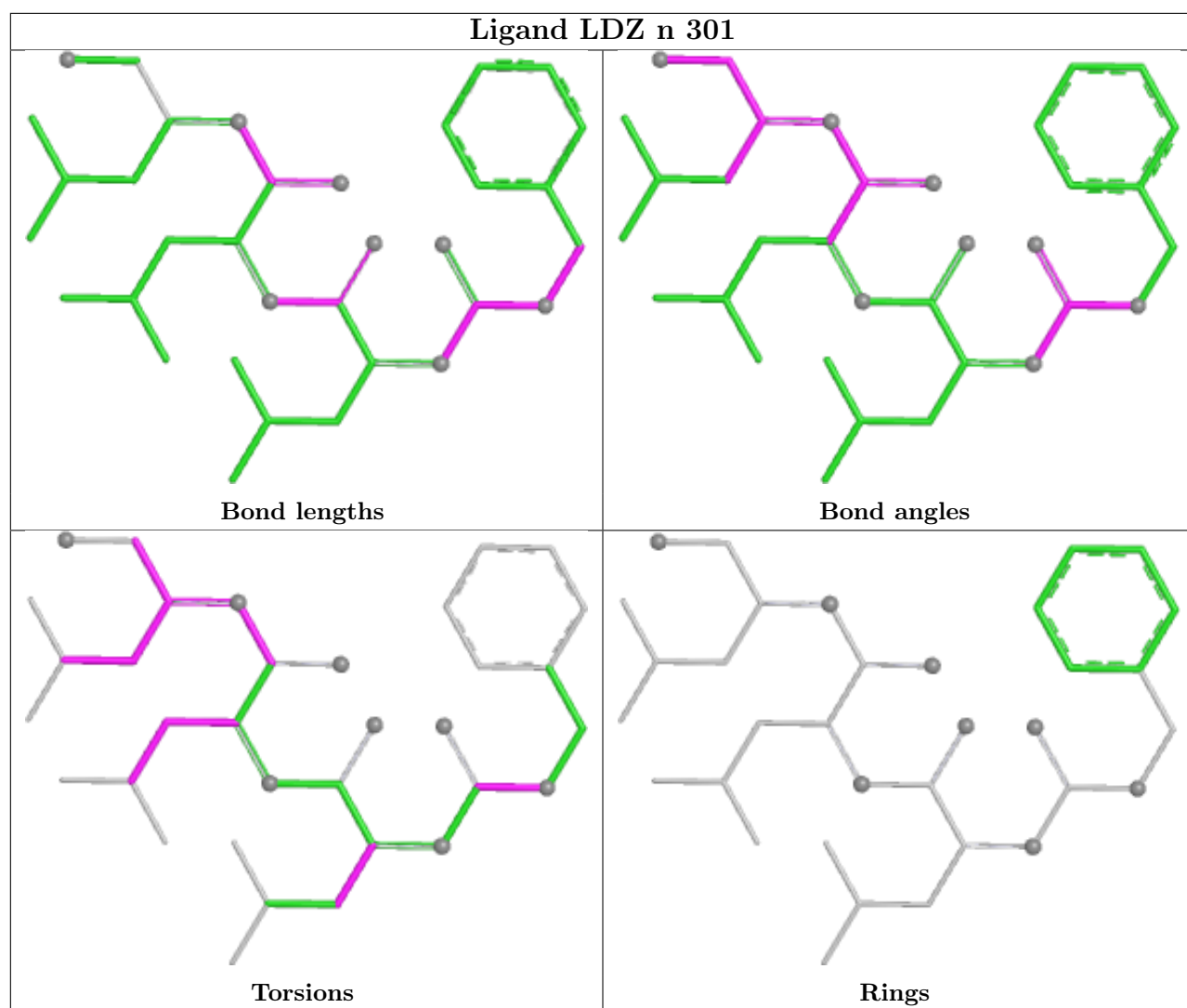
No monomer is involved in short contacts.

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

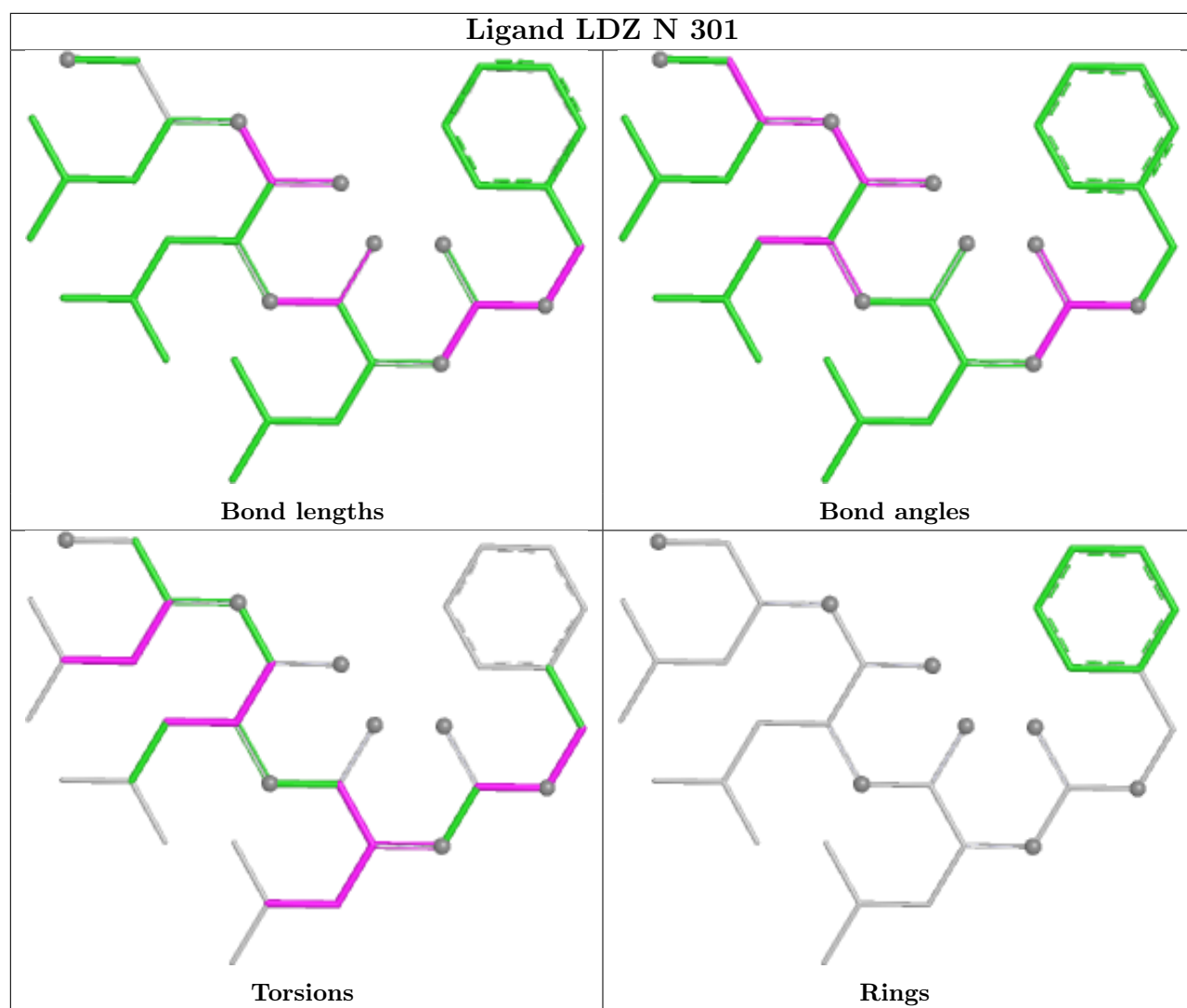


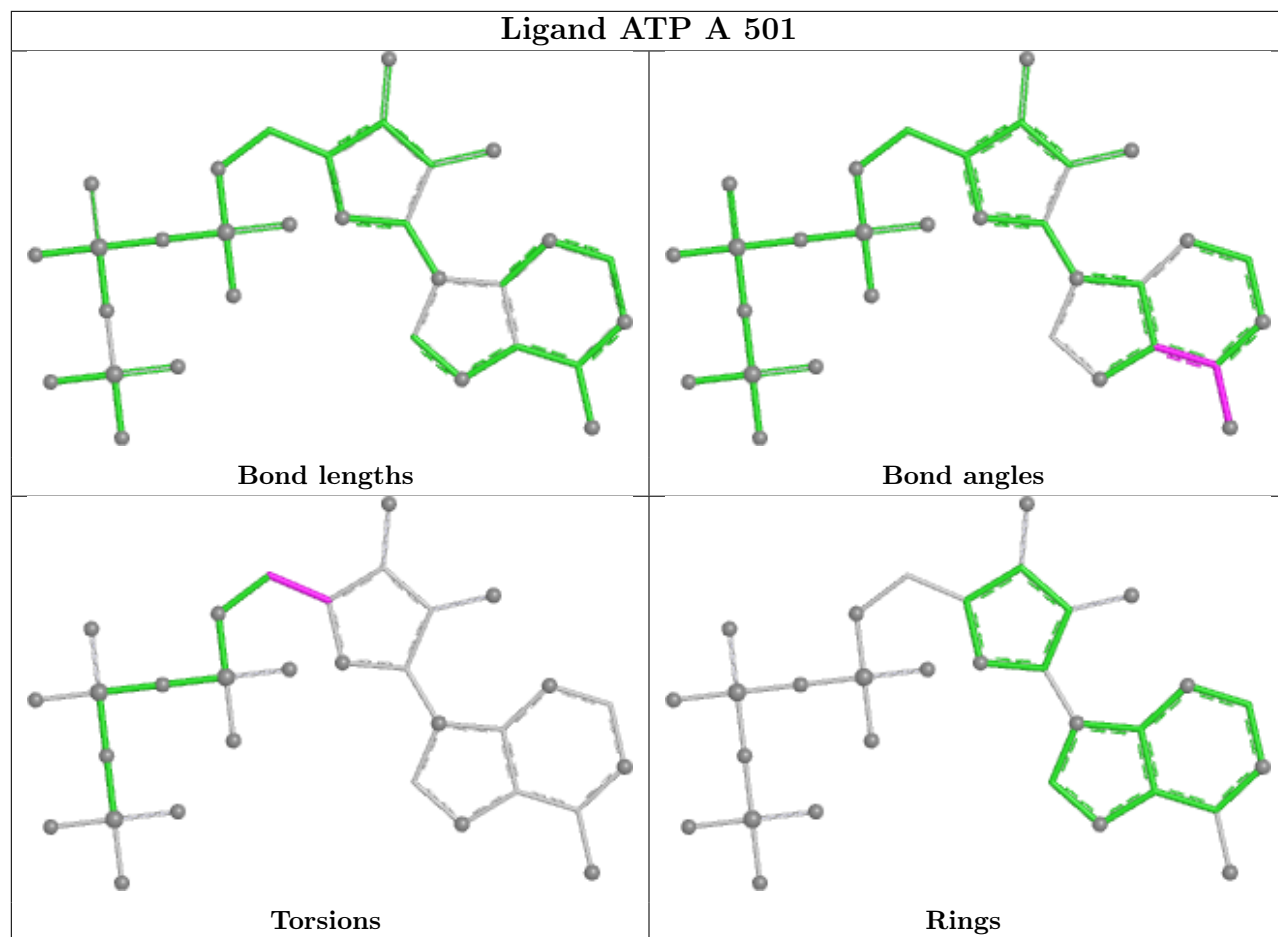


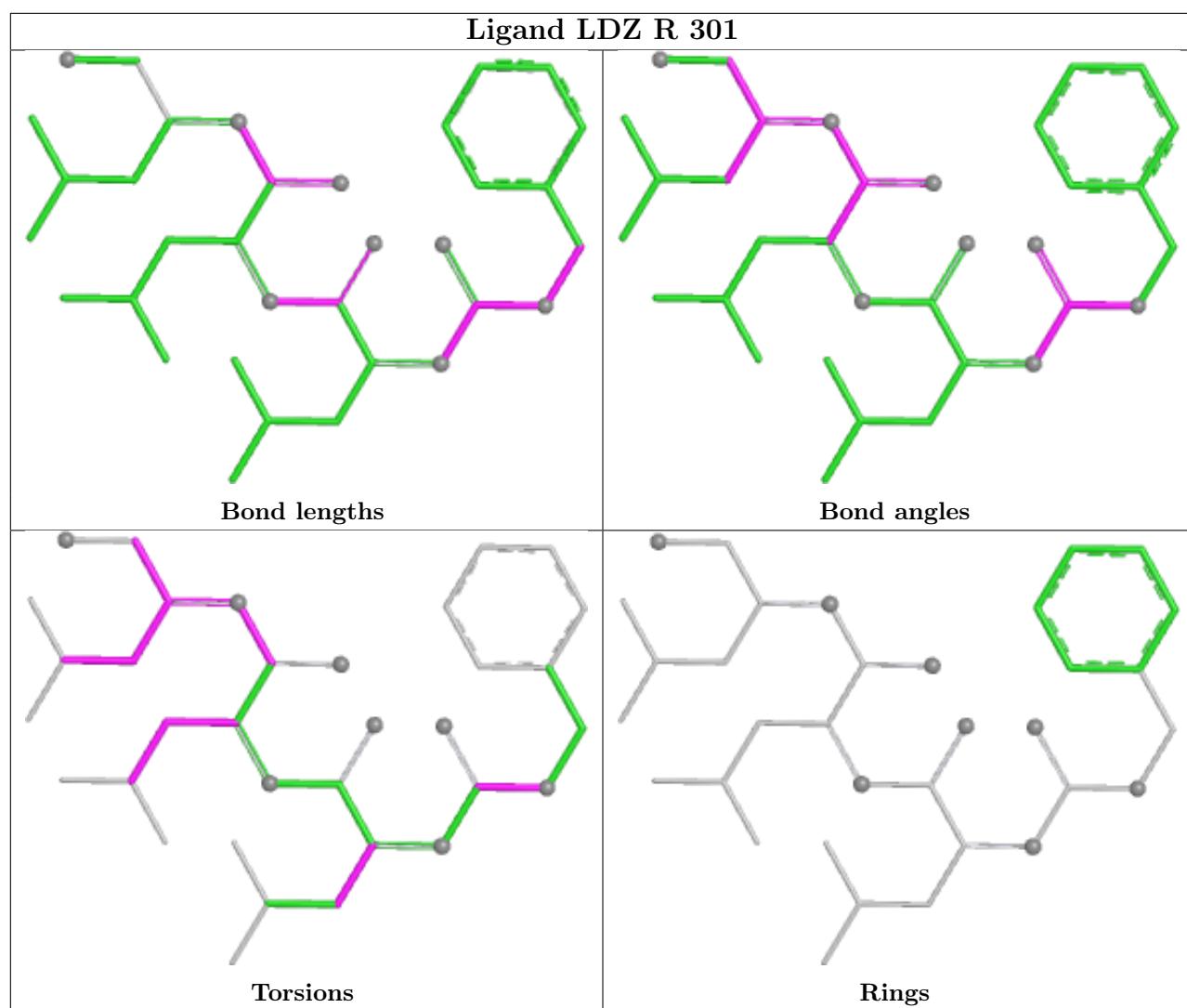


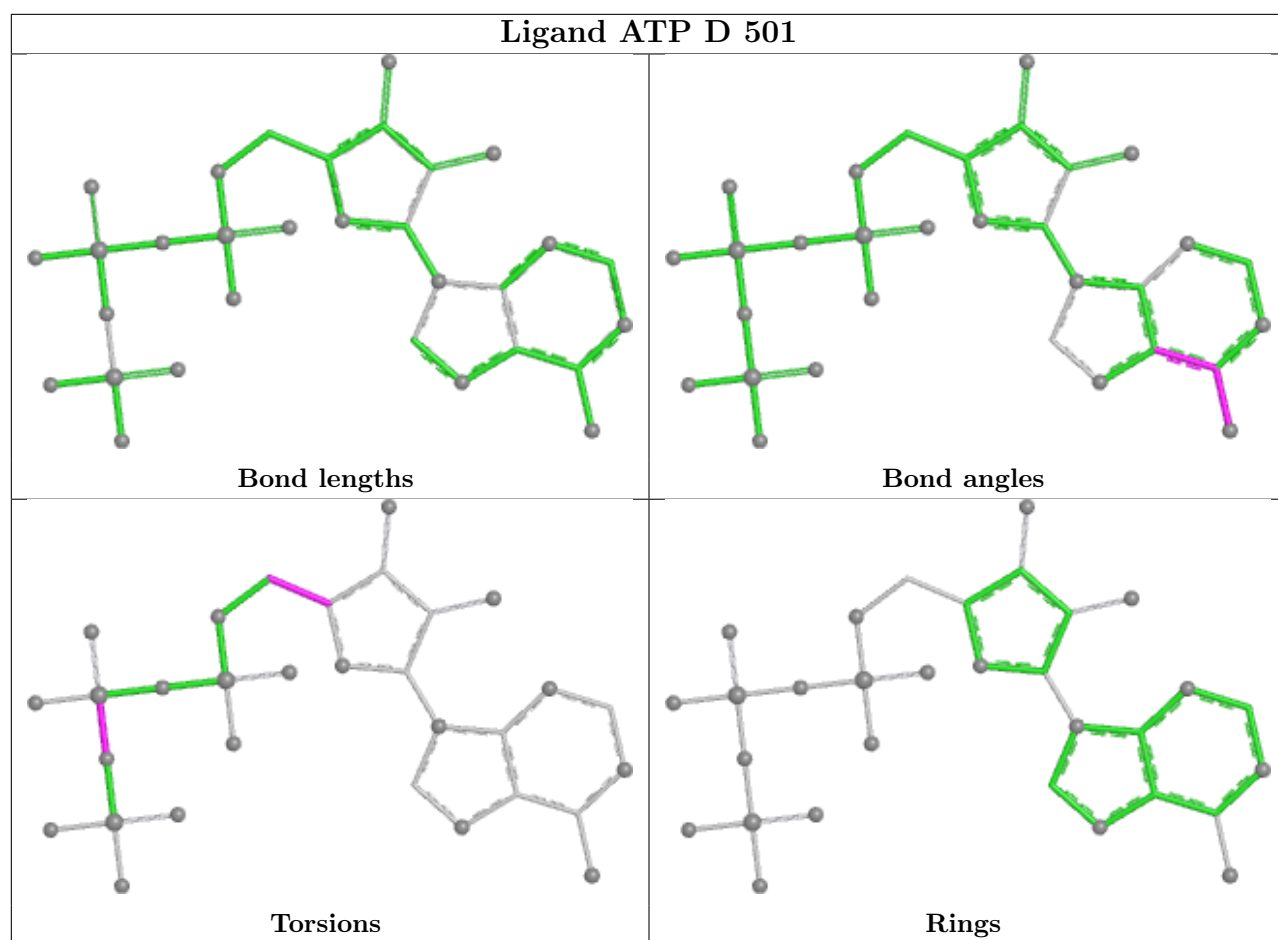


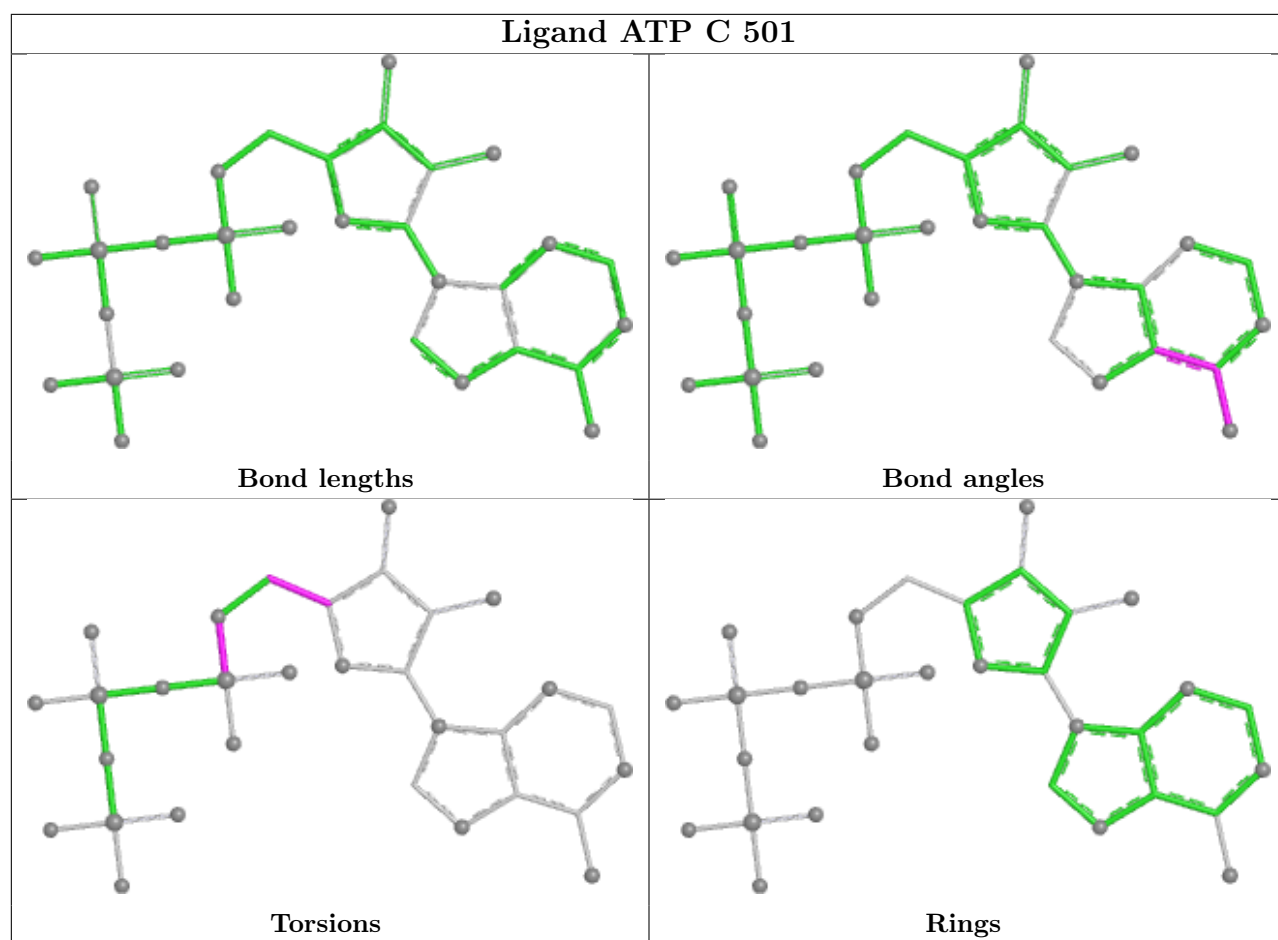


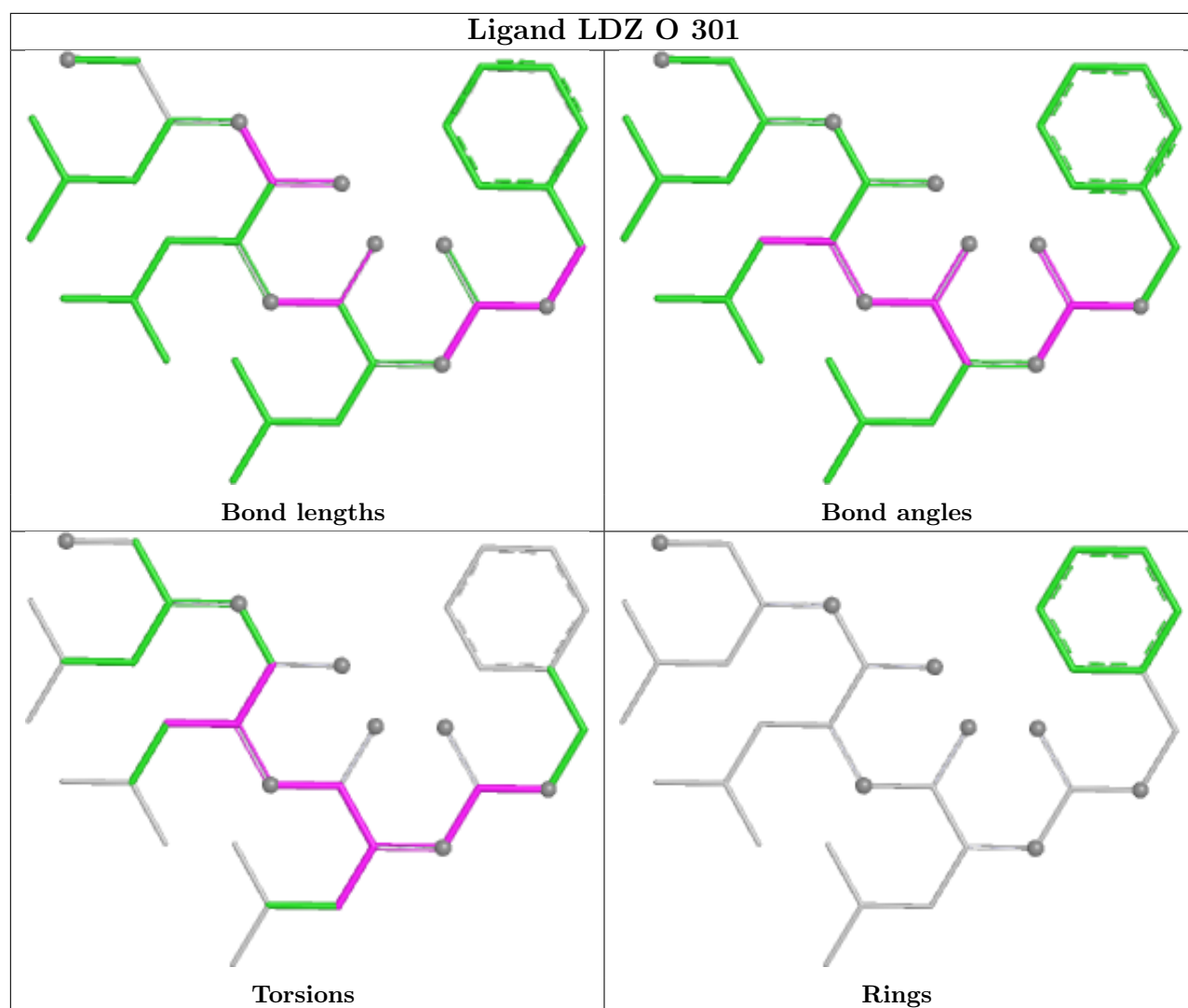












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

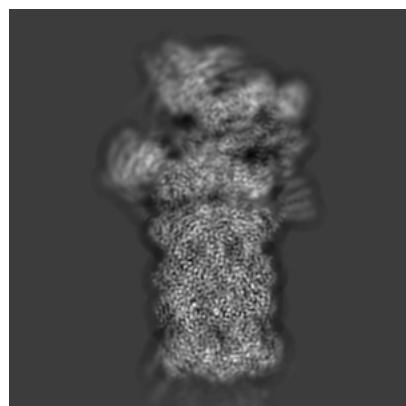
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27018. These allow visual inspection of the internal detail of the map and identification of artifacts.

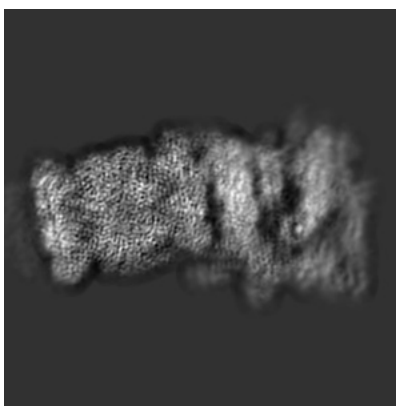
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

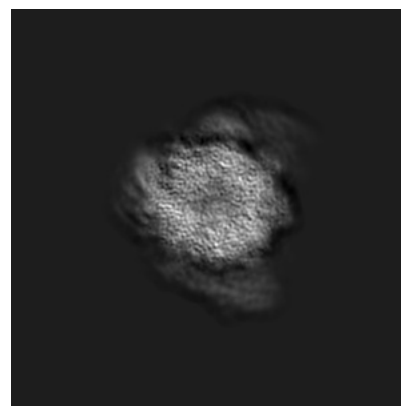
#### 6.1.1 Primary map



X

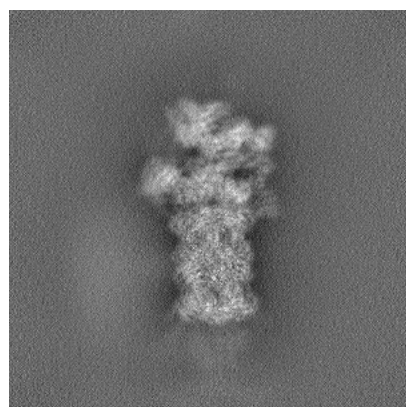


Y

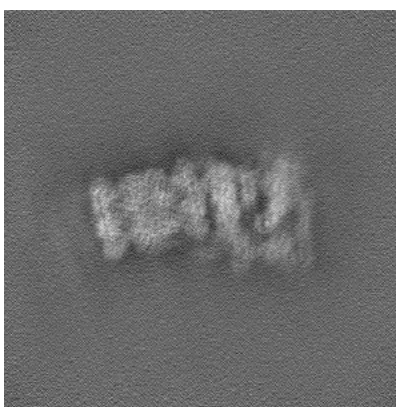


Z

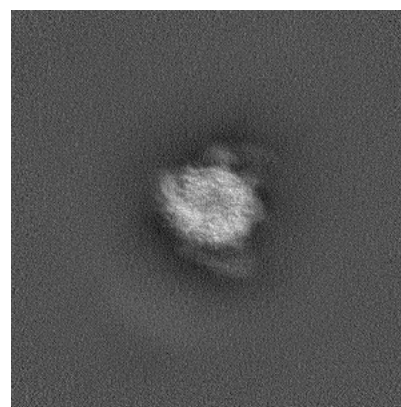
#### 6.1.2 Raw map



X



Y

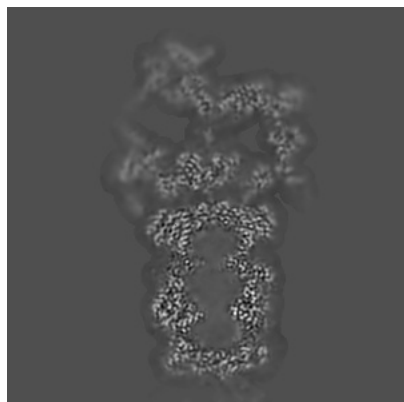


Z

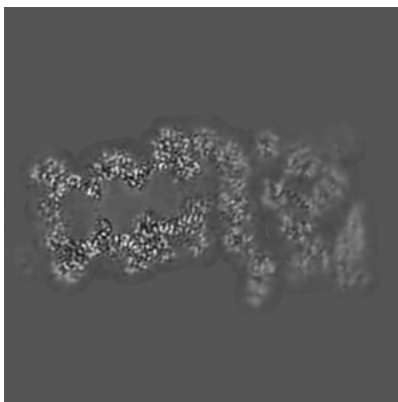
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

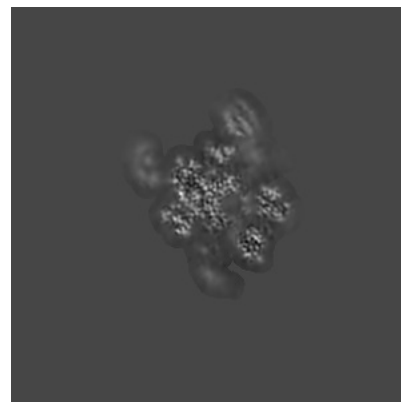
### 6.2.1 Primary map



X Index: 170

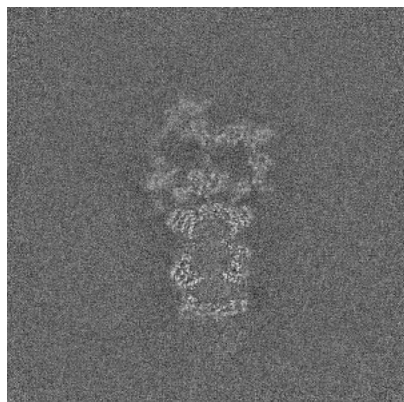


Y Index: 170

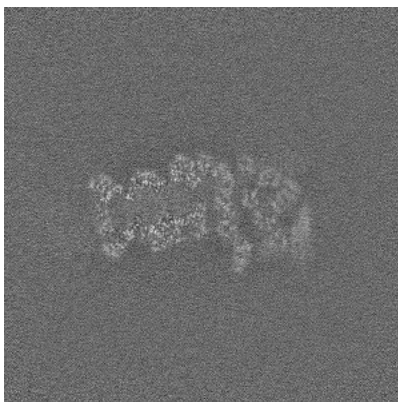


Z Index: 170

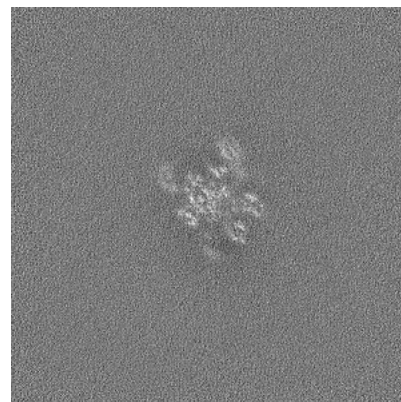
### 6.2.2 Raw map



X Index: 256



Y Index: 256



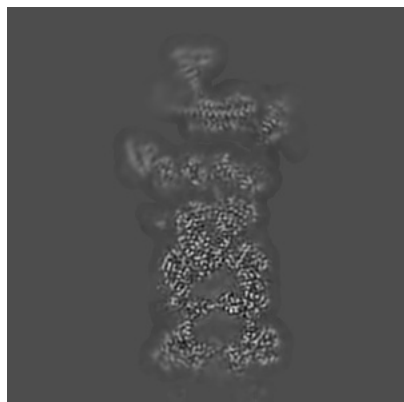
Z Index: 256

The images above show central slices of the map in three orthogonal directions.



## 6.3 Largest variance slices [i](#)

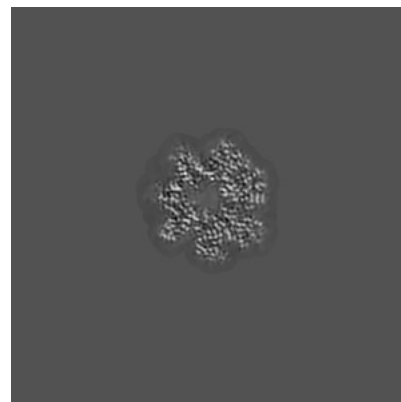
### 6.3.1 Primary map



X Index: 153

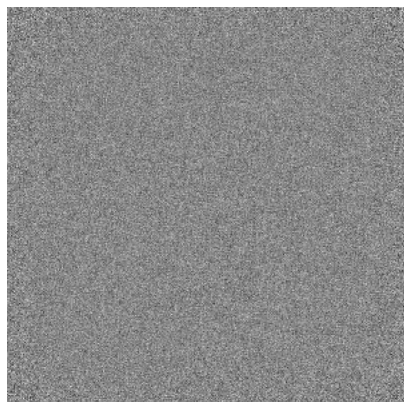


Y Index: 193

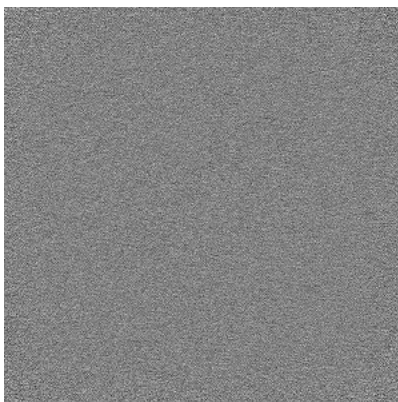


Z Index: 80

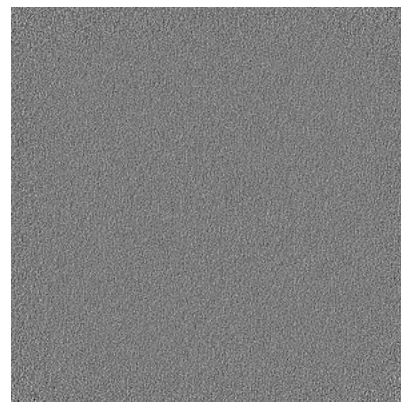
### 6.3.2 Raw map



X Index: 0



Y Index: 0

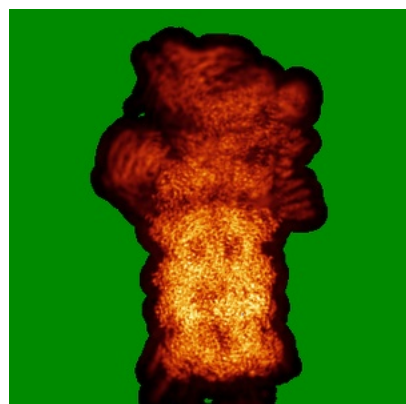


Z Index: 511

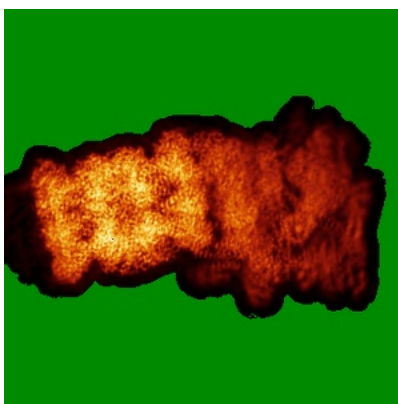
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

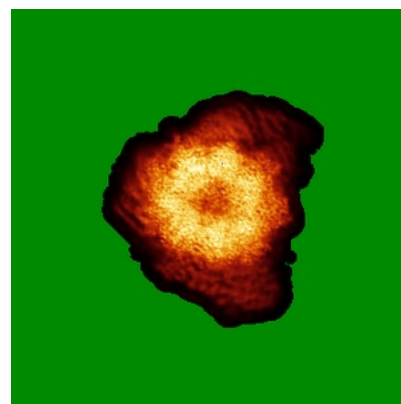
### 6.4.1 Primary map



X

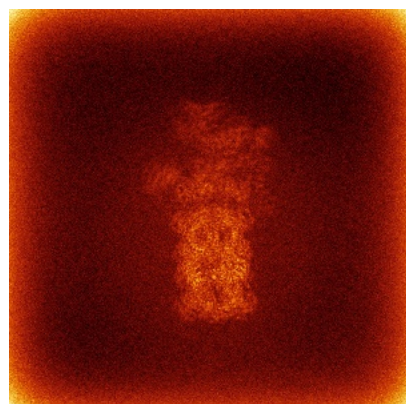


Y

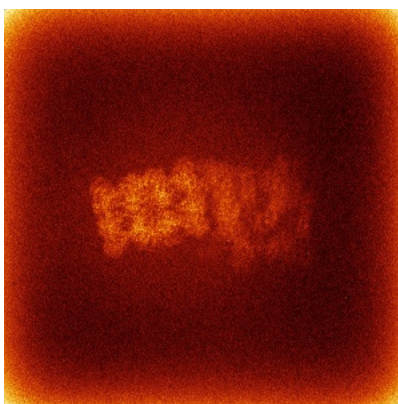


Z

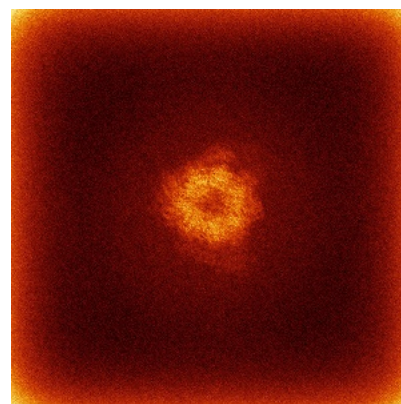
### 6.4.2 Raw map



X



Y

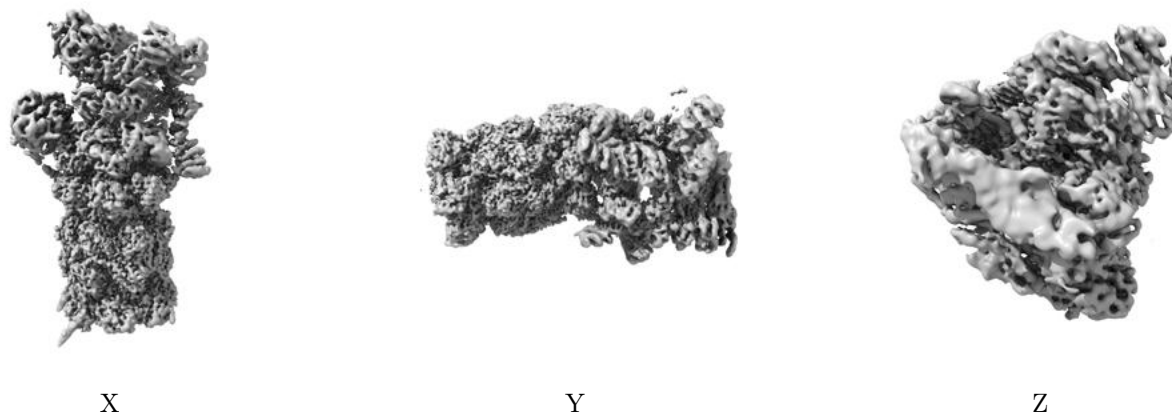


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

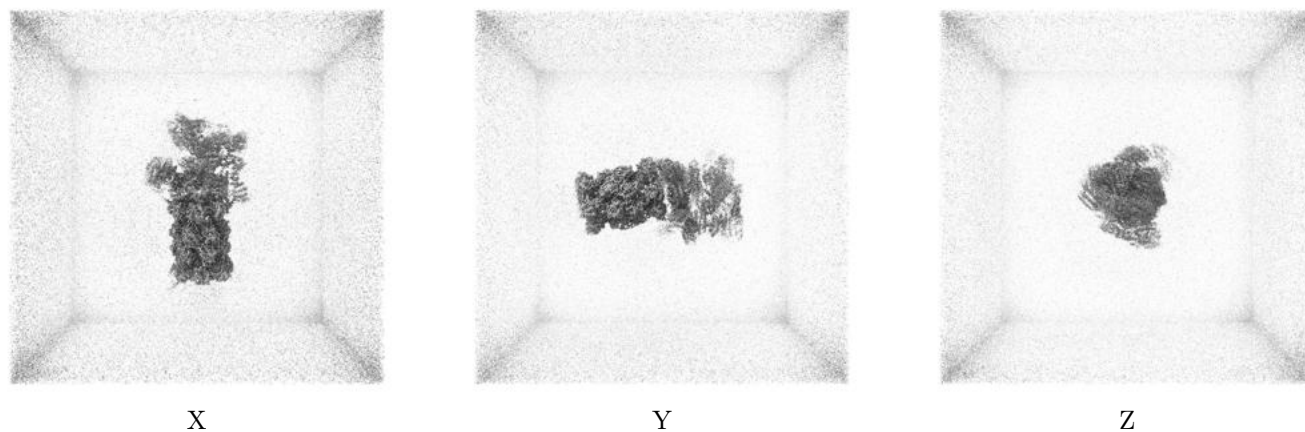
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

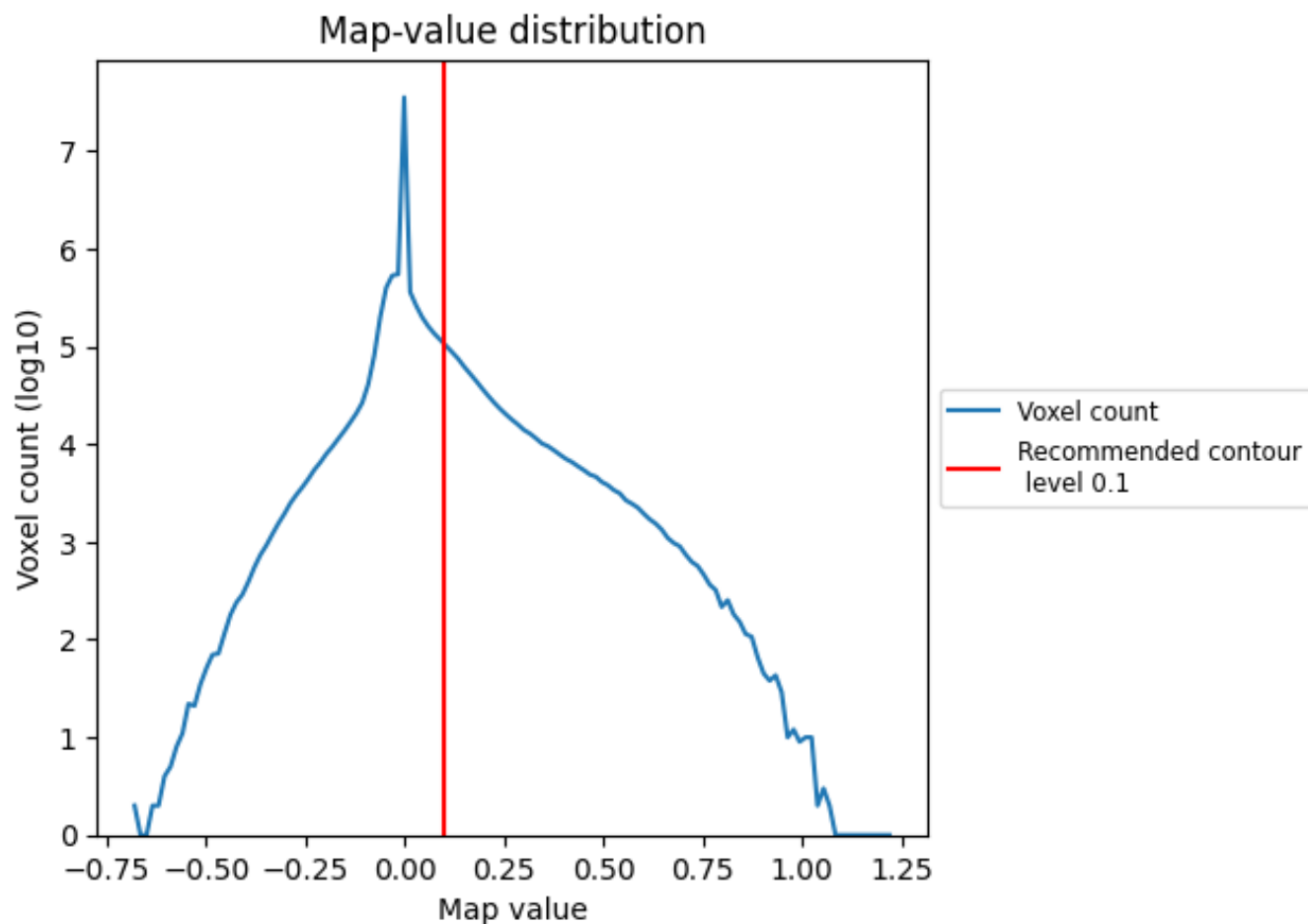
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

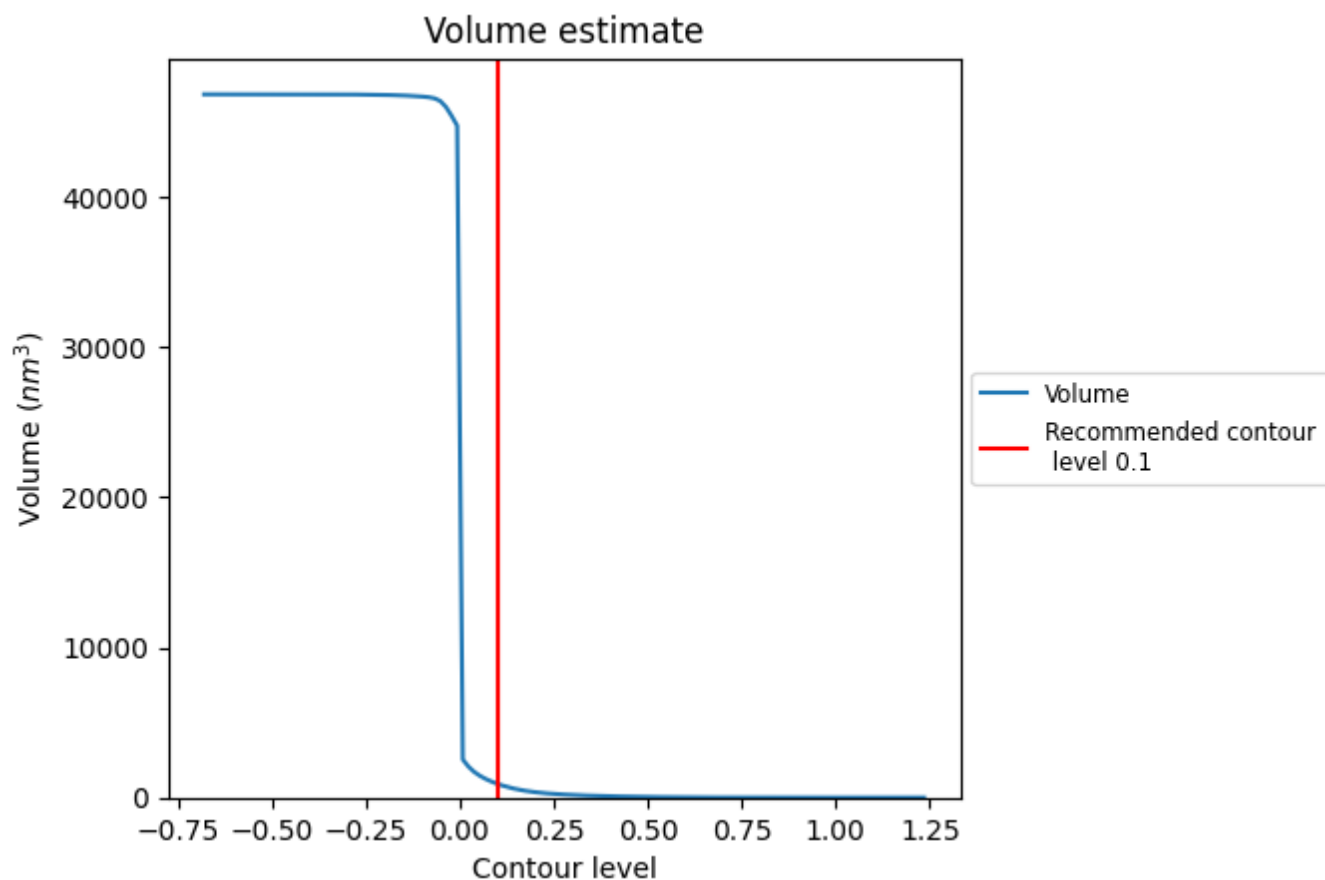
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

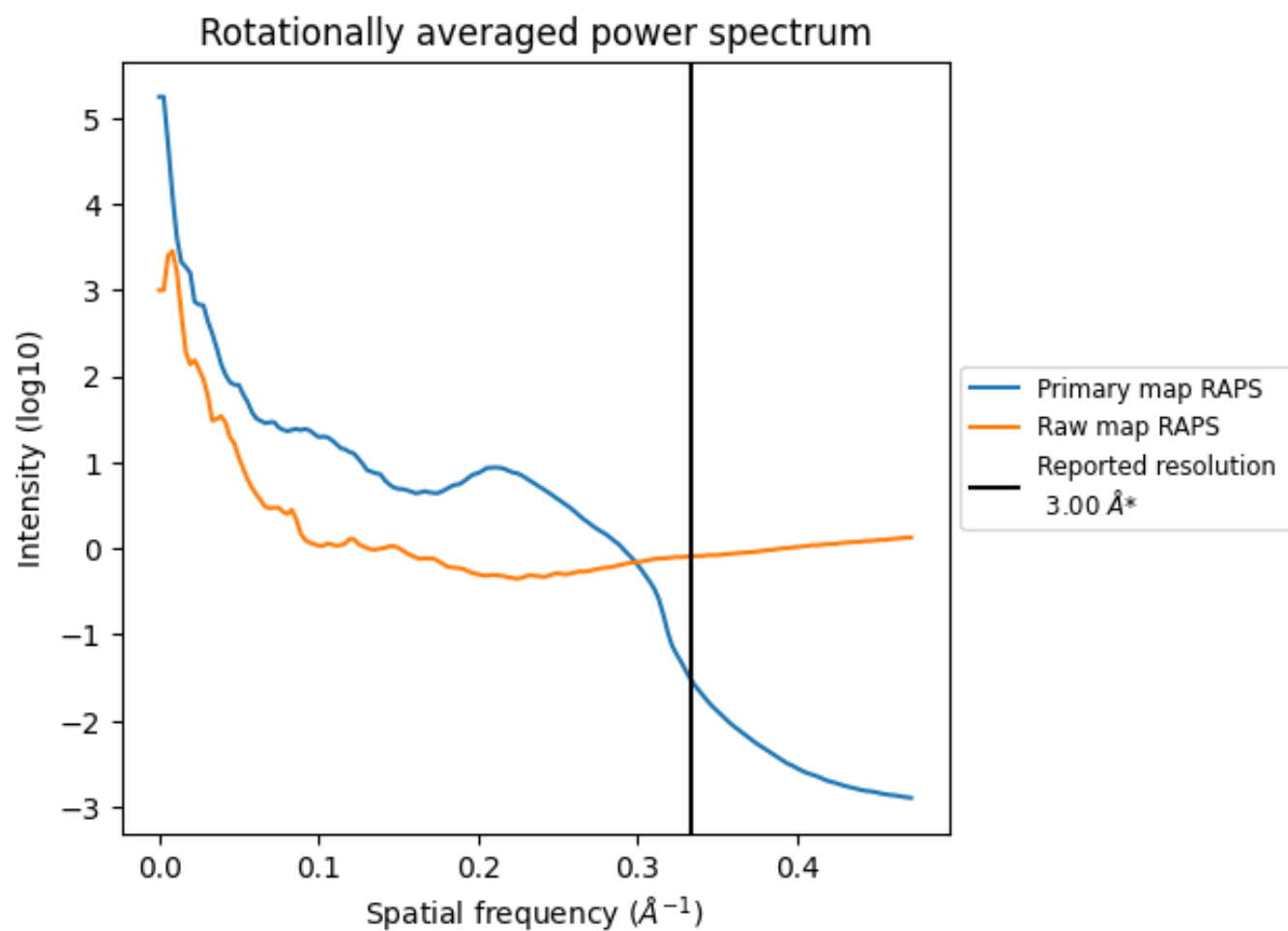
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 915  $\text{nm}^3$ ; this corresponds to an approximate mass of 827 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

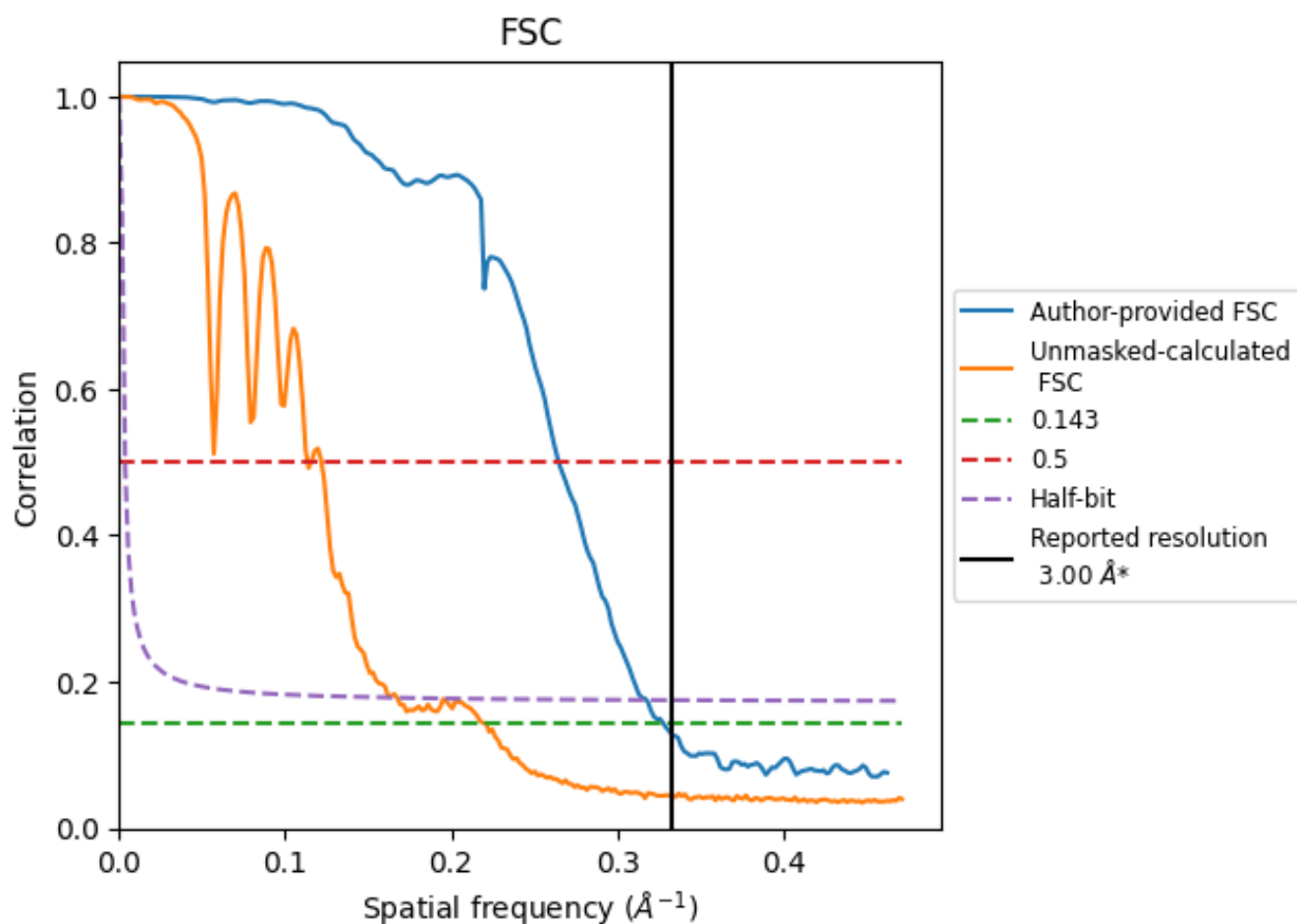


\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.05	3.78	3.15
Unmasked-calculated*	4.52	8.80	5.97

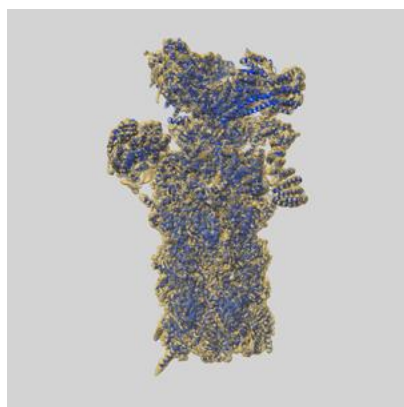
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.52 differs from the reported value 3.0 by more than 10 %



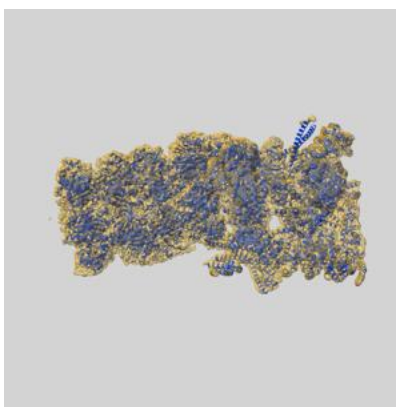
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27018 and PDB model 8CVT. Per-residue inclusion information can be found in section [3](#) on page [12](#).

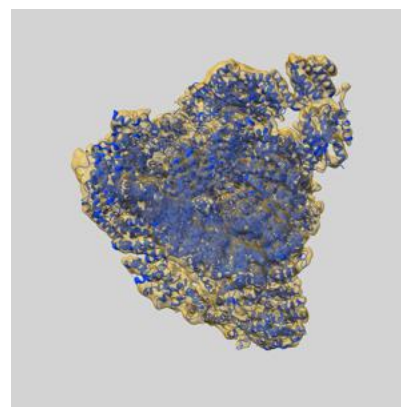
### 9.1 Map-model overlay [i](#)



X



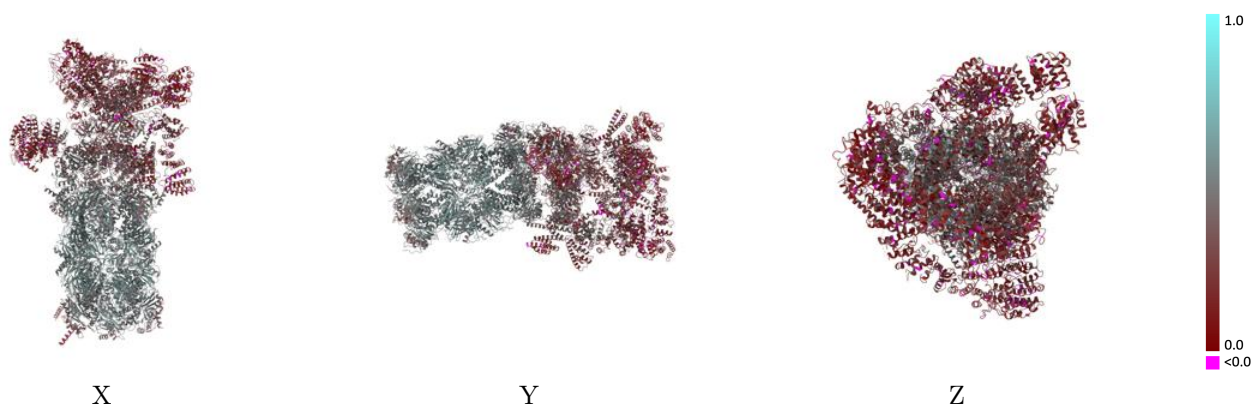
Y



Z

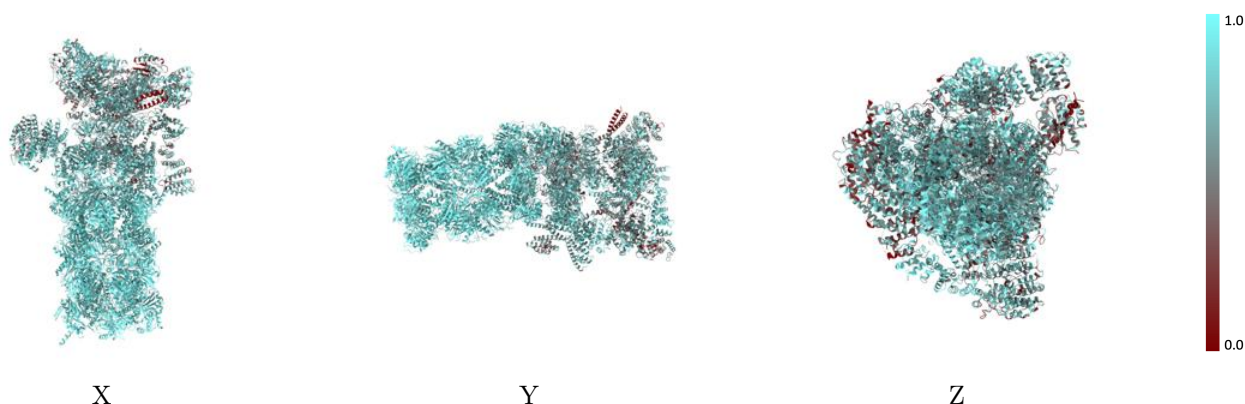
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



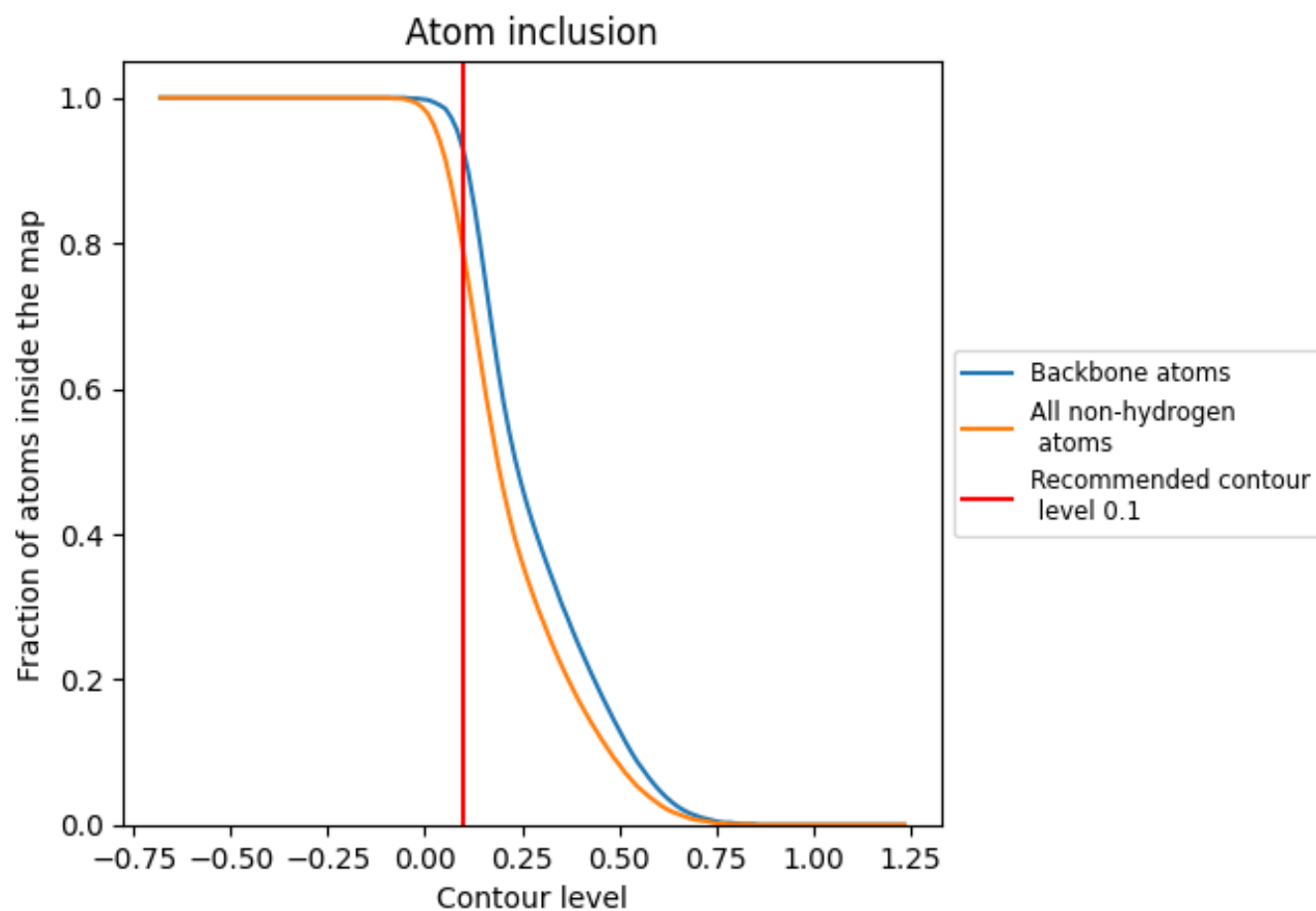
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

























The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7850	 0.3760
A	 0.7510	 0.3770
B	 0.7520	 0.3790
C	 0.8000	 0.3780
D	 0.7300	 0.3490
E	 0.5960	 0.2150
F	 0.7010	 0.3270
G	 0.8900	 0.4870
H	 0.9250	 0.4980
I	 0.8830	 0.4860
J	 0.8980	 0.4890
K	 0.8720	 0.4810
L	 0.9080	 0.4940
M	 0.8760	 0.4730
N	 0.9270	 0.5340
O	 0.9190	 0.5220
P	 0.9290	 0.5310
Q	 0.9210	 0.5350
R	 0.9220	 0.5360
S	 0.9390	 0.5350
T	 0.9330	 0.5310
U	 0.7050	 0.2050
V	 0.5590	 0.1920
W	 0.6350	 0.2210
X	 0.6590	 0.3040
Y	 0.7390	 0.3020
Z	 0.6780	 0.2770
a	 0.6720	 0.1950
b	 0.4950	 0.1800
c	 0.6340	 0.2680
d	 0.4930	 0.1770
e	 0.6000	 0.2260
f	 0.6920	 0.1850
g	 0.9000	 0.4780
h	 0.9140	 0.4860



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Chain	Atom inclusion	Q-score
i	 0.8790	 0.4450
j	 0.8790	 0.4460
k	 0.8690	 0.4680
l	 0.9110	 0.4880
m	 0.8920	 0.4850
n	 0.9170	 0.5270
o	 0.9270	 0.5350
p	 0.9330	 0.5320
q	 0.9350	 0.5350
r	 0.9450	 0.5430
s	 0.9400	 0.5500
t	 0.9450	 0.5480