



Full wwPDB EM Validation Report ⓘ

Apr 21, 2026 – 10:43 AM JST

PDB ID : 9K4P / pdb_00009k4p
EMDB ID : EMD-62066
Title : Structure of substrate-engaged human 26S proteasome RP-CP subcomplex in state EA2.3
Authors : Wu, Z.; Chen, E.; Mao, Y.
Deposited on : 2024-10-21
Resolution : 4.80 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

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

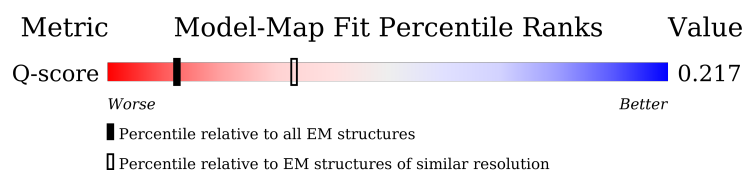
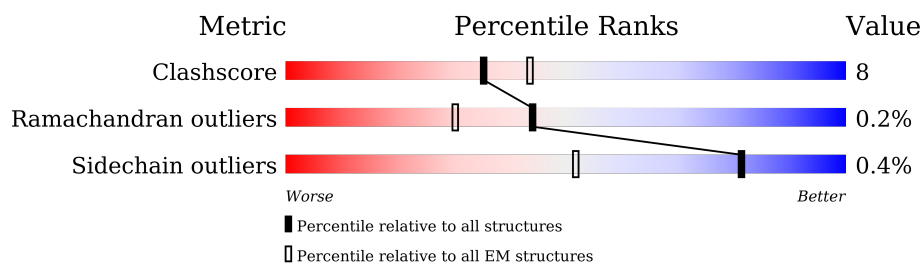
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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	1575 (4.30 - 5.30)

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 ≥ 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	

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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	

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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	u	76	
33	z	76	
34	v	10	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 106531 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	394	Total	C	N	O	S	0	0
			3096	1951	543	584	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	384	Total	C	N	O	S	0	0
			3018	1901	515	587	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	389	Total	C	N	O	S	0	0
			3097	1947	552	581	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	415	Total	C	N	O	S	0	0
			3251	2038	561	634	18		

- 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	1	0
			1958	1236	336	376	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		

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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	818	Total	C	N	O	S	0	0
			6373	4047	1084	1197	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	444	Total	C	N	O	S	0	0
			3612	2301	645	653	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		

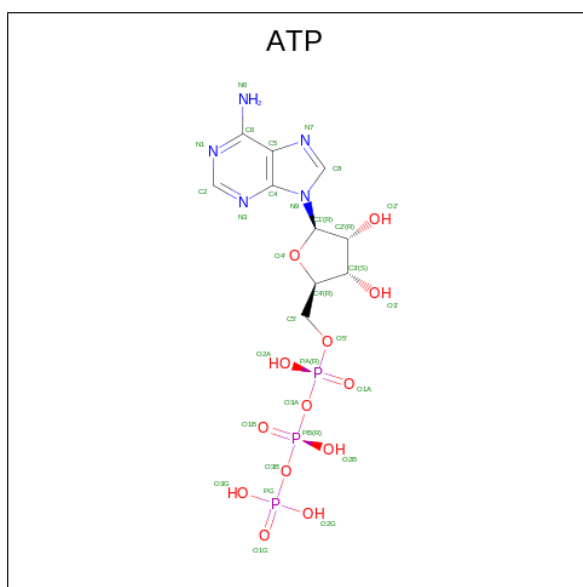
- Molecule 33 is a protein called Ubiquitin.

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

- Molecule 34 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	v	10	Total	C	N	O	0	0
			53	32	11	10		

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

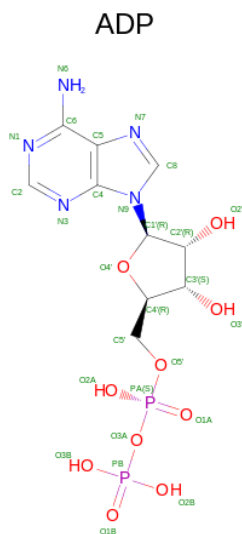


Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
36	B	2	Total	Mg	0
			2	2	
36	D	1	Total	Mg	0
			1	1	
36	E	1	Total	Mg	0
			1	1	
36	F	1	Total	Mg	0
			1	1	

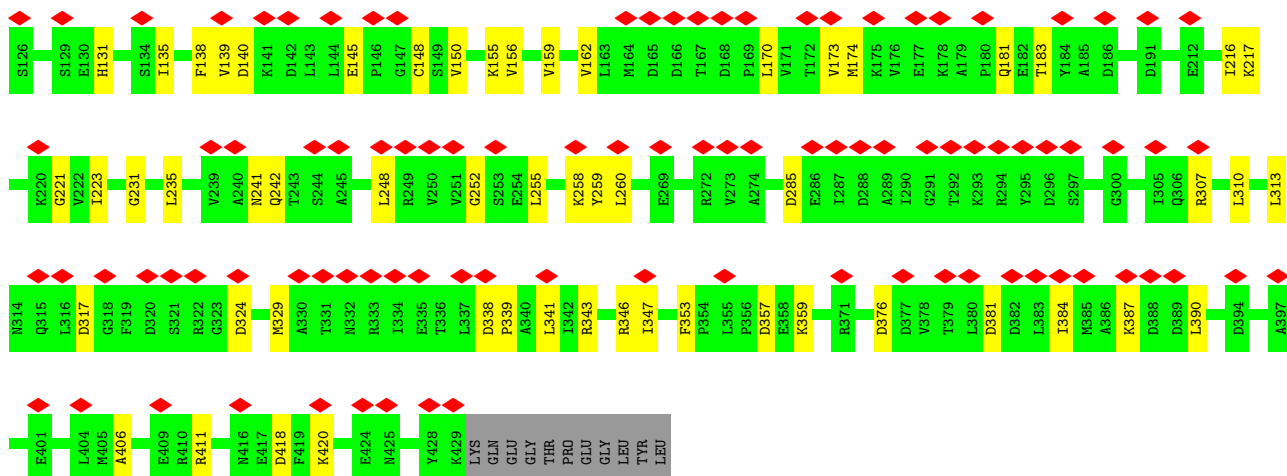
- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



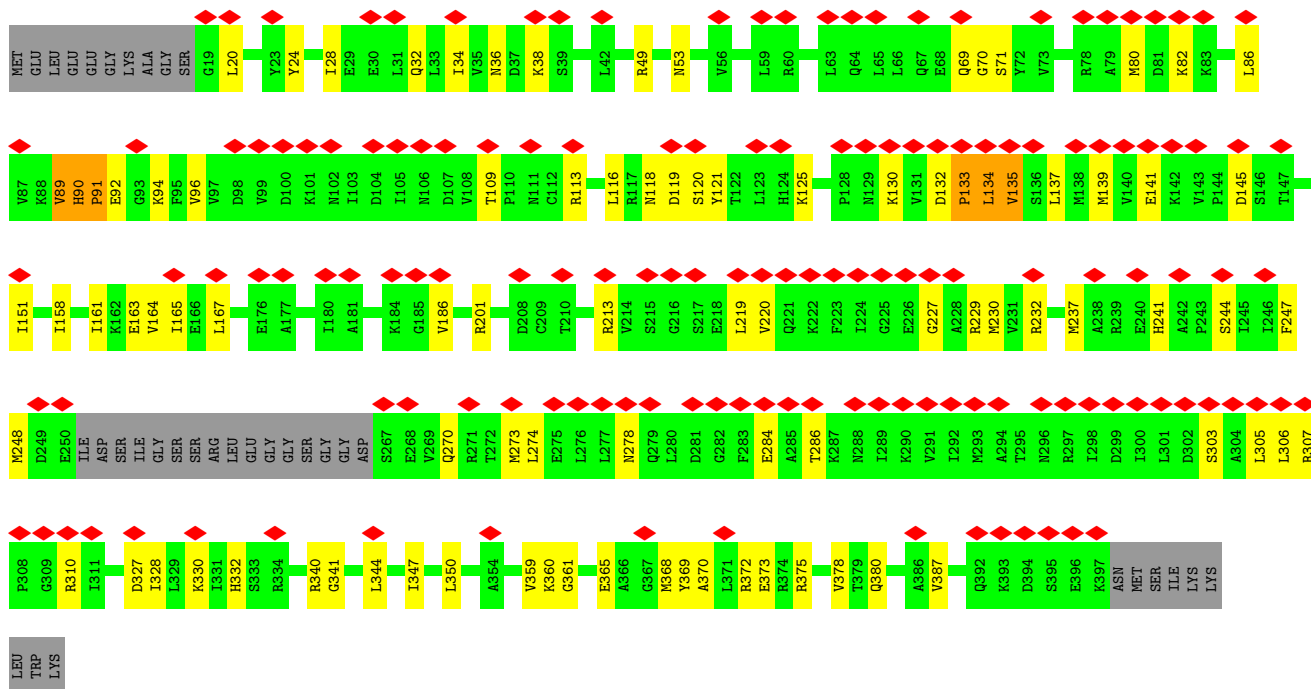
Mol	Chain	Residues	Atoms					AltConf
37	C	1	Total 27	C 10	N 5	O 10	P 2	0
37	F	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

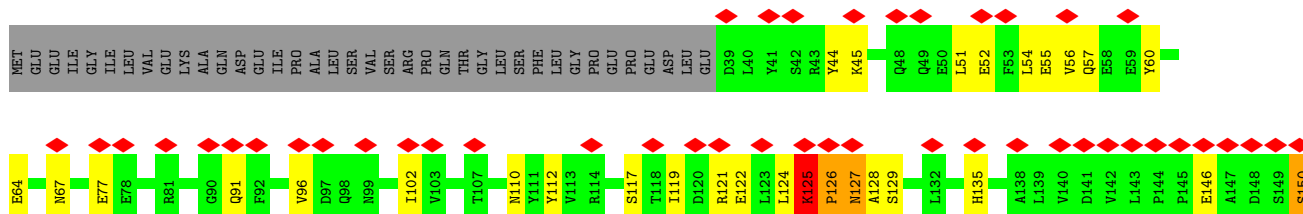
Mol	Chain	Residues	Atoms	AltConf
38	c	1	Total Zn 1 1	0

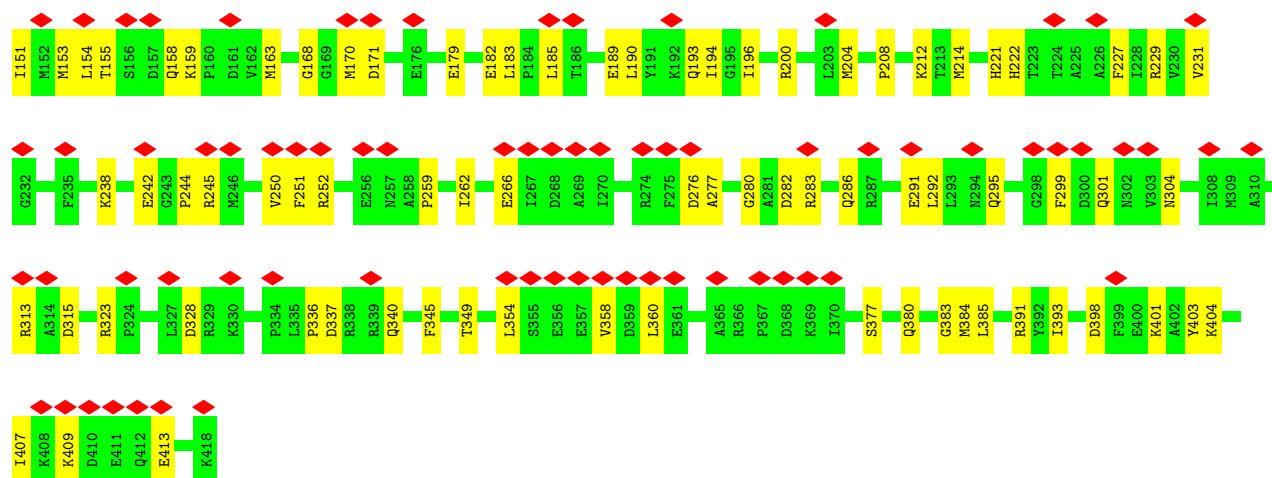


• Molecule 3: 26S proteasome regulatory subunit 8

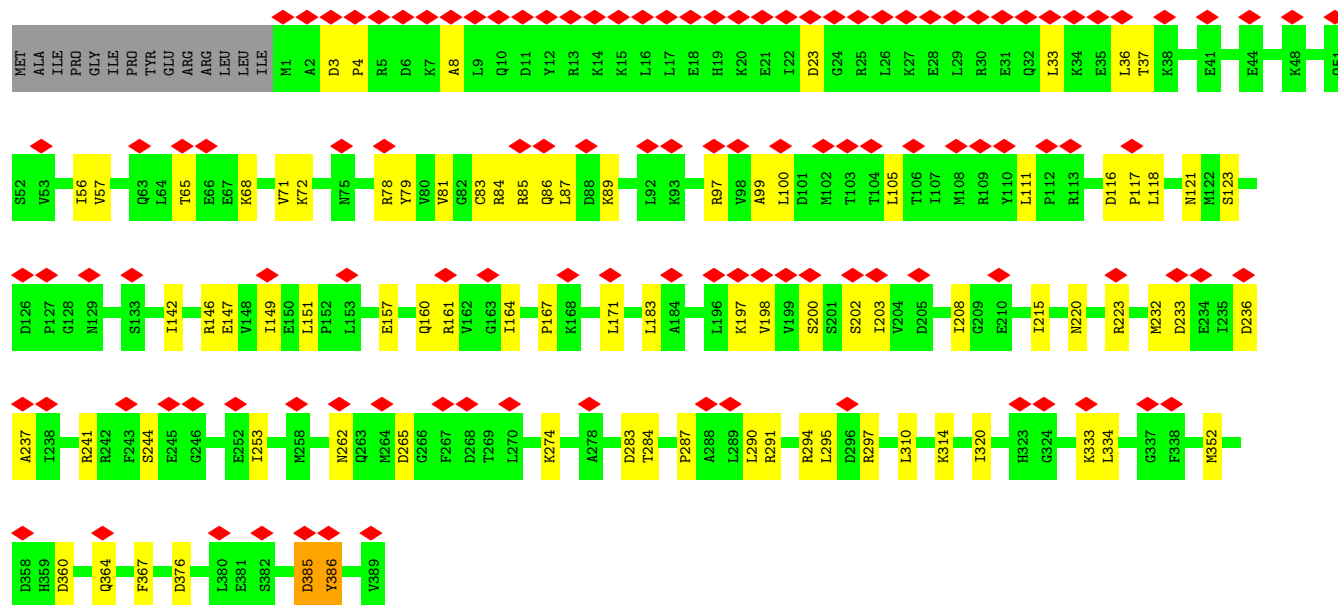
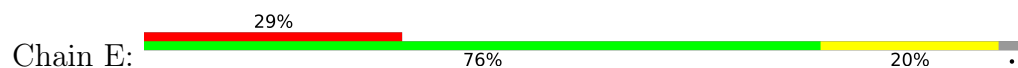


• Molecule 4: 26S proteasome regulatory subunit 6B

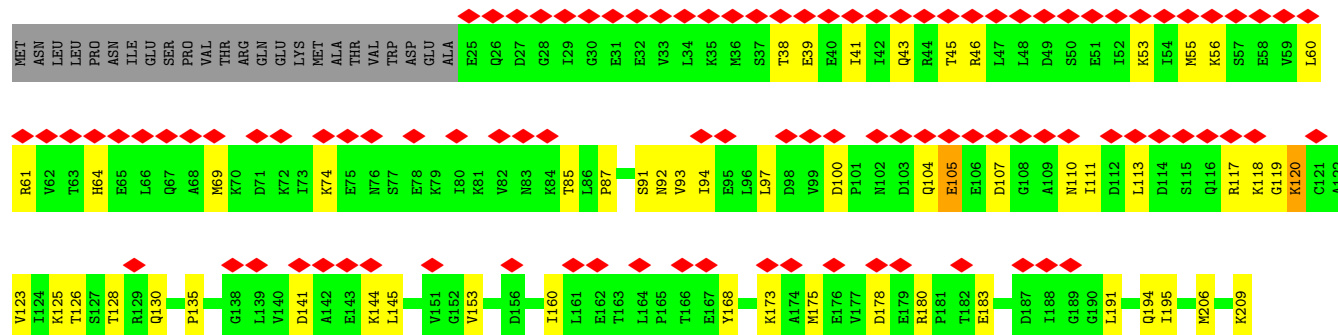


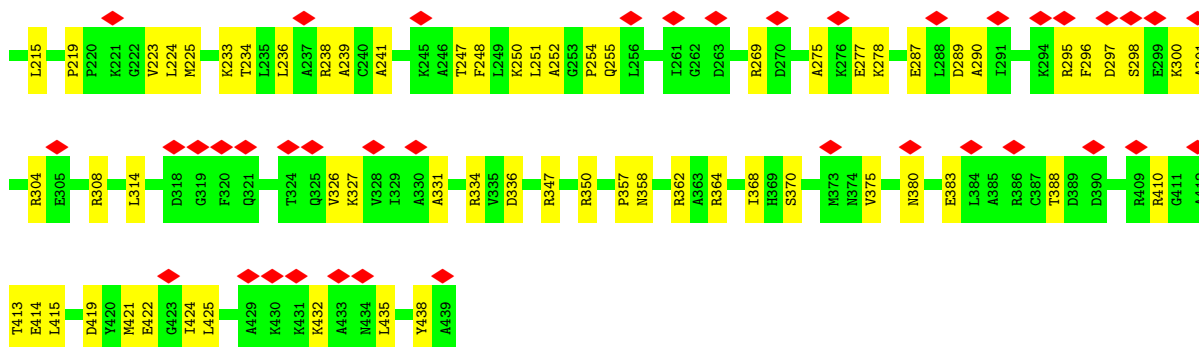


• Molecule 5: Proteasome 26S subunit, ATPase 6

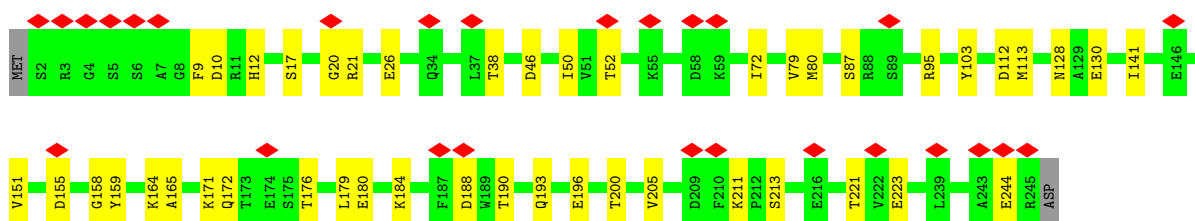
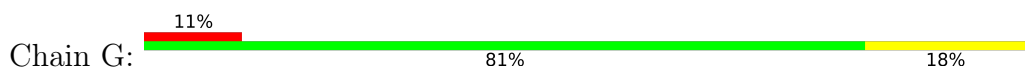


• Molecule 6: 26S proteasome regulatory subunit 6A

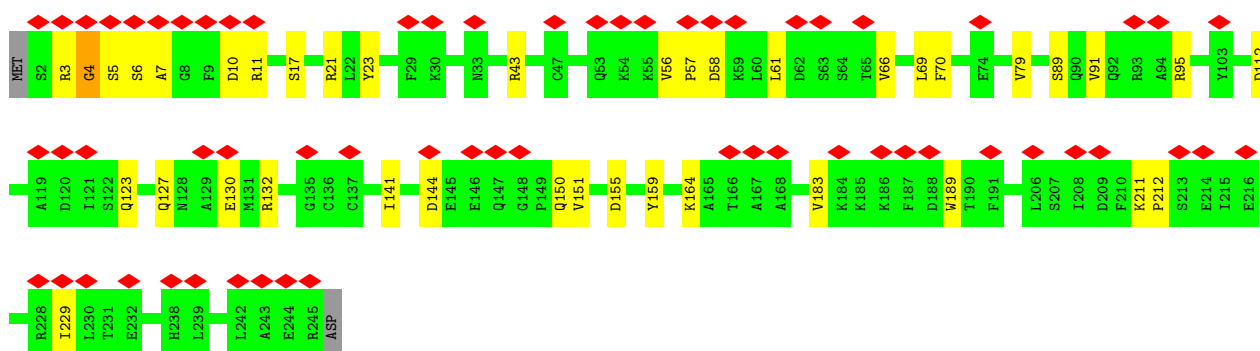
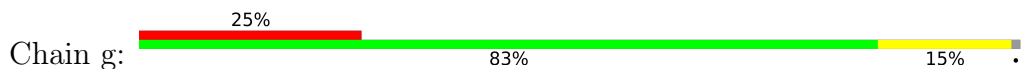




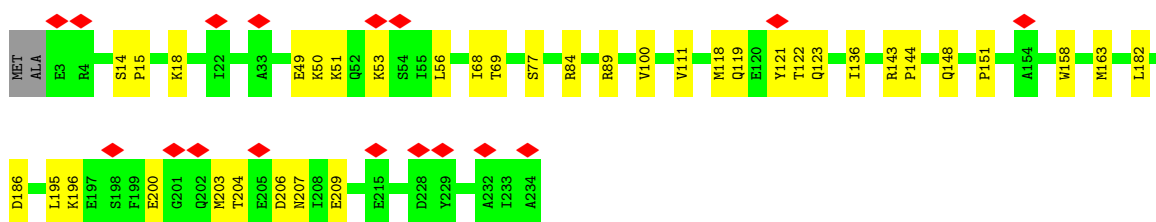
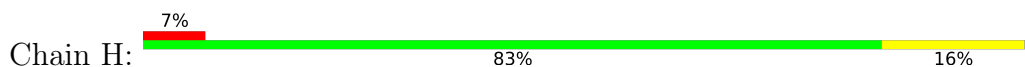
• Molecule 7: Proteasome subunit alpha type-6



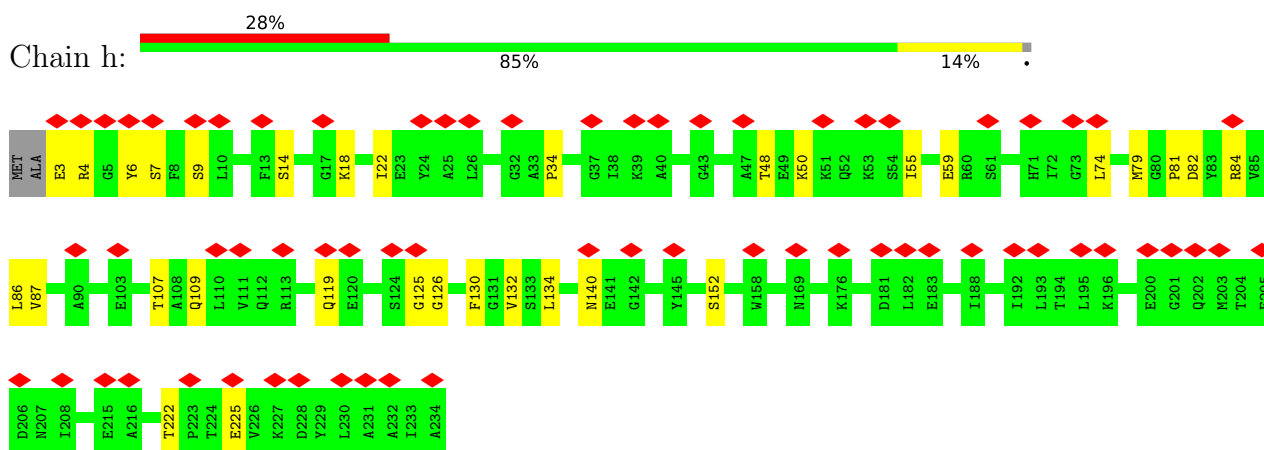
• Molecule 7: Proteasome subunit alpha type-6



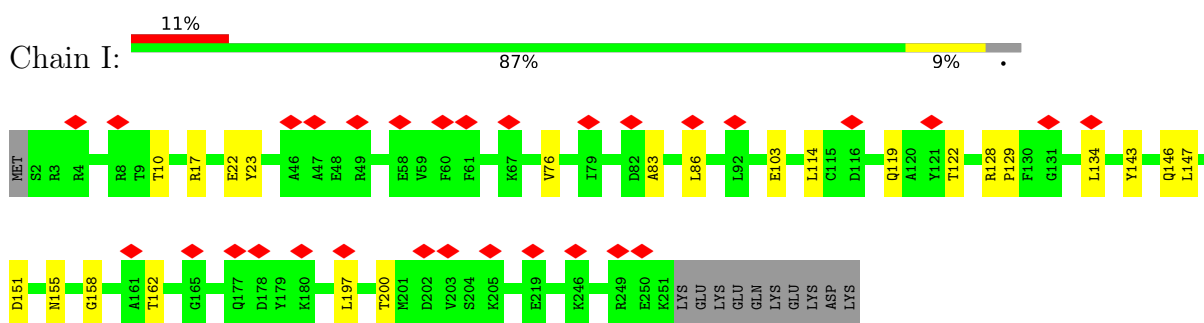
• Molecule 8: Proteasome subunit alpha type-2



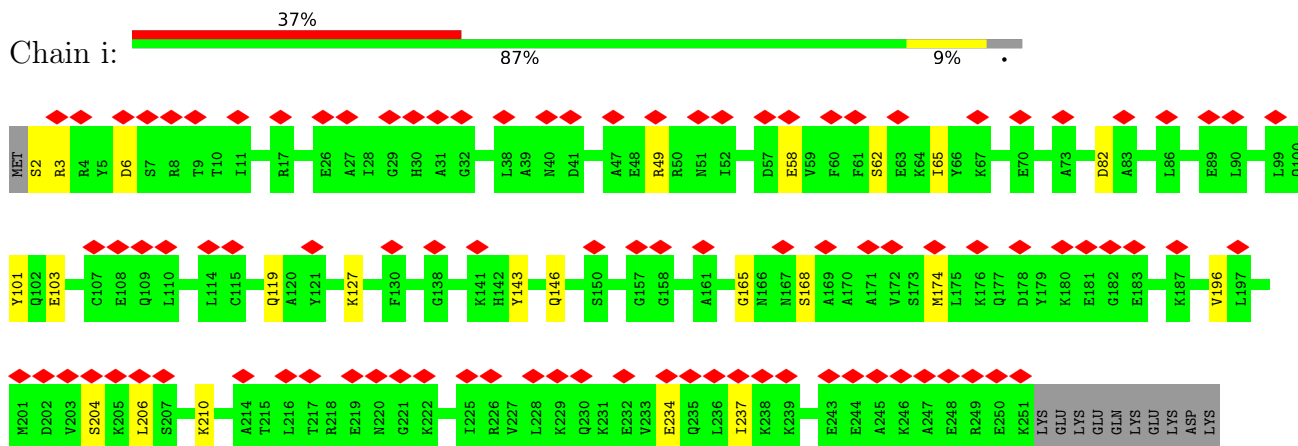
• Molecule 8: Proteasome subunit alpha type-2



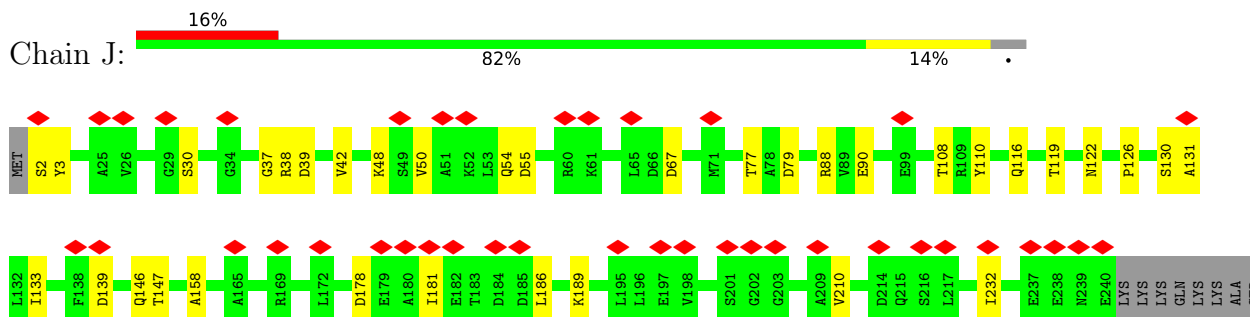
• Molecule 9: Proteasome subunit alpha type-4

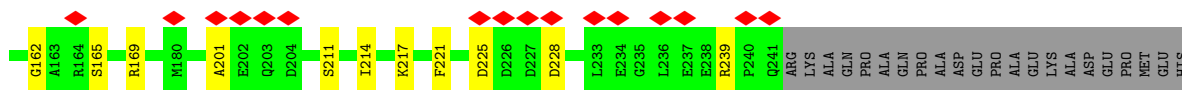


• Molecule 9: Proteasome subunit alpha type-4

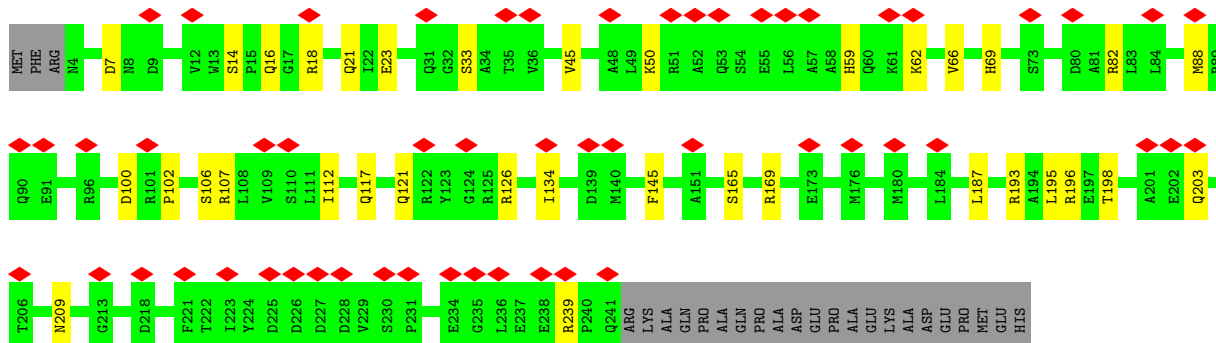
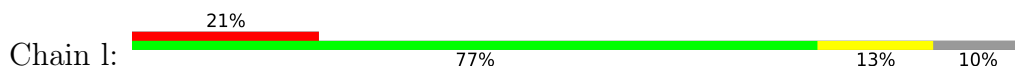


• Molecule 10: Proteasome subunit alpha type-7

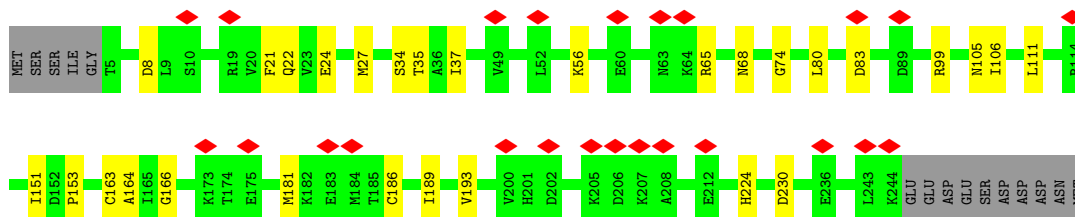
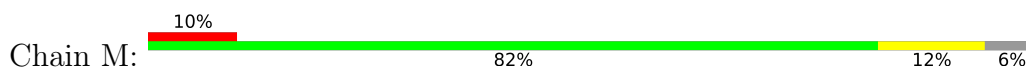




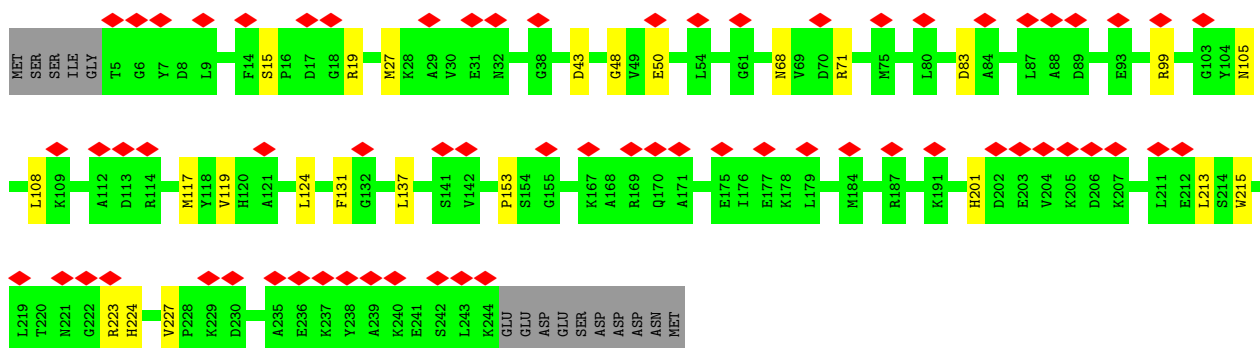
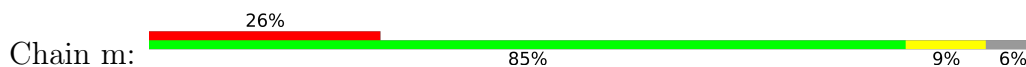
• Molecule 12: Proteasome subunit alpha type-1



• Molecule 13: Proteasome subunit alpha type-3

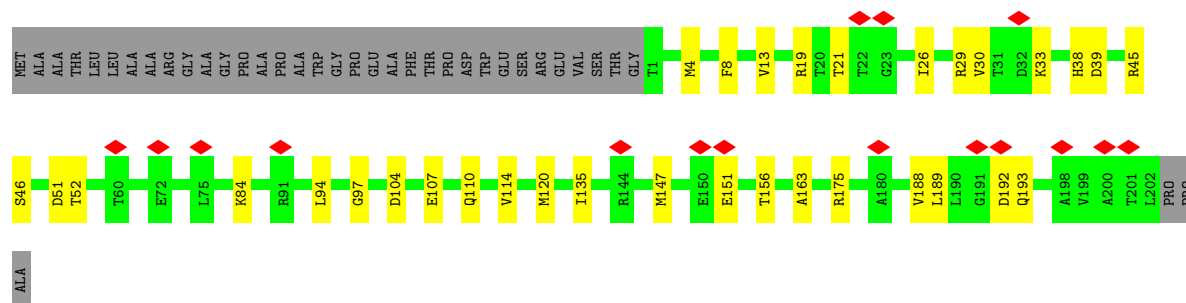


• Molecule 13: Proteasome subunit alpha type-3

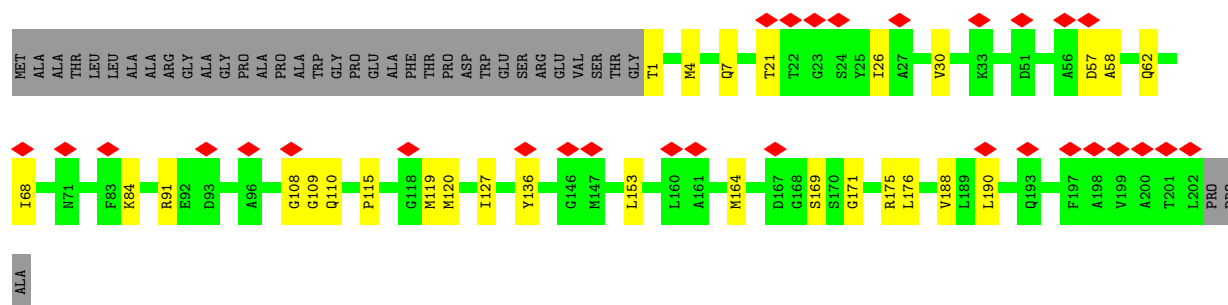
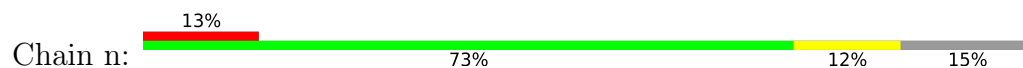


• Molecule 14: Proteasome subunit beta type-6

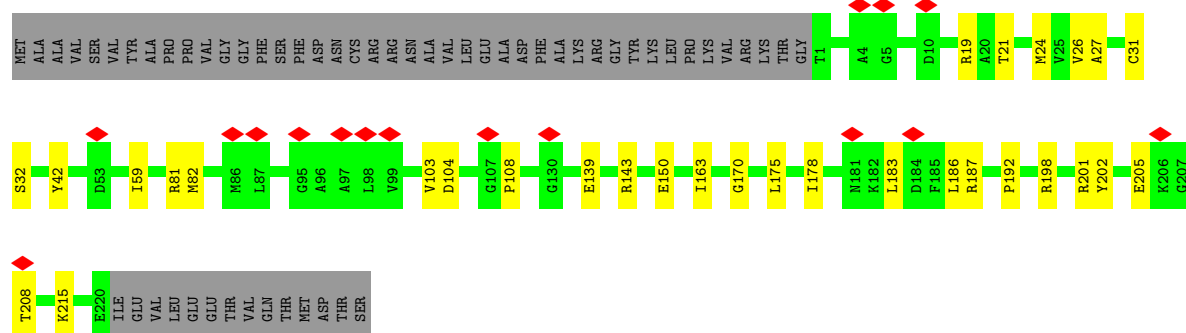




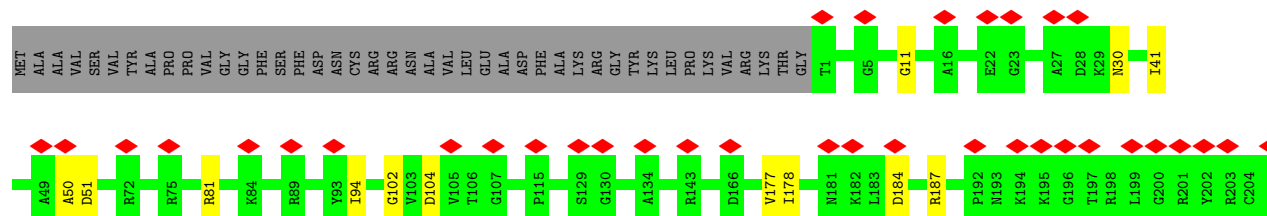
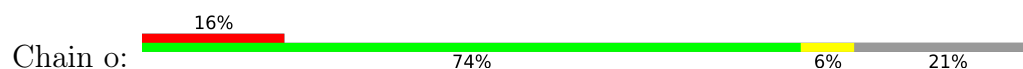
• Molecule 14: Proteasome subunit beta type-6

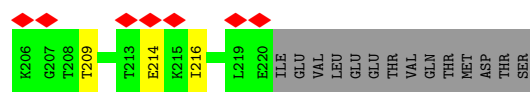


• Molecule 15: Proteasome subunit beta type-7

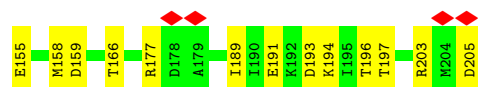
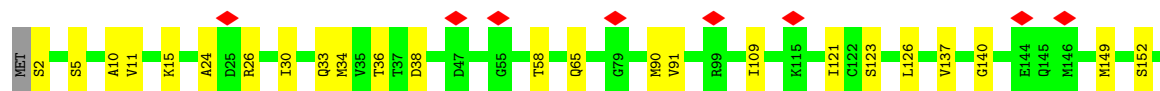
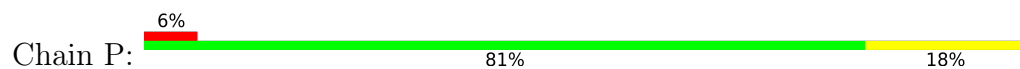


• Molecule 15: Proteasome subunit beta type-7

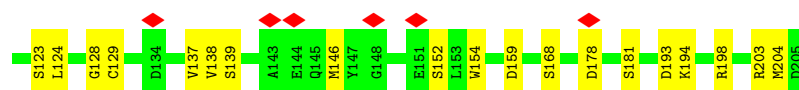
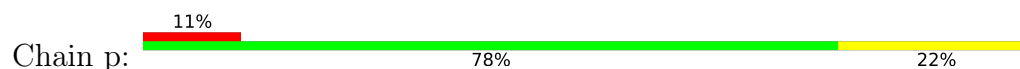




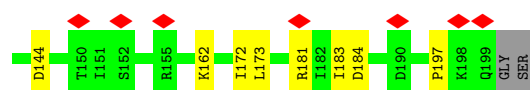
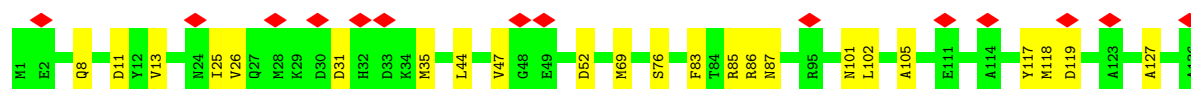
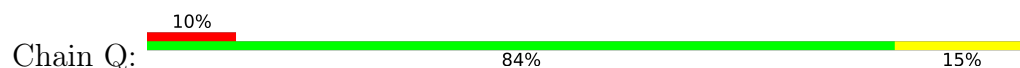
- Molecule 16: Proteasome subunit beta type-3



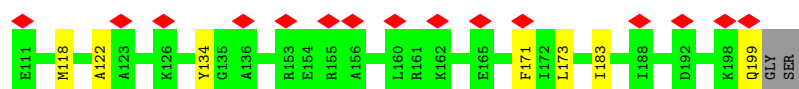
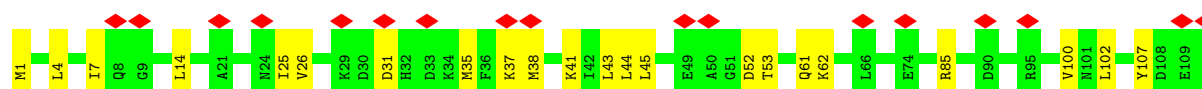
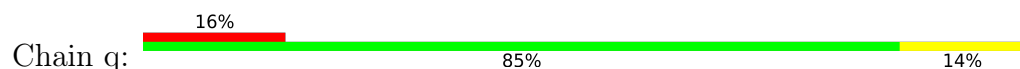
- Molecule 16: Proteasome subunit beta type-3



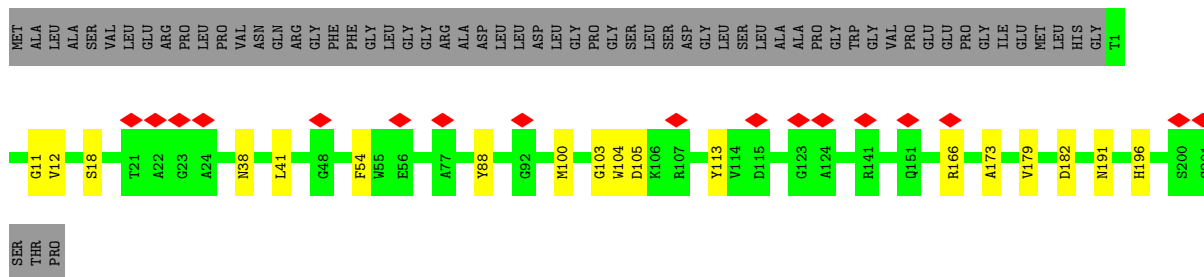
- Molecule 17: Proteasome subunit beta type-2



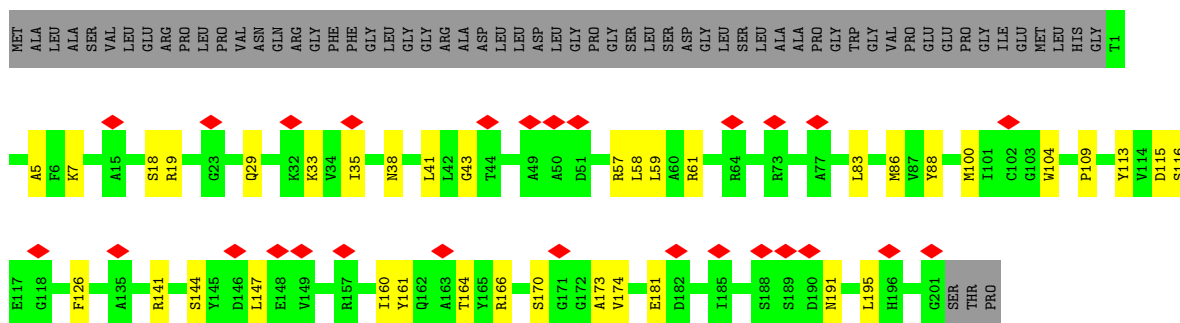
- Molecule 17: Proteasome subunit beta type-2



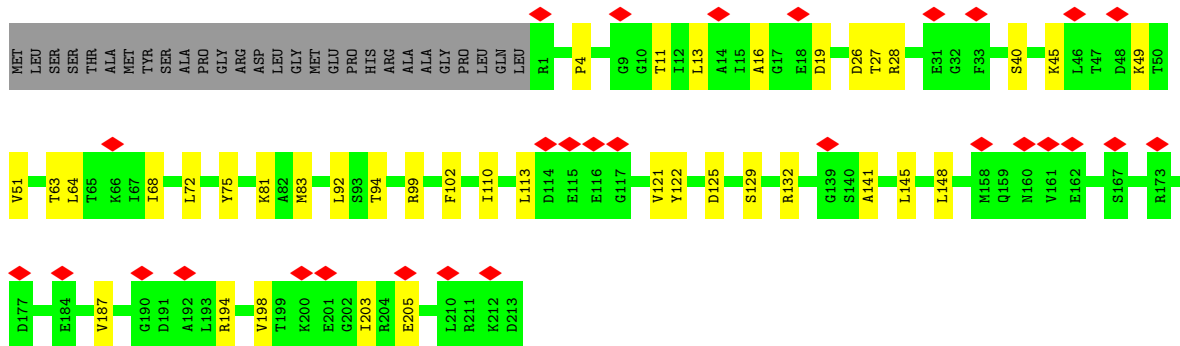
- Molecule 18: Proteasome subunit beta type-5



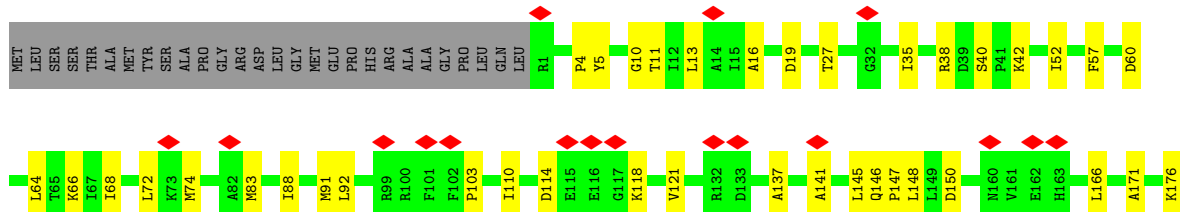
• Molecule 18: Proteasome subunit beta type-5



• Molecule 19: Proteasome subunit beta type-1

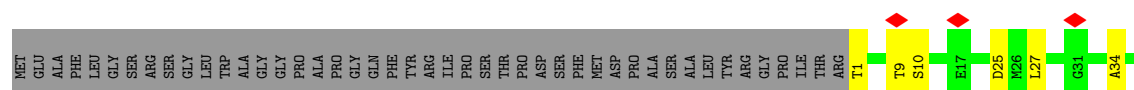


• Molecule 19: Proteasome subunit beta type-1

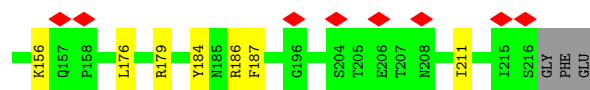
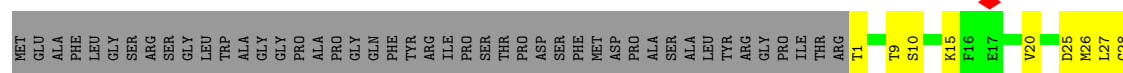




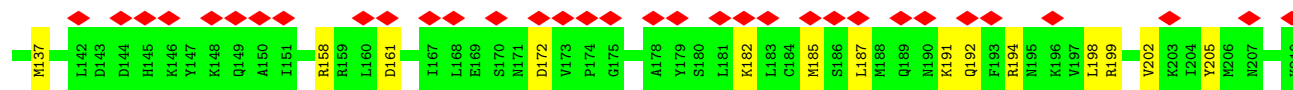
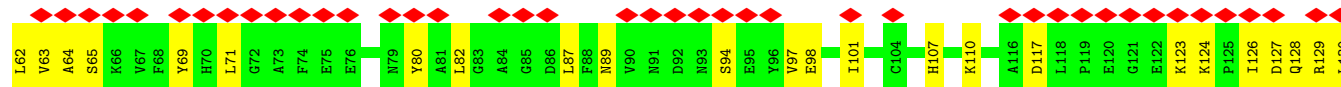
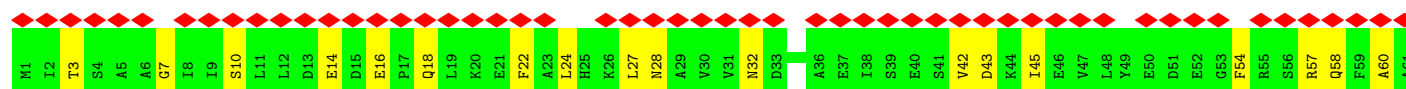
- Molecule 20: Proteasome subunit beta type-4

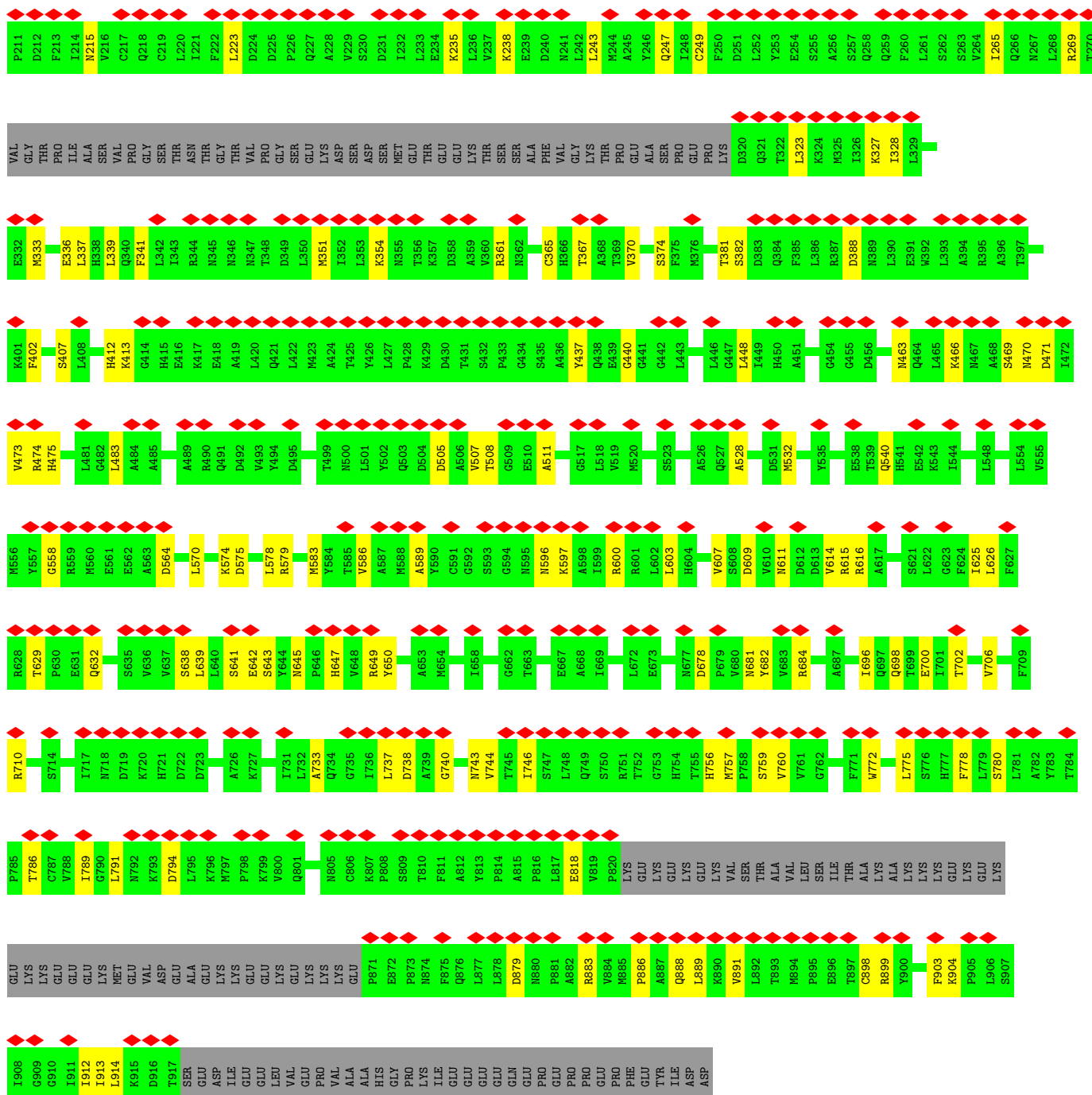


- Molecule 20: Proteasome subunit beta type-4

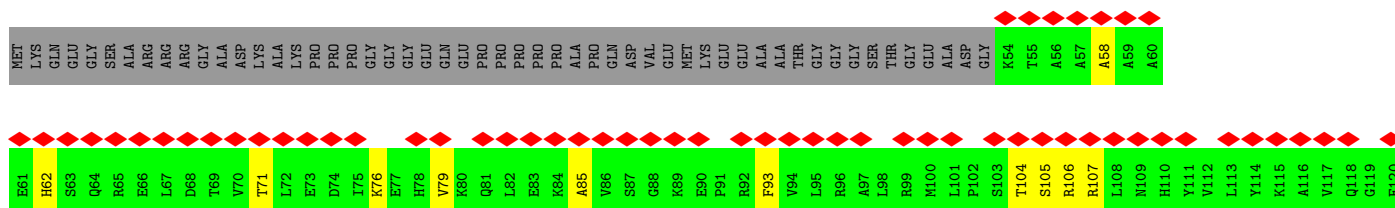


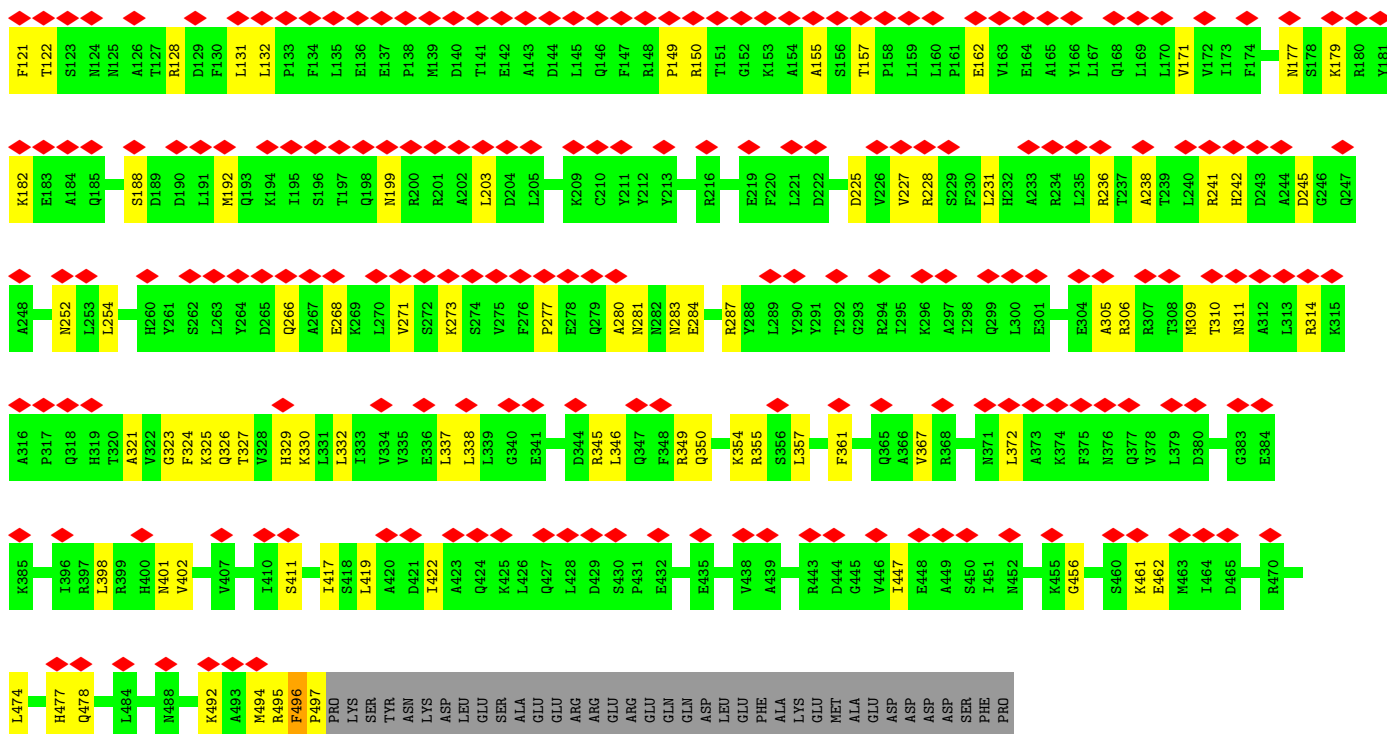
- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1



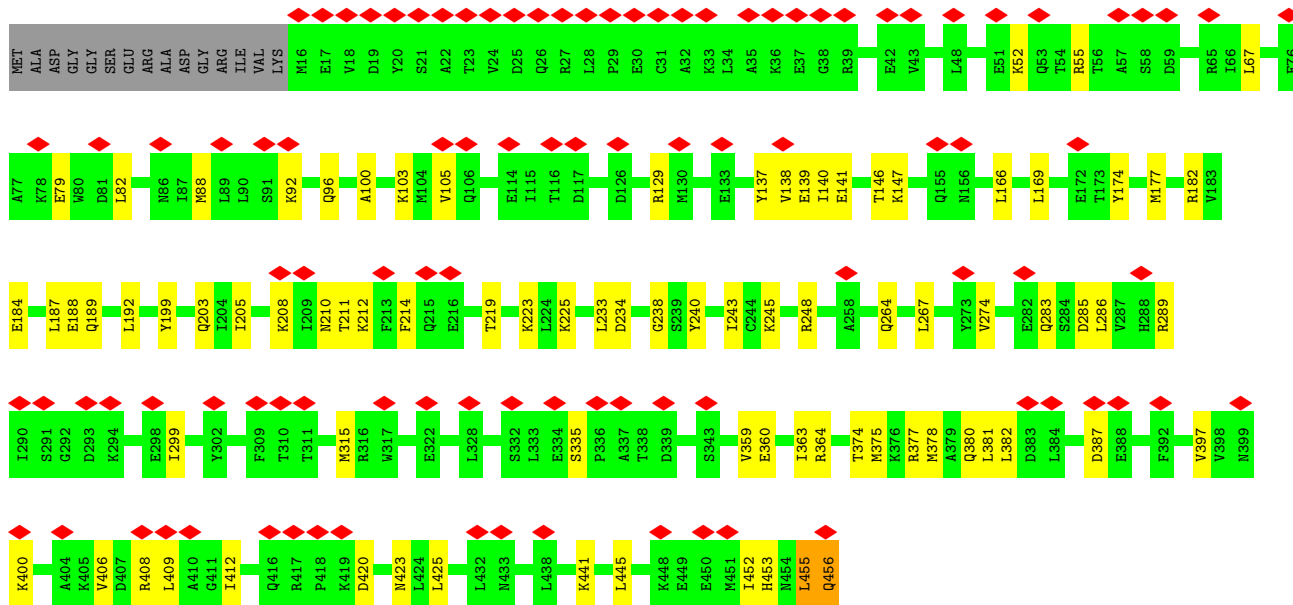
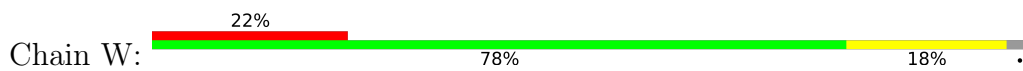


• Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

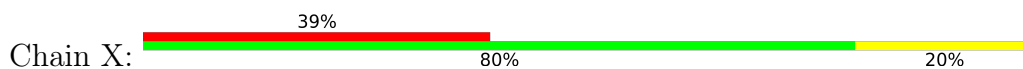


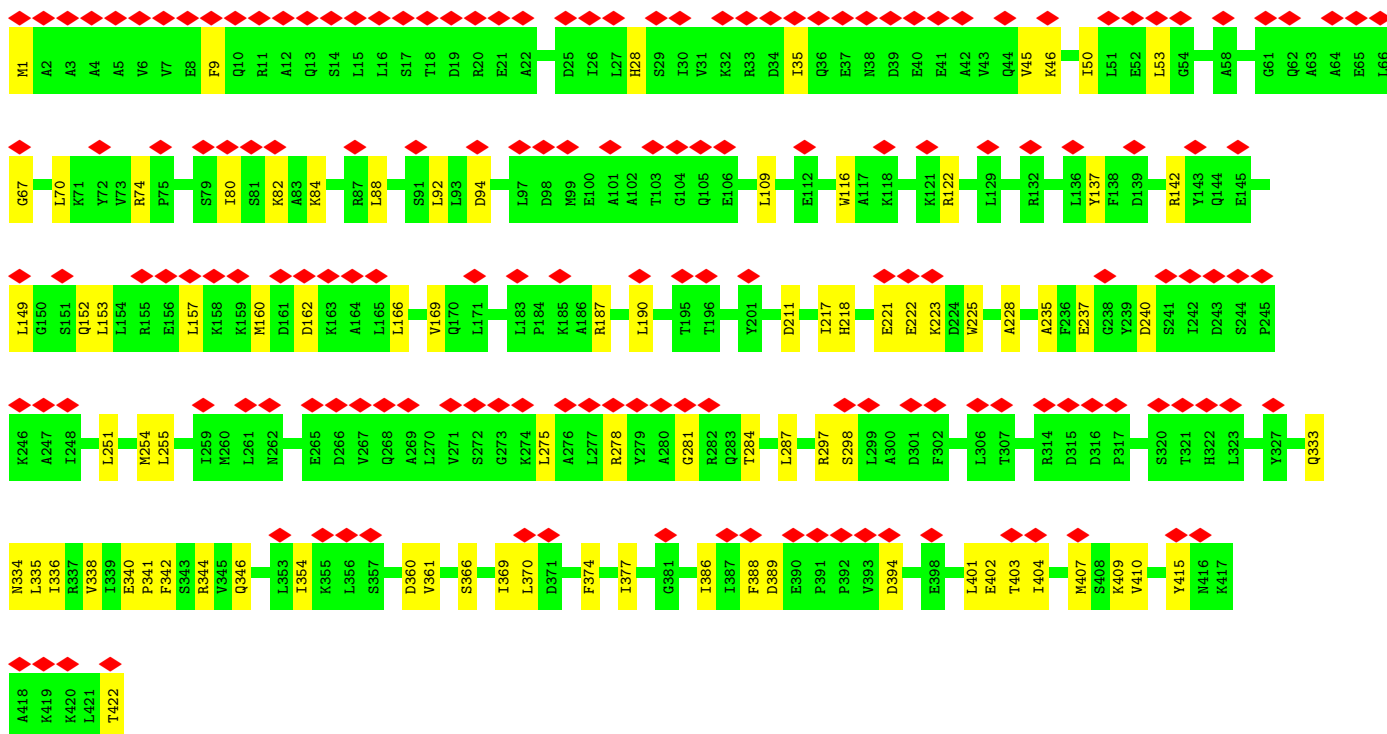


• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

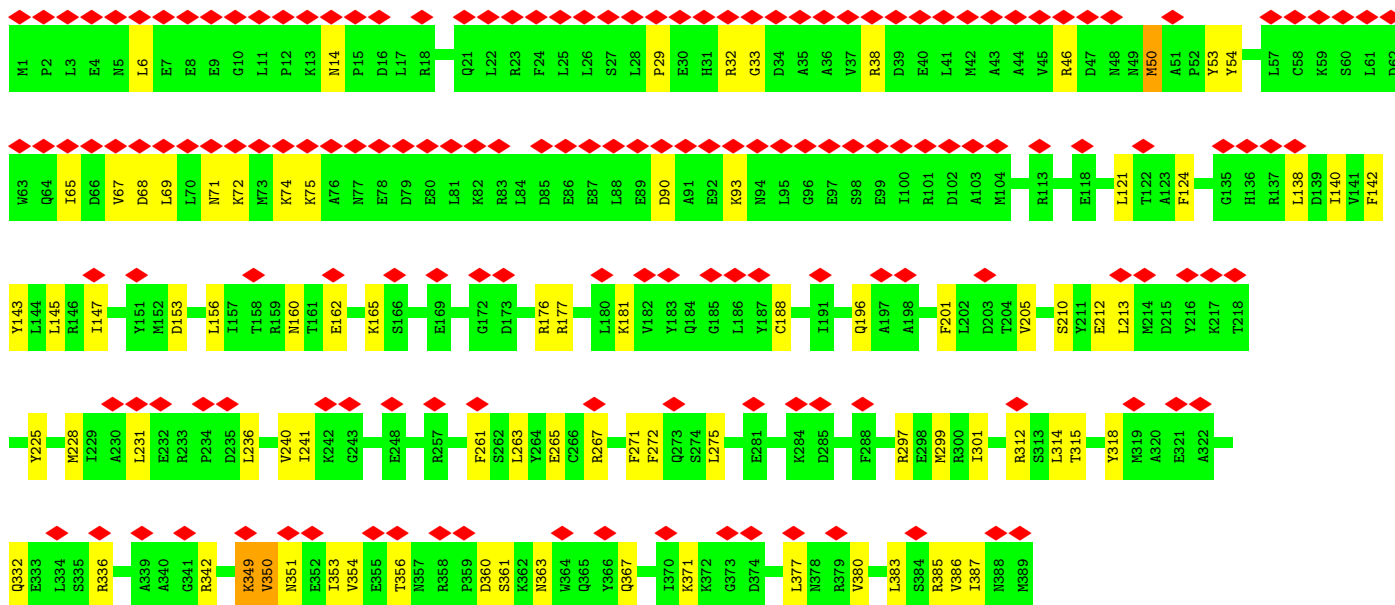
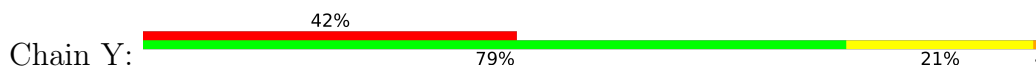


• Molecule 24: 26S proteasome non-ATPase regulatory subunit 11



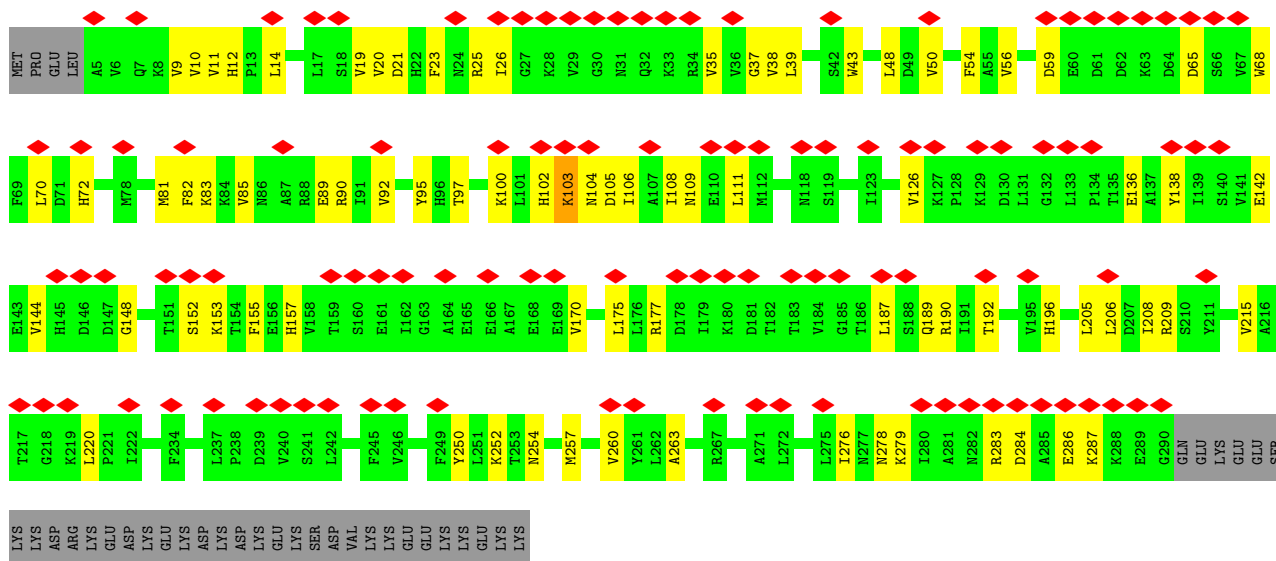


- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6



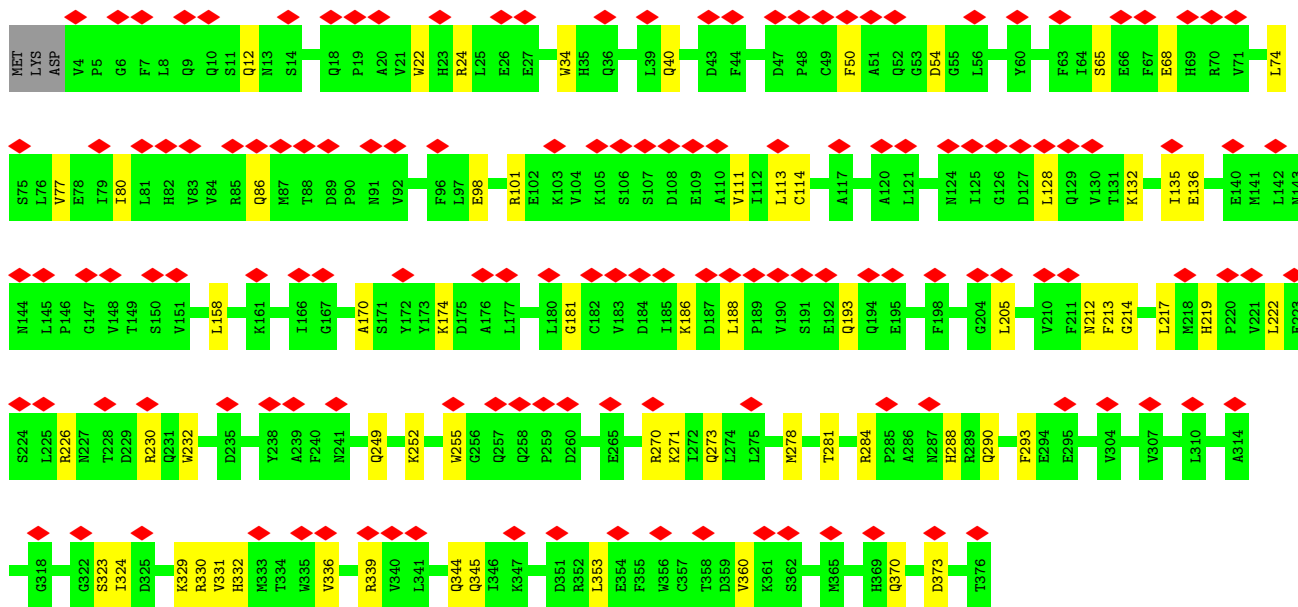
- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7





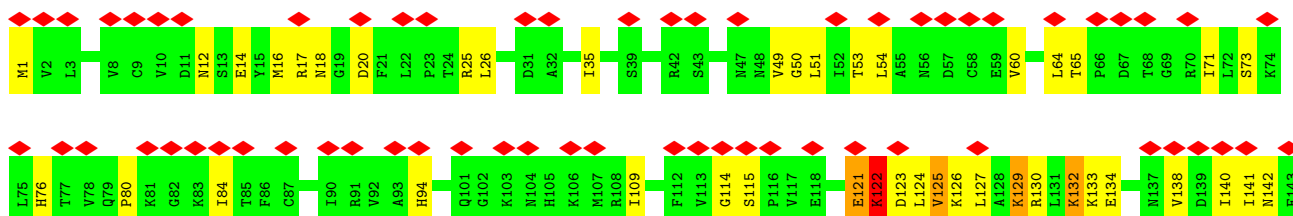
• Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

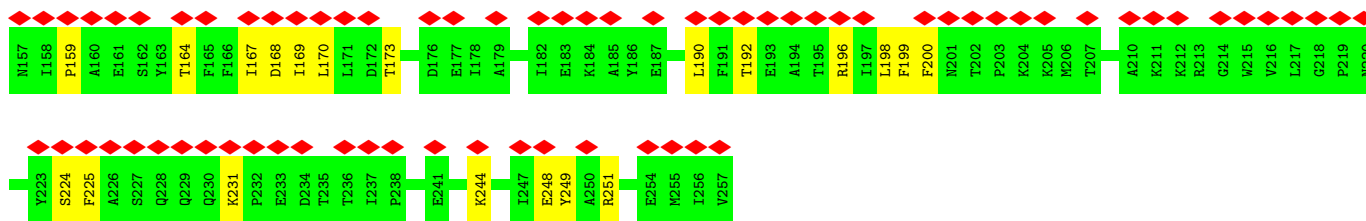
Chain a:



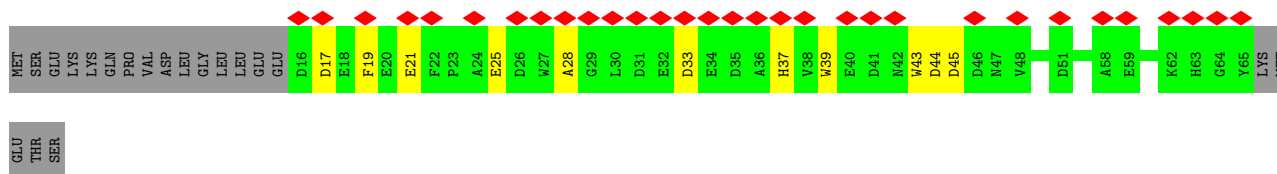
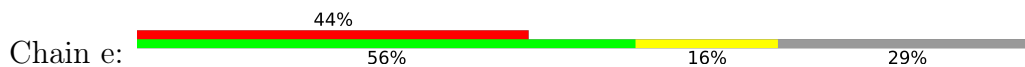
• Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

Chain b:

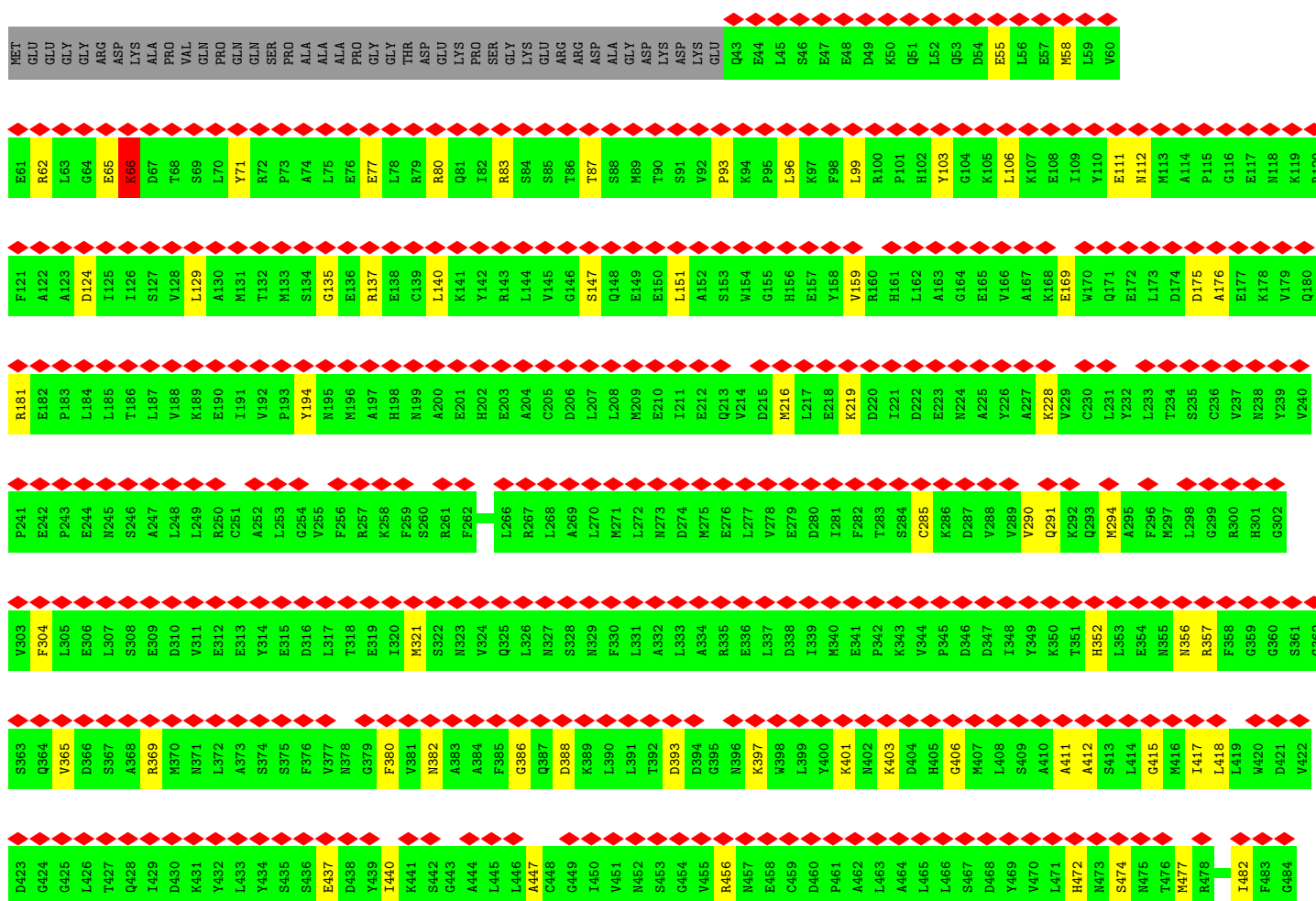
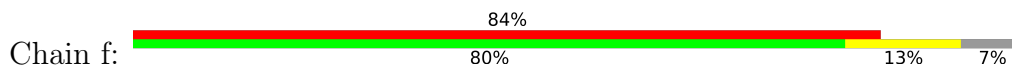


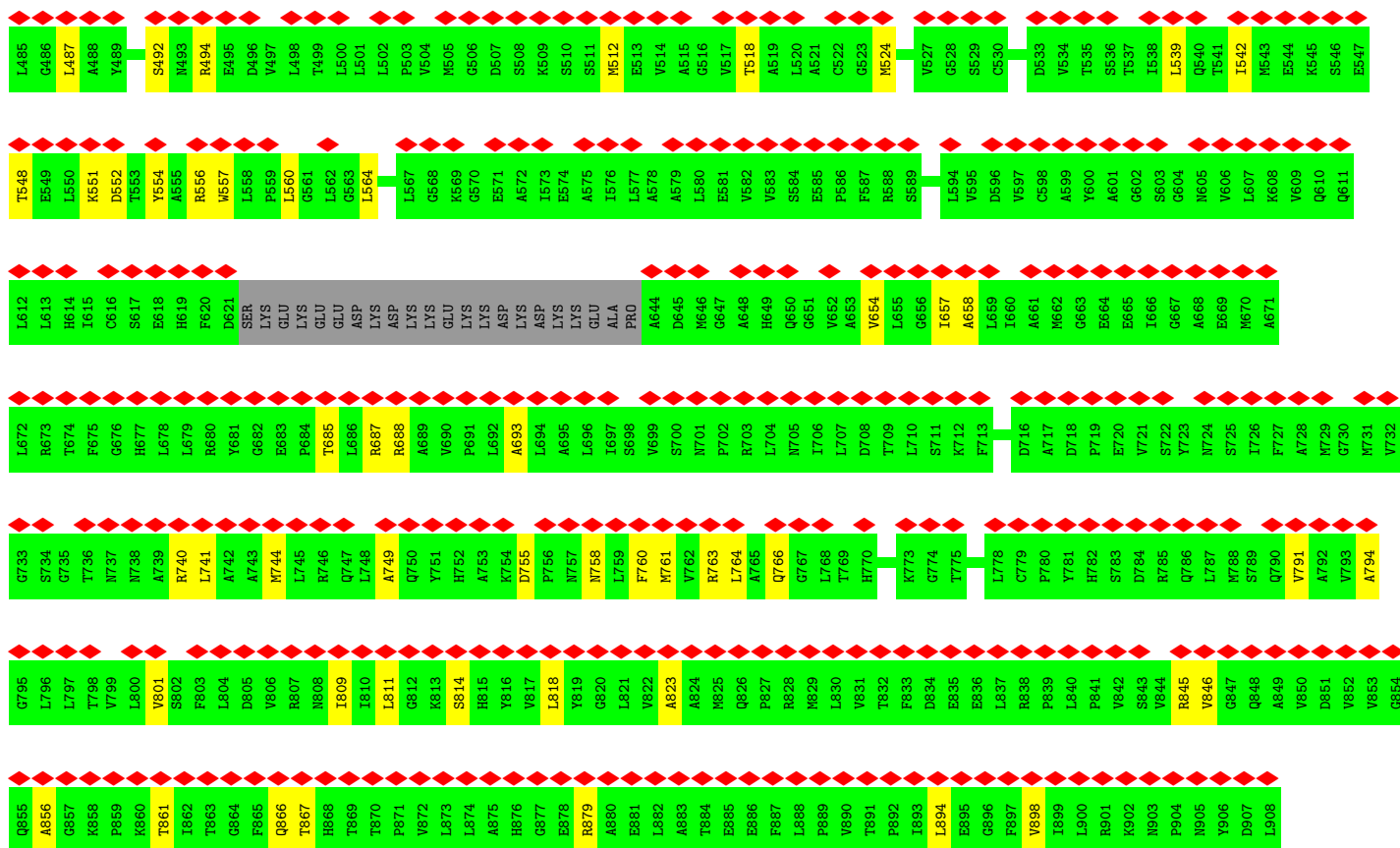


• Molecule 31: 26S proteasome complex subunit SEM1

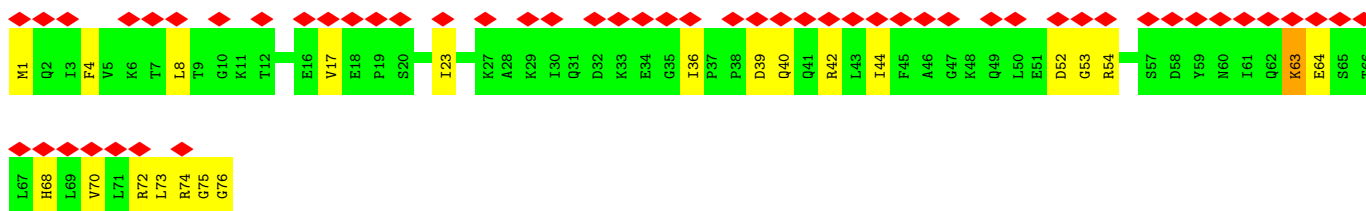


• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2

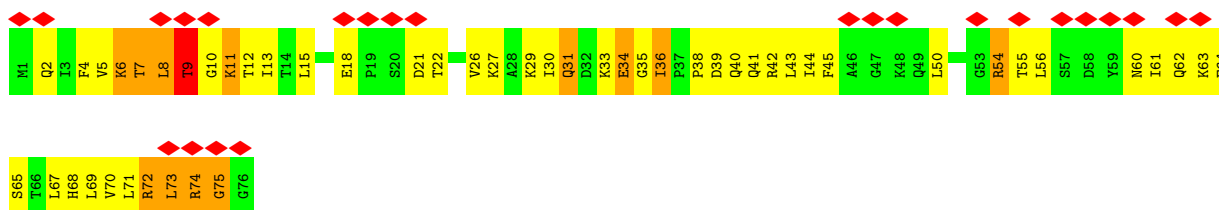




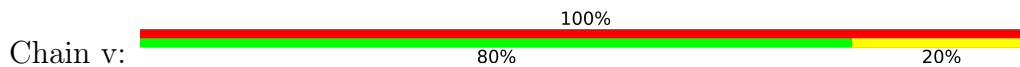
• Molecule 33: Ubiquitin



• Molecule 33: Ubiquitin



• Molecule 34: Substrate



X19	X20	X21	X22	X23	X24	X25	X26	X27	X28
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5842	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	0.020	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0049	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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/3148	0.48	0/4250
2	B	0.18	0/3061	0.46	0/4129
3	C	0.23	0/2902	0.54	0/3904
4	D	0.23	0/3089	0.53	0/4168
5	E	0.19	0/3145	0.50	0/4233
6	F	0.20	0/3292	0.48	0/4435
7	G	0.17	0/1923	0.42	0/2601
7	g	0.19	0/1914	0.45	0/2590
8	H	0.15	0/1844	0.38	0/2499
8	h	0.16	0/1844	0.37	0/2497
9	I	0.15	0/1991	0.37	0/2685
9	i	0.14	0/1985	0.36	0/2677
10	J	0.17	0/1906	0.39	0/2573
10	j	0.15	0/1887	0.42	0/2549
11	K	0.16	0/1804	0.43	0/2436
11	k	0.14	0/1809	0.37	0/2444
12	L	0.14	0/1901	0.34	0/2570
12	l	0.14	0/1896	0.37	0/2565
13	M	0.16	0/1911	0.41	0/2573
13	m	0.13	0/1916	0.36	0/2580
14	N	0.14	0/1540	0.36	0/2085
14	n	0.14	0/1536	0.35	0/2080
15	O	0.15	0/1676	0.39	0/2271
15	o	0.15	0/1686	0.39	1/2282 (0.0%)
16	P	0.17	0/1616	0.47	0/2180
16	p	0.17	0/1620	0.45	0/2184
17	Q	0.13	0/1621	0.35	0/2194
17	q	0.14	0/1621	0.36	0/2194
18	R	0.14	0/1590	0.36	0/2147
18	r	0.13	0/1590	0.35	0/2147
19	S	0.14	0/1671	0.39	0/2252
19	s	0.15	0/1684	0.40	0/2268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.15	0/1716	0.37	0/2323
20	t	0.14	0/1720	0.37	0/2328
21	U	0.17	0/6488	0.47	0/8782
22	V	0.16	0/3681	0.40	0/4969
23	W	0.15	0/3644	0.41	0/4901
24	X	0.17	0/3381	0.48	0/4558
25	Y	0.20	0/3261	0.51	1/4393 (0.0%)
26	Z	0.19	0/2324	0.51	0/3150
27	a	0.18	0/3053	0.51	0/4133
28	b	0.26	0/1478	0.61	0/2001
29	c	0.25	0/2302	0.54	0/3110
30	d	0.24	0/2162	0.56	3/2919 (0.1%)
31	e	0.19	0/437	0.52	0/595
32	f	0.20	0/6640	0.49	0/8988
33	u	0.26	0/607	0.67	2/816 (0.2%)
33	z	0.65	0/607	0.90	2/816 (0.2%)
34	v	0.03	0/8	0.06	0/8
All	All	0.18	0/108128	0.45	9/146032 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	u	75	GLY	CA-C-N	-8.35	106.66	121.70
33	u	75	GLY	C-N-CA	-8.35	106.66	121.70
30	d	198	LEU	N-CA-C	-6.77	104.77	113.16
30	d	67	ASP	CA-C-N	6.17	124.13	120.24
30	d	67	ASP	C-N-CA	6.17	124.13	120.24
25	Y	50	MET	CB-CG-SD	5.71	129.83	112.70
15	o	11	GLY	N-CA-C	5.40	117.33	110.20
33	z	6	LYS	CA-C-N	-5.13	115.91	123.00
33	z	6	LYS	C-N-CA	-5.13	115.91	123.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3096	0	3139	77	0
2	B	3018	0	3081	60	0
3	C	2864	0	2971	73	0
4	D	3039	0	3076	88	0
5	E	3097	0	3173	67	0
6	F	3251	0	3318	89	0
7	G	1889	0	1885	26	0
7	g	1880	0	1875	31	0
8	H	1805	0	1784	23	0
8	h	1805	0	1798	22	0
9	I	1958	0	1960	17	0
9	i	1955	0	1955	14	0
10	J	1880	0	1892	25	0
10	j	1861	0	1865	19	0
11	K	1777	0	1762	19	0
11	k	1782	0	1766	19	0
12	L	1866	0	1852	23	0
12	l	1861	0	1839	24	0
13	M	1876	0	1861	20	0
13	m	1881	0	1868	17	0
14	N	1514	0	1487	21	0
14	n	1510	0	1483	18	0
15	O	1649	0	1659	21	0
15	o	1659	0	1681	12	0
16	P	1587	0	1598	27	0
16	p	1591	0	1609	34	0
17	Q	1588	0	1584	25	0
17	q	1588	0	1584	21	0
18	R	1559	0	1523	13	0
18	r	1559	0	1523	24	0
19	S	1641	0	1639	25	0
19	s	1654	0	1656	38	0
20	T	1683	0	1662	18	0
20	t	1687	0	1666	28	0
21	U	6373	0	6411	122	0
22	V	3612	0	3682	75	0
23	W	3596	0	3713	58	0
24	X	3335	0	3435	55	0
25	Y	3202	0	3204	57	0
26	Z	2281	0	2312	61	0
27	a	2995	0	3012	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	b	1458	0	1504	82	0
29	c	2260	0	2276	72	0
30	d	2116	0	2146	39	0
31	e	425	0	328	14	0
32	f	6529	0	6541	71	0
33	u	601	0	629	34	0
33	z	601	0	629	96	0
34	v	53	0	21	2	0
35	A	31	0	12	3	0
35	B	31	0	12	1	0
35	D	31	0	12	6	0
35	E	31	0	12	0	0
36	B	2	0	0	0	0
36	D	1	0	0	0	0
36	E	1	0	0	0	0
36	F	1	0	0	0	0
37	C	27	0	12	0	0
37	F	27	0	12	1	0
38	c	1	0	0	0	0
All	All	106531	0	106989	1677	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 8.

All (1677) 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)
33:u:4:PHE:CE2	33:u:64:GLU:HG2	1.58	1.37
33:u:4:PHE:HE2	33:u:64:GLU:CG	1.58	1.17
33:u:63:LYS:HE3	33:u:64:GLU:HB2	1.37	1.06
33:u:63:LYS:HE3	33:u:64:GLU:CB	1.85	1.05
33:u:63:LYS:CE	33:u:64:GLU:HB3	1.90	1.01
29:c:89:PRO:CB	33:u:70:VAL:HG11	1.90	1.01
33:u:63:LYS:HE2	33:u:64:GLU:HB3	1.44	0.97
33:u:64:GLU:CD	33:u:64:GLU:O	2.08	0.96
7:g:5:SER:HB3	7:g:11:ARG:HH21	1.32	0.94
33:u:4:PHE:HE2	33:u:64:GLU:HG2	0.77	0.93
33:u:63:LYS:CE	33:u:64:GLU:CB	2.47	0.92
29:c:96:LEU:HD12	33:u:8:LEU:HD22	1.52	0.91
29:c:89:PRO:HB2	33:u:70:VAL:HG11	1.52	0.88
4:D:126:PRO:HD2	4:D:128:ALA:HB2	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:89:PRO:HB3	33:u:70:VAL:HG11	1.58	0.84
28:b:133:LYS:HE3	33:z:7:THR:HG21	1.60	0.81
22:V:355:ARG:HH21	31:e:28:ALA:HA	1.47	0.80
28:b:133:LYS:CE	33:z:7:THR:HG21	2.14	0.77
33:u:64:GLU:O	33:u:64:GLU:OE1	2.03	0.76
28:b:126:LYS:HA	28:b:129:LYS:HD2	1.66	0.76
33:z:30:ILE:HG22	33:z:36:ILE:HG13	1.68	0.76
33:z:7:THR:HG23	33:z:11:LYS:HE2	1.69	0.75
33:z:34:GLU:HB2	33:z:36:ILE:HD11	1.67	0.75
28:b:133:LYS:HG2	33:z:7:THR:OG1	1.87	0.74
28:b:132:LYS:HB3	33:z:34:GLU:HB3	1.68	0.74
25:Y:188:CYS:SG	25:Y:196:GLN:NE2	2.60	0.74
28:b:125:VAL:HG22	28:b:129:LYS:NZ	2.03	0.73
24:X:298:SER:HA	24:X:334:ASN:HD21	1.52	0.73
33:z:45:PHE:HB2	33:z:50:LEU:HD11	1.69	0.73
7:g:5:SER:HB3	7:g:11:ARG:NH2	2.03	0.72
28:b:129:LYS:HB2	33:z:36:ILE:HD12	1.71	0.71
3:C:230:MET:HG3	3:C:232:ARG:H	1.56	0.70
25:Y:240:VAL:HG23	25:Y:241:ILE:HG13	1.74	0.70
23:W:203:GLN:HE21	23:W:233:LEU:HD21	1.56	0.70
22:V:323:GLY:HA3	31:e:25:GLU:HB2	1.72	0.70
3:C:134:LEU:HD22	3:C:237:MET:HB3	1.74	0.70
4:D:124:LEU:C	4:D:126:PRO:HD3	2.17	0.69
32:f:55:GLU:HA	32:f:58:MET:HE2	1.73	0.69
1:A:396:ALA:HA	1:A:401:ARG:HD2	1.73	0.69
6:F:175:MET:HE3	6:F:250:LYS:HG3	1.73	0.69
3:C:369:TYR:HA	3:C:372:ARG:HE	1.57	0.69
13:M:35:THR:HA	13:M:166:GLY:HA3	1.74	0.69
19:S:27:THR:HB	19:S:40:SER:H	1.58	0.68
27:a:344:GLN:HE22	27:a:345:GLN:HE21	1.41	0.68
19:s:176:LYS:HE2	19:s:208:VAL:HG11	1.74	0.68
33:z:36:ILE:HB	33:z:41:GLN:HE21	1.59	0.68
27:a:284:ARG:HD3	27:a:288:HIS:H	1.57	0.68
11:k:221:GLN:HB2	11:k:224:GLN:HG2	1.76	0.68
2:B:95:GLU:HA	2:B:98:LYS:HE3	1.76	0.68
17:Q:25:ILE:HG22	17:Q:26:VAL:HG13	1.76	0.68
4:D:121:ARG:HG3	4:D:124:LEU:HD22	1.75	0.68
4:D:125:LYS:N	4:D:126:PRO:HD3	2.08	0.68
3:C:38:LYS:HE2	4:D:54:LEU:HD22	1.74	0.68
4:D:67:ASN:ND2	21:U:607:VAL:O	2.27	0.68
4:D:96:VAL:HG23	4:D:102:ILE:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:163:ILE:HG12	15:O:170:GLY:HA2	1.76	0.67
25:Y:315:THR:HA	25:Y:353:ILE:HA	1.75	0.67
32:f:557:TRP:HA	32:f:560:LEU:HD12	1.77	0.67
7:g:5:SER:CB	7:g:11:ARG:HH21	2.05	0.67
10:j:36:ARG:HH21	10:j:157:LYS:HG2	1.60	0.67
28:b:126:LYS:HE2	33:z:72:ARG:H	1.60	0.66
28:b:132:LYS:HZ1	28:b:163:LYS:HD2	1.58	0.66
4:D:163:MET:SD	4:D:222:HIS:NE2	2.65	0.66
19:s:27:THR:HB	19:s:40:SER:H	1.60	0.66
33:u:72:ARG:HD3	33:u:74:ARG:HD2	1.78	0.66
15:o:216:ILE:HD11	16:p:194:LYS:HD2	1.78	0.66
16:P:2:SER:N	16:P:5:SER:HG	1.94	0.65
30:d:192:THR:HG23	30:d:196:ARG:HH21	1.61	0.65
35:A:501:ATP:H5'1	2:B:343:ARG:HH12	1.61	0.65
5:E:352:MET:HE1	6:F:219:PRO:HA	1.77	0.65
24:X:366:SER:O	24:X:370:LEU:HB2	1.96	0.65
3:C:20:LEU:HD12	21:U:137:MET:HB3	1.78	0.65
3:C:164:VAL:HG12	3:C:165:ILE:HG13	1.79	0.65
7:G:180:GLU:OE1	7:G:184:LYS:NZ	2.30	0.64
28:b:25:ARG:HH22	28:b:145:GLU:HG3	1.61	0.64
17:q:118:MET:HE1	17:q:122:ALA:HA	1.79	0.64
17:q:25:ILE:HG22	17:q:26:VAL:HG13	1.77	0.64
1:A:396:ALA:HA	1:A:401:ARG:HH11	1.63	0.64
29:c:53:VAL:HA	29:c:77:GLN:HE22	1.62	0.64
6:F:85:THR:HG22	6:F:87:PRO:HD2	1.80	0.64
21:U:243:LEU:HG	21:U:913:ILE:HG23	1.79	0.64
16:p:14:MET:HE3	16:p:15:LYS:H	1.63	0.64
18:r:19:ARG:HH21	18:r:29:GLN:HE22	1.45	0.64
5:E:84:ARG:HB2	5:E:87:LEU:HD23	1.79	0.64
28:b:129:LYS:CE	33:z:36:ILE:HG23	2.28	0.64
4:D:159:LYS:HD2	4:D:221:HIS:HA	1.79	0.63
27:a:214:GLY:HA2	27:a:217:LEU:HD13	1.79	0.63
19:S:110:ILE:HB	19:S:122:TYR:HB2	1.81	0.63
25:Y:349:LYS:O	25:Y:351:ASN:N	2.31	0.63
7:g:89:SER:HA	13:m:117:MET:HE1	1.81	0.63
33:z:31:GLN:HA	33:z:36:ILE:H	1.63	0.63
17:Q:197:PRO:HD2	17:q:199:GLN:H	1.63	0.63
20:t:96:MET:HE1	20:t:106:LEU:HB2	1.80	0.63
26:Z:20:VAL:HG13	29:c:212:LEU:HD23	1.80	0.63
29:c:115:HIS:HB3	29:c:118:PHE:HB2	1.81	0.63
32:f:382:ASN:ND2	32:f:388:ASP:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:861:THR:HB	32:f:879:ARG:HH11	1.61	0.63
33:z:44:ILE:HB	33:z:68:HIS:HB3	1.80	0.63
22:V:417:ILE:HG22	25:Y:349:LYS:HD3	1.80	0.63
8:h:86:LEU:HD13	8:h:134:LEU:HD11	1.79	0.63
4:D:383:GLY:HA3	5:E:164:ILE:HG21	1.81	0.63
25:Y:210:SER:HB3	25:Y:213:LEU:HD23	1.79	0.63
1:A:55:LEU:HD11	2:B:76:GLU:HG2	1.81	0.63
20:T:25:ASP:OD1	20:T:41:ARG:NH2	2.32	0.63
1:A:156:LYS:HE2	2:B:114:GLU:HG2	1.79	0.62
21:U:625:ILE:HG13	21:U:626:LEU:HG	1.81	0.62
32:f:140:LEU:HD22	32:f:169:GLU:HB2	1.81	0.62
19:S:4:PRO:O	20:T:100:ARG:NH2	2.26	0.62
32:f:77:GLU:HA	32:f:80:ARG:HG2	1.81	0.62
1:A:390:THR:HA	2:B:216:ILE:HD11	1.80	0.62
21:U:158:ARG:NH2	21:U:192:GLN:OE1	2.29	0.62
24:X:237:GLU:HA	24:X:240:ASP:HB2	1.82	0.62
26:Z:284:ASP:OD1	26:Z:287:LYS:NZ	2.33	0.62
28:b:133:LYS:NZ	33:z:34:GLU:HG3	2.14	0.62
22:V:349:ARG:NH2	31:e:39:TRP:O	2.32	0.62
27:a:111:VAL:HA	27:a:114:CYS:HB2	1.81	0.62
27:a:249:GLN:HA	27:a:252:LYS:HB2	1.80	0.62
11:K:203:LYS:HB2	11:K:210:LEU:HD22	1.81	0.62
21:U:402:PHE:HB2	21:U:437:TYR:HB3	1.81	0.62
4:D:204:MET:HE1	4:D:212:LYS:HD2	1.82	0.62
22:V:461:LYS:NZ	22:V:462:GLU:O	2.32	0.62
15:o:214:GLU:HG2	16:p:198:ARG:HG2	1.80	0.62
33:u:23:ILE:HB	33:u:52:ASP:HA	1.81	0.62
25:Y:231:LEU:HG	25:Y:236:LEU:HD12	1.82	0.62
29:c:59:GLY:HA3	29:c:69:VAL:HA	1.81	0.62
23:W:360:GLU:HG2	23:W:364:ARG:HE	1.65	0.62
16:p:2:SER:N	16:p:5:SER:HG	1.98	0.61
3:C:53:ASN:HD21	21:U:643:SER:HA	1.64	0.61
23:W:245:LYS:HE2	23:W:248:ARG:HH12	1.65	0.61
1:A:306:LEU:O	1:A:312:ARG:NH1	2.34	0.61
3:C:132:ASP:CG	3:C:133:PRO:HD2	2.25	0.61
28:b:16:MET:HA	28:b:25:ARG:HD2	1.82	0.61
29:c:178:THR:HA	29:c:181:LEU:HB3	1.82	0.61
17:q:4:LEU:HD22	17:q:45:LEU:HD23	1.83	0.61
1:A:44:GLN:OE1	1:A:47:GLN:NE2	2.33	0.61
16:P:123:SER:HB3	16:P:137:VAL:HB	1.82	0.61
12:l:16:GLN:HE21	12:l:18:ARG:HE	1.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:45:LYS:HG3	21:U:187:LEU:HD13	1.82	0.61
7:G:21:ARG:NH2	7:G:26:GLU:OE1	2.33	0.61
5:E:241:ARG:NH2	5:E:283:ASP:O	2.34	0.61
23:W:274:VAL:O	23:W:283:GLN:NE2	2.33	0.61
24:X:409:LYS:NZ	29:c:260:GLU:OE1	2.34	0.61
12:l:33:SER:OG	12:l:62:LYS:NZ	2.33	0.61
16:p:35:VAL:HG12	16:p:36:THR:HG23	1.80	0.61
16:P:36:THR:HG22	17:Q:127:ALA:HB2	1.83	0.61
28:b:122:LYS:HE2	33:z:75:GLY:O	2.00	0.61
32:f:539:LEU:HD12	32:f:542:ILE:HD11	1.83	0.61
11:K:36:THR:HA	11:K:171:GLY:HA3	1.83	0.60
29:c:63:ASP:O	29:c:139:ARG:NH1	2.34	0.60
1:A:113:ILE:HG22	1:A:121:PHE:H	1.65	0.60
21:U:14:GLU:HG2	30:d:73:ARG:HD2	1.82	0.60
22:V:225:ASP:OD1	22:V:228:ARG:NH1	2.34	0.60
30:d:30:LEU:HD12	30:d:31:LEU:HG	1.83	0.60
15:o:50:ALA:HB2	16:p:129:CYS:HB2	1.82	0.60
15:o:177:VAL:HB	15:o:184:ASP:HB2	1.83	0.60
33:z:43:LEU:HB3	33:z:50:LEU:HD12	1.81	0.60
21:U:733:ALA:O	21:U:737:LEU:HB2	2.02	0.60
24:X:297:ARG:O	24:X:334:ASN:ND2	2.34	0.60
33:z:18:GLU:H	33:z:21:ASP:HB2	1.66	0.60
22:V:281:ASN:ND2	31:e:17:ASP:OD1	2.34	0.60
28:b:157:VAL:HG21	28:b:170:LEU:HB2	1.83	0.60
30:d:114:GLU:HA	30:d:117:THR:HG22	1.82	0.60
17:q:1:MET:HE2	17:q:134:TYR:HB2	1.84	0.60
33:z:43:LEU:HB2	33:z:50:LEU:HB2	1.83	0.60
2:B:150:VAL:HG12	2:B:162:VAL:HG23	1.83	0.60
28:b:129:LYS:HB2	33:z:36:ILE:CD1	2.30	0.60
28:b:130:ARG:NH1	33:z:8:LEU:HB2	2.17	0.60
13:m:50:GLU:OE2	13:m:201:HIS:ND1	2.34	0.60
7:g:5:SER:HA	7:g:23:TYR:OH	2.02	0.60
33:z:15:LEU:HD11	33:z:30:ILE:HG13	1.83	0.60
20:T:122:LEU:HG	20:T:137:LEU:HD12	1.84	0.60
20:t:108:ASN:HB3	20:t:110:MET:HE3	1.83	0.60
6:F:314:LEU:HD22	6:F:347:ARG:HD3	1.83	0.60
14:N:114:VAL:HG22	14:N:120:MET:HE1	1.84	0.60
21:U:94:SER:HA	21:U:98:GLU:HG3	1.83	0.60
22:V:345:ARG:NH2	31:e:45:ASP:OD1	2.35	0.60
22:V:277:PRO:HG2	22:V:280:ALA:HB2	1.84	0.60
29:c:123:SER:HB2	29:c:126:ASP:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:135:ALA:HB3	33:u:36:ILE:HD11	1.83	0.60
5:E:65:THR:HG1	5:E:68:LYS:H	1.49	0.59
2:B:313:LEU:O	2:B:346:ARG:NH2	2.34	0.59
10:J:42:VAL:HG22	10:J:210:VAL:HG12	1.84	0.59
21:U:772:TRP:HB3	21:U:775:LEU:HB2	1.83	0.59
25:Y:265:GLU:O	25:Y:267:ARG:NH1	2.35	0.59
29:c:123:SER:HB2	29:c:126:ASP:CG	2.27	0.59
3:C:145:ASP:HA	3:C:201:ARG:HG2	1.83	0.59
27:a:370:GLN:O	30:d:251:ARG:NH2	2.35	0.59
32:f:228:LYS:HZ3	32:f:856:ALA:HA	1.68	0.59
15:o:94:ILE:HG12	16:p:99:ARG:HH22	1.67	0.59
7:G:155:ASP:OD1	7:G:159:TYR:N	2.35	0.59
21:U:558:GLY:H	21:U:589:ALA:HA	1.68	0.59
25:Y:32:ARG:O	25:Y:38:ARG:NH2	2.36	0.59
1:A:309:PHE:H	6:F:238:ARG:HD3	1.67	0.59
4:D:56:VAL:HA	21:U:600:ARG:HE	1.67	0.59
6:F:375:VAL:HG22	6:F:415:LEU:HD12	1.85	0.59
11:K:235:GLU:HA	11:K:238:ILE:HG22	1.84	0.59
21:U:351:MET:HG3	21:U:818:GLU:HA	1.83	0.59
24:X:74:ARG:HH22	24:X:116:TRP:HB2	1.67	0.59
11:k:142:LEU:HB3	11:k:153:LEU:HD11	1.83	0.59
33:z:6:LYS:HA	33:z:11:LYS:O	2.02	0.59
29:c:89:PRO:HB2	33:u:70:VAL:HG21	1.85	0.59
29:c:254:ASN:ND2	29:c:279:ASP:OD1	2.35	0.59
33:z:63:LYS:HG3	33:z:64:GLU:HG3	1.85	0.59
20:T:193:THR:HG23	20:T:195:LYS:H	1.67	0.59
21:U:700:GLU:H	21:U:706:VAL:HG21	1.68	0.59
33:u:63:LYS:CE	33:u:64:GLU:HB2	2.20	0.59
21:U:643:SER:O	21:U:649:ARG:NH1	2.36	0.59
26:Z:126:VAL:HB	29:c:212:LEU:HD21	1.84	0.59
26:Z:142:GLU:OE2	26:Z:153:LYS:NZ	2.36	0.59
7:G:244:GLU:O	23:W:52:LYS:NZ	2.35	0.59
25:Y:69:LEU:HA	25:Y:72:LYS:HG2	1.85	0.59
1:A:300:LEU:HD13	6:F:290:ALA:HB2	1.85	0.58
1:A:400:ARG:HA	1:A:400:ARG:CZ	2.32	0.58
4:D:313:ARG:NH2	4:D:315:ASP:OD2	2.34	0.58
5:E:202:SER:HA	6:F:269:ARG:HH22	1.68	0.58
6:F:364:ARG:HH21	6:F:368:ILE:HG13	1.68	0.58
15:O:21:THR:HG22	15:O:26:VAL:HG22	1.83	0.58
21:U:611:ASN:HB3	21:U:614:VAL:HG12	1.85	0.58
4:D:182:GLU:HA	4:D:185:LEU:HB2	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:253:ILE:HG21	6:F:308:ARG:HH22	1.68	0.58
17:Q:44:LEU:HD11	17:Q:102:LEU:HD23	1.84	0.58
24:X:187:ARG:HH21	24:X:217:ILE:HG22	1.68	0.58
32:f:96:LEU:HD13	32:f:129:LEU:HD13	1.85	0.58
33:u:4:PHE:CD2	33:u:64:GLU:HG2	2.32	0.58
33:z:7:THR:O	33:z:9:THR:N	2.36	0.58
35:D:501:ATP:O3G	5:E:294:ARG:NH1	2.36	0.58
12:L:117:GLN:NE2	13:M:83:ASP:OD1	2.36	0.58
16:P:15:LYS:HE3	16:P:121:ILE:HG12	1.84	0.58
21:U:7:GLY:O	30:d:77:GLN:NE2	2.36	0.58
22:V:372:LEU:HD11	22:V:402:VAL:HG21	1.84	0.58
32:f:548:THR:HA	32:f:551:LYS:HE3	1.84	0.58
2:B:145:GLU:HG2	2:B:148:CYS:HB2	1.85	0.58
26:Z:81:MET:HE1	29:c:94:LYS:HB3	1.85	0.58
26:Z:138:TYR:HB3	26:Z:155:PHE:HB3	1.84	0.58
28:b:132:LYS:CB	33:z:34:GLU:HB3	2.33	0.58
1:A:210:LYS:NZ	1:A:313:GLY:O	2.36	0.58
7:G:165:ALA:HB1	7:G:179:LEU:HD13	1.85	0.58
26:Z:26:ILE:HD11	26:Z:35:VAL:HG22	1.85	0.58
26:Z:82:PHE:HA	26:Z:85:VAL:HG12	1.85	0.58
3:C:90:HIS:ND1	3:C:91:PRO:HD3	2.19	0.58
10:J:30:SER:OG	10:J:48:LYS:NZ	2.36	0.58
12:L:33:SER:OG	12:L:62:LYS:NZ	2.36	0.58
26:Z:136:GLU:OE2	26:Z:157:HIS:ND1	2.35	0.58
16:p:58:THR:O	17:q:85:ARG:NH2	2.37	0.58
18:r:161:TYR:HB2	18:r:195:LEU:HD13	1.86	0.58
33:z:36:ILE:HB	33:z:41:GLN:NE2	2.18	0.58
2:B:96:ARG:HH22	3:C:82:LYS:HE2	1.69	0.58
7:G:9:PHE:HB3	7:G:12:HIS:HB2	1.86	0.58
10:J:88:ARG:HG2	17:Q:69:MET:HE1	1.86	0.58
13:M:34:SER:HG	13:M:65:ARG:HH12	1.50	0.58
30:d:149:ASN:HB3	30:d:199:PHE:CZ	2.39	0.58
3:C:89:VAL:HB	3:C:92:GLU:HB2	1.85	0.58
21:U:65:SER:HB3	21:U:80:TYR:HB2	1.86	0.58
25:Y:360:ASP:HB2	25:Y:363:ASN:HB2	1.86	0.58
30:d:49:ILE:HD12	30:d:52:ARG:HH21	1.69	0.58
8:h:14:SER:HB3	8:h:18:LYS:H	1.69	0.58
5:E:171:LEU:HD22	5:E:295:LEU:HD13	1.84	0.57
29:c:198:ARG:C	29:c:200:TYR:H	2.11	0.57
21:U:333:MET:O	21:U:337:LEU:HB2	2.04	0.57
23:W:67:LEU:HD22	23:W:100:ALA:HB1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:124:LEU:HA	28:b:127:LEU:HD12	1.85	0.57
20:t:27:LEU:HD22	20:t:184:TYR:HB2	1.86	0.57
1:A:118:PHE:O	1:A:120:LYS:NZ	2.37	0.57
8:H:204:THR:OG1	8:H:206:ASP:OD1	2.21	0.57
13:M:80:LEU:H	13:M:133:CYS:HB3	1.69	0.57
19:S:49:LYS:HD2	19:S:113:LEU:HB2	1.87	0.57
25:Y:225:TYR:HA	25:Y:228:MET:HE3	1.86	0.57
33:z:42:ARG:HB2	33:z:70:VAL:HB	1.85	0.57
6:F:180:ARG:HH22	6:F:248:PHE:HB3	1.69	0.57
23:W:285:ASP:HB3	23:W:289:ARG:HH22	1.70	0.57
19:s:148:LEU:HD23	19:s:178:VAL:HG12	1.86	0.57
5:E:85:ARG:HH22	29:c:49:VAL:HG12	1.69	0.57
12:L:165:SER:OG	12:L:169:ARG:NH1	2.38	0.57
26:Z:70:LEU:HD11	26:Z:108:ILE:HG23	1.87	0.57
2:B:235:LEU:HD13	2:B:353:PHE:HZ	1.70	0.57
24:X:297:ARG:NH1	24:X:333:GLN:O	2.37	0.57
25:Y:350:VAL:HG23	25:Y:351:ASN:H	1.69	0.57
29:c:60:GLU:OE1	29:c:68:ARG:NH2	2.38	0.57
29:c:89:PRO:HB2	33:u:70:VAL:CG1	2.32	0.57
15:O:19:ARG:NH2	19:s:213:ASP:OD2	2.35	0.57
7:g:56:VAL:HG23	7:g:61:LEU:HD22	1.87	0.57
8:H:89:ARG:NH1	8:H:121:TYR:OH	2.38	0.57
22:V:177:ASN:O	22:V:179:LYS:NZ	2.37	0.57
4:D:190:LEU:HA	4:D:193:GLN:HE21	1.70	0.57
16:P:155:GLU:H	16:P:158:MET:HE3	1.70	0.57
19:S:28:ARG:NH1	19:S:187:VAL:O	2.37	0.57
25:Y:90:ASP:HA	25:Y:93:LYS:HB2	1.86	0.57
28:b:163:LYS:HE3	33:z:34:GLU:C	2.30	0.57
32:f:437:GLU:HB3	32:f:440:ILE:HB	1.87	0.57
14:n:84:LYS:HD2	14:n:120:MET:HB2	1.87	0.57
19:s:198:VAL:HG22	19:s:203:ILE:HG12	1.86	0.57
14:n:7:GLN:NE2	14:n:109:GLY:O	2.38	0.57
18:r:100:MET:HE1	18:r:113:TYR:HD1	1.70	0.57
4:D:119:ILE:O	4:D:121:ARG:NH1	2.38	0.56
22:V:284:GLU:OE2	22:V:287:ARG:NH1	2.38	0.56
32:f:151:LEU:HB3	32:f:159:VAL:HG22	1.86	0.56
12:l:66:VAL:HG21	12:l:88:MET:HE2	1.86	0.56
16:p:67:LEU:HG	16:p:90:MET:HE1	1.85	0.56
3:C:373:GLU:HG3	3:C:375:ARG:HG3	1.85	0.56
6:F:410:ARG:NH2	6:F:419:ASP:OD2	2.38	0.56
7:G:80:MET:HE2	7:G:87:SER:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:143:ARG:NH1	8:H:144:PRO:O	2.38	0.56
27:a:370:GLN:OE1	30:d:244:LYS:NZ	2.37	0.56
8:h:79:MET:H	8:h:132:VAL:HG12	1.70	0.56
22:V:281:ASN:HA	25:Y:385:ARG:HH22	1.69	0.56
26:Z:83:LYS:NZ	26:Z:89:GLU:O	2.38	0.56
27:a:98:GLU:HG2	27:a:101:ARG:HH21	1.69	0.56
30:d:99:LEU:HB3	30:d:133:ILE:HD11	1.87	0.56
9:i:143:TYR:HB2	9:i:146:GLN:HE21	1.68	0.56
11:k:100:TRP:O	18:r:57:ARG:NH2	2.38	0.56
33:z:45:PHE:HB3	33:z:50:LEU:HD21	1.86	0.56
3:C:49:ARG:NH1	21:U:639:LEU:O	2.38	0.56
10:J:119:THR:HG22	10:J:126:PRO:HB3	1.86	0.56
32:f:685:THR:HA	32:f:688:ARG:HD2	1.87	0.56
6:F:153:VAL:HG22	6:F:160:ILE:HG22	1.88	0.56
25:Y:14:ASN:HB3	25:Y:143:TYR:HE1	1.71	0.56
25:Y:67:VAL:O	25:Y:71:ASN:ND2	2.37	0.56
25:Y:142:PHE:HE2	25:Y:176:ARG:HD2	1.70	0.56
20:t:27:LEU:HD11	20:t:34:ALA:HB1	1.88	0.56
13:M:8:ASP:HB3	13:M:21:PHE:HD2	1.71	0.56
16:P:2:SER:N	16:P:5:SER:OG	2.39	0.56
12:l:7:ASP:O	12:l:21:GLN:NE2	2.35	0.56
10:J:38:ARG:NH2	10:J:178:ASP:O	2.39	0.56
21:U:463:ASN:OD1	21:U:466:LYS:NZ	2.39	0.56
30:d:131:VAL:HG23	30:d:134:LYS:HE2	1.86	0.56
4:D:336:PRO:HB3	4:D:340:GLN:HB2	1.87	0.56
5:E:56:ILE:HB	5:E:100:LEU:HB2	1.88	0.56
33:z:27:LYS:HA	33:z:30:ILE:HD12	1.87	0.56
3:C:90:HIS:CG	3:C:91:PRO:HD3	2.41	0.56
6:F:153:VAL:HA	6:F:160:ILE:HA	1.88	0.56
8:H:118:MET:HE1	8:H:151:PRO:HA	1.88	0.56
22:V:105:SER:OG	22:V:106:ARG:NH1	2.39	0.56
26:Z:205:LEU:HD22	27:a:353:LEU:HD11	1.88	0.56
32:f:216:MET:HA	32:f:219:LYS:HE2	1.87	0.56
9:i:206:LEU:HA	9:i:210:LYS:HD2	1.86	0.56
14:n:115:PRO:HD2	14:n:119:MET:HB3	1.88	0.56
33:z:34:GLU:CB	33:z:36:ILE:HD11	2.35	0.56
22:V:58:ALA:O	22:V:62:HIS:ND1	2.39	0.56
33:z:45:PHE:HE1	33:z:65:SER:HB3	1.71	0.56
3:C:90:HIS:CD2	3:C:90:HIS:H	2.24	0.55
4:D:154:LEU:HB3	4:D:158:GLN:HG3	1.88	0.55
23:W:129:ARG:NH1	23:W:146:THR:OG1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:422:THR:O	26:Z:279:LYS:NZ	2.39	0.55
25:Y:301:ILE:HG21	25:Y:342:ARG:HH11	1.71	0.55
10:j:116:GLN:NE2	10:j:120:GLN:OE1	2.39	0.55
12:l:100:ASP:OD1	19:s:66:LYS:NZ	2.37	0.55
4:D:122:GLU:OE1	29:c:282:ARG:NH2	2.40	0.55
23:W:409:LEU:HD21	24:X:344:ARG:HG2	1.89	0.55
5:E:203:ILE:HD11	5:E:215:ILE:HB	1.88	0.55
9:I:155:ASN:OD1	10:J:77:THR:OG1	2.25	0.55
17:Q:52:ASP:OD1	18:R:88:TYR:OH	2.24	0.55
19:S:194:ARG:HH12	19:S:205:GLU:HB3	1.71	0.55
29:c:71:ASP:OD2	29:c:104:ARG:NH2	2.39	0.55
1:A:277:ILE:HG12	1:A:321:THR:HB	1.88	0.55
4:D:345:PHE:HB3	4:D:360:LEU:HD23	1.89	0.55
5:E:244:SER:HB2	6:F:300:LYS:HD3	1.87	0.55
11:K:52:LYS:NZ	11:K:64:ILE:O	2.40	0.55
19:S:68:ILE:HD11	19:S:92:LEU:HD13	1.88	0.55
21:U:243:LEU:HD22	21:U:903:PHE:HD2	1.69	0.55
24:X:344:ARG:HG3	24:X:386:ILE:HG12	1.87	0.55
8:H:68:ILE:HG22	8:H:69:THR:HG23	1.89	0.55
22:V:150:ARG:NH1	22:V:157:THR:O	2.40	0.55
24:X:369:ILE:HG13	24:X:374:PHE:HB3	1.88	0.55
33:z:60:ASN:OD1	33:z:62:GLN:NE2	2.40	0.55
4:D:170:MET:HE3	35:D:501:ATP:HN61	1.72	0.55
6:F:61:ARG:HH12	33:u:54:ARG:HA	1.70	0.55
10:J:146:GLN:NE2	10:J:147:THR:O	2.40	0.55
17:Q:162:LYS:O	18:r:141:ARG:NH2	2.40	0.55
14:n:58:ALA:O	14:n:62:GLN:NE2	2.40	0.55
19:s:13:LEU:HD22	19:s:145:LEU:HD13	1.87	0.55
25:Y:360:ASP:OD2	25:Y:363:ASN:ND2	2.40	0.55
27:a:205:LEU:O	27:a:271:LYS:NZ	2.38	0.55
33:z:6:LYS:O	33:z:69:LEU:N	2.39	0.55
3:C:70:GLY:O	3:C:118:ASN:ND2	2.39	0.55
28:b:14:GLU:HB2	28:b:17:ARG:HH21	1.71	0.55
28:b:126:LYS:HE2	33:z:72:ARG:N	2.22	0.55
7:g:69:LEU:HD11	7:g:229:ILE:HD13	1.89	0.55
33:z:73:LEU:HD12	33:z:74:ARG:HG3	1.89	0.55
3:C:227:GLY:HA3	3:C:229:ARG:HH11	1.71	0.55
5:E:86:GLN:NE2	6:F:104:GLN:HB3	2.22	0.55
6:F:117:ARG:NH2	6:F:135:PRO:O	2.40	0.55
21:U:57:ARG:NH1	21:U:58:GLN:OE1	2.40	0.55
2:B:90:GLU:HG3	2:B:92:GLN:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:197:LEU:HA	9:I:200:THR:HG22	1.88	0.54
12:L:225:ASP:H	12:L:228:ASP:HB2	1.72	0.54
24:X:149:LEU:HD12	24:X:152:GLN:HE21	1.72	0.54
28:b:142:ASN:ND2	28:b:146:GLU:OE1	2.40	0.54
29:c:125:VAL:HG21	34:v:25:LYS:HD2	1.89	0.54
19:s:52:ILE:HG13	19:s:110:ILE:HG12	1.89	0.54
5:E:161:ARG:NH2	23:W:139:GLU:OE2	2.39	0.54
23:W:234:ASP:O	23:W:238:GLY:N	2.40	0.54
23:W:456:GLN:HB2	26:Z:100:LYS:NZ	2.23	0.54
20:t:122:LEU:HG	20:t:137:LEU:HD12	1.88	0.54
1:A:166:VAL:HG22	1:A:168:GLU:HG3	1.89	0.54
4:D:57:GLN:HA	4:D:60:TYR:HB3	1.90	0.54
7:G:190:THR:OG1	7:G:193:GLN:OE1	2.24	0.54
8:H:14:SER:OG	8:H:18:LYS:N	2.39	0.54
12:L:146:GLN:NE2	12:L:156:CYS:SG	2.80	0.54
28:b:132:LYS:HZ2	33:z:34:GLU:HA	1.72	0.54
32:f:135:GLY:O	32:f:137:ARG:NH1	2.39	0.54
10:j:119:THR:HA	10:j:126:PRO:HG3	1.89	0.54
5:E:236:ASP:O	6:F:304:ARG:NH2	2.41	0.54
22:V:494:MET:HE3	22:V:496:PHE:HZ	1.72	0.54
32:f:285:CYS:O	32:f:291:GLN:NE2	2.40	0.54
19:s:88:ILE:HA	19:s:91:MET:HE2	1.89	0.54
2:B:49:LEU:HG	2:B:51:LEU:HD23	1.89	0.54
3:C:137:LEU:HD11	3:C:220:VAL:HG13	1.90	0.54
6:F:275:ALA:HB1	6:F:326:VAL:HG11	1.90	0.54
9:I:86:LEU:HD22	9:I:114:LEU:HD11	1.90	0.54
9:I:143:TYR:HB2	9:I:146:GLN:HE21	1.72	0.54
19:S:194:ARG:NH2	19:S:205:GLU:OE1	2.41	0.54
26:Z:14:LEU:HA	29:c:39:LEU:HD13	1.88	0.54
1:A:394:MET:HA	1:A:397:ILE:HD12	1.90	0.54
2:B:105:THR:OG1	3:C:120:SER:OG	2.26	0.54
2:B:223:ILE:HG13	2:B:329:MET:HB3	1.90	0.54
2:B:252:GLY:HA2	2:B:255:LEU:HD23	1.90	0.54
6:F:233:LYS:N	37:F:501:ADP:O2A	2.40	0.54
15:O:42:TYR:HE2	15:O:183:LEU:HD11	1.73	0.54
15:O:163:ILE:HD13	15:O:192:PRO:HG3	1.88	0.54
15:O:215:LYS:HB3	16:P:197:THR:HB	1.89	0.54
21:U:98:GLU:HA	21:U:101:ILE:HG12	1.90	0.54
22:V:245:ASP:N	22:V:245:ASP:OD1	2.40	0.54
29:c:44:HIS:ND1	29:c:112:TYR:OH	2.39	0.54
33:z:22:THR:HA	33:z:55:THR:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:135:VAL:HG12	3:C:139:MET:HE1	1.89	0.54
21:U:89:ASN:HB2	21:U:97:VAL:HG21	1.89	0.54
32:f:492:SER:HB2	32:f:494:ARG:HD3	1.90	0.54
15:o:51:ASP:OD1	16:p:99:ARG:NH2	2.40	0.54
3:C:350:LEU:HB3	3:C:387:VAL:HG11	1.90	0.54
25:Y:386:VAL:HG23	25:Y:387:ILE:HD12	1.90	0.54
28:b:130:ARG:HH21	33:z:71:LEU:HD13	1.73	0.54
19:s:16:ALA:HB2	19:s:121:VAL:HG23	1.90	0.54
16:P:34:MET:HB3	18:r:166:ARG:HH11	1.73	0.53
21:U:678:ASP:O	21:U:684:ARG:NH1	2.33	0.53
24:X:67:GLY:HA2	24:X:109:LEU:HD21	1.89	0.53
24:X:401:LEU:HA	24:X:404:ILE:HD12	1.90	0.53
3:C:274:LEU:O	3:C:278:ASN:ND2	2.41	0.53
6:F:180:ARG:NH1	6:F:241:ALA:O	2.41	0.53
24:X:297:ARG:HH12	24:X:336:ILE:HB	1.72	0.53
28:b:129:LYS:HE2	33:z:36:ILE:HG23	1.88	0.53
32:f:755:ASP:OD2	32:f:758:ASN:ND2	2.39	0.53
10:j:71:MET:HE2	10:j:133:ILE:HG12	1.89	0.53
2:B:181:GLN:O	2:B:241:ASN:ND2	2.42	0.53
4:D:168:GLY:O	35:D:501:ATP:N6	2.33	0.53
4:D:292:LEU:HA	4:D:295:GLN:HG2	1.89	0.53
6:F:61:ARG:NH1	33:u:53:GLY:O	2.42	0.53
21:U:505:ASP:HB3	21:U:508:THR:HG22	1.90	0.53
23:W:79:GLU:HB3	23:W:82:LEU:HB2	1.90	0.53
33:z:38:PRO:HA	33:z:41:GLN:HB2	1.90	0.53
2:B:135:ILE:HA	2:B:159:VAL:HB	1.91	0.53
8:h:7:SER:O	9:i:127:LYS:NZ	2.40	0.53
8:h:119:GLN:NE2	9:i:82:ASP:OD1	2.40	0.53
19:S:13:LEU:HD12	19:S:145:LEU:HD13	1.90	0.53
21:U:596:ASN:O	21:U:600:ARG:HB2	2.08	0.53
28:b:20:ASP:OD1	28:b:20:ASP:N	2.42	0.53
10:j:196:LEU:HA	10:j:199:VAL:HB	1.90	0.53
11:k:36:THR:HA	11:k:171:GLY:HA3	1.90	0.53
4:D:259:PRO:HB3	4:D:304:ASN:HB2	1.90	0.53
5:E:33:LEU:O	5:E:37:THR:OG1	2.24	0.53
23:W:146:THR:HG21	23:W:169:LEU:HD21	1.89	0.53
28:b:126:LYS:HG2	33:z:40:GLN:HE21	1.73	0.53
11:k:117:SER:HB3	11:k:156:MET:HE1	1.89	0.53
2:B:71:TYR:HA	2:B:74:MET:HG3	1.91	0.53
4:D:60:TYR:HB2	21:U:603:LEU:HD11	1.90	0.53
15:O:31:CYS:O	15:O:187:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:35:MET:SD	17:Q:181:ARG:NH1	2.80	0.53
22:V:252:ASN:ND2	22:V:284:GLU:OE1	2.41	0.53
27:a:278:MET:HG2	27:a:339:ARG:HH22	1.73	0.53
16:p:159:ASP:OD1	16:p:159:ASP:N	2.40	0.53
2:B:107:MET:HB2	3:C:96:VAL:HB	1.90	0.53
4:D:117:SER:HA	4:D:121:ARG:HH12	1.74	0.53
11:K:41:GLN:NE2	11:K:151:PRO:O	2.40	0.53
14:N:38:HIS:ND1	14:N:39:ASP:OD1	2.36	0.53
24:X:221:GLU:O	24:X:223:LYS:NZ	2.37	0.53
28:b:126:LYS:HE3	33:z:40:GLN:HG2	1.89	0.53
10:J:90:GLU:HG3	10:J:110:TYR:CZ	2.44	0.53
16:P:189:ILE:HB	16:P:196:THR:HB	1.91	0.53
22:V:496:PHE:H	22:V:497:PRO:HD2	1.74	0.53
23:W:174:TYR:O	23:W:182:ARG:NH2	2.41	0.53
25:Y:54:TYR:HE2	25:Y:65:ILE:HG23	1.74	0.53
26:Z:215:VAL:HA	26:Z:220:LEU:HB2	1.90	0.53
19:s:192:ALA:HA	19:s:209:SER:HA	1.91	0.53
20:t:15:LYS:HG2	20:t:20:VAL:HG22	1.91	0.53
23:W:210:ASN:HD21	23:W:212:LYS:HE3	1.74	0.52
32:f:415:GLY:HA3	32:f:447:ALA:HB1	1.91	0.52
8:h:130:PHE:HB3	8:h:132:VAL:HG22	1.91	0.52
14:n:1:THR:N	14:n:169:SER:O	2.42	0.52
19:s:11:THR:HG21	19:s:141:ALA:HB3	1.90	0.52
1:A:427:PRO:HA	1:A:430:MET:HE1	1.92	0.52
4:D:150:SER:HB3	4:D:250:VAL:HG12	1.92	0.52
10:J:189:LYS:HA	10:J:232:ILE:HD11	1.91	0.52
21:U:43:ASP:N	21:U:43:ASP:OD1	2.42	0.52
21:U:126:ILE:HB	21:U:130:LEU:HD21	1.91	0.52
21:U:235:LYS:HA	21:U:238:LYS:HD2	1.90	0.52
24:X:211:ASP:HB2	24:X:235:ALA:HB2	1.91	0.52
32:f:654:VAL:HA	32:f:657:ILE:HD12	1.90	0.52
1:A:192:GLU:HB2	1:A:196:LEU:HD23	1.90	0.52
12:L:201:ALA:O	12:L:239:ARG:NH2	2.42	0.52
23:W:147:LYS:NZ	23:W:184:GLU:OE1	2.42	0.52
28:b:133:LYS:HZ2	33:z:34:GLU:HG3	1.74	0.52
1:A:391:GLU:HA	1:A:394:MET:HE2	1.91	0.52
2:B:252:GLY:N	2:B:285:ASP:O	2.36	0.52
4:D:146:GLU:OE2	4:D:252:ARG:NH1	2.41	0.52
10:J:108:THR:HG23	10:J:133:ILE:HD12	1.90	0.52
11:k:200:ILE:HD13	11:k:203:LYS:HZ1	1.73	0.52
13:m:215:TRP:CD1	13:m:227:VAL:HG22	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:p:74:TYR:OH	16:p:80:ARG:NH2	2.42	0.52
19:s:4:PRO:O	20:t:100:ARG:NH2	2.38	0.52
20:t:25:ASP:HA	20:t:187:PHE:HA	1.90	0.52
33:u:44:ILE:HB	33:u:68:HIS:HB2	1.91	0.52
3:C:133:PRO:O	3:C:134:LEU:C	2.52	0.52
6:F:357:PRO:O	6:F:362:ARG:NH1	2.42	0.52
14:n:4:MET:HG2	14:n:127:ILE:HG22	1.91	0.52
5:E:65:THR:HG1	5:E:68:LYS:N	2.08	0.52
5:E:123:SER:O	5:E:197:LYS:NZ	2.42	0.52
15:O:175:LEU:HB2	15:O:186:LEU:HB2	1.92	0.52
27:a:270:ARG:NH1	27:a:273:GLN:OE1	2.41	0.52
7:g:5:SER:O	7:g:11:ARG:NE	2.42	0.52
4:D:208:PRO:HB2	5:E:291:ARG:HD3	1.90	0.52
6:F:432:LYS:HD2	6:F:435:LEU:HB3	1.91	0.52
16:P:65:GLN:OE1	17:Q:86:ARG:NH2	2.42	0.52
7:g:4:GLY:O	7:g:5:SER:HB2	2.10	0.52
12:l:134:ILE:HB	12:l:145:PHE:HB2	1.92	0.52
12:l:203:GLN:O	12:l:239:ARG:NH1	2.43	0.52
14:n:91:ARG:NH1	20:t:1:THR:OG1	2.43	0.52
33:z:56:LEU:HA	33:z:61:ILE:HD12	1.91	0.52
4:D:354:LEU:HD22	4:D:358:VAL:HG11	1.92	0.52
7:G:38:THR:O	7:G:52:THR:OG1	2.21	0.52
16:P:177:ARG:NH2	19:s:150:ASP:OD2	2.34	0.52
21:U:45:ILE:HG23	21:U:60:ALA:HB1	1.92	0.52
22:V:287:ARG:HH21	31:e:21:GLU:H	1.58	0.52
24:X:255:LEU:HD12	24:X:287:LEU:HD13	1.91	0.52
32:f:176:ALA:HA	32:f:181:ARG:HH22	1.75	0.52
2:B:183:THR:OG1	2:B:242:GLN:OE1	2.27	0.52
3:C:213:ARG:HB3	3:C:247:PHE:HB3	1.92	0.52
3:C:303:SER:HA	3:C:306:LEU:HB2	1.91	0.52
4:D:171:ASP:OD1	4:D:171:ASP:N	2.42	0.52
4:D:345:PHE:O	4:D:349:THR:OG1	2.28	0.52
6:F:168:TYR:O	6:F:173:LYS:NZ	2.43	0.52
6:F:225:MET:HE2	6:F:331:ALA:HB2	1.91	0.52
6:F:422:GLU:HG3	6:F:425:LEU:HD12	1.91	0.52
21:U:172:ASP:OD1	21:U:172:ASP:N	2.42	0.52
21:U:743:ASN:O	21:U:786:THR:OG1	2.27	0.52
23:W:267:LEU:HD23	23:W:299:ILE:HD12	1.90	0.52
24:X:377:ILE:HB	24:X:388:PHE:HE2	1.75	0.52
11:k:52:LYS:NZ	11:k:64:ILE:O	2.43	0.52
17:q:35:MET:HE2	17:q:45:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:358:ASN:O	6:F:362:ARG:NH2	2.43	0.52
14:N:4:MET:HE1	14:N:156:THR:HA	1.91	0.52
25:Y:46:ARG:HE	25:Y:69:LEU:HD21	1.75	0.52
26:Z:192:THR:O	26:Z:196:HIS:ND1	2.32	0.52
29:c:100:LYS:HA	29:c:105:PRO:HB3	1.92	0.52
30:d:248:GLU:HA	30:d:251:ARG:HD3	1.92	0.52
14:n:115:PRO:HG3	20:t:36:PHE:HZ	1.74	0.52
19:s:35:ILE:O	20:t:151:ARG:NH2	2.39	0.52
3:C:165:ILE:HD11	3:C:186:VAL:HG21	1.92	0.51
5:E:237:ALA:HB1	6:F:308:ARG:HG3	1.91	0.51
13:M:134:SER:HB2	13:M:153:PRO:HD3	1.92	0.51
32:f:99:LEU:HD22	32:f:106:LEU:HD11	1.91	0.51
8:h:74:LEU:HD21	8:h:87:VAL:HG22	1.91	0.51
13:m:71:ARG:HD2	13:m:223:ARG:HH12	1.74	0.51
16:p:193:ASP:OD1	16:p:193:ASP:N	2.42	0.51
1:A:295:VAL:HG11	2:B:307:ARG:HH21	1.75	0.51
2:B:406:ALA:HA	2:B:411:ARG:HH21	1.74	0.51
3:C:86:LEU:HD21	3:C:94:LYS:HE2	1.91	0.51
4:D:126:PRO:O	4:D:127:ASN:C	2.52	0.51
21:U:45:ILE:HG21	21:U:64:ALA:HB2	1.93	0.51
2:B:170:LEU:HD23	3:C:229:ARG:HH21	1.75	0.51
4:D:349:THR:HG21	4:D:360:LEU:HD21	1.92	0.51
6:F:289:ASP:OD1	6:F:289:ASP:N	2.42	0.51
13:M:230:ASP:N	13:M:230:ASP:OD1	2.43	0.51
29:c:191:ALA:HB1	29:c:196:LEU:HD23	1.91	0.51
12:l:14:SER:OG	12:l:18:ARG:N	2.39	0.51
4:D:413:GLU:OE1	8:H:53:LYS:NZ	2.42	0.51
23:W:359:VAL:HG23	23:W:382:LEU:HD22	1.91	0.51
13:M:37:ILE:HD11	13:M:193:VAL:HG13	1.92	0.51
21:U:388:ASP:OD1	21:U:388:ASP:N	2.43	0.51
32:f:369:ARG:HG3	32:f:763:ARG:HH22	1.75	0.51
12:l:117:GLN:NE2	13:m:83:ASP:OD1	2.43	0.51
19:s:5:TYR:OH	19:s:103:PRO:O	2.28	0.51
1:A:269:ALA:O	32:f:352:HIS:NE2	2.44	0.51
2:B:117:ASP:OD1	2:B:117:ASP:N	2.44	0.51
17:Q:144:ASP:OD2	18:r:166:ARG:NH2	2.43	0.51
33:z:35:GLY:C	33:z:36:ILE:HD13	2.36	0.51
33:z:38:PRO:O	33:z:42:ARG:NH1	2.44	0.51
1:A:324:PRO:HA	1:A:327:LEU:HD13	1.92	0.51
8:H:111:VAL:HG22	8:H:136:ILE:HD12	1.93	0.51
26:Z:39:LEU:HB2	26:Z:95:TYR:HD2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:HD21	32:f:687:ARG:HH12	1.76	0.51
7:G:10:ASP:OD1	7:G:10:ASP:N	2.44	0.51
17:Q:26:VAL:HG12	17:q:171:PHE:HA	1.93	0.51
24:X:160:MET:HE3	24:X:162:ASP:HB2	1.92	0.51
2:B:58:CYS:SG	2:B:59:ARG:N	2.84	0.51
6:F:97:LEU:O	6:F:120:LYS:HA	2.11	0.51
6:F:277:GLU:OE1	6:F:278:LYS:NZ	2.38	0.51
21:U:24:LEU:O	21:U:28:ASN:ND2	2.44	0.51
21:U:327:LYS:HA	21:U:333:MET:HE1	1.92	0.51
7:g:183:VAL:HG22	7:g:189:TRP:HH2	1.76	0.51
19:S:72:LEU:HD23	19:S:83:MET:HE2	1.93	0.51
24:X:70:LEU:HD13	24:X:109:LEU:HD23	1.92	0.51
24:X:360:ASP:OD1	24:X:360:ASP:N	2.43	0.51
29:c:126:ASP:OD1	33:u:76:GLY:N	2.43	0.51
21:U:643:SER:OG	21:U:645:ASN:O	2.28	0.50
21:U:681:ASN:OD1	21:U:682:TYR:N	2.45	0.50
21:U:710:ARG:NH2	21:U:738:ASP:OD1	2.44	0.50
22:V:325:LYS:O	22:V:329:HIS:ND1	2.41	0.50
7:g:155:ASP:OD1	7:g:159:TYR:N	2.44	0.50
12:l:107:ARG:NH2	20:t:74:GLU:OE2	2.44	0.50
16:p:106:GLU:HG3	16:p:139:SER:HB2	1.91	0.50
5:E:57:VAL:HG13	5:E:97:ARG:HD3	1.93	0.50
19:S:122:TYR:OH	19:S:132:ARG:NH2	2.44	0.50
20:T:209:TRP:HB2	14:n:190:LEU:HD13	1.92	0.50
21:U:16:GLU:OE2	21:U:18:GLN:NE2	2.44	0.50
22:V:345:ARG:HH21	31:e:43:TRP:HA	1.75	0.50
29:c:133:PHE:HZ	33:u:73:LEU:HD13	1.77	0.50
17:q:4:LEU:HD13	17:q:45:LEU:HB3	1.92	0.50
33:u:40:GLN:HA	33:u:72:ARG:HB2	1.94	0.50
5:E:4:PRO:HG2	5:E:8:ALA:H	1.75	0.50
21:U:191:LYS:HA	21:U:194:ARG:HB3	1.92	0.50
21:U:888:GLN:HA	21:U:891:VAL:HG22	1.94	0.50
27:a:186:LYS:HB3	27:a:193:GLN:HE22	1.75	0.50
30:d:114:GLU:O	30:d:118:GLU:HB2	2.10	0.50
30:d:199:PHE:O	30:d:200:PHE:HB2	2.11	0.50
10:j:52:LYS:HG3	10:j:53:LEU:HD12	1.93	0.50
13:m:27:MET:HE1	13:m:153:PRO:HD2	1.92	0.50
33:z:30:ILE:HB	33:z:41:GLN:HE22	1.76	0.50
1:A:300:LEU:HD11	6:F:287:GLU:HB3	1.93	0.50
2:B:381:ASP:HA	2:B:384:ILE:HD12	1.92	0.50
3:C:90:HIS:HE1	4:D:110:ASN:H	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:66:LYS:N	32:f:71:TYR:OH	2.44	0.50
32:f:760:PHE:HD1	32:f:763:ARG:HH21	1.58	0.50
4:D:200:ARG:HH12	4:D:301:GLN:HA	1.76	0.50
10:J:130:SER:OG	10:J:147:THR:O	2.25	0.50
21:U:10:SER:OG	30:d:77:GLN:NE2	2.45	0.50
21:U:124:LYS:HB2	21:U:126:ILE:HG12	1.94	0.50
21:U:333:MET:O	21:U:337:LEU:CB	2.59	0.50
21:U:381:THR:HG22	21:U:412:HIS:HA	1.93	0.50
32:f:290:VAL:HG12	32:f:294:MET:HE1	1.94	0.50
33:u:39:ASP:O	33:u:42:ARG:NH1	2.44	0.50
33:z:50:LEU:HA	33:z:54:ARG:NH1	2.26	0.50
6:F:38:THR:HG22	6:F:39:GLU:HG2	1.94	0.50
9:I:119:GLN:NE2	10:J:79:ASP:OD1	2.45	0.50
21:U:583:MET:HA	21:U:586:VAL:HG12	1.92	0.50
22:V:85:ALA:HB2	22:V:93:PHE:HB2	1.93	0.50
27:a:65:SER:HA	27:a:68:GLU:HB2	1.93	0.50
14:n:21:THR:HG22	14:n:26:ILE:HA	1.93	0.50
5:E:56:ILE:O	5:E:100:LEU:N	2.44	0.50
9:I:151:ASP:OD1	9:I:155:ASN:N	2.44	0.50
26:Z:37:GLY:HA2	26:Z:56:VAL:HG12	1.93	0.50
27:a:34:TRP:HD1	28:b:18:ASN:HA	1.76	0.50
27:a:290:GLN:O	27:a:330:ARG:NH2	2.45	0.50
16:p:97:GLU:HG2	16:p:98:LYS:HG2	1.92	0.50
18:r:58:LEU:HD12	18:r:61:ARG:HD3	1.92	0.50
7:G:103:TYR:O	15:O:81:ARG:NH2	2.45	0.50
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.94	0.50
1:A:140:VAL:HG12	1:A:152:PRO:HA	1.92	0.50
6:F:93:VAL:HG21	6:F:145:LEU:HD11	1.94	0.50
21:U:199:ARG:HE	21:U:223:LEU:HD11	1.76	0.50
22:V:199:ASN:OD1	22:V:241:ARG:NH2	2.44	0.50
25:Y:29:PRO:HB3	25:Y:32:ARG:HH21	1.77	0.50
30:d:72:GLU:HA	30:d:75:MET:HG2	1.94	0.50
32:f:93:PRO:HB2	32:f:96:LEU:HD23	1.94	0.50
32:f:411:ALA:HB2	32:f:440:ILE:HD13	1.94	0.50
7:g:144:ASP:OD2	7:g:150:GLN:NE2	2.45	0.50
2:B:118:ASP:OD1	2:B:118:ASP:N	2.45	0.49
35:D:501:ATP:O2G	5:E:294:ARG:NH2	2.45	0.49
5:E:167:PRO:HB3	5:E:297:ARG:HH12	1.76	0.49
8:H:148:GLN:OE1	8:H:158:TRP:NE1	2.40	0.49
9:I:122:THR:HG22	9:I:129:PRO:HB3	1.93	0.49
21:U:3:THR:O	22:V:266:GLN:NE2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:121:PHE:HB3	22:V:128:ARG:HD2	1.93	0.49
22:V:357:LEU:O	22:V:361:PHE:N	2.37	0.49
24:X:251:LEU:HA	24:X:254:MET:HE2	1.94	0.49
24:X:354:ILE:HG21	24:X:361:VAL:HG21	1.94	0.49
26:Z:254:ASN:HA	26:Z:257:MET:HE2	1.95	0.49
27:a:252:LYS:HA	27:a:255:TRP:HE3	1.77	0.49
8:h:6:TYR:HB2	8:h:126:GLY:HA3	1.94	0.49
13:m:119:VAL:HA	13:m:131:PHE:HE2	1.76	0.49
20:t:126:ASP:OD1	20:t:130:VAL:N	2.45	0.49
13:M:8:ASP:O	13:M:22:GLN:NE2	2.40	0.49
22:V:494:MET:HE3	22:V:496:PHE:CZ	2.47	0.49
27:a:24:ARG:NH1	27:a:40:GLN:OE1	2.45	0.49
28:b:133:LYS:HG3	33:z:11:LYS:CE	2.42	0.49
29:c:192:LEU:HA	29:c:195:GLY:O	2.12	0.49
10:J:39:ASP:OD1	10:J:39:ASP:N	2.45	0.49
11:K:82:ILE:HG22	11:K:86:LYS:HZ1	1.77	0.49
12:L:34:ALA:HA	12:L:162:GLY:HA3	1.94	0.49
28:b:133:LYS:NZ	33:z:36:ILE:HG13	2.28	0.49
32:f:397:LYS:HZ3	32:f:401:LYS:HD3	1.76	0.49
33:u:1:MET:N	33:u:17:VAL:O	2.36	0.49
1:A:279:ALA:HB2	2:B:310:LEU:HG	1.94	0.49
3:C:89:VAL:O	3:C:90:HIS:C	2.55	0.49
5:E:310:LEU:HD11	5:E:314:LYS:HE3	1.94	0.49
8:H:50:LYS:HD2	8:H:209:GLU:HB2	1.94	0.49
16:P:152:SER:HG	19:s:181:SER:HG	1.51	0.49
21:U:629:THR:OG1	21:U:632:GLN:OE1	2.25	0.49
29:c:79:GLY:HA2	29:c:84:VAL:HA	1.95	0.49
32:f:83:ARG:O	32:f:87:THR:OG1	2.30	0.49
18:r:35:ILE:N	18:r:43:GLY:O	2.46	0.49
33:z:2:GLN:H	33:z:63:LYS:HD2	1.78	0.49
33:z:30:ILE:HG21	33:z:69:LEU:CD2	2.42	0.49
33:z:41:GLN:H	33:z:72:ARG:HH12	1.59	0.49
4:D:385:LEU:HD21	4:D:401:LYS:HD2	1.95	0.49
5:E:284:THR:HG22	6:F:297:ASP:HB2	1.93	0.49
22:V:305:ALA:O	22:V:309:MET:HG3	2.12	0.49
24:X:402:GLU:OE2	24:X:403:THR:OG1	2.30	0.49
29:c:34:SER:OG	29:c:70:ILE:O	2.26	0.49
29:c:263:ASP:HB3	29:c:265:MET:HE1	1.93	0.49
32:f:761:MET:HG2	32:f:764:LEU:HD12	1.95	0.49
2:B:109:VAL:HG11	3:C:94:LYS:HZ2	1.78	0.49
3:C:53:ASN:ND2	21:U:642:GLU:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:MET:HE1	3:C:86:LEU:HB2	1.94	0.49
5:E:287:PRO:HA	5:E:290:LEU:HB2	1.94	0.49
16:P:205:ASP:OD1	16:P:205:ASP:N	2.45	0.49
24:X:1:MET:HE1	24:X:35:ILE:HG12	1.95	0.49
24:X:9:PHE:CE2	24:X:45:VAL:HG13	2.48	0.49
26:Z:9:VAL:HG12	26:Z:48:LEU:HB3	1.95	0.49
28:b:121:GLU:O	28:b:122:LYS:C	2.55	0.49
1:A:78:TRP:HZ3	2:B:98:LYS:HD2	1.77	0.49
1:A:224:LEU:N	35:A:501:ATP:O2A	2.44	0.49
1:A:239:ARG:HA	1:A:273:PHE:HB3	1.94	0.49
1:A:307:ASP:OD2	1:A:333:ARG:NH2	2.46	0.49
2:B:174:MET:HG3	2:B:248:LEU:HD22	1.93	0.49
13:M:181:MET:SD	13:M:181:MET:N	2.85	0.49
21:U:126:ILE:HD12	21:U:130:LEU:HD11	1.95	0.49
22:V:122:THR:HG21	22:V:155:ALA:HB1	1.95	0.49
17:q:38:MET:HE3	17:q:44:LEU:HB2	1.94	0.49
4:D:337:ASP:OD1	4:D:337:ASP:N	2.45	0.49
6:F:141:ASP:OD1	6:F:144:LYS:NZ	2.43	0.49
7:G:158:GLY:O	8:H:84:ARG:NH2	2.45	0.49
22:V:419:LEU:HD12	22:V:456:GLY:HA2	1.95	0.49
31:e:37:HIS:HD2	31:e:39:TRP:HB2	1.78	0.49
20:t:152:GLU:OE1	20:t:156:LYS:NZ	2.44	0.49
1:A:335:GLY:N	1:A:338:ASP:OD1	2.37	0.49
4:D:77:GLU:OE2	26:Z:177:ARG:NH2	2.46	0.49
17:Q:13:VAL:HG11	17:Q:105:ALA:HB1	1.94	0.49
21:U:574:LYS:O	21:U:579:ARG:NH2	2.46	0.49
24:X:297:ARG:HD2	24:X:333:GLN:HB3	1.93	0.49
26:Z:59:ASP:OD1	26:Z:59:ASP:N	2.45	0.49
27:a:373:ASP:OD1	27:a:373:ASP:N	2.46	0.49
28:b:12:ASN:OD1	28:b:53:THR:OG1	2.31	0.49
7:g:43:ARG:HH21	7:g:164:LYS:HG2	1.77	0.49
7:g:123:GLN:NE2	8:h:82:ASP:OD1	2.46	0.49
19:s:145:LEU:HD22	19:s:178:VAL:HB	1.94	0.49
5:E:333:LYS:HG3	5:E:334:LEU:HD12	1.95	0.49
6:F:43:GLN:HA	6:F:46:ARG:HG2	1.95	0.49
15:O:143:ARG:NH2	15:O:150:GLU:OE1	2.46	0.49
24:X:9:PHE:HE2	24:X:45:VAL:HG13	1.77	0.49
32:f:393:ASP:OD1	32:f:393:ASP:N	2.45	0.49
17:q:43:LEU:HB2	17:q:183:ILE:HD11	1.94	0.49
1:A:240:VAL:O	1:A:275:ASP:N	2.42	0.48
21:U:205:TYR:HB3	21:U:215:ASN:HD22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:124:PHE:HD1	25:Y:140:ILE:HG23	1.77	0.48
27:a:278:MET:HA	27:a:281:THR:HG22	1.95	0.48
15:o:102:GLY:HA2	15:o:178:ILE:HG21	1.95	0.48
18:r:115:ASP:OD1	18:r:116:SER:N	2.45	0.48
1:A:240:VAL:N	1:A:273:PHE:O	2.44	0.48
3:C:113:ARG:HH11	3:C:130:LYS:HE3	1.77	0.48
4:D:179:GLU:HA	4:D:183:LEU:HB3	1.95	0.48
5:E:320:ILE:HG23	6:F:215:LEU:HD21	1.94	0.48
21:U:194:ARG:O	21:U:198:LEU:HB2	2.14	0.48
21:U:564:ASP:OD1	21:U:564:ASP:N	2.46	0.48
23:W:264:GLN:OE1	23:W:335:SER:OG	2.29	0.48
26:Z:103:LYS:HA	26:Z:103:LYS:HD2	1.72	0.48
28:b:124:LEU:HD13	28:b:156:PHE:HB2	1.95	0.48
18:R:41:LEU:HD23	18:R:103:GLY:HA3	1.94	0.48
22:V:104:THR:HG22	22:V:107:ARG:HH12	1.79	0.48
22:V:326:GLN:HE22	31:e:28:ALA:HB2	1.78	0.48
22:V:338:LEU:HG	22:V:398:LEU:HD12	1.95	0.48
23:W:425:LEU:HD23	26:Z:252:LYS:HG3	1.95	0.48
26:Z:175:LEU:HB3	29:c:217:LEU:HD11	1.94	0.48
27:a:54:ASP:N	27:a:54:ASP:OD1	2.42	0.48
32:f:356:ASN:ND2	32:f:749:ALA:O	2.46	0.48
4:D:401:LYS:HA	4:D:404:LYS:HE2	1.95	0.48
9:I:158:GLY:O	10:J:54:GLN:NE2	2.47	0.48
12:L:42:THR:O	12:L:217:LYS:NZ	2.42	0.48
21:U:471:ASP:HA	21:U:474:ARG:HB2	1.95	0.48
24:X:222:GLU:HG2	24:X:225:TRP:HZ2	1.78	0.48
29:c:27:THR:HG21	29:c:65:TYR:HA	1.95	0.48
9:i:204:SER:O	9:i:210:LYS:NZ	2.47	0.48
4:D:153:MET:HG2	4:D:227:PHE:HB3	1.95	0.48
6:F:178:ASP:N	6:F:178:ASP:OD1	2.45	0.48
17:Q:31:ASP:OD1	17:Q:31:ASP:N	2.46	0.48
19:S:16:ALA:HB2	19:S:121:VAL:HG23	1.94	0.48
25:Y:275:LEU:HD11	25:Y:299:MET:HB3	1.96	0.48
27:a:50:PHE:O	27:a:86:GLN:NE2	2.46	0.48
28:b:129:LYS:NZ	28:b:129:LYS:HB3	2.23	0.48
30:d:82:TYR:HE2	30:d:98:LEU:HD23	1.78	0.48
18:r:7:LYS:HD2	18:r:109:PRO:HB2	1.96	0.48
35:D:501:ATP:O3G	5:E:291:ARG:NE	2.47	0.48
5:E:23:ASP:HA	6:F:55:MET:HE1	1.96	0.48
21:U:82:LEU:O	21:U:129:ARG:NE	2.46	0.48
30:d:26:LEU:HD21	30:d:55:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:196:ARG:O	30:d:199:PHE:HD1	1.97	0.48
7:g:57:PRO:HD2	7:g:61:LEU:HD13	1.95	0.48
9:i:49:ARG:NH2	9:i:58:GLU:OE2	2.46	0.48
10:j:96:LEU:HB2	17:q:62:LYS:HG3	1.94	0.48
1:A:100:LYS:O	1:A:114:ASN:N	2.43	0.48
6:F:195:ILE:HG22	6:F:236:LEU:HD21	1.95	0.48
9:I:103:GLU:OE2	17:Q:76:SER:OG	2.29	0.48
23:W:240:TYR:HA	23:W:243:ILE:HD12	1.96	0.48
28:b:133:LYS:HG3	33:z:11:LYS:NZ	2.29	0.48
19:s:114:ASP:OD1	19:s:118:LYS:N	2.36	0.48
2:B:155:LYS:HD3	2:B:156:VAL:HG13	1.95	0.48
5:E:117:PRO:HG3	6:F:94:ILE:HA	1.96	0.48
8:H:49:GLU:HG3	8:H:195:LEU:HD22	1.95	0.48
8:H:123:GLN:NE2	9:I:128:ARG:O	2.47	0.48
15:O:24:MET:SD	15:O:24:MET:N	2.85	0.48
21:U:616:ARG:HH21	21:U:650:TYR:HE2	1.62	0.48
23:W:211:THR:HA	23:W:214:PHE:HD2	1.78	0.48
24:X:218:HIS:HD2	24:X:228:ALA:HB2	1.78	0.48
26:Z:70:LEU:HD12	26:Z:111:LEU:HD22	1.96	0.48
28:b:26:LEU:HD11	28:b:80:PRO:HG3	1.95	0.48
30:d:3:GLU:H	30:d:25:ARG:HD3	1.79	0.48
12:l:7:ASP:OD1	12:l:7:ASP:N	2.45	0.48
33:z:26:VAL:HG21	33:z:56:LEU:HD21	1.96	0.48
1:A:73:ALA:HB2	2:B:140:ASP:H	1.79	0.48
23:W:375:MET:HA	23:W:378:MET:HE2	1.96	0.48
27:a:74:LEU:HD22	27:a:113:LEU:HD21	1.96	0.48
32:f:740:ARG:HG2	32:f:744:MET:HE1	1.96	0.48
12:l:165:SER:OG	12:l:169:ARG:NH1	2.47	0.48
3:C:151:ILE:HG21	3:C:158:ILE:HD11	1.96	0.48
9:I:76:VAL:HG12	9:I:134:LEU:HG	1.95	0.48
19:S:125:ASP:OD1	19:S:129:SER:N	2.47	0.48
20:T:56:ASP:O	20:T:108:ASN:ND2	2.45	0.48
22:V:492:LYS:O	22:V:495:ARG:NH2	2.47	0.48
25:Y:50:MET:SD	25:Y:53:TYR:HB3	2.54	0.48
28:b:123:ASP:O	28:b:127:LEU:HG	2.14	0.48
30:d:4:GLN:NE2	30:d:21:GLU:OE2	2.46	0.48
15:o:30:ASN:O	15:o:187:ARG:NH2	2.43	0.48
6:F:252:ALA:HB3	6:F:255:GLN:HB2	1.95	0.47
11:K:105:GLU:OE2	19:S:75:TYR:OH	2.29	0.47
14:N:19:ARG:O	14:N:33:LYS:NZ	2.46	0.47
14:N:45:ARG:NH2	14:N:52:THR:OG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:105:VAL:HG13	23:W:141:GLU:HG3	1.94	0.47
28:b:130:ARG:HH12	33:z:8:LEU:HB2	1.79	0.47
32:f:352:HIS:O	32:f:357:ARG:NH1	2.47	0.47
7:g:69:LEU:HB3	7:g:79:VAL:HG23	1.95	0.47
13:m:99:ARG:NH1	13:m:105:ASN:OD1	2.47	0.47
19:s:145:LEU:HD21	19:s:182:ALA:HB2	1.96	0.47
20:t:25:ASP:OD1	20:t:41:ARG:NH2	2.39	0.47
1:A:48:VAL:HG11	2:B:65:LEU:HB3	1.95	0.47
3:C:49:ARG:HE	4:D:64:GLU:HG2	1.79	0.47
3:C:340:ARG:O	3:C:380:GLN:NE2	2.47	0.47
5:E:360:ASP:N	5:E:360:ASP:OD1	2.47	0.47
6:F:91:SER:HA	6:F:126:THR:HA	1.96	0.47
7:G:211:LYS:HD3	7:G:213:SER:H	1.79	0.47
14:N:147:MET:HE3	14:N:151:GLU:HB3	1.94	0.47
18:R:100:MET:HE1	18:R:113:TYR:HB2	1.96	0.47
23:W:187:LEU:HB3	23:W:225:LYS:HE2	1.96	0.47
23:W:420:ASP:HB3	23:W:423:ASN:HB2	1.95	0.47
26:Z:260:VAL:HG13	29:c:292:MET:HE1	1.96	0.47
7:g:211:LYS:HG2	7:g:212:PRO:HD2	1.95	0.47
11:k:141:LEU:H	11:k:156:MET:HB3	1.79	0.47
1:A:189:GLU:O	1:A:193:THR:OG1	2.32	0.47
7:G:112:ASP:OD1	7:G:113:MET:N	2.47	0.47
7:G:128:ASN:HB3	7:G:130:GLU:HG2	1.95	0.47
16:P:159:ASP:OD1	16:P:159:ASP:N	2.43	0.47
20:T:56:ASP:HB2	20:T:107:TRP:HB3	1.96	0.47
22:V:309:MET:HE1	22:V:332:LEU:HB2	1.94	0.47
27:a:135:ILE:HG12	27:a:158:LEU:HD13	1.95	0.47
17:q:41:LYS:HD3	17:q:107:TYR:HD2	1.79	0.47
21:U:570:LEU:HD22	21:U:578:LEU:HD21	1.97	0.47
21:U:607:VAL:O	21:U:615:ARG:NH1	2.43	0.47
22:V:321:ALA:HB1	22:V:324:PHE:HB3	1.96	0.47
26:Z:12:HIS:ND1	26:Z:50:VAL:O	2.28	0.47
26:Z:38:VAL:N	26:Z:54:PHE:O	2.43	0.47
28:b:51:LEU:HD23	28:b:71:ILE:HG23	1.96	0.47
28:b:73:SER:O	28:b:76:HIS:ND1	2.43	0.47
29:c:183:HIS:CG	29:c:184:LEU:H	2.32	0.47
2:B:102:LEU:HD22	2:B:138:PHE:HZ	1.79	0.47
2:B:357:ASP:OD2	2:B:359:LYS:NZ	2.39	0.47
3:C:38:LYS:HZ3	4:D:51:LEU:HA	1.79	0.47
6:F:223:VAL:HG12	6:F:350:ARG:HB2	1.96	0.47
20:T:27:LEU:HD11	20:T:34:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:219:THR:O	23:W:223:LYS:N	2.42	0.47
25:Y:177:ARG:HG2	25:Y:181:LYS:HE3	1.97	0.47
17:q:37:LYS:O	17:q:61:GLN:NE2	2.46	0.47
18:r:144:SER:HB3	18:r:147:LEU:HG	1.96	0.47
3:C:28:ILE:HB	4:D:44:TYR:HE1	1.79	0.47
12:L:72:ILE:HD11	12:L:132:LEU:HD22	1.95	0.47
28:b:179:LEU:HG	28:b:181:ASP:H	1.80	0.47
32:f:846:VAL:O	32:f:866:GLN:N	2.45	0.47
33:u:4:PHE:CE2	33:u:64:GLU:CG	2.49	0.47
1:A:278:ASP:N	1:A:278:ASP:OD1	2.47	0.47
1:A:328:ASP:HB3	1:A:331:LEU:HD23	1.97	0.47
2:B:338:ASP:HB3	2:B:341:LEU:HG	1.95	0.47
4:D:391:ARG:HG2	4:D:393:ILE:H	1.79	0.47
14:N:192:ASP:OD1	14:N:192:ASP:N	2.48	0.47
16:P:30:ILE:HD12	16:P:33:GLN:HE21	1.79	0.47
20:T:45:VAL:HB	20:T:49:THR:HB	1.97	0.47
21:U:337:LEU:HD21	21:U:789:ILE:HG21	1.96	0.47
22:V:281:ASN:HA	25:Y:385:ARG:HH12	1.79	0.47
22:V:346:LEU:HA	22:V:349:ARG:HD3	1.96	0.47
25:Y:332:GLN:OE1	25:Y:336:ARG:NE	2.47	0.47
28:b:132:LYS:HE2	28:b:162:GLY:N	2.29	0.47
29:c:279:ASP:OD1	29:c:279:ASP:N	2.47	0.47
10:j:212:ARG:H	10:j:215:GLN:HG2	1.80	0.47
14:n:164:MET:HG2	14:n:171:GLY:HA2	1.95	0.47
19:s:4:PRO:HB3	20:t:103:MET:HE1	1.96	0.47
33:z:31:GLN:HB2	33:z:36:ILE:H	1.80	0.47
3:C:284:GLU:HG3	3:C:286:THR:H	1.80	0.47
4:D:214:MET:HG3	35:D:501:ATP:H2'	1.97	0.47
12:L:68:ASN:OD1	12:L:69:HIS:ND1	2.37	0.47
15:O:42:TYR:HB2	15:O:178:ILE:HD11	1.97	0.47
18:R:191:ASN:OD1	16:p:203:ARG:NH2	2.39	0.47
21:U:540:GLN:O	29:c:208:ARG:NH2	2.48	0.47
9:i:2:SER:OG	9:i:3:ARG:N	2.48	0.47
33:z:42:ARG:HG2	33:z:72:ARG:NH2	2.30	0.47
2:B:86:LYS:HD3	2:B:88:LEU:HD13	1.96	0.47
6:F:206:MET:SD	6:F:327:LYS:NZ	2.73	0.47
6:F:247:THR:HG21	6:F:278:LYS:HG3	1.97	0.47
11:K:82:ILE:O	11:K:86:LYS:NZ	2.48	0.47
12:L:48:ALA:HB3	12:L:211:SER:HB3	1.95	0.47
25:Y:145:LEU:HG	25:Y:160:ASN:HB3	1.97	0.47
26:Z:109:ASN:HD22	26:Z:155:PHE:HE1	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:31:ILE:HD11	11:k:158:PRO:HD2	1.97	0.47
25:Y:72:LYS:HA	25:Y:75:LYS:HG2	1.96	0.47
7:g:112:ASP:OD1	7:g:112:ASP:N	2.48	0.47
16:p:30:ILE:HG22	16:p:31:GLN:H	1.80	0.47
6:F:41:ILE:O	6:F:45:THR:OG1	2.27	0.46
7:G:164:LYS:N	8:H:56:LEU:O	2.42	0.46
7:G:172:GLN:O	7:G:176:THR:OG1	2.25	0.46
22:V:76:LYS:HD3	22:V:149:PRO:HB3	1.97	0.46
26:Z:10:VAL:O	26:Z:50:VAL:N	2.48	0.46
28:b:132:LYS:HE2	28:b:162:GLY:H	1.80	0.46
11:k:129:ASP:N	11:k:129:ASP:OD1	2.46	0.46
33:z:6:LYS:HD2	33:z:11:LYS:O	2.16	0.46
10:J:2:SER:OG	10:J:3:TYR:N	2.48	0.46
16:P:26:ARG:HE	16:P:38:ASP:HA	1.81	0.46
20:T:211:ILE:HG23	14:n:30:VAL:HG11	1.98	0.46
19:s:183:ALA:HB2	19:s:210:LEU:HD13	1.97	0.46
3:C:91:PRO:HD2	3:C:92:GLU:HG2	1.96	0.46
13:M:8:ASP:OD1	13:M:8:ASP:N	2.47	0.46
22:V:131:LEU:HD22	22:V:171:VAL:HG11	1.97	0.46
26:Z:187:LEU:HD21	29:c:293:THR:HA	1.97	0.46
29:c:196:LEU:HD22	29:c:200:TYR:HE2	1.80	0.46
32:f:741:LEU:HA	32:f:744:MET:HE2	1.97	0.46
32:f:763:ARG:HA	32:f:766:GLN:HG2	1.97	0.46
10:j:90:GLU:HG3	10:j:110:TYR:CZ	2.50	0.46
16:p:123:SER:HB3	16:p:137:VAL:HB	1.97	0.46
19:s:184:GLU:HA	19:s:211:ARG:HH11	1.80	0.46
1:A:69:ASP:HB2	1:A:72:LEU:H	1.80	0.46
5:E:85:ARG:NH2	29:c:46:ARG:O	2.49	0.46
6:F:107:ASP:HB3	29:c:76:PRO:HB3	1.97	0.46
6:F:334:ARG:NE	6:F:336:ASP:OD1	2.47	0.46
6:F:364:ARG:HE	6:F:368:ILE:HG13	1.79	0.46
13:M:186:CYS:HA	13:M:189:ILE:HB	1.96	0.46
14:N:8:PHE:HE1	14:N:13:VAL:HG23	1.81	0.46
21:U:202:VAL:HA	21:U:205:TYR:HB2	1.96	0.46
26:Z:189:GLN:HE21	26:Z:190:ARG:HE	1.64	0.46
28:b:25:ARG:NH2	28:b:145:GLU:H	2.14	0.46
29:c:269:GLN:HA	29:c:272:ILE:HG22	1.97	0.46
20:t:92:LEU:HD12	20:t:112:ILE:HD11	1.95	0.46
1:A:272:ILE:O	1:A:318:LEU:N	2.48	0.46
6:F:298:SER:OG	6:F:301:ALA:O	2.32	0.46
19:S:26:ASP:OD1	19:S:26:ASP:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:265:ILE:HG23	21:U:269:ARG:HH12	1.80	0.46
22:V:71:THR:HG22	22:V:107:ARG:HE	1.81	0.46
26:Z:35:VAL:HB	26:Z:97:THR:HB	1.96	0.46
26:Z:170:VAL:HA	29:c:152:LYS:HG3	1.97	0.46
10:j:222:PRO:HA	10:j:225:ILE:HB	1.97	0.46
1:A:400:ARG:HA	1:A:400:ARG:NE	2.29	0.46
6:F:111:ILE:HG12	6:F:113:LEU:H	1.81	0.46
7:G:171:LYS:HD2	7:G:205:VAL:HG11	1.98	0.46
23:W:397:VAL:HG11	24:X:341:PRO:HB3	1.98	0.46
24:X:70:LEU:HD12	24:X:92:LEU:HD23	1.98	0.46
29:c:89:PRO:CB	33:u:70:VAL:CG1	2.78	0.46
32:f:417:ILE:HG22	32:f:418:LEU:HD12	1.98	0.46
7:g:123:GLN:NE2	7:g:127:GLN:OE1	2.43	0.46
1:A:188:ARG:HA	1:A:191:VAL:HG12	1.98	0.46
4:D:238:LYS:HA	5:E:208:ILE:HB	1.98	0.46
5:E:79:TYR:HB3	5:E:105:LEU:HD21	1.98	0.46
5:E:385:ASP:O	5:E:386:TYR:CG	2.69	0.46
18:R:54:PHE:HE2	19:S:94:THR:HA	1.81	0.46
26:Z:283:ARG:HA	26:Z:286:GLU:HG3	1.97	0.46
32:f:552:ASP:O	32:f:556:ARG:NH1	2.49	0.46
33:z:42:ARG:HG2	33:z:72:ARG:CZ	2.45	0.46
6:F:107:ASP:HA	6:F:110:ASN:HB2	1.98	0.46
21:U:249:CYS:HB3	21:U:328:ILE:HB	1.97	0.46
22:V:283:ASN:HB3	31:e:19:PHE:HD1	1.81	0.46
23:W:199:TYR:O	23:W:203:GLN:HG3	2.16	0.46
28:b:54:LEU:HD13	28:b:84:ILE:HG13	1.98	0.46
8:h:22:ILE:HG21	8:h:152:SER:HB2	1.97	0.46
9:i:101:TYR:HB3	9:i:103:GLU:HG2	1.96	0.46
19:s:60:ASP:OD1	20:t:97:TYR:OH	2.33	0.46
19:s:137:ALA:N	19:s:146:GLN:OE1	2.46	0.46
3:C:327:ASP:N	3:C:327:ASP:OD1	2.45	0.46
3:C:330:LYS:HB2	3:C:344:LEU:HD21	1.98	0.46
4:D:125:LYS:N	4:D:126:PRO:CD	2.79	0.46
5:E:99:ALA:HB2	5:E:111:LEU:HD11	1.98	0.46
13:M:68:ASN:OD1	13:M:224:HIS:ND1	2.38	0.46
21:U:42:VAL:HA	21:U:45:ILE:HD13	1.98	0.46
22:V:311:ASN:HA	22:V:314:ARG:HG2	1.98	0.46
25:Y:377:LEU:HA	25:Y:380:VAL:HG22	1.98	0.46
10:j:168:VAL:HG23	10:j:194:ALA:HB1	1.98	0.46
3:C:248:MET:HG3	3:C:273:MET:HE3	1.98	0.46
9:I:17:ARG:NE	9:I:22:GLU:OE2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:117:GLN:O	12:L:120:THR:OG1	2.30	0.46
15:O:59:ILE:HD12	15:O:82:MET:HE3	1.97	0.46
16:P:158:MET:HE1	16:P:166:THR:HG21	1.98	0.46
21:U:440:GLY:HA2	21:U:473:VAL:HG13	1.97	0.46
26:Z:187:LEU:HG	29:c:293:THR:HG22	1.98	0.46
27:a:188:LEU:O	27:a:193:GLN:NE2	2.49	0.46
32:f:894:LEU:HA	32:f:898:VAL:HG21	1.98	0.46
7:g:17:SER:OG	7:g:21:ARG:N	2.46	0.46
20:T:109:THR:HG23	20:T:126:ASP:HA	1.98	0.45
22:V:311:ASN:OD1	22:V:314:ARG:NH1	2.48	0.45
24:X:281:GLY:H	24:X:284:THR:HG22	1.81	0.45
25:Y:201:PHE:O	25:Y:205:VAL:N	2.48	0.45
26:Z:43:TRP:HB3	26:Z:90:ARG:HH21	1.82	0.45
29:c:196:LEU:HD22	29:c:200:TYR:CE2	2.52	0.45
30:d:52:ARG:HH22	30:d:92:SER:HB3	1.81	0.45
33:z:13:ILE:HB	33:z:33:LYS:NZ	2.31	0.45
2:B:76:GLU:HA	2:B:79:ILE:HG22	1.98	0.45
2:B:106:PRO:HB3	3:C:121:TYR:HB2	1.98	0.45
2:B:317:ASP:HB2	2:B:346:ARG:HG2	1.98	0.45
4:D:276:ASP:N	4:D:282:ASP:OD2	2.48	0.45
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.97	0.45
14:N:189:LEU:HD22	14:N:193:GLN:HB3	1.97	0.45
18:R:196:HIS:CD2	16:p:204:MET:HE2	2.51	0.45
19:S:11:THR:HG21	19:S:141:ALA:HB3	1.98	0.45
23:W:453:HIS:HA	26:Z:103:LYS:HZ3	1.80	0.45
27:a:212:ASN:OD1	27:a:213:PHE:N	2.46	0.45
27:a:290:GLN:HB3	27:a:330:ARG:HH21	1.81	0.45
10:j:160:ALA:O	10:j:169:ARG:NH2	2.49	0.45
16:p:47:ASP:OD1	16:p:47:ASP:N	2.48	0.45
18:r:58:LEU:HD21	18:r:86:MET:HE2	1.98	0.45
19:s:213:ASP:OD1	19:s:213:ASP:N	2.48	0.45
1:A:111:TYR:HE2	1:A:125:LEU:HG	1.81	0.45
11:K:77:ALA:HB3	11:K:142:LEU:HB2	1.96	0.45
13:M:24:GLU:HA	13:M:27:MET:HE2	1.99	0.45
13:M:106:ILE:HG12	13:M:111:LEU:HB2	1.98	0.45
22:V:238:ALA:O	22:V:242:HIS:N	2.50	0.45
22:V:327:THR:HA	22:V:330:LYS:HD2	1.98	0.45
24:X:157:LEU:HB3	24:X:166:LEU:HG	1.99	0.45
8:h:109:GLN:NE2	16:p:78:GLU:OE1	2.43	0.45
21:U:756:HIS:HB3	21:U:759:SER:HB3	1.96	0.45
22:V:227:VAL:HG12	22:V:231:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:153:ASP:HB3	25:Y:156:LEU:HB3	1.97	0.45
7:g:70:PHE:HD2	7:g:91:VAL:HG21	1.82	0.45
12:l:106:SER:OG	20:t:79:ASP:OD2	2.34	0.45
20:t:37:ARG:O	20:t:186:ARG:NH1	2.49	0.45
4:D:385:LEU:HD23	4:D:398:ASP:HA	1.99	0.45
5:E:220:ASN:OD1	5:E:223:ARG:NH2	2.50	0.45
6:F:60:LEU:O	6:F:64:HIS:ND1	2.42	0.45
23:W:452:ILE:HG12	26:Z:100:LYS:HE2	1.98	0.45
27:a:323:SER:O	27:a:332:HIS:N	2.46	0.45
29:c:88:ASP:N	29:c:88:ASP:OD1	2.49	0.45
29:c:251:LEU:HD11	29:c:283:HIS:HB3	1.98	0.45
10:j:31:THR:OG1	10:j:163:ARG:O	2.35	0.45
12:l:45:VAL:HG23	12:l:187:LEU:HD23	1.98	0.45
13:m:68:ASN:OD1	13:m:224:HIS:ND1	2.45	0.45
13:m:213:LEU:HB2	13:m:227:VAL:HG21	1.98	0.45
16:p:204:MET:SD	16:p:204:MET:N	2.86	0.45
17:q:31:ASP:OD1	17:q:31:ASP:N	2.48	0.45
2:B:387:LYS:HB3	2:B:390:LEU:HD23	1.98	0.45
5:E:72:LYS:HA	5:E:78:ARG:HA	1.99	0.45
8:H:51:LYS:NZ	8:H:200:GLU:O	2.50	0.45
8:H:196:LYS:NZ	8:H:203:MET:SD	2.86	0.45
12:L:69:HIS:CE1	12:L:102:PRO:HB3	2.51	0.45
26:Z:206:LEU:HA	26:Z:209:ARG:HG2	1.99	0.45
27:a:222:LEU:HD12	27:a:226:ARG:HH21	1.81	0.45
30:d:132:TYR:HE1	30:d:159:PRO:HG2	1.80	0.45
3:C:241:HIS:O	3:C:244:SER:OG	2.31	0.45
10:J:122:ASN:ND2	11:K:132:ALA:O	2.50	0.45
15:O:205:GLU:O	15:O:208:THR:OG1	2.30	0.45
23:W:315:MET:HE2	23:W:315:MET:HB2	1.83	0.45
26:Z:11:VAL:HA	26:Z:50:VAL:HB	1.99	0.45
26:Z:19:VAL:O	26:Z:23:PHE:N	2.46	0.45
26:Z:48:LEU:HD21	26:Z:92:VAL:HG21	1.98	0.45
32:f:412:ALA:HA	32:f:447:ALA:HB2	1.98	0.45
7:g:58:ASP:OD1	7:g:58:ASP:N	2.48	0.45
1:A:425:ALA:HA	2:B:339:PRO:HB2	1.98	0.45
2:B:173:VAL:HG13	3:C:232:ARG:HD2	1.99	0.45
4:D:409:LYS:HD3	4:D:409:LYS:HA	1.81	0.45
12:L:10:VAL:HG13	12:L:11:THR:HG23	1.99	0.45
17:Q:119:ASP:OD1	17:Q:119:ASP:N	2.49	0.45
24:X:394:ASP:HB3	25:Y:361:SER:HB3	1.98	0.45
32:f:403:LYS:HG3	32:f:406:GLY:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:r:19:ARG:O	18:r:33:LYS:NZ	2.44	0.45
5:E:147:GLU:HA	5:E:151:LEU:HD12	1.97	0.45
20:T:177:TYR:CZ	20:T:185:ASN:HB2	2.52	0.45
22:V:121:PHE:O	22:V:128:ARG:NH1	2.49	0.45
25:Y:314:LEU:O	25:Y:354:VAL:N	2.48	0.45
30:d:149:ASN:HB3	30:d:199:PHE:CE2	2.52	0.45
32:f:111:GLU:HG2	32:f:112:ASN:H	1.82	0.45
11:k:42:THR:OG1	11:k:45:GLY:O	2.31	0.45
12:l:195:LEU:O	12:l:198:THR:OG1	2.32	0.45
1:A:401:ARG:CZ	1:A:401:ARG:HB3	2.46	0.45
2:B:411:ARG:NH2	2:B:418:ASP:OD2	2.50	0.45
6:F:370:SER:HB2	6:F:375:VAL:HG21	1.99	0.45
8:H:77:SER:HB3	8:H:163:MET:HE1	1.99	0.45
8:H:119:GLN:O	8:H:122:THR:OG1	2.26	0.45
29:c:90:VAL:HG12	33:u:44:ILE:HG21	1.99	0.45
29:c:104:ARG:NH2	29:c:106:GLU:OE1	2.50	0.45
1:A:306:LEU:HB3	1:A:336:ARG:HG2	1.99	0.44
3:C:270:GLN:HG2	3:C:305:LEU:HD12	1.99	0.44
4:D:194:ILE:HG22	4:D:196:ILE:HG23	1.99	0.44
6:F:100:ASP:OD1	6:F:100:ASP:N	2.45	0.44
10:J:158:ALA:HB3	11:K:58:LEU:HD13	1.99	0.44
11:K:38:ILE:HG23	11:K:181:LEU:HD11	1.99	0.44
23:W:214:PHE:HD1	23:W:223:LYS:HG2	1.81	0.44
23:W:286:LEU:HD22	23:W:289:ARG:HH12	1.82	0.44
23:W:387:ASP:OD1	23:W:387:ASP:N	2.49	0.44
27:a:77:VAL:HA	27:a:80:ILE:HG22	1.98	0.44
32:f:291:GLN:HA	32:f:294:MET:HE2	1.99	0.44
32:f:304:PHE:HD1	32:f:321:MET:HG2	1.82	0.44
16:p:178:ASP:HB3	16:p:181:SER:HB2	1.99	0.44
1:A:258:ARG:HH12	6:F:255:GLN:HG3	1.82	0.44
4:D:127:ASN:ND2	4:D:252:ARG:HG3	2.32	0.44
16:P:149:MET:HE3	19:s:147:PRO:HB2	1.99	0.44
28:b:141:ILE:HA	28:b:171:VAL:HB	1.99	0.44
16:p:11:VAL:HG23	16:p:54:ALA:HB2	1.99	0.44
21:U:161:ASP:OD1	21:U:161:ASP:N	2.49	0.44
21:U:323:LEU:HG	21:U:327:LYS:HG3	1.98	0.44
11:k:200:ILE:HA	11:k:203:LYS:HZ3	1.81	0.44
16:p:138:VAL:HG11	16:p:146:MET:HB3	1.98	0.44
19:s:166:LEU:HD21	19:s:171:ALA:HB2	1.99	0.44
1:A:417:ILE:O	1:A:421:ALA:HB2	2.17	0.44
4:D:200:ARG:HD2	4:D:299:PHE:HD2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:36:LEU:HG	6:F:69:MET:HE1	2.00	0.44
6:F:295:ARG:NH2	6:F:296:PHE:O	2.51	0.44
8:H:196:LYS:HG3	8:H:203:MET:HE1	2.00	0.44
21:U:794:ASP:OD1	21:U:794:ASP:N	2.49	0.44
22:V:306:ARG:O	22:V:310:THR:OG1	2.33	0.44
23:W:380:GLN:HG3	23:W:381:LEU:HD12	1.98	0.44
26:Z:68:TRP:CD1	26:Z:104:ASN:HD21	2.36	0.44
27:a:293:PHE:HB3	27:a:329:LYS:HB3	1.98	0.44
28:b:140:ILE:HD13	28:b:157:VAL:HG22	2.00	0.44
32:f:175:ASP:N	32:f:175:ASP:OD1	2.50	0.44
3:C:368:MET:HG2	3:C:372:ARG:NH2	2.32	0.44
5:E:142:ILE:HG12	5:E:183:LEU:HD11	1.98	0.44
9:I:76:VAL:HG11	9:I:83:ALA:HB1	1.98	0.44
21:U:82:LEU:HG	21:U:129:ARG:HE	1.82	0.44
24:X:407:MET:HA	24:X:410:VAL:HG22	1.98	0.44
28:b:49:VAL:N	28:b:65:THR:O	2.43	0.44
1:A:296:GLN:HA	1:A:299:MET:HG2	1.99	0.44
1:A:382:GLY:HA3	35:A:501:ATP:C6	2.52	0.44
3:C:134:LEU:O	3:C:137:LEU:N	2.48	0.44
5:E:146:ARG:HA	5:E:149:ILE:HG12	1.98	0.44
22:V:417:ILE:HD12	22:V:422:ILE:HB	2.00	0.44
24:X:82:LYS:HB3	24:X:122:ARG:HH22	1.83	0.44
25:Y:212:GLU:HG2	25:Y:213:LEU:HD22	1.99	0.44
28:b:132:LYS:NZ	33:z:34:GLU:HA	2.32	0.44
1:A:103:ASN:HA	1:A:136:GLU:HG2	2.00	0.44
1:A:308:GLY:HA3	6:F:234:THR:HG21	1.99	0.44
3:C:307:ARG:HB3	3:C:310:ARG:HG2	2.00	0.44
3:C:332:HIS:NE2	3:C:360:LYS:HB2	2.33	0.44
5:E:116:ASP:O	5:E:118:LEU:N	2.50	0.44
7:G:46:ASP:OD1	7:G:46:ASP:N	2.49	0.44
21:U:374:SER:HB3	21:U:407:SER:HB3	1.98	0.44
22:V:477:HIS:ND1	30:d:249:TYR:OH	2.40	0.44
32:f:124:ASP:OD2	32:f:147:SER:OG	2.36	0.44
18:r:18:SER:OG	18:r:173:ALA:N	2.51	0.44
33:z:74:ARG:H	33:z:74:ARG:NE	2.15	0.44
5:E:3:ASP:OD1	5:E:3:ASP:N	2.48	0.44
17:Q:47:VAL:HG23	17:Q:101:ASN:HB2	2.00	0.44
18:R:12:VAL:HB	18:R:179:VAL:HB	1.99	0.44
23:W:441:LYS:HE3	23:W:445:LEU:HD11	2.00	0.44
25:Y:33:GLY:HA2	25:Y:38:ARG:HH22	1.82	0.44
32:f:809:ILE:HG23	32:f:814:SER:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:234:GLU:HA	9:i:237:ILE:HG12	2.00	0.44
19:s:38:ARG:NH1	19:s:191:ASP:OD1	2.49	0.44
33:z:61:ILE:HG21	33:z:67:LEU:HD21	1.99	0.44
1:A:124:ASP:OD1	1:A:124:ASP:N	2.50	0.44
3:C:119:ASP:OD1	3:C:119:ASP:N	2.51	0.44
3:C:341:GLY:HA2	25:Y:6:LEU:HD11	2.00	0.44
16:P:58:THR:HA	17:Q:85:ARG:HH21	1.83	0.44
19:S:45:LYS:HG3	19:S:51:VAL:HG22	1.99	0.44
19:S:64:LEU:HD21	19:S:92:LEU:HD11	1.99	0.44
21:U:182:LYS:HG2	21:U:185:MET:HE2	1.99	0.44
21:U:247:GLN:HG2	21:U:913:ILE:HG22	2.00	0.44
28:b:121:GLU:O	28:b:124:LEU:HG	2.18	0.44
29:c:96:LEU:CD1	33:u:8:LEU:HB3	2.48	0.44
30:d:164:THR:HA	30:d:167:ILE:HG12	1.99	0.44
32:f:564:LEU:HD21	32:f:794:ALA:HB1	2.00	0.44
20:t:56:ASP:H	20:t:107:TRP:HD1	1.64	0.44
4:D:102:ILE:HG13	4:D:112:TYR:HD1	1.83	0.43
4:D:242:GLU:OE1	4:D:245:ARG:NH2	2.50	0.43
4:D:315:ASP:N	4:D:315:ASP:OD1	2.51	0.43
5:E:233:ASP:OD1	5:E:233:ASP:N	2.51	0.43
6:F:224:LEU:N	6:F:350:ARG:O	2.51	0.43
10:J:131:ALA:H	10:J:147:THR:HG1	1.66	0.43
16:P:193:ASP:OD1	16:P:193:ASP:N	2.51	0.43
19:S:99:ARG:HH21	19:S:102:PHE:HD2	1.64	0.43
28:b:180:ALA:HA	28:b:183:LEU:HB2	1.99	0.43
29:c:198:ARG:C	29:c:200:TYR:N	2.75	0.43
7:g:123:GLN:HG3	8:h:81:PRO:HB2	2.00	0.43
11:k:196:LYS:O	11:k:200:ILE:HG12	2.17	0.43
1:A:171:ASP:OD1	1:A:171:ASP:N	2.51	0.43
5:E:83:CYS:HB2	5:E:89:LYS:HE2	2.00	0.43
12:L:44:ALA:HB2	12:L:142:PRO:HB3	2.00	0.43
12:L:93:LEU:HD23	12:L:93:LEU:HA	1.88	0.43
14:N:26:ILE:HG22	20:t:179:ARG:HH11	1.83	0.43
16:P:11:VAL:HG12	16:P:24:ALA:HA	1.99	0.43
21:U:528:ALA:O	21:U:532:MET:HG3	2.18	0.43
22:V:231:LEU:HD23	22:V:254:LEU:HG	2.00	0.43
23:W:166:LEU:HG	23:W:189:GLN:HG2	1.99	0.43
32:f:62:ARG:HA	32:f:65:GLU:HG3	2.00	0.43
12:l:69:HIS:CE1	12:l:102:PRO:HB3	2.53	0.43
12:l:193:ARG:HG2	12:l:196:ARG:HH12	1.83	0.43
1:A:157:ILE:HD12	1:A:157:ILE:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:116:GLN:NE2	11:K:84:ASP:OD1	2.44	0.43
21:U:32:ASN:O	22:V:236:ARG:NH1	2.51	0.43
22:V:76:LYS:HA	22:V:79:VAL:HG12	1.99	0.43
22:V:128:ARG:HH21	22:V:132:LEU:HD11	1.83	0.43
23:W:147:LYS:HE3	23:W:188:GLU:HG3	2.01	0.43
25:Y:297:ARG:NH1	31:e:44:ASP:OD2	2.50	0.43
27:a:128:LEU:O	27:a:132:LYS:NZ	2.50	0.43
28:b:121:GLU:OE2	28:b:124:LEU:HD11	2.18	0.43
32:f:472:HIS:CD2	32:f:474:SER:HB3	2.54	0.43
8:h:222:THR:HG22	8:h:225:GLU:HG2	2.00	0.43
9:i:119:GLN:NE2	10:j:79:ASP:OD1	2.48	0.43
11:k:98:ASN:OD1	18:r:61:ARG:NH2	2.51	0.43
11:k:117:SER:OG	12:l:82:ARG:NH1	2.42	0.43
19:s:72:LEU:HA	19:s:83:MET:HE3	2.00	0.43
3:C:24:TYR:O	4:D:44:TYR:OH	2.35	0.43
4:D:91:GLN:HA	4:D:129:SER:HA	1.99	0.43
5:E:72:LYS:HG3	5:E:78:ARG:HG2	1.99	0.43
6:F:421:MET:HA	6:F:424:ILE:HD12	1.98	0.43
10:J:139:ASP:OD1	10:J:139:ASP:N	2.49	0.43
14:N:51:ASP:HB3	14:N:94:LEU:HD22	2.00	0.43
21:U:337:LEU:HG	21:U:789:ILE:HD13	2.00	0.43
21:U:361:ARG:NH1	21:U:365:CYS:SG	2.92	0.43
22:V:354:LYS:HD3	31:e:33:ASP:HA	2.00	0.43
24:X:153:LEU:HD23	24:X:169:VAL:HG11	2.01	0.43
28:b:126:LYS:HE3	33:z:40:GLN:CG	2.48	0.43
28:b:129:LYS:CD	33:z:71:LEU:HD21	2.48	0.43
12:l:88:MET:HB3	12:l:112:ILE:HD11	2.00	0.43
15:o:209:THR:HG21	16:p:168:SER:HB2	2.01	0.43
18:r:59:LEU:HD12	18:r:83:LEU:HB2	1.98	0.43
2:B:54:PRO:HD2	2:B:61:LYS:HG3	2.01	0.43
4:D:155:THR:HG23	4:D:159:LYS:HE2	2.01	0.43
6:F:92:ASN:N	6:F:125:LYS:O	2.52	0.43
10:J:186:LEU:HD23	10:J:189:LYS:HD2	2.01	0.43
14:N:104:ASP:OD1	14:N:104:ASP:N	2.52	0.43
21:U:696:ILE:HD11	21:U:746:ILE:HG22	2.00	0.43
22:V:411:SER:HB3	22:V:447:ILE:HG12	2.00	0.43
25:Y:367:GLN:O	25:Y:371:LYS:NZ	2.43	0.43
11:k:13:ASN:HB3	12:l:126:ARG:HG2	2.00	0.43
18:r:104:TRP:NE1	18:r:181:GLU:OE1	2.52	0.43
33:z:30:ILE:HG21	33:z:69:LEU:HD22	2.00	0.43
1:A:85:GLN:HA	1:A:88:GLN:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:125:LYS:HA	4:D:125:LYS:HD2	1.52	0.43
13:M:134:SER:OG	13:M:151:ILE:O	2.29	0.43
16:P:10:ALA:HA	16:P:140:GLY:HA3	1.99	0.43
16:P:91:VAL:HG21	16:P:109:ILE:HD11	2.01	0.43
21:U:62:LEU:HD22	21:U:87:LEU:HG	2.01	0.43
21:U:107:HIS:HA	21:U:110:LYS:HE3	2.00	0.43
21:U:123:LYS:NZ	21:U:128:GLN:OE1	2.41	0.43
26:Z:250:TYR:O	26:Z:254:ASN:ND2	2.51	0.43
28:b:94:HIS:NE2	28:b:134:GLU:OE1	2.52	0.43
28:b:129:LYS:HG2	28:b:130:ARG:N	2.34	0.43
29:c:27:THR:OG1	29:c:28:ALA:N	2.51	0.43
32:f:791:VAL:HG12	32:f:823:ALA:HB1	2.00	0.43
7:g:3:ARG:O	7:g:4:GLY:C	2.61	0.43
7:g:130:GLU:OE1	8:h:3:GLU:N	2.51	0.43
17:q:37:LYS:C	17:q:61:GLN:HE22	2.26	0.43
17:q:52:ASP:OD1	18:r:88:TYR:OH	2.30	0.43
2:B:139:VAL:HG21	2:B:159:VAL:HG12	1.99	0.43
6:F:118:LYS:O	6:F:119:GLY:C	2.60	0.43
18:R:11:GLY:HA2	18:R:104:TRP:HZ3	1.83	0.43
21:U:71:LEU:HD11	22:V:273:LYS:HD2	2.00	0.43
28:b:125:VAL:HG22	28:b:129:LYS:HZ3	1.78	0.43
28:b:125:VAL:HG13	33:z:40:GLN:HE22	1.84	0.43
28:b:134:GLU:HG3	33:z:9:THR:HB	2.00	0.43
19:s:10:GLY:HA3	19:s:42:LYS:HE2	2.01	0.43
19:s:68:ILE:HD11	19:s:92:LEU:HD13	2.01	0.43
33:z:7:THR:O	33:z:8:LEU:C	2.61	0.43
33:z:50:LEU:CD2	33:z:54:ARG:HH12	2.32	0.43
3:C:328:ILE:HG22	3:C:359:VAL:HG11	2.01	0.43
4:D:231:VAL:HG13	5:E:262:ASN:HD22	1.84	0.43
5:E:167:PRO:O	5:E:274:LYS:NZ	2.52	0.43
6:F:97:LEU:HD11	6:F:123:VAL:HG23	2.01	0.43
21:U:904:LYS:HE2	21:U:912:ILE:HG22	2.01	0.43
23:W:203:GLN:HG3	23:W:233:LEU:HD11	2.00	0.43
23:W:214:PHE:HB3	23:W:223:LYS:HZ3	1.84	0.43
23:W:406:VAL:HG23	24:X:342:PHE:HB3	2.01	0.43
27:a:219:HIS:HB3	27:a:222:LEU:HG	2.01	0.43
1:A:94:GLN:HG2	1:A:95:VAL:H	1.84	0.43
1:A:323:ARG:HE	1:A:326:THR:HG21	1.84	0.43
2:B:258:LYS:HE2	2:B:259:TYR:CZ	2.54	0.43
5:E:71:VAL:HG13	5:E:81:VAL:HG11	2.01	0.43
5:E:198:VAL:HG12	5:E:200:SER:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:200:SER:HB2	5:E:232:MET:HE3	2.00	0.43
6:F:175:MET:O	6:F:250:LYS:NZ	2.41	0.43
6:F:191:LEU:HB3	6:F:194:GLN:HB2	1.99	0.43
13:M:74:GLY:HA3	13:M:224:HIS:CD2	2.54	0.43
15:O:198:ARG:HD3	15:O:202:TYR:HE2	1.83	0.43
18:R:105:ASP:OD1	18:R:105:ASP:N	2.50	0.43
21:U:448:LEU:HA	21:U:483:LEU:HD23	2.01	0.43
23:W:455:LEU:H	23:W:455:LEU:HG	1.62	0.43
26:Z:148:GLY:HA3	27:a:181:GLY:HA3	1.99	0.43
27:a:360:VAL:HG22	29:c:308:VAL:HG13	2.00	0.43
32:f:487:LEU:HA	32:f:524:MET:HE1	2.01	0.43
14:n:175:ARG:HG2	14:n:188:VAL:HG22	2.00	0.43
33:z:27:LYS:HD3	33:z:41:GLN:HB3	2.01	0.43
1:A:368:ILE:HD12	1:A:409:PHE:HE2	1.84	0.43
3:C:134:LEU:O	3:C:135:VAL:C	2.61	0.43
4:D:380:GLN:NE2	5:E:167:PRO:HG3	2.34	0.43
7:G:50:ILE:HG21	7:G:79:VAL:HB	2.01	0.43
14:N:21:THR:HG22	14:N:26:ILE:HG12	2.01	0.43
15:O:32:SER:HA	15:O:187:ARG:HH22	1.84	0.43
17:Q:11:ASP:N	17:Q:11:ASP:OD1	2.51	0.43
22:V:398:LEU:HA	22:V:401:ASN:HB2	2.01	0.43
23:W:245:LYS:HD3	23:W:248:ARG:HH22	1.82	0.43
25:Y:162:GLU:HA	25:Y:165:LYS:HE3	2.01	0.43
25:Y:241:ILE:HG12	25:Y:261:PHE:HE1	1.83	0.43
28:b:1:MET:SD	28:b:1:MET:N	2.91	0.43
28:b:130:ARG:NH2	33:z:71:LEU:HD22	2.33	0.43
29:c:196:LEU:C	29:c:198:ARG:H	2.26	0.43
20:t:28:GLY:HA3	20:t:39:ILE:HD11	2.00	0.43
4:D:244:PRO:HB3	4:D:291:GLU:HG3	2.00	0.42
8:H:203:MET:HA	8:H:207:ASN:HD21	1.84	0.42
15:O:27:ALA:O	19:s:185:ARG:NH1	2.51	0.42
18:R:166:ARG:NH1	16:p:34:MET:O	2.52	0.42
18:R:182:ASP:OD1	18:R:182:ASP:N	2.45	0.42
23:W:453:HIS:HA	26:Z:103:LYS:HE2	2.00	0.42
25:Y:383:LEU:HA	25:Y:386:VAL:HG22	2.01	0.42
26:Z:65:ASP:OD1	26:Z:65:ASP:N	2.49	0.42
27:a:324:ILE:HG13	27:a:331:VAL:HG13	2.01	0.42
30:d:51:ALA:HA	30:d:54:ILE:HG12	2.00	0.42
30:d:143:LEU:HD12	30:d:151:VAL:HG21	2.00	0.42
32:f:386:GLY:HA2	32:f:418:LEU:HG	2.01	0.42
7:g:61:LEU:HD21	7:g:66:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:q:102:LEU:HB2	17:q:118:MET:HG3	2.01	0.42
4:D:155:THR:H	4:D:158:GLN:HB2	1.84	0.42
10:J:67:ASP:OD1	10:J:67:ASP:N	2.52	0.42
20:T:124:TYR:HE1	20:T:139:THR:HG22	1.84	0.42
22:V:461:LYS:HD2	22:V:461:LYS:HA	1.87	0.42
19:s:19:ASP:OD1	19:s:19:ASP:N	2.52	0.42
33:z:50:LEU:HA	33:z:54:ARG:CZ	2.50	0.42
6:F:61:ARG:NH1	33:u:54:ARG:HA	2.33	0.42
16:P:203:ARG:HH12	18:r:191:ASN:HD21	1.67	0.42
17:Q:83:PHE:O	17:Q:87:ASN:ND2	2.45	0.42
18:R:38:ASN:OD1	18:R:41:LEU:N	2.51	0.42
27:a:136:GLU:OE2	27:a:136:GLU:N	2.51	0.42
28:b:35:ILE:HD12	28:b:184:ILE:HD13	2.00	0.42
28:b:129:LYS:CG	33:z:71:LEU:HD21	2.49	0.42
29:c:117:GLY:N	29:c:146:ASP:OD1	2.45	0.42
16:p:124:LEU:HD23	16:p:128:GLY:HA2	2.02	0.42
19:s:193:LEU:N	19:s:208:VAL:O	2.52	0.42
33:z:45:PHE:CD1	33:z:61:ILE:HG12	2.53	0.42
4:D:189:GLU:O	4:D:193:GLN:HG3	2.18	0.42
11:K:15:PHE:HE2	12:L:127:PRO:HD2	1.84	0.42
17:Q:13:VAL:HB	17:Q:183:ILE:HB	2.01	0.42
17:Q:117:TYR:O	17:Q:118:MET:HE2	2.19	0.42
20:T:136:SER:OG	20:T:147:GLN:OE1	2.37	0.42
22:V:283:ASN:ND2	31:e:17:ASP:O	2.53	0.42
25:Y:71:ASN:HA	25:Y:74:LYS:HG2	2.02	0.42
25:Y:312:ARG:HA	25:Y:356:THR:HG22	2.02	0.42
28:b:122:LYS:HE2	33:z:75:GLY:C	2.44	0.42
28:b:129:LYS:HE3	33:z:36:ILE:HG23	1.99	0.42
29:c:177:THR:HG23	29:c:179:SER:H	1.84	0.42
30:d:66:LYS:HD2	30:d:68:ILE:HD11	2.01	0.42
30:d:190:LEU:HD22	30:d:192:THR:HG22	2.00	0.42
32:f:380:PHE:HZ	32:f:818:LEU:HD12	1.83	0.42
1:A:213:LEU:HD21	1:A:340:LYS:HG2	2.00	0.42
3:C:370:ALA:HB2	3:C:378:VAL:HG13	2.02	0.42
6:F:53:LYS:O	6:F:56:LYS:HG3	2.20	0.42
10:J:37:GLY:HA2	10:J:181:ILE:HB	2.02	0.42
11:K:36:THR:HG21	11:K:173:ALA:HB3	2.02	0.42
14:N:175:ARG:HG2	14:N:188:VAL:HG22	2.01	0.42
19:S:198:VAL:HG22	19:S:203:ILE:HG12	2.02	0.42
21:U:791:LEU:O	21:U:914:LEU:N	2.33	0.42
23:W:103:LYS:HA	23:W:103:LYS:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:408:ARG:HH21	24:X:346:GLN:NE2	2.17	0.42
26:Z:276:ILE:HA	26:Z:279:LYS:HG3	2.01	0.42
30:d:224:SER:OG	30:d:225:PHE:N	2.53	0.42
31:e:17:ASP:OD1	31:e:17:ASP:N	2.50	0.42
32:f:560:LEU:HD21	32:f:801:VAL:HG21	2.01	0.42
8:h:4:ARG:CZ	10:j:5:ARG:HH22	2.33	0.42
17:q:7:ILE:N	17:q:14:LEU:O	2.44	0.42
1:A:365:GLU:HB3	1:A:368:ILE:HG23	2.00	0.42
4:D:328:ASP:OD1	4:D:328:ASP:N	2.53	0.42
27:a:230:ARG:HG3	27:a:232:TRP:HE1	1.83	0.42
13:m:43:ASP:OD1	13:m:43:ASP:N	2.53	0.42
19:s:57:PHE:HZ	20:t:128:LEU:HB3	1.84	0.42
20:t:9:THR:OG1	20:t:10:SER:N	2.51	0.42
33:z:41:GLN:N	33:z:72:ARG:HH22	2.18	0.42
1:A:194:PRO:HG2	1:A:316:LYS:HE3	2.02	0.42
1:A:236:CYS:SG	32:f:352:HIS:HE1	2.43	0.42
1:A:300:LEU:HD22	6:F:254:PRO:HD3	2.02	0.42
4:D:52:GLU:HG3	21:U:596:ASN:HD21	1.85	0.42
6:F:128:THR:HG23	6:F:130:GLN:HG2	2.01	0.42
6:F:183:GLU:HB2	6:F:239:ALA:HA	2.01	0.42
8:H:100:VAL:HG12	16:P:90:MET:HE1	2.02	0.42
12:L:157:ARG:NH1	13:M:56:LYS:O	2.52	0.42
23:W:374:THR:HG22	23:W:412:ILE:HG13	2.02	0.42
24:X:35:ILE:HD12	24:X:46:LYS:HD2	2.01	0.42
24:X:275:LEU:HD11	24:X:278:ARG:HH21	1.83	0.42
26:Z:65:ASP:HB2	26:Z:104:ASN:HB2	2.02	0.42
28:b:184:ILE:HA	28:b:187:PRO:HD2	2.01	0.42
7:g:5:SER:CB	7:g:11:ARG:NH2	2.74	0.42
9:i:165:GLY:O	9:i:168:SER:OG	2.30	0.42
11:k:196:LYS:HG3	11:k:241:ILE:HG13	2.02	0.42
13:m:15:SER:OG	13:m:19:ARG:N	2.44	0.42
33:z:50:LEU:HD11	33:z:67:LEU:HD22	2.02	0.42
2:B:231:GLY:N	35:B:502:ATP:O2B	2.53	0.42
4:D:380:GLN:HE21	4:D:384:MET:HE3	1.84	0.42
5:E:117:PRO:O	5:E:121:ASN:N	2.42	0.42
5:E:295:LEU:HD23	5:E:295:LEU:HA	1.90	0.42
12:L:45:VAL:HG12	12:L:214:ILE:HG12	2.02	0.42
21:U:341:PHE:HZ	21:U:883:ARG:HB3	1.84	0.42
21:U:471:ASP:HB2	21:U:507:VAL:HG13	2.00	0.42
24:X:190:LEU:HD13	24:X:217:ILE:HD12	2.01	0.42
30:d:91:GLU:OE2	30:d:96:HIS:NE2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:103:TYR:HA	32:f:106:LEU:HB2	2.01	0.42
32:f:482:ILE:HD12	32:f:518:THR:HG23	2.02	0.42
8:h:9:SER:HA	8:h:125:GLY:HA2	2.02	0.42
13:m:215:TRP:HD1	13:m:227:VAL:HG22	1.85	0.42
17:q:53:THR:HG22	17:q:100:VAL:HG12	2.00	0.42
33:z:15:LEU:HD13	33:z:29:LYS:HB2	2.01	0.42
3:C:347:ILE:HD12	3:C:350:LEU:HD12	2.01	0.42
6:F:74:LYS:HA	6:F:74:LYS:HD3	1.89	0.42
21:U:757:MET:HA	21:U:760:VAL:HB	2.02	0.42
22:V:182:LYS:HE2	22:V:182:LYS:HB2	1.89	0.42
23:W:88:MET:HB2	23:W:92:LYS:HE2	2.02	0.42
28:b:16:MET:HE2	28:b:25:ARG:HH11	1.84	0.42
28:b:133:LYS:HE2	33:z:7:THR:HG21	1.95	0.42
29:c:195:GLY:O	29:c:196:LEU:HB2	2.19	0.42
12:l:209:ASN:OD1	12:l:209:ASN:N	2.53	0.42
18:r:5:ALA:N	18:r:126:PHE:O	2.49	0.42
33:z:5:VAL:HG21	33:z:30:ILE:HD11	2.01	0.42
33:z:31:GLN:HA	33:z:36:ILE:N	2.30	0.42
6:F:128:THR:O	6:F:130:GLN:NE2	2.37	0.42
17:Q:173:LEU:HD23	17:q:173:LEU:HD23	2.01	0.42
21:U:382:SER:O	21:U:382:SER:OG	2.38	0.42
21:U:886:PRO:HA	21:U:889:LEU:HB2	2.02	0.42
22:V:188:SER:O	22:V:192:MET:HG3	2.20	0.42
27:a:252:LYS:HA	27:a:252:LYS:HD2	1.89	0.42
30:d:170:LEU:HA	30:d:173:THR:HG22	2.02	0.42
32:f:658:ALA:HB2	32:f:693:ALA:HB1	2.02	0.42
13:m:108:LEU:HD11	13:m:137:LEU:HB3	2.02	0.42
4:D:280:GLY:H	4:D:283:ARG:HG3	1.85	0.41
6:F:105:GLU:OE2	6:F:110:ASN:HA	2.19	0.41
6:F:233:LYS:HD3	6:F:331:ALA:HB1	2.01	0.41
13:M:99:ARG:NH2	13:M:105:ASN:OD1	2.47	0.41
15:O:104:ASP:N	15:O:104:ASP:OD1	2.53	0.41
17:Q:8:GLN:HA	17:Q:13:VAL:HA	2.02	0.41
21:U:82:LEU:HD11	21:U:127:ASP:HB3	2.01	0.41
21:U:469:SER:OG	21:U:470:ASN:N	2.53	0.41
22:V:162:GLU:HG3	22:V:203:LEU:HG	2.01	0.41
24:X:28:HIS:CE1	24:X:53:LEU:HD11	2.55	0.41
26:Z:72:HIS:HE1	28:b:60:VAL:HB	1.84	0.41
29:c:198:ARG:O	29:c:200:TYR:N	2.53	0.41
29:c:253:LYS:HD2	29:c:253:LYS:HA	1.87	0.41
16:p:15:LYS:HE3	16:p:154:TRP:HE1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:t:26:MET:SD	20:t:26:MET:N	2.93	0.41
19:S:148:LEU:HD22	16:p:152:SER:HB3	2.02	0.41
21:U:69:TYR:OH	22:V:236:ARG:NH2	2.48	0.41
22:V:346:LEU:O	22:V:350:GLN:NE2	2.51	0.41
24:X:335:LEU:HA	24:X:338:VAL:HG22	2.02	0.41
24:X:389:ASP:OD1	24:X:389:ASP:N	2.47	0.41
25:Y:350:VAL:HG23	25:Y:351:ASN:N	2.34	0.41
30:d:45:LYS:HA	30:d:48:LEU:HB2	2.01	0.41
32:f:472:HIS:CD2	32:f:477:MET:HB2	2.55	0.41
16:p:7:ASN:ND2	16:p:29:GLY:O	2.52	0.41
19:s:64:LEU:HD21	19:s:92:LEU:HD11	2.01	0.41
5:E:86:GLN:NE2	6:F:104:GLN:O	2.46	0.41
5:E:157:GLU:HA	5:E:160:GLN:NE2	2.36	0.41
6:F:175:MET:HE2	6:F:251:LEU:HA	2.00	0.41
6:F:209:LYS:HB2	6:F:209:LYS:HE2	1.88	0.41
14:N:29:ARG:NH2	15:O:139:GLU:OE1	2.53	0.41
19:S:19:ASP:OD1	19:S:19:ASP:N	2.53	0.41
20:T:136:SER:HB2	20:T:150:LEU:HD13	2.03	0.41
21:U:483:LEU:HD22	21:U:778:PHE:CE1	2.55	0.41
23:W:377:ARG:HA	23:W:380:GLN:HG2	2.01	0.41
25:Y:138:LEU:HD13	25:Y:176:ARG:HG3	2.02	0.41
27:a:170:ALA:O	27:a:174:LYS:HB2	2.20	0.41
28:b:25:ARG:NH1	28:b:114:GLY:O	2.53	0.41
32:f:66:LYS:HB2	32:f:66:LYS:HE3	1.63	0.41
32:f:99:LEU:HB2	32:f:129:LEU:HD11	2.02	0.41
32:f:456:ARG:HD2	32:f:494:ARG:HH12	1.85	0.41
10:j:46:GLU:HG3	10:j:199:VAL:HG22	2.02	0.41
20:t:142:GLY:HA2	20:t:176:LEU:HD21	2.02	0.41
7:G:221:THR:HG22	7:G:223:GLU:H	1.86	0.41
17:Q:184:ASP:OD1	17:Q:184:ASP:N	2.52	0.41
21:U:22:PHE:CD2	30:d:30:LEU:HD13	2.55	0.41
21:U:367:THR:HA	21:U:370:VAL:HG22	2.01	0.41
21:U:698:GLN:HG2	21:U:702:THR:HG21	2.01	0.41
21:U:879:ASP:OD1	21:U:879:ASP:N	2.48	0.41
24:X:415:TYR:HB2	25:Y:383:LEU:HD11	2.03	0.41
26:Z:263:ALA:HB1	29:c:288:VAL:HB	2.02	0.41
30:d:231:LYS:HA	30:d:231:LYS:HD2	1.78	0.41
10:j:136:PHE:HE1	10:j:142:PRO:HB3	1.84	0.41
33:z:4:PHE:HB3	33:z:12:THR:HB	2.02	0.41
33:z:6:LYS:HD2	33:z:11:LYS:C	2.45	0.41
33:z:6:LYS:N	33:z:67:LEU:O	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PRO:HA	1:A:75:PRO:HD3	1.94	0.41
2:B:324:ASP:OD1	2:B:324:ASP:N	2.50	0.41
3:C:219:LEU:HD23	4:D:286:GLN:HG3	2.02	0.41
5:E:376:ASP:OD1	5:E:376:ASP:N	2.53	0.41
21:U:638:SER:O	21:U:641:SER:OG	2.33	0.41
22:V:417:ILE:HA	25:Y:349:LYS:HD3	2.03	0.41
25:Y:272:PHE:HA	25:Y:275:LEU:HB3	2.03	0.41
26:Z:105:ASP:HA	26:Z:108:ILE:HD13	2.03	0.41
28:b:132:LYS:HB3	33:z:34:GLU:OE1	2.21	0.41
8:h:3:GLU:O	8:h:4:ARG:HB3	2.20	0.41
14:n:127:ILE:HD11	14:n:136:TYR:CE1	2.55	0.41
15:o:41:ILE:HD13	15:o:102:GLY:HA3	2.02	0.41
3:C:125:LYS:NZ	4:D:112:TYR:OH	2.42	0.41
3:C:161:ILE:HD12	3:C:161:ILE:HA	1.94	0.41
3:C:163:GLU:HG2	3:C:167:LEU:HD22	2.03	0.41
3:C:361:GLY:O	3:C:365:GLU:HB2	2.21	0.41
4:D:55:GLU:HG3	21:U:600:ARG:HH21	1.84	0.41
4:D:377:SER:O	4:D:380:GLN:N	2.54	0.41
7:G:17:SER:OG	7:G:20:GLY:N	2.53	0.41
18:R:18:SER:OG	18:R:173:ALA:N	2.49	0.41
21:U:413:LYS:HD2	21:U:780:SER:HB2	2.02	0.41
22:V:122:THR:H	22:V:150:ARG:HH21	1.69	0.41
22:V:268:GLU:HA	22:V:271:VAL:HG12	2.02	0.41
24:X:94:ASP:OD1	24:X:94:ASP:N	2.54	0.41
28:b:129:LYS:HB3	28:b:129:LYS:HZ1	1.85	0.41
16:p:14:MET:HE3	16:p:15:LYS:N	2.34	0.41
19:s:74:MET:HE3	19:s:74:MET:O	2.20	0.41
33:z:30:ILE:HG22	33:z:36:ILE:CG1	2.45	0.41
1:A:269:ALA:HA	1:A:314:ASN:O	2.21	0.41
4:D:251:PHE:HE1	4:D:262:ILE:HG21	1.85	0.41
5:E:364:GLN:HA	5:E:367:PHE:HD2	1.84	0.41
8:H:15:PRO:HA	9:I:23:TYR:CZ	2.56	0.41
11:K:148:GLU:OE1	19:S:81:LYS:NZ	2.52	0.41
21:U:475:HIS:ND1	21:U:511:ALA:HB2	2.36	0.41
28:b:133:LYS:O	33:z:11:LYS:HG2	2.20	0.41
29:c:126:ASP:OD1	29:c:126:ASP:N	2.53	0.41
29:c:245:VAL:HA	29:c:248:MET:HB2	2.03	0.41
32:f:845:ARG:HG2	32:f:867:THR:HG22	2.03	0.41
7:g:95:ARG:HD3	14:n:68:ILE:HG22	2.02	0.41
9:i:174:MET:SD	9:i:196:VAL:HG22	2.60	0.41
10:j:169:ARG:O	10:j:173:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:46:VAL:HG21	11:k:153:LEU:HB2	2.03	0.41
18:r:38:ASN:HD21	18:r:41:LEU:HD12	1.86	0.41
18:r:164:THR:HG22	18:r:170:SER:HB3	2.03	0.41
1:A:97:ARG:HE	2:B:131:HIS:CD2	2.39	0.41
2:B:376:ASP:OD1	2:B:376:ASP:N	2.54	0.41
3:C:34:ILE:HD12	4:D:51:LEU:HD11	2.01	0.41
3:C:69:GLN:HG3	3:C:118:ASN:HD21	1.85	0.41
3:C:141:GLU:O	4:D:323:ARG:NH1	2.54	0.41
9:I:10:THR:OG1	9:I:122:THR:O	2.30	0.41
11:K:157:ASP:OD2	11:K:159:SER:OG	2.38	0.41
21:U:597:LYS:HD2	21:U:597:LYS:HA	1.92	0.41
21:U:898:CYS:SG	21:U:899:ARG:N	2.94	0.41
22:V:417:ILE:HA	25:Y:349:LYS:CG	2.51	0.41
22:V:474:LEU:O	22:V:478:GLN:NE2	2.53	0.41
24:X:404:ILE:HA	24:X:407:MET:SD	2.60	0.41
26:Z:208:ILE:HG23	27:a:353:LEU:HD21	2.03	0.41
27:a:12:GLN:HG3	27:a:22:TRP:HB3	2.03	0.41
28:b:18:ASN:HD21	28:b:25:ARG:NH2	2.19	0.41
28:b:129:LYS:O	28:b:133:LYS:HD3	2.21	0.41
30:d:18:LYS:HB2	30:d:18:LYS:HE2	1.87	0.41
7:g:132:ARG:HE	13:m:124:LEU:HD23	1.85	0.41
8:h:50:LYS:NZ	8:h:59:GLU:O	2.45	0.41
12:l:121:GLN:HE22	13:m:131:PHE:HD1	1.68	0.41
14:n:108:GLY:O	14:n:110:GLN:NE2	2.54	0.41
1:A:57:LYS:HE3	1:A:57:LYS:HB3	1.92	0.41
1:A:108:ASP:OD2	1:A:110:LYS:NZ	2.52	0.41
1:A:386:ARG:HD3	2:B:217:LYS:NZ	2.36	0.41
3:C:71:SER:OG	3:C:116:LEU:O	2.32	0.41
3:C:90:HIS:CE1	4:D:110:ASN:H	2.39	0.41
4:D:227:PHE:HE2	4:D:229:ARG:HB2	1.86	0.41
4:D:266:GLU:OE2	5:E:262:ASN:ND2	2.53	0.41
6:F:362:ARG:NE	6:F:388:THR:O	2.54	0.41
7:G:188:ASP:OD1	7:G:188:ASP:N	2.54	0.41
9:I:147:LEU:HD21	9:I:162:THR:HG22	2.02	0.41
9:I:158:GLY:HA3	10:J:55:ASP:HB3	2.02	0.41
10:J:50:VAL:HB	10:J:54:GLN:HB2	2.03	0.41
12:L:93:LEU:O	12:L:97:PHE:HB2	2.21	0.41
14:N:46:SER:OG	14:N:97:GLY:O	2.28	0.41
14:N:84:LYS:HB2	14:N:120:MET:SD	2.61	0.41
16:P:191:GLU:OE1	16:P:194:LYS:NZ	2.41	0.41
20:T:1:THR:N	20:T:105:PRO:O	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:9:THR:OG1	20:T:10:SER:N	2.54	0.41
21:U:117:ASP:OD1	21:U:117:ASP:N	2.53	0.41
25:Y:68:ASP:OD1	25:Y:68:ASP:N	2.53	0.41
25:Y:314:LEU:HD11	25:Y:318:TYR:CD2	2.55	0.41
29:c:194:HIS:NE2	34:v:21:UNK:O	2.44	0.41
30:d:168:ASP:OD1	30:d:169:ILE:N	2.53	0.41
32:f:159:VAL:HG21	32:f:194:TYR:CE2	2.56	0.41
32:f:761:MET:HE2	32:f:811:LEU:HD21	2.03	0.41
8:h:34:PRO:O	8:h:48:THR:OG1	2.31	0.41
8:h:81:PRO:HG3	8:h:84:ARG:HH21	1.86	0.41
8:h:107:THR:H	8:h:140:ASN:ND2	2.18	0.41
9:i:6:ASP:N	9:i:6:ASP:OD1	2.52	0.41
10:j:192:ILE:HD12	10:j:206:ILE:HD12	2.03	0.41
13:m:48:GLY:HA2	13:m:213:LEU:HD23	2.03	0.41
18:r:160:ILE:HG21	18:r:174:VAL:HG23	2.03	0.41
33:z:13:ILE:HD12	33:z:15:LEU:HD21	2.03	0.41
33:z:15:LEU:HD22	33:z:29:LYS:HB3	2.03	0.41
1:A:65:ILE:HG13	1:A:74:PRO:HB3	2.03	0.41
1:A:420:TYR:O	1:A:424:SER:OG	2.37	0.41
3:C:32:GLN:NE2	3:C:36:ASN:OD1	2.54	0.41
4:D:277:ALA:HA	4:D:283:ARG:HG2	2.03	0.41
16:P:126:LEU:HD23	16:P:126:LEU:HA	1.97	0.41
21:U:336:GLU:HA	21:U:339:LEU:HB3	2.03	0.41
23:W:400:LYS:NZ	24:X:340:GLU:OE2	2.39	0.41
24:X:80:ILE:HB	24:X:84:LYS:HE3	2.03	0.41
24:X:137:TYR:HA	24:X:142:ARG:HE	1.86	0.41
27:a:278:MET:HB2	27:a:336:VAL:HG13	2.03	0.41
28:b:16:MET:HE1	28:b:114:GLY:HA3	2.03	0.41
28:b:109:ILE:HD12	28:b:138:VAL:HG22	2.01	0.41
30:d:75:MET:HA	30:d:78:LEU:HD12	2.03	0.41
32:f:512:MET:HE1	32:f:554:TYR:HB2	2.02	0.41
33:z:45:PHE:CE1	33:z:65:SER:HB3	2.54	0.41
1:A:98:CYS:HA	1:A:141:GLY:HA2	2.03	0.40
1:A:181:LYS:HA	1:A:184:ILE:HD12	2.03	0.40
2:B:420:LYS:HD2	2:B:420:LYS:HA	1.96	0.40
3:C:69:GLN:NE2	4:D:135:HIS:O	2.51	0.40
6:F:120:LYS:HB3	6:F:120:LYS:HE3	1.77	0.40
8:H:182:LEU:HD22	8:H:186:ASP:HB3	2.02	0.40
12:L:65:HIS:HD2	12:L:221:PHE:HB3	1.87	0.40
14:N:120:MET:HA	14:N:120:MET:HE3	2.03	0.40
14:N:135:ILE:HD13	14:N:163:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:103:VAL:HG22	15:O:108:PRO:HB3	2.03	0.40
15:O:201:ARG:HD3	15:O:201:ARG:HA	1.91	0.40
17:Q:172:ILE:HG23	17:Q:173:LEU:HG	2.04	0.40
21:U:575:ASP:HB3	21:U:578:LEU:HB3	2.03	0.40
23:W:55:ARG:HD2	23:W:96:GLN:HA	2.03	0.40
26:Z:102:HIS:N	26:Z:105:ASP:OD2	2.43	0.40
28:b:84:ILE:HD12	28:b:115:SER:HB2	2.03	0.40
5:E:265:ASP:OD2	5:E:291:ARG:NH2	2.54	0.40
6:F:380:ASN:HB3	6:F:383:GLU:HB3	2.04	0.40
6:F:413:THR:OG1	6:F:414:GLU:OE1	2.29	0.40
11:K:13:ASN:HB3	12:L:126:ARG:HB3	2.03	0.40
12:L:6:TYR:O	12:L:20:HIS:ND1	2.54	0.40
21:U:54:PHE:HB3	21:U:57:ARG:HB3	2.02	0.40
21:U:609:ASP:O	21:U:615:ARG:NH1	2.40	0.40
23:W:192:LEU:HD23	23:W:192:LEU:HA	1.85	0.40
23:W:205:ILE:HG23	23:W:208:LYS:HD2	2.03	0.40
23:W:360:GLU:HA	23:W:363:ILE:HG22	2.04	0.40
26:Z:106:ILE:HA	26:Z:155:PHE:HZ	1.86	0.40
7:g:10:ASP:OD1	7:g:10:ASP:N	2.54	0.40
12:l:18:ARG:NH1	12:l:23:GLU:OE1	2.55	0.40
12:l:50:LYS:HB3	12:l:59:HIS:HB3	2.03	0.40
16:p:38:ASP:OD1	16:p:38:ASP:N	2.53	0.40
1:A:248:LYS:HA	2:B:260:LEU:HB2	2.03	0.40
2:B:70:ASP:HA	2:B:73:LEU:HG	2.03	0.40
4:D:403:TYR:O	4:D:407:ILE:HG12	2.21	0.40
5:E:117:PRO:HD3	6:F:94:ILE:HG23	2.02	0.40
6:F:438:TYR:OH	11:K:19:GLY:O	2.33	0.40
7:G:72:ILE:HG23	7:G:95:ARG:HA	2.03	0.40
14:N:30:VAL:HG11	20:t:211:ILE:HG23	2.04	0.40
21:U:27:LEU:HD23	21:U:63:VAL:HG11	2.03	0.40
21:U:354:LYS:HD2	21:U:354:LYS:HA	1.87	0.40
21:U:616:ARG:HG3	21:U:647:HIS:HB3	2.03	0.40
24:X:50:ILE:HG21	24:X:88:LEU:HD21	2.03	0.40
29:c:279:ASP:HB2	29:c:283:HIS:HB2	2.03	0.40
11:k:146:VAL:HG11	11:k:222:PRO:HA	2.03	0.40
14:n:57:ASP:OD2	15:o:81:ARG:NH1	2.47	0.40
16:p:25:ASP:OD1	16:p:25:ASP:N	2.52	0.40
2:B:116:ILE:HB	2:B:120:HIS:O	2.21	0.40
7:G:196:GLU:O	7:G:200:THR:OG1	2.35	0.40
13:M:163:CYS:SG	13:M:164:ALA:N	2.95	0.40
21:U:740:GLY:HA3	21:U:744:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:337:LEU:HD22	22:V:367:VAL:HG11	2.04	0.40
23:W:137:TYR:HD1	23:W:138:VAL:HG13	1.87	0.40
25:Y:121:LEU:HD21	25:Y:147:ILE:HG21	2.04	0.40
25:Y:263:LEU:HB3	25:Y:271:PHE:CE1	2.56	0.40
29:c:195:GLY:HA3	29:c:200:TYR:CE1	2.57	0.40
29:c:270:LEU:HA	29:c:273:LYS:HG2	2.03	0.40
8:h:55:ILE:HD12	8:h:55:ILE:HA	1.96	0.40
14:n:153:LEU:HD22	14:n:176:LEU:HD13	2.03	0.40
15:o:104:ASP:OD1	15:o:104:ASP:N	2.52	0.40
33:z:6:LYS:HE2	33:z:10:GLY:HA2	2.04	0.40
1:A:73:ALA:HB3	2:B:138:PHE:HA	2.03	0.40
2:B:221:GLY:HA3	2:B:347:ILE:HG22	2.03	0.40
4:D:159:LYS:HD3	4:D:159:LYS:HA	1.86	0.40
5:E:237:ALA:O	6:F:308:ARG:NE	2.43	0.40
14:N:107:GLU:HB3	14:N:110:GLN:NE2	2.37	0.40
19:S:63:THR:OG1	20:T:94:ARG:NH1	2.55	0.40
22:V:495:ARG:O	26:Z:278:ASN:ND2	2.45	0.40
23:W:140:ILE:HG12	23:W:177:MET:HE1	2.03	0.40
26:Z:21:ASP:OD2	26:Z:25:ARG:NH2	2.55	0.40
26:Z:144:VAL:HA	26:Z:152:SER:HB3	2.03	0.40
28:b:50:GLY:N	28:b:64:LEU:HD12	2.36	0.40
29:c:184:LEU:HG	29:c:185:ASN:N	2.35	0.40
9:i:62:SER:OG	9:i:65:ILE:O	2.28	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	392/433 (90%)	347 (88%)	44 (11%)	1 (0%)	36	71
2	B	382/440 (87%)	351 (92%)	30 (8%)	1 (0%)	36	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	359/398 (90%)	328 (91%)	27 (8%)	4 (1%)	11	45
4	D	378/418 (90%)	340 (90%)	35 (9%)	3 (1%)	16	52
5	E	387/403 (96%)	348 (90%)	37 (10%)	2 (0%)	24	63
6	F	413/439 (94%)	376 (91%)	37 (9%)	0	100	100
7	G	242/246 (98%)	229 (95%)	13 (5%)	0	100	100
7	g	242/246 (98%)	223 (92%)	17 (7%)	2 (1%)	16	52
8	H	230/234 (98%)	218 (95%)	12 (5%)	0	100	100
8	h	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
9	I	249/261 (95%)	240 (96%)	9 (4%)	0	100	100
9	i	248/261 (95%)	242 (98%)	6 (2%)	0	100	100
10	J	237/248 (96%)	224 (94%)	13 (6%)	0	100	100
10	j	237/248 (96%)	221 (93%)	16 (7%)	0	100	100
11	K	232/241 (96%)	219 (94%)	12 (5%)	1 (0%)	30	67
11	k	232/241 (96%)	224 (97%)	8 (3%)	0	100	100
12	L	236/263 (90%)	224 (95%)	12 (5%)	0	100	100
12	l	236/263 (90%)	224 (95%)	12 (5%)	0	100	100
13	M	238/255 (93%)	234 (98%)	4 (2%)	0	100	100
13	m	238/255 (93%)	235 (99%)	3 (1%)	0	100	100
14	N	200/239 (84%)	192 (96%)	8 (4%)	0	100	100
14	n	200/239 (84%)	193 (96%)	7 (4%)	0	100	100
15	O	218/277 (79%)	210 (96%)	8 (4%)	0	100	100
15	o	218/277 (79%)	209 (96%)	9 (4%)	0	100	100
16	P	202/205 (98%)	188 (93%)	14 (7%)	0	100	100
16	p	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
17	Q	197/201 (98%)	189 (96%)	8 (4%)	0	100	100
17	q	197/201 (98%)	189 (96%)	8 (4%)	0	100	100
18	R	199/263 (76%)	194 (98%)	5 (2%)	0	100	100
18	r	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
19	S	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
19	s	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
20	T	214/264 (81%)	203 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	t	214/264 (81%)	204 (95%)	10 (5%)	0	100	100
21	U	812/953 (85%)	756 (93%)	56 (7%)	0	100	100
22	V	442/534 (83%)	426 (96%)	15 (3%)	1 (0%)	43	78
23	W	439/456 (96%)	432 (98%)	7 (2%)	0	100	100
24	X	420/422 (100%)	399 (95%)	21 (5%)	0	100	100
25	Y	387/389 (100%)	357 (92%)	29 (8%)	1 (0%)	36	71
26	Z	284/324 (88%)	257 (90%)	27 (10%)	0	100	100
27	a	371/376 (99%)	346 (93%)	25 (7%)	0	100	100
28	b	189/377 (50%)	168 (89%)	20 (11%)	1 (0%)	24	63
29	c	285/310 (92%)	255 (90%)	28 (10%)	2 (1%)	18	55
30	d	255/350 (73%)	220 (86%)	35 (14%)	0	100	100
31	e	48/70 (69%)	39 (81%)	9 (19%)	0	100	100
32	f	840/908 (92%)	803 (96%)	36 (4%)	1 (0%)	48	83
33	u	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
33	z	74/76 (97%)	56 (76%)	15 (20%)	3 (4%)	2	17
34	v	1/10 (10%)	0	1 (100%)	0	100	100
All	All	13441/15038 (89%)	12612 (94%)	806 (6%)	23 (0%)	44	78

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	ARG
3	C	134	LEU
4	D	125	LYS
5	E	386	TYR
11	K	130	PRO
33	z	8	LEU
33	z	9	THR
3	C	133	PRO
4	D	126	PRO
25	Y	350	VAL
29	c	183	HIS
29	c	199	HIS
7	g	4	GLY
7	g	7	ALA
33	z	75	GLY

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Mol	Chain	Res	Type
22	V	496	PHE
32	f	66	LYS
3	C	91	PRO
5	E	385	ASP
28	b	122	LYS
4	D	150	SER
2	B	87	PRO
3	C	135	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	337/372 (91%)	334 (99%)	3 (1%)	70	77
2	B	339/385 (88%)	338 (100%)	1 (0%)	86	84
3	C	314/346 (91%)	311 (99%)	3 (1%)	68	76
4	D	333/366 (91%)	330 (99%)	3 (1%)	70	77
5	E	341/353 (97%)	341 (100%)	0	100	100
6	F	357/379 (94%)	355 (99%)	2 (1%)	78	81
7	G	205/210 (98%)	205 (100%)	0	100	100
7	g	202/210 (96%)	201 (100%)	1 (0%)	81	82
8	H	188/191 (98%)	188 (100%)	0	100	100
8	h	188/191 (98%)	188 (100%)	0	100	100
9	I	207/221 (94%)	207 (100%)	0	100	100
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	201/211 (95%)	201 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
21	U	696/816 (85%)	696 (100%)	0	100	100
22	V	390/460 (85%)	390 (100%)	0	100	100
23	W	406/416 (98%)	404 (100%)	2 (0%)	81	82
24	X	362/362 (100%)	362 (100%)	0	100	100
25	Y	344/344 (100%)	343 (100%)	1 (0%)	86	84
26	Z	257/295 (87%)	256 (100%)	1 (0%)	84	83
27	a	333/336 (99%)	333 (100%)	0	100	100
28	b	167/312 (54%)	161 (96%)	6 (4%)	31	52
29	c	252/268 (94%)	248 (98%)	4 (2%)	55	69
30	d	231/294 (79%)	231 (100%)	0	100	100
31	e	44/63 (70%)	44 (100%)	0	100	100
32	f	711/763 (93%)	709 (100%)	2 (0%)	86	84
33	u	68/68 (100%)	67 (98%)	1 (2%)	57	71
33	z	68/68 (100%)	57 (84%)	11 (16%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	v	1/1 (100%)	1 (100%)	0	100	100
All	All	11505/12751 (90%)	11464 (100%)	41 (0%)	81	83

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	400	ARG
1	A	401	ARG
1	A	403	ILE
2	B	125	THR
3	C	89	VAL
3	C	90	HIS
3	C	109	THR
4	D	125	LYS
4	D	127	ASN
4	D	151	ILE
6	F	105	GLU
6	F	120	LYS
23	W	455	LEU
23	W	456	GLN
25	Y	349	LYS
26	Z	103	LYS
28	b	121	GLU
28	b	122	LYS
28	b	125	VAL
28	b	129	LYS
28	b	132	LYS
28	b	163	LYS
29	c	107	MET
29	c	126	ASP
29	c	184	LEU
29	c	198	ARG
32	f	66	LYS
32	f	365	VAL
7	g	6	SER
33	u	63	LYS
33	z	7	THR
33	z	9	THR
33	z	11	LYS
33	z	31	GLN
33	z	34	GLU
33	z	36	ILE

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Mol	Chain	Res	Type
33	z	39	ASP
33	z	54	ARG
33	z	72	ARG
33	z	73	LEU
33	z	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	247	GLN
3	C	41	ASN
3	C	53	ASN
3	C	64	GLN
3	C	90	HIS
3	C	171	HIS
3	C	337	ASN
3	C	343	ASN
3	C	377	HIS
3	C	380	GLN
4	D	127	ASN
4	D	193	GLN
4	D	278	GLN
4	D	353	ASN
4	D	380	GLN
5	E	39	GLN
5	E	280	ASN
5	E	339	ASN
6	F	102	ASN
6	F	208	HIS
6	F	316	GLN
6	F	436	GLN
7	G	12	HIS
7	G	33	ASN
7	G	34	GLN
7	G	75	ASN
7	G	90	GLN
8	H	95	GLN
8	H	102	GLN
9	I	142	HIS
10	J	18	GLN
10	J	54	GLN

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Mol	Chain	Res	Type
11	K	41	GLN
11	K	155	HIS
11	K	221	GLN
12	L	4	ASN
12	L	86	ASN
13	M	143	ASN
14	N	28	ASN
15	O	91	GLN
15	O	116	HIS
15	O	153	ASN
15	O	165	ASN
15	O	172	ASN
17	Q	61	GLN
17	Q	65	GLN
17	Q	168	GLN
19	S	108	ASN
20	T	157	GLN
21	U	28	ASN
21	U	115	ASN
21	U	258	GLN
21	U	541	HIS
21	U	718	ASN
21	U	743	ASN
22	V	81	GLN
22	V	247	GLN
22	V	381	GLN
22	V	427	GLN
22	V	473	GLN
23	W	203	GLN
24	X	13	GLN
24	X	44	GLN
24	X	334	ASN
25	Y	64	GLN
25	Y	160	ASN
25	Y	196	GLN
25	Y	365	GLN
25	Y	378	ASN
25	Y	388	ASN
26	Z	72	HIS
26	Z	77	ASN
26	Z	109	ASN
27	a	12	GLN

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Mol	Chain	Res	Type
27	a	86	GLN
27	a	129	GLN
27	a	143	ASN
27	a	193	GLN
27	a	249	GLN
27	a	288	HIS
27	a	345	GLN
28	b	158	ASN
29	c	197	ASN
29	c	232	GLN
30	d	88	GLN
32	f	238	ASN
32	f	323	ASN
32	f	378	ASN
32	f	402	ASN
32	f	614	HIS
32	f	737	ASN
32	f	752	HIS
32	f	866	GLN
7	g	128	ASN
7	g	150	GLN
9	i	95	GLN
9	i	102	GLN
9	i	146	GLN
10	j	85	ASN
10	j	122	ASN
10	j	154	HIS
10	j	200	GLN
11	k	221	GLN
12	l	90	GLN
14	n	66	HIS
14	n	110	GLN
15	o	80	ASN
17	q	61	GLN
18	r	10	HIS
18	r	29	GLN
18	r	85	ASN
18	r	196	HIS
33	z	25	ASN
33	z	31	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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$
35	ATP	D	501	36	29,33,33	0.31	0	44,52,52	0.46	0
37	ADP	C	501	-	27,29,29	1.38	4 (14%)	42,45,45	2.02	9 (21%)
37	ADP	F	501	36	27,29,29	1.35	4 (14%)	42,45,45	1.99	10 (23%)
35	ATP	B	502	36	29,33,33	0.27	0	44,52,52	0.46	1 (2%)
35	ATP	E	401	36	29,33,33	0.29	0	44,52,52	0.49	1 (2%)
35	ATP	A	501	36	29,33,33	0.31	0	44,52,52	0.45	0

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
35	ATP	D	501	36	-	5/22/38/38	0/3/3/3
37	ADP	C	501	-	-	4/16/32/32	0/3/3/3
37	ADP	F	501	36	-	7/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	B	502	36	-	4/22/38/38	0/3/3/3
35	ATP	E	401	36	-	4/22/38/38	0/3/3/3
35	ATP	A	501	36	-	7/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C	501	ADP	C5-C4	4.71	1.47	1.39
37	F	501	ADP	C5-C4	4.43	1.47	1.39
37	F	501	ADP	C5-C6	2.68	1.48	1.41
37	C	501	ADP	C5-C6	2.63	1.48	1.41
37	F	501	ADP	C8-N7	2.44	1.36	1.31
37	C	501	ADP	C5-N7	-2.37	1.34	1.39
37	C	501	ADP	C8-N7	2.22	1.35	1.31
37	F	501	ADP	C5-N7	-2.15	1.35	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	501	ADP	C5-C4-N3	-6.90	117.75	126.75
37	F	501	ADP	C5-C4-N3	-5.91	119.03	126.75
37	C	501	ADP	N3-C4-N9	5.53	136.19	127.08
37	F	501	ADP	N3-C4-N9	4.59	134.65	127.08
37	F	501	ADP	PA-O3A-PB	-4.31	118.04	132.83
37	C	501	ADP	C2-N3-C4	3.99	121.17	111.75
37	F	501	ADP	C2-N3-C4	3.85	120.85	111.75
37	F	501	ADP	C4-C5-N7	-3.30	106.60	110.62
37	F	501	ADP	N3-C2-N1	-3.28	123.48	128.60
37	C	501	ADP	PA-O3A-PB	-3.25	121.66	132.83
37	C	501	ADP	C4-C5-N7	-3.11	106.83	110.62
37	C	501	ADP	N3-C2-N1	-2.92	124.04	128.60
37	F	501	ADP	C5-N7-C8	2.77	107.44	103.51
37	F	501	ADP	C4-N9-C8	2.75	108.70	105.73
37	C	501	ADP	C5-N7-C8	2.57	107.16	103.51
37	C	501	ADP	C3'-C2'-C1'	2.39	105.97	101.43
37	F	501	ADP	C6-C5-N7	2.34	136.38	132.02
37	F	501	ADP	N9-C8-N7	-2.17	110.94	113.91
37	C	501	ADP	C4-N9-C8	2.16	108.06	105.73
35	B	502	ATP	PB-O3B-PG	2.02	139.76	132.83
35	E	401	ATP	PB-O3B-PG	2.01	139.74	132.83

There are no chirality outliers.

All (31) torsion outliers are listed below:

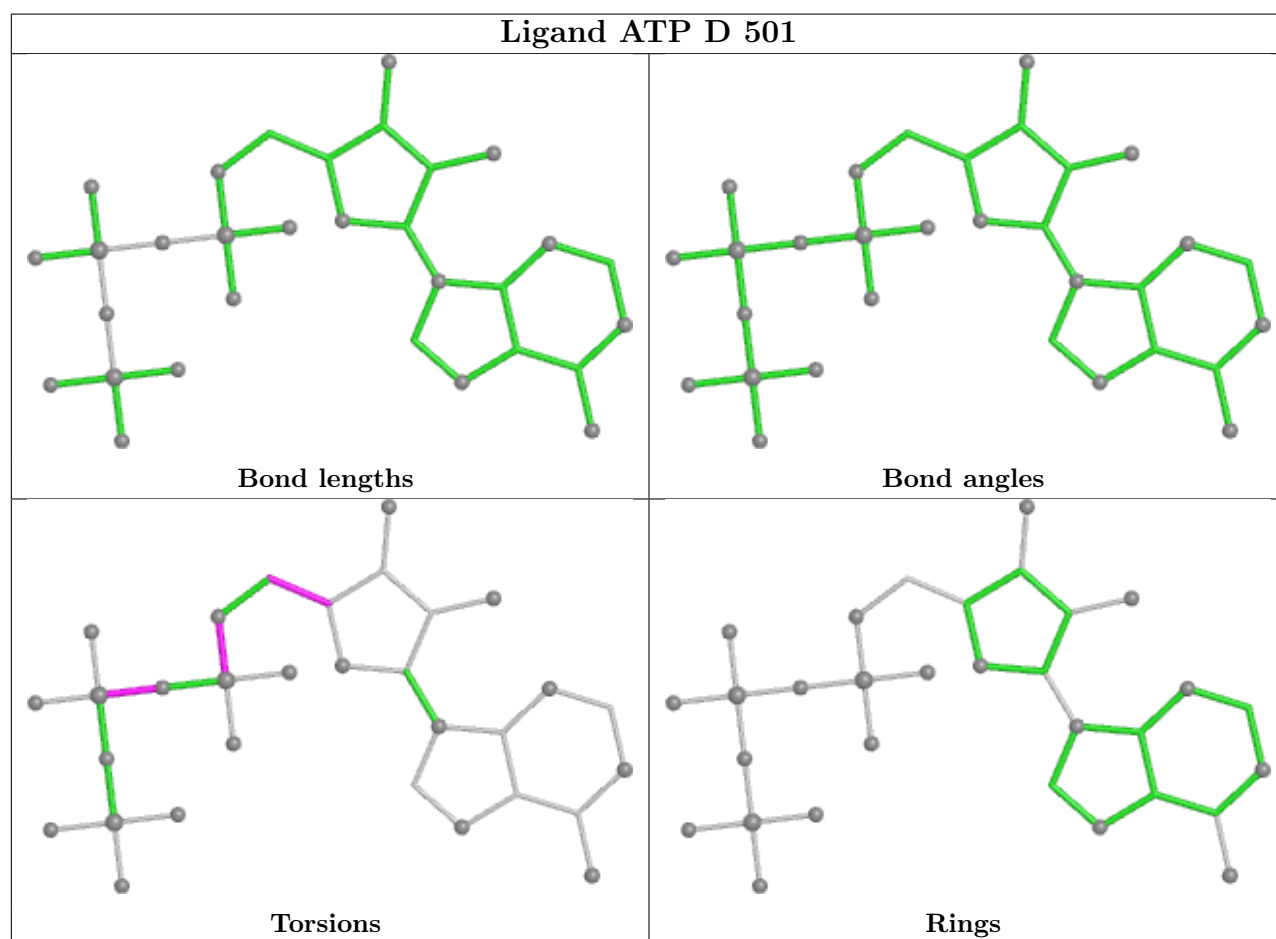
Mol	Chain	Res	Type	Atoms
35	A	501	ATP	C5'-O5'-PA-O1A
35	A	501	ATP	C5'-O5'-PA-O2A
35	B	502	ATP	C5'-O5'-PA-O1A
35	B	502	ATP	C5'-O5'-PA-O2A
35	B	502	ATP	C5'-O5'-PA-O3A
35	D	501	ATP	C5'-O5'-PA-O1A
35	D	501	ATP	C5'-O5'-PA-O3A
35	E	401	ATP	C5'-O5'-PA-O1A
35	E	401	ATP	C5'-O5'-PA-O3A
37	F	501	ADP	C5'-O5'-PA-O1A
35	D	501	ATP	O4'-C4'-C5'-O5'
35	E	401	ATP	O4'-C4'-C5'-O5'
35	E	401	ATP	C3'-C4'-C5'-O5'
37	F	501	ADP	O4'-C4'-C5'-O5'
37	F	501	ADP	C3'-C4'-C5'-O5'
37	F	501	ADP	C2'-C1'-N9-C8
37	C	501	ADP	PA-O3A-PB-O1B
37	F	501	ADP	C2'-C1'-N9-C4
37	C	501	ADP	C5'-O5'-PA-O3A
35	D	501	ATP	PA-O3A-PB-O2B
35	D	501	ATP	C5'-O5'-PA-O2A
37	C	501	ADP	C5'-O5'-PA-O2A
35	A	501	ATP	PA-O3A-PB-O1B
35	A	501	ATP	PA-O3A-PB-O2B
35	B	502	ATP	PA-O3A-PB-O1B
37	F	501	ADP	C4'-C5'-O5'-PA
37	C	501	ADP	C4'-C5'-O5'-PA
35	A	501	ATP	C5'-O5'-PA-O3A
37	F	501	ADP	C5'-O5'-PA-O3A
35	A	501	ATP	PG-O3B-PB-O1B
35	A	501	ATP	PG-O3B-PB-O2B

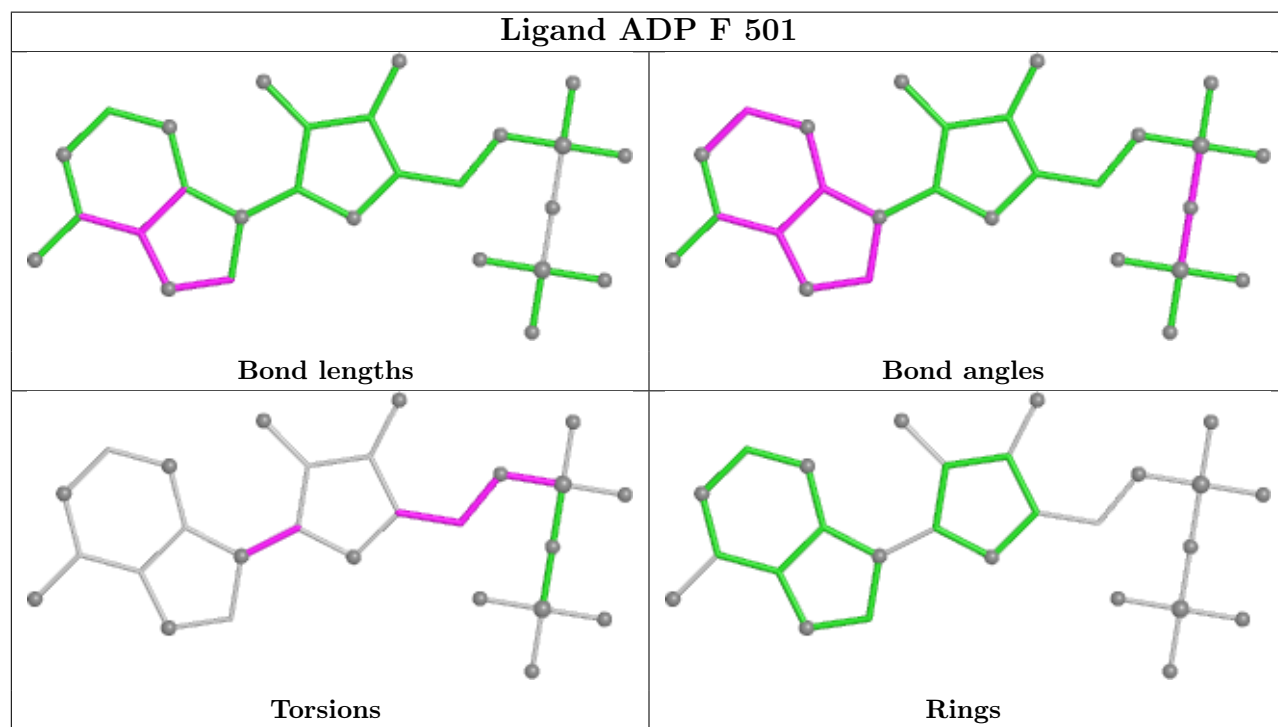
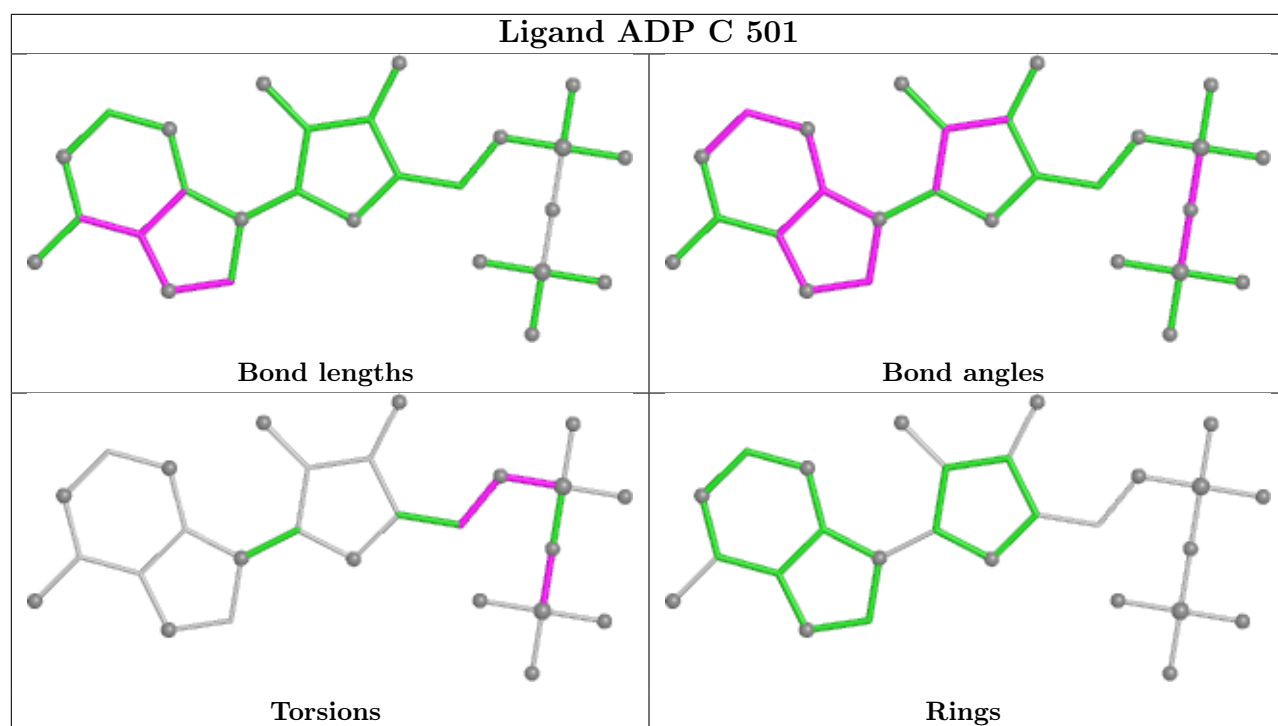
There are no ring outliers.

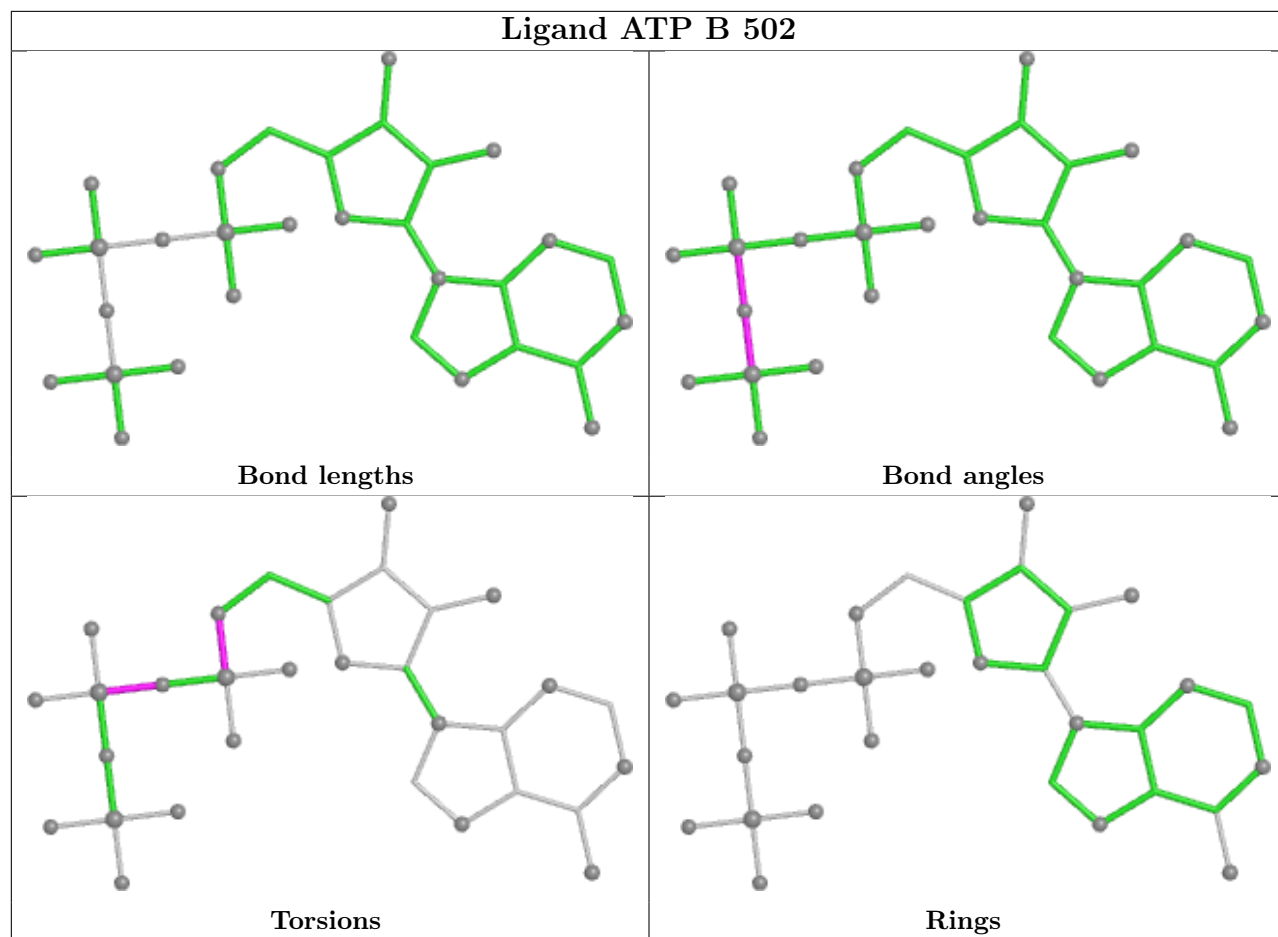
4 monomers are involved in 11 short contacts:

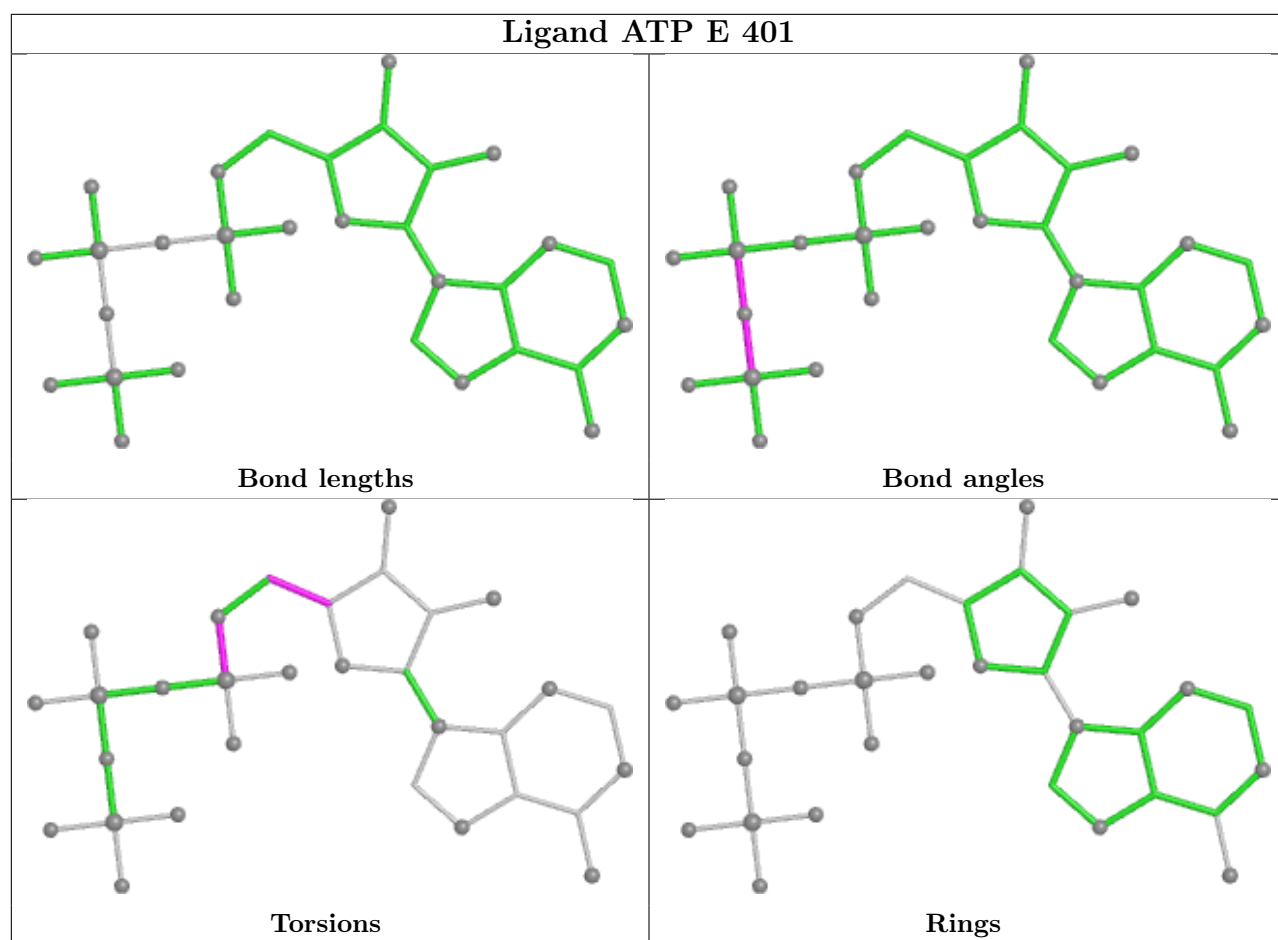
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	D	501	ATP	6	0
37	F	501	ADP	1	0
35	B	502	ATP	1	0
35	A	501	ATP	3	0

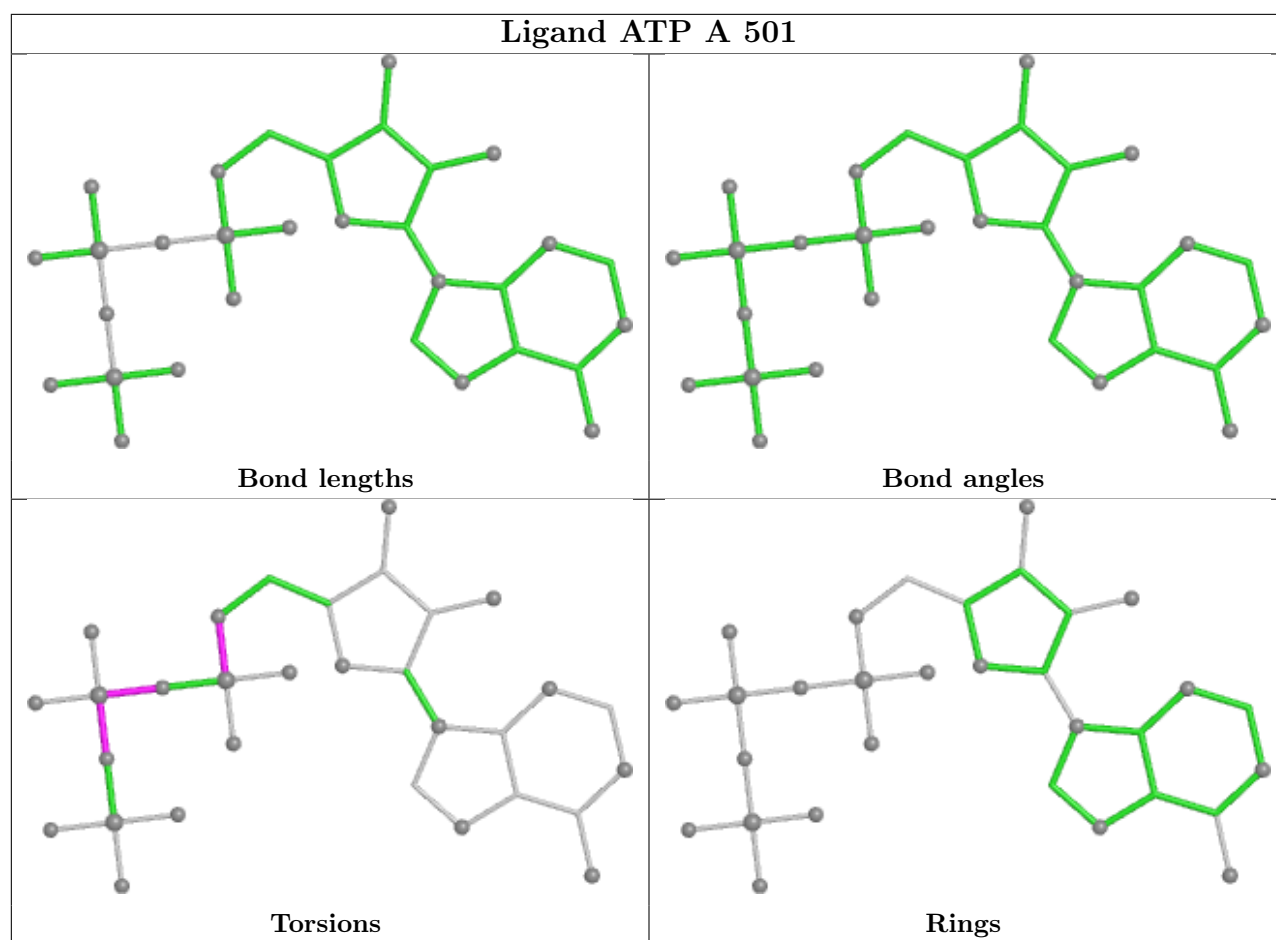
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.











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.

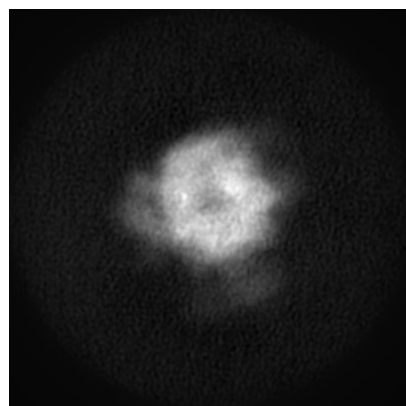
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62066. 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](#)

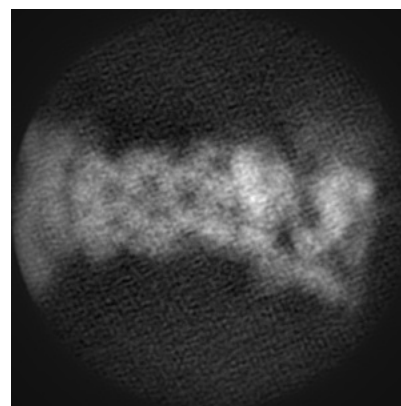
6.1.1 Primary map



X

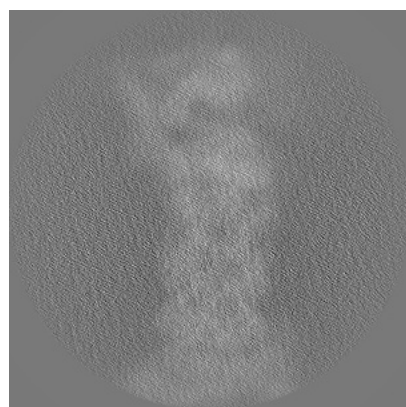


Y

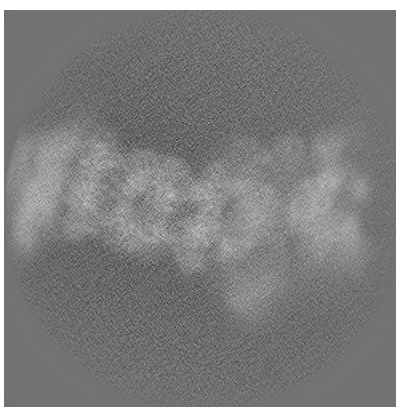


Z

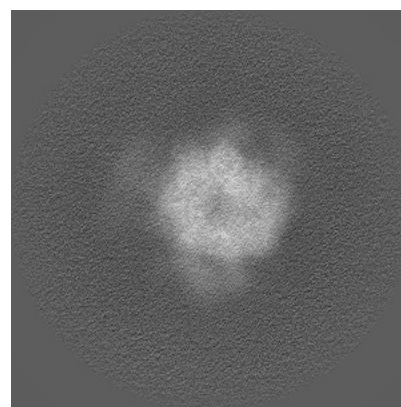
6.1.2 Raw map



X



Y

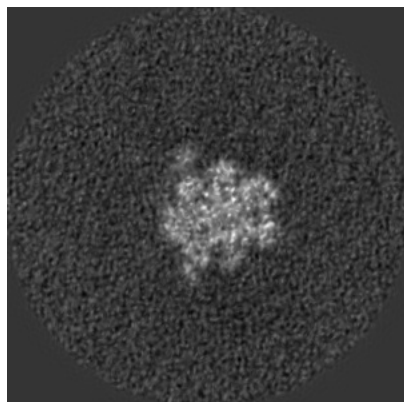


Z

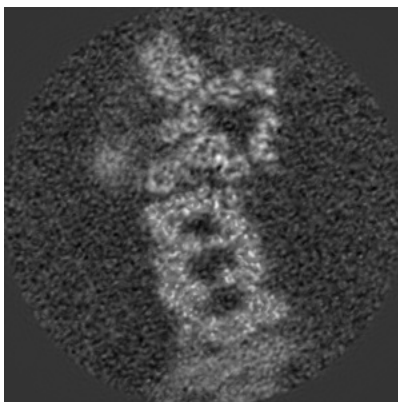
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

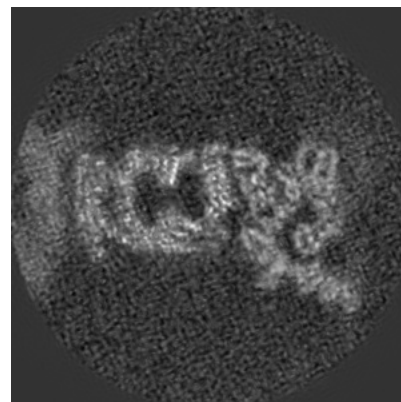
6.2.1 Primary map



X Index: 300

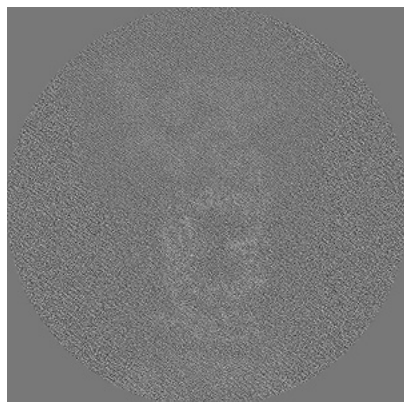


Y Index: 300

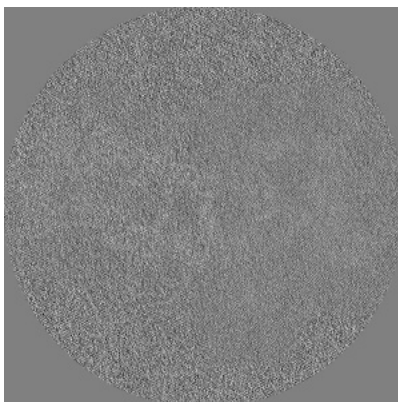


Z Index: 300

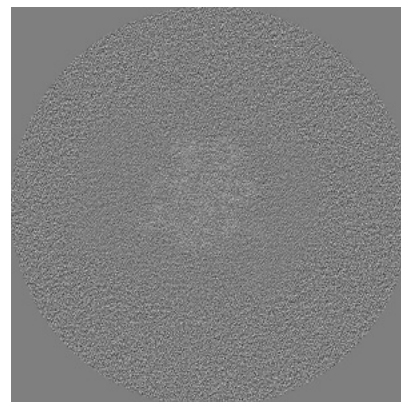
6.2.2 Raw map



X Index: 300



Y Index: 300

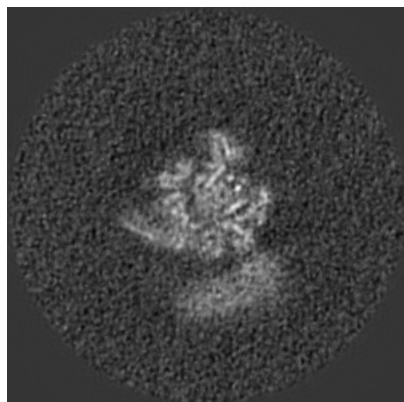


Z Index: 300

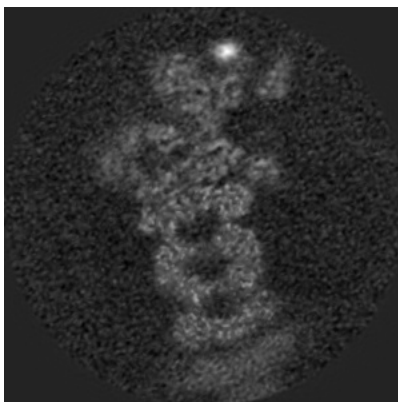
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

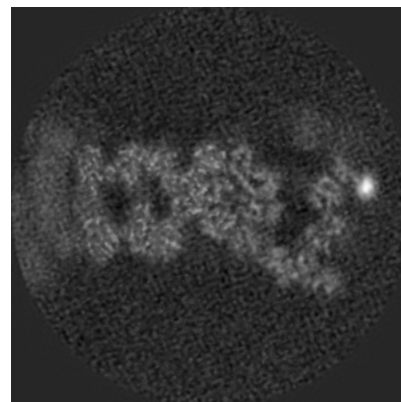
6.3.1 Primary map



X Index: 364

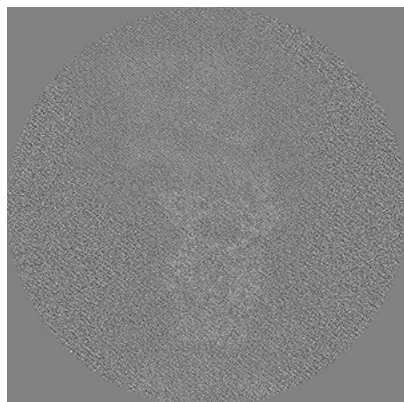


Y Index: 329

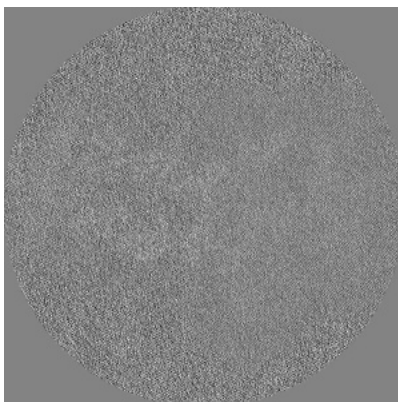


Z Index: 332

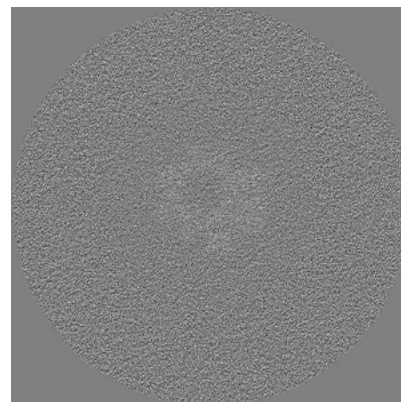
6.3.2 Raw map



X Index: 274



Y Index: 312

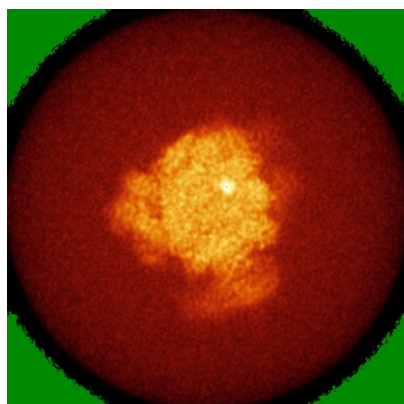


Z Index: 258

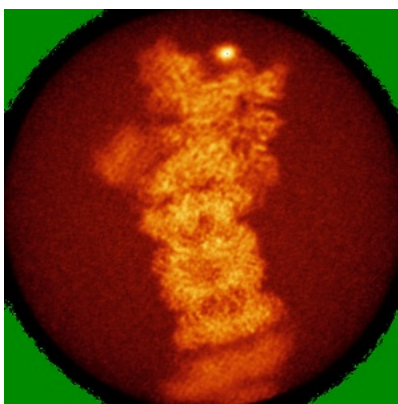
The images above show the largest variance slices of the map in three orthogonal directions.

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

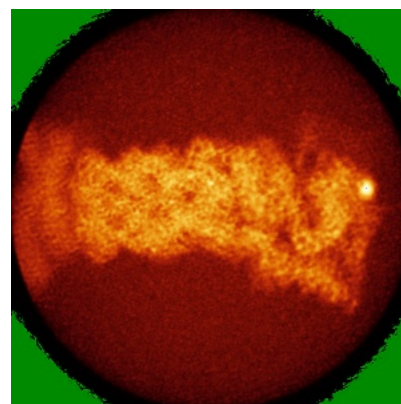
6.4.1 Primary map



X

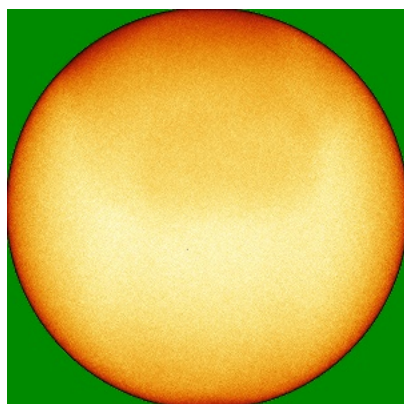


Y

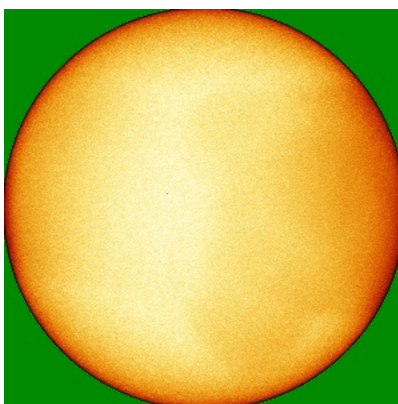


Z

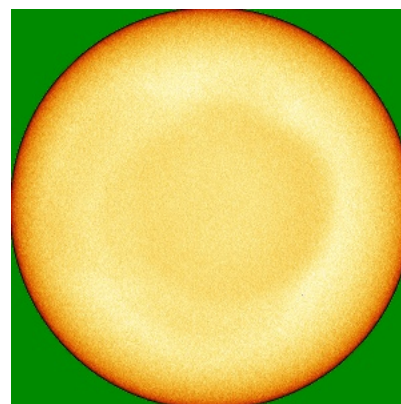
6.4.2 Raw map



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



X



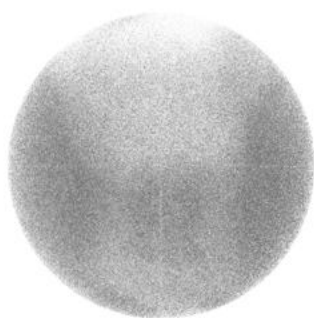
Y



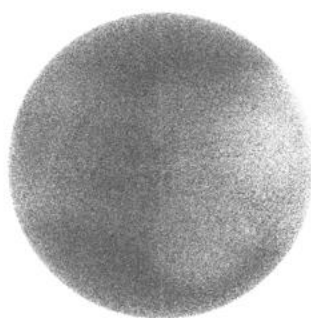
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0049. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

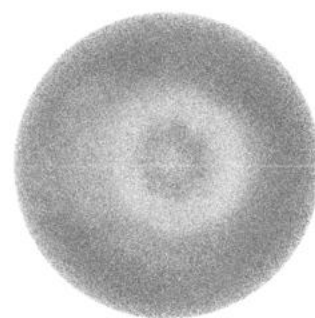
6.5.2 Raw map



X



Y



Z

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.

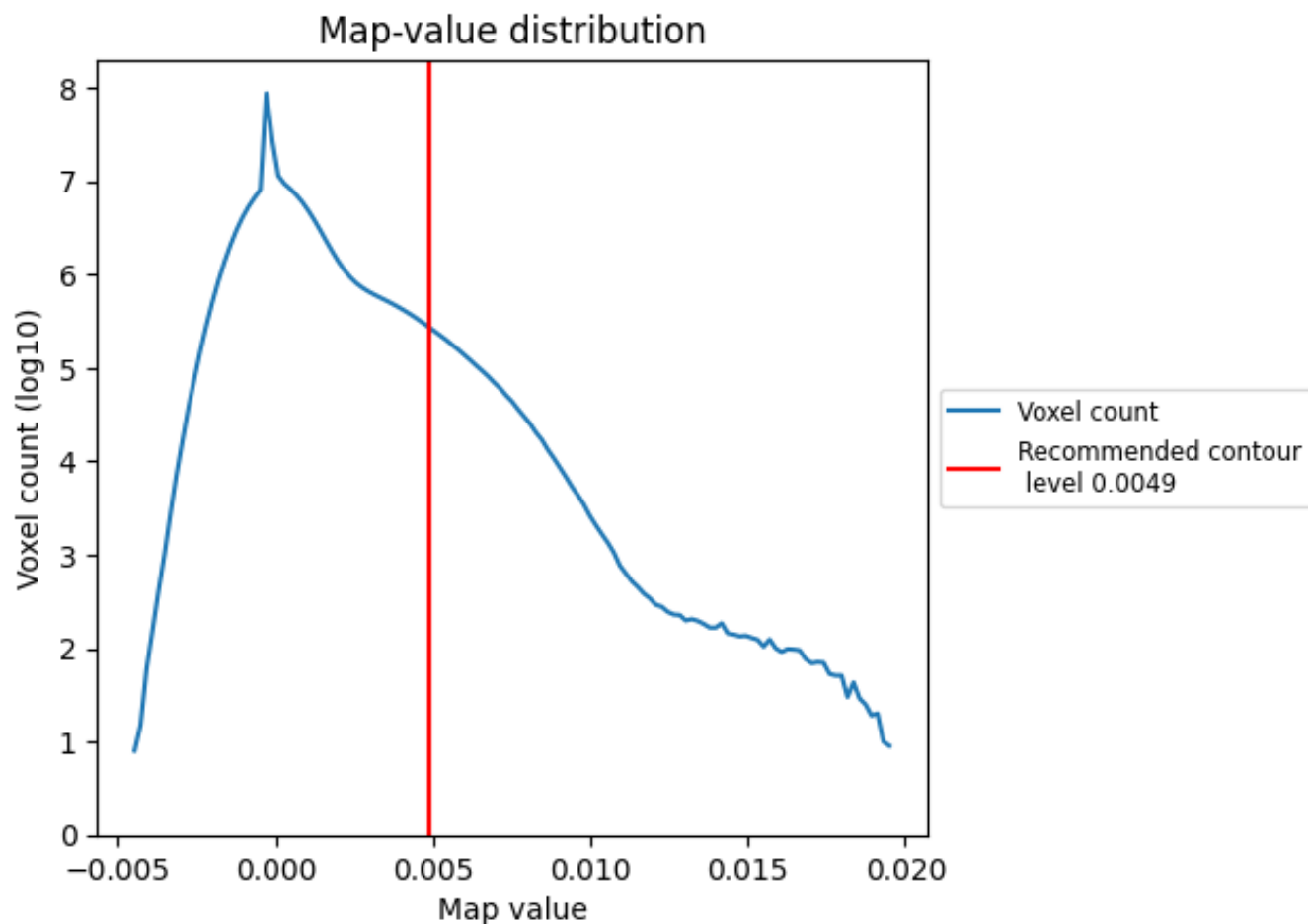
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

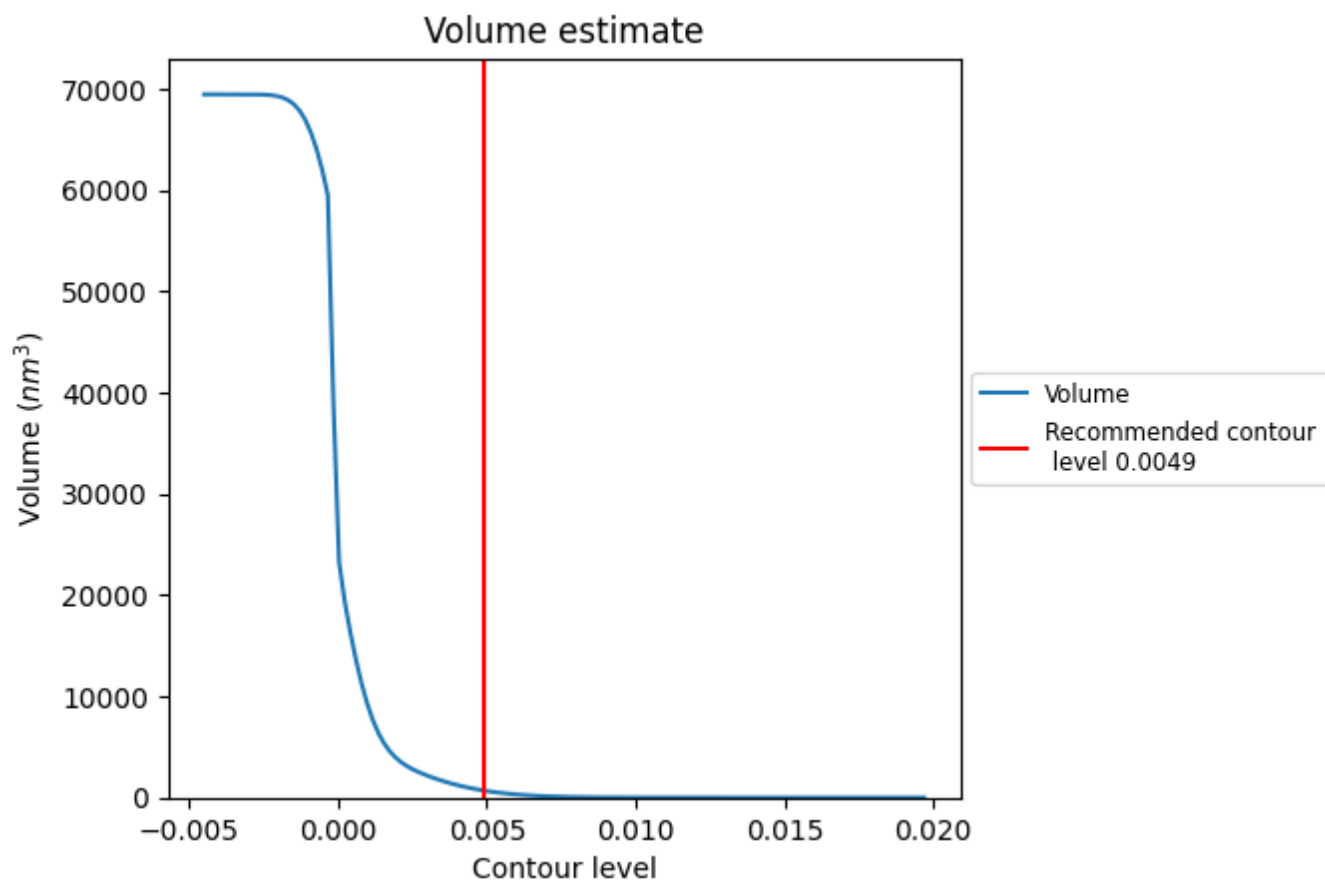
This section contains the results of statistical analysis of the map.

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.

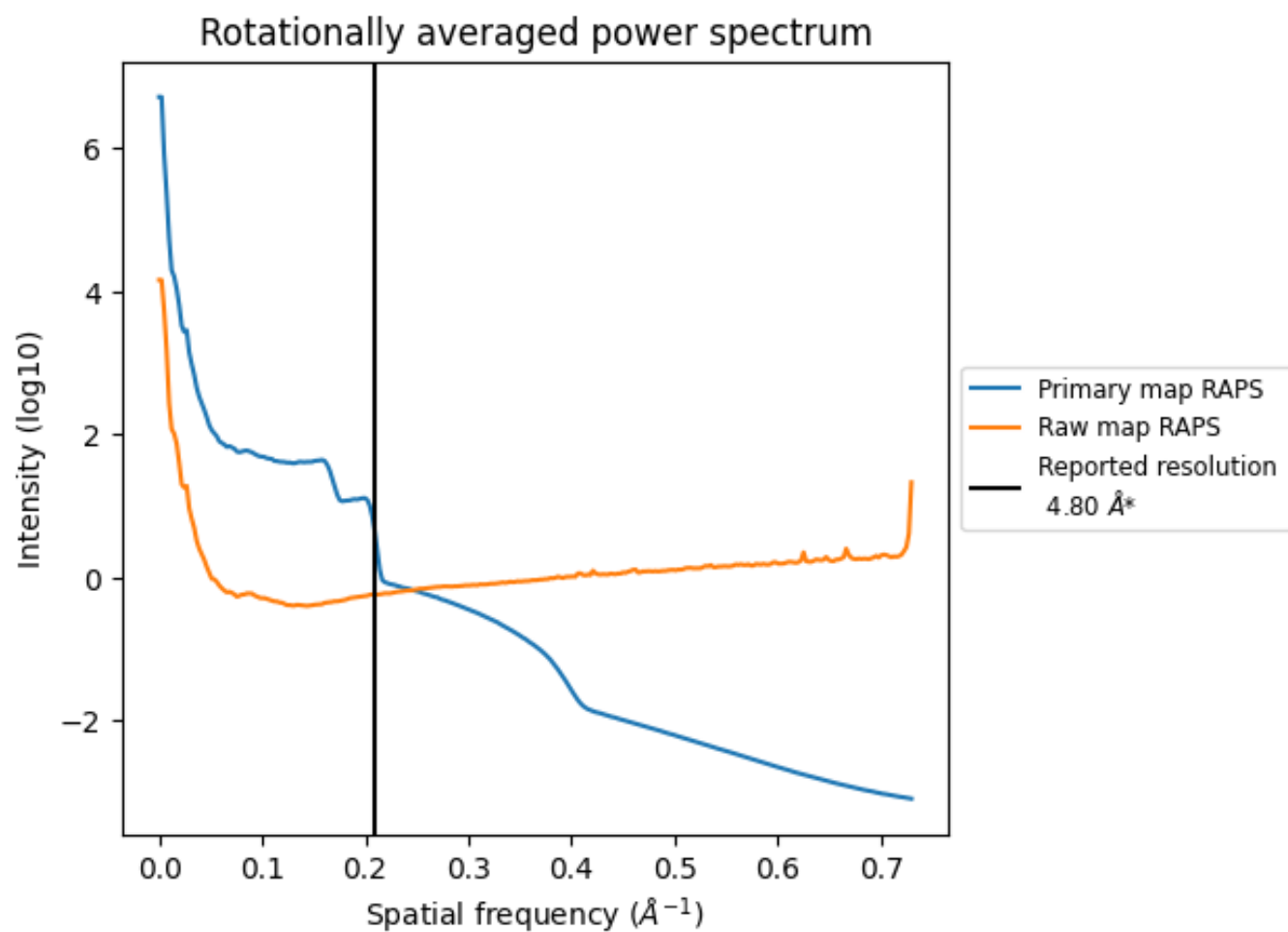
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 694 nm³; this corresponds to an approximate mass of 627 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 ⓘ

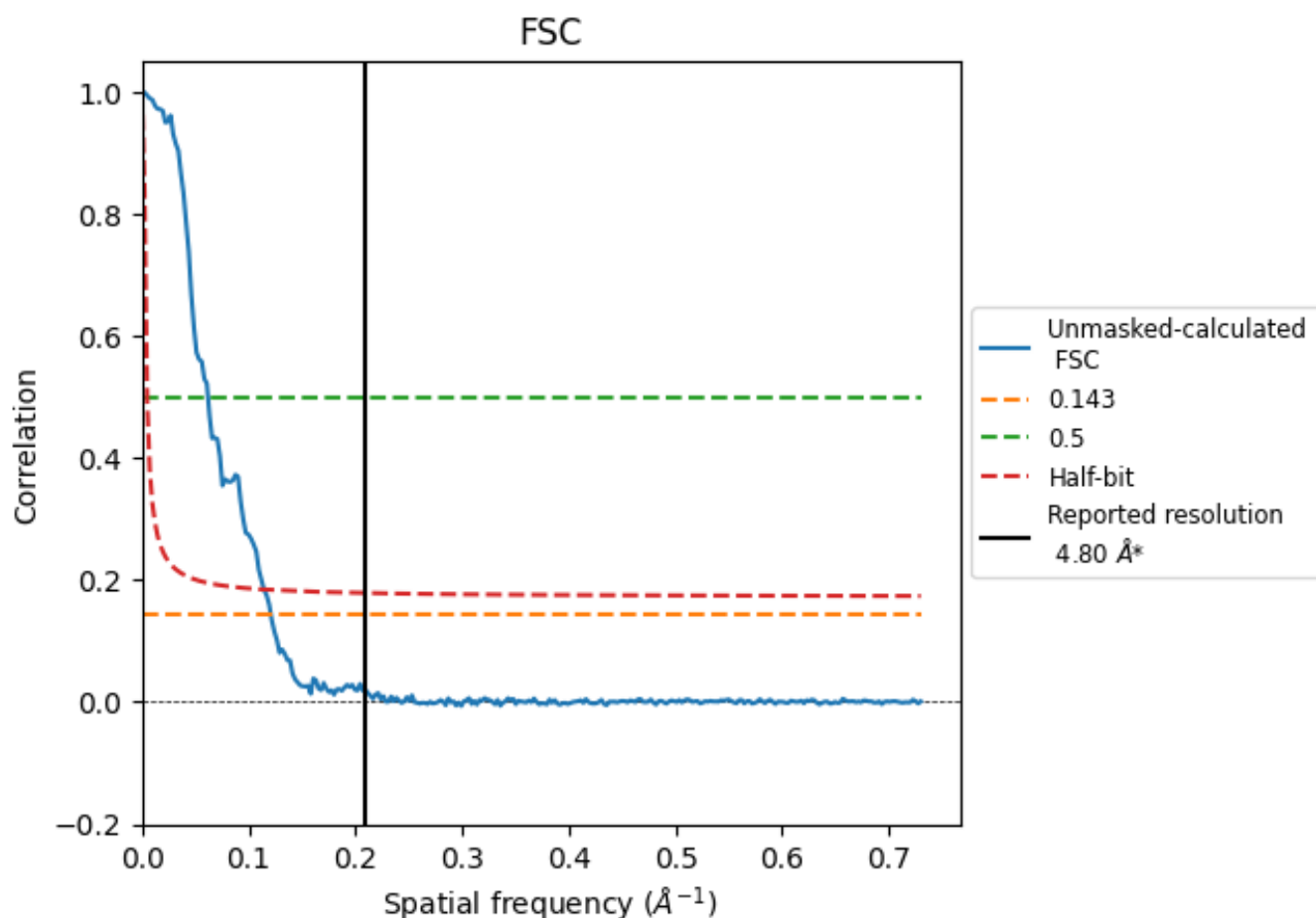


*Reported resolution corresponds to spatial frequency of 0.208 \AA^{-1}

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 0.208 \AA^{-1}

8.2 Resolution estimates [i](#)

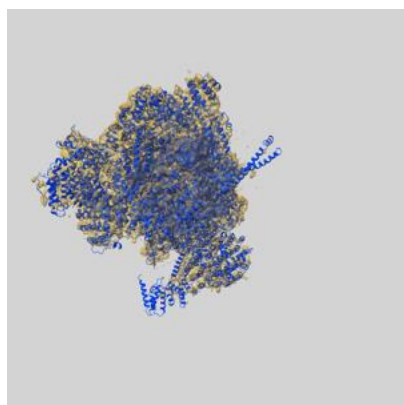
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.28	16.18	8.75

*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 8.28 differs from the reported value 4.8 by more than 10 %

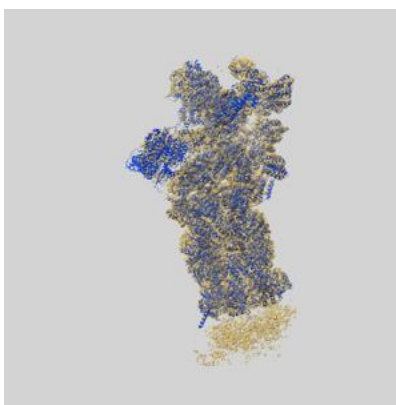
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62066 and PDB model 9K4P. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

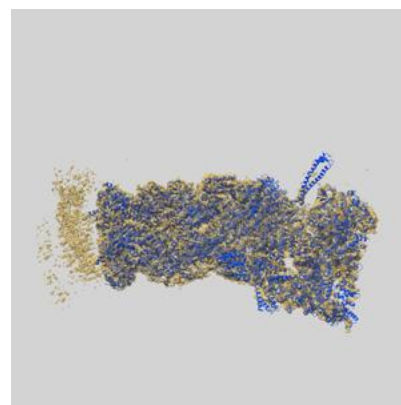
9.1 Map-model overlay [i](#)



X



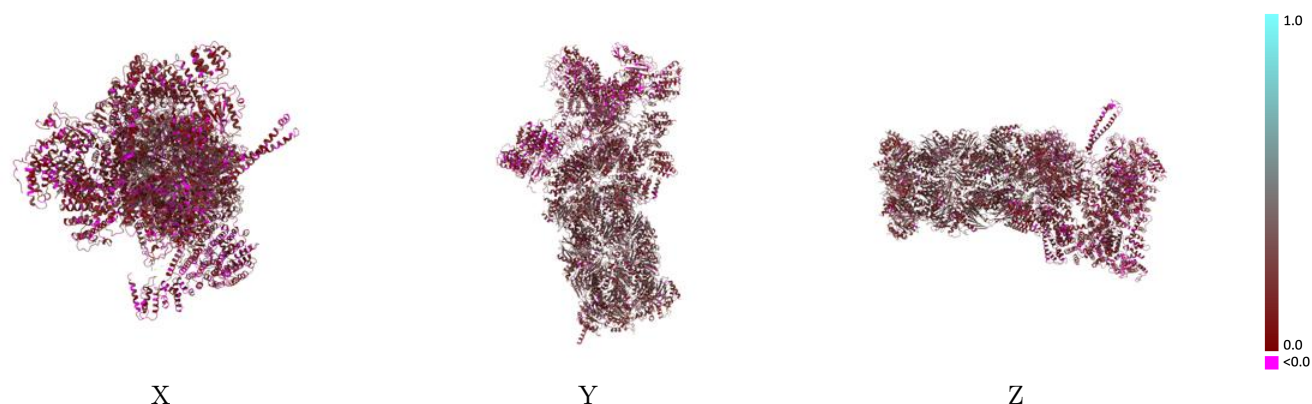
Y



Z

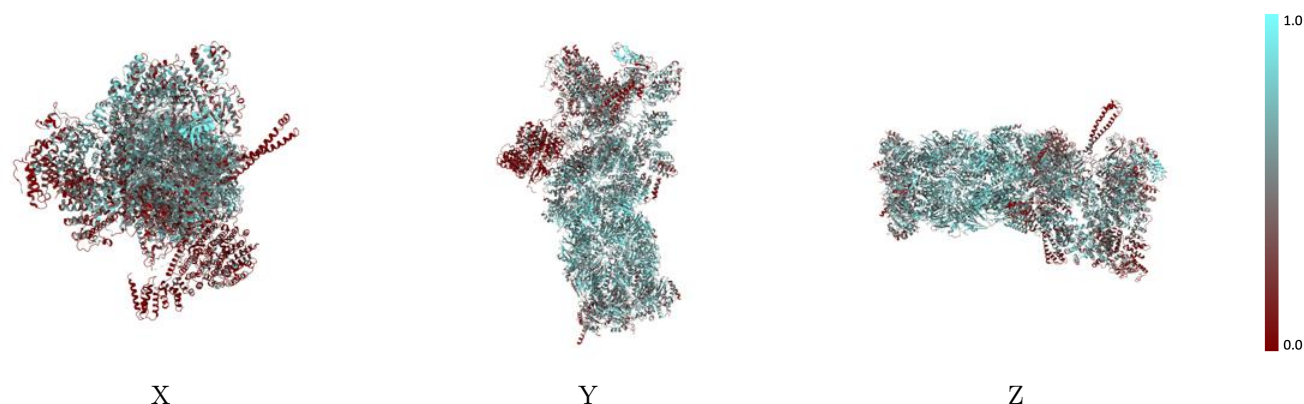
The images above show the 3D surface view of the map at the recommended contour level 0.0049 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



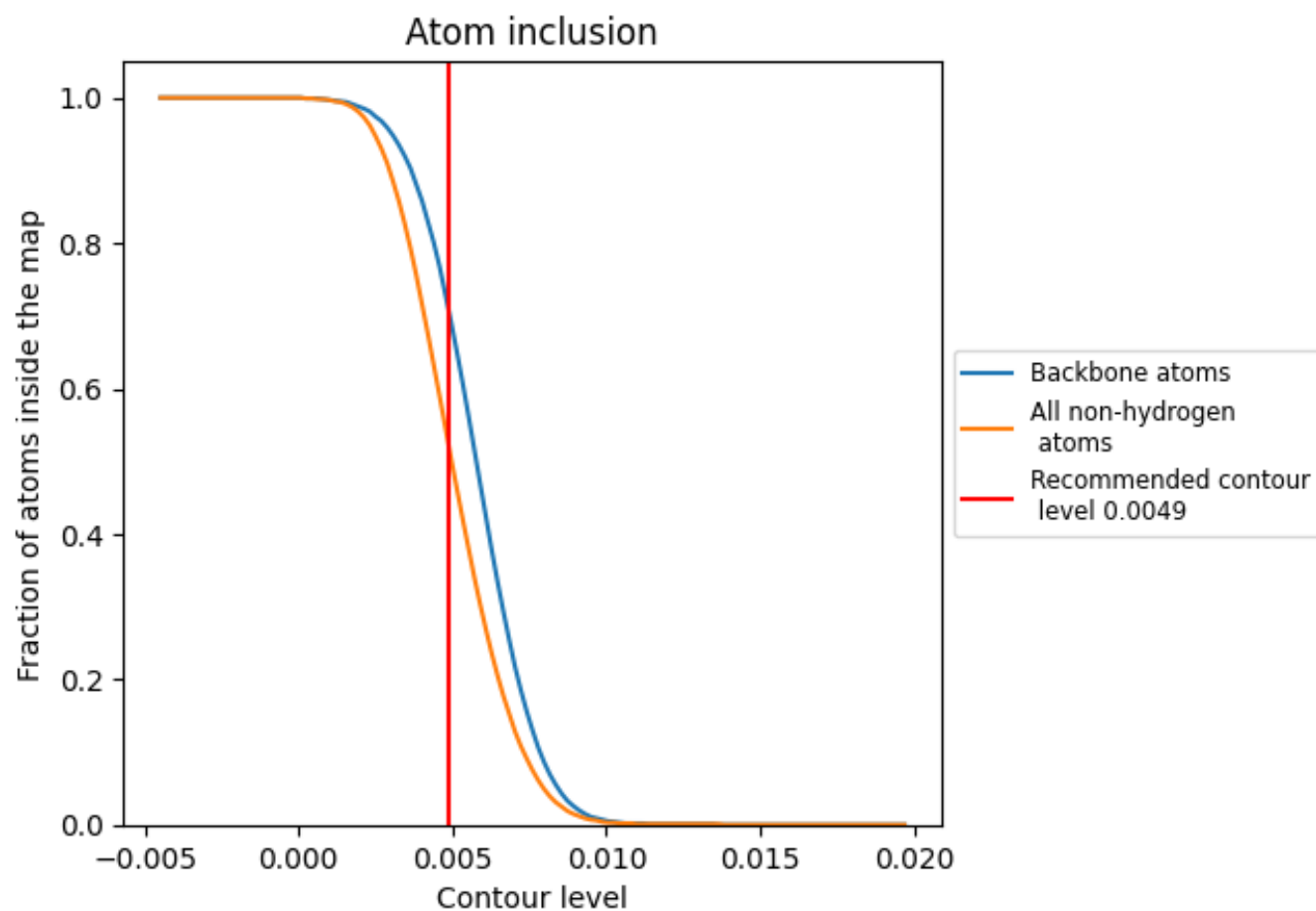
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0049).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 52% 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 (0.0049) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5150	 0.2170
A	 0.4990	 0.2080
B	 0.4730	 0.2020
C	 0.5010	 0.1870
D	 0.5320	 0.1950
E	 0.5260	 0.2030
F	 0.4900	 0.2040
G	 0.6850	 0.2620
H	 0.6820	 0.2810
I	 0.6630	 0.2530
J	 0.6290	 0.2520
K	 0.6420	 0.2750
L	 0.6840	 0.2790
M	 0.6830	 0.2680
N	 0.7130	 0.2820
O	 0.7390	 0.2950
P	 0.6910	 0.2750
Q	 0.6710	 0.2800
R	 0.7100	 0.2790
S	 0.6510	 0.2920
T	 0.7040	 0.2810
U	 0.3610	 0.1520
V	 0.3410	 0.1640
W	 0.5570	 0.1970
X	 0.4750	 0.1820
Y	 0.4780	 0.1550
Z	 0.4700	 0.1670
a	 0.5070	 0.1620
b	 0.4420	 0.1450
c	 0.4780	 0.1690
d	 0.2650	 0.1320
e	 0.3220	 0.1350
f	 0.1140	 0.1200
g	 0.5360	 0.2680
h	 0.5350	 0.2750



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Chain	Atom inclusion	Q-score
i	 0.4750	 0.2550
j	 0.4620	 0.2500
k	 0.4820	 0.2540
l	 0.5800	 0.2770
m	 0.5390	 0.2780
n	 0.6330	 0.2920
o	 0.6080	 0.2870
p	 0.6610	 0.2830
q	 0.6280	 0.2860
r	 0.6810	 0.2790
s	 0.6710	 0.2810
t	 0.6890	 0.2820
u	 0.2750	 0.1100
v	 0.0190	 -0.0510
z	 0.6940	 0.0730