



## Full wwPDB EM Validation Report ⓘ

Apr 20, 2026 – 03:29 PM JST

PDB ID : 9K56 / pdb\_00009k56  
EMDB ID : EMD-62082  
Title : Structure of substrate-engaged single-cap human proteasome in state EA1  
Authors : Wu, Z.; Chen, E.; Mao, Y.  
Deposited on : 2024-10-21  
Resolution : 3.80 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>.

---

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

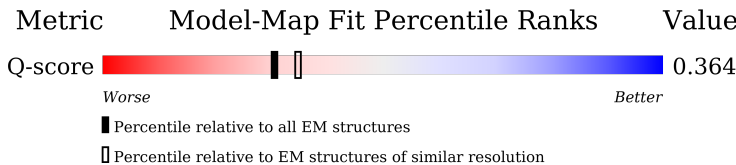
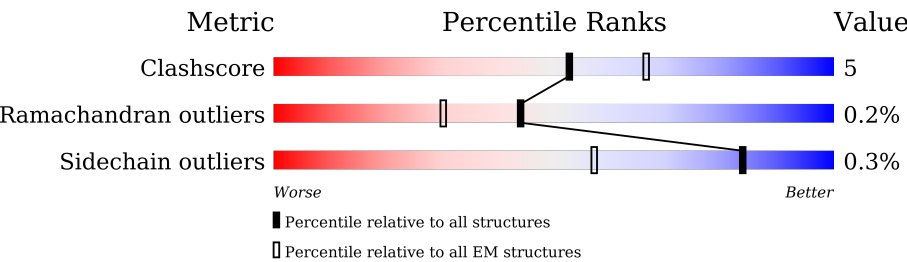
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 ( 3.30 - 4.30 )

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	
2	B	440	
3	C	398	
4	D	418	











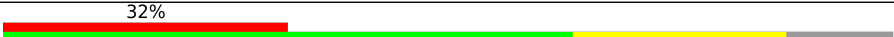

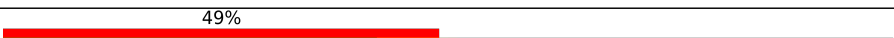
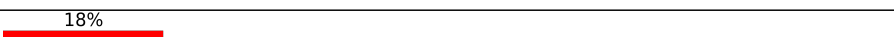

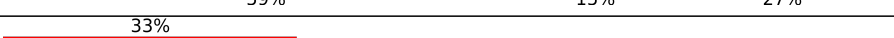

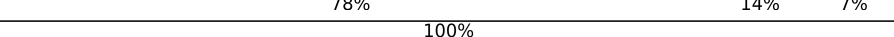
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
18	r	263	
19	S	241	
19	s	241	
20	T	264	
20	t	264	
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	
33	w	76	

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 105968 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	413	Total	C	N	O	S	0	0
			3240	2042	567	613	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	388	Total	C	N	O	S	0	0
			3042	1915	519	593	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	363	Total	C	N	O	S	0	0
			2864	1808	515	525	16		

- 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
			3039	1923	524	579	13		

- Molecule 5 is a protein called Proteasome 26S subunit, ATPase 6.

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
			2858	1802	496	545	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	244	Total	C	N	O	S	0	0
			1889	1198	316	362	13		
7	g	244	Total	C	N	O	S	0	0
			1880	1193	318	356	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1805	1152	305	342	6		
8	h	232	Total	C	N	O	S	0	0
			1805	1154	307	338	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	250	Total	C	N	O	S	0	0
			1955	1234	336	375	10		
9	i	250	Total	C	N	O	S	0	0
			1955	1234	336	375	10		

- 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
			1880	1179	333	363	5		
10	j	239	Total	C	N	O	S	0	0
			1861	1168	332	356	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	234	Total	C	N	O	S	0	0
			1777	1117	295	354	11		
11	k	234	Total	C	N	O	S	0	0
			1782	1119	295	357	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
			1866	1169	336	350	11		
12	l	238	Total	C	N	O	S	0	0
			1861	1165	335	350	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
			1876	1191	321	353	11		
13	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		
14	n	202	Total	C	N	O	S	0	0
			1510	947	258	293	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1649	1038	279	320	12		
15	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1587	1010	264	294	19		
16	p	204	Total	C	N	O	S	0	0
			1591	1013	265	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
			1588	1017	270	292	9		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	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
			1559	982	274	294	9		
18	r	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1041	281	309	10		
19	s	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	216	Total	C	N	O	S	0	0
			1683	1062	291	318	12		
20	t	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	868	Total	C	N	O	S	0	0
			6787	4303	1153	1285	46		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	472	Total	C	N	O	S	0	0
			3754	2387	673	681	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	441	Total	C	N	O	S	0	0
			3596	2277	613	682	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	422	Total	C	N	O	S	0	0
			3335	2116	567	639	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	389	Total	C	N	O	S	0	0
			3202	2041	545	598	18		

- 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	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- 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	50	Total	C	N	O	0	0
			425	260	65	100		

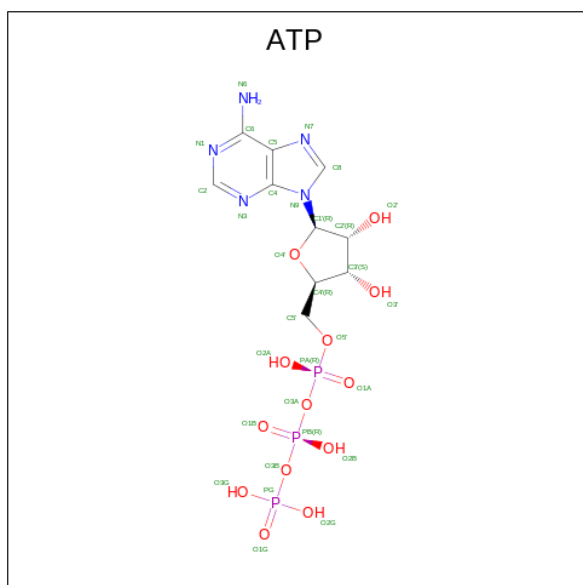
- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	844	Total	C	N	O	S	0	0
			6529	4126	1108	1250	45		

- Molecule 33 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	w	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



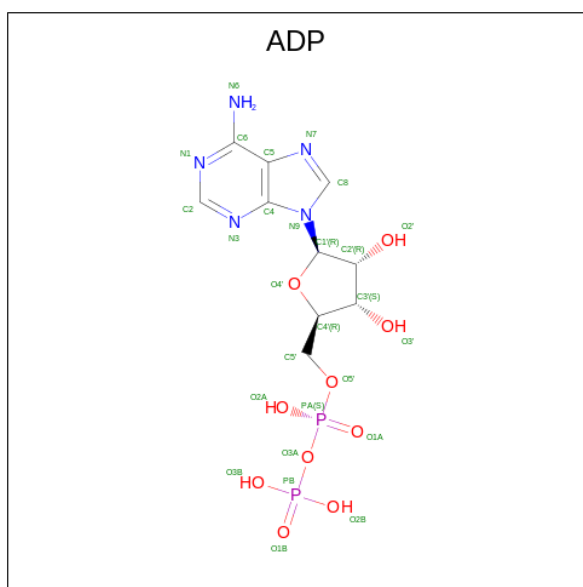
*Continued from previous page...*

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

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
35	A	1	Total	Mg	0
			1	1	
35	B	1	Total	Mg	0
			1	1	
35	D	1	Total	Mg	0
			1	1	
35	E	1	Total	Mg	0
			1	1	
35	F	1	Total	Mg	0
			1	1	

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
36	C	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	

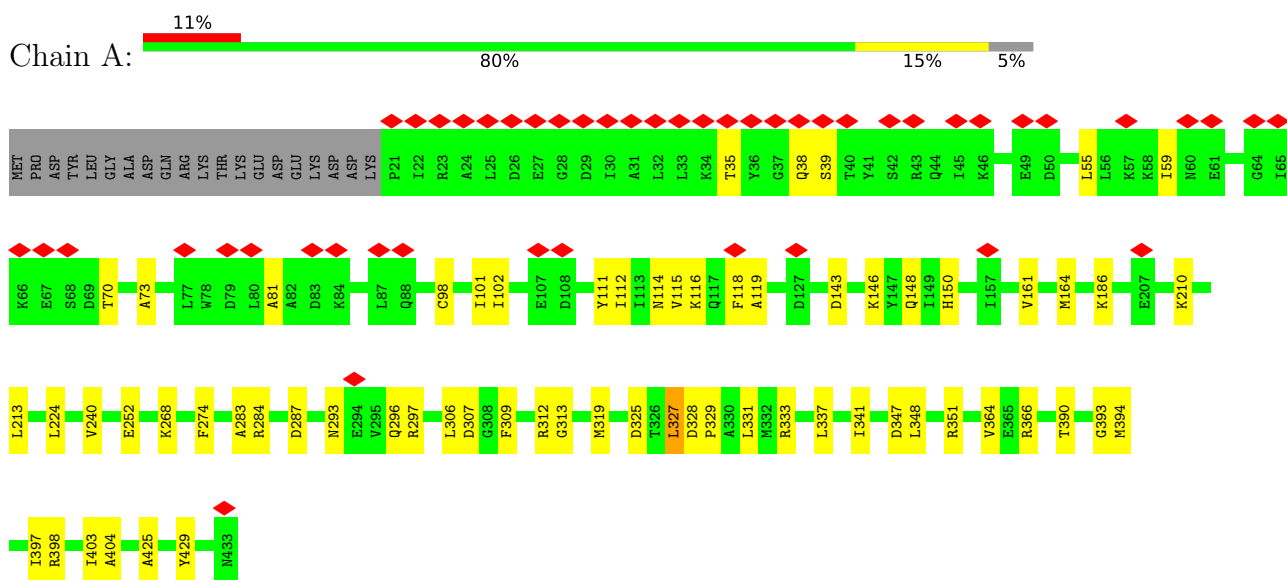
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

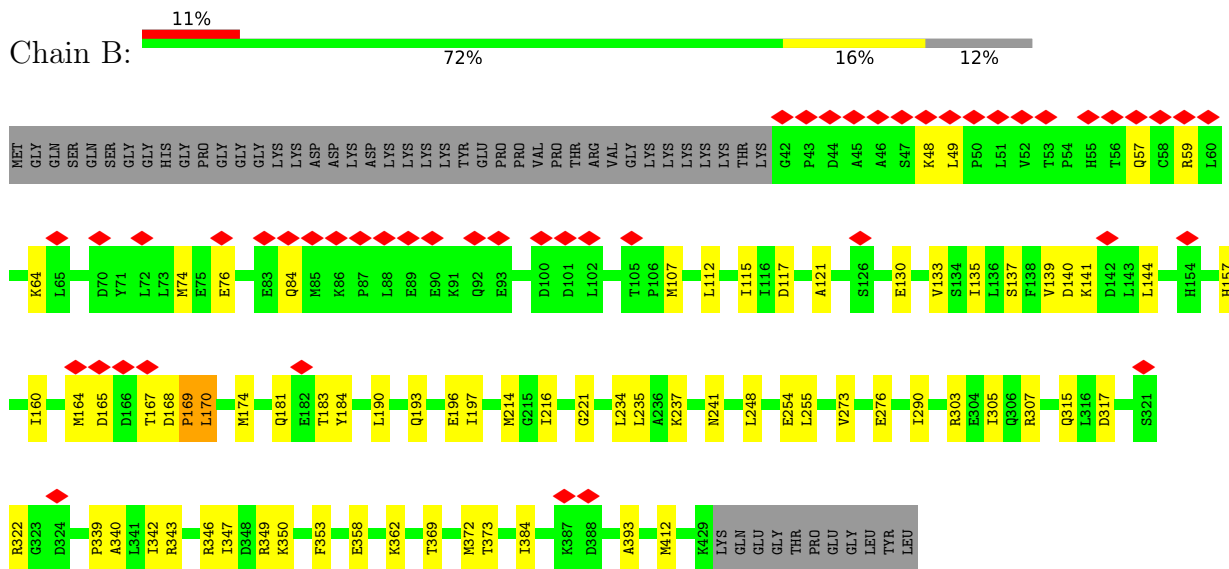
### 3 Residue-property plots [i](#)

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

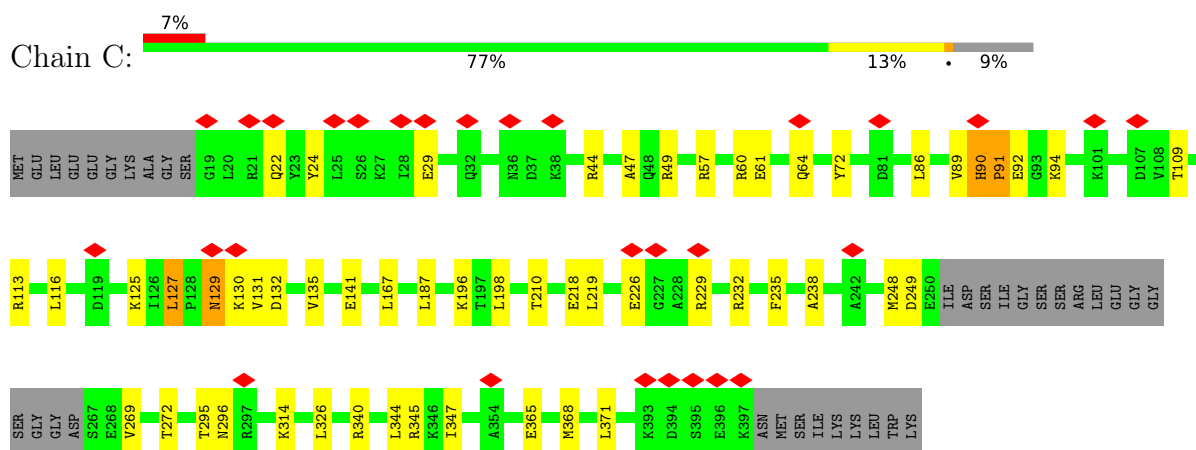
- Molecule 1: 26S proteasome regulatory subunit 7



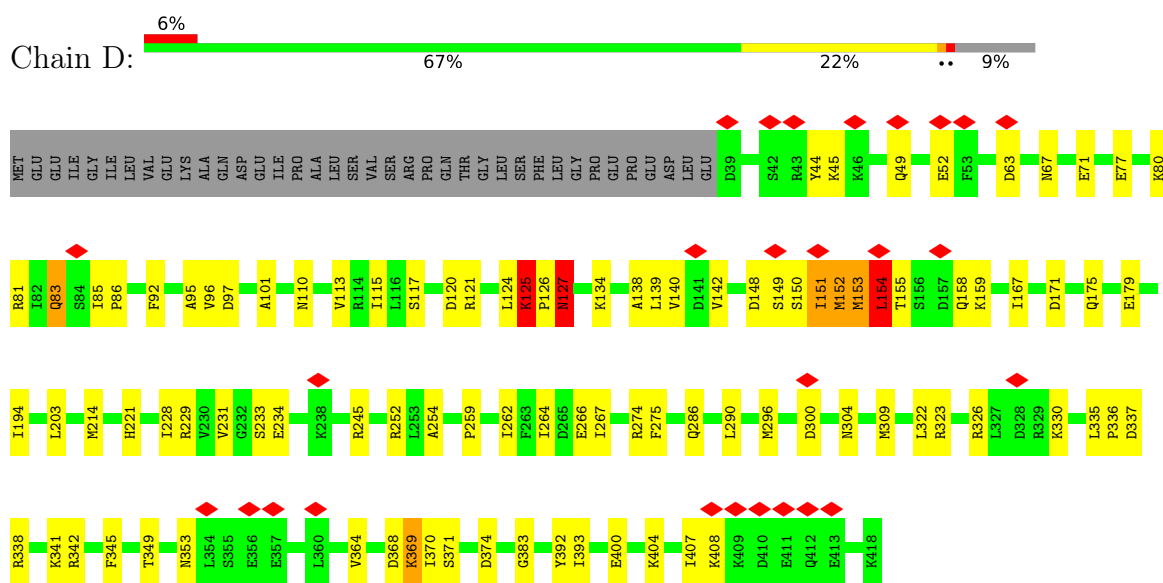
- Molecule 2: 26S proteasome regulatory subunit 4



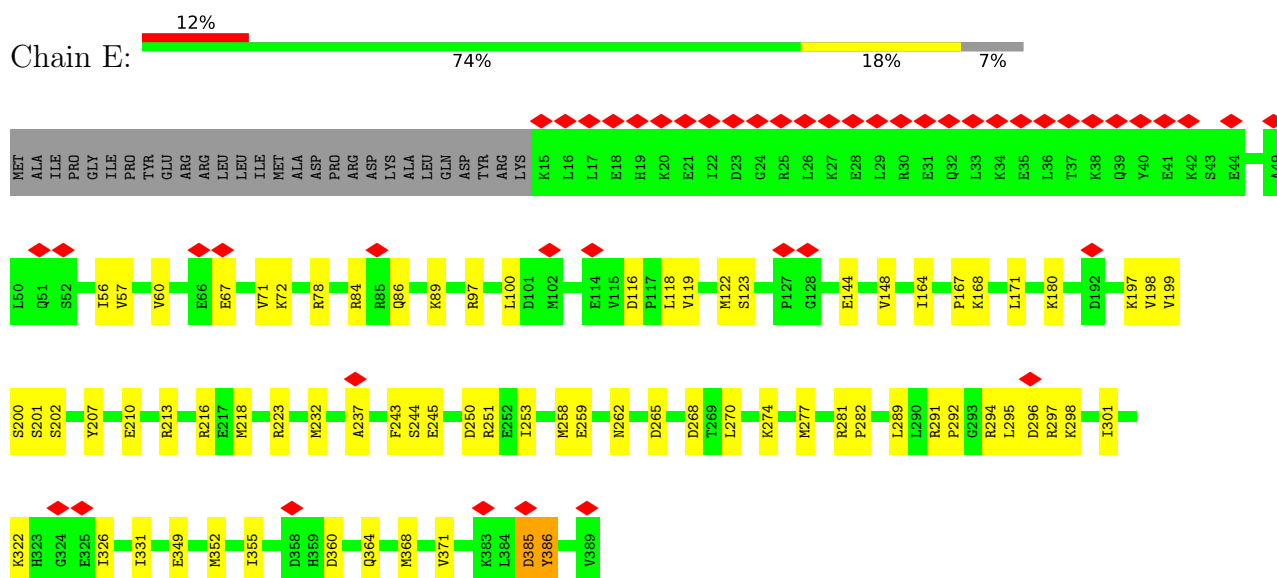
- Molecule 3: 26S proteasome regulatory subunit 8



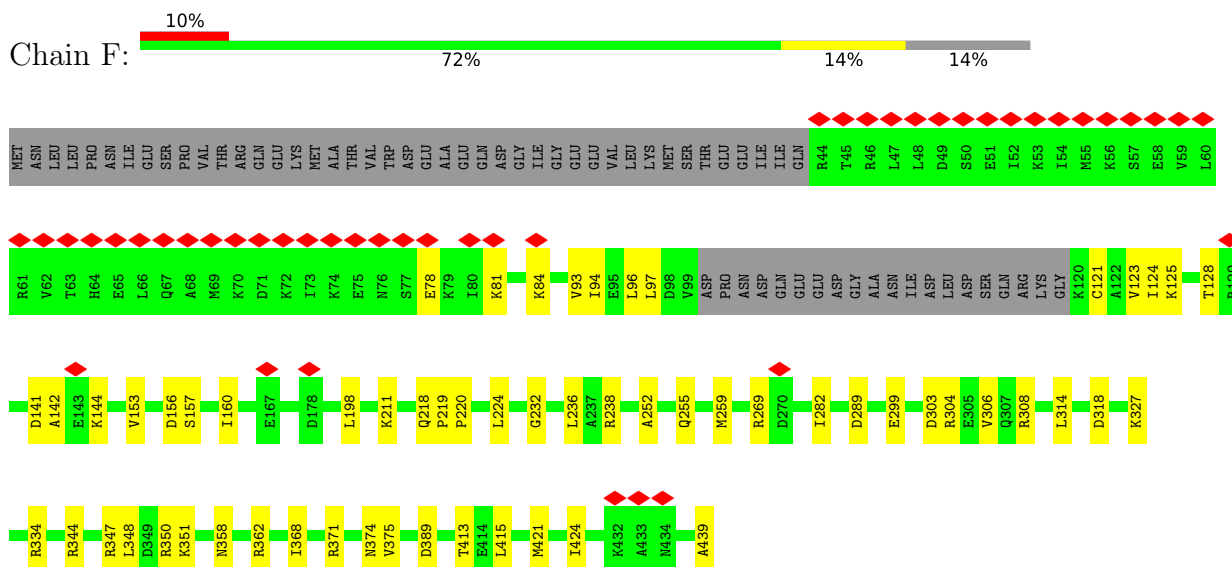
• Molecule 4: 26S proteasome regulatory subunit 6B



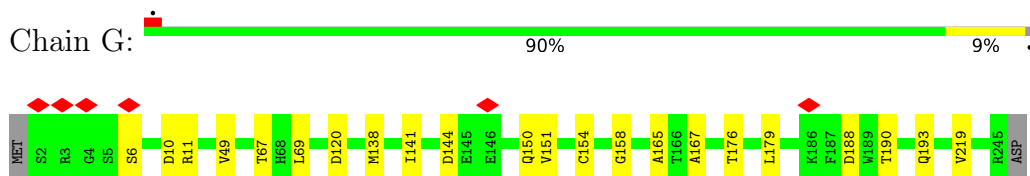
• Molecule 5: Proteasome 26S subunit, ATPase 6



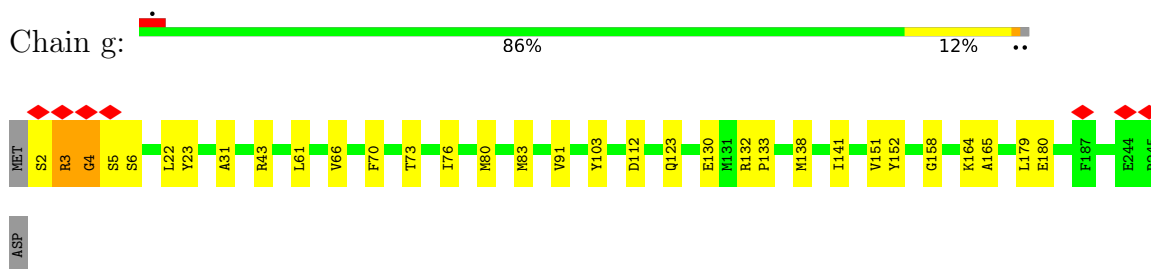
- Molecule 6: 26S proteasome regulatory subunit 6A



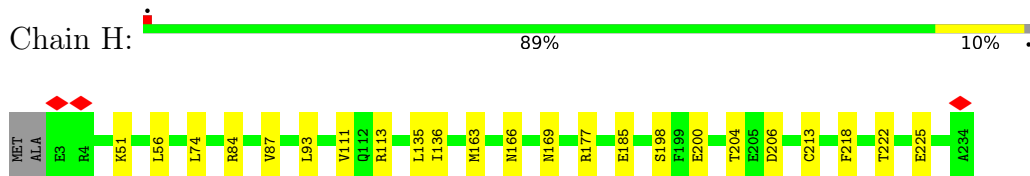
- Molecule 7: Proteasome subunit alpha type-6



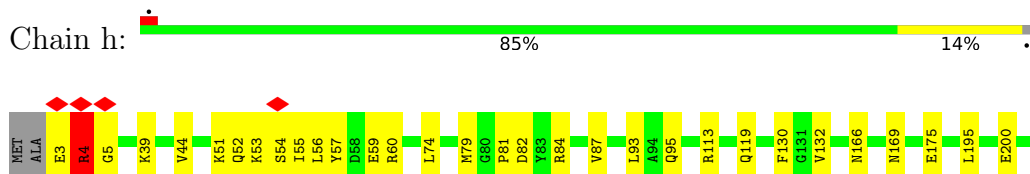
- Molecule 7: Proteasome subunit alpha type-6




- Molecule 8: Proteasome subunit alpha type-2



- Molecule 8: Proteasome subunit alpha type-2

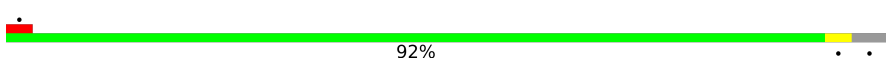


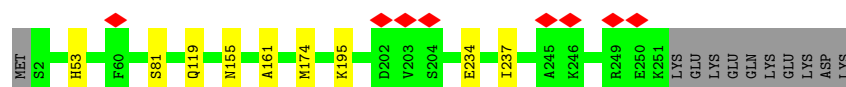
- Molecule 9: Proteasome subunit alpha type-4

Chain I:  88% 7% . .




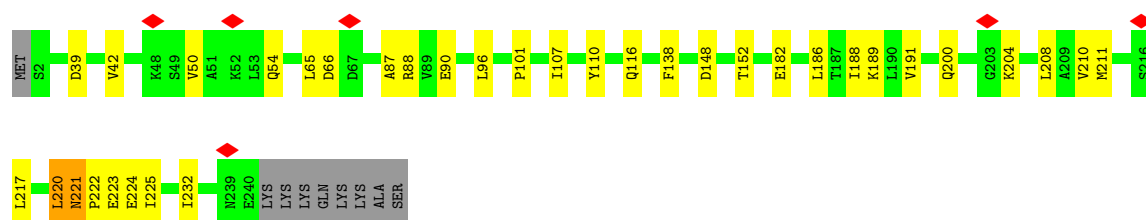
- Molecule 9: Proteasome subunit alpha type-4

Chain i:  92% . .




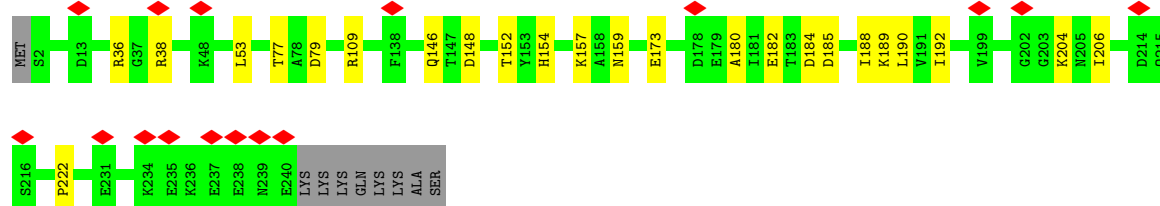
- Molecule 10: Proteasome subunit alpha type-7

Chain J:  82% 13% . .

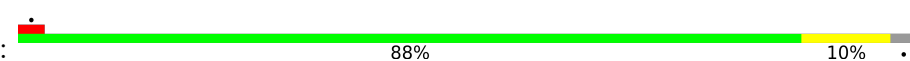


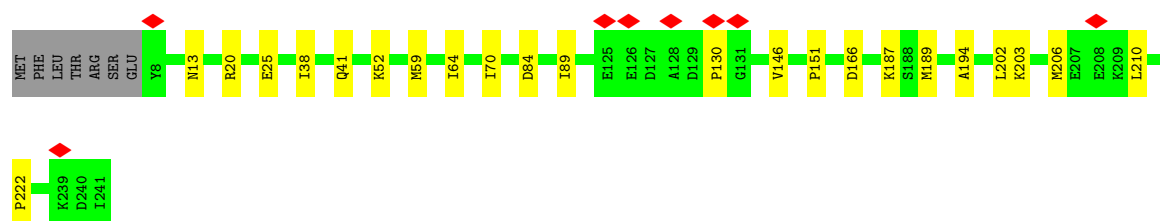
- Molecule 10: Proteasome subunit alpha type-7

Chain j:  6% 87% 10% .

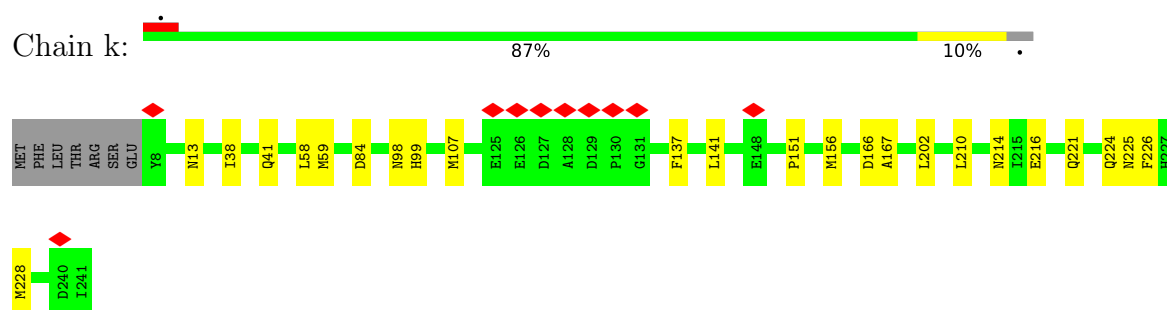


- Molecule 11: Proteasome subunit alpha type-5

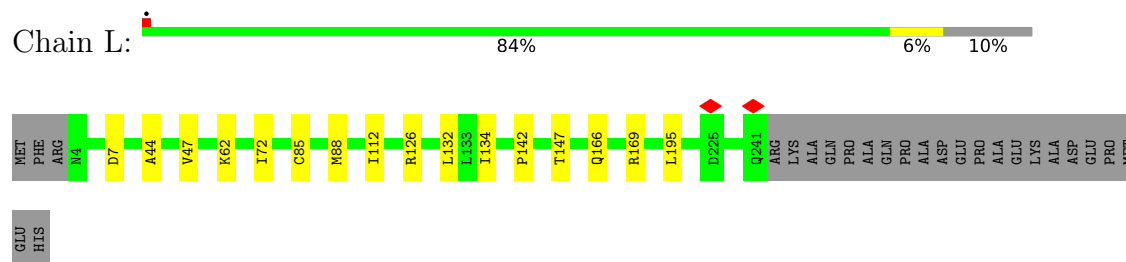
Chain K:  88% 10% .



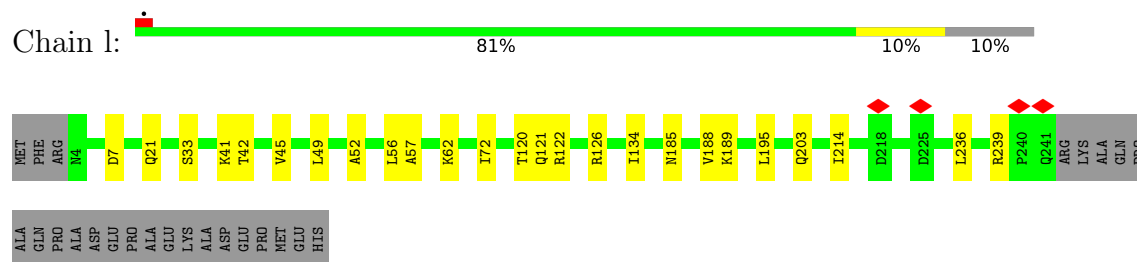
- Molecule 11: Proteasome subunit alpha type-5



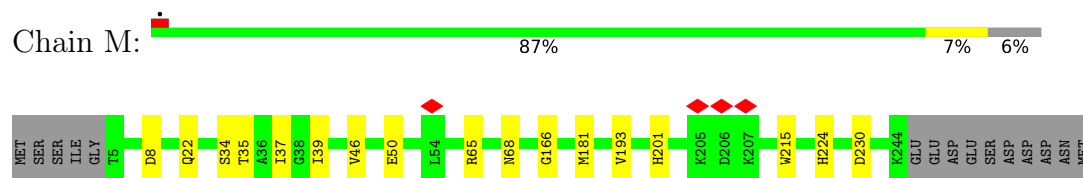
- Molecule 12: Proteasome subunit alpha type-1



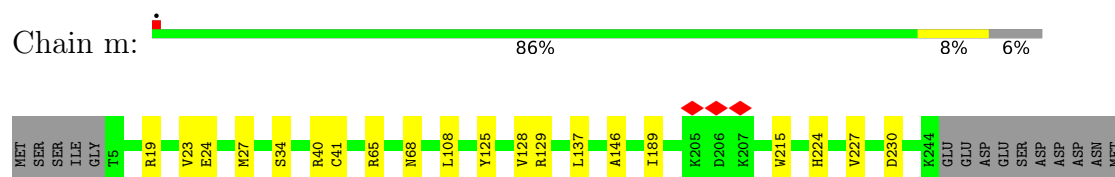
- Molecule 12: Proteasome subunit alpha type-1



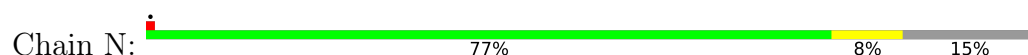
- Molecule 13: Proteasome subunit alpha type-3

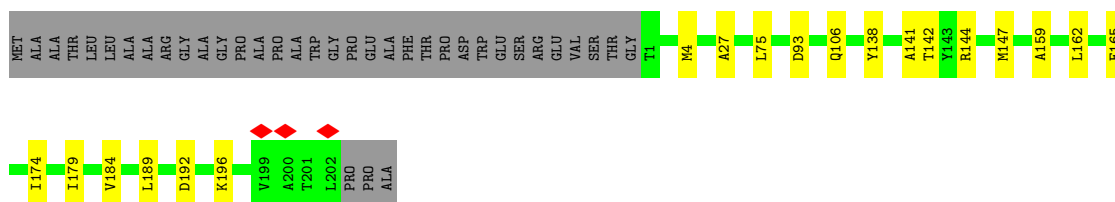


- Molecule 13: Proteasome subunit alpha type-3

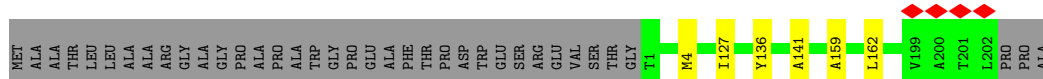
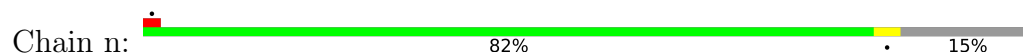


- Molecule 14: Proteasome subunit beta type-6

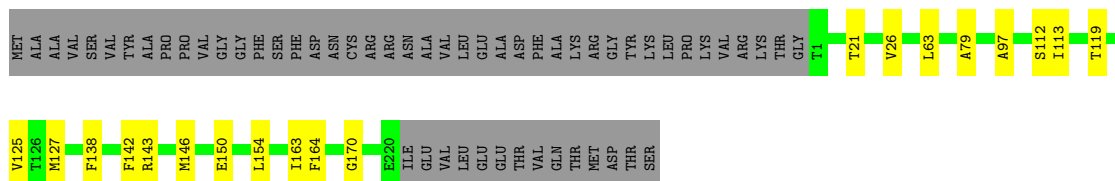




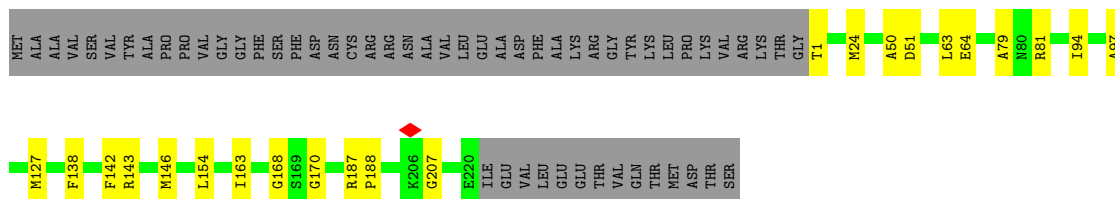
- Molecule 14: Proteasome subunit beta type-6



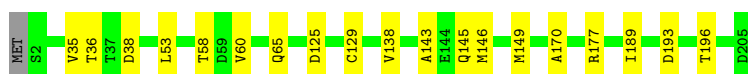
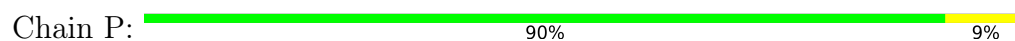
- Molecule 15: Proteasome subunit beta type-7



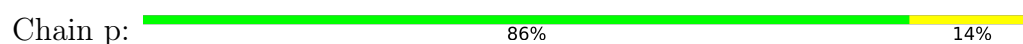
- Molecule 15: Proteasome subunit beta type-7



- Molecule 16: Proteasome subunit beta type-3



- Molecule 16: Proteasome subunit beta type-3



- Molecule 17: Proteasome subunit beta type-2

Chain Q:  85% 14%



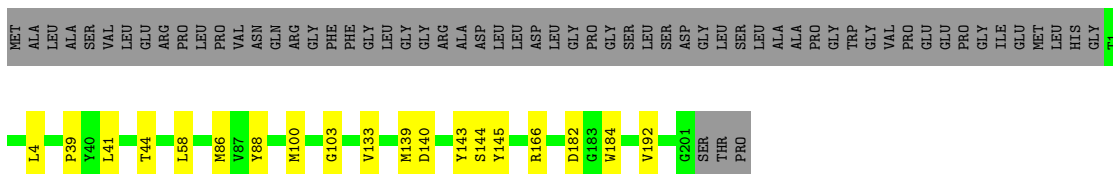
- Molecule 17: Proteasome subunit beta type-2

Chain q:  89% 10%



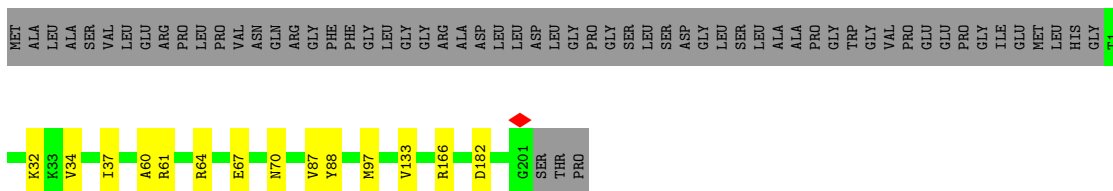
- Molecule 18: Proteasome subunit beta type-5

Chain R:  69% 7% 24%

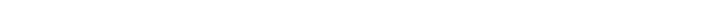


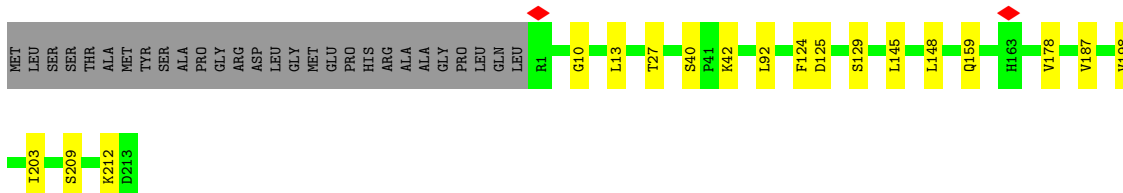
- Molecule 18: Proteasome subunit beta type-5

Chain r:  71% 5% 24%

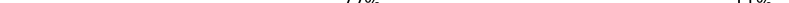


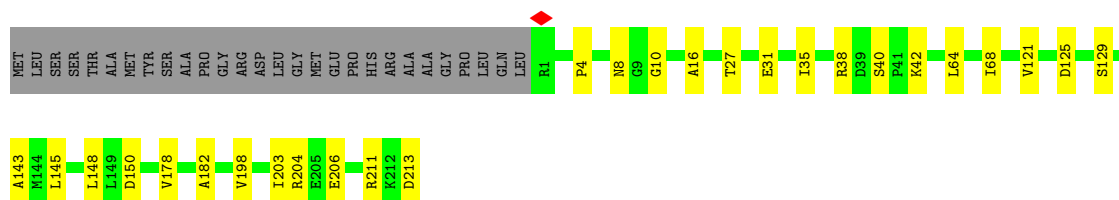
- Molecule 19: Proteasome subunit beta type-1

Chain S:  81% 7% 12%



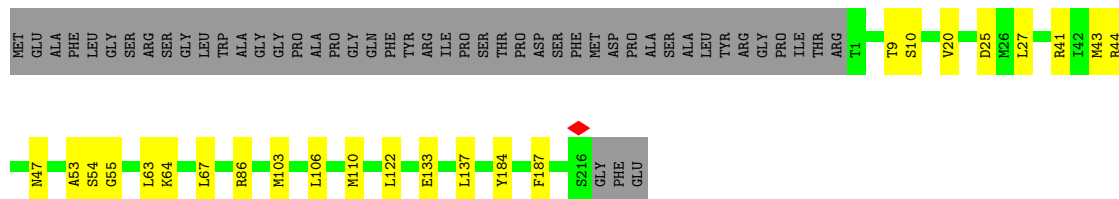
- Molecule 19: Proteasome subunit beta type-1

Chain s: 



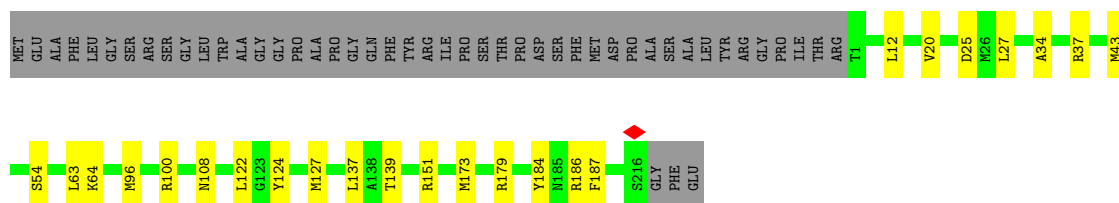
• Molecule 20: Proteasome subunit beta type-4

Chain T: 73% 9% 18%



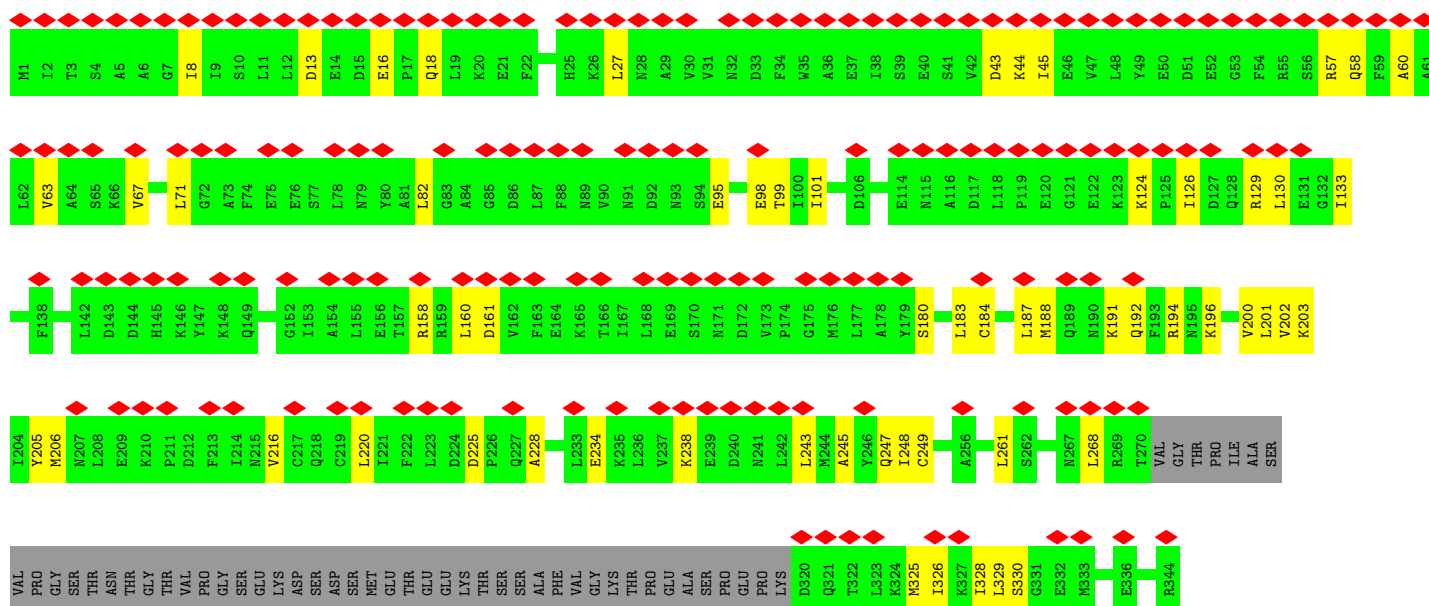
• Molecule 20: Proteasome subunit beta type-4

Chain t: 73% 9% 18%

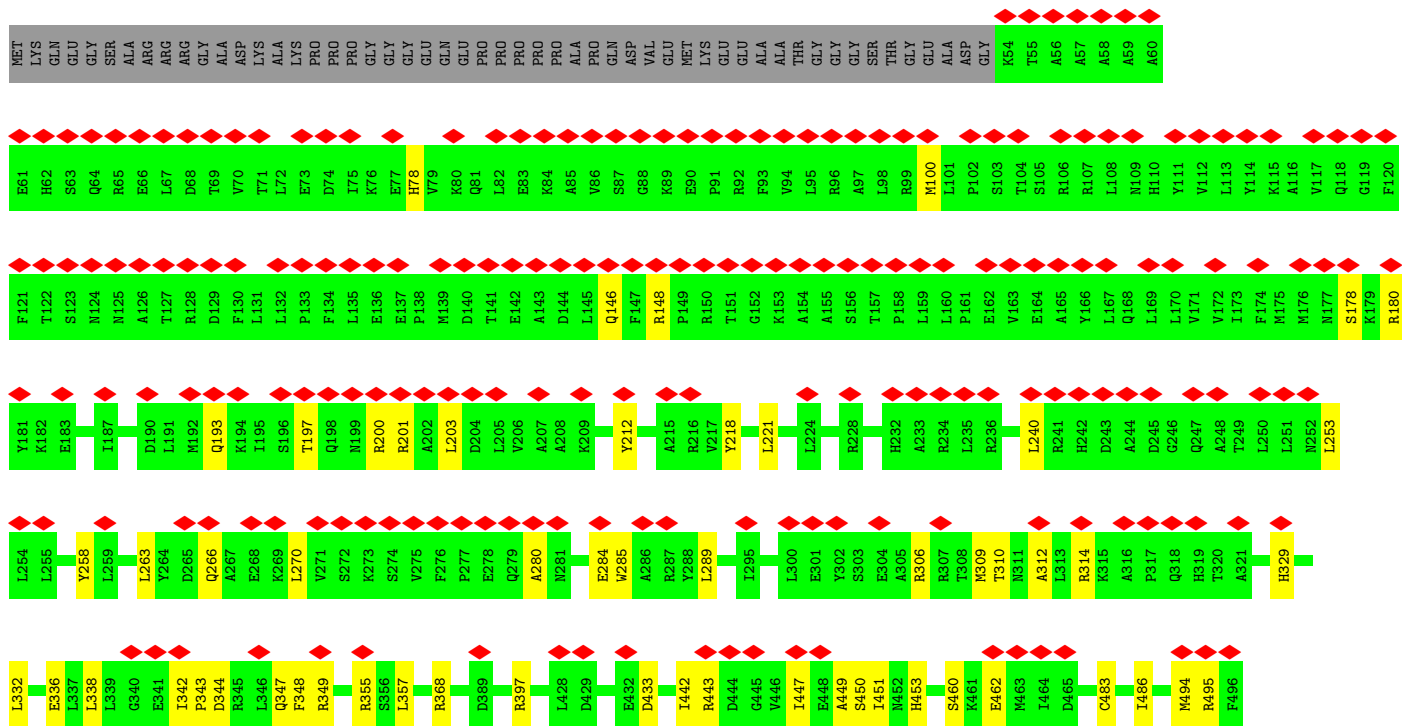
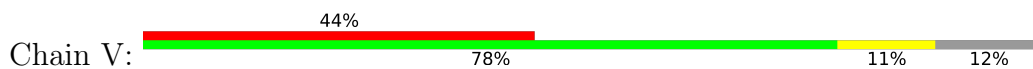


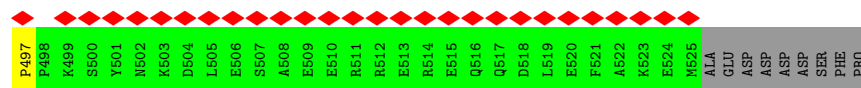
• Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

Chain U: 35% 74% 17% 9%

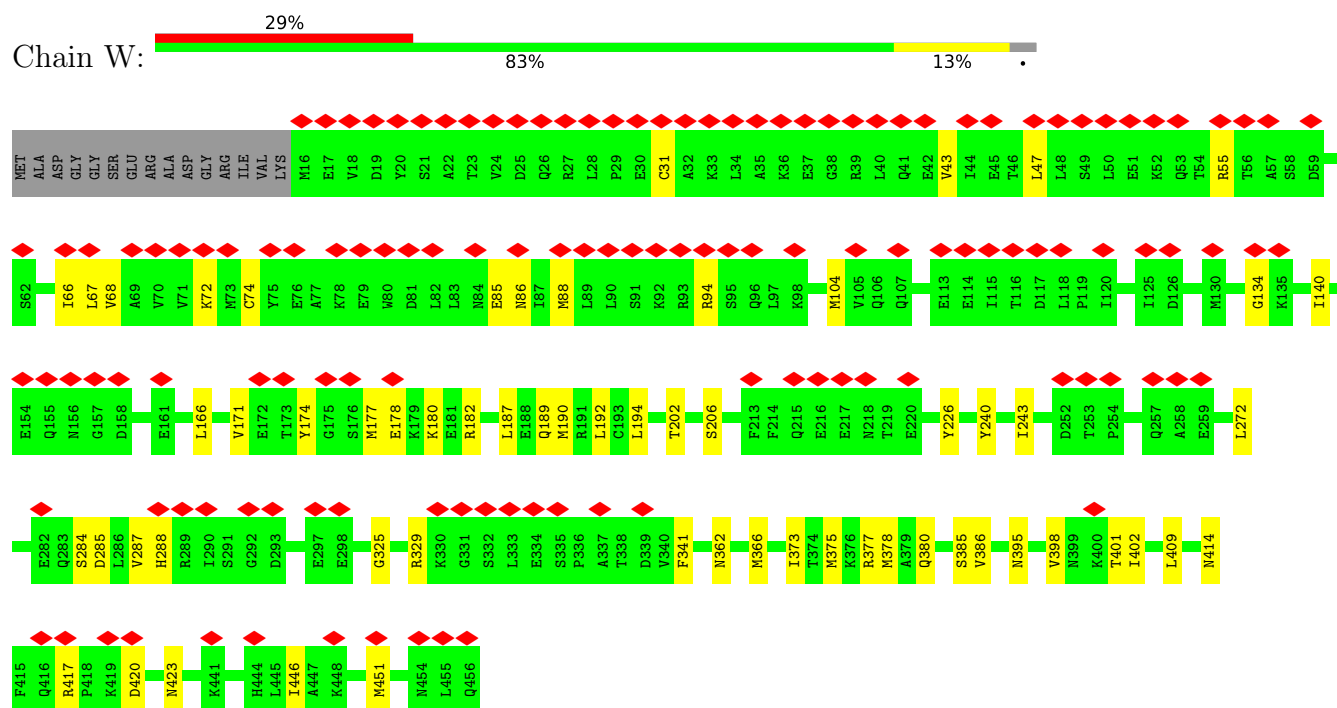


- Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

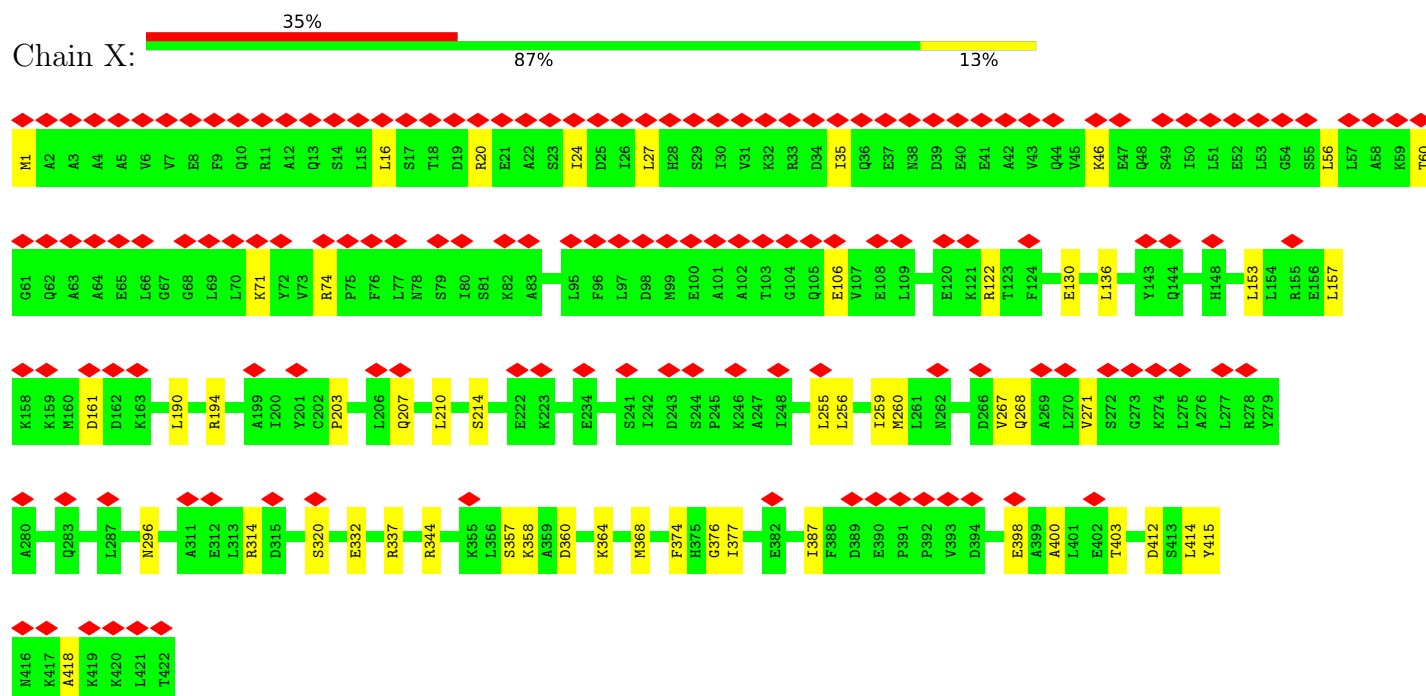




- Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

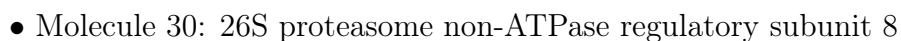


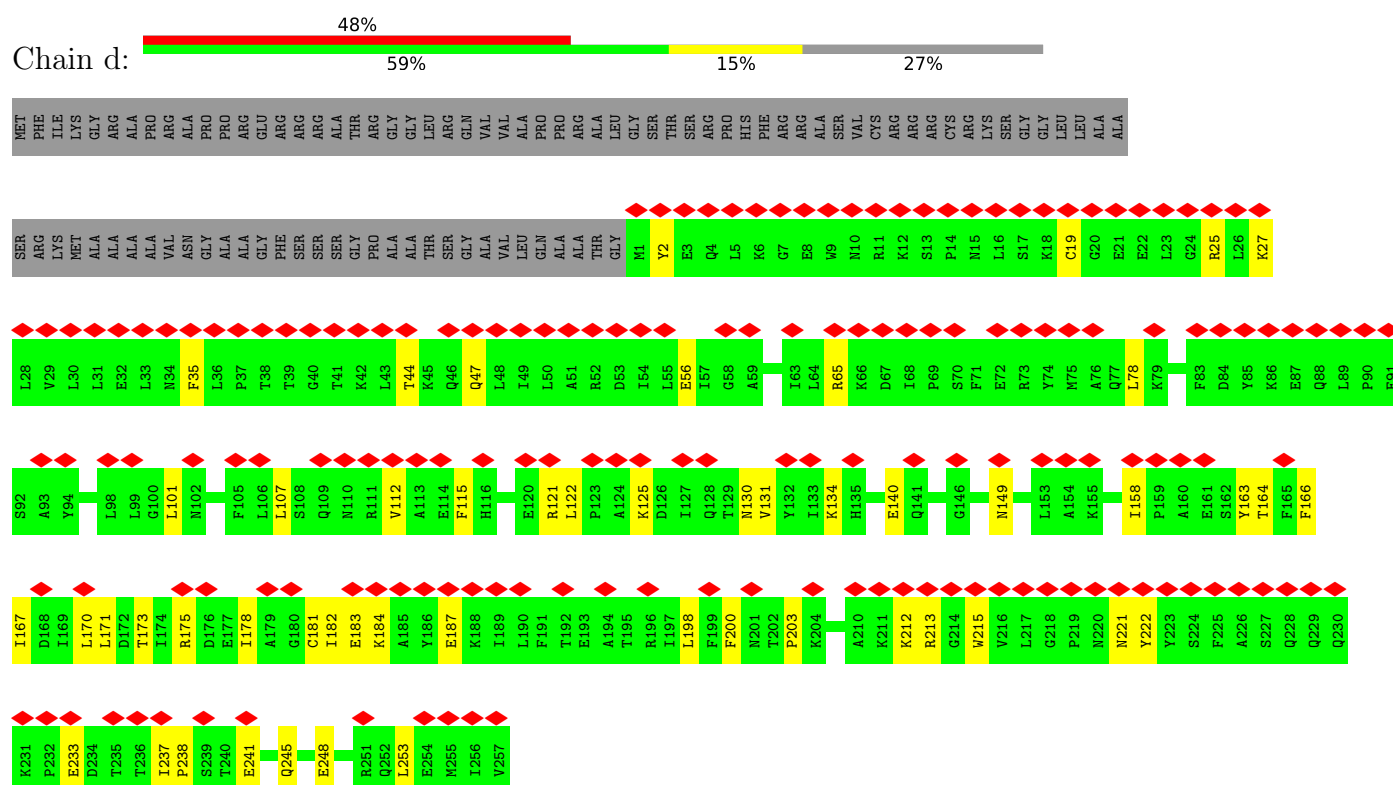
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11



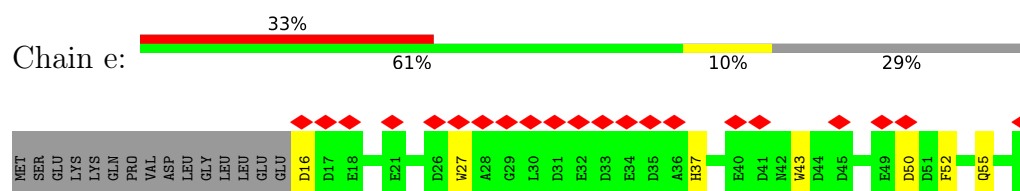
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6



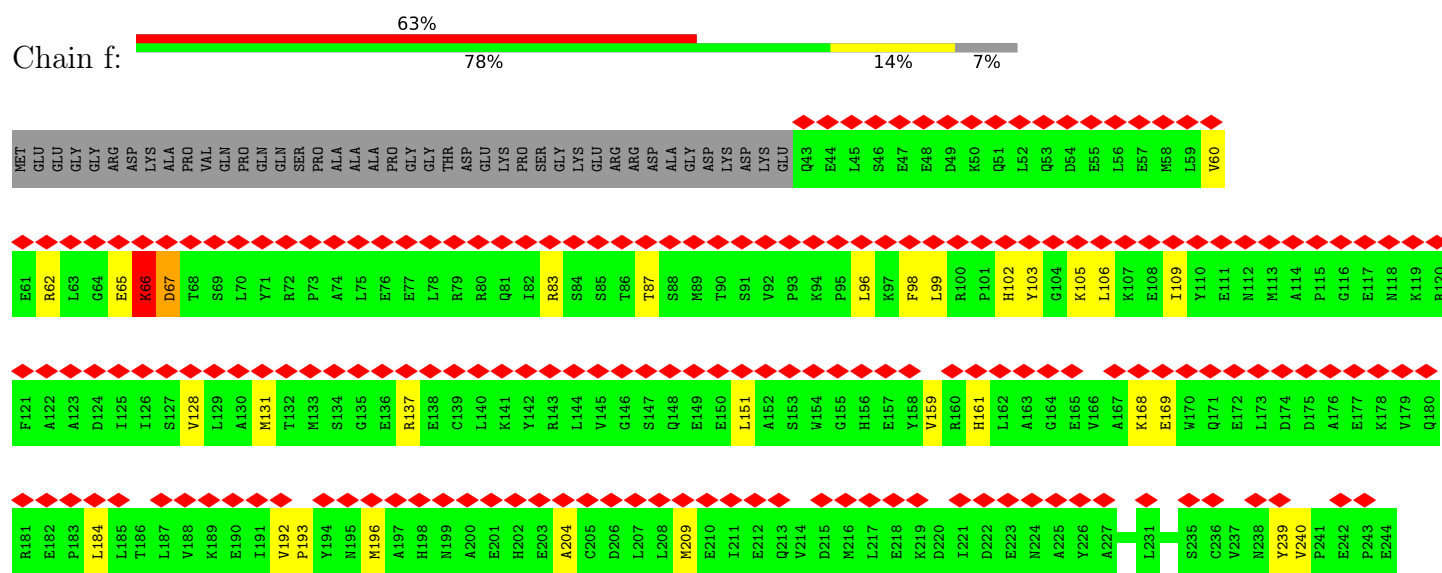


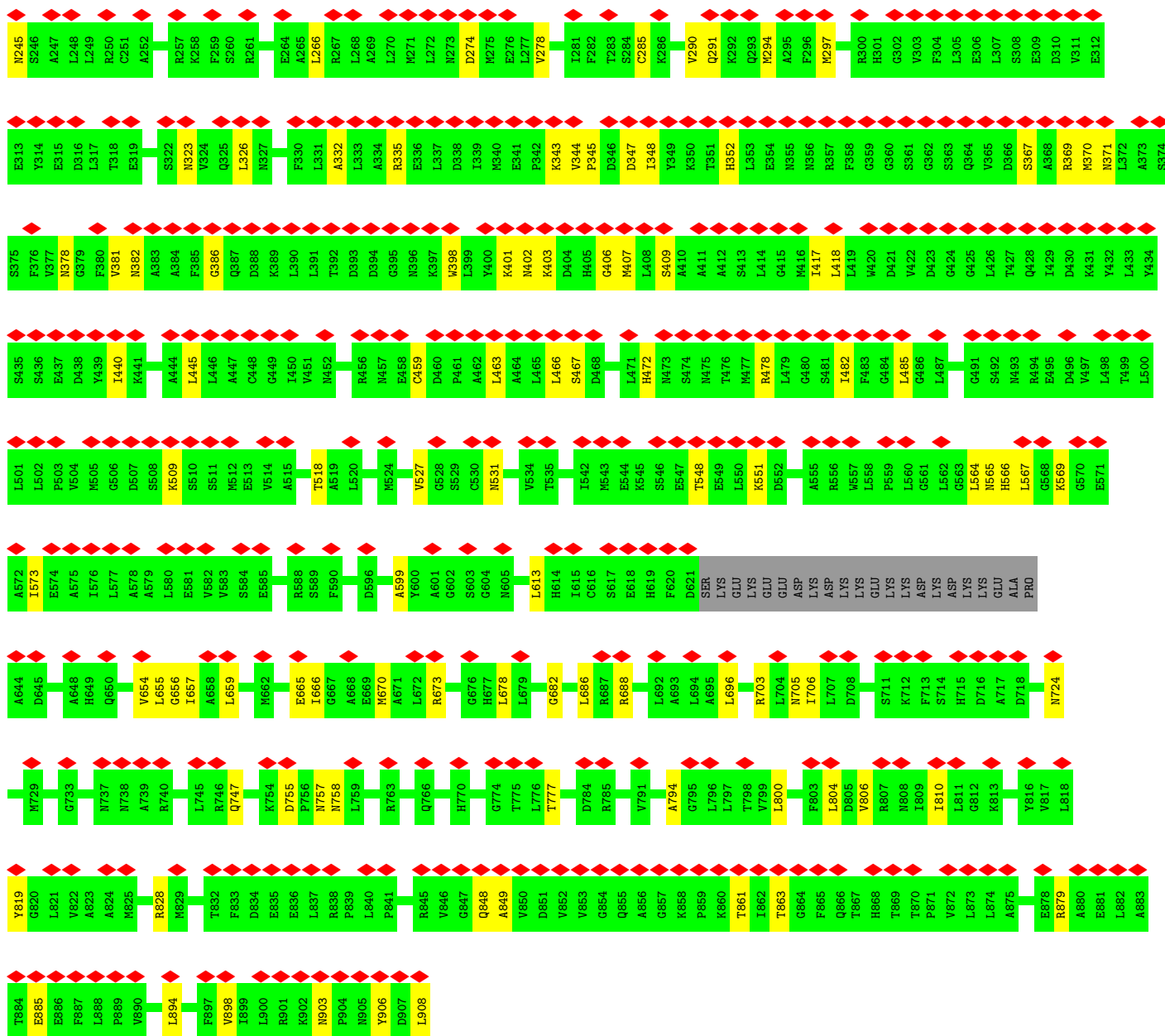


• Molecule 31: 26S proteasome complex subunit SEM1

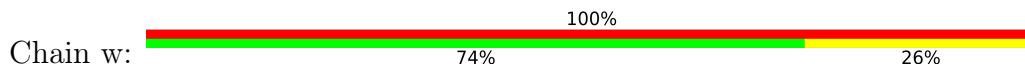


• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2





### • Molecule 33: Ubiquitin



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24241	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 ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.023	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00601	Depositor
Map size (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, 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	0.20	0/3294	0.59	2/4447 (0.0%)
2	B	0.21	0/3086	0.51	0/4164
3	C	0.23	0/2902	0.52	0/3904
4	D	0.28	0/3089	0.54	0/4168
5	E	0.19	0/2904	0.51	0/3924
6	F	0.17	0/2896	0.48	0/3912
7	G	0.16	0/1923	0.45	0/2601
7	g	0.20	0/1914	0.46	0/2590
8	H	0.16	0/1844	0.43	0/2499
8	h	0.20	0/1844	0.41	0/2497
9	I	0.23	0/1985	0.48	0/2677
9	i	0.17	0/1985	0.46	0/2677
10	J	0.18	0/1906	0.48	0/2573
10	j	0.16	0/1887	0.44	0/2549
11	K	0.16	0/1804	0.40	0/2436
11	k	0.12	0/1809	0.35	0/2444
12	L	0.15	0/1901	0.38	0/2570
12	l	0.14	0/1896	0.41	0/2565
13	M	0.14	0/1911	0.39	0/2573
13	m	0.13	0/1916	0.37	0/2580
14	N	0.14	0/1540	0.35	0/2085
14	n	0.14	0/1536	0.35	0/2080
15	O	0.16	0/1676	0.41	0/2271
15	o	0.16	0/1686	0.43	0/2282
16	P	0.16	0/1616	0.46	0/2180
16	p	0.17	0/1620	0.45	0/2184
17	Q	0.14	0/1621	0.42	2/2194 (0.1%)
17	q	0.14	0/1621	0.37	0/2194
18	R	0.16	0/1590	0.42	0/2147
18	r	0.15	0/1590	0.39	0/2147
19	S	0.15	0/1671	0.45	0/2252
19	s	0.18	0/1684	0.45	0/2268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
20	T	0.15	0/1716	0.38	0/2323
20	t	0.15	0/1720	0.39	0/2328
21	U	0.16	0/6903	0.48	2/9324 (0.0%)
22	V	0.16	0/3824	0.42	0/5170
23	W	0.16	0/3644	0.43	0/4901
24	X	0.18	0/3381	0.48	0/4558
25	Y	0.17	0/3261	0.48	3/4393 (0.1%)
26	Z	0.21	0/2324	0.56	0/3150
27	a	0.22	0/3053	0.61	4/4133 (0.1%)
28	b	0.22	0/1478	0.61	0/2001
29	c	0.26	0/2302	0.63	0/3110
30	d	0.21	0/2162	0.55	0/2919
31	e	0.20	0/437	0.62	0/595
32	f	0.18	0/6640	0.47	0/8988
33	w	0.13	0/607	0.36	0/816
All	All	0.18	0/107599	0.47	13/145343 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	LEU	CA-C-N	10.85	135.21	120.67
1	A	327	LEU	C-N-CA	10.85	135.21	120.67
17	Q	23	SER	CA-C-N	6.53	134.00	121.54
17	Q	23	SER	C-N-CA	6.53	134.00	121.54
27	a	146	PRO	CA-N-CD	-5.52	104.27	112.00
27	a	135	ILE	CA-C-N	-5.34	111.69	121.52
27	a	135	ILE	C-N-CA	-5.34	111.69	121.52
21	U	95	GLU	CA-C-N	5.23	128.67	120.82
21	U	95	GLU	C-N-CA	5.23	128.67	120.82
25	Y	91	ALA	CA-C-N	-5.14	112.15	121.14
25	Y	91	ALA	C-N-CA	-5.14	112.15	121.14
27	a	146	PRO	N-CD-CG	-5.07	95.60	103.20
25	Y	92	GLU	N-CA-CB	5.02	118.58	110.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3240	0	3287	53	0
2	B	3042	0	3101	53	0
3	C	2864	0	2971	47	0
4	D	3039	0	3076	80	0
5	E	2860	0	2828	59	0
6	F	2858	0	2853	44	0
7	G	1889	0	1885	14	0
7	g	1880	0	1875	23	0
8	H	1805	0	1784	15	0
8	h	1805	0	1798	25	0
9	I	1955	0	1955	11	0
9	i	1955	0	1955	7	0
10	J	1880	0	1892	25	0
10	j	1861	0	1865	16	0
11	K	1777	0	1762	13	0
11	k	1782	0	1766	15	0
12	L	1866	0	1852	11	0
12	l	1861	0	1839	16	0
13	M	1876	0	1861	10	0
13	m	1881	0	1868	13	0
14	N	1514	0	1487	13	0
14	n	1510	0	1483	6	0
15	O	1649	0	1659	12	0
15	o	1659	0	1681	14	0
16	P	1587	0	1598	14	0
16	p	1591	0	1609	18	0
17	Q	1588	0	1584	20	0
17	q	1588	0	1584	17	0
18	R	1559	0	1523	14	0
18	r	1559	0	1523	10	0
19	S	1641	0	1639	10	0
19	s	1654	0	1656	18	0
20	T	1683	0	1662	14	0
20	t	1687	0	1666	17	0
21	U	6787	0	6858	103	0
22	V	3754	0	3749	45	0
23	W	3596	0	3713	35	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	X	3335	0	3435	35	0
25	Y	3202	0	3204	28	0
26	Z	2281	0	2312	60	0
27	a	2995	0	3012	45	0
28	b	1458	0	1505	27	0
29	c	2260	0	2276	45	0
30	d	2116	0	2146	41	0
31	e	425	0	328	7	0
32	f	6529	0	6541	86	0
33	w	601	0	629	12	0
34	A	31	0	12	2	0
34	B	31	0	12	1	0
34	D	31	0	12	2	0
34	E	31	0	12	1	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	D	1	0	0	0	0
35	E	1	0	0	0	0
35	F	1	0	0	0	0
36	C	27	0	12	1	0
36	F	27	0	12	1	0
37	c	1	0	0	0	0
All	All	105968	0	106207	1122	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.

All (1122) 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)
29:c:197:ASN:HB2	29:c:198:ARG:CZ	1.90	1.02
29:c:197:ASN:HB2	29:c:198:ARG:NH2	1.74	1.01
4:D:154:LEU:HB2	4:D:158:GLN:HG3	1.43	0.96
1:A:274:PHE:HB2	1:A:319:MET:HG2	1.60	0.83
29:c:191:ALA:HB1	29:c:196:LEU:HD13	1.63	0.79
4:D:154:LEU:HB2	4:D:158:GLN:CG	2.13	0.78
3:C:89:VAL:HB	3:C:92:GLU:HB3	1.64	0.78
10:J:220:LEU:HD11	10:J:224:GLU:HB3	1.67	0.76
29:c:197:ASN:CB	29:c:198:ARG:NH2	2.52	0.71
30:d:178:ILE:O	30:d:182:ILE:HB	1.90	0.71
32:f:666:ILE:HG22	32:f:670:MET:HE1	1.73	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:41:LYS:HD2	12:l:42:THR:HG23	1.74	0.70
30:d:183:GLU:HA	30:d:215:TRP:HE1	1.57	0.69
10:J:204:LYS:HD2	10:J:222:PRO:HB3	1.74	0.69
7:g:130:GLU:HG2	8:h:5:GLY:HA2	1.73	0.69
24:X:314:ARG:HH22	24:X:320:SER:HB3	1.58	0.69
3:C:90:HIS:CG	3:C:91:PRO:HD3	2.28	0.68
1:A:297:ARG:HH12	6:F:306:VAL:HG21	1.58	0.68
2:B:74:MET:HE1	32:f:613:LEU:HD12	1.76	0.68
9:I:143:TYR:HB2	9:I:146:GLN:HE21	1.59	0.68
3:C:90:HIS:CE1	4:D:110:ASN:H	2.11	0.67
24:X:398:GLU:OE1	25:Y:365:GLN:NE2	2.28	0.67
8:h:3:GLU:N	13:m:125:TYR:HB3	2.10	0.67
19:s:8:ASN:ND2	19:s:31:GLU:OE2	2.27	0.67
32:f:402:ASN:HB2	32:f:407:MET:HB3	1.77	0.67
5:E:281:ARG:HB3	5:E:386:TYR:CD2	2.31	0.66
18:R:44:THR:HB	18:R:100:MET:H	1.60	0.66
24:X:332:GLU:HG2	24:X:368:MET:HE1	1.77	0.66
6:F:224:LEU:HB2	6:F:348:LEU:HD23	1.77	0.66
29:c:197:ASN:CB	29:c:198:ARG:CZ	2.70	0.66
5:E:198:VAL:HG12	5:E:200:SER:H	1.60	0.66
3:C:90:HIS:HE1	4:D:110:ASN:H	1.44	0.66
1:A:101:ILE:HD11	1:A:111:TYR:HB3	1.78	0.65
27:a:14:SER:HB2	27:a:18:GLN:HG2	1.77	0.65
32:f:102:HIS:HB3	32:f:105:LYS:HE3	1.77	0.65
23:W:190:MET:HE2	23:W:206:SER:HA	1.78	0.65
7:g:2:SER:C	7:g:4:GLY:H	2.04	0.65
21:U:328:ILE:HG13	21:U:329:LEU:HG	1.78	0.65
4:D:150:SER:HB3	4:D:228:ILE:HG23	1.79	0.64
1:A:119:ALA:HB2	6:F:128:THR:HG23	1.80	0.64
4:D:335:LEU:HD11	4:D:371:SER:HA	1.80	0.64
21:U:509:GLY:HA3	21:U:544:ILE:HG22	1.78	0.64
19:S:159:GLN:NE2	15:o:207:GLY:O	2.31	0.64
3:C:44:ARG:O	22:V:495:ARG:NH1	2.31	0.63
23:W:373:ILE:HD11	23:W:377:ARG:HG2	1.79	0.63
19:S:148:LEU:HD23	19:S:178:VAL:HG12	1.81	0.63
26:Z:111:LEU:O	26:Z:114:ARG:NH1	2.30	0.62
26:Z:128:PRO:HG3	29:c:216:MET:HB3	1.80	0.62
23:W:401:THR:HG23	23:W:402:ILE:HD12	1.82	0.62
16:p:27:ARG:HB2	16:p:183:MET:HB2	1.80	0.62
15:O:63:LEU:HD11	15:O:79:ALA:HB2	1.81	0.62
3:C:196:LYS:NZ	3:C:295:THR:O	2.32	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:46:ARG:NH2	29:c:147:PRO:O	2.33	0.62
23:W:140:ILE:HG12	23:W:177:MET:HB3	1.81	0.62
21:U:234:GLU:HG2	21:U:238:LYS:HE3	1.80	0.62
26:Z:9:VAL:HG12	26:Z:48:LEU:HD23	1.82	0.61
32:f:459:CYS:HB3	33:w:66:THR:HB	1.82	0.61
5:E:122:MET:HE1	5:E:218:MET:HE2	1.82	0.61
19:s:4:PRO:O	20:t:100:ARG:NH2	2.32	0.61
19:s:27:THR:HB	19:s:40:SER:H	1.65	0.61
19:s:148:LEU:HD23	19:s:178:VAL:HG12	1.82	0.61
3:C:90:HIS:ND1	3:C:91:PRO:HD3	2.15	0.61
3:C:90:HIS:CD2	3:C:90:HIS:H	2.15	0.61
13:M:34:SER:HG	13:M:65:ARG:HH12	1.48	0.61
28:b:25:ARG:NH2	28:b:145:GLU:OE1	2.25	0.61
24:X:71:LYS:HG2	24:X:74:ARG:HH12	1.66	0.61
28:b:157:VAL:HG21	28:b:170:LEU:HB2	1.81	0.61
32:f:103:TYR:HA	32:f:106:LEU:HB2	1.83	0.61
23:W:47:LEU:HD22	23:W:66:ILE:HG23	1.83	0.60
26:Z:136:GLU:OE2	26:Z:157:HIS:ND1	2.34	0.60
26:Z:73:ASP:H	28:b:63:THR:HG21	1.66	0.60
27:a:112:ILE:HB	27:a:151:VAL:HG21	1.84	0.60
4:D:266:GLU:HG3	5:E:258:MET:HB3	1.83	0.60
33:w:22:THR:HG22	33:w:55:THR:HG22	1.82	0.60
5:E:265:ASP:OD2	5:E:291:ARG:NH2	2.34	0.60
11:k:210:LEU:HA	11:k:214:ASN:HD21	1.66	0.60
25:Y:237:ARG:HH12	25:Y:242:LYS:HE3	1.65	0.60
2:B:59:ARG:NH1	32:f:209:MET:SD	2.75	0.60
4:D:353:ASN:ND2	4:D:392:TYR:O	2.34	0.60
24:X:203:PRO:HB2	24:X:207:GLN:HB2	1.82	0.60
16:p:35:VAL:HG12	16:p:36:THR:HG23	1.83	0.60
1:A:55:LEU:HD11	2:B:76:GLU:HG2	1.83	0.60
27:a:227:ASN:O	27:a:231:GLN:NE2	2.35	0.60
8:H:111:VAL:HG22	8:H:136:ILE:HD12	1.83	0.59
9:I:53:HIS:CG	9:I:54:LYS:H	2.19	0.59
1:A:186:LYS:HE3	1:A:341:ILE:HG22	1.84	0.59
8:H:177:ARG:HH22	24:X:161:ASP:H	1.48	0.59
20:T:25:ASP:HA	20:T:187:PHE:HA	1.84	0.59
21:U:628:ARG:NH1	21:U:749:GLN:OE1	2.36	0.59
26:Z:97:THR:HG23	26:Z:99:PRO:HD3	1.83	0.59
30:d:178:ILE:HD11	30:d:198:LEU:HD11	1.84	0.59
11:K:20:ARG:NE	11:K:25:GLU:OE1	2.33	0.59
26:Z:109:ASN:ND2	26:Z:140:SER:OG	2.35	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:THR:HA	2:B:216:ILE:HD11	1.85	0.59
2:B:84:GLN:NE2	21:U:825:LYS:O	2.35	0.59
32:f:777:THR:HB	32:f:828:ARG:HD2	1.85	0.59
16:p:58:THR:O	17:q:85:ARG:NH2	2.36	0.59
22:V:306:ARG:HH12	22:V:332:LEU:HB2	1.66	0.59
10:j:38:ARG:NH1	10:j:182:GLU:O	2.34	0.59
21:U:440:GLY:HA2	21:U:473:VAL:HG13	1.85	0.58
18:r:32:LYS:NZ	18:r:34:VAL:O	2.35	0.58
30:d:19:CYS:SG	30:d:65:ARG:NH2	2.76	0.58
1:A:307:ASP:OD2	1:A:333:ARG:NH2	2.36	0.58
27:a:165:THR:HG22	27:a:166:ILE:H	1.69	0.58
15:o:63:LEU:HD11	15:o:79:ALA:HB2	1.84	0.58
4:D:152:MET:O	4:D:153:MET:HB2	2.03	0.58
11:K:203:LYS:HB2	11:K:210:LEU:HD22	1.84	0.58
1:A:148:GLN:NE2	1:A:150:HIS:CE1	2.71	0.58
26:Z:138:TYR:HA	26:Z:157:HIS:HA	1.85	0.58
27:a:255:TRP:O	27:a:258:GLN:NE2	2.37	0.58
5:E:245:GLU:OE1	5:E:251:ARG:NE	2.29	0.58
5:E:282:PRO:HD2	5:E:386:TYR:HB3	1.85	0.58
27:a:70:ARG:HE	28:b:17:ARG:HD2	1.68	0.58
27:a:119:GLY:HA3	27:a:158:LEU:HD11	1.85	0.58
2:B:221:GLY:HA3	2:B:347:ILE:HA	1.86	0.58
2:B:369:THR:HA	2:B:372:MET:HE3	1.86	0.58
3:C:60:ARG:NH2	4:D:71:GLU:OE2	2.37	0.58
28:b:17:ARG:HG2	28:b:80:PRO:HG2	1.83	0.58
4:D:400:GLU:OE2	4:D:404:LYS:NZ	2.38	0.57
21:U:522:GLY:O	21:U:559:ARG:NH2	2.37	0.57
22:V:494:MET:SD	26:Z:278:ASN:ND2	2.77	0.57
3:C:340:ARG:HE	25:Y:6:LEU:HD13	1.69	0.57
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.86	0.57
16:P:65:GLN:OE1	17:Q:86:ARG:NH2	2.38	0.57
23:W:325:GLY:O	23:W:329:ARG:HB2	2.05	0.57
3:C:29:GLU:OE1	22:V:201:ARG:NH2	2.36	0.57
6:F:318:ASP:HB3	6:F:347:ARG:HG2	1.87	0.57
26:Z:244:GLU:HA	26:Z:247:LYS:HE2	1.87	0.57
2:B:358:GLU:HG3	10:J:200:GLN:HE21	1.70	0.57
4:D:338:ARG:NH1	4:D:364:VAL:O	2.38	0.57
9:I:161:ALA:HB1	9:I:175:LEU:HD13	1.87	0.57
20:T:43:MET:HG3	20:T:64:LYS:HG3	1.86	0.57
22:V:497:PRO:HG2	26:Z:278:ASN:HB3	1.87	0.57
22:V:306:ARG:HH11	22:V:336:GLU:HG3	1.70	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:478:ARG:HH12	32:f:509:LYS:HD2	1.70	0.57
17:q:168:GLN:NE2	17:q:175:LEU:O	2.38	0.57
9:I:52:ILE:O	9:I:53:HIS:C	2.47	0.57
22:V:349:ARG:NH2	31:e:37:HIS:O	2.33	0.57
9:i:119:GLN:NE2	10:j:79:ASP:OD1	2.38	0.57
13:M:34:SER:OG	13:M:65:ARG:NH1	2.35	0.56
18:R:39:PRO:HA	18:R:184:TRP:HE1	1.70	0.56
26:Z:10:VAL:HG13	26:Z:163:GLY:HA3	1.87	0.56
11:k:221:GLN:HB2	11:k:224:GLN:HG2	1.86	0.56
18:R:192:VAL:HG11	16:p:205:ASP:HB3	1.86	0.56
23:W:285:ASP:HA	23:W:288:HIS:CE1	2.40	0.56
30:d:2:TYR:O	30:d:25:ARG:NH2	2.38	0.56
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.87	0.56
6:F:421:MET:HA	6:F:424:ILE:HD12	1.85	0.56
21:U:158:ARG:NH2	21:U:192:GLN:OE1	2.39	0.56
26:Z:189:GLN:HA	26:Z:192:THR:HG22	1.87	0.56
32:f:655:LEU:HD11	32:f:800:LEU:HD13	1.86	0.56
7:g:5:SER:HB3	7:g:23:TYR:OH	2.04	0.56
7:g:43:ARG:HH21	7:g:164:LYS:HG2	1.70	0.56
3:C:47:ALA:HB3	22:V:495:ARG:HH22	1.71	0.56
5:E:123:SER:O	5:E:197:LYS:NZ	2.38	0.56
10:J:50:VAL:HB	10:J:54:GLN:HB2	1.87	0.56
20:T:25:ASP:OD1	20:T:41:ARG:NH2	2.38	0.56
25:Y:188:CYS:SG	25:Y:196:GLN:NE2	2.78	0.56
1:A:284:ARG:O	6:F:334:ARG:NH1	2.38	0.56
23:W:240:TYR:HA	23:W:243:ILE:HD12	1.88	0.56
34:E:401:ATP:O3G	6:F:347:ARG:NH2	2.38	0.56
22:V:442:ILE:HD13	30:d:184:LYS:HZ1	1.71	0.56
4:D:342:ARG:HB3	4:D:364:VAL:HG11	1.88	0.56
10:J:220:LEU:HD13	10:J:225:ILE:HG13	1.88	0.56
14:N:165:GLU:OE2	20:t:37:ARG:NH1	2.39	0.56
27:a:33:LEU:HD13	27:a:36:GLN:HB2	1.87	0.56
2:B:141:LYS:HA	2:B:144:LEU:HD23	1.88	0.56
4:D:83:GLN:HB3	4:D:140:VAL:CG1	2.36	0.56
24:X:16:LEU:O	24:X:20:ARG:NH1	2.39	0.56
21:U:542:GLU:OE1	21:U:546:ARG:NH1	2.39	0.55
22:V:178:SER:O	22:V:180:ARG:NH1	2.39	0.55
25:Y:301:ILE:HG13	25:Y:343:LEU:HD12	1.87	0.55
24:X:1:MET:HE1	24:X:35:ILE:HG12	1.88	0.55
24:X:106:GLU:HB3	24:X:136:LEU:HD21	1.88	0.55
1:A:293:ASN:O	1:A:297:ARG:NE	2.39	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:GLN:O	2:B:241:ASN:ND2	2.40	0.55
25:Y:12:PRO:O	25:Y:146:ARG:NH1	2.40	0.55
28:b:1:MET:SD	28:b:2:VAL:N	2.79	0.55
8:h:175:GLU:OE2	9:i:53:HIS:NE2	2.35	0.55
16:p:65:GLN:OE1	17:q:86:ARG:NH2	2.39	0.55
2:B:317:ASP:HB2	2:B:346:ARG:HG2	1.88	0.55
17:Q:38:MET:O	17:Q:65:GLN:NE2	2.39	0.55
32:f:285:CYS:O	32:f:291:GLN:NE2	2.39	0.55
32:f:345:PRO:HA	32:f:348:ILE:HD12	1.88	0.55
1:A:364:VAL:HG12	1:A:404:ALA:HB3	1.86	0.55
10:J:96:LEU:HD13	17:Q:62:LYS:HB2	1.89	0.55
8:h:95:GLN:NE2	15:o:64:GLU:OE2	2.35	0.55
10:J:221:ASN:HD21	10:J:223:GLU:HB3	1.71	0.55
32:f:151:LEU:HB3	32:f:159:VAL:HG22	1.88	0.55
14:n:4:MET:HG3	14:n:127:ILE:HG22	1.88	0.55
3:C:248:MET:HE2	3:C:269:VAL:HG13	1.88	0.55
23:W:74:CYS:SG	23:W:86:ASN:ND2	2.79	0.55
12:l:189:LYS:HD2	12:l:236:LEU:HD13	1.89	0.55
2:B:133:VAL:HG11	2:B:157:HIS:HB2	1.89	0.55
10:J:220:LEU:CD1	10:J:224:GLU:HB3	2.37	0.55
7:g:158:GLY:O	8:h:84:ARG:NH2	2.40	0.55
1:A:148:GLN:HE22	1:A:150:HIS:CE1	2.25	0.54
4:D:167:ILE:HG12	4:D:214:MET:HE3	1.89	0.54
15:O:163:ILE:HG12	15:O:170:GLY:HA2	1.87	0.54
21:U:834:SER:HB2	21:U:836:THR:HG23	1.88	0.54
33:w:6:LYS:HA	33:w:12:THR:HA	1.89	0.54
1:A:347:ASP:O	1:A:351:ARG:NH1	2.41	0.54
10:j:146:GLN:OE1	10:j:159:ASN:ND2	2.40	0.54
12:l:120:THR:O	13:m:129:ARG:NH1	2.41	0.54
4:D:267:ILE:HD11	4:D:309:MET:HB3	1.89	0.54
27:a:33:LEU:HA	28:b:18:ASN:HD22	1.72	0.54
15:o:146:MET:HE1	15:o:154:LEU:HD22	1.88	0.54
3:C:86:LEU:HD21	3:C:94:LYS:HD3	1.89	0.54
9:i:234:GLU:HA	9:i:237:ILE:HG12	1.90	0.54
4:D:86:PRO:HB2	4:D:134:LYS:HD2	1.90	0.54
7:G:120:ASP:OD1	8:H:84:ARG:NH1	2.41	0.54
23:W:68:VAL:HG12	23:W:72:LYS:HE2	1.89	0.54
4:D:368:ASP:O	4:D:370:ILE:HD12	2.08	0.54
7:G:158:GLY:O	8:H:84:ARG:NH2	2.40	0.54
11:k:141:LEU:H	11:k:156:MET:HB3	1.71	0.54
5:E:199:VAL:HG23	5:E:201:SER:H	1.73	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:94:ILE:HD11	6:F:125:LYS:HB2	1.88	0.54
11:K:166:ASP:OD2	11:K:187:LYS:NZ	2.40	0.54
19:S:209:SER:OG	19:S:212:LYS:NZ	2.40	0.54
30:d:241:GLU:OE2	30:d:245:GLN:NE2	2.41	0.54
20:t:27:LEU:HD22	20:t:184:TYR:HB2	1.89	0.54
1:A:161:VAL:HA	1:A:164:MET:HE3	1.89	0.54
19:s:204:ARG:NH1	19:s:206:GLU:OE2	2.40	0.54
6:F:141:ASP:OD1	6:F:144:LYS:NZ	2.38	0.54
17:Q:27:GLN:O	17:q:170:ARG:NH1	2.40	0.54
23:W:375:MET:HA	23:W:378:MET:HE2	1.90	0.54
32:f:567:LEU:O	32:f:569:LYS:NZ	2.40	0.54
2:B:181:GLN:HG2	2:B:237:LYS:HE2	1.90	0.54
9:I:86:LEU:HD22	9:I:114:LEU:HD11	1.90	0.54
11:K:52:LYS:NZ	11:K:64:ILE:O	2.41	0.54
20:T:27:LEU:HD22	20:T:184:TYR:HB2	1.90	0.54
21:U:900:TYR:HB3	21:U:914:LEU:HG	1.90	0.54
23:W:409:LEU:HD23	24:X:344:ARG:HH21	1.73	0.54
25:Y:298:GLU:O	25:Y:302:HIS:ND1	2.32	0.54
32:f:659:LEU:HB3	32:f:696:LEU:HD21	1.89	0.54
8:H:213:CYS:HB2	8:H:218:PHE:HD1	1.73	0.53
21:U:243:LEU:HG	21:U:913:ILE:HG12	1.90	0.53
24:X:255:LEU:HD22	24:X:267:VAL:HG13	1.90	0.53
1:A:283:ALA:O	1:A:296:GLN:NE2	2.41	0.53
3:C:125:LYS:HZ2	4:D:96:VAL:HG11	1.73	0.53
4:D:153:MET:O	4:D:155:THR:N	2.40	0.53
10:J:96:LEU:HD11	17:Q:58:GLU:HB3	1.89	0.53
20:T:63:LEU:HD21	20:T:106:LEU:HD13	1.90	0.53
21:U:99:THR:HG23	22:V:240:LEU:HD13	1.90	0.53
21:U:772:TRP:HB3	21:U:775:LEU:HB2	1.89	0.53
4:D:117:SER:HA	4:D:121:ARG:HH22	1.72	0.53
15:O:146:MET:HE1	15:O:154:LEU:HD22	1.90	0.53
28:b:14:GLU:O	28:b:17:ARG:NH2	2.41	0.53
29:c:69:VAL:O	29:c:208:ARG:NH2	2.41	0.53
29:c:163:ILE:HG12	29:c:174:PRO:HG3	1.91	0.53
33:w:40:GLN:HG2	33:w:72:ARG:HB3	1.89	0.53
2:B:273:VAL:HA	2:B:276:GLU:HG2	1.91	0.53
5:E:232:MET:HB3	5:E:277:MET:HG2	1.90	0.53
10:J:101:PRO:HG2	10:J:138:PHE:HE2	1.74	0.53
27:a:281:THR:HG21	27:a:333:MET:HE2	1.91	0.53
17:Q:144:ASP:OD2	18:r:166:ARG:NH2	2.42	0.53
7:g:80:MET:HE3	7:g:138:MET:HB2	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:358:ASN:O	6:F:362:ARG:NH1	2.41	0.53
22:V:289:LEU:HB3	22:V:312:ALA:HB2	1.91	0.53
12:l:122:ARG:HE	13:m:128:VAL:HG12	1.74	0.53
13:m:34:SER:OG	13:m:65:ARG:NH1	2.37	0.53
5:E:253:ILE:HG13	6:F:308:ARG:HH22	1.74	0.53
26:Z:234:PHE:HE2	27:a:349:MET:HG2	1.73	0.53
19:s:145:LEU:HD22	19:s:178:VAL:HB	1.91	0.53
4:D:67:ASN:ND2	21:U:607:VAL:O	2.41	0.53
13:M:37:ILE:HD11	13:M:193:VAL:HG13	1.90	0.53
5:E:213:ARG:HG2	5:E:216:ARG:HH22	1.74	0.53
21:U:497:LEU:HB3	21:U:516:LEU:HD22	1.90	0.53
24:X:377:ILE:HB	25:Y:358:ARG:HH12	1.74	0.53
3:C:61:GLU:OE2	3:C:64:GLN:NE2	2.42	0.52
9:I:53:HIS:CG	9:I:54:LYS:N	2.76	0.52
31:e:50:ASP:OD1	31:e:55:GLN:NE2	2.35	0.52
8:H:222:THR:OG1	8:H:225:GLU:OE1	2.23	0.52
16:P:145:GLN:HE22	19:s:143:ALA:HB1	1.73	0.52
22:V:258:TYR:HE2	22:V:270:LEU:HD12	1.74	0.52
22:V:450:SER:OG	22:V:451:ILE:N	2.39	0.52
27:a:370:GLN:NE2	30:d:248:GLU:OE2	2.42	0.52
30:d:171:LEU:HD22	30:d:175:ARG:HH12	1.74	0.52
32:f:398:TRP:HA	32:f:401:LYS:HD3	1.91	0.52
30:d:175:ARG:HH21	30:d:198:LEU:HD22	1.73	0.52
2:B:196:GLU:OE2	2:B:349:ARG:NH1	2.42	0.52
3:C:89:VAL:O	3:C:90:HIS:C	2.52	0.52
6:F:318:ASP:OD2	6:F:344:ARG:NH2	2.42	0.52
26:Z:48:LEU:HD21	26:Z:120:VAL:HG11	1.91	0.52
27:a:197:ALA:HB2	27:a:222:LEU:HD22	1.90	0.52
32:f:849:ALA:HB2	32:f:879:ARG:HB2	1.90	0.52
1:A:116:LYS:HE3	2:B:130:GLU:H	1.75	0.52
21:U:906:LEU:HD13	21:U:912:ILE:HD13	1.92	0.52
30:d:215:TRP:HE3	30:d:222:TYR:HB3	1.74	0.52
32:f:894:LEU:HA	32:f:898:VAL:HG21	1.90	0.52
12:l:185:ASN:OD1	12:l:189:LYS:NZ	2.42	0.52
16:p:7:ASN:ND2	16:p:29:GLY:O	2.32	0.52
6:F:97:LEU:HB2	6:F:121:CYS:HB2	1.91	0.52
8:H:166:ASN:OD1	8:H:169:ASN:ND2	2.35	0.52
9:I:21:VAL:HG12	9:I:25:MET:HE1	1.92	0.52
26:Z:17:LEU:HD22	29:c:36:LEU:HB3	1.90	0.52
27:a:286:ALA:HA	27:a:289:ARG:HE	1.74	0.52
30:d:56:GLU:HA	30:d:78:LEU:HD11	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:LEU:HA	2:B:237:LYS:HD3	1.91	0.52
4:D:124:LEU:C	4:D:126:PRO:HD2	2.35	0.52
5:E:281:ARG:HB3	5:E:386:TYR:CE2	2.45	0.52
21:U:707:ASN:HA	21:U:710:ARG:HB2	1.92	0.52
34:A:501:ATP:O1G	2:B:343:ARG:NH2	2.43	0.52
26:Z:94:TRP:HB3	26:Z:112:MET:HE3	1.91	0.52
32:f:266:LEU:HD11	32:f:278:VAL:HG13	1.91	0.52
10:j:109:ARG:NH2	18:r:70:ASN:OD1	2.42	0.52
17:Q:68:LYS:HD3	17:Q:74:GLU:HG2	1.91	0.52
1:A:366:ARG:NH1	32:f:906:TYR:OH	2.43	0.52
3:C:57:ARG:NH1	21:U:642:GLU:OE1	2.43	0.51
6:F:198:LEU:HD13	6:F:236:LEU:HD13	1.92	0.51
27:a:34:TRP:HZ3	27:a:64:ILE:HG23	1.74	0.51
11:k:167:ALA:HB3	12:l:56:LEU:HD13	1.92	0.51
17:q:25:ILE:HG22	17:q:26:VAL:HG13	1.92	0.51
21:U:898:CYS:SG	21:U:899:ARG:N	2.83	0.51
28:b:24:THR:HB	28:b:27:GLN:NE2	2.24	0.51
32:f:548:THR:HA	32:f:551:LYS:HE3	1.92	0.51
11:k:41:GLN:NE2	11:k:151:PRO:O	2.43	0.51
8:H:93:LEU:HD13	8:H:113:ARG:HB3	1.91	0.51
16:P:177:ARG:NH2	19:s:150:ASP:OD2	2.40	0.51
24:X:376:GLY:O	25:Y:358:ARG:NH2	2.44	0.51
32:f:371:ASN:ND2	32:f:401:LYS:O	2.43	0.51
18:r:87:VAL:HG11	18:r:97:MET:HE1	1.92	0.51
10:J:220:LEU:HD11	10:J:224:GLU:OE1	2.10	0.51
21:U:27:LEU:HD13	21:U:63:VAL:HG11	1.93	0.51
21:U:599:ILE:HD13	21:U:625:ILE:HD11	1.92	0.51
5:E:171:LEU:HD22	5:E:295:LEU:HD13	1.91	0.51
12:L:72:ILE:HG22	12:L:134:ILE:HG12	1.92	0.51
21:U:700:GLU:H	21:U:706:VAL:HG21	1.75	0.51
22:V:212:TYR:HA	22:V:253:LEU:HD11	1.93	0.51
25:Y:210:SER:HB3	25:Y:213:LEU:HD23	1.92	0.51
32:f:531:ASN:O	32:f:565:ASN:ND2	2.43	0.51
32:f:654:VAL:HA	32:f:657:ILE:HD12	1.93	0.51
16:p:149:MET:HE1	16:p:173:ASN:HB2	1.93	0.51
21:U:490:ARG:HH11	21:U:491:GLN:H	1.59	0.51
26:Z:135:THR:HG21	26:Z:162:ILE:HD11	1.93	0.51
30:d:198:LEU:HD12	30:d:200:PHE:HE2	1.75	0.51
2:B:135:ILE:HG22	2:B:139:VAL:HG11	1.92	0.51
3:C:226:GLU:OE2	3:C:229:ARG:NH1	2.43	0.51
4:D:337:ASP:OD1	4:D:337:ASP:N	2.43	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:322:LYS:HD3	5:E:326:ILE:HG13	1.93	0.51
7:G:165:ALA:HB3	8:H:56:LEU:HD22	1.92	0.51
16:P:138:VAL:HG11	16:P:146:MET:HB3	1.92	0.51
18:R:133:VAL:HG21	17:q:137:PHE:HB3	1.92	0.51
21:U:13:ASP:OD1	21:U:44:LYS:NZ	2.43	0.51
25:Y:142:PHE:HE2	25:Y:176:ARG:HD2	1.75	0.51
5:E:72:LYS:HB2	5:E:78:ARG:HG2	1.93	0.51
9:I:180:LYS:HB2	9:I:184:MET:HE3	1.93	0.51
15:O:138:PHE:O	15:O:142:PHE:HB2	2.11	0.51
3:C:365:GLU:HA	3:C:368:MET:HE2	1.92	0.51
5:E:168:LYS:HD3	5:E:270:LEU:HD23	1.93	0.51
6:F:81:LYS:HA	6:F:84:LYS:HG2	1.93	0.51
26:Z:12:HIS:ND1	26:Z:50:VAL:O	2.35	0.51
26:Z:16:LEU:HB3	29:c:216:MET:HE1	1.93	0.51
10:j:36:ARG:HH21	10:j:157:LYS:HG2	1.75	0.51
4:D:233:SER:OG	5:E:259:GLU:OE1	2.29	0.51
9:i:161:ALA:HB3	10:j:53:LEU:HD23	1.93	0.51
1:A:210:LYS:NZ	1:A:313:GLY:O	2.33	0.50
1:A:309:PHE:H	6:F:238:ARG:HD3	1.76	0.50
5:E:167:PRO:O	5:E:274:LYS:NZ	2.40	0.50
21:U:666:LYS:HA	21:U:669:ILE:HD12	1.94	0.50
24:X:374:PHE:HZ	24:X:387:ILE:HG12	1.75	0.50
1:A:148:GLN:NE2	1:A:150:HIS:HE1	2.10	0.50
2:B:64:LYS:NZ	32:f:239:TYR:OH	2.44	0.50
3:C:371:LEU:HD12	4:D:194:ILE:HD12	1.93	0.50
4:D:245:ARG:HE	5:E:78:ARG:HH12	1.58	0.50
21:U:576:PRO:HA	21:U:579:ARG:HE	1.76	0.50
22:V:342:ILE:HD12	22:V:343:PRO:HD2	1.93	0.50
27:a:54:ASP:HA	27:a:57:ILE:HG22	1.94	0.50
32:f:294:MET:HA	32:f:297:MET:HG3	1.93	0.50
22:V:449:ALA:HB3	22:V:460:SER:HA	1.93	0.50
24:X:27:LEU:HD12	24:X:56:LEU:HD12	1.92	0.50
26:Z:167:ALA:HB2	29:c:46:ARG:HG2	1.93	0.50
26:Z:172:VAL:HG13	29:c:217:LEU:HD21	1.92	0.50
32:f:417:ILE:HG22	32:f:418:LEU:HD12	1.92	0.50
7:g:2:SER:C	7:g:4:GLY:N	2.68	0.50
12:l:52:ALA:HB1	12:l:57:ALA:HB3	1.93	0.50
6:F:282:ILE:HG22	6:F:327:LYS:HB2	1.93	0.50
19:S:10:GLY:HA3	19:S:42:LYS:HE2	1.93	0.50
27:a:124:ASN:HB2	27:a:125:ILE:HD12	1.93	0.50
32:f:472:HIS:O	32:f:478:ARG:NH2	2.38	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:482:ILE:HD12	32:f:518:THR:HG23	1.94	0.50
11:k:98:ASN:OD1	18:r:61:ARG:NH2	2.45	0.50
13:M:50:GLU:OE2	13:M:201:HIS:ND1	2.36	0.50
23:W:55:ARG:NH1	23:W:94:ARG:O	2.44	0.50
23:W:174:TYR:O	23:W:182:ARG:NH2	2.45	0.50
28:b:22:LEU:HB3	28:b:23:PRO:HD3	1.92	0.50
29:c:291:LEU:O	29:c:295:ASN:ND2	2.45	0.50
32:f:99:LEU:HD22	32:f:106:LEU:HD11	1.93	0.50
32:f:573:ILE:HD13	32:f:599:ALA:HB2	1.94	0.50
8:H:74:LEU:HD12	8:H:87:VAL:HG22	1.93	0.50
17:Q:137:PHE:HB3	18:r:133:VAL:HG21	1.93	0.50
19:S:198:VAL:HG22	19:S:203:ILE:HG12	1.92	0.50
21:U:67:VAL:O	21:U:71:LEU:HB2	2.11	0.50
21:U:424:ALA:HA	21:U:427:LEU:HD13	1.93	0.50
21:U:749:GLN:NE2	21:U:750:SER:O	2.41	0.50
26:Z:193:ASN:HA	26:Z:196:HIS:HB3	1.94	0.50
30:d:212:LYS:HD2	30:d:213:ARG:HG2	1.94	0.50
4:D:175:GLN:NE2	4:D:179:GLU:OE2	2.40	0.50
10:J:90:GLU:HG3	10:J:110:TYR:CZ	2.46	0.50
3:C:167:LEU:HD21	25:Y:95:LEU:HD22	1.93	0.50
21:U:714:SER:O	21:U:718:ASN:ND2	2.45	0.50
29:c:267:PRO:HA	29:c:270:LEU:HD23	1.93	0.50
8:h:81:PRO:HA	8:h:84:ARG:HE	1.77	0.50
10:J:42:VAL:HG22	10:J:210:VAL:HG12	1.94	0.49
21:U:57:ARG:NH1	21:U:58:GLN:OE1	2.45	0.49
19:s:198:VAL:HG22	19:s:203:ILE:HG12	1.93	0.49
4:D:149:SER:O	4:D:150:SER:C	2.55	0.49
18:R:58:LEU:HB3	18:R:86:MET:HE1	1.94	0.49
28:b:24:THR:HB	28:b:27:GLN:HE22	1.77	0.49
32:f:755:ASP:OD2	32:f:758:ASN:ND2	2.39	0.49
11:k:13:ASN:HB2	12:l:126:ARG:HG2	1.93	0.49
19:s:35:ILE:O	20:t:151:ARG:NH2	2.39	0.49
3:C:344:LEU:HA	3:C:347:ILE:HD12	1.94	0.49
12:L:166:GLN:OE1	12:L:169:ARG:NH2	2.45	0.49
14:N:75:LEU:HD22	14:N:106:GLN:HE21	1.77	0.49
22:V:355:ARG:NE	31:e:27:TRP:O	2.44	0.49
25:Y:2:PRO:HG2	25:Y:5:ASN:HB2	1.93	0.49
27:a:115:LYS:HD3	27:a:118:ILE:HD12	1.92	0.49
32:f:240:VAL:O	32:f:245:ASN:ND2	2.43	0.49
15:o:138:PHE:O	15:o:142:PHE:HB2	2.13	0.49
1:A:287:ASP:OD1	1:A:287:ASP:N	2.45	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:144:ARG:H	14:N:147:MET:HE3	1.78	0.49
4:D:336:PRO:O	4:D:369:LYS:NZ	2.45	0.49
6:F:289:ASP:OD1	6:F:289:ASP:N	2.44	0.49
28:b:107:MET:HB3	28:b:136:VAL:HG13	1.94	0.49
32:f:378:ASN:OD1	32:f:382:ASN:ND2	2.46	0.49
32:f:386:GLY:HA2	32:f:418:LEU:HG	1.95	0.49
32:f:848:GLN:N	32:f:863:THR:O	2.44	0.49
5:E:148:VAL:HG23	5:E:167:PRO:HD2	1.95	0.49
14:N:93:ASP:OD1	14:N:93:ASP:N	2.46	0.49
15:o:1:THR:N	15:o:168:GLY:O	2.45	0.49
18:r:182:ASP:OD1	18:r:182:ASP:N	2.45	0.49
6:F:156:ASP:OD2	6:F:157:SER:N	2.46	0.49
21:U:410:VAL:HG23	21:U:448:LEU:HD13	1.94	0.49
7:G:49:VAL:HG22	7:G:219:VAL:HG22	1.95	0.49
21:U:416:GLU:OE1	21:U:450:HIS:NE2	2.45	0.49
29:c:155:VAL:O	29:c:156:VAL:C	2.55	0.49
8:h:59:GLU:HG2	8:h:60:ARG:HD3	1.93	0.49
14:n:127:ILE:HD11	14:n:136:TYR:CD1	2.47	0.49
16:p:30:ILE:HG22	16:p:31:GLN:H	1.77	0.49
33:w:40:GLN:HE22	33:w:71:LEU:HB3	1.77	0.49
1:A:366:ARG:NH2	32:f:908:LEU:OXT	2.45	0.49
21:U:469:SER:OG	21:U:470:ASN:N	2.44	0.49
24:X:256:LEU:HD12	24:X:260:MET:HE1	1.94	0.49
26:Z:61:ASP:H	28:b:91:ARG:HH22	1.60	0.49
26:Z:193:ASN:ND2	26:Z:193:ASN:O	2.44	0.49
27:a:290:GLN:HG2	27:a:330:ARG:HE	1.77	0.49
19:S:92:LEU:HD23	19:S:124:PHE:HE2	1.78	0.49
24:X:194:ARG:HG2	24:X:210:LEU:HD21	1.95	0.49
26:Z:78:MET:HB2	29:c:98:MET:HE2	1.95	0.49
16:p:12:MET:HB2	16:p:138:VAL:HG12	1.93	0.49
1:A:429:TYR:HE2	2:B:340:ALA:HB2	1.77	0.48
6:F:96:LEU:HD11	6:F:142:ALA:HB1	1.95	0.48
21:U:584:TYR:OH	21:U:768:GLN:NE2	2.43	0.48
8:h:204:THR:OG1	8:h:206:ASP:OD1	2.29	0.48
12:l:203:GLN:O	12:l:239:ARG:NH1	2.46	0.48
5:E:67:GLU:OE2	5:E:89:LYS:NZ	2.45	0.48
21:U:8:ILE:HG13	30:d:35:PHE:HZ	1.77	0.48
23:W:194:LEU:HG	23:W:202:THR:HG21	1.94	0.48
32:f:369:ARG:NH1	32:f:757:ASN:OD1	2.46	0.48
8:h:51:LYS:NZ	8:h:200:GLU:O	2.47	0.48
8:h:74:LEU:HD21	8:h:87:VAL:HG22	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:180:ALA:HB1	10:j:190:LEU:HD11	1.95	0.48
19:s:125:ASP:OD1	19:s:129:SER:N	2.46	0.48
3:C:295:THR:OG1	3:C:296:ASN:N	2.46	0.48
4:D:171:ASP:OD1	4:D:171:ASP:N	2.45	0.48
7:G:167:ALA:HB3	7:G:176:THR:HG23	1.95	0.48
17:Q:152:SER:OG	17:Q:155:ARG:NE	2.40	0.48
12:l:121:GLN:HG3	13:m:129:ARG:HG2	1.95	0.48
4:D:92:PHE:HE2	4:D:125:LYS:HD2	1.78	0.48
5:E:144:GLU:OE2	5:E:297:ARG:NH1	2.47	0.48
6:F:94:ILE:HD12	6:F:123:VAL:HG12	1.95	0.48
28:b:95:LEU:O	28:b:99:HIS:ND1	2.41	0.48
33:w:7:THR:HG22	33:w:69:LEU:HD23	1.95	0.48
5:E:180:LYS:HG2	5:E:301:ILE:HD12	1.93	0.48
16:P:35:VAL:HG12	16:P:36:THR:HG23	1.95	0.48
16:P:145:GLN:NE2	19:s:143:ALA:HB1	2.29	0.48
8:h:4:ARG:HE	8:h:5:GLY:N	2.10	0.48
13:m:215:TRP:CD1	13:m:227:VAL:HG22	2.48	0.48
1:A:73:ALA:HA	2:B:140:ASP:HB3	1.96	0.48
4:D:341:LYS:NZ	4:D:370:ILE:O	2.38	0.48
12:L:132:LEU:HB2	12:L:147:THR:HB	1.96	0.48
13:M:230:ASP:N	13:M:230:ASP:OD1	2.46	0.48
29:c:151:VAL:HG23	29:c:152:LYS:H	1.78	0.48
7:g:80:MET:HG2	7:g:138:MET:HA	1.94	0.48
20:t:27:LEU:HD11	20:t:34:ALA:HB1	1.95	0.48
33:w:27:LYS:HB3	33:w:38:PRO:HB3	1.96	0.48
1:A:210:LYS:HB2	1:A:312:ARG:HH21	1.78	0.48
6:F:224:LEU:HB3	6:F:351:LYS:HG2	1.96	0.48
19:S:27:THR:HB	19:S:40:SER:H	1.78	0.48
22:V:78:HIS:NE2	22:V:100:MET:SD	2.86	0.48
2:B:48:LYS:HE3	32:f:673:ARG:HD3	1.96	0.48
2:B:373:THR:OG1	2:B:412:MET:O	2.32	0.48
5:E:243:PHE:HE2	6:F:304:ARG:HE	1.61	0.48
31:e:50:ASP:OD1	31:e:50:ASP:N	2.42	0.48
10:j:192:ILE:HD12	10:j:206:ILE:HD12	1.96	0.48
6:F:439:ALA:HB1	12:L:62:LYS:HE3	1.96	0.48
20:T:44:ARG:NH2	20:T:47:ASN:OD1	2.47	0.48
21:U:200:VAL:HA	21:U:203:LYS:HZ3	1.79	0.48
23:W:67:LEU:HB3	23:W:104:MET:SD	2.54	0.48
23:W:451:MET:HE2	26:Z:101:LEU:HD22	1.96	0.48
29:c:165:ALA:HA	29:c:168:MET:HE2	1.96	0.48
10:j:154:HIS:HB3	11:k:59:MET:HE1	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:190:THR:OG1	7:G:193:GLN:OE1	2.22	0.48
21:U:742:HIS:O	21:U:883:ARG:NE	2.47	0.48
21:U:798:PRO:O	21:U:880:ASN:ND2	2.47	0.48
21:U:857:ASP:OD1	21:U:857:ASP:N	2.47	0.48
29:c:163:ILE:HD13	29:c:201:TYR:HE2	1.78	0.48
30:d:131:VAL:HG23	30:d:134:LYS:HE2	1.96	0.48
4:D:45:LYS:HB3	21:U:187:LEU:HG	1.96	0.47
4:D:150:SER:HB2	4:D:229:ARG:O	2.14	0.47
11:K:38:ILE:HD12	11:K:202:LEU:HG	1.96	0.47
11:K:146:VAL:HG11	11:K:222:PRO:HA	1.97	0.47
22:V:348:PHE:HE1	22:V:357:LEU:HB3	1.78	0.47
27:a:193:GLN:HB3	27:a:225:LEU:HD21	1.95	0.47
20:t:37:ARG:O	20:t:186:ARG:NH1	2.47	0.47
5:E:364:GLN:NE2	5:E:368:MET:SD	2.88	0.47
18:R:140:ASP:OD2	17:q:169:LYS:NZ	2.45	0.47
21:U:216:VAL:HG23	21:U:220:LEU:HD23	1.96	0.47
26:Z:65:ASP:OD1	26:Z:65:ASP:N	2.48	0.47
28:b:91:ARG:HH12	28:b:95:LEU:HD13	1.79	0.47
32:f:678:LEU:HD22	32:f:686:LEU:HD21	1.96	0.47
32:f:861:THR:O	32:f:879:ARG:NH1	2.46	0.47
4:D:214:MET:HE1	34:D:501:ATP:C5	2.48	0.47
4:D:374:ASP:HB3	5:E:292:PRO:HG2	1.96	0.47
6:F:314:LEU:HD22	6:F:347:ARG:HD3	1.95	0.47
10:J:116:GLN:NE2	11:K:84:ASP:OD1	2.40	0.47
20:T:53:ALA:HB2	20:T:110:MET:HG3	1.96	0.47
23:W:171:VAL:HG12	23:W:182:ARG:HG3	1.96	0.47
26:Z:62:ASP:OD1	26:Z:63:LYS:N	2.47	0.47
26:Z:180:LYS:HG2	26:Z:182:THR:HG23	1.96	0.47
31:e:16:ASP:OD1	31:e:16:ASP:N	2.47	0.47
32:f:65:GLU:O	32:f:66:LYS:C	2.57	0.47
2:B:342:ILE:HG22	2:B:350:LYS:HE3	1.97	0.47
17:Q:143:LEU:O	17:Q:147:TYR:HB2	2.15	0.47
21:U:261:LEU:HG	21:U:329:LEU:HD22	1.95	0.47
21:U:770:TRP:O	29:c:179:SER:OG	2.32	0.47
23:W:187:LEU:HD21	23:W:226:TYR:HB2	1.95	0.47
26:Z:242:LEU:HA	30:d:233:GLU:HG2	1.96	0.47
27:a:290:GLN:O	27:a:330:ARG:NH2	2.47	0.47
7:g:112:ASP:OD1	7:g:112:ASP:N	2.46	0.47
12:l:33:SER:OG	12:l:62:LYS:NZ	2.34	0.47
20:t:96:MET:HE3	20:t:127:MET:HA	1.94	0.47
10:J:188:ILE:HD12	10:J:208:LEU:HD21	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:48:ASN:HB2	25:Y:50:MET:HE3	1.97	0.47
3:C:198:LEU:HD23	36:C:501:ADP:H5'2	1.96	0.47
5:E:202:SER:HA	6:F:269:ARG:HH22	1.80	0.47
5:E:277:MET:HE2	5:E:295:LEU:HD21	1.97	0.47
12:L:88:MET:HG3	12:L:112:ILE:HD11	1.96	0.47
22:V:443:ARG:HD2	30:d:181:CYS:HB3	1.97	0.47
23:W:272:LEU:HD22	23:W:341:PHE:HE2	1.79	0.47
26:Z:231:GLN:HE21	27:a:341:LEU:HD23	1.79	0.47
26:Z:263:ALA:HB1	29:c:288:VAL:HG13	1.96	0.47
32:f:656:GLY:HA2	32:f:659:LEU:HG	1.95	0.47
19:s:64:LEU:O	19:s:68:ILE:HG12	2.14	0.47
1:A:98:CYS:O	1:A:116:LYS:NZ	2.48	0.47
2:B:235:LEU:HD13	2:B:353:PHE:HZ	1.80	0.47
4:D:335:LEU:HG	4:D:369:LYS:NZ	2.30	0.47
12:L:47:VAL:HG12	12:L:195:LEU:HD22	1.97	0.47
15:O:143:ARG:NH2	15:O:150:GLU:OE1	2.48	0.47
21:U:126:ILE:HD12	21:U:130:LEU:HD11	1.96	0.47
21:U:220:LEU:HD11	21:U:228:ALA:HB3	1.97	0.47
21:U:268:LEU:HD23	21:U:325:MET:HB3	1.97	0.47
21:U:497:LEU:HD23	21:U:516:LEU:HB2	1.96	0.47
21:U:583:MET:HA	21:U:586:VAL:HG12	1.96	0.47
22:V:447:ILE:HD11	22:V:460:SER:HB2	1.96	0.47
25:Y:202:LEU:HA	25:Y:205:VAL:HG23	1.97	0.47
26:Z:190:ARG:HH12	29:c:297:VAL:HG22	1.80	0.47
28:b:12:ASN:OD1	28:b:53:THR:OG1	2.28	0.47
28:b:24:THR:O	28:b:25:ARG:C	2.58	0.47
7:g:103:TYR:O	15:o:81:ARG:NH2	2.48	0.47
9:i:155:ASN:OD1	10:j:77:THR:OG1	2.32	0.47
12:l:72:ILE:HG22	12:l:134:ILE:HG12	1.95	0.47
15:o:163:ILE:HG12	15:o:170:GLY:HA2	1.97	0.47
17:q:169:LYS:HZ2	17:q:170:ARG:HB2	1.80	0.47
1:A:240:VAL:HB	1:A:274:PHE:HD1	1.79	0.47
4:D:153:MET:HE1	4:D:229:ARG:HE	1.80	0.47
9:I:197:LEU:HA	9:I:200:THR:HG22	1.96	0.47
21:U:43:ASP:N	21:U:43:ASP:OD1	2.47	0.47
22:V:433:ASP:HB3	30:d:149:ASN:HD21	1.80	0.47
25:Y:379:ARG:HH12	25:Y:383:LEU:HB2	1.80	0.47
7:g:70:PHE:HD2	7:g:91:VAL:HG21	1.78	0.47
19:s:16:ALA:HB2	19:s:121:VAL:HG23	1.96	0.47
3:C:132:ASP:HB2	3:C:135:VAL:HG23	1.97	0.47
4:D:77:GLU:OE2	29:c:152:LYS:HE3	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:126:PRO:O	4:D:127:ASN:C	2.58	0.47
10:J:148:ASP:OD1	10:J:152:THR:N	2.44	0.47
10:J:182:GLU:HB2	10:J:186:LEU:HD12	1.97	0.47
15:O:164:PHE:O	19:s:38:ARG:NH2	2.47	0.47
21:U:505:ASP:HB3	21:U:508:THR:HG22	1.97	0.47
24:X:24:ILE:HD11	24:X:60:THR:HG21	1.95	0.47
26:Z:66:SER:OG	26:Z:103:LYS:NZ	2.48	0.47
32:f:403:LYS:HG3	32:f:406:GLY:H	1.78	0.47
5:E:277:MET:HE1	5:E:289:LEU:HD21	1.97	0.47
8:H:135:LEU:HG	8:H:163:MET:HE3	1.97	0.47
24:X:415:TYR:HA	24:X:418:ALA:HB3	1.97	0.47
25:Y:262:SER:HA	25:Y:267:ARG:HG3	1.97	0.47
26:Z:262:LEU:O	26:Z:266:ILE:HG12	2.15	0.47
32:f:564:LEU:HD21	32:f:794:ALA:HB1	1.96	0.47
18:R:166:ARG:NH1	16:p:34:MET:O	2.48	0.46
29:c:225:TRP:O	29:c:226:MET:HE2	2.15	0.46
15:o:50:ALA:HB2	16:p:129:CYS:HB2	1.97	0.46
10:J:188:ILE:HA	10:J:191:VAL:HG22	1.97	0.46
21:U:82:LEU:O	21:U:129:ARG:NE	2.48	0.46
26:Z:238:PRO:HG2	29:c:309:PHE:HB3	1.98	0.46
2:B:315:GLN:O	2:B:322:ARG:NH1	2.48	0.46
4:D:63:ASP:HB3	21:U:607:VAL:HG11	1.96	0.46
34:D:501:ATP:O2G	5:E:294:ARG:NH2	2.43	0.46
7:G:6:SER:OG	7:G:11:ARG:NH1	2.48	0.46
19:S:125:ASP:OD1	19:S:129:SER:N	2.49	0.46
26:Z:191:ILE:HG21	27:a:375:LEU:HD22	1.95	0.46
1:A:224:LEU:HD13	34:A:501:ATP:H2'	1.97	0.46
4:D:127:ASN:HD22	4:D:252:ARG:HD3	1.80	0.46
23:W:166:LEU:HD13	23:W:189:GLN:HG2	1.97	0.46
16:p:53:LEU:HB3	16:p:60:VAL:HG22	1.98	0.46
17:q:52:ASP:OD1	18:r:88:TYR:OH	2.28	0.46
24:X:296:ASN:O	24:X:337:ARG:NH1	2.49	0.46
26:Z:186:THR:HG21	30:d:253:LEU:HD23	1.97	0.46
28:b:20:ASP:OD1	28:b:20:ASP:N	2.48	0.46
32:f:65:GLU:O	32:f:67:ASP:N	2.48	0.46
32:f:96:LEU:HD11	32:f:128:VAL:HG12	1.98	0.46
7:g:165:ALA:HB3	8:h:56:LEU:HD22	1.98	0.46
18:r:64:ARG:NH1	18:r:67:GLU:OE1	2.49	0.46
23:W:395:ASN:HA	23:W:398:VAL:HG22	1.97	0.46
26:Z:61:ASP:H	28:b:91:ARG:NH2	2.13	0.46
16:p:123:SER:HB3	16:p:137:VAL:HB	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:t:122:LEU:HG	20:t:137:LEU:HD12	1.98	0.46
1:A:35:THR:O	1:A:39:SER:OG	2.34	0.46
2:B:303:ARG:O	2:B:307:ARG:NH1	2.49	0.46
24:X:414:LEU:O	24:X:418:ALA:CB	2.63	0.46
30:d:164:THR:HA	30:d:167:ILE:HG12	1.98	0.46
2:B:174:MET:HE2	2:B:248:LEU:HD22	1.97	0.46
4:D:369:LYS:HD2	4:D:369:LYS:HA	1.69	0.46
8:H:51:LYS:NZ	8:H:200:GLU:O	2.48	0.46
10:J:189:LYS:HA	10:J:232:ILE:HD11	1.98	0.46
11:K:70:ILE:HD11	11:K:89:ILE:HD12	1.98	0.46
17:Q:197:PRO:HD2	17:q:199:GLN:H	1.80	0.46
27:a:273:GLN:HB3	27:a:310:LEU:HD11	1.96	0.46
32:f:66:LYS:O	32:f:67:ASP:C	2.58	0.46
3:C:187:LEU:HB3	3:C:314:LYS:HG2	1.98	0.46
6:F:93:VAL:HA	6:F:124:ILE:HG22	1.96	0.46
6:F:232:GLY:HA2	36:F:501:ADP:H5'2	1.98	0.46
11:K:189:MET:HE2	11:K:194:ALA:HA	1.97	0.46
21:U:124:LYS:HG2	21:U:126:ILE:HG23	1.98	0.46
21:U:625:ILE:HG13	21:U:626:LEU:HG	1.97	0.46
24:X:412:ASP:HA	25:Y:379:ARG:HH21	1.81	0.46
26:Z:190:ARG:HH21	26:Z:194:GLN:HG3	1.80	0.46
32:f:705:ASN:OD1	32:f:706:ILE:N	2.49	0.46
5:E:56:ILE:HB	5:E:100:LEU:HB2	1.98	0.46
22:V:306:ARG:O	22:V:310:THR:OG1	2.27	0.46
25:Y:13:LYS:HE2	25:Y:212:GLU:HA	1.99	0.46
27:a:292:THR:HG23	27:a:295:GLU:H	1.81	0.46
32:f:688:ARG:O	32:f:724:ASN:ND2	2.37	0.46
11:k:166:ASP:OD1	11:k:166:ASP:N	2.42	0.46
5:E:326:ILE:HA	5:E:364:GLN:HG3	1.98	0.45
11:K:202:LEU:O	11:K:206:MET:HB2	2.16	0.45
21:U:483:LEU:HD11	21:U:781:LEU:HD11	1.98	0.45
26:Z:214:LYS:HA	26:Z:218:GLY:HA3	1.98	0.45
32:f:407:MET:HE1	32:f:440:ILE:HG12	1.98	0.45
11:k:99:HIS:HB2	11:k:107:MET:HE3	1.97	0.45
12:l:45:VAL:HG22	12:l:214:ILE:HG12	1.98	0.45
1:A:38:GLN:HG2	2:B:57:GLN:HB2	1.98	0.45
4:D:231:VAL:HG23	5:E:262:ASN:HD22	1.80	0.45
5:E:60:VAL:HA	5:E:71:VAL:HG12	1.98	0.45
5:E:349:GLU:OE2	6:F:350:ARG:NH1	2.48	0.45
20:T:122:LEU:HG	20:T:137:LEU:HD12	1.98	0.45
11:k:225:ASN:OD1	11:k:226:PHE:N	2.48	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:GLU:OE2	3:C:232:ARG:NH2	2.48	0.45
21:U:180:SER:HA	21:U:183:LEU:HD12	1.98	0.45
21:U:202:VAL:HB	21:U:206:MET:HE1	1.98	0.45
27:a:28:LEU:HB3	27:a:33:LEU:HD11	1.99	0.45
27:a:194:GLN:HB2	27:a:226:ARG:HG2	1.97	0.45
12:l:45:VAL:HG11	12:l:188:VAL:HG22	1.99	0.45
33:w:44:ILE:HB	33:w:68:HIS:HB2	1.99	0.45
25:Y:300:ARG:NH1	25:Y:333:GLU:OE2	2.47	0.45
4:D:393:ILE:HD12	23:W:134:GLY:HA2	1.98	0.45
22:V:280:ALA:HB3	22:V:285:TRP:CD1	2.52	0.45
26:Z:21:ASP:OD1	26:Z:22:HIS:N	2.48	0.45
27:a:11:SER:HB2	27:a:56:LEU:HD13	1.99	0.45
29:c:27:THR:OG1	29:c:175:ARG:NH2	2.49	0.45
32:f:367:SER:HA	32:f:370:MET:HG2	1.99	0.45
8:h:119:GLN:HG3	9:i:81:SER:HB2	1.98	0.45
13:m:23:VAL:HG12	13:m:27:MET:HE1	1.99	0.45
1:A:268:LYS:HG2	32:f:352:HIS:HB3	1.99	0.45
10:J:204:LYS:HE2	10:J:222:PRO:O	2.17	0.45
22:V:280:ALA:HB1	22:V:284:GLU:HB2	1.99	0.45
28:b:14:GLU:HB3	28:b:82:GLY:H	1.82	0.45
30:d:112:VAL:HA	30:d:115:PHE:HB3	1.97	0.45
16:p:47:ASP:OD1	16:p:47:ASP:N	2.45	0.45
21:U:191:LYS:HA	21:U:194:ARG:HB3	1.99	0.45
3:C:218:GLU:HB3	4:D:275:PHE:HB2	1.98	0.45
16:P:189:ILE:HB	16:P:196:THR:HB	1.99	0.45
20:T:86:ARG:NH1	20:T:133:GLU:OE2	2.50	0.45
28:b:100:ARG:HH12	28:b:105:HIS:HB2	1.80	0.45
32:f:274:ASP:OD1	32:f:274:ASP:N	2.47	0.45
12:l:49:LEU:HG	12:l:195:LEU:HD21	1.99	0.45
15:o:143:ARG:H	15:o:146:MET:HE3	1.82	0.45
33:w:39:ASP:O	33:w:42:ARG:NH1	2.46	0.45
3:C:219:LEU:HD12	4:D:290:LEU:HG	1.99	0.45
4:D:264:ILE:HB	4:D:309:MET:HG2	1.98	0.45
4:D:345:PHE:O	4:D:349:THR:OG1	2.23	0.45
16:P:149:MET:HG2	16:P:170:ALA:HA	1.99	0.45
21:U:16:GLU:OE1	30:d:27:LYS:NZ	2.49	0.45
22:V:309:MET:HE1	22:V:332:LEU:HA	1.98	0.45
27:a:84:VAL:HA	27:a:87:MET:HG3	1.98	0.45
29:c:146:ASP:HB3	29:c:156:VAL:HB	1.99	0.45
32:f:83:ARG:O	32:f:87:THR:OG1	2.34	0.45
32:f:291:GLN:HA	32:f:294:MET:HE2	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:254:ALA:HB2	4:D:262:ILE:HD11	1.98	0.45
6:F:389:ASP:OD1	6:F:389:ASP:N	2.44	0.45
32:f:60:VAL:HG11	32:f:105:LYS:NZ	2.32	0.45
32:f:343:LYS:HG3	32:f:348:ILE:HD11	1.98	0.45
10:j:185:ASP:OD1	10:j:185:ASP:N	2.49	0.45
1:A:325:ASP:OD1	1:A:325:ASP:N	2.49	0.44
3:C:49:ARG:HH21	21:U:639:LEU:HG	1.81	0.44
21:U:376:MET:HA	21:U:739:ALA:HA	1.98	0.44
21:U:475:HIS:CE1	21:U:507:VAL:HG22	2.52	0.44
20:t:124:TYR:HB2	20:t:137:LEU:HD13	1.99	0.44
2:B:197:ILE:HG13	2:B:235:LEU:HD21	1.98	0.44
4:D:97:ASP:OD1	4:D:97:ASP:N	2.51	0.44
10:J:65:LEU:HD13	10:J:88:ARG:HG3	1.99	0.44
16:P:125:ASP:OD1	16:P:129:CYS:N	2.40	0.44
18:R:139:MET:O	18:R:143:TYR:HB2	2.18	0.44
20:T:43:MET:HE1	20:T:67:LEU:HD23	1.99	0.44
23:W:377:ARG:NH2	23:W:380:GLN:OE1	2.51	0.44
29:c:75:MET:HE1	29:c:87:VAL:HA	1.98	0.44
32:f:169:GLU:HG3	32:f:184:LEU:HD11	1.99	0.44
13:m:68:ASN:OD1	13:m:224:HIS:ND1	2.48	0.44
2:B:183:THR:OG1	2:B:184:TYR:N	2.49	0.44
6:F:153:VAL:HG22	6:F:160:ILE:HG22	1.99	0.44
21:U:45:ILE:HG23	21:U:60:ALA:HB1	1.98	0.44
25:Y:52:PRO:HA	25:Y:55:GLU:HG2	1.99	0.44
27:a:115:LYS:HB3	27:a:134:THR:HG23	1.98	0.44
32:f:98:PHE:O	32:f:102:HIS:ND1	2.40	0.44
13:m:19:ARG:NH2	13:m:24:GLU:OE1	2.50	0.44
4:D:49:GLN:NE2	4:D:52:GLU:OE1	2.48	0.44
6:F:252:ALA:HB3	6:F:255:GLN:HB2	1.98	0.44
26:Z:170:VAL:HG11	29:c:150:SER:HB2	1.99	0.44
27:a:54:ASP:OD1	27:a:54:ASP:N	2.48	0.44
10:J:87:ALA:HB1	10:J:107:ILE:HD11	1.98	0.44
13:M:68:ASN:OD1	13:M:224:HIS:ND1	2.51	0.44
19:S:187:VAL:HG21	15:o:24:MET:HE3	2.00	0.44
21:U:764:LEU:O	21:U:767:THR:OG1	2.35	0.44
30:d:101:LEU:HG	30:d:166:PHE:HE2	1.82	0.44
20:t:124:TYR:HE1	20:t:139:THR:HG22	1.83	0.44
1:A:347:ASP:OD1	1:A:348:LEU:N	2.46	0.44
3:C:113:ARG:HB2	3:C:127:LEU:HB2	2.00	0.44
4:D:296:MET:HE3	4:D:326:ARG:HB3	1.99	0.44
21:U:632:GLN:O	21:U:635:SER:OG	2.34	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:130:ASP:OD1	26:Z:130:ASP:N	2.50	0.44
33:w:24:GLU:HG2	33:w:52:ASP:HB3	1.99	0.44
3:C:57:ARG:NH2	21:U:643:SER:O	2.45	0.44
18:R:144:SER:OG	18:R:145:TYR:N	2.50	0.44
22:V:342:ILE:HD13	22:V:368:ARG:HD3	1.99	0.44
24:X:35:ILE:HD12	24:X:46:LYS:HD2	1.99	0.44
25:Y:300:ARG:HH21	31:e:52:PHE:HB2	1.82	0.44
29:c:196:LEU:HD12	29:c:200:TYR:HE2	1.83	0.44
32:f:703:ARG:HB2	32:f:706:ILE:HG12	2.00	0.44
8:h:39:LYS:HG3	8:h:44:VAL:HG22	2.00	0.44
14:n:4:MET:HE1	14:n:159:ALA:HB3	2.00	0.44
17:q:53:THR:HG22	17:q:100:VAL:HG12	2.00	0.44
1:A:284:ARG:HH21	6:F:334:ARG:HG3	1.83	0.44
3:C:248:MET:HE1	3:C:272:THR:HB	1.99	0.44
16:P:58:THR:O	17:Q:85:ARG:NH2	2.51	0.44
22:V:483:CYS:HA	22:V:486:ILE:HG22	2.00	0.44
23:W:272:LEU:HD23	23:W:272:LEU:HA	1.88	0.44
27:a:277:LEU:HD21	27:a:296:ILE:HG23	1.98	0.44
8:h:93:LEU:HD13	8:h:113:ARG:HB3	1.98	0.44
1:A:115:VAL:HG21	1:A:118:PHE:HB2	1.98	0.44
17:q:22:ALA:HA	17:q:27:GLN:HA	1.99	0.44
20:t:12:LEU:HD12	20:t:173:MET:HE2	2.00	0.44
1:A:143:ASP:OD1	1:A:143:ASP:N	2.51	0.43
3:C:219:LEU:HD13	4:D:286:GLN:HG3	2.00	0.43
3:C:249:ASP:OD1	3:C:249:ASP:N	2.49	0.43
4:D:115:ILE:HG22	4:D:139:LEU:HD12	2.00	0.43
7:G:10:ASP:OD1	7:G:10:ASP:N	2.50	0.43
7:G:144:ASP:HB2	7:G:150:GLN:HE22	1.83	0.43
7:G:165:ALA:HB1	7:G:179:LEU:HD13	2.00	0.43
13:M:39:ILE:HG23	13:M:181:MET:HE3	2.00	0.43
21:U:622:LEU:HD13	21:U:637:VAL:HG22	2.00	0.43
22:V:344:ASP:O	22:V:347:GLN:NE2	2.44	0.43
5:E:171:LEU:HD21	5:E:298:LYS:HG2	2.00	0.43
17:Q:44:LEU:HD11	17:Q:102:LEU:HD22	1.99	0.43
21:U:247:GLN:HE22	21:U:912:ILE:HA	1.83	0.43
21:U:899:ARG:O	21:U:917:THR:OG1	2.33	0.43
29:c:27:THR:HB	29:c:175:ARG:HB3	2.00	0.43
29:c:143:VAL:HG22	29:c:159:ALA:HB2	1.99	0.43
7:g:3:ARG:O	7:g:3:ARG:HG2	2.19	0.43
20:t:43:MET:HE2	20:t:64:LYS:HG3	2.00	0.43
33:w:44:ILE:O	33:w:68:HIS:N	2.51	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:THR:HA	2:B:164:MET:HE2	1.99	0.43
21:U:249:CYS:HB3	21:U:328:ILE:HB	2.00	0.43
21:U:388:ASP:OD1	21:U:388:ASP:N	2.49	0.43
24:X:357:SER:OG	24:X:358:LYS:N	2.52	0.43
27:a:112:ILE:HD12	27:a:151:VAL:HG11	2.00	0.43
29:c:163:ILE:HD12	29:c:163:ILE:HA	1.94	0.43
7:g:123:GLN:NE2	8:h:82:ASP:OD1	2.50	0.43
17:q:44:LEU:HD11	17:q:102:LEU:HD22	2.00	0.43
2:B:117:ASP:OD2	32:f:747:GLN:NE2	2.36	0.43
4:D:234:GLU:OE2	5:E:216:ARG:NH1	2.52	0.43
4:D:267:ILE:HD12	4:D:267:ILE:H	1.84	0.43
10:J:39:ASP:OD1	10:J:39:ASP:N	2.51	0.43
17:Q:102:LEU:HB2	17:Q:118:MET:HB2	1.98	0.43
18:R:182:ASP:OD1	18:R:182:ASP:N	2.50	0.43
22:V:338:LEU:HD21	22:V:397:ARG:HG3	1.99	0.43
24:X:268:GLN:HA	24:X:271:VAL:HG22	2.00	0.43
28:b:72:LEU:O	28:b:76:HIS:ND1	2.47	0.43
30:d:178:ILE:HA	30:d:181:CYS:SG	2.59	0.43
2:B:167:THR:O	2:B:168:ASP:HB2	2.18	0.43
2:B:169:PRO:O	2:B:170:LEU:C	2.61	0.43
4:D:159:LYS:HD2	4:D:221:HIS:HA	1.99	0.43
16:P:143:ALA:HA	16:P:146:MET:HE2	2.01	0.43
23:W:85:GLU:HA	23:W:88:MET:HE2	1.99	0.43
4:D:203:LEU:HD13	4:D:322:LEU:HD21	2.01	0.43
6:F:375:VAL:HG22	6:F:415:LEU:HD12	1.99	0.43
21:U:482:GLY:HA2	21:U:519:VAL:HG13	2.01	0.43
21:U:568:GLU:OE2	21:U:572:ARG:NE	2.50	0.43
22:V:453:HIS:N	30:d:187:GLU:OE2	2.52	0.43
26:Z:121:LEU:HD11	26:Z:138:TYR:HD1	1.84	0.43
27:a:289:ARG:NH1	27:a:334:THR:O	2.48	0.43
32:f:566:HIS:HB2	32:f:573:ILE:HD12	2.00	0.43
32:f:682:GLY:HA2	32:f:686:LEU:HD23	2.00	0.43
7:g:61:LEU:HD21	7:g:66:VAL:HG11	2.01	0.43
15:o:51:ASP:HB3	15:o:94:ILE:HG23	2.01	0.43
19:s:211:ARG:NH2	19:s:213:ASP:OD2	2.51	0.43
20:t:54:SER:O	20:t:108:ASN:ND2	2.43	0.43
1:A:394:MET:O	1:A:398:ARG:HG2	2.18	0.43
4:D:113:VAL:HB	4:D:138:ALA:HA	2.01	0.43
7:G:188:ASP:OD1	7:G:188:ASP:N	2.52	0.43
17:Q:119:ASP:OD1	17:Q:123:ALA:N	2.43	0.43
21:U:770:TRP:HA	29:c:180:ASN:HB3	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:174:MET:SD	9:i:195:LYS:NZ	2.88	0.43
19:s:10:GLY:HA3	19:s:42:LYS:HE2	2.01	0.43
3:C:235:PHE:HA	3:C:238:ALA:HB3	2.00	0.43
14:N:138:TYR:O	14:N:142:THR:OG1	2.34	0.43
21:U:245:ALA:HA	21:U:248:ILE:HG22	1.99	0.43
21:U:325:MET:HA	21:U:328:ILE:HG12	2.00	0.43
25:Y:195:LYS:HA	25:Y:230:ALA:HB1	1.99	0.43
7:g:22:LEU:HD13	8:h:79:MET:HE1	2.00	0.43
15:O:113:ILE:HG12	15:O:119:THR:HG22	2.01	0.43
18:R:4:LEU:HB2	18:R:139:MET:HE1	2.01	0.43
20:T:20:VAL:HG11	20:T:122:LEU:HD13	2.00	0.43
32:f:655:LEU:HD22	32:f:804:LEU:HD11	2.00	0.43
2:B:112:LEU:HD11	2:B:144:LEU:HD12	2.01	0.43
3:C:72:TYR:N	3:C:116:LEU:O	2.49	0.43
6:F:78:GLU:HA	6:F:81:LYS:HG3	2.01	0.43
8:H:204:THR:OG1	8:H:206:ASP:OD1	2.32	0.43
14:N:27:ALA:O	20:t:179:ARG:NH1	2.47	0.43
14:N:162:LEU:HD11	14:n:141:ALA:HB2	2.01	0.43
16:P:193:ASP:OD1	16:P:193:ASP:N	2.50	0.43
21:U:596:ASN:HA	21:U:599:ILE:HG22	2.01	0.43
28:b:58:CYS:HB3	28:b:92:VAL:HG21	2.00	0.43
32:f:527:VAL:HG12	32:f:564:LEU:HG	1.99	0.43
20:t:25:ASP:HA	20:t:187:PHE:HA	1.99	0.43
4:D:95:ALA:HA	4:D:101:ALA:HA	2.01	0.42
10:J:211:MET:HB2	10:J:217:LEU:HD13	1.99	0.42
21:U:701:ILE:HG21	21:U:810:THR:HA	2.01	0.42
21:U:750:SER:OG	21:U:754:HIS:O	2.34	0.42
23:W:414:ASN:HB2	23:W:417:ARG:HD3	2.00	0.42
28:b:3:LEU:HB3	28:b:105:HIS:ND1	2.34	0.42
7:g:132:ARG:HA	7:g:133:PRO:HD3	1.86	0.42
13:m:230:ASP:OD1	13:m:230:ASP:N	2.51	0.42
2:B:190:LEU:HD13	2:B:193:GLN:HE21	1.83	0.42
4:D:274:ARG:HD3	5:E:245:GLU:HB3	2.00	0.42
5:E:57:VAL:HG13	5:E:97:ARG:HD3	2.01	0.42
5:E:207:TYR:HD2	5:E:210:GLU:HG3	1.85	0.42
9:I:201:MET:HE3	9:I:206:LEU:HD11	2.00	0.42
15:O:143:ARG:H	15:O:146:MET:HE3	1.84	0.42
17:Q:52:ASP:OD1	18:R:88:TYR:OH	2.31	0.42
21:U:202:VAL:HA	21:U:205:TYR:HB2	2.00	0.42
22:V:343:PRO:O	31:e:43:TRP:NE1	2.46	0.42
24:X:255:LEU:O	24:X:259:ILE:HG12	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:151:THR:HG23	27:a:146:PRO:HB2	1.99	0.42
29:c:87:VAL:HG11	29:c:133:PHE:HZ	1.85	0.42
30:d:115:PHE:CE1	30:d:140:GLU:HG2	2.54	0.42
11:k:216:GLU:HB2	11:k:228:MET:HE1	2.01	0.42
1:A:81:ALA:HB3	2:B:137:SER:HB2	2.01	0.42
4:D:407:ILE:HG13	4:D:408:LYS:H	1.84	0.42
20:T:54:SER:OG	20:T:55:GLY:N	2.52	0.42
21:U:16:GLU:HB3	30:d:27:LYS:HZ3	1.84	0.42
22:V:200:ARG:HB3	22:V:203:LEU:HB2	2.02	0.42
8:h:52:GLN:HB3	8:h:57:TYR:HD2	1.85	0.42
5:E:237:ALA:HB1	6:F:308:ARG:HG3	2.01	0.42
6:F:219:PRO:HA	6:F:220:PRO:HD3	1.93	0.42
11:K:59:MET:HE3	11:K:59:MET:HB3	1.82	0.42
22:V:497:PRO:HG3	26:Z:279:LYS:HE2	2.01	0.42
28:b:151:GLU:OE1	28:b:152:LYS:HG3	2.19	0.42
32:f:445:LEU:HD11	32:f:466:LEU:HA	2.01	0.42
8:h:166:ASN:HB3	8:h:169:ASN:HD21	1.83	0.42
16:p:143:ALA:HA	16:p:146:MET:HE2	2.01	0.42
3:C:130:LYS:HD2	3:C:131:VAL:N	2.34	0.42
4:D:300:ASP:OD1	4:D:300:ASP:N	2.52	0.42
5:E:244:SER:OG	6:F:299:GLU:OE2	2.33	0.42
12:L:7:ASP:OD1	12:L:7:ASP:N	2.53	0.42
13:M:46:VAL:HG22	13:M:215:TRP:HB3	2.01	0.42
19:S:13:LEU:HD12	19:S:145:LEU:HD13	2.01	0.42
21:U:248:ILE:HD12	21:U:248:ILE:HA	1.88	0.42
26:Z:139:ILE:N	26:Z:156:GLU:O	2.51	0.42
27:a:159:SER:OG	27:a:175:ASP:OD2	2.35	0.42
13:m:41:CYS:HB3	13:m:189:ILE:HG13	2.02	0.42
5:E:385:ASP:O	5:E:386:TYR:CB	2.67	0.42
22:V:218:TYR:HA	22:V:221:LEU:HD12	2.01	0.42
22:V:263:LEU:HB3	22:V:266:GLN:NE2	2.35	0.42
23:W:31:CYS:HA	23:W:43:VAL:HG11	2.02	0.42
24:X:403:THR:HG22	29:c:249:LEU:HA	2.00	0.42
32:f:131:MET:HE1	32:f:161:HIS:HB3	2.01	0.42
8:h:82:ASP:HB3	8:h:130:PHE:HD1	1.84	0.42
16:p:86:THR:HG22	16:p:90:MET:HE2	2.01	0.42
33:w:23:ILE:HD13	33:w:50:LEU:HB3	2.01	0.42
1:A:102:ILE:HD11	1:A:114:ASN:HB2	2.02	0.42
2:B:290:ILE:HG12	2:B:305:ILE:HG23	2.01	0.42
3:C:141:GLU:O	4:D:323:ARG:NH1	2.52	0.42
5:E:355:ILE:HD11	6:F:211:LYS:HG2	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:185:GLU:HG3	24:X:122:ARG:HH21	1.85	0.42
22:V:193:GLN:O	22:V:197:THR:OG1	2.29	0.42
24:X:130:GLU:HB3	24:X:153:LEU:HD21	2.02	0.42
32:f:62:ARG:HA	32:f:65:GLU:OE2	2.19	0.42
32:f:885:GLU:OE2	32:f:903:ASN:ND2	2.52	0.42
8:h:52:GLN:HE21	8:h:57:TYR:HD2	1.66	0.42
10:j:185:ASP:O	10:j:189:LYS:HG2	2.20	0.42
11:k:84:ASP:HB3	11:k:137:PHE:HD1	1.85	0.42
1:A:293:ASN:ND2	6:F:303:ASP:OD2	2.53	0.42
4:D:383:GLY:HA3	5:E:164:ILE:HD13	2.01	0.42
5:E:223:ARG:NH1	5:E:268:ASP:OD2	2.53	0.42
7:G:138:MET:HB2	7:G:154:CYS:HB3	2.02	0.42
8:H:166:ASN:HD22	8:H:198:SER:HB3	1.83	0.42
15:O:63:LEU:HD23	15:O:63:LEU:HA	1.94	0.42
17:Q:27:GLN:HG3	17:q:172:ILE:HG22	2.01	0.42
27:a:239:ALA:HB2	27:a:247:ARG:HD2	2.01	0.42
32:f:348:ILE:HD13	32:f:381:VAL:HG21	2.01	0.42
1:A:327:LEU:HD23	1:A:331:LEU:HD22	2.01	0.42
4:D:124:LEU:HD21	4:D:142:VAL:HG12	2.01	0.42
5:E:331:ILE:HG23	5:E:371:VAL:HG21	2.01	0.42
5:E:360:ASP:OD1	5:E:360:ASP:N	2.52	0.42
7:G:67:THR:HG22	7:G:69:LEU:H	1.84	0.42
24:X:400:ALA:O	24:X:403:THR:OG1	2.30	0.42
32:f:193:PRO:HA	32:f:196:MET:HG2	2.00	0.42
4:D:150:SER:CB	4:D:228:ILE:HG23	2.48	0.42
11:K:13:ASN:HB3	12:L:126:ARG:HB3	2.02	0.42
12:L:44:ALA:HB2	12:L:142:PRO:HB3	2.02	0.42
15:O:97:ALA:HB1	15:O:127:MET:HE2	2.02	0.42
22:V:314:ARG:HH11	25:Y:385:ARG:HD3	1.85	0.42
24:X:360:ASP:OD1	24:X:360:ASP:N	2.53	0.42
24:X:364:LYS:HA	24:X:364:LYS:HD2	1.76	0.42
30:d:107:LEU:HD11	30:d:140:GLU:HB2	2.02	0.42
30:d:237:ILE:HG23	30:d:238:PRO:HD3	2.02	0.42
7:g:112:ASP:HB3	7:g:152:TYR:CZ	2.55	0.42
1:A:59:ILE:HD11	2:B:76:GLU:HB3	2.02	0.41
2:B:115:ILE:HD12	2:B:121:ALA:HB2	2.03	0.41
5:E:144:GLU:O	5:E:297:ARG:NH2	2.52	0.41
13:M:35:THR:HA	13:M:166:GLY:HA3	2.02	0.41
17:Q:25:ILE:HG22	17:Q:26:VAL:HG13	2.01	0.41
21:U:101:ILE:HG22	21:U:133:ILE:HD11	2.02	0.41
21:U:672:LEU:HA	21:U:675:MET:HE2	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:25:VAL:HG23	29:c:175:ARG:HA	2.03	0.41
30:d:170:LEU:HA	30:d:173:THR:HG22	2.02	0.41
15:o:187:ARG:HA	15:o:188:PRO:HA	1.85	0.41
17:q:31:ASP:OD1	17:q:31:ASP:N	2.53	0.41
3:C:90:HIS:CD2	3:C:90:HIS:N	2.87	0.41
4:D:81:ARG:HE	29:c:154:LYS:HG2	1.84	0.41
5:E:250:ASP:OD1	5:E:250:ASP:N	2.45	0.41
14:N:192:ASP:O	14:N:196:LYS:NZ	2.53	0.41
16:P:53:LEU:HB3	16:P:60:VAL:HG22	2.02	0.41
27:a:70:ARG:NE	28:b:17:ARG:HD2	2.34	0.41
32:f:409:SER:O	32:f:819:TYR:OH	2.37	0.41
2:B:343:ARG:HE	2:B:346:ARG:NH1	2.18	0.41
3:C:90:HIS:CB	3:C:91:PRO:HD3	2.50	0.41
4:D:150:SER:O	4:D:151:ILE:C	2.63	0.41
21:U:671:LEU:O	21:U:674:PRO:HD2	2.19	0.41
23:W:178:GLU:HG3	23:W:180:LYS:H	1.86	0.41
26:Z:39:LEU:H	26:Z:94:TRP:HA	1.85	0.41
26:Z:82:PHE:HA	26:Z:85:VAL:HG12	2.01	0.41
27:a:43:ASP:HA	27:a:46:GLN:HG2	2.02	0.41
30:d:221:ASN:OD1	30:d:222:TYR:N	2.53	0.41
32:f:344:VAL:HG13	32:f:347:ASP:H	1.85	0.41
17:q:38:MET:HE3	17:q:44:LEU:HB3	2.02	0.41
2:B:393:ALA:HB2	34:B:501:ATP:H5'1	2.02	0.41
3:C:24:TYR:OH	4:D:44:TYR:N	2.54	0.41
4:D:259:PRO:HB3	4:D:304:ASN:HB2	2.02	0.41
21:U:373:ASN:HA	21:U:376:MET:HG2	2.02	0.41
21:U:376:MET:HA	21:U:740:GLY:H	1.84	0.41
22:V:443:ARG:HH11	30:d:181:CYS:HB3	1.84	0.41
23:W:362:ASN:O	23:W:366:MET:HG2	2.19	0.41
25:Y:13:LYS:HG2	25:Y:212:GLU:HB2	2.01	0.41
26:Z:73:ASP:OD1	26:Z:77:ASN:ND2	2.53	0.41
26:Z:193:ASN:O	26:Z:197:GLY:N	2.37	0.41
30:d:125:LYS:HB3	30:d:130:ASN:HD22	1.85	0.41
30:d:200:PHE:HB2	30:d:203:PRO:HD3	2.03	0.41
32:f:290:VAL:HG12	32:f:294:MET:HE1	2.02	0.41
32:f:332:ALA:HA	32:f:335:ARG:HG2	2.03	0.41
1:A:328:ASP:HA	1:A:329:PRO:HD3	1.97	0.41
6:F:368:ILE:HG23	6:F:371:ARG:HH22	1.86	0.41
10:J:66:ASP:HA	17:Q:69:MET:HE3	2.03	0.41
14:N:141:ALA:HB2	14:n:162:LEU:HD11	2.03	0.41
21:U:18:GLN:HG2	30:d:27:LYS:HZ2	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:329:HIS:HA	22:V:332:LEU:HG	2.01	0.41
27:a:100:THR:HA	27:a:103:LYS:HG2	2.01	0.41
28:b:20:ASP:OD2	28:b:25:ARG:NH2	2.53	0.41
4:D:155:THR:HG23	4:D:159:LYS:NZ	2.35	0.41
6:F:374:ASN:ND2	6:F:413:THR:O	2.54	0.41
14:N:4:MET:HE1	14:N:159:ALA:HB3	2.02	0.41
14:N:174:ILE:HB	14:N:189:LEU:HB2	2.02	0.41
20:T:103:MET:HE2	20:T:103:MET:HB2	1.94	0.41
21:U:225:ASP:OD1	21:U:225:ASP:N	2.52	0.41
21:U:326:ILE:O	21:U:330:SER:OG	2.37	0.41
22:V:442:ILE:HG21	30:d:184:LYS:HZ3	1.84	0.41
24:X:414:LEU:O	24:X:418:ALA:HB3	2.20	0.41
26:Z:234:PHE:CE2	27:a:349:MET:HG2	2.55	0.41
32:f:66:LYS:HG2	32:f:67:ASP:H	1.86	0.41
32:f:192:VAL:HG13	32:f:204:ALA:HB1	2.03	0.41
32:f:323:ASN:HB3	32:f:326:LEU:HB2	2.03	0.41
32:f:665:GLU:HG3	32:f:666:ILE:HG13	2.02	0.41
32:f:806:VAL:HG23	32:f:810:ILE:HB	2.02	0.41
7:g:180:GLU:HG2	8:h:55:ILE:HG22	2.03	0.41
8:h:3:GLU:O	8:h:5:GLY:N	2.53	0.41
8:h:130:PHE:HB3	8:h:132:VAL:HG12	2.02	0.41
2:B:49:LEU:HD23	32:f:666:ILE:HG23	2.03	0.41
3:C:326:LEU:HD22	3:C:345:ARG:HE	1.85	0.41
5:E:84:ARG:HH21	5:E:86:GLN:HE21	1.69	0.41
5:E:349:GLU:HA	5:E:352:MET:HB2	2.03	0.41
21:U:160:LEU:HD11	21:U:196:LYS:HB3	2.03	0.41
21:U:201:LEU:HD23	21:U:201:LEU:HA	1.96	0.41
22:V:146:GLN:HG3	22:V:148:ARG:HG2	2.03	0.41
22:V:462:GLU:OE2	25:Y:357:ASN:ND2	2.53	0.41
8:h:195:LEU:HD23	8:h:195:LEU:HA	1.95	0.41
10:j:173:GLU:HG2	11:k:58:LEU:HD23	2.02	0.41
1:A:146:LYS:NZ	1:A:148:GLN:HG2	2.35	0.41
3:C:340:ARG:HH21	25:Y:6:LEU:HD22	1.83	0.41
4:D:322:LEU:HD22	4:D:330:LYS:HE3	2.03	0.41
11:K:41:GLN:NE2	11:K:151:PRO:O	2.54	0.41
18:R:41:LEU:HD23	18:R:103:GLY:HA3	2.03	0.41
23:W:284:SER:HA	23:W:287:VAL:HG22	2.02	0.41
29:c:115:HIS:HB3	29:c:118:PHE:HB2	2.02	0.41
7:g:165:ALA:HB1	7:g:179:LEU:HD13	2.02	0.41
20:t:20:VAL:HG11	20:t:122:LEU:HD13	2.02	0.41
1:A:306:LEU:O	1:A:312:ARG:NH1	2.54	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ASP:C	2:B:167:THR:H	2.29	0.41
3:C:22:GLN:NE2	21:U:98:GLU:OE1	2.53	0.41
3:C:130:LYS:HD2	3:C:131:VAL:HG12	2.02	0.41
4:D:124:LEU:O	4:D:125:LYS:CB	2.69	0.41
9:I:38:LEU:HD23	9:I:160:LYS:HG2	2.03	0.41
13:M:8:ASP:O	13:M:22:GLN:NE2	2.45	0.41
16:P:38:ASP:OD1	16:P:38:ASP:N	2.52	0.41
18:R:166:ARG:NE	17:q:144:ASP:OD2	2.44	0.41
21:U:161:ASP:OD1	21:U:161:ASP:N	2.53	0.41
21:U:184:CYS:HA	21:U:188:MET:SD	2.60	0.41
21:U:366:HIS:CE1	21:U:395:ARG:HD2	2.56	0.41
21:U:381:THR:HG22	21:U:412:HIS:HA	2.02	0.41
23:W:420:ASP:OD1	23:W:423:ASN:ND2	2.50	0.41
26:Z:14:LEU:HD22	29:c:43:LYS:HD3	2.03	0.41
30:d:44:THR:O	30:d:47:GLN:NE2	2.54	0.41
32:f:137:ARG:HE	32:f:168:LYS:NZ	2.19	0.41
32:f:463:LEU:O	32:f:467:SER:OG	2.32	0.41
10:j:204:LYS:NZ	10:j:222:PRO:O	2.54	0.41
14:n:127:ILE:HD11	14:n:136:TYR:HD1	1.86	0.41
16:p:138:VAL:HG11	16:p:146:MET:HB3	2.03	0.41
18:r:37:ILE:HG23	18:r:60:ALA:HB2	2.03	0.41
1:A:397:ILE:HD11	2:B:214:MET:HB2	2.03	0.41
5:E:119:VAL:HA	5:E:122:MET:HE2	2.03	0.41
14:N:196:LYS:HE2	14:N:196:LYS:HB2	1.83	0.41
21:U:465:LEU:HD11	21:U:477:GLY:HA3	2.03	0.41
21:U:611:ASN:HB3	21:U:614:VAL:HG12	2.02	0.41
23:W:385:SER:OG	23:W:386:VAL:N	2.54	0.41
27:a:151:VAL:HA	27:a:154:ARG:HD3	2.02	0.41
29:c:160:PHE:CE1	29:c:196:LEU:HD11	2.57	0.41
32:f:60:VAL:HG13	32:f:109:ILE:HG21	2.03	0.41
10:j:184:ASP:O	10:j:188:ILE:HG12	2.21	0.41
12:l:7:ASP:O	12:l:21:GLN:NE2	2.44	0.41
13:m:108:LEU:HD11	13:m:137:LEU:HB3	2.03	0.41
15:o:97:ALA:HB1	15:o:127:MET:HE2	2.03	0.41
4:D:139:LEU:HD23	4:D:139:LEU:HA	1.78	0.40
29:c:100:LYS:HE2	29:c:105:PRO:HB3	2.04	0.40
11:k:38:ILE:HD12	11:k:202:LEU:HG	2.03	0.40
1:A:102:ILE:HD12	1:A:112:ILE:HG22	2.02	0.40
1:A:252:GLU:HG2	6:F:259:MET:HE2	2.03	0.40
1:A:425:ALA:HA	2:B:339:PRO:HB2	2.02	0.40
5:E:84:ARG:HH21	5:E:86:GLN:NE2	2.19	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:116:ASP:O	5:E:118:LEU:N	2.54	0.40
5:E:168:LYS:N	5:E:296:ASP:OD2	2.53	0.40
12:L:85:CYS:HA	12:L:88:MET:HE3	2.03	0.40
20:T:9:THR:OG1	20:T:10:SER:N	2.53	0.40
24:X:153:LEU:O	24:X:157:LEU:HB2	2.21	0.40
25:Y:155:ASP:OD1	25:Y:156:LEU:N	2.54	0.40
26:Z:68:TRP:HE1	26:Z:111:LEU:HD22	1.86	0.40
27:a:148:VAL:HG13	27:a:152:HIS:HB2	2.02	0.40
10:j:148:ASP:OD1	10:j:152:THR:N	2.54	0.40
1:A:213:LEU:HD22	1:A:337:LEU:HD12	2.04	0.40
2:B:362:LYS:HB3	2:B:384:ILE:HD11	2.03	0.40
4:D:77:GLU:O	4:D:80:LYS:HG2	2.21	0.40
12:L:112:ILE:HD13	12:L:112:ILE:HA	1.91	0.40
15:O:21:THR:HG22	15:O:26:VAL:HA	2.04	0.40
15:O:112:SER:HB3	15:O:125:VAL:HG11	2.02	0.40
21:U:365:CYS:HA	21:U:368:ALA:HB3	2.03	0.40
21:U:492:ASP:OD1	21:U:493:VAL:N	2.54	0.40
7:g:31:ALA:HB1	7:g:83:MET:HE3	2.03	0.40
20:t:63:LEU:HD23	20:t:63:LEU:HA	1.93	0.40
2:B:107:MET:HE1	2:B:160:ILE:HD12	2.03	0.40
2:B:255:LEU:HD23	2:B:290:ILE:HD12	2.04	0.40
4:D:120:ASP:OD1	29:c:282:ARG:NH2	2.54	0.40
4:D:124:LEU:O	4:D:125:LYS:HB2	2.21	0.40
5:E:84:ARG:HG2	29:c:50:PRO:HG3	2.03	0.40
6:F:303:ASP:OD1	6:F:303:ASP:N	2.54	0.40
14:N:179:ILE:HG12	14:N:184:VAL:HG22	2.03	0.40
17:Q:83:PHE:O	17:Q:87:ASN:ND2	2.53	0.40
23:W:192:LEU:HD23	23:W:192:LEU:HA	1.84	0.40
26:Z:26:ILE:HD11	26:Z:35:VAL:HG22	2.02	0.40
26:Z:79:TYR:HE1	26:Z:90:ARG:HA	1.87	0.40
26:Z:209:ARG:NH2	27:a:354:GLU:HA	2.36	0.40
27:a:341:LEU:HD13	27:a:345:GLN:HB2	2.02	0.40
30:d:121:ARG:HE	30:d:121:ARG:HB3	1.66	0.40
7:g:73:THR:HG22	7:g:76:ILE:HB	2.04	0.40
19:s:145:LEU:HD21	19:s:182:ALA:HB2	2.04	0.40
1:A:393:GLY:HA2	2:B:214:MET:HE2	2.04	0.40
5:E:295:LEU:HD23	5:E:295:LEU:HA	1.92	0.40
22:V:495:ARG:HA	22:V:495:ARG:HD2	1.98	0.40
23:W:446:ILE:HG13	26:Z:226:ILE:HD11	2.03	0.40
24:X:190:LEU:HD21	24:X:214:SER:HA	2.04	0.40
30:d:101:LEU:HG	30:d:166:PHE:CE2	2.56	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:158:ILE:HG21	30:d:163:TYR:HB2	2.04	0.40
32:f:466:LEU:HB3	32:f:485:LEU:HD23	2.03	0.40
13:m:40:ARG:NE	13:m:146:ALA:O	2.50	0.40
16:p:67:LEU:HD11	16:p:91:VAL:HG22	2.03	0.40

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	A	411/433 (95%)	371 (90%)	40 (10%)	0	100	100
2	B	386/440 (88%)	355 (92%)	30 (8%)	1 (0%)	36	67
3	C	359/398 (90%)	334 (93%)	23 (6%)	2 (1%)	21	54
4	D	378/418 (90%)	330 (87%)	43 (11%)	5 (1%)	9	38
5	E	373/403 (93%)	340 (91%)	31 (8%)	2 (0%)	24	57
6	F	372/439 (85%)	351 (94%)	21 (6%)	0	100	100
7	G	242/246 (98%)	231 (96%)	11 (4%)	0	100	100
7	g	242/246 (98%)	225 (93%)	16 (7%)	1 (0%)	30	62
8	H	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
8	h	230/234 (98%)	217 (94%)	10 (4%)	3 (1%)	9	38
9	I	248/261 (95%)	239 (96%)	7 (3%)	2 (1%)	16	48
9	i	248/261 (95%)	243 (98%)	5 (2%)	0	100	100
10	J	237/248 (96%)	229 (97%)	8 (3%)	0	100	100
10	j	237/248 (96%)	227 (96%)	10 (4%)	0	100	100
11	K	232/241 (96%)	222 (96%)	9 (4%)	1 (0%)	30	62
11	k	232/241 (96%)	224 (97%)	8 (3%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	236/263 (90%)	233 (99%)	3 (1%)	0	100	100
12	l	236/263 (90%)	228 (97%)	8 (3%)	0	100	100
13	M	238/255 (93%)	236 (99%)	2 (1%)	0	100	100
13	m	238/255 (93%)	234 (98%)	4 (2%)	0	100	100
14	N	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
14	n	200/239 (84%)	194 (97%)	6 (3%)	0	100	100
15	O	218/277 (79%)	213 (98%)	5 (2%)	0	100	100
15	o	218/277 (79%)	214 (98%)	4 (2%)	0	100	100
16	P	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
16	p	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
17	Q	197/201 (98%)	193 (98%)	4 (2%)	0	100	100
17	q	197/201 (98%)	193 (98%)	4 (2%)	0	100	100
18	R	199/263 (76%)	192 (96%)	7 (4%)	0	100	100
18	r	199/263 (76%)	196 (98%)	3 (2%)	0	100	100
19	S	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
19	s	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
20	T	214/264 (81%)	210 (98%)	4 (2%)	0	100	100
20	t	214/264 (81%)	208 (97%)	6 (3%)	0	100	100
21	U	864/953 (91%)	819 (95%)	45 (5%)	0	100	100
22	V	470/534 (88%)	453 (96%)	17 (4%)	0	100	100
23	W	439/456 (96%)	431 (98%)	8 (2%)	0	100	100
24	X	420/422 (100%)	399 (95%)	21 (5%)	0	100	100
25	Y	387/389 (100%)	375 (97%)	12 (3%)	0	100	100
26	Z	284/324 (88%)	250 (88%)	34 (12%)	0	100	100
27	a	371/376 (99%)	339 (91%)	32 (9%)	0	100	100
28	b	189/377 (50%)	170 (90%)	18 (10%)	1 (0%)	24	57
29	c	285/310 (92%)	252 (88%)	30 (10%)	3 (1%)	11	41
30	d	255/350 (73%)	220 (86%)	35 (14%)	0	100	100
31	e	48/70 (69%)	40 (83%)	8 (17%)	0	100	100
32	f	840/908 (92%)	800 (95%)	39 (5%)	1 (0%)	48	79
33	w	74/76 (97%)	72 (97%)	2 (3%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	13413/14952 (90%)	12709 (95%)	682 (5%)	22 (0%)	44	73

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	91	PRO
3	C	129	ASN
4	D	125	LYS
5	E	386	TYR
28	b	23	PRO
32	f	66	LYS
4	D	154	LEU
5	E	385	ASP
29	c	156	VAL
29	c	157	ILE
7	g	4	GLY
8	h	4	ARG
8	h	53	LYS
8	h	54	SER
4	D	127	ASN
9	I	53	HIS
4	D	85	ILE
4	D	152	MET
2	B	169	PRO
11	K	130	PRO
9	I	203	VAL
29	c	155	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	A	352/372 (95%)	351 (100%)	1 (0%)	86	84
2	B	341/385 (89%)	340 (100%)	1 (0%)	86	84
3	C	314/346 (91%)	309 (98%)	5 (2%)	55	68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	333/366 (91%)	325 (98%)	8 (2%)	43	62
5	E	298/353 (84%)	298 (100%)	0	100	100
6	F	296/379 (78%)	295 (100%)	1 (0%)	86	84
7	G	205/210 (98%)	205 (100%)	0	100	100
7	g	202/210 (96%)	200 (99%)	2 (1%)	68	74
8	H	188/191 (98%)	188 (100%)	0	100	100
8	h	188/191 (98%)	187 (100%)	1 (0%)	81	81
9	I	206/221 (93%)	204 (99%)	2 (1%)	68	74
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	201/211 (95%)	199 (99%)	2 (1%)	68	74
10	j	196/211 (93%)	196 (100%)	0	100	100
11	K	193/203 (95%)	193 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/224 (90%)	202 (100%)	0	100	100
12	l	201/224 (90%)	201 (100%)	0	100	100
13	M	196/212 (92%)	196 (100%)	0	100	100
13	m	198/212 (93%)	198 (100%)	0	100	100
14	N	157/181 (87%)	157 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	179/228 (78%)	179 (100%)	0	100	100
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	172 (100%)	0	100	100
16	p	173/174 (99%)	173 (100%)	0	100	100
17	Q	168/171 (98%)	168 (100%)	0	100	100
17	q	168/171 (98%)	168 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	156/202 (77%)	156 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	178/199 (89%)	178 (100%)	0	100	100
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	179 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U	742/816 (91%)	742 (100%)	0	100	100
22	V	391/460 (85%)	391 (100%)	0	100	100
23	W	406/416 (98%)	406 (100%)	0	100	100
24	X	362/362 (100%)	362 (100%)	0	100	100
25	Y	344/344 (100%)	344 (100%)	0	100	100
26	Z	257/295 (87%)	257 (100%)	0	100	100
27	a	333/336 (99%)	333 (100%)	0	100	100
28	b	167/312 (54%)	166 (99%)	1 (1%)	78	79
29	c	252/268 (94%)	248 (98%)	4 (2%)	55	68
30	d	231/294 (79%)	230 (100%)	1 (0%)	84	83
31	e	44/63 (70%)	44 (100%)	0	100	100
32	f	711/763 (93%)	709 (100%)	2 (0%)	86	84
33	w	68/68 (100%)	68 (100%)	0	100	100
All	All	11395/12682 (90%)	11364 (100%)	31 (0%)	84	84

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	403	ILE
2	B	170	LEU
3	C	90	HIS
3	C	109	THR
3	C	127	LEU
3	C	129	ASN
3	C	210	THR
4	D	83	GLN
4	D	125	LYS
4	D	127	ASN
4	D	148	ASP
4	D	151	ILE
4	D	153	MET
4	D	154	LEU
4	D	369	LYS
6	F	218	GLN
9	I	52	ILE
9	I	203	VAL
10	J	220	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	J	221	ASN
28	b	24	THR
29	c	155	VAL
29	c	157	ILE
29	c	196	LEU
29	c	198	ARG
30	d	122	LEU
32	f	66	LYS
32	f	67	ASP
7	g	3	ARG
7	g	6	SER
8	h	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	94	GLN
1	A	148	GLN
1	A	150	HIS
1	A	203	ASN
1	A	247	GLN
1	A	296	GLN
2	B	57	GLN
2	B	242	GLN
3	C	32	GLN
3	C	67	GLN
3	C	90	HIS
3	C	129	ASN
3	C	205	HIS
4	D	83	GLN
4	D	127	ASN
4	D	221	HIS
4	D	353	ASN
4	D	412	GLN
4	D	414	HIS
5	E	307	GLN
5	E	339	ASN
6	F	321	GLN
6	F	417	HIS
7	G	75	ASN
7	G	150	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	H	88	HIS
10	J	175	ASN
10	J	215	GLN
10	J	221	ASN
11	K	13	ASN
11	K	186	HIS
11	K	204	GLN
12	L	69	HIS
12	L	143	HIS
14	N	77	HIS
14	N	106	GLN
17	Q	32	HIS
17	Q	82	ASN
17	Q	101	ASN
17	Q	168	GLN
18	R	162	GLN
20	T	3	ASN
21	U	258	GLN
21	U	259	GLN
21	U	267	ASN
21	U	355	ASN
21	U	421	GLN
21	U	698	GLN
22	V	260	HIS
22	V	299	GLN
22	V	401	ASN
22	V	427	GLN
22	V	473	GLN
23	W	362	ASN
24	X	170	GLN
24	X	178	HIS
24	X	346	GLN
25	Y	94	ASN
25	Y	160	ASN
25	Y	344	HIS
26	Z	24	ASN
26	Z	109	ASN
26	Z	194	GLN
26	Z	223	ASN
26	Z	256	GLN
27	a	18	GLN
27	a	164	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
27	a	169	HIS
27	a	249	GLN
29	c	101	GLN
29	c	172	HIS
29	c	237	HIS
29	c	241	ASN
29	c	295	ASN
30	d	60	GLN
32	f	156	HIS
32	f	171	GLN
32	f	329	ASN
7	g	128	ASN
9	i	40	ASN
9	i	177	GLN
10	j	175	ASN
10	j	215	GLN
14	n	158	ASN
15	o	116	HIS
17	q	82	ASN
18	r	85	ASN
18	r	162	GLN
19	s	146	GLN
19	s	151	ASN
33	w	68	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	ATP	D	501	35	29,33,33	0.29	0	44,52,52	0.51	1 (2%)
36	ADP	C	501	-	27,29,29	1.36	4 (14%)	42,45,45	2.05	9 (21%)
34	ATP	E	401	35	29,33,33	0.27	0	44,52,52	0.44	1 (2%)
36	ADP	F	501	35	27,29,29	1.36	4 (14%)	42,45,45	1.98	11 (26%)
34	ATP	B	501	35	29,33,33	0.28	0	44,52,52	0.45	1 (2%)
34	ATP	A	501	35	29,33,33	0.28	0	44,52,52	0.46	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	ATP	D	501	35	-	7/22/38/38	0/3/3/3
36	ADP	C	501	-	-	2/16/32/32	0/3/3/3
34	ATP	E	401	35	-	4/22/38/38	0/3/3/3
36	ADP	F	501	35	-	7/16/32/32	0/3/3/3
34	ATP	B	501	35	-	5/22/38/38	0/3/3/3
34	ATP	A	501	35	-	2/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	501	ADP	C5-C4	4.59	1.47	1.39
36	F	501	ADP	C5-C4	4.48	1.47	1.39
36	C	501	ADP	C5-C6	2.68	1.48	1.41
36	F	501	ADP	C5-C6	2.66	1.48	1.41
36	F	501	ADP	C8-N7	2.44	1.36	1.31
36	C	501	ADP	C8-N7	2.32	1.36	1.31
36	C	501	ADP	C5-N7	-2.27	1.34	1.39
36	F	501	ADP	C5-N7	-2.18	1.34	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	501	ADP	C5-C4-N3	-6.72	117.98	126.75
36	F	501	ADP	C5-C4-N3	-6.18	118.69	126.75
36	C	501	ADP	N3-C4-N9	5.30	135.82	127.08
36	F	501	ADP	N3-C4-N9	4.75	134.91	127.08
36	C	501	ADP	C2-N3-C4	4.05	121.32	111.75
36	F	501	ADP	C2-N3-C4	3.86	120.86	111.75
36	F	501	ADP	PA-O3A-PB	-3.85	119.61	132.83
36	C	501	ADP	PA-O3A-PB	-3.66	120.28	132.83
36	F	501	ADP	C4-C5-N7	-3.31	106.59	110.62
36	C	501	ADP	C4-C5-N7	-3.17	106.76	110.62
36	C	501	ADP	N3-C2-N1	-3.11	123.73	128.60
36	F	501	ADP	N3-C2-N1	-3.11	123.74	128.60
36	C	501	ADP	C5-N7-C8	2.75	107.41	103.51
36	F	501	ADP	C5-N7-C8	2.74	107.40	103.51
36	C	501	ADP	C3'-C2'-C1'	2.71	106.58	101.43
36	F	501	ADP	C4-N9-C8	2.51	108.45	105.73
36	F	501	ADP	C3'-C2'-C1'	2.40	105.98	101.43
36	C	501	ADP	C4-N9-C8	2.30	108.22	105.73
36	F	501	ADP	C6-C5-N7	2.20	136.11	132.02
34	A	501	ATP	PB-O3B-PG	2.04	139.84	132.83
34	B	501	ATP	PB-O3B-PG	2.02	139.77	132.83
34	D	501	ATP	PB-O3B-PG	2.02	139.77	132.83
34	E	401	ATP	PB-O3B-PG	2.02	139.76	132.83
36	F	501	ADP	N9-C8-N7	-2.01	111.17	113.91

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	D	501	ATP	C5'-O5'-PA-O1A
34	D	501	ATP	C5'-O5'-PA-O2A
34	D	501	ATP	C5'-O5'-PA-O3A
36	C	501	ADP	C5'-O5'-PA-O3A
36	F	501	ADP	C3'-C4'-C5'-O5'
34	B	501	ATP	C3'-C4'-C5'-O5'
34	D	501	ATP	O4'-C4'-C5'-O5'
36	F	501	ADP	O4'-C4'-C5'-O5'
34	D	501	ATP	O4'-C1'-N9-C8
34	D	501	ATP	O4'-C1'-N9-C4
34	B	501	ATP	O4'-C4'-C5'-O5'
34	B	501	ATP	PB-O3B-PG-O1G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
34	D	501	ATP	C3'-C4'-C5'-O5'
34	E	401	ATP	O4'-C4'-C5'-O5'
34	B	501	ATP	C5'-O5'-PA-O3A
34	A	501	ATP	PA-O3A-PB-O2B
34	E	401	ATP	PA-O3A-PB-O2B
36	F	501	ADP	C2'-C1'-N9-C8
36	C	501	ADP	C5'-O5'-PA-O1A
34	E	401	ATP	C3'-C4'-C5'-O5'
36	F	501	ADP	O4'-C1'-N9-C4
36	F	501	ADP	O4'-C1'-N9-C8
36	F	501	ADP	C2'-C1'-N9-C4
34	B	501	ATP	PA-O3A-PB-O1B
34	A	501	ATP	PA-O3A-PB-O1B
34	E	401	ATP	C5'-O5'-PA-O1A
36	F	501	ADP	C5'-O5'-PA-O1A

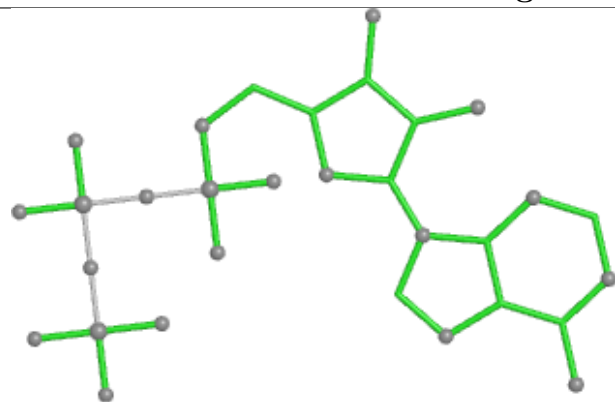
There are no ring outliers.

6 monomers are involved in 8 short contacts:

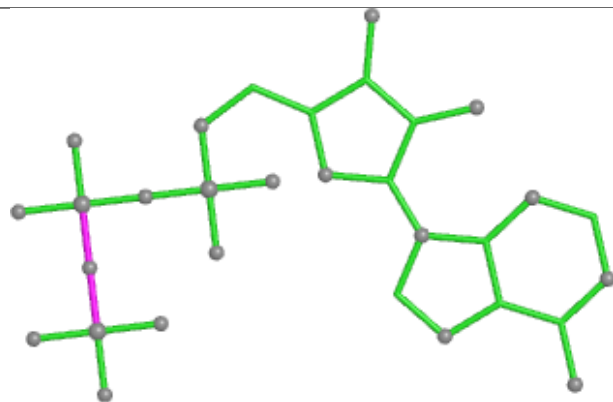
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	D	501	ATP	2	0
36	C	501	ADP	1	0
34	E	401	ATP	1	0
36	F	501	ADP	1	0
34	B	501	ATP	1	0
34	A	501	ATP	2	0

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

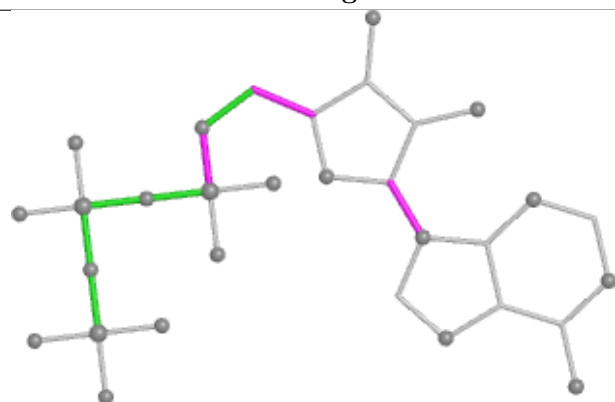
## Ligand ATP D 501



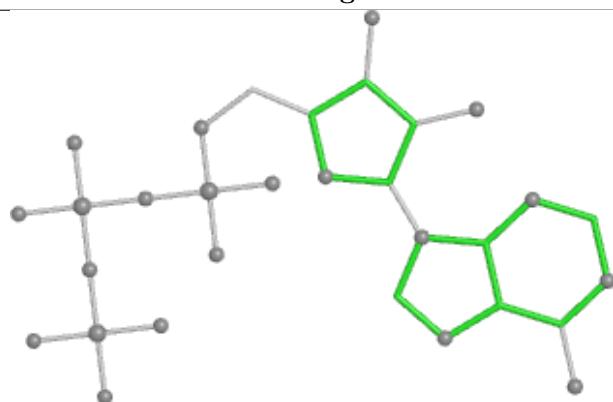
Bond lengths



Bond angles

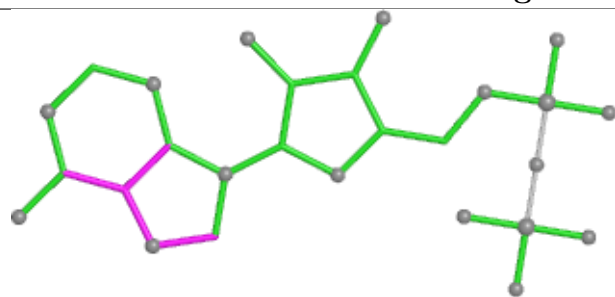


Torsions

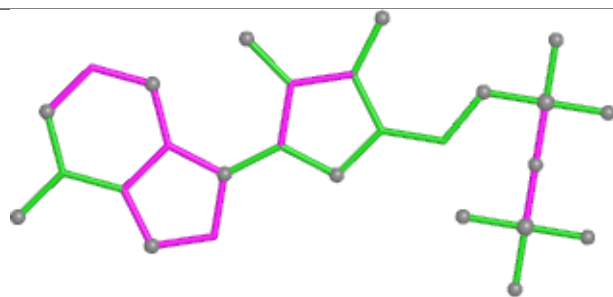


Rings

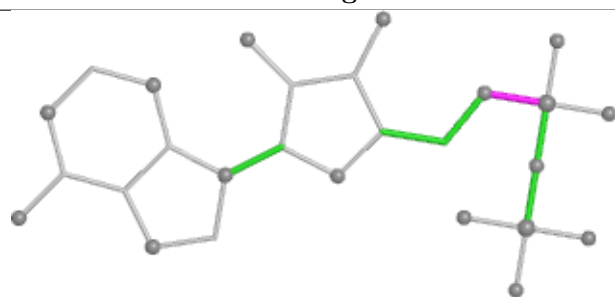
## Ligand ADP C 501



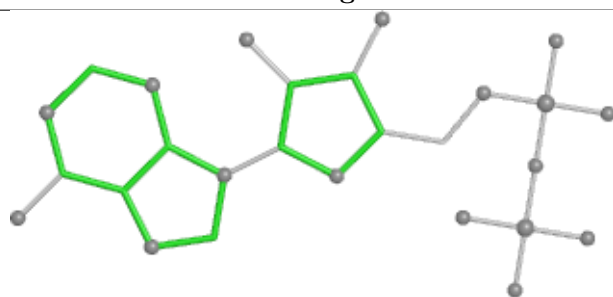
Bond lengths



Bond angles

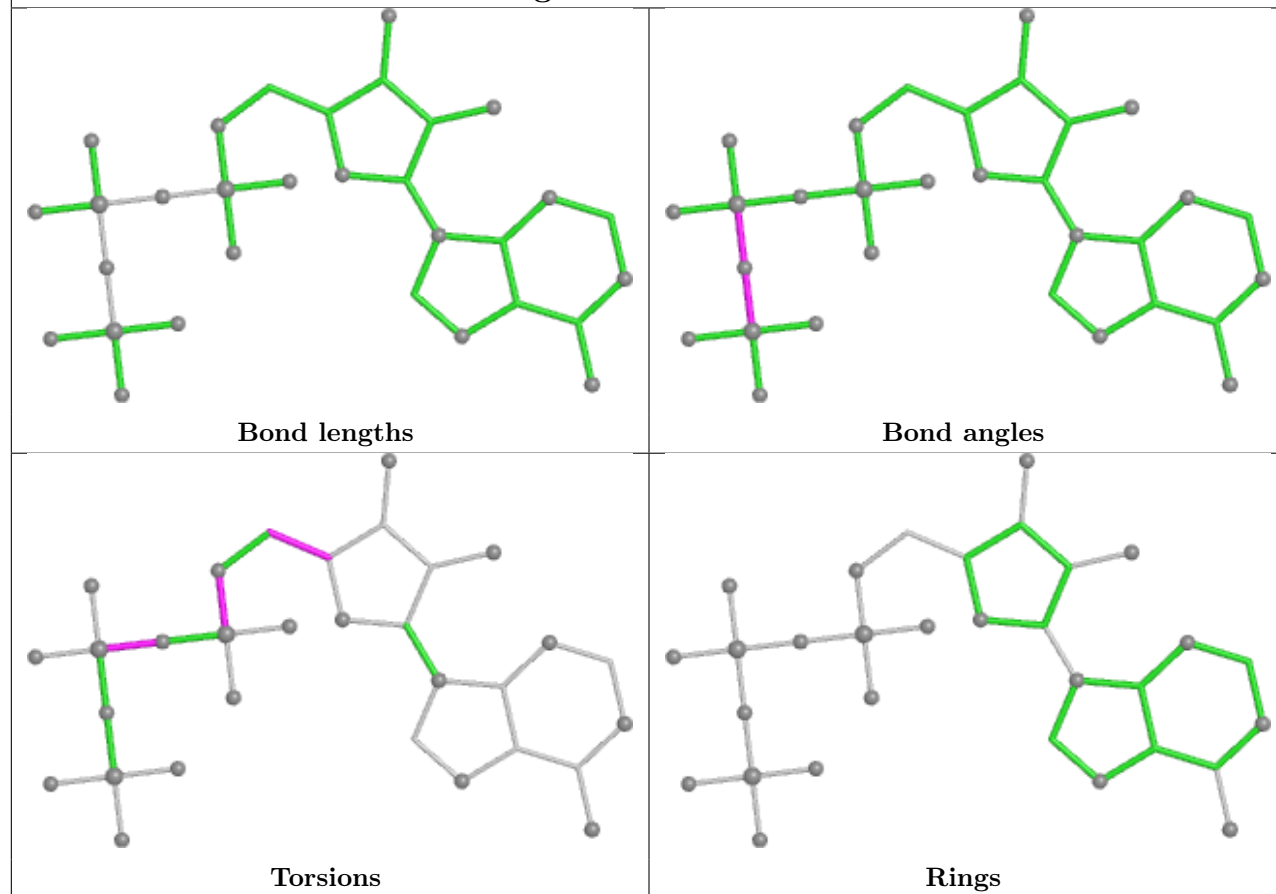


Torsions

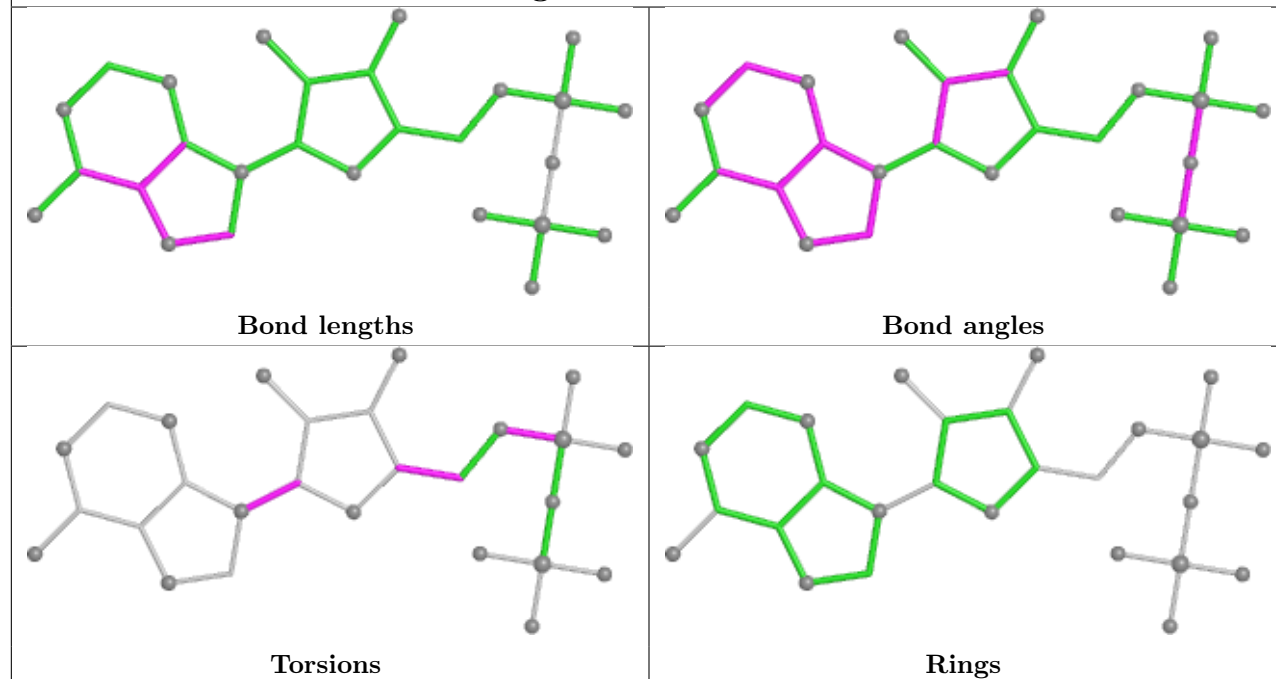


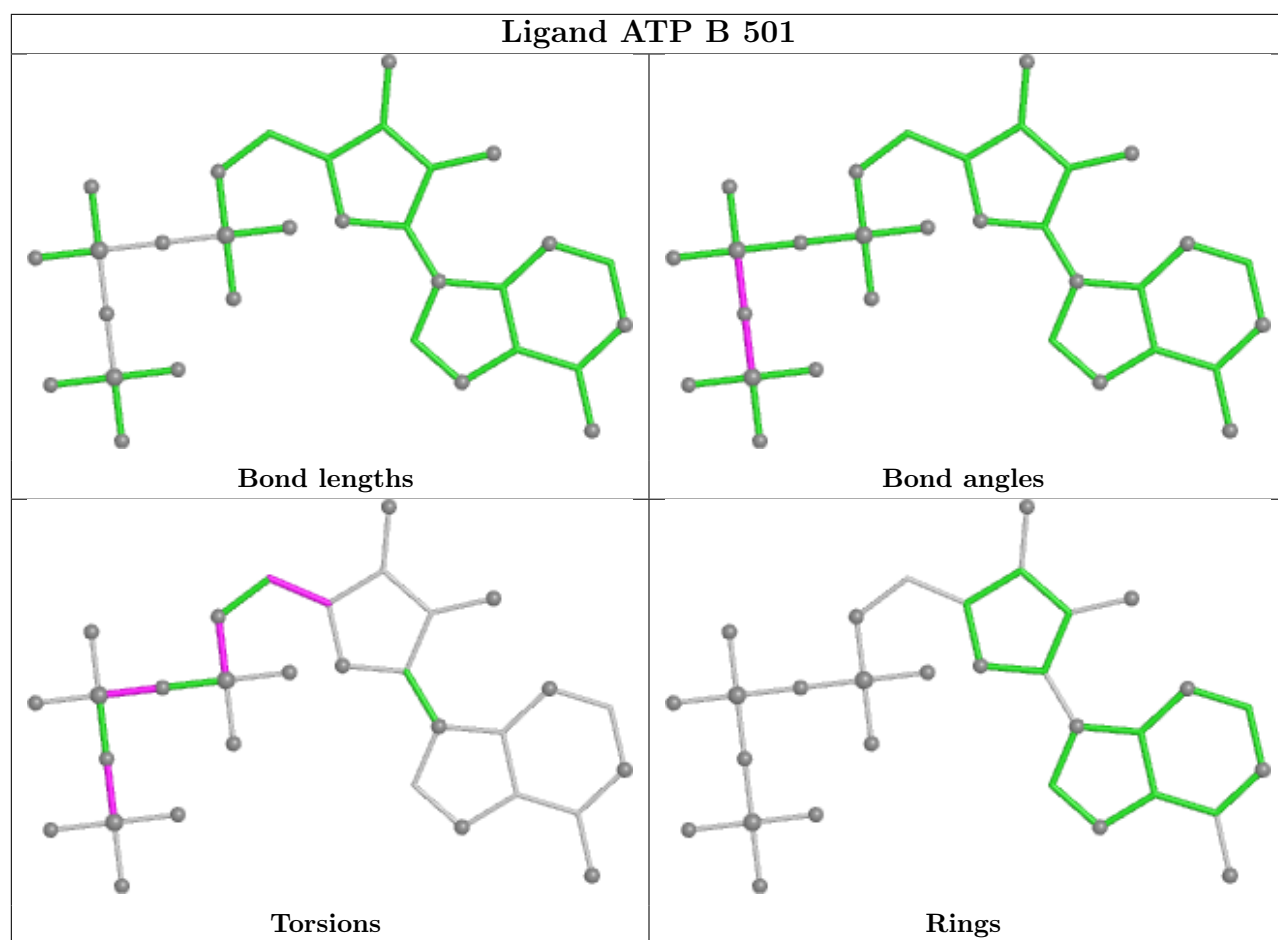
Rings

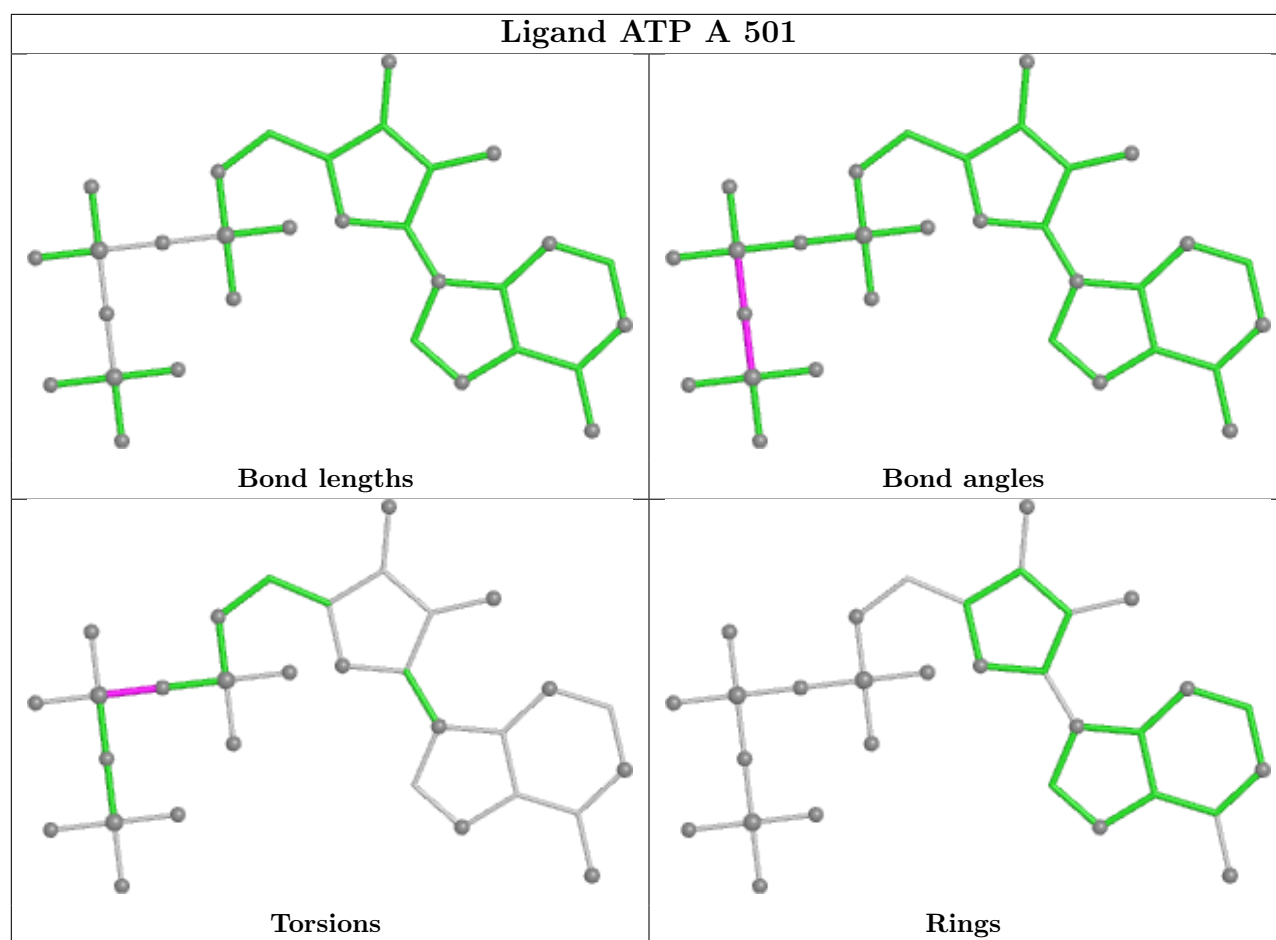
## Ligand ATP E 401



## Ligand ADP F 501







## 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.

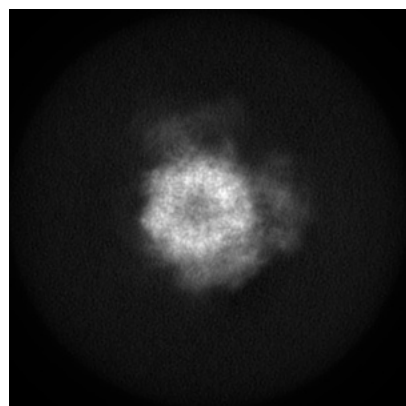
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62082. These allow visual inspection of the internal detail of the map and identification of artifacts.

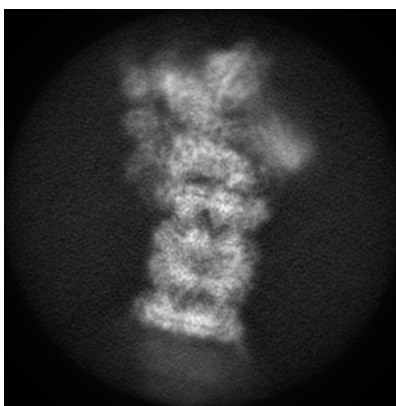
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

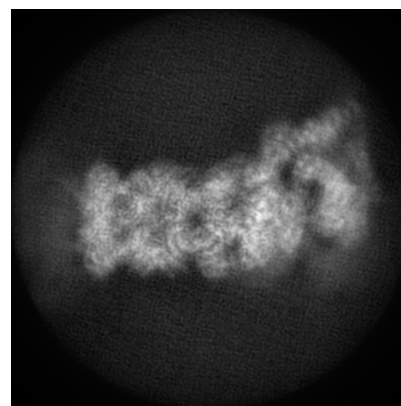
#### 6.1.1 Primary map



X

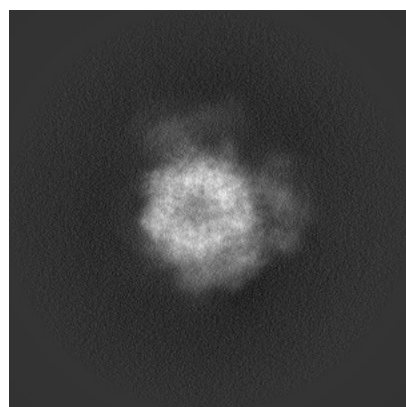


Y

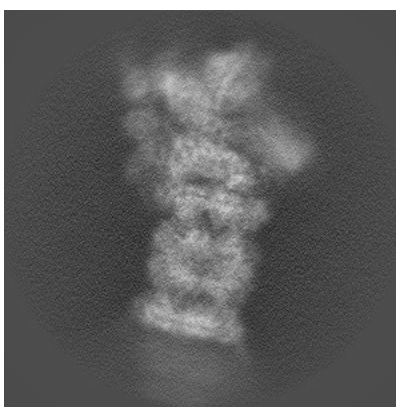


Z

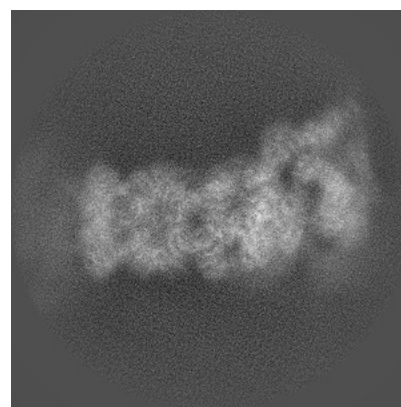
#### 6.1.2 Raw map



X



Y

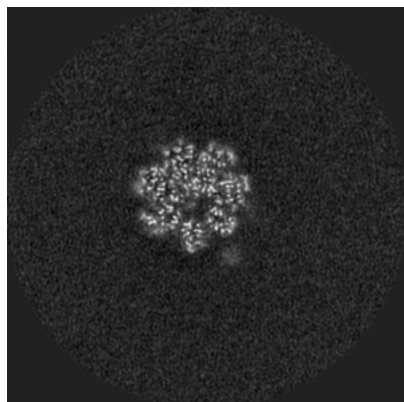


Z

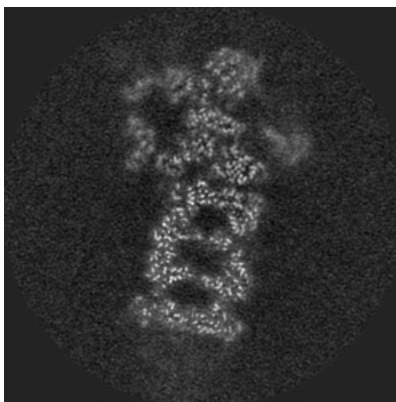
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

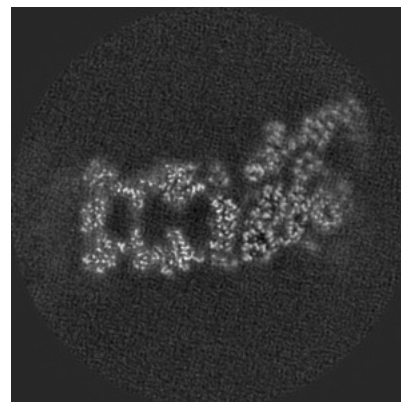
### 6.2.1 Primary map



X Index: 300

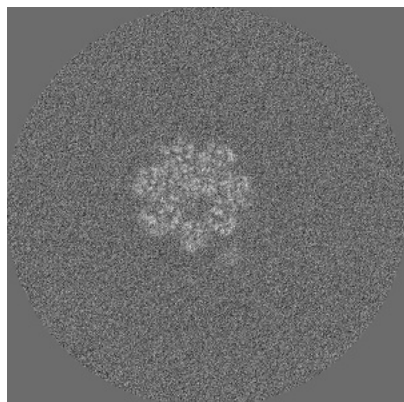


Y Index: 300

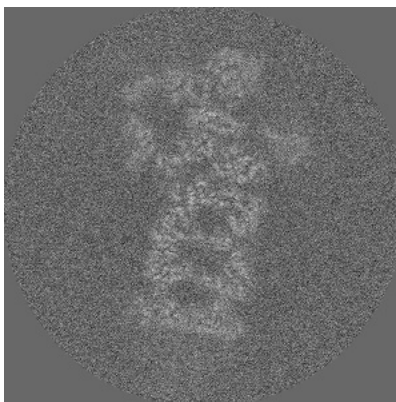


Z Index: 300

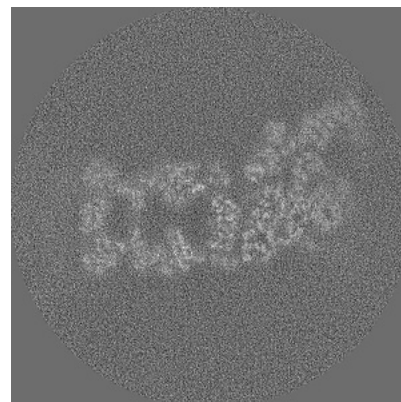
### 6.2.2 Raw map



X Index: 300



Y Index: 300

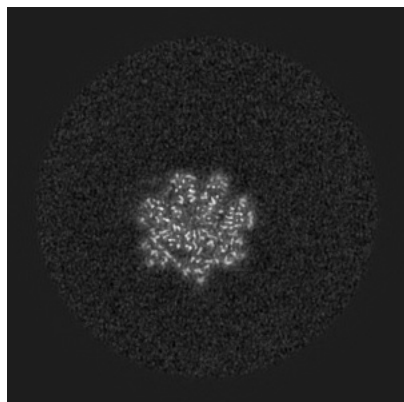


Z Index: 300

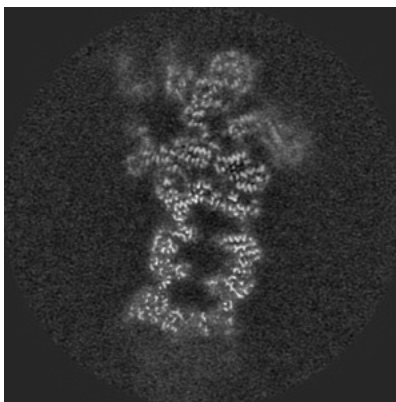
The images above show central slices of the map in three orthogonal directions.

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

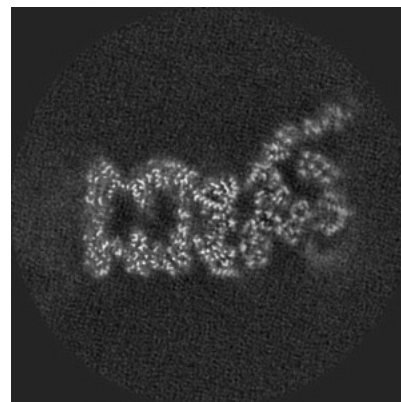
### 6.3.1 Primary map



X Index: 139

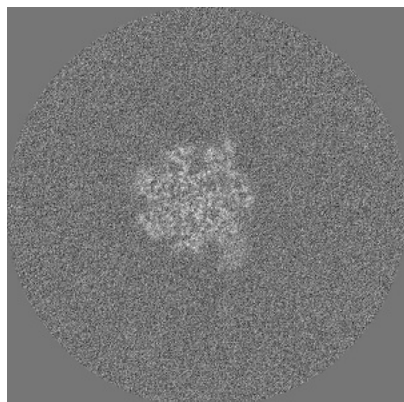


Y Index: 287

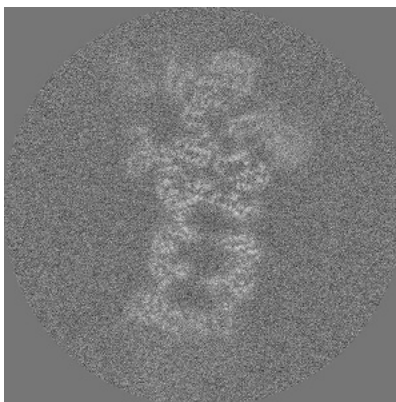


Z Index: 280

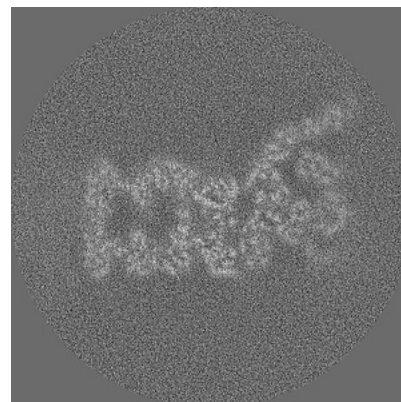
### 6.3.2 Raw map



X Index: 311



Y Index: 288

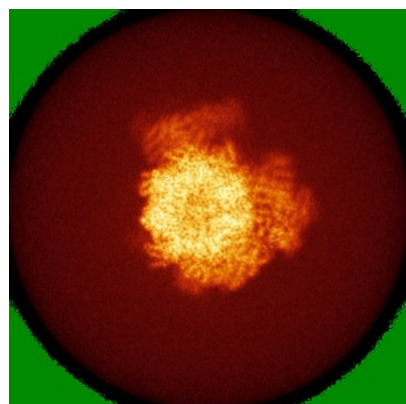


Z Index: 281

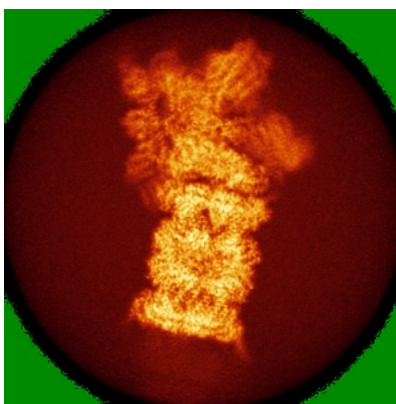
The images above show the largest variance slices of the map in three orthogonal directions.

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

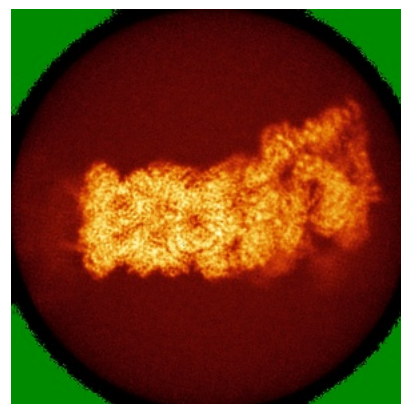
### 6.4.1 Primary map



X

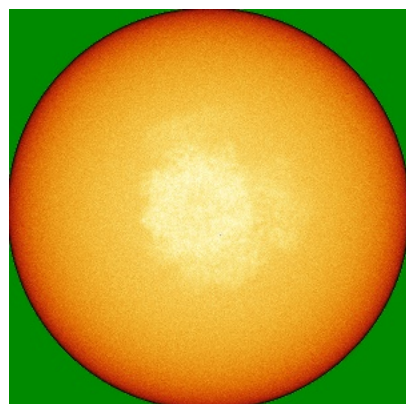


Y

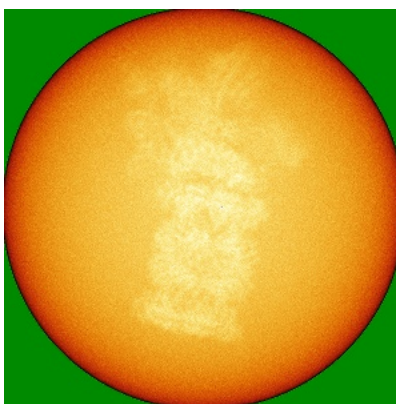


Z

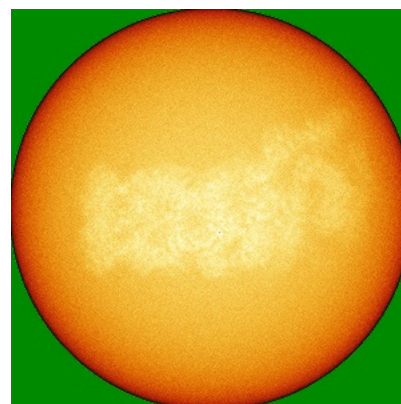
### 6.4.2 Raw map



X



Y

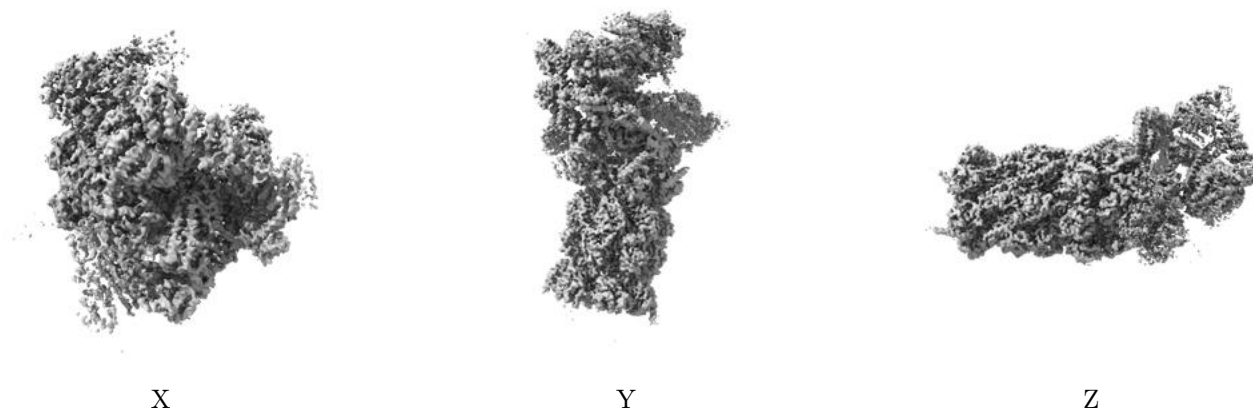


Z

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.

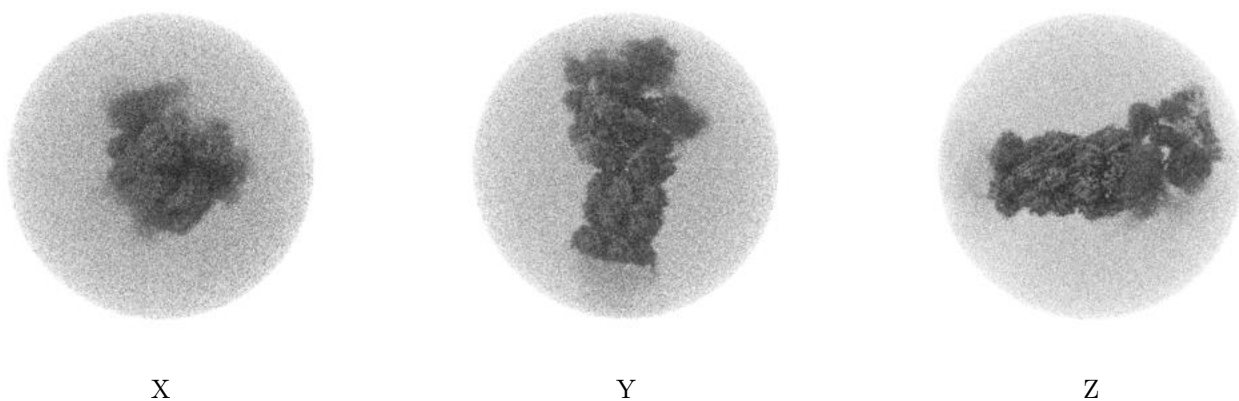
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00601. 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.

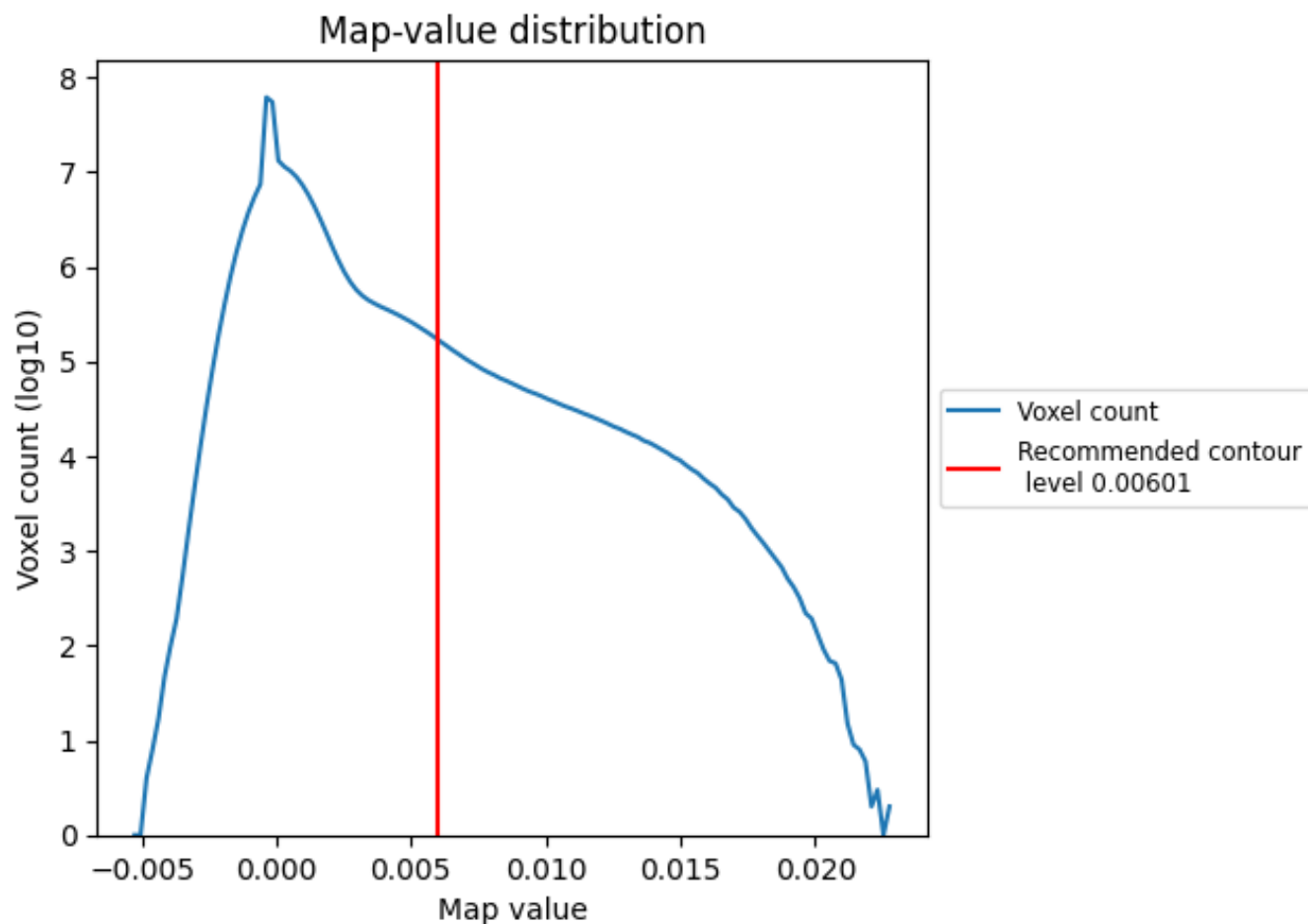
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

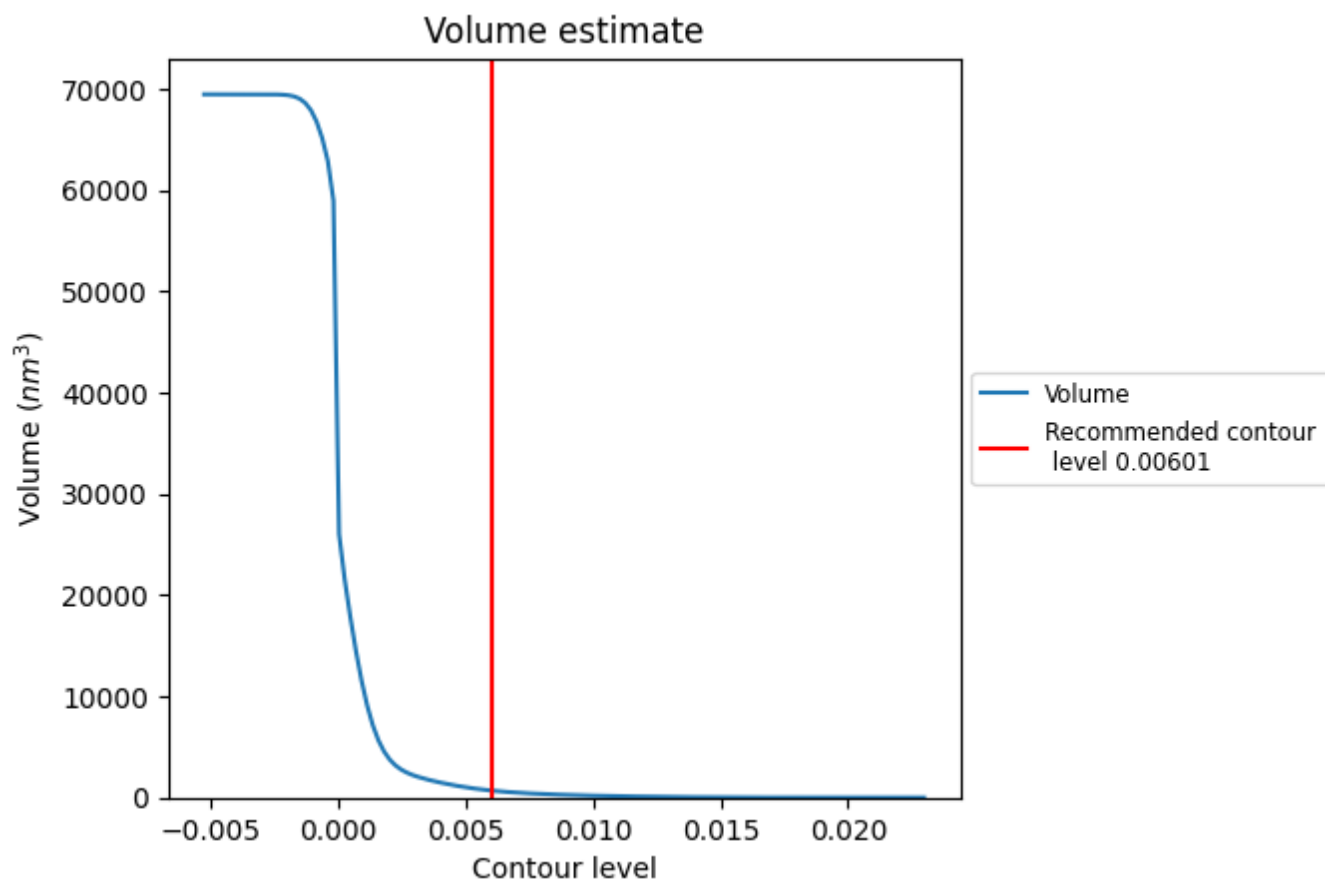
This section contains the results of statistical analysis of the map.

### 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.

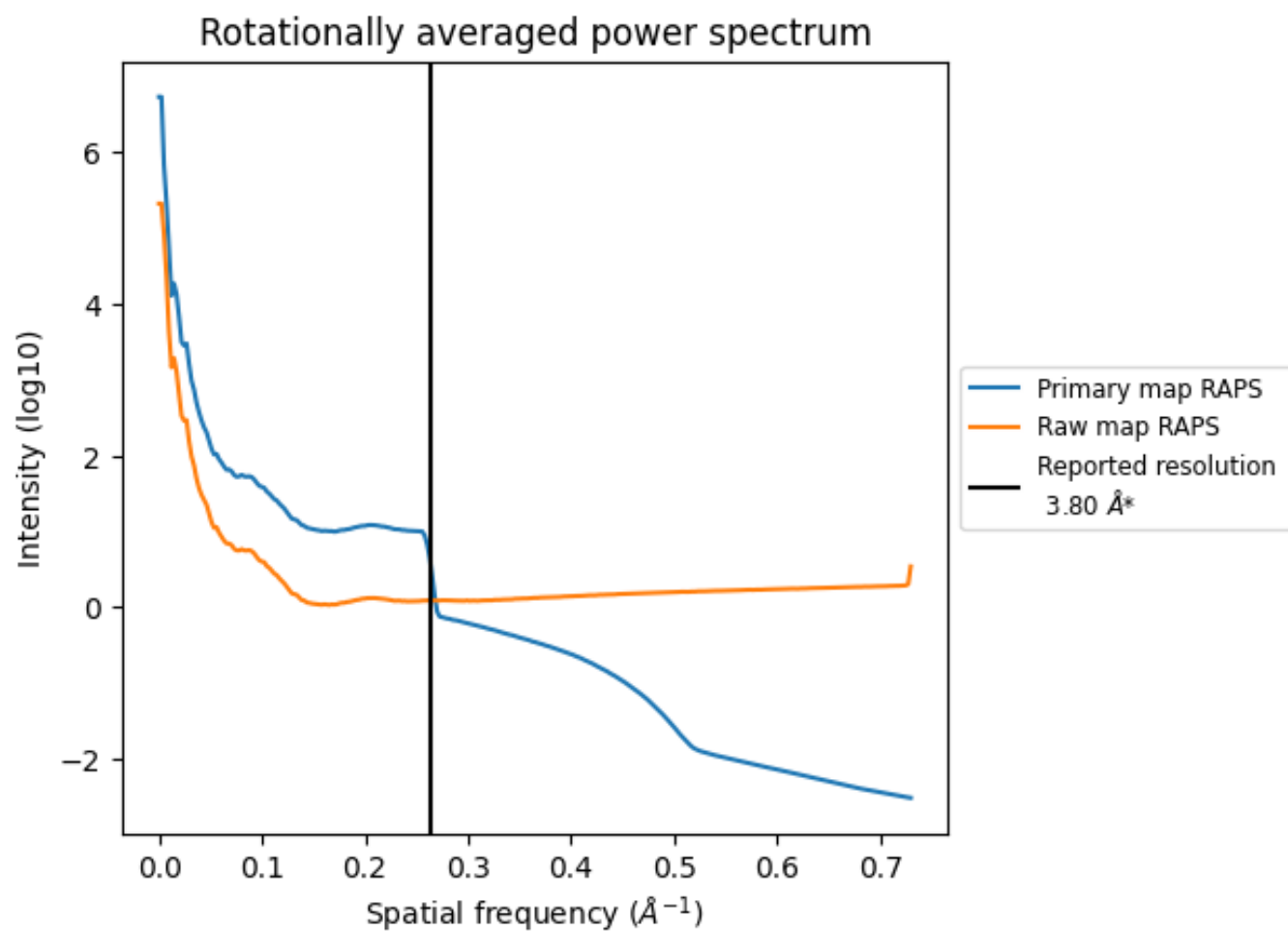
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 691 nm<sup>3</sup>; this corresponds to an approximate mass of 624 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 ⓘ

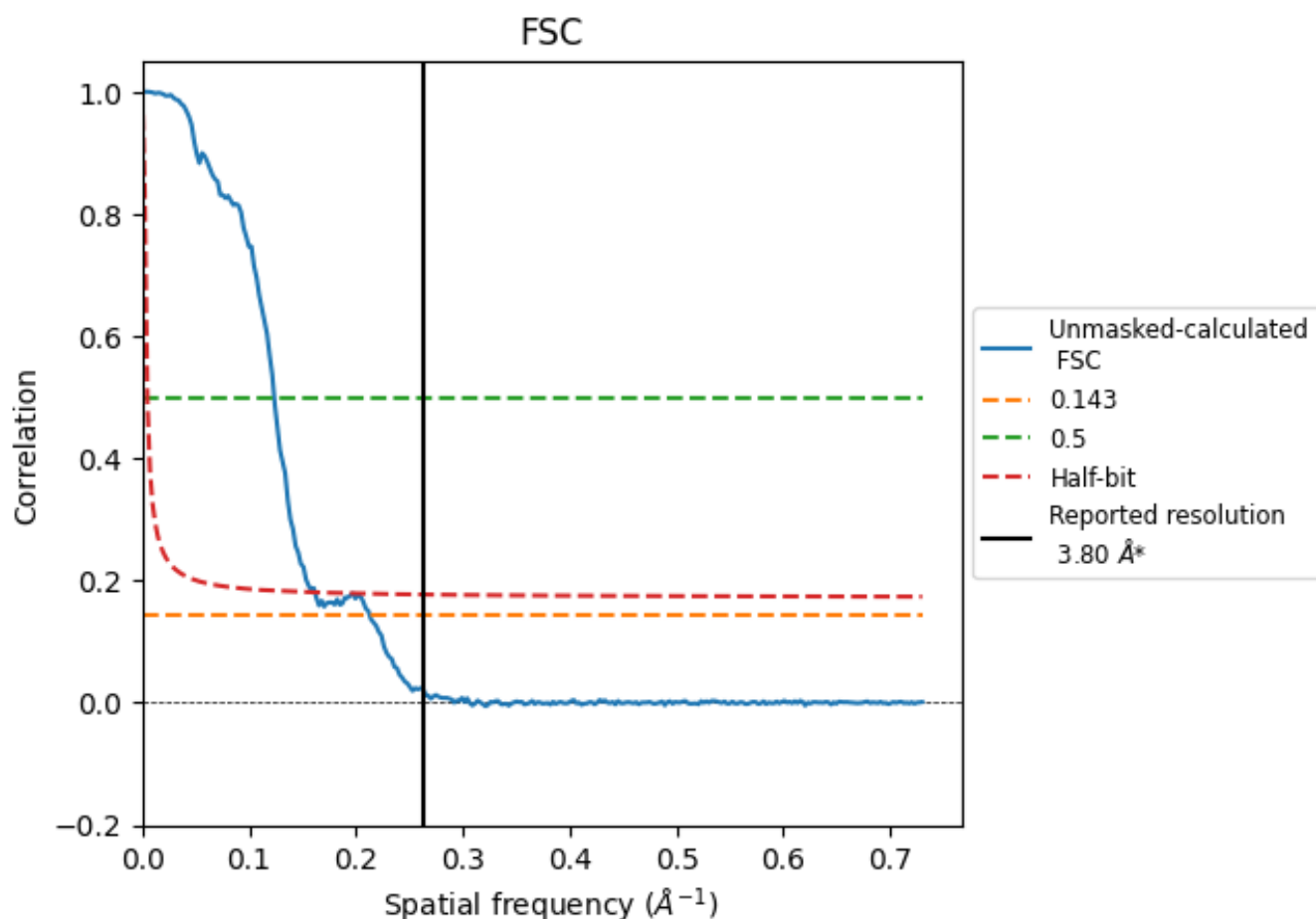


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 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 0.263  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

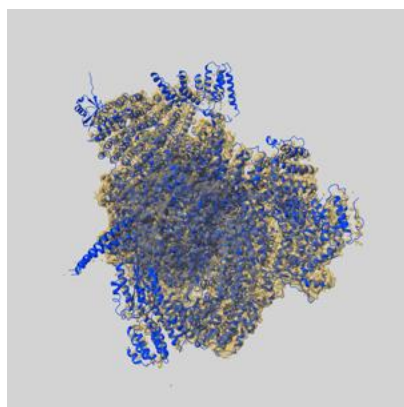
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.70	8.10	6.18

\*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 4.70 differs from the reported value 3.8 by more than 10 %

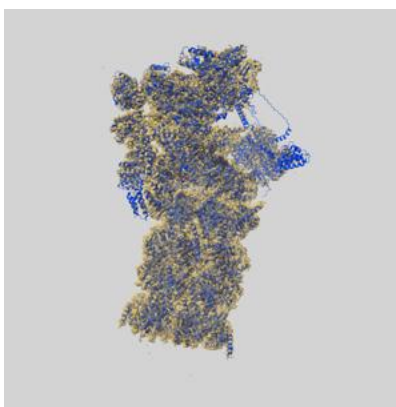
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62082 and PDB model 9K56. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

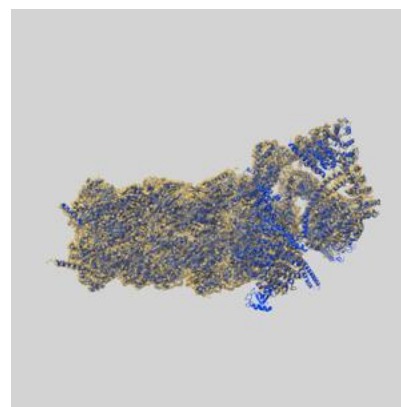
### 9.1 Map-model overlay [i](#)



X



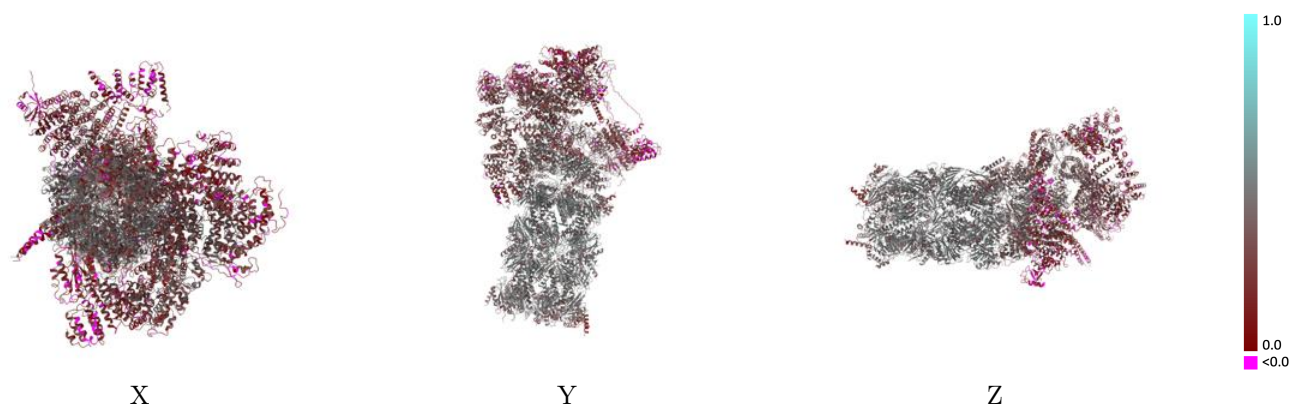
Y



Z

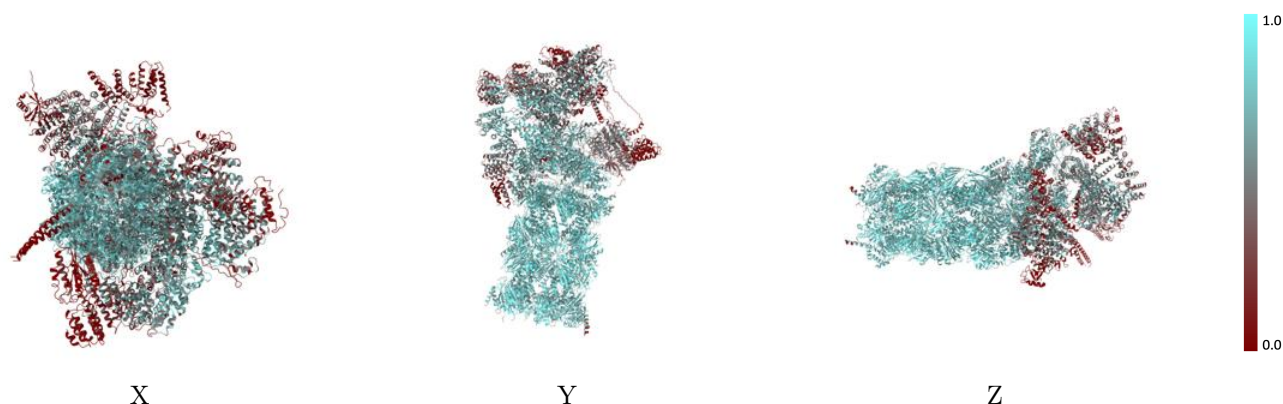
The images above show the 3D surface view of the map at the recommended contour level 0.00601 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



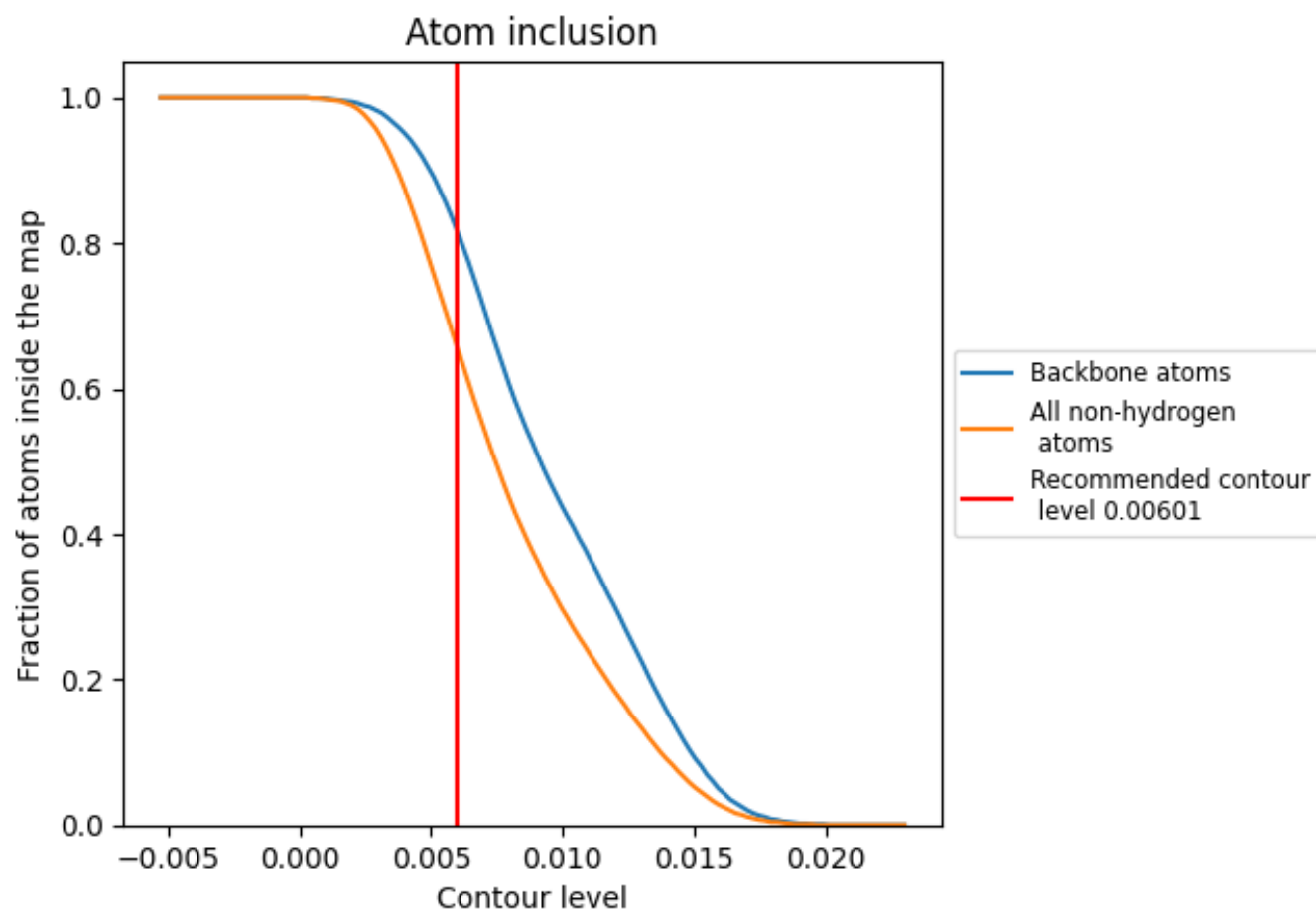
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00601).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 66% 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 (0.00601) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6560	 0.3640
A	 0.6970	 0.3780
B	 0.6690	 0.3800
C	 0.7100	 0.3960
D	 0.6820	 0.3860
E	 0.6920	 0.3870
F	 0.6930	 0.3950
G	 0.8290	 0.4600
H	 0.8330	 0.4610
I	 0.8100	 0.4450
J	 0.7870	 0.4220
K	 0.8030	 0.4590
L	 0.8520	 0.4750
M	 0.8200	 0.4520
N	 0.8700	 0.4700
O	 0.8740	 0.4740
P	 0.8700	 0.4660
Q	 0.8590	 0.4670
R	 0.8850	 0.4660
S	 0.8540	 0.4620
T	 0.8650	 0.4700
U	 0.4570	 0.2380
V	 0.3980	 0.2540
W	 0.5180	 0.2880
X	 0.4900	 0.2930
Y	 0.6690	 0.3230
Z	 0.4820	 0.2670
a	 0.3410	 0.2200
b	 0.0950	 0.1520
c	 0.5860	 0.3360
d	 0.3080	 0.1870
e	 0.4250	 0.2720
f	 0.2760	 0.1890
g	 0.8250	 0.4370
h	 0.8370	 0.4370



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
i	 0.7840	 0.4200
j	 0.7410	 0.3780
k	 0.7870	 0.4270
l	 0.8460	 0.4380
m	 0.8280	 0.4360
n	 0.8640	 0.4630
o	 0.8470	 0.4600
p	 0.8570	 0.4570
q	 0.8500	 0.4660
r	 0.8760	 0.4620
s	 0.8470	 0.4580
t	 0.8660	 0.4650
w	 0.0020	 0.0530