



Full wwPDB EM Validation Report ⓘ

Apr 20, 2026 – 06:01 PM JST

PDB ID : 9K55 / pdb_00009k55
EMDB ID : EMD-62081
Title : Structure of substrate-engaged human 26S proteasome RP-CP subcomplex in state ED2.3
Authors : Wu, Z.; Chen, E.; Mao, Y.
Deposited on : 2024-10-21
Resolution : 7.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

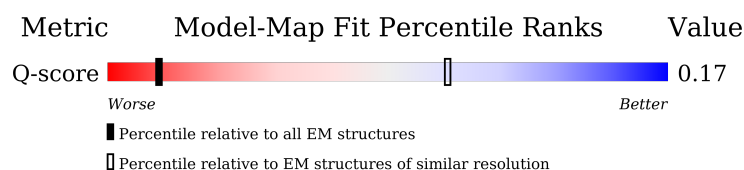
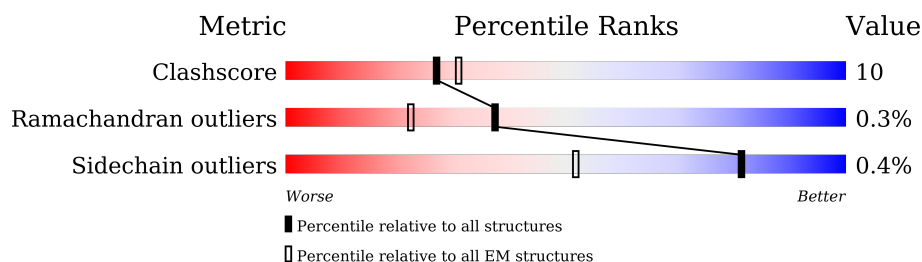
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	483 (6.50 - 7.50)

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	<div> <div>37%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>5%</div> </div> </div>
2	B	440	<div> <div>32%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>7%</div> </div> </div>
3	C	398	<div> <div>27%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>...</div> </div> </div>
4	D	418	<div> <div>22%</div> <div> <div></div> <div>64%</div> <div>25%</div> <div>9%</div> </div> </div>

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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	v	36	
34	w	76	
34	x	76	
34	z	76	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 108111 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	413	Total	C	N	O	S	0	0
			3229	2034	566	611	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	411	Total	C	N	O	S	0	0
			3207	2022	548	622	15		

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

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

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

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

- Molecule 5 is a protein called 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	395	Total	C	N	O	S	0	0
			3098	1951	533	596	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	240	Total	C	N	O	S	0	0
			1867	1187	312	355	13		
7	g	244	Total	C	N	O	S	0	0
			1879	1193	318	355	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
			1801	1149	304	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	248	Total	C	N	O	S	0	0
			1933	1222	330	371	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
			1861	1166	327	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	238	Total	C	N	O	S	0	0
			1813	1139	302	361	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	240	Total	C	N	O	S	0	0
			1876	1175	338	352	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	242	Total	C	N	O	S	1	0
			1893	1202	323	356	12		
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	203	Total	C	N	O	S	0	0
			1521	954	259	296	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
			1645	1035	278	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	1	0
			1591	1019	270	292	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1578	1012	267	290	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
18	r	201	Total	C	N	O	S	0	0
			1549	977	270	293	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
			1650	1044	283	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	878	Total	C	N	O	S	0	0
			6867	4352	1163	1306	46		

- 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		

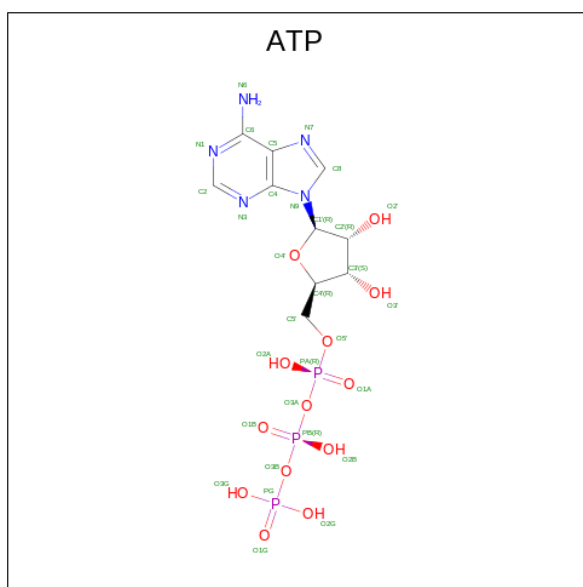
- Molecule 33 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	v	36	Total	C	N	O	0	0
			180	108	36	36		

- Molecule 34 is a protein called Ubiquitin.

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

- 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	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	F	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	A	1	Total	Mg	0
			1	1	
36	B	1	Total	Mg	0
			1	1	
36	C	1	Total	Mg	0
			1	1	
36	D	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	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

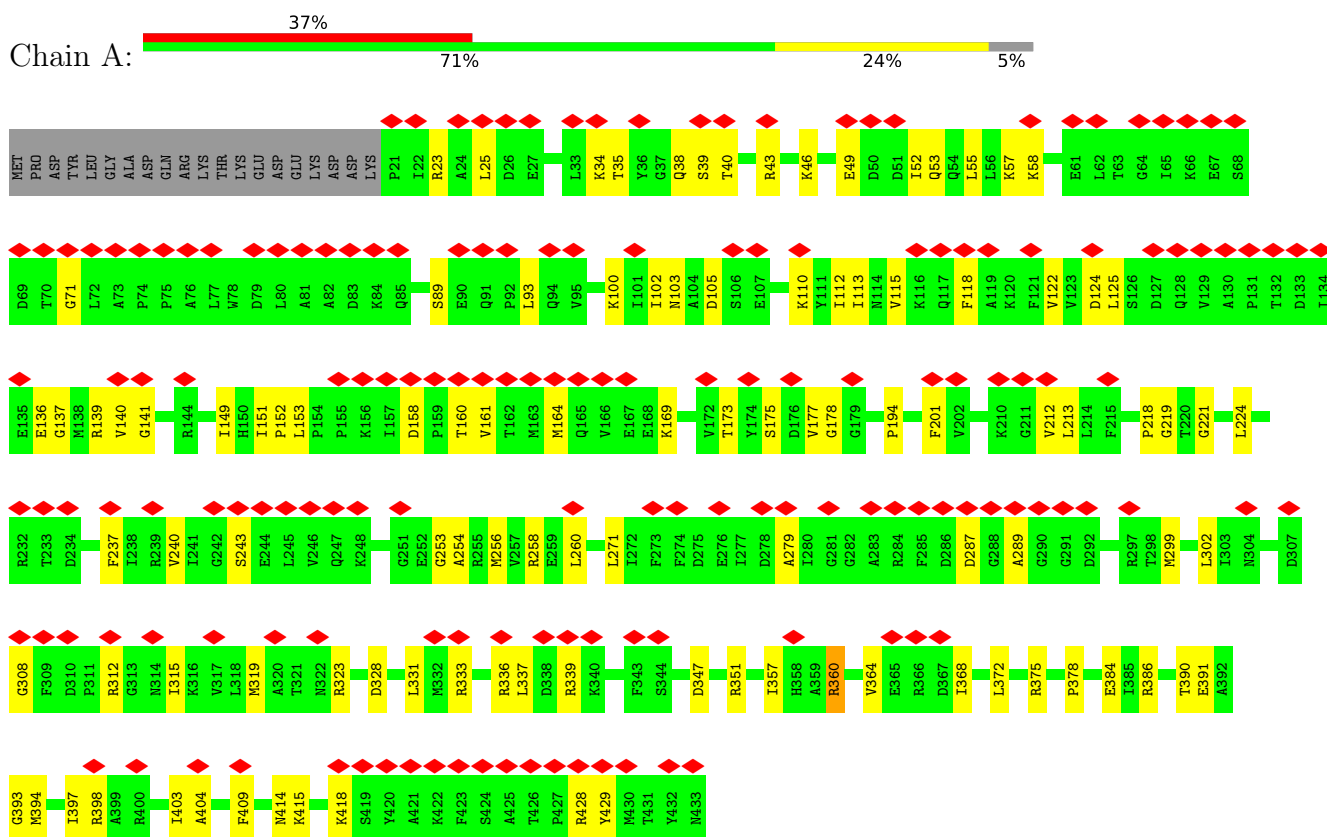
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

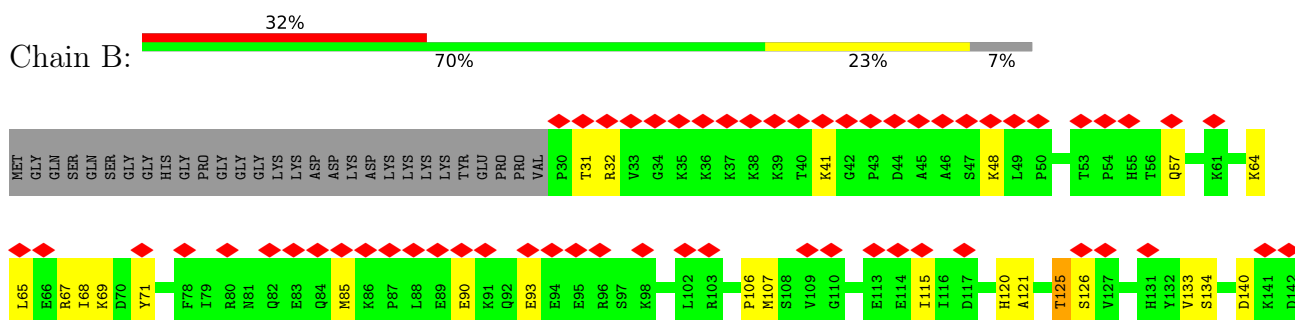
3 Residue-property plots

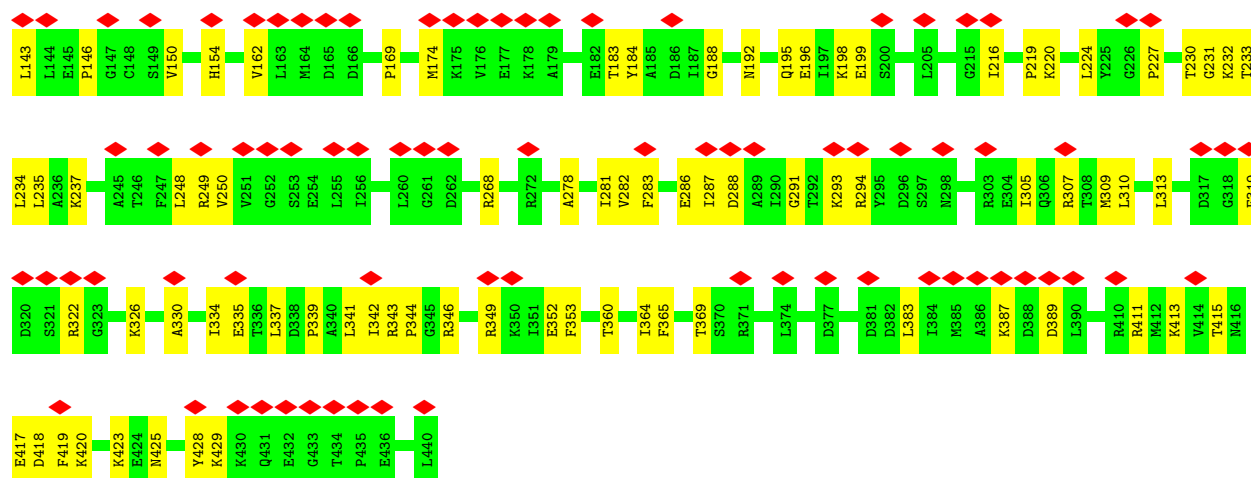
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 26S proteasome regulatory subunit 7



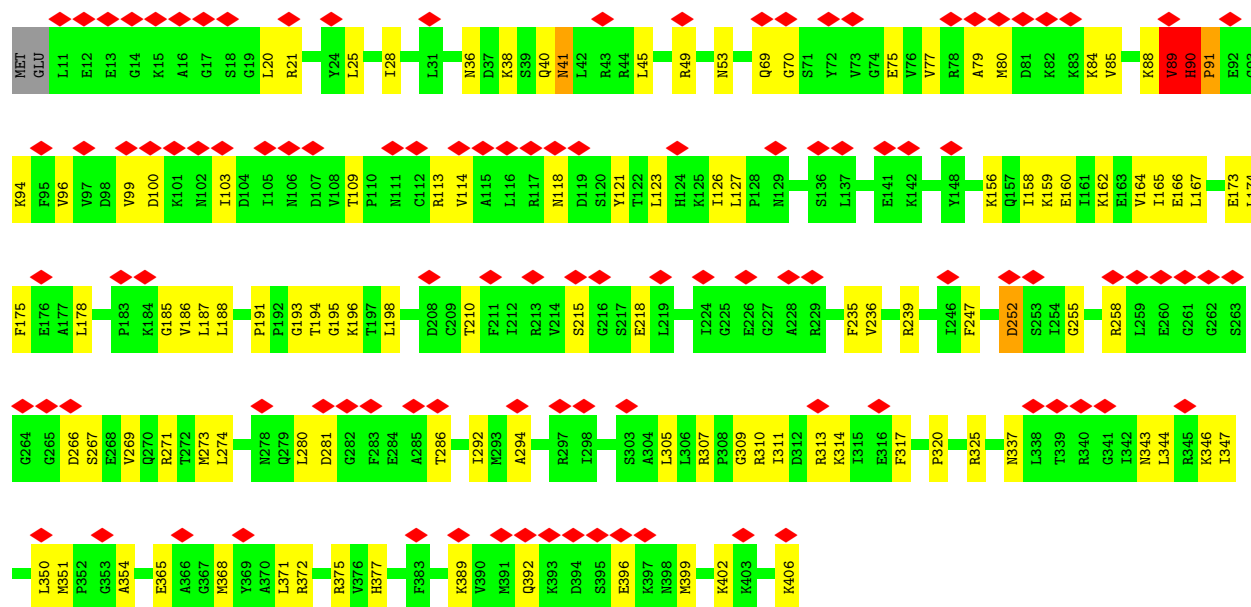
• Molecule 2: 26S proteasome regulatory subunit 4





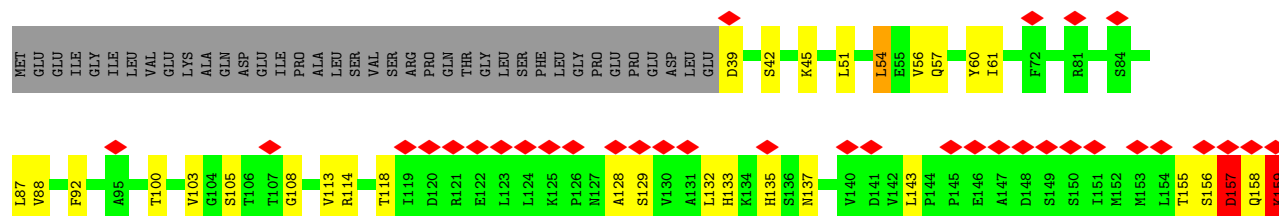
• Molecule 3: 26S proteasome regulatory subunit 8

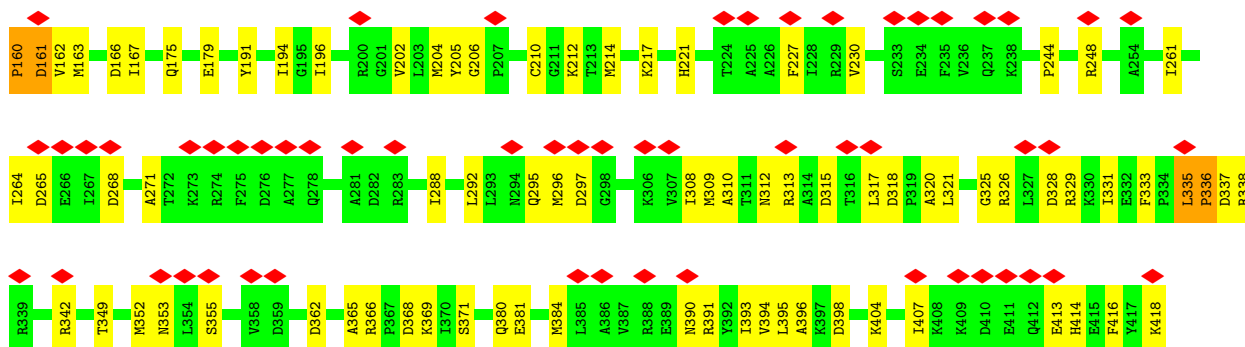
Chain C: 27% 72% 26% ...



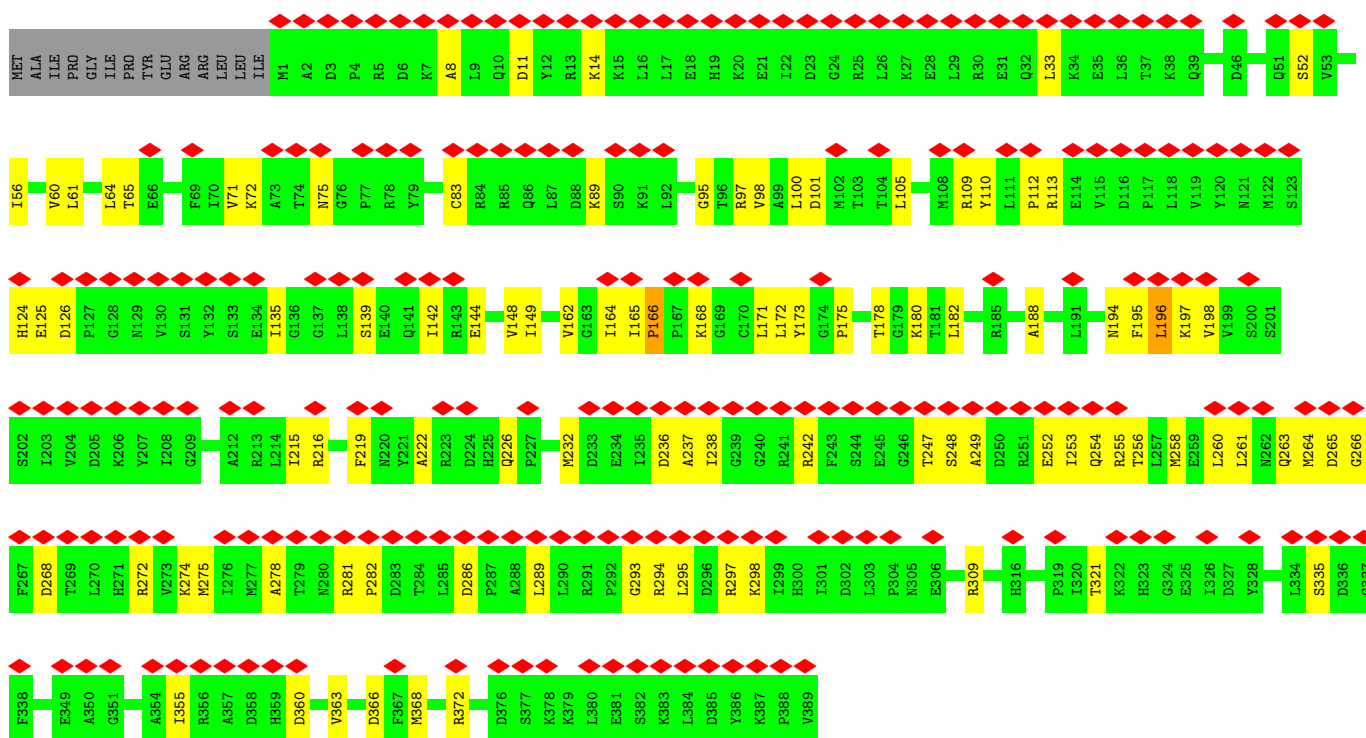
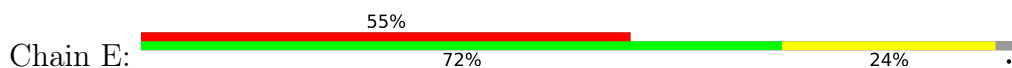
• Molecule 4: 26S proteasome regulatory subunit 6B

Chain D: 22% 64% 25% 9%

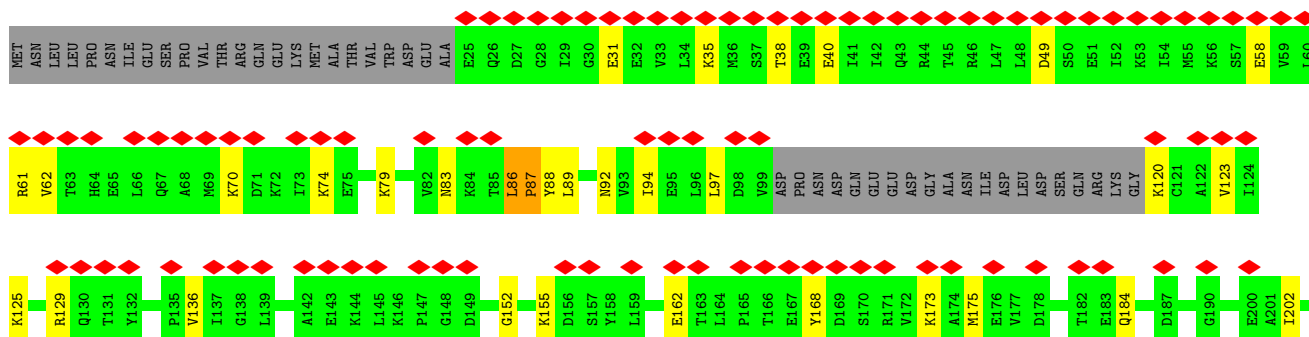
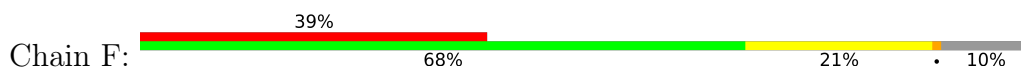


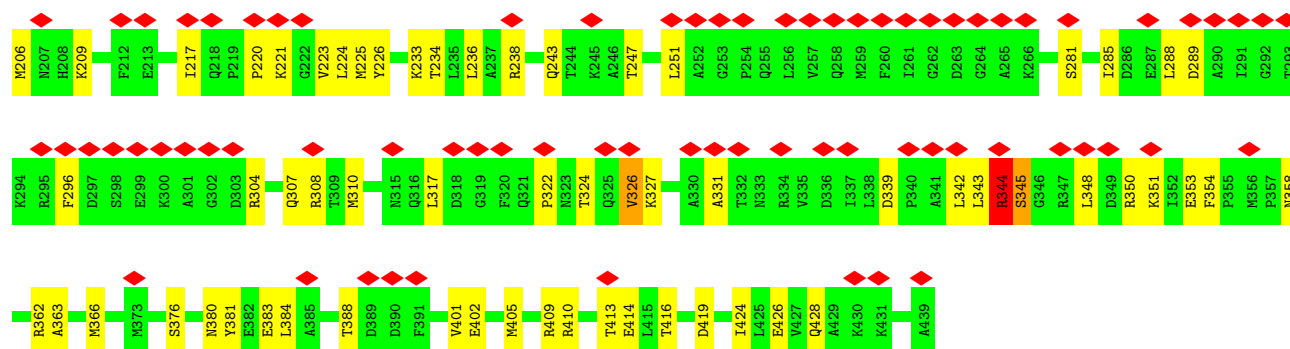


• Molecule 5: Proteasome 26S subunit, ATPase 6

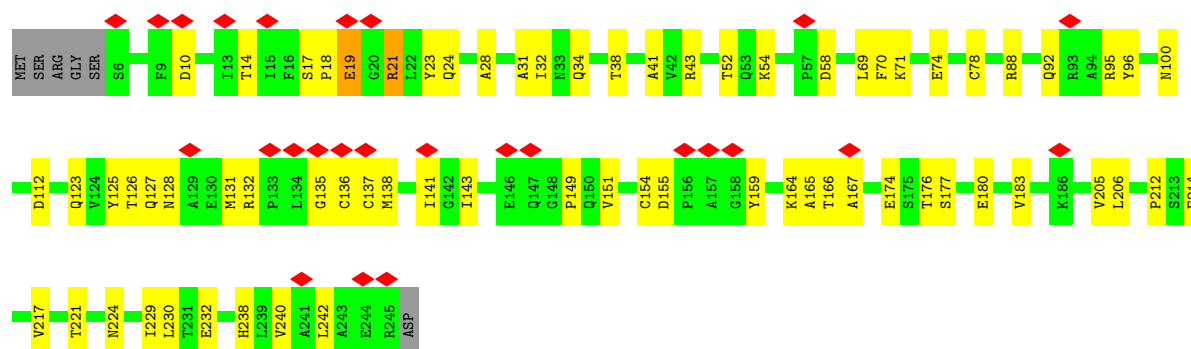


• Molecule 6: 26S proteasome regulatory subunit 6A

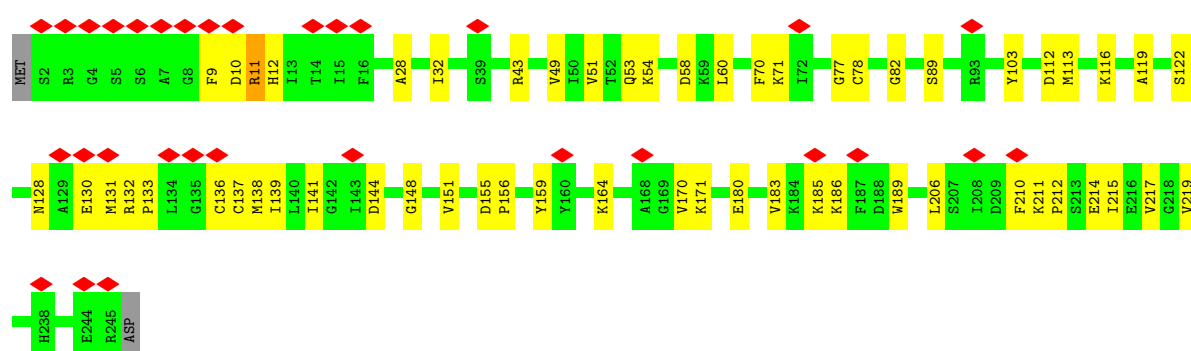
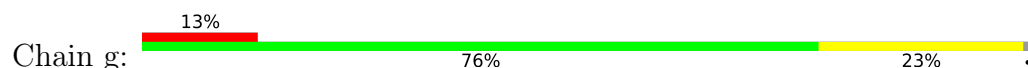




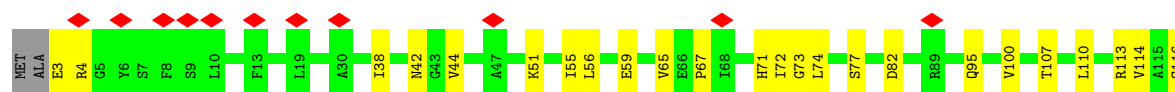
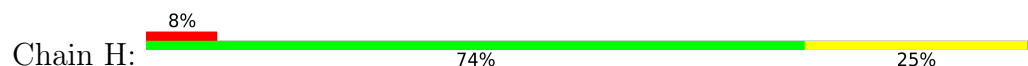
• Molecule 7: Proteasome subunit alpha type-6

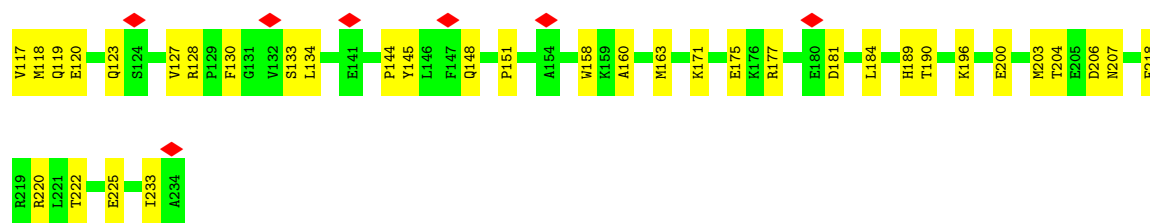


• Molecule 7: Proteasome subunit alpha type-6

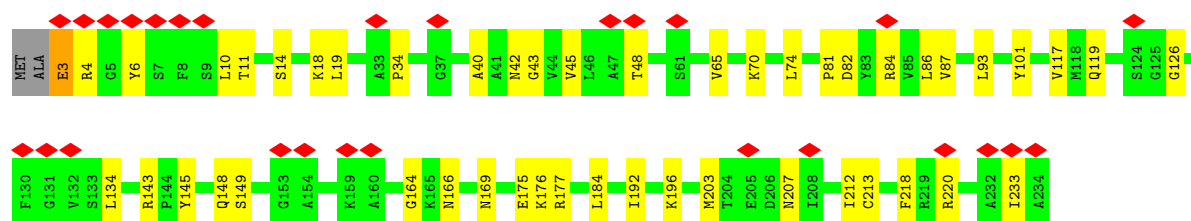
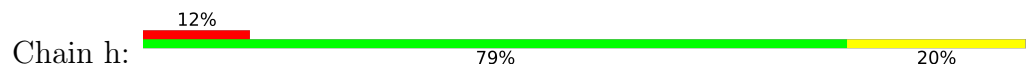


• Molecule 8: Proteasome subunit alpha type-2

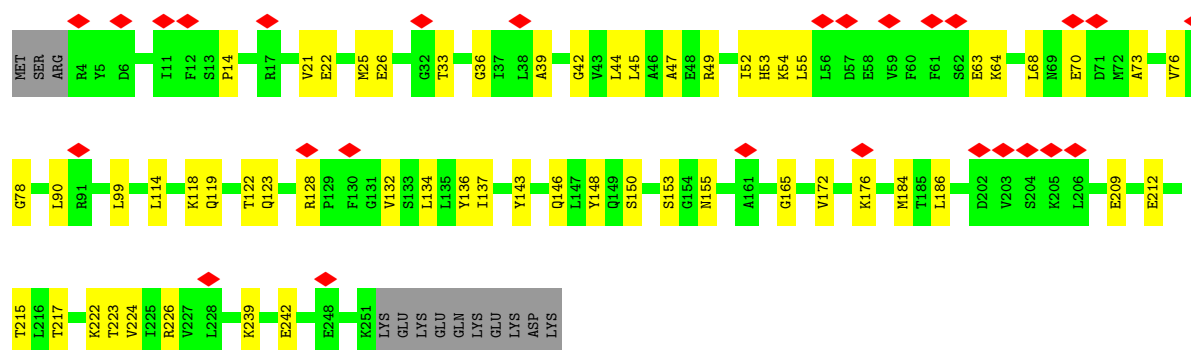




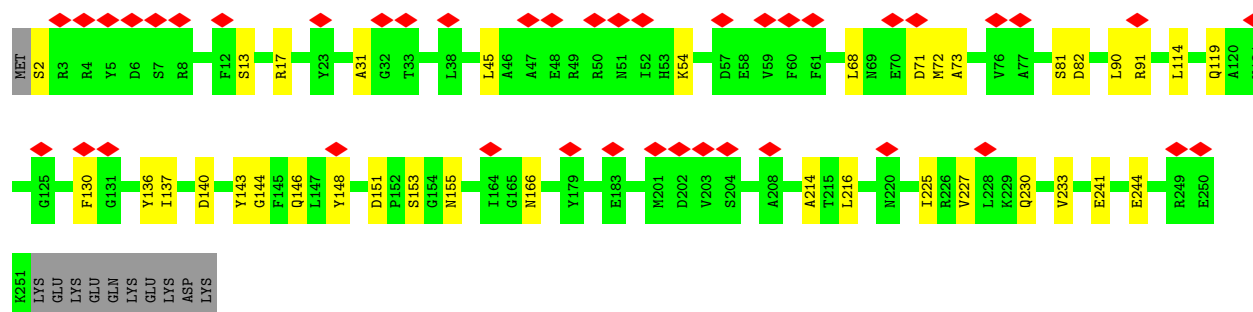
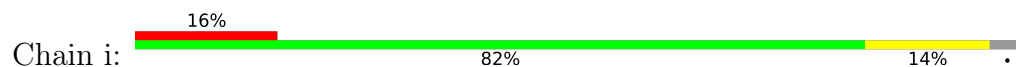
• Molecule 8: Proteasome subunit alpha type-2



• Molecule 9: Proteasome subunit alpha type-4

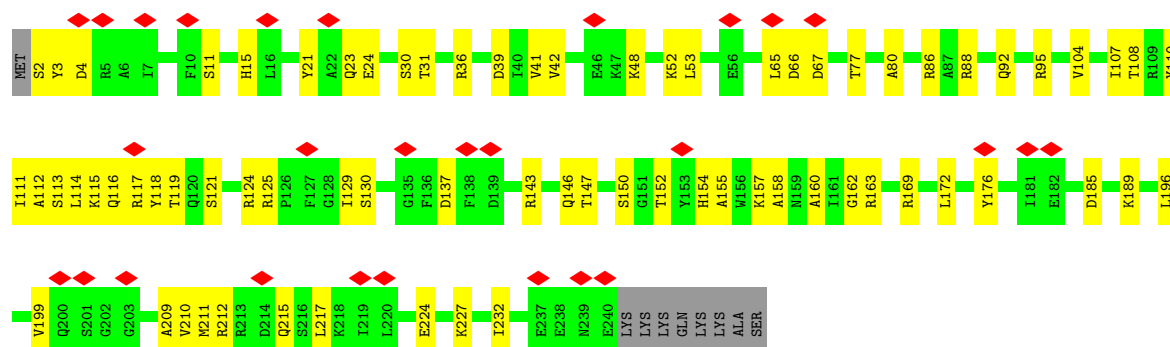


• Molecule 9: Proteasome subunit alpha type-4

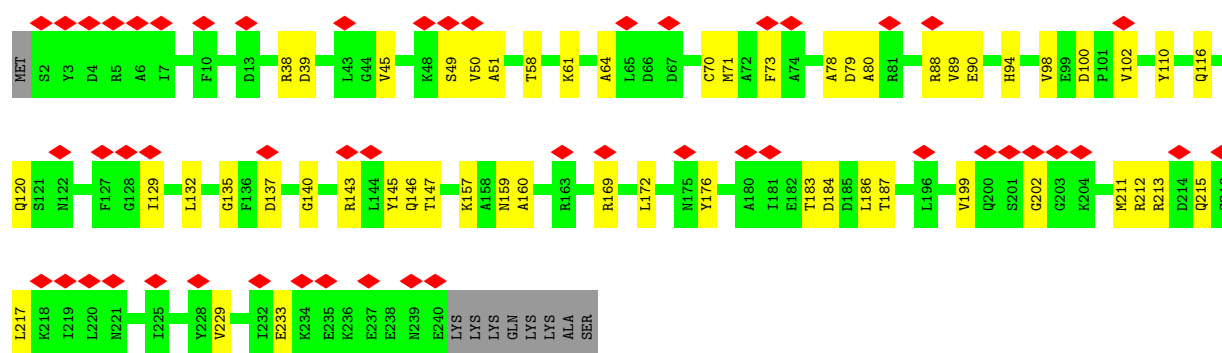
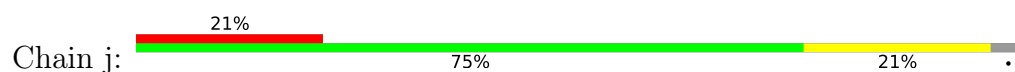


• Molecule 10: Proteasome subunit alpha type-7

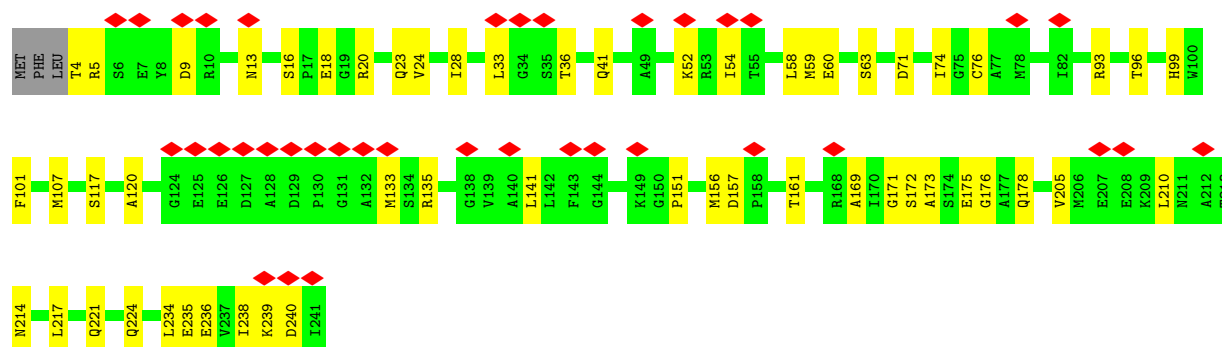
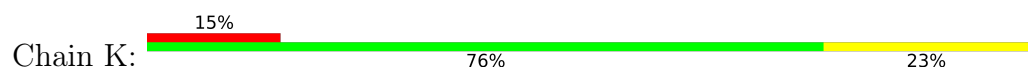




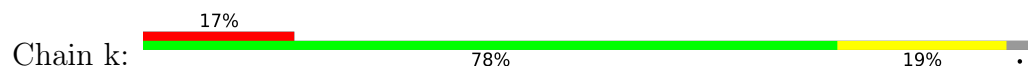
• Molecule 10: Proteasome subunit alpha type-7

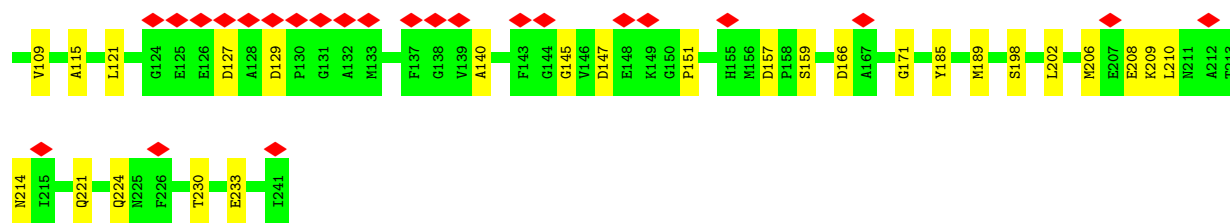


• Molecule 11: Proteasome subunit alpha type-5

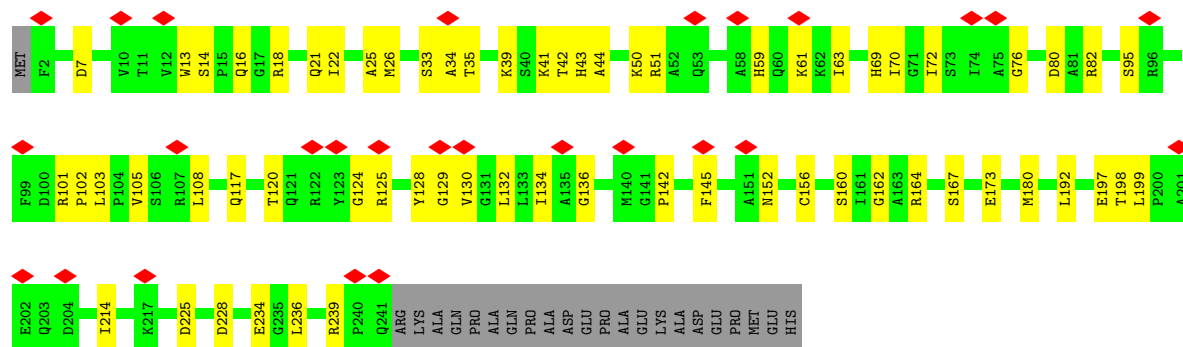


• Molecule 11: Proteasome subunit alpha type-5

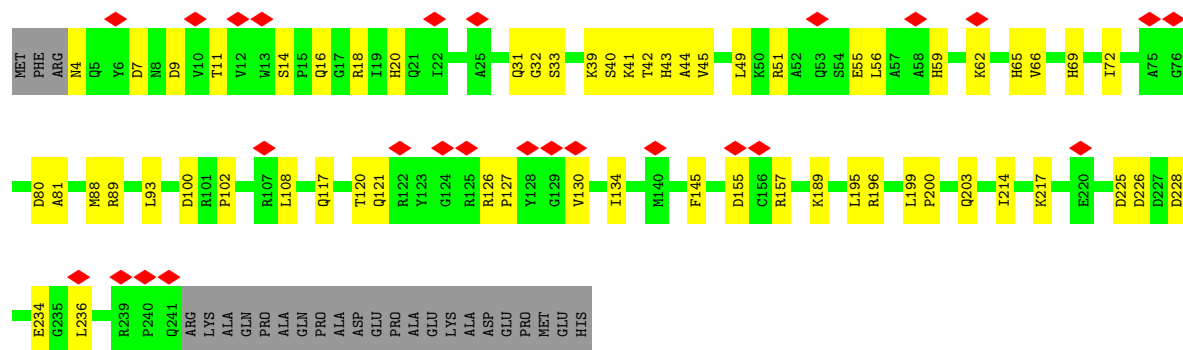




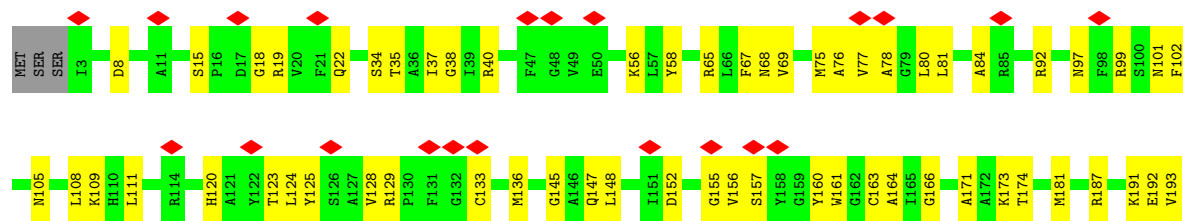
• Molecule 12: Proteasome subunit alpha type-1



• Molecule 12: Proteasome subunit alpha type-1

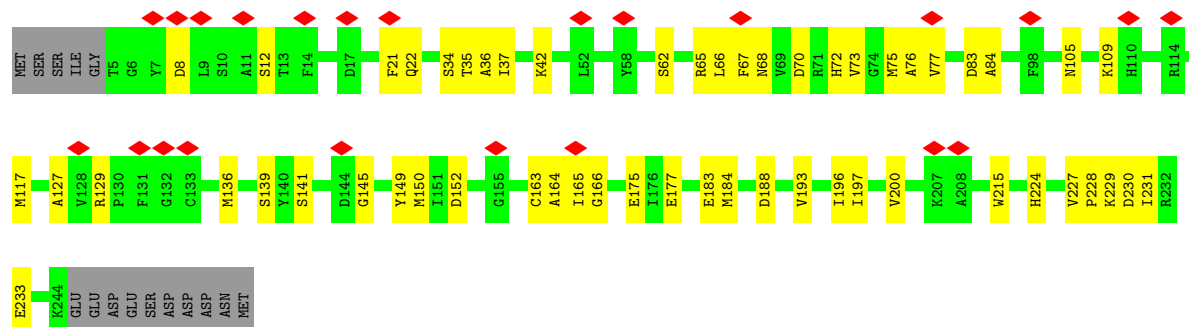
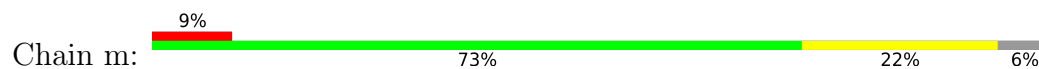


• Molecule 13: Proteasome subunit alpha type-3

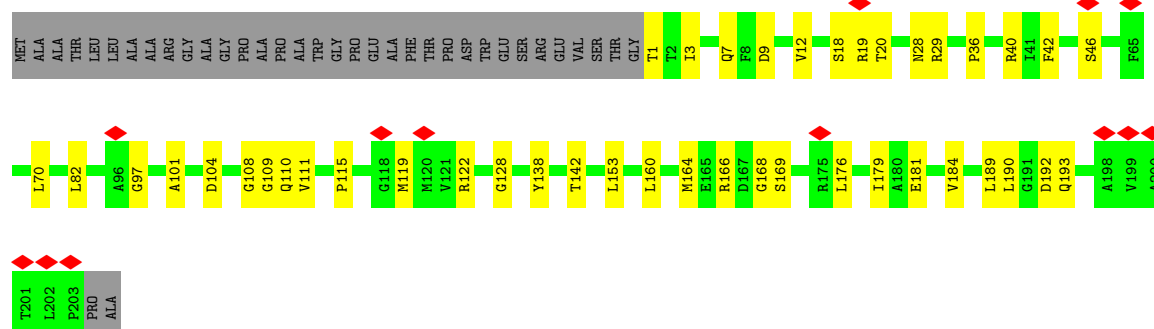




• Molecule 13: Proteasome subunit alpha type-3



• Molecule 14: Proteasome subunit beta type-6

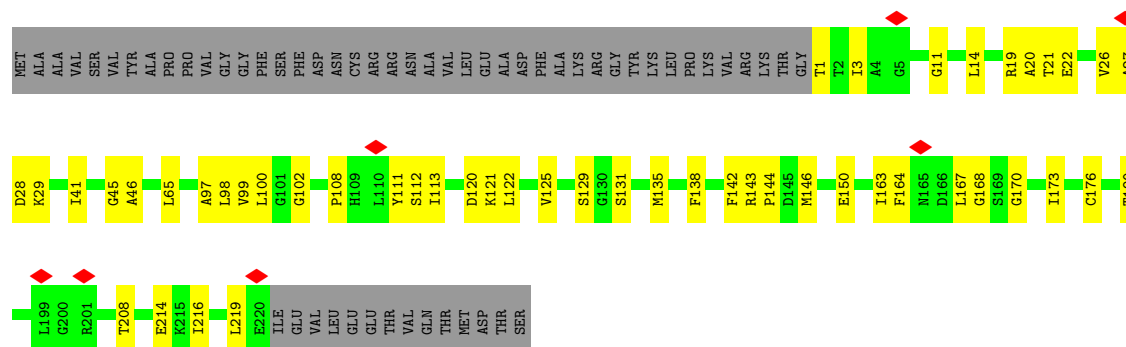


• Molecule 14: Proteasome subunit beta type-6

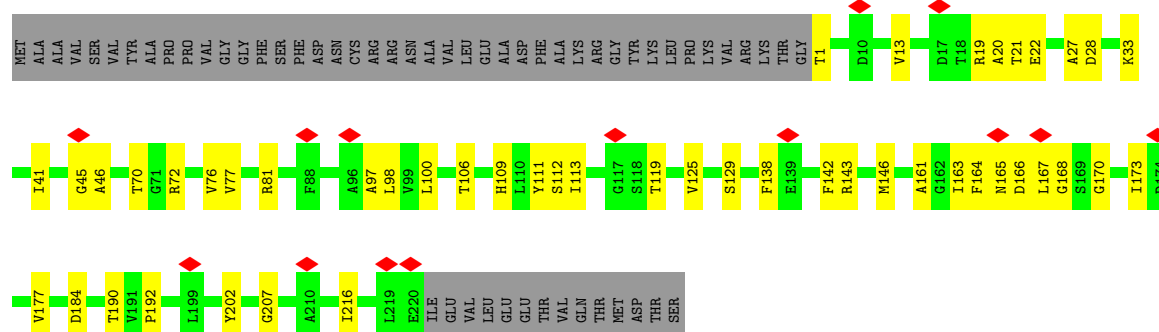


• Molecule 15: Proteasome subunit beta type-7

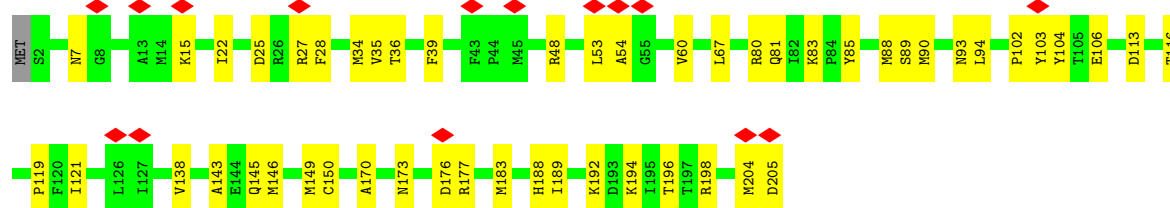
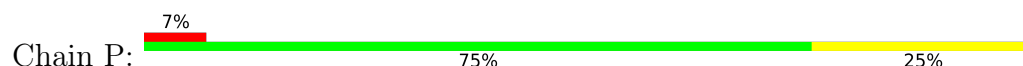




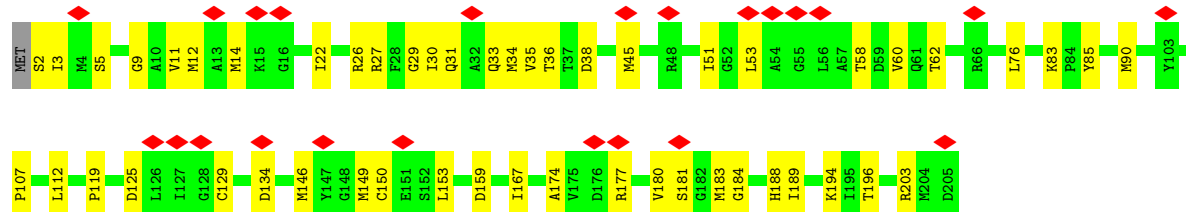
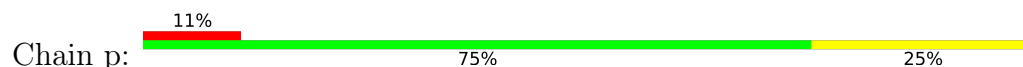
- Molecule 15: Proteasome subunit beta type-7



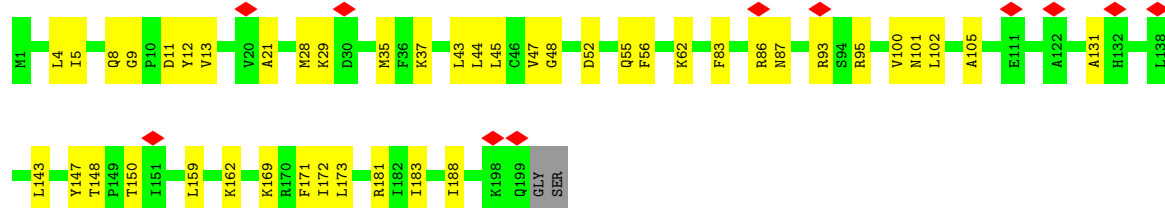
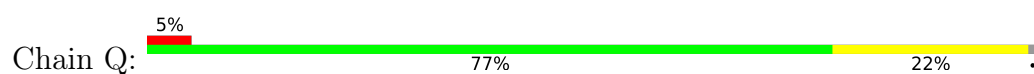
- Molecule 16: Proteasome subunit beta type-3



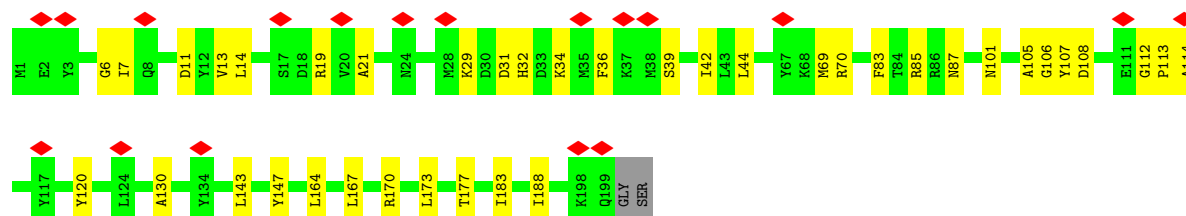
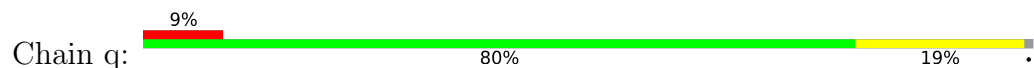
- Molecule 16: Proteasome subunit beta type-3



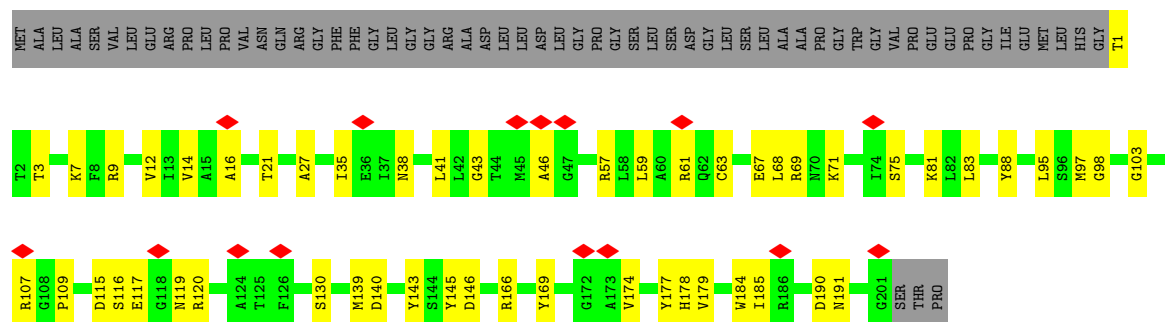
- Molecule 17: Proteasome subunit beta type-2



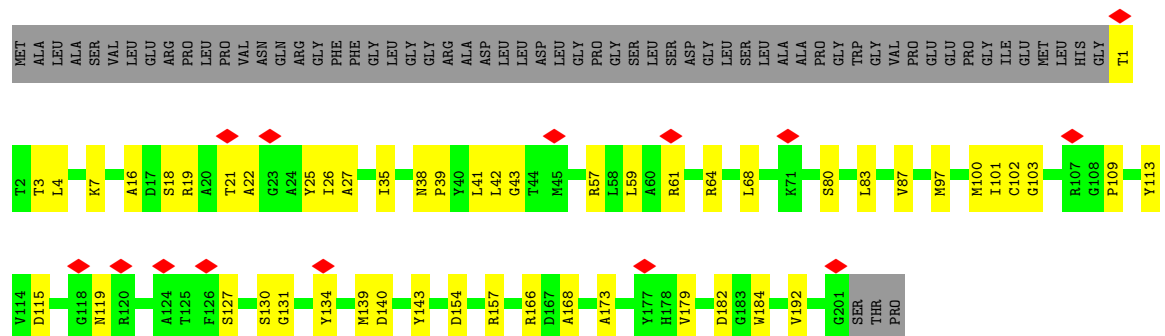
• Molecule 17: Proteasome subunit beta type-2



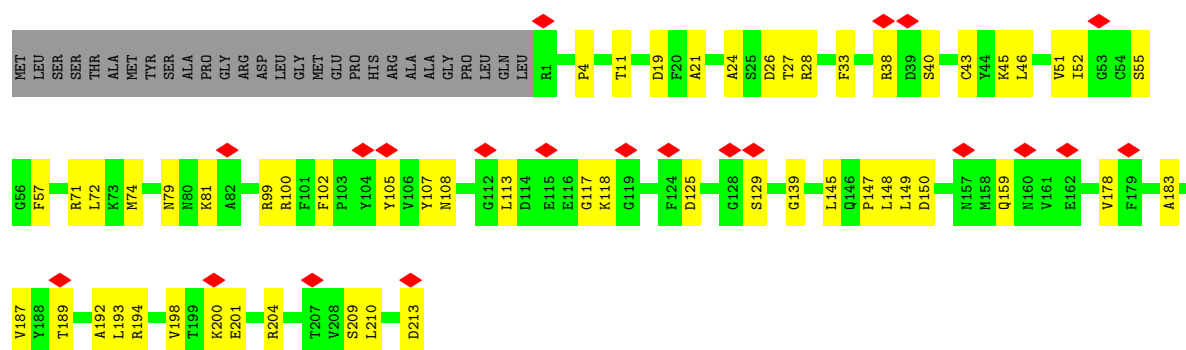
• Molecule 18: Proteasome subunit beta type-5



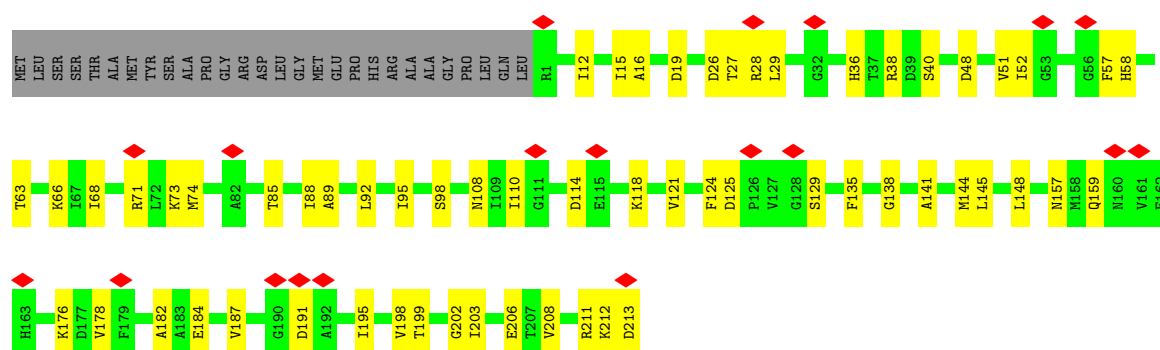
• Molecule 18: Proteasome subunit beta type-5



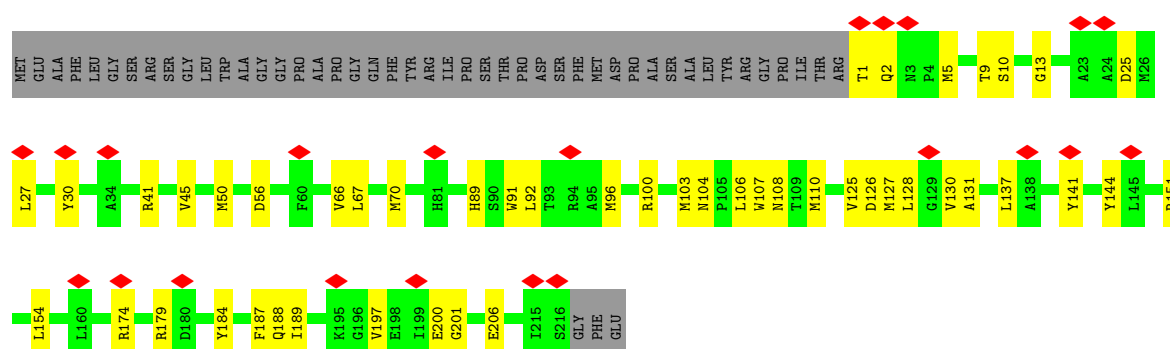
• Molecule 19: Proteasome subunit beta type-1



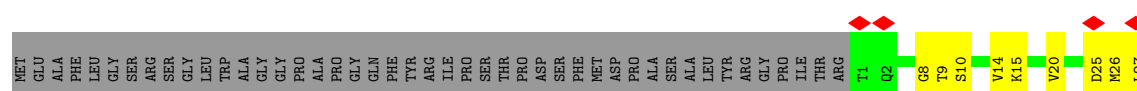
• Molecule 19: Proteasome subunit beta type-1

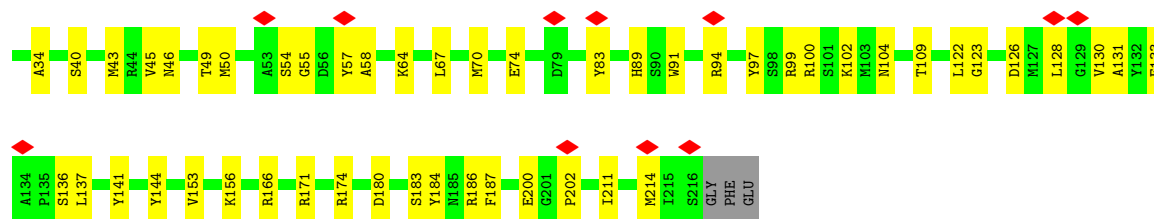


• Molecule 20: Proteasome subunit beta type-4

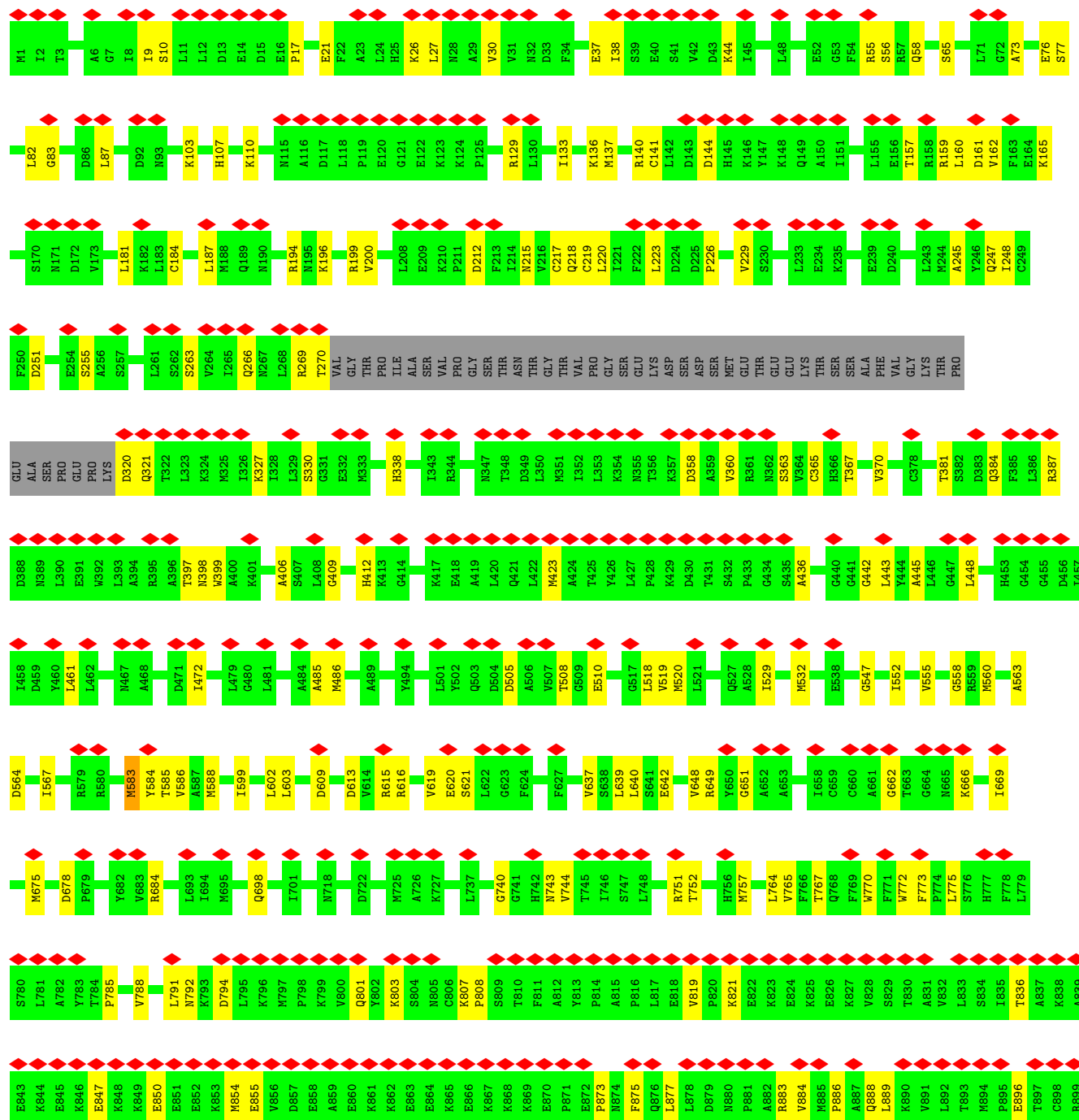
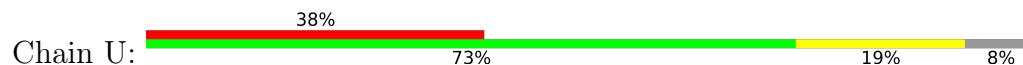


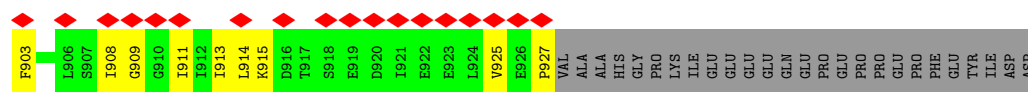
• Molecule 20: Proteasome subunit beta type-4



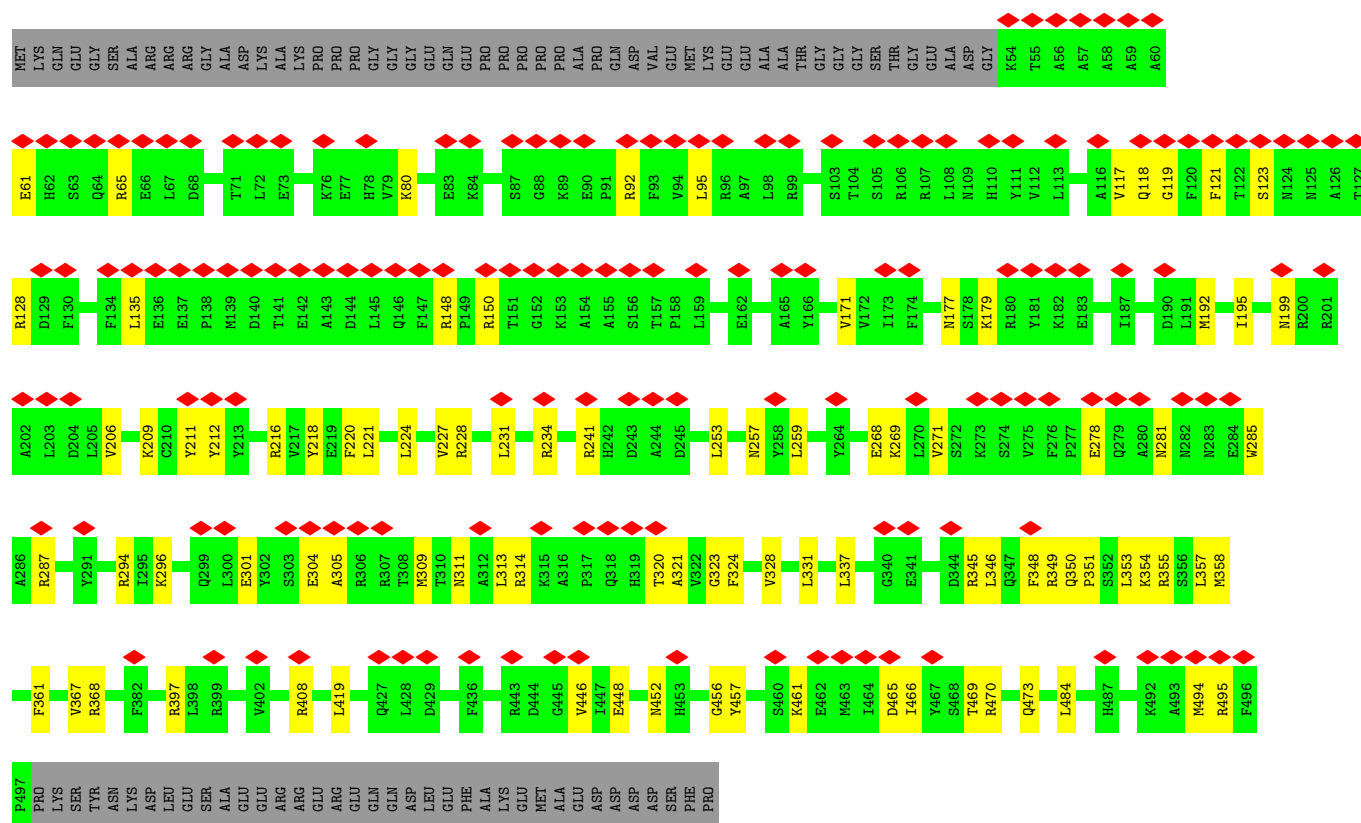


- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

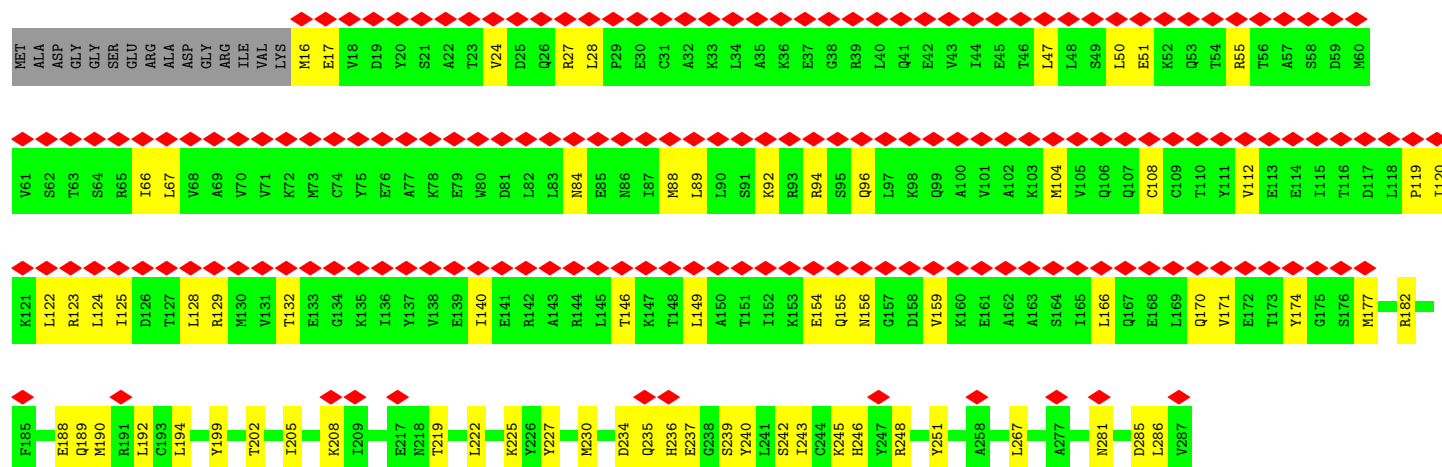
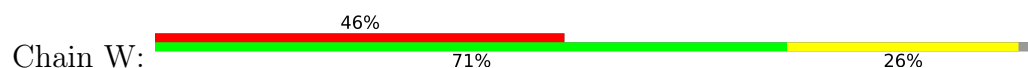


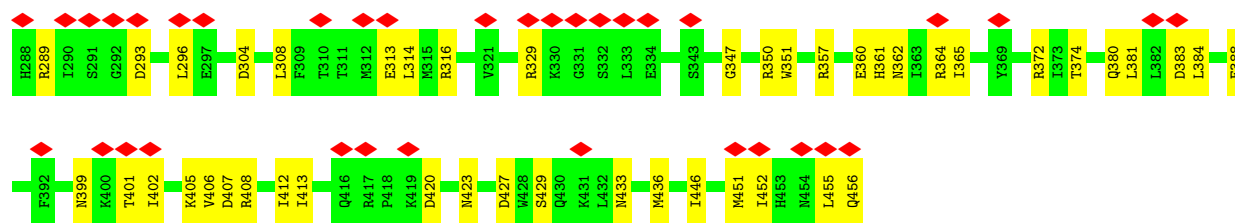


- Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

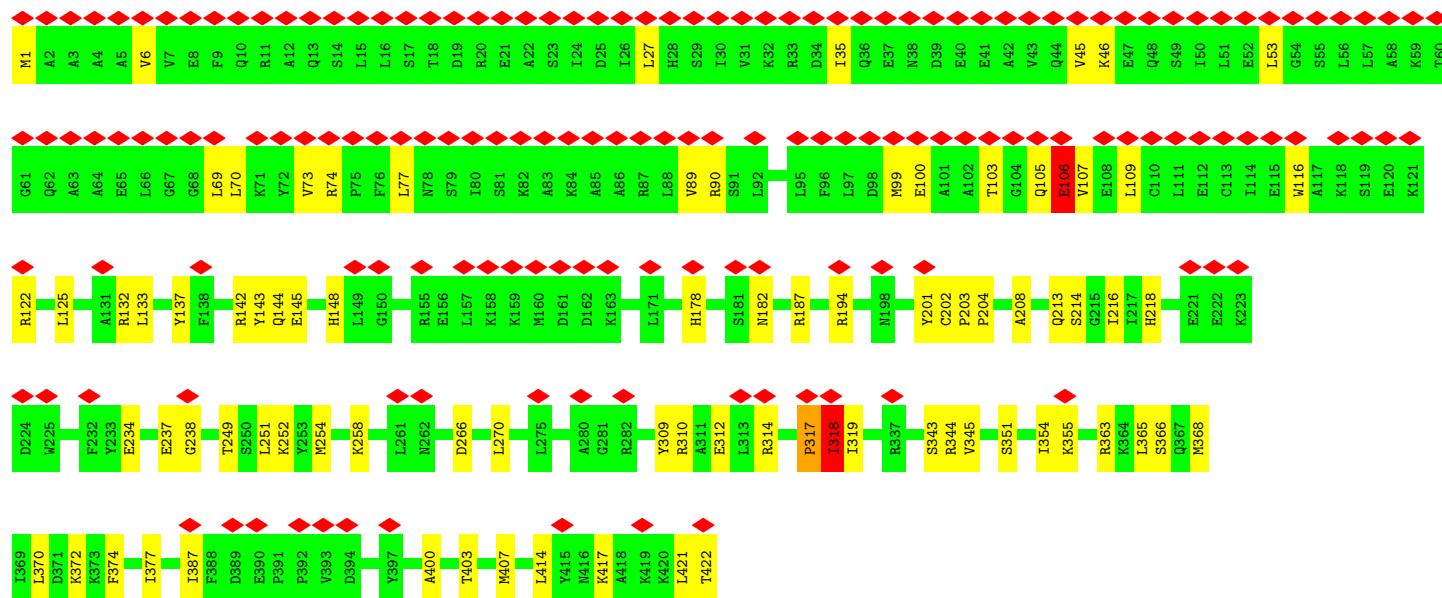
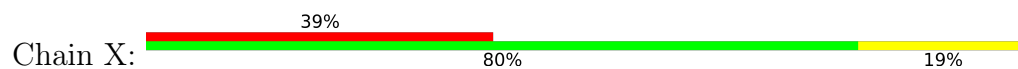


- Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

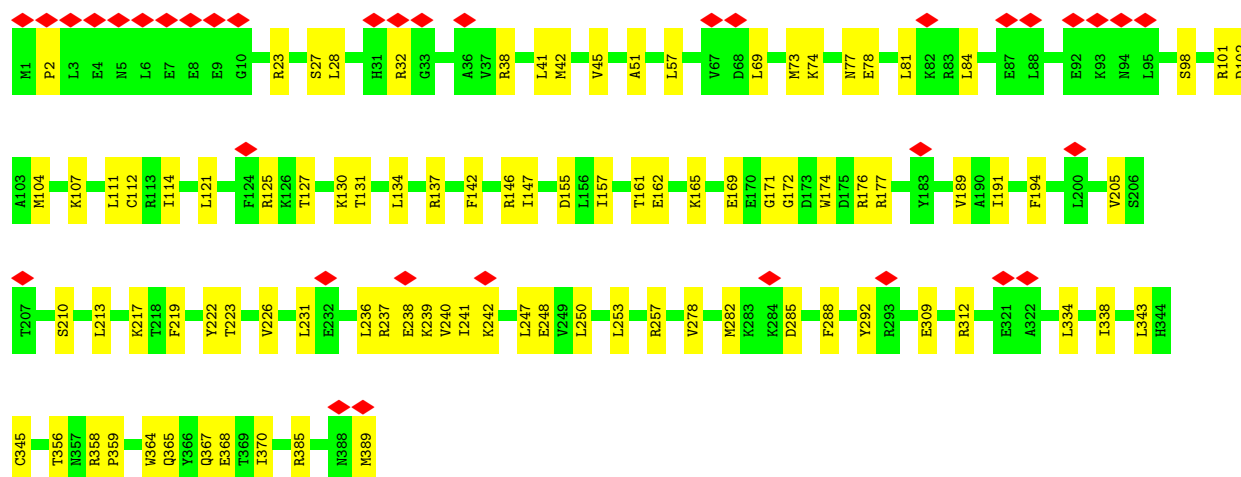
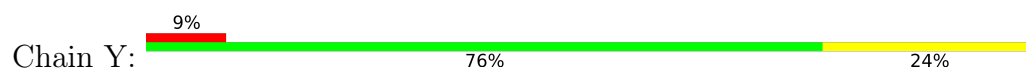




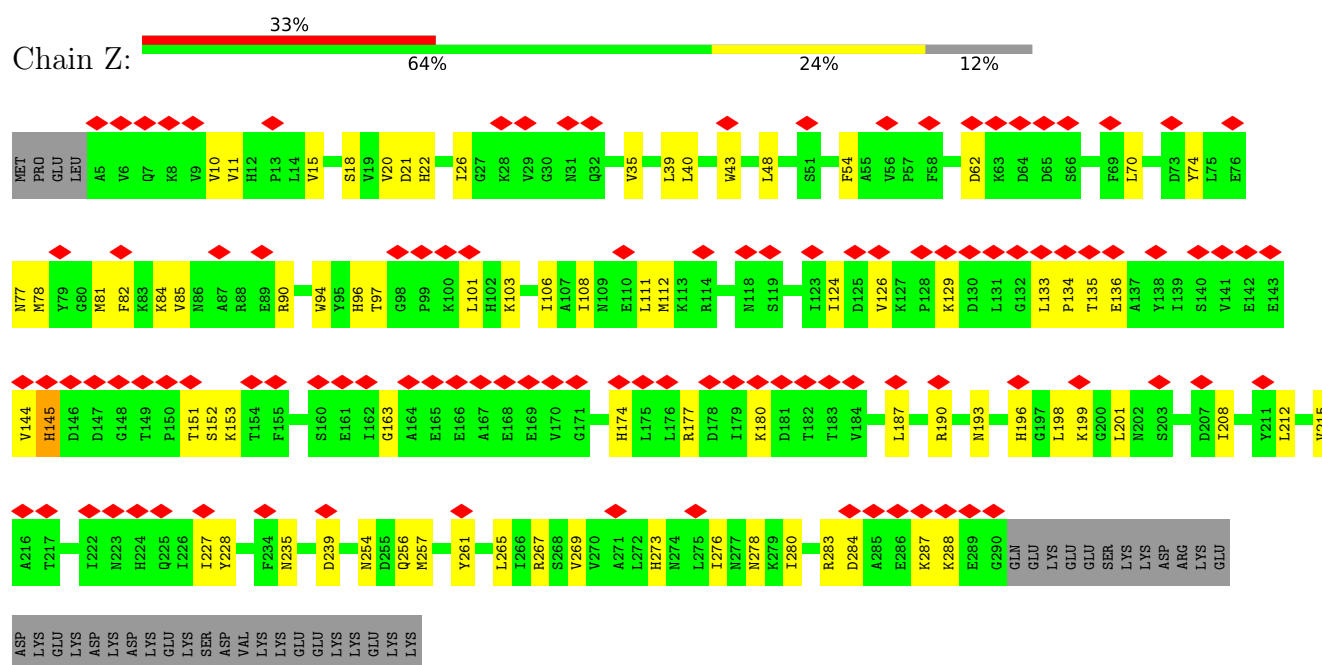
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11



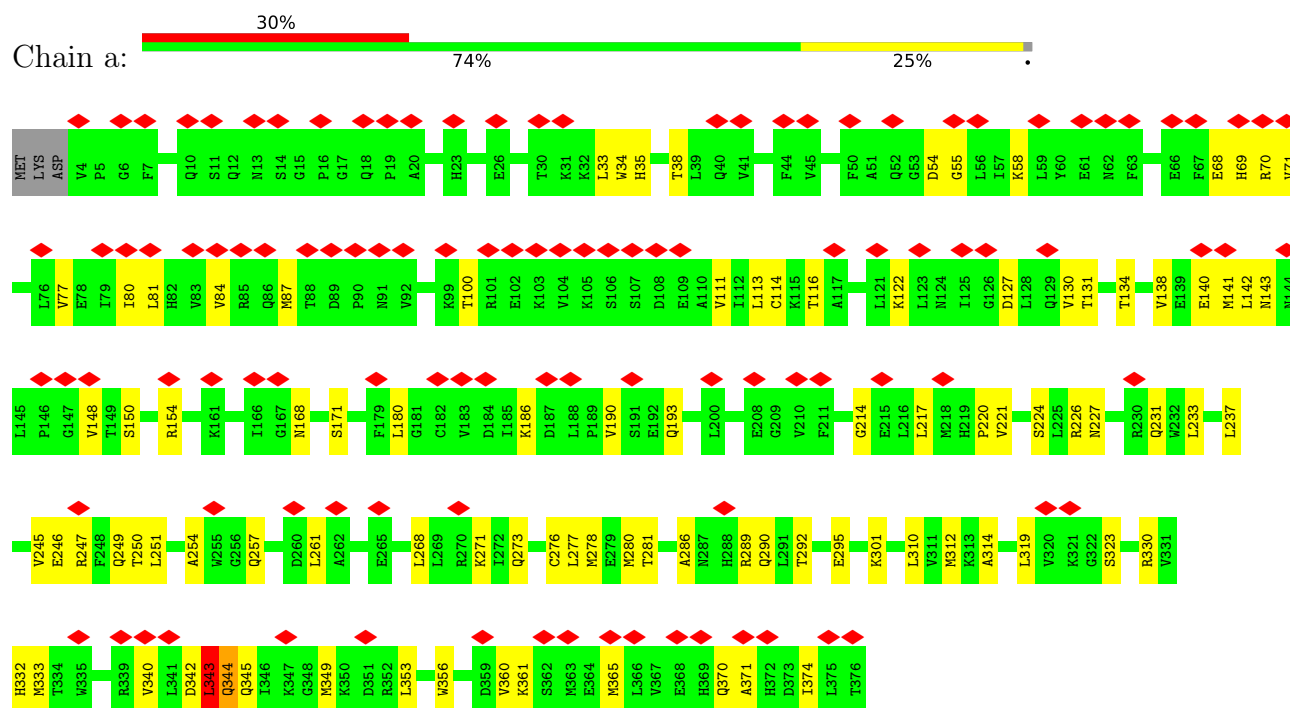
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6



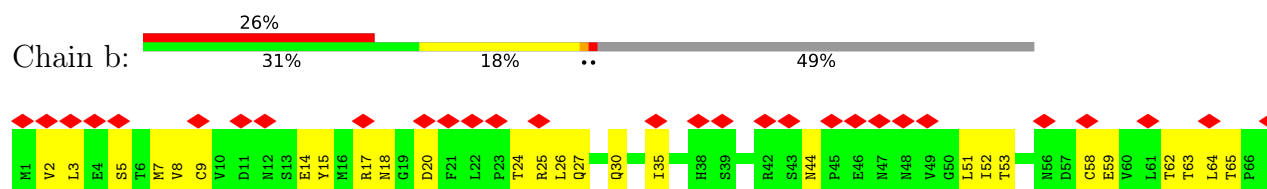
- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

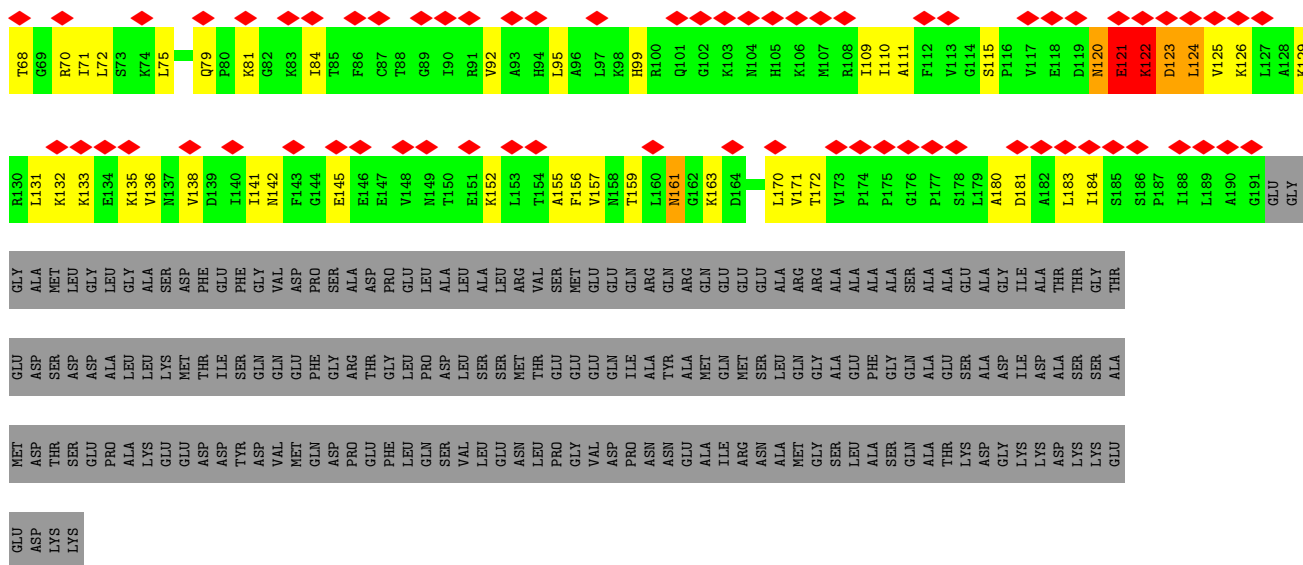


- Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

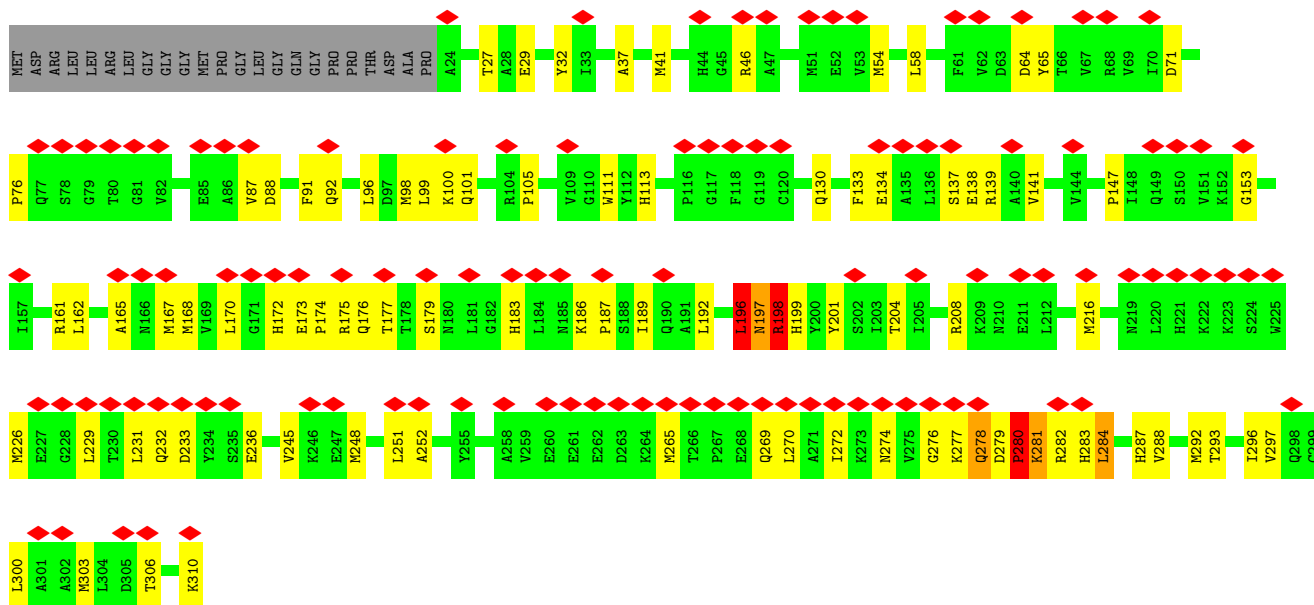


- Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

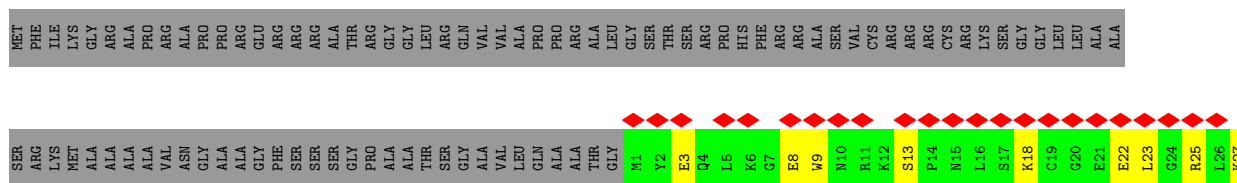
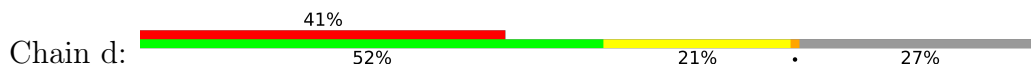




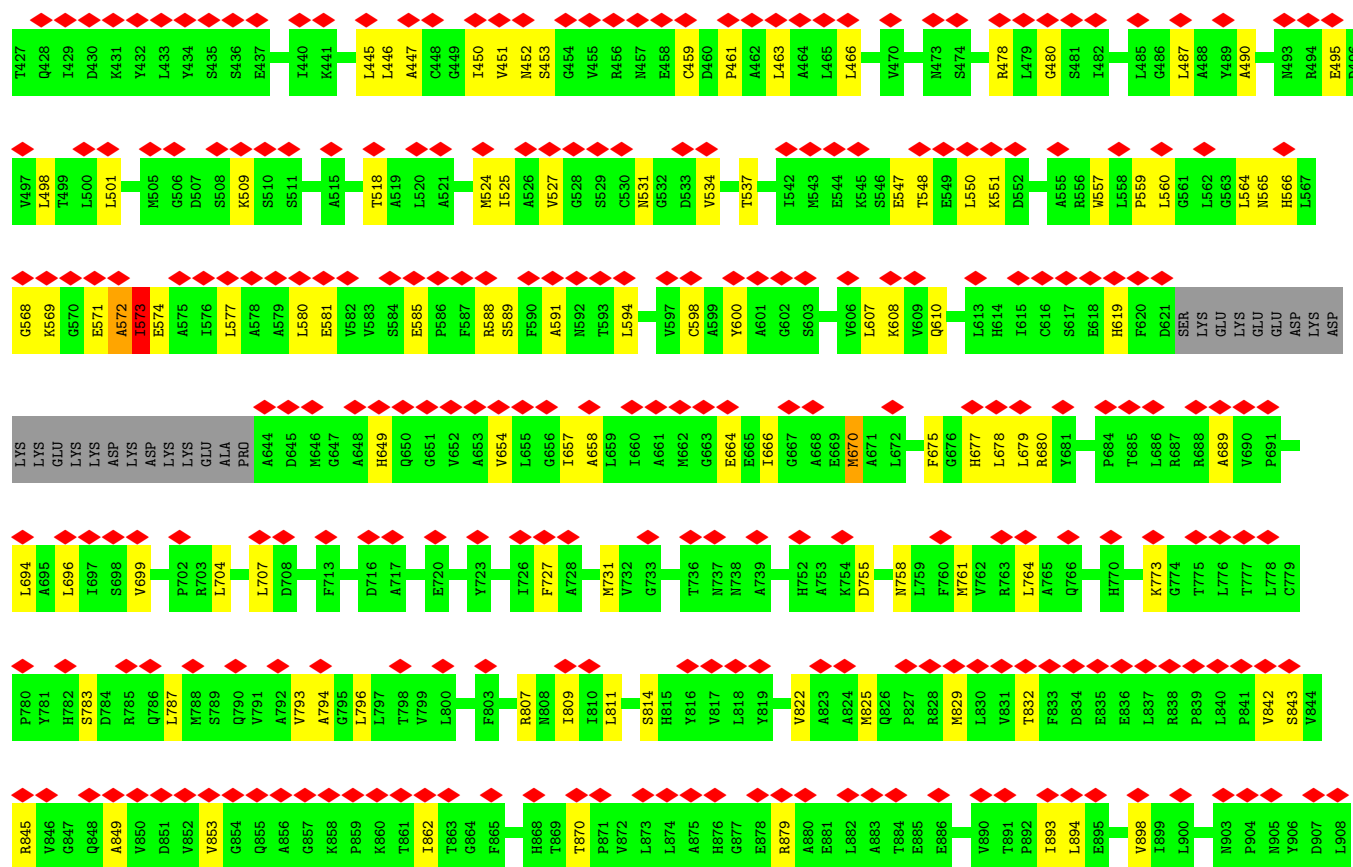
- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14



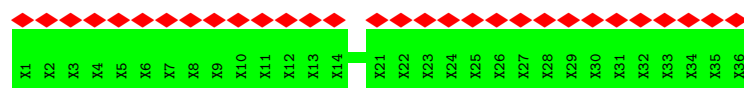
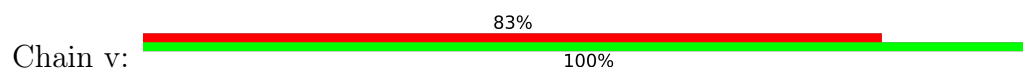
- Molecule 30: 26S proteasome non-ATPase regulatory subunit 8



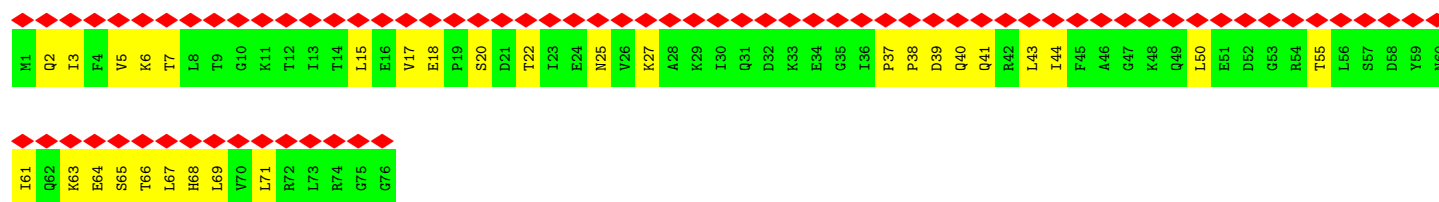




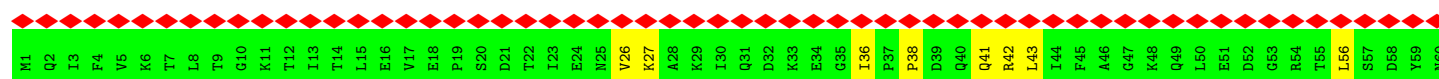
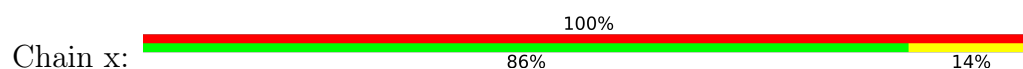
• Molecule 33: Substrate

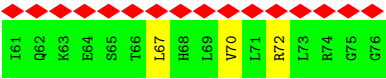


• Molecule 34: Ubiquitin

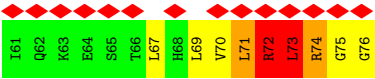
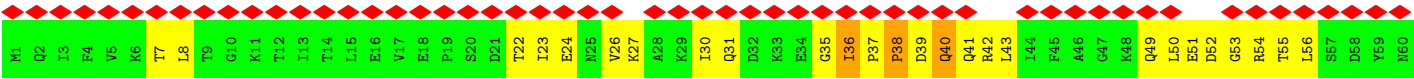
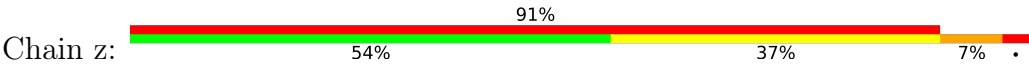


• Molecule 34: Ubiquitin





● Molecule 34: Ubiquitin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6192	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS 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	0.017	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00578	Depositor
Map size (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/3283	0.48	0/4433
2	B	0.21	0/3254	0.57	1/4388 (0.0%)
3	C	0.24	0/3146	0.54	0/4226
4	D	0.25	0/3090	0.58	1/4168 (0.0%)
5	E	0.25	1/3145 (0.0%)	0.58	1/4233 (0.0%)
6	F	0.23	0/3137	0.51	0/4223
7	G	0.24	0/1901	0.52	1/2572 (0.0%)
7	g	0.18	0/1913	0.44	0/2589
8	H	0.19	0/1840	0.49	0/2495
8	h	0.17	0/1844	0.41	0/2497
9	I	0.22	0/1963	0.55	2/2650 (0.1%)
9	i	0.17	0/1985	0.43	0/2677
10	J	0.17	0/1887	0.45	0/2553
10	j	0.19	0/1887	0.46	0/2549
11	K	0.19	0/1841	0.42	0/2486
11	k	0.16	0/1809	0.41	0/2444
12	L	0.18	0/1911	0.43	0/2584
12	l	0.16	0/1896	0.38	0/2565
13	M	0.20	0/1931	0.47	0/2600
13	m	0.18	0/1916	0.44	0/2580
14	N	0.15	0/1548	0.36	0/2097
14	n	0.15	0/1536	0.34	0/2080
15	O	0.17	0/1672	0.44	0/2267
15	o	0.17	0/1686	0.42	0/2282
16	P	0.21	0/1616	0.53	0/2180
16	p	0.20	0/1620	0.50	0/2184
17	Q	0.17	0/1627	0.41	0/2202
17	q	0.17	0/1611	0.40	0/2182
18	R	0.19	0/1590	0.41	0/2147
18	r	0.17	0/1580	0.44	0/2135
19	S	0.20	0/1671	0.47	0/2252
19	s	0.18	0/1680	0.43	0/2264

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.19	0/1716	0.45	0/2323
20	t	0.18	0/1720	0.44	0/2328
21	U	0.18	0/6984	0.48	0/9435
22	V	0.17	0/3681	0.44	0/4969
23	W	0.18	0/3644	0.45	0/4901
24	X	0.20	0/3381	0.44	2/4558 (0.0%)
25	Y	0.17	0/3261	0.44	0/4393
26	Z	0.24	0/2324	0.61	0/3150
27	a	0.23	0/3053	0.59	0/4133
28	b	0.30	0/1478	0.59	0/2001
29	c	0.30	0/2302	0.67	0/3110
30	d	0.24	0/2162	0.54	0/2919
31	e	0.23	0/437	0.60	0/595
32	f	0.23	0/6640	0.55	4/8988 (0.0%)
34	w	0.16	0/607	0.43	0/816
34	x	0.11	0/607	0.28	0/816
34	z	0.54	0/607	0.70	0/816
All	All	0.21	1/109620 (0.0%)	0.49	12/148035 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	281	ARG	C-N	6.81	1.41	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	166	PRO	N-CA-C	6.19	118.25	110.70
24	X	317	PRO	N-CA-C	-6.12	99.86	112.47
2	B	85	MET	CB-CG-SD	6.02	130.77	112.70
9	I	26	GLU	N-CA-CB	5.74	119.75	110.40
7	G	92	GLN	N-CA-CB	5.60	118.97	110.28
4	D	54	LEU	CA-CB-CG	5.53	135.64	116.30
32	f	670	MET	CG-SD-CE	-5.48	88.85	100.90
9	I	52	ILE	O-C-N	5.24	126.02	121.98
32	f	689	ALA	CA-C-N	5.24	123.54	120.24
32	f	689	ALA	C-N-CA	5.24	123.54	120.24
24	X	203	PRO	N-CA-C	-5.04	104.55	110.70
32	f	670	MET	CA-CB-CG	-5.01	104.08	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3229	0	3261	82	0
2	B	3207	0	3278	80	0
3	C	3105	0	3219	88	0
4	D	3040	0	3076	81	0
5	E	3097	0	3174	67	0
6	F	3098	0	3187	67	0
7	G	1867	0	1867	45	0
7	g	1879	0	1872	36	0
8	H	1801	0	1773	44	0
8	h	1805	0	1798	31	0
9	I	1933	0	1923	41	0
9	i	1955	0	1955	28	0
10	J	1861	0	1846	47	0
10	j	1861	0	1865	34	0
11	K	1813	0	1796	43	0
11	k	1782	0	1766	31	0
12	L	1876	0	1856	43	0
12	l	1861	0	1839	41	0
13	M	1893	0	1885	44	0
13	m	1881	0	1868	36	0
14	N	1521	0	1494	27	0
14	n	1510	0	1483	25	0
15	O	1645	0	1648	33	0
15	o	1659	0	1681	30	0
16	P	1587	0	1598	37	0
16	p	1591	0	1609	37	0
17	Q	1591	0	1589	30	0
17	q	1578	0	1569	30	0
18	R	1559	0	1523	37	0
18	r	1549	0	1506	34	0
19	S	1641	0	1639	39	0
19	s	1650	0	1645	42	0
20	T	1683	0	1662	29	0
20	t	1687	0	1666	38	0
21	U	6867	0	6929	122	0
22	V	3612	0	3682	63	0
23	W	3596	0	3713	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	X	3335	0	3435	58	0
25	Y	3202	0	3204	64	0
26	Z	2281	0	2312	61	0
27	a	2995	0	3012	67	0
28	b	1458	0	1502	84	0
29	c	2260	0	2276	74	0
30	d	2116	0	2146	52	0
31	e	425	0	328	12	0
32	f	6529	0	6541	100	0
33	v	180	0	46	0	0
34	w	601	0	629	21	0
34	x	601	0	629	6	0
34	z	601	0	629	73	0
35	A	31	0	12	6	0
35	B	31	0	12	2	0
35	C	31	0	12	3	0
35	F	31	0	12	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	F	1	0	0	0	0
37	D	27	0	12	0	0
38	c	1	0	0	0	0
All	All	108111	0	108489	2145	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 10.

All (2145) 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)
34:z:42:ARG:HD3	34:z:49:GLN:HG3	1.34	1.08
28:b:163:LYS:HB3	34:z:42:ARG:HH22	1.10	1.05
34:z:27:LYS:HB3	34:z:38:PRO:HA	1.41	1.01
29:c:279:ASP:HA	29:c:283:HIS:HB3	1.43	0.97
28:b:132:LYS:HE2	34:z:42:ARG:HB2	1.46	0.94
30:d:200:PHE:HB3	30:d:203:PRO:HG2	1.50	0.93
29:c:192:LEU:HA	29:c:196:LEU:HB2	1.53	0.88
28:b:163:LYS:HB3	34:z:42:ARG:NH2	1.89	0.86
28:b:129:LYS:HD2	34:z:70:VAL:HB	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:103:THR:HA	24:X:106:GLU:HB2	1.57	0.84
19:S:43:CYS:H	19:S:194:ARG:HH21	1.27	0.82
28:b:163:LYS:HA	34:z:52:ASP:H	1.45	0.81
34:z:7:THR:HB	34:z:71:LEU:HG	1.63	0.80
30:d:147:SER:HB3	30:d:150:LYS:HZ2	1.49	0.78
34:z:8:LEU:HD13	34:z:73:LEU:HB2	1.66	0.78
9:I:99:LEU:HG	17:Q:86:ARG:HH12	1.49	0.77
30:d:248:GLU:HB3	30:d:252:GLN:HE22	1.50	0.76
18:R:97:MET:H	18:R:116:SER:HB3	1.49	0.76
34:z:42:ARG:HD3	34:z:49:GLN:CG	2.16	0.75
28:b:132:LYS:CE	34:z:42:ARG:HB2	2.17	0.75
16:P:149:MET:HE1	16:P:170:ALA:HA	1.68	0.75
34:z:8:LEU:HD13	34:z:73:LEU:CB	2.18	0.74
34:z:8:LEU:HB2	34:z:71:LEU:HB3	1.69	0.73
20:T:108:ASN:HB3	20:T:110:MET:HE3	1.70	0.73
7:G:88:ARG:HH12	13:M:157:SER:H	1.34	0.73
22:V:117:VAL:O	22:V:121:PHE:HB2	1.88	0.73
32:f:333:LEU:HD21	32:f:829:MET:HG2	1.69	0.73
15:o:70:THR:HG23	15:o:72:ARG:H	1.54	0.72
4:D:155:THR:HA	4:D:159:LYS:HE3	1.70	0.72
12:l:88:MET:HE1	12:l:108:LEU:HD21	1.72	0.72
9:i:143:TYR:HB2	9:i:146:GLN:HE21	1.53	0.72
34:z:22:THR:HA	34:z:55:THR:HA	1.72	0.72
8:h:6:TYR:HH	9:i:2:SER:N	1.87	0.71
34:z:41:GLN:HB2	34:z:69:LEU:HD11	1.72	0.71
9:I:143:TYR:HB2	9:I:146:GLN:HE21	1.55	0.71
21:U:619:VAL:HG11	21:U:648:VAL:HG13	1.73	0.71
28:b:132:LYS:O	34:z:40:GLN:HA	1.91	0.71
17:q:183:ILE:HG12	17:q:188:ILE:HG12	1.72	0.71
24:X:202:CYS:O	24:X:204:PRO:HD3	1.91	0.70
1:A:43:ARG:HA	1:A:46:LYS:HG2	1.74	0.70
29:c:278:GLN:H	29:c:282:ARG:HH21	1.40	0.70
23:W:401:THR:HG23	23:W:402:ILE:HD12	1.74	0.70
11:k:210:LEU:HA	11:k:214:ASN:HD21	1.56	0.70
12:l:14:SER:HB3	12:l:18:ARG:H	1.57	0.70
28:b:121:GLU:O	28:b:124:LEU:HG	1.91	0.70
32:f:398:TRP:HA	32:f:401:LYS:HD3	1.73	0.69
34:z:30:ILE:HB	34:z:41:GLN:HE22	1.55	0.69
21:U:10:SER:HB2	30:d:73:ARG:HD3	1.73	0.69
7:g:71:LYS:HA	7:g:77:GLY:HA2	1.74	0.69
3:C:90:HIS:ND1	3:C:91:PRO:HD3	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:14:SER:HB3	8:h:18:LYS:H	1.56	0.69
28:b:157:VAL:HG21	28:b:170:LEU:HB2	1.73	0.69
4:D:335:LEU:CB	4:D:336:PRO:HD3	2.24	0.68
4:D:156:SER:O	4:D:157:ASP:HB3	1.93	0.68
29:c:173:GLU:HG3	29:c:175:ARG:HD2	1.74	0.68
2:B:224:LEU:HD21	2:B:235:LEU:HD11	1.75	0.68
21:U:619:VAL:HG23	21:U:651:GLY:HA3	1.75	0.68
16:p:146:MET:HE3	16:p:174:ALA:HB2	1.75	0.68
27:a:180:LEU:HD11	27:a:221:VAL:HG21	1.76	0.68
19:S:4:PRO:HB2	20:T:100:ARG:HH21	1.59	0.68
19:S:52:ILE:HD11	19:S:108:ASN:HB3	1.75	0.68
26:Z:145:HIS:NE2	26:Z:152:SER:HB3	2.09	0.68
21:U:792:ASN:HB3	21:U:914:LEU:HB3	1.76	0.67
5:E:286:ASP:HB3	5:E:289:LEU:HB2	1.76	0.67
11:K:41:GLN:HE21	11:K:151:PRO:HB2	1.60	0.67
21:U:903:PHE:HB2	21:U:915:LYS:HB2	1.75	0.67
11:K:36:THR:HA	11:K:171:GLY:HA3	1.76	0.67
12:l:121:GLN:HG3	13:m:129:ARG:HG2	1.76	0.67
7:G:17:SER:OG	7:G:21:ARG:HG3	1.95	0.67
22:V:484:LEU:HA	26:Z:267:ARG:HH12	1.57	0.67
5:E:52:SER:HB3	6:F:136:VAL:HB	1.77	0.67
31:e:25:GLU:HG3	31:e:27:TRP:H	1.59	0.67
11:k:101:PHE:HD1	18:r:57:ARG:HG2	1.58	0.67
19:S:11:THR:HA	19:S:139:GLY:HA3	1.76	0.67
3:C:113:ARG:HG3	3:C:127:LEU:HB2	1.75	0.66
7:G:88:ARG:HH22	13:M:156:VAL:HA	1.59	0.66
28:b:133:LYS:HD2	34:z:40:GLN:HB3	1.75	0.66
19:s:195:ILE:HB	19:s:206:GLU:HB3	1.77	0.66
24:X:105:GLN:HG2	24:X:105:GLN:O	1.95	0.66
3:C:99:VAL:HA	3:C:123:LEU:HB2	1.75	0.66
12:L:199:LEU:HB2	12:L:239:ARG:HH22	1.59	0.66
32:f:822:VAL:HA	32:f:825:MET:HE3	1.77	0.66
3:C:198:LEU:HD11	35:C:501:ATP:H2'	1.78	0.66
16:p:146:MET:O	16:p:150:CYS:HB2	1.96	0.66
10:J:112:ALA:HA	10:J:115:LYS:HE2	1.77	0.66
15:O:100:LEU:HB3	15:O:111:TYR:HB2	1.77	0.66
9:I:63:GLU:HG3	9:I:64:LYS:HG3	1.77	0.66
28:b:120:ASN:ND2	28:b:123:ASP:HB3	2.11	0.66
29:c:165:ALA:HA	29:c:168:MET:HE3	1.77	0.65
29:c:197:ASN:HA	29:c:201:TYR:HA	1.78	0.65
7:G:18:PRO:O	7:G:19:GLU:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:411:ARG:HH22	2:B:415:THR:H	1.43	0.65
4:D:92:PHE:HA	4:D:103:VAL:HG12	1.79	0.65
1:A:279:ALA:HB1	2:B:307:ARG:HG3	1.78	0.65
3:C:188:LEU:HB3	3:C:317:PHE:HE2	1.61	0.65
25:Y:278:VAL:O	25:Y:282:MET:HB2	1.96	0.65
30:d:197:ILE:HG13	30:d:198:LEU:HG	1.78	0.65
34:z:27:LYS:HE3	34:z:42:ARG:HH21	1.61	0.65
24:X:178:HIS:HE1	24:X:318:ILE:HG12	1.60	0.65
28:b:53:THR:HG22	28:b:59:GLU:H	1.62	0.65
16:p:45:MET:HE1	16:p:51:ILE:HB	1.78	0.65
4:D:160:PRO:HB3	4:D:221:HIS:CG	2.31	0.65
13:m:35:THR:HA	13:m:166:GLY:HA3	1.78	0.65
3:C:195:GLY:HA2	3:C:198:LEU:HD13	1.79	0.65
27:a:278:MET:HA	27:a:281:THR:HG22	1.78	0.65
3:C:159:LYS:HA	3:C:162:LYS:HD2	1.79	0.64
4:D:268:ASP:HB3	4:D:312:ASN:H	1.62	0.64
9:I:33:THR:HA	9:I:165:GLY:HA3	1.78	0.64
28:b:3:LEU:HD23	28:b:44:ASN:HD21	1.63	0.64
11:K:16:SER:HB3	11:K:20:ARG:H	1.63	0.64
17:Q:148:THR:HG22	17:Q:150:THR:H	1.62	0.64
28:b:126:LYS:HA	28:b:129:LYS:HE2	1.80	0.64
34:w:38:PRO:HA	34:w:41:GLN:HE21	1.62	0.64
6:F:343:LEU:HD13	6:F:348:LEU:HB3	1.80	0.64
21:U:889:LEU:HD13	21:U:909:GLY:H	1.62	0.64
32:f:231:LEU:HB3	32:f:853:VAL:HG22	1.79	0.64
21:U:58:GLN:HB2	21:U:87:LEU:HD12	1.80	0.63
28:b:30:GLN:HG3	28:b:75:LEU:HD13	1.79	0.63
34:w:22:THR:HA	34:w:55:THR:HA	1.79	0.63
2:B:174:MET:HE3	2:B:249:ARG:HG3	1.80	0.63
22:V:281:ASN:HA	25:Y:385:ARG:HH21	1.64	0.63
2:B:120:HIS:HA	2:B:134:SER:HA	1.80	0.63
13:M:35:THR:HA	13:M:166:GLY:HA3	1.80	0.63
19:S:148:LEU:HD12	16:p:149:MET:HA	1.80	0.63
23:W:47:LEU:HD12	23:W:66:ILE:HG23	1.80	0.63
29:c:192:LEU:HA	29:c:196:LEU:CB	2.26	0.63
12:l:196:ARG:HH12	12:l:236:LEU:HB3	1.63	0.63
18:r:64:ARG:HH22	18:r:68:LEU:HD13	1.63	0.63
4:D:394:VAL:HG12	4:D:396:ALA:H	1.63	0.63
7:G:138:MET:HB3	7:G:154:CYS:HB2	1.79	0.63
1:A:312:ARG:HB3	1:A:315:ILE:HD13	1.80	0.63
4:D:204:MET:HG3	4:D:331:ILE:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:146:MET:O	16:P:150:CYS:HB2	1.99	0.63
21:U:140:ARG:O	21:U:144:ASP:HB2	1.99	0.63
3:C:307:ARG:HG2	3:C:310:ARG:HG2	1.81	0.62
22:V:121:PHE:HB3	22:V:128:ARG:HD2	1.81	0.62
12:l:49:LEU:HB2	12:l:195:LEU:HD11	1.81	0.62
6:F:307:GLN:HA	6:F:310:MET:HG3	1.81	0.62
16:P:15:LYS:HE2	16:P:119:PRO:HB2	1.81	0.62
13:m:76:ALA:H	13:m:136:MET:HB3	1.64	0.62
9:I:78:GLY:HA3	9:I:132:VAL:HG22	1.81	0.62
30:d:41:THR:HG22	30:d:44:THR:H	1.63	0.62
27:a:289:ARG:HB2	27:a:333:MET:HB3	1.80	0.62
11:K:133:MET:HE2	11:K:135:ARG:HH11	1.64	0.62
29:c:279:ASP:N	29:c:280:PRO:HD2	2.15	0.62
6:F:220:PRO:HG2	6:F:350:ARG:HH11	1.64	0.62
15:o:177:VAL:HB	15:o:184:ASP:HB2	1.82	0.62
3:C:99:VAL:HG12	3:C:123:LEU:HD12	1.80	0.62
28:b:65:THR:HG21	28:b:70:ARG:HD3	1.81	0.62
30:d:198:LEU:HD13	30:d:213:ARG:HH22	1.63	0.62
19:s:68:ILE:HD11	19:s:92:LEU:HD13	1.82	0.62
6:F:225:MET:HE2	6:F:233:LYS:HG2	1.82	0.62
29:c:189:ILE:HA	29:c:192:LEU:HG	1.82	0.62
9:i:119:GLN:NE2	10:j:79:ASP:OD1	2.33	0.62
1:A:178:GLY:O	35:A:501:ATP:N6	2.29	0.62
10:J:52:LYS:HG3	10:J:53:LEU:HG	1.81	0.62
14:N:179:ILE:HG12	14:N:184:VAL:HG22	1.81	0.62
11:k:101:PHE:CD1	18:r:57:ARG:HG2	2.34	0.62
15:O:14:LEU:HB2	15:O:176:CYS:HB3	1.82	0.62
29:c:196:LEU:O	29:c:198:ARG:N	2.33	0.62
3:C:258:ARG:HD3	3:C:274:LEU:HD21	1.81	0.61
18:R:38:ASN:OD1	18:R:41:LEU:N	2.33	0.61
8:h:176:LYS:HD2	8:h:177:ARG:HE	1.65	0.61
34:z:52:ASP:C	34:z:54:ARG:H	2.08	0.61
28:b:163:LYS:HA	34:z:52:ASP:N	2.15	0.61
21:U:26:LYS:HZ2	30:d:36:LEU:HB2	1.64	0.61
23:W:329:ARG:HE	23:W:351:TRP:HE1	1.46	0.61
17:Q:4:LEU:HD22	17:Q:45:LEU:HD23	1.81	0.61
23:W:408:ARG:HD3	24:X:345:VAL:HG23	1.83	0.61
34:z:75:GLY:O	34:z:76:GLY:C	2.43	0.61
8:h:34:PRO:HA	8:h:164:GLY:HA3	1.83	0.61
16:p:53:LEU:HG	16:p:107:PRO:HB3	1.82	0.61
24:X:249:THR:HA	24:X:252:LYS:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:t:27:LEU:HD22	20:t:184:TYR:HB2	1.82	0.61
5:E:101:ASP:HB3	5:E:105:LEU:H	1.64	0.61
21:U:532:MET:HG3	21:U:552:ILE:HG22	1.83	0.61
28:b:133:LYS:HA	34:z:40:GLN:HA	1.80	0.61
15:o:173:ILE:HB	15:o:190:THR:HB	1.82	0.61
28:b:121:GLU:O	28:b:122:LYS:C	2.44	0.61
29:c:279:ASP:O	29:c:280:PRO:C	2.43	0.61
12:l:41:LYS:HG3	12:l:42:THR:HG23	1.82	0.61
18:R:7:LYS:HG2	18:R:12:VAL:HG22	1.83	0.61
25:Y:359:PRO:HB2	25:Y:364:TRP:HB2	1.83	0.61
3:C:158:ILE:HG22	3:C:162:LYS:HE3	1.82	0.61
9:i:13:SER:HG	9:i:17:ARG:H	1.47	0.61
9:i:45:LEU:HD11	9:i:137:ILE:HD13	1.83	0.61
10:j:183:THR:HB	10:j:186:LEU:HB2	1.82	0.61
32:f:96:LEU:HD13	32:f:129:LEU:HD13	1.83	0.60
2:B:287:ILE:O	2:B:291:GLY:N	2.34	0.60
4:D:118:THR:O	29:c:277:LYS:NZ	2.33	0.60
26:Z:26:ILE:HD11	26:Z:35:VAL:HG22	1.83	0.60
8:h:81:PRO:HB3	8:h:84:ARG:HH21	1.66	0.60
3:C:247:PHE:HD1	3:C:292:ILE:HG13	1.67	0.60
12:l:55:GLU:HG2	12:l:56:LEU:HG	1.83	0.60
21:U:801:GLN:HB3	21:U:877:LEU:HB3	1.83	0.60
23:W:125:ILE:HG23	23:W:129:ARG:HH21	1.66	0.60
29:c:174:PRO:O	29:c:176:GLN:NE2	2.33	0.60
3:C:389:LYS:O	3:C:392:GLN:NE2	2.35	0.60
4:D:335:LEU:HB3	4:D:336:PRO:HD3	1.83	0.60
9:I:119:GLN:O	9:I:123:GLN:HB2	2.01	0.60
21:U:751:ARG:HE	21:U:908:ILE:HG23	1.67	0.60
2:B:339:PRO:HA	2:B:342:ILE:HG12	1.82	0.60
6:F:94:ILE:HD11	6:F:125:LYS:HB2	1.84	0.60
7:G:127:GLN:HE22	8:H:127:VAL:HB	1.66	0.60
20:T:45:VAL:H	20:T:50:MET:HA	1.66	0.60
32:f:548:THR:HA	32:f:551:LYS:HE3	1.82	0.60
7:g:123:GLN:NE2	8:h:82:ASP:OD1	2.35	0.60
26:Z:212:LEU:HD21	27:a:353:LEU:HD13	1.82	0.60
27:a:361:LYS:HG2	27:a:365:MET:HE1	1.84	0.60
30:d:198:LEU:O	30:d:205:LYS:NZ	2.35	0.60
32:f:761:MET:HA	32:f:764:LEU:HB2	1.82	0.60
7:g:9:PHE:HB3	7:g:12:HIS:HB2	1.83	0.60
34:z:43:LEU:HB3	34:z:50:LEU:HD12	1.83	0.60
6:F:209:LYS:HD2	6:F:324:THR:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:182:ASN:ND2	25:Y:248:GLU:OE2	2.35	0.60
30:d:3:GLU:O	30:d:25:ARG:NH1	2.35	0.60
5:E:295:LEU:HD13	5:E:298:LYS:HD3	1.82	0.59
15:O:1:THR:O	15:O:129:SER:N	2.35	0.59
15:O:46:ALA:HB3	15:O:97:ALA:HB3	1.84	0.59
23:W:205:ILE:HA	23:W:208:LYS:HZ3	1.66	0.59
28:b:120:ASN:ND2	28:b:123:ASP:CB	2.65	0.59
1:A:243:SER:OG	2:B:268:ARG:NH2	2.34	0.59
2:B:183:THR:HG22	2:B:184:TYR:H	1.67	0.59
21:U:649:ARG:HB3	21:U:675:MET:HE1	1.84	0.59
26:Z:144:VAL:O	26:Z:145:HIS:HB2	2.01	0.59
7:g:138:MET:HE3	7:g:139:ILE:H	1.67	0.59
34:z:37:PRO:HB2	34:z:40:GLN:HG2	1.84	0.59
6:F:362:ARG:NH2	6:F:388:THR:O	2.35	0.59
10:J:42:VAL:HG22	10:J:210:VAL:HG12	1.84	0.59
11:K:93:ARG:HD3	18:R:68:LEU:HB3	1.84	0.59
16:P:177:ARG:NH1	18:r:26:ILE:O	2.36	0.59
25:Y:338:ILE:HG13	25:Y:343:LEU:HD23	1.84	0.59
30:d:49:ILE:HG23	30:d:52:ARG:HH21	1.67	0.59
13:M:211:LEU:O	13:M:232:ARG:NH2	2.35	0.59
21:U:662:GLY:O	21:U:698:GLN:NE2	2.35	0.59
2:B:417:GLU:HA	2:B:420:LYS:HD2	1.83	0.59
3:C:36:ASN:OD1	3:C:40:GLN:NE2	2.35	0.59
6:F:251:LEU:HB2	6:F:285:ILE:HG12	1.84	0.59
28:b:163:LYS:CA	34:z:52:ASP:H	2.15	0.59
14:n:14:LEU:HB2	14:n:177:ALA:HB3	1.84	0.59
16:p:58:THR:O	17:q:85:ARG:NH2	2.36	0.59
20:T:141:TYR:HA	20:T:144:TYR:HD2	1.68	0.59
29:c:288:VAL:HG12	29:c:292:MET:HE3	1.84	0.59
13:m:34:SER:OG	13:m:65:ARG:NH1	2.35	0.59
34:z:23:ILE:HB	34:z:52:ASP:HA	1.83	0.59
7:G:88:ARG:NH2	13:M:155:GLY:O	2.35	0.59
25:Y:101:ARG:HA	25:Y:104:MET:HE2	1.84	0.59
9:i:13:SER:OG	9:i:17:ARG:N	2.35	0.59
12:l:196:ARG:HG3	12:l:199:LEU:HD12	1.83	0.59
21:U:505:ASP:HB3	21:U:508:THR:HG22	1.83	0.59
27:a:247:ARG:HE	27:a:251:LEU:HB2	1.66	0.59
29:c:197:ASN:C	29:c:199:HIS:N	2.58	0.59
1:A:34:LYS:HD3	3:C:173:GLU:HG3	1.84	0.59
8:H:51:LYS:NZ	8:H:200:GLU:O	2.35	0.59
22:V:228:ARG:NH2	22:V:257:ASN:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:116:THR:OG1	27:a:154:ARG:NH1	2.35	0.59
32:f:378:ASN:ND2	32:f:392:THR:OG1	2.36	0.59
10:j:140:GLY:O	10:j:213:ARG:NH1	2.36	0.59
3:C:281:ASP:OD2	3:C:307:ARG:NH2	2.35	0.59
4:D:191:TYR:HA	4:D:196:ILE:HD12	1.85	0.59
29:c:58:LEU:HB3	29:c:71:ASP:HB3	1.85	0.59
15:o:20:ALA:HB3	15:o:28:ASP:HB3	1.83	0.59
5:E:97:ARG:NH2	5:E:112:PRO:O	2.35	0.58
10:J:31:THR:HA	10:J:162:GLY:HA3	1.84	0.58
11:K:210:LEU:HA	11:K:214:ASN:HD21	1.68	0.58
27:a:186:LYS:HG2	27:a:193:GLN:HE22	1.66	0.58
28:b:163:LYS:HE3	34:z:38:PRO:C	2.27	0.58
11:k:103:TYR:HB3	11:k:105:GLU:HG2	1.84	0.58
16:p:30:ILE:HG22	16:p:31:GLN:HG2	1.84	0.58
3:C:255:GLY:H	3:C:273:MET:HE2	1.67	0.58
6:F:79:LYS:O	6:F:83:ASN:HB2	2.03	0.58
20:T:66:VAL:HG12	20:T:70:MET:HE1	1.85	0.58
27:a:190:VAL:HA	27:a:193:GLN:HB2	1.85	0.58
1:A:224:LEU:HD11	35:A:501:ATP:H2'	1.85	0.58
22:V:206:VAL:HA	22:V:209:LYS:HE3	1.85	0.58
28:b:25:ARG:NH1	28:b:145:GLU:OE1	2.33	0.58
29:c:141:VAL:HG22	29:c:161:ARG:HB2	1.84	0.58
30:d:203:PRO:C	30:d:205:LYS:H	2.10	0.58
3:C:235:PHE:HZ	3:C:286:THR:HG21	1.69	0.58
4:D:204:MET:HB3	4:D:212:LYS:HZ2	1.68	0.58
9:I:53:HIS:CD2	9:I:55:LEU:H	2.21	0.58
19:S:159:GLN:NE2	15:o:207:GLY:O	2.37	0.58
21:U:770:TRP:HA	29:c:179:SER:HB3	1.84	0.58
22:V:337:LEU:HD22	22:V:367:VAL:HG11	1.86	0.58
23:W:451:MET:HE2	26:Z:101:LEU:HD23	1.84	0.58
20:t:99:ARG:NH1	20:t:104:ASN:O	2.35	0.58
28:b:133:LYS:HA	34:z:40:GLN:CA	2.34	0.58
12:l:81:ALA:HB2	12:l:130:VAL:HG21	1.86	0.58
5:E:173:TYR:HE1	5:E:298:LYS:HB3	1.69	0.58
5:E:309:ARG:NH1	5:E:335:SER:O	2.37	0.58
7:G:132:ARG:HH12	7:G:135:GLY:H	1.51	0.58
26:Z:10:VAL:HG13	26:Z:163:GLY:HA3	1.86	0.58
26:Z:129:LYS:HE2	29:c:216:MET:HB3	1.86	0.58
28:b:133:LYS:HE2	34:z:36:ILE:HG23	1.85	0.58
13:m:184:MET:HE2	13:m:188:ASP:HB2	1.85	0.58
15:o:138:PHE:O	15:o:142:PHE:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:28:ARG:NH1	19:s:187:VAL:O	2.36	0.58
1:A:253:GLY:HA2	1:A:256:MET:HE3	1.85	0.58
1:A:323:ARG:HB2	2:B:294:ARG:HH21	1.68	0.58
5:E:109:ARG:NH1	5:E:110:TYR:O	2.37	0.58
10:J:66:ASP:OD2	10:J:95:ARG:NH2	2.36	0.58
19:S:27:THR:O	19:S:40:SER:N	2.35	0.58
21:U:9:ILE:O	21:U:44:LYS:NZ	2.37	0.58
34:z:27:LYS:HB3	34:z:38:PRO:CA	2.24	0.58
3:C:351:MET:HG2	3:C:354:ALA:HB2	1.85	0.58
19:S:24:ALA:HB1	19:S:193:LEU:HD11	1.86	0.58
21:U:82:LEU:O	21:U:129:ARG:NH2	2.36	0.58
27:a:140:GLU:O	27:a:143:ASN:ND2	2.36	0.58
1:A:390:THR:HA	2:B:216:ILE:HD13	1.86	0.58
14:N:40:ARG:NH2	14:N:181:GLU:O	2.36	0.58
21:U:583:MET:O	21:U:586:VAL:HG12	2.04	0.58
23:W:316:ARG:NH1	23:W:383:ASP:OD1	2.37	0.58
29:c:32:TYR:HB3	29:c:208:ARG:HD2	1.85	0.58
2:B:411:ARG:NH2	2:B:418:ASP:OD2	2.37	0.57
6:F:58:GLU:OE1	6:F:61:ARG:NH2	2.37	0.57
17:Q:183:ILE:HG12	17:Q:188:ILE:HG12	1.85	0.57
18:R:14:VAL:HB	18:R:177:TYR:HB2	1.86	0.57
22:V:355:ARG:HA	22:V:358:MET:HE3	1.85	0.57
15:o:161:ALA:O	15:o:165:ASN:ND2	2.37	0.57
19:s:57:PHE:HZ	20:t:128:LEU:HB3	1.69	0.57
20:t:180:ASP:HB3	20:t:183:SER:HB3	1.85	0.57
1:A:158:ASP:OD2	1:A:160:THR:OG1	2.20	0.57
7:G:131:MET:HE1	13:M:124:LEU:HD13	1.86	0.57
29:c:134:GLU:OE1	29:c:161:ARG:NH1	2.36	0.57
32:f:807:ARG:HA	32:f:811:LEU:HD12	1.87	0.57
7:g:82:GLY:HA3	7:g:136:CYS:HA	1.86	0.57
13:m:109:LYS:HA	13:m:149:TYR:HE2	1.69	0.57
19:s:27:THR:O	19:s:40:SER:N	2.36	0.57
11:K:221:GLN:HB2	11:K:224:GLN:HG2	1.87	0.57
12:L:41:LYS:HG3	12:L:42:THR:HG23	1.86	0.57
13:M:37:ILE:HD11	13:M:193:VAL:HG13	1.85	0.57
13:M:197:ILE:HG21	13:M:211:LEU:HD13	1.86	0.57
27:a:122:LYS:HD3	27:a:130:VAL:HG13	1.86	0.57
19:s:52:ILE:HD11	19:s:108:ASN:HD21	1.69	0.57
2:B:281:ILE:HG22	2:B:326:LYS:HB2	1.87	0.57
28:b:15:TYR:O	28:b:25:ARG:NH1	2.36	0.57
28:b:163:LYS:HE2	34:z:52:ASP:OD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:211:MET:HB2	10:j:217:LEU:HD12	1.85	0.57
3:C:396:GLU:HG3	3:C:402:LYS:HZ2	1.68	0.57
29:c:161:ARG:NH1	29:c:162:LEU:O	2.37	0.57
13:M:68:ASN:OD1	13:M:224:HIS:ND1	2.38	0.57
18:R:139:MET:O	18:R:143:TYR:HB2	2.05	0.57
21:U:902:PRO:HA	21:U:915:LYS:H	1.68	0.57
23:W:166:LEU:HD22	23:W:192:LEU:HD12	1.85	0.57
25:Y:309:GLU:HA	25:Y:358:ARG:HH22	1.68	0.57
7:G:123:GLN:NE2	8:H:82:ASP:OD1	2.37	0.57
21:U:884:VAL:HA	21:U:888:GLN:HE21	1.68	0.57
28:b:51:LEU:HD23	28:b:71:ILE:HG23	1.87	0.57
11:k:221:GLN:HB2	11:k:224:GLN:HG2	1.85	0.57
19:s:145:LEU:HD22	19:s:178:VAL:HB	1.86	0.57
34:w:43:LEU:HB3	34:w:50:LEU:HD12	1.87	0.57
4:D:161:ASP:HB2	4:D:217:LYS:HD2	1.86	0.57
6:F:343:LEU:O	6:F:344:ARG:C	2.47	0.57
9:I:222:LYS:NZ	9:I:223:THR:OG1	2.38	0.57
27:a:273:GLN:HB3	27:a:310:LEU:HD11	1.87	0.57
30:d:248:GLU:O	30:d:252:GLN:NE2	2.37	0.57
32:f:879:ARG:HH12	32:f:893:ILE:HG23	1.70	0.57
6:F:168:TYR:HB2	6:F:173:LYS:HE2	1.86	0.57
10:j:89:VAL:HG23	17:q:70:ARG:HH22	1.70	0.57
5:E:144:GLU:O	5:E:297:ARG:NH2	2.38	0.57
18:R:179:VAL:HA	18:R:184:TRP:HA	1.87	0.57
27:a:113:LEU:O	27:a:154:ARG:NH1	2.37	0.57
34:z:42:ARG:HA	34:z:42:ARG:HE	1.70	0.57
6:F:288:LEU:HD23	6:F:331:ALA:H	1.70	0.56
9:I:22:GLU:HA	9:I:25:MET:HG3	1.86	0.56
12:L:95:SER:OG	12:L:101:ARG:NH1	2.38	0.56
20:T:110:MET:HB2	20:T:125:VAL:HB	1.86	0.56
22:V:345:ARG:HA	22:V:348:PHE:HD2	1.69	0.56
24:X:407:MET:HE3	29:c:252:ALA:HB1	1.86	0.56
25:Y:231:LEU:HG	25:Y:236:LEU:HD12	1.86	0.56
26:Z:177:ARG:HA	26:Z:180:LYS:HD3	1.86	0.56
28:b:2:VAL:O	28:b:44:ASN:ND2	2.38	0.56
32:f:339:ILE:O	32:f:773:LYS:NZ	2.35	0.56
13:m:42:LYS:NZ	13:m:183:GLU:OE1	2.37	0.56
5:E:8:ALA:HB1	6:F:40:GLU:HG3	1.88	0.56
5:E:60:VAL:HA	5:E:71:VAL:HG12	1.87	0.56
5:E:171:LEU:HB3	5:E:298:LYS:HG2	1.88	0.56
6:F:322:PRO:O	6:F:327:LYS:NZ	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:143:LEU:O	17:Q:147:TYR:HB2	2.04	0.56
21:U:443:LEU:HD22	21:U:461:LEU:HG	1.87	0.56
26:Z:84:LYS:HE3	29:c:76:PRO:HG3	1.87	0.56
27:a:70:ARG:HH21	28:b:17:ARG:HA	1.70	0.56
29:c:270:LEU:O	29:c:274:ASN:ND2	2.38	0.56
30:d:203:PRO:C	30:d:205:LYS:N	2.61	0.56
8:h:119:GLN:NE2	9:i:82:ASP:OD1	2.38	0.56
13:m:73:VAL:HG22	13:m:139:SER:HB3	1.86	0.56
34:z:27:LYS:HZ1	34:z:42:ARG:HA	1.70	0.56
1:A:213:LEU:HA	1:A:319:MET:HB2	1.86	0.56
5:E:260:LEU:HD13	5:E:264:MET:HE3	1.86	0.56
12:L:76:GLY:HA3	12:L:130:VAL:HA	1.86	0.56
13:M:187:ARG:O	13:M:191:LYS:NZ	2.35	0.56
17:Q:44:LEU:HD11	17:Q:102:LEU:HD12	1.87	0.56
20:T:25:ASP:HA	20:T:187:PHE:HA	1.87	0.56
20:T:27:LEU:HD22	20:T:184:TYR:HB2	1.86	0.56
23:W:357:ARG:NH1	23:W:360:GLU:OE2	2.39	0.56
24:X:234:GLU:HA	24:X:237:GLU:HB2	1.88	0.56
28:b:131:LEU:HD22	28:b:136:VAL:HB	1.87	0.56
12:l:65:HIS:O	12:l:89:ARG:NH2	2.35	0.56
18:r:38:ASN:OD1	18:r:41:LEU:N	2.38	0.56
22:V:473:GLN:NE2	26:Z:256:GLN:OE1	2.33	0.56
7:g:113:MET:HA	7:g:116:LYS:HG2	1.87	0.56
14:n:84:LYS:HD3	14:n:120:MET:HB2	1.86	0.56
18:R:9:ARG:NH1	18:R:145:TYR:O	2.39	0.56
5:E:175:PRO:O	5:E:180:LYS:NZ	2.36	0.56
19:S:147:PRO:HG3	16:p:177:ARG:HG2	1.87	0.56
25:Y:250:LEU:HD13	25:Y:257:ARG:HG3	1.86	0.56
26:Z:254:ASN:HA	26:Z:257:MET:HE2	1.88	0.56
28:b:120:ASN:CG	28:b:123:ASP:HB3	2.31	0.56
29:c:27:THR:HG23	29:c:176:GLN:HB2	1.88	0.56
20:t:54:SER:HB2	20:t:109:THR:HB	1.88	0.56
1:A:375:ARG:HH21	11:K:176:GLY:H	1.54	0.56
3:C:344:LEU:HA	3:C:347:ILE:HD12	1.87	0.56
4:D:248:ARG:HG2	4:D:295:GLN:HE22	1.71	0.56
6:F:363:ALA:HA	6:F:366:MET:HE2	1.88	0.56
21:U:194:ARG:NH2	21:U:218:GLN:OE1	2.39	0.56
21:U:409:GLY:HA3	21:U:445:ALA:HB1	1.87	0.56
25:Y:78:GLU:HA	25:Y:81:LEU:HB2	1.88	0.56
26:Z:70:LEU:HD11	26:Z:108:ILE:HG13	1.88	0.56
26:Z:177:ARG:NH2	29:c:153:GLY:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:77:VAL:HG11	13:m:84:ALA:HB1	1.87	0.56
16:P:15:LYS:HE3	16:P:121:ILE:HG12	1.88	0.56
21:U:141:CYS:HA	21:U:144:ASP:HB3	1.87	0.56
23:W:293:ASP:HB2	23:W:296:LEU:HD23	1.86	0.56
19:s:114:ASP:OD1	19:s:118:LYS:N	2.38	0.56
1:A:140:VAL:HA	1:A:152:PRO:HA	1.87	0.56
4:D:100:THR:HA	4:D:114:ARG:HA	1.87	0.56
5:E:219:PHE:HA	5:E:222:ALA:HB3	1.86	0.56
10:J:117:ARG:HD2	10:J:118:TYR:HD1	1.70	0.56
15:O:138:PHE:O	15:O:142:PHE:HB2	2.05	0.56
15:O:214:GLU:HG3	16:P:198:ARG:HG2	1.88	0.56
19:S:43:CYS:N	19:S:194:ARG:HH21	2.01	0.56
21:U:217:CYS:SG	21:U:752:THR:OG1	2.59	0.56
23:W:16:MET:HE3	23:W:17:GLU:H	1.69	0.56
24:X:107:VAL:HG23	24:X:133:LEU:HD11	1.88	0.56
25:Y:210:SER:HB3	25:Y:213:LEU:HD23	1.88	0.56
25:Y:345:CYS:HA	25:Y:356:THR:HA	1.87	0.56
27:a:356:TRP:HZ3	29:c:310:LYS:HG2	1.70	0.56
28:b:180:ALA:HB1	28:b:183:LEU:HB2	1.87	0.56
32:f:727:PHE:HA	32:f:761:MET:HE2	1.86	0.56
12:l:117:GLN:NE2	13:m:83:ASP:OD1	2.39	0.56
1:A:122:VAL:HB	6:F:88:TYR:HB2	1.88	0.56
13:M:8:ASP:O	13:M:22:GLN:NE2	2.39	0.56
22:V:494:MET:SD	26:Z:278:ASN:ND2	2.79	0.56
32:f:569:LYS:NZ	32:f:572:ALA:HB3	2.20	0.56
7:g:155:ASP:OD1	7:g:159:TYR:N	2.38	0.56
20:t:25:ASP:HA	20:t:187:PHE:HA	1.87	0.56
4:D:355:SER:HB3	4:D:393:ILE:HD11	1.88	0.55
27:a:227:ASN:O	27:a:231:GLN:NE2	2.39	0.55
27:a:342:ASP:O	27:a:344:GLN:N	2.39	0.55
5:E:75:ASN:ND2	6:F:129:ARG:O	2.39	0.55
15:O:208:THR:O	19:s:159:GLN:NE2	2.38	0.55
21:U:836:THR:HG22	32:f:607:LEU:HD21	1.86	0.55
23:W:455:LEU:HD21	26:Z:103:LYS:HG2	1.88	0.55
28:b:133:LYS:HD2	34:z:40:GLN:CB	2.37	0.55
32:f:344:VAL:HG23	32:f:391:LEU:HD22	1.88	0.55
14:n:174:ILE:HB	14:n:189:LEU:HB2	1.88	0.55
2:B:125:THR:OG1	2:B:126:SER:N	2.40	0.55
3:C:167:LEU:HD11	3:C:174:LEU:HD12	1.89	0.55
6:F:339:ASP:HB3	6:F:342:LEU:HD13	1.89	0.55
21:U:788:VAL:HG13	21:U:884:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:298:LEU:HB3	32:f:321:MET:HE1	1.86	0.55
32:f:501:LEU:HD22	32:f:518:THR:HG23	1.89	0.55
15:o:100:LEU:HB3	15:o:111:TYR:HB2	1.88	0.55
17:q:143:LEU:O	17:q:147:TYR:HB2	2.07	0.55
1:A:141:GLY:N	1:A:151:ILE:O	2.35	0.55
18:R:21:THR:HA	18:R:27:ALA:H	1.71	0.55
27:a:254:ALA:HA	27:a:261:LEU:HD23	1.88	0.55
28:b:132:LYS:HE2	34:z:42:ARG:HD2	1.88	0.55
29:c:278:GLN:H	29:c:282:ARG:NH2	2.03	0.55
14:N:115:PRO:HD2	14:N:119:MET:HB2	1.88	0.55
30:d:87:GLU:HA	30:d:89:LEU:HD23	1.88	0.55
9:i:68:LEU:H	9:i:73:ALA:HA	1.72	0.55
34:z:24:GLU:HB3	34:z:52:ASP:HB3	1.86	0.55
2:B:150:VAL:HA	2:B:162:VAL:HA	1.87	0.55
21:U:896:GLU:O	21:U:901:GLN:NE2	2.39	0.55
22:V:296:LYS:HB3	22:V:301:GLU:HB3	1.87	0.55
32:f:459:CYS:HB3	34:w:66:THR:HG21	1.88	0.55
32:f:463:LEU:HB3	34:w:6:LYS:HZ1	1.72	0.55
8:H:107:THR:HB	8:H:145:TYR:HD2	1.72	0.55
25:Y:172:GLY:HA2	25:Y:177:ARG:HH22	1.72	0.55
32:f:654:VAL:HA	32:f:657:ILE:HD12	1.87	0.55
11:k:41:GLN:NE2	11:k:151:PRO:O	2.40	0.55
34:x:27:LYS:HB3	34:x:38:PRO:HB3	1.88	0.55
8:H:65:VAL:O	8:H:220:ARG:NH1	2.38	0.55
12:L:14:SER:HB2	12:L:18:ARG:H	1.70	0.55
21:U:58:GLN:NE2	21:U:83:GLY:O	2.40	0.55
24:X:365:LEU:HA	24:X:368:MET:HG3	1.89	0.55
26:Z:196:HIS:HA	26:Z:199:LYS:HB2	1.89	0.55
20:t:141:TYR:HA	20:t:144:TYR:HD2	1.70	0.55
4:D:160:PRO:HB3	4:D:221:HIS:CD2	2.41	0.55
17:Q:83:PHE:O	17:Q:87:ASN:ND2	2.40	0.55
22:V:448:GLU:HB2	22:V:461:LYS:HE3	1.88	0.55
32:f:151:LEU:HB3	32:f:159:VAL:HG22	1.88	0.55
18:r:154:ASP:OD1	18:r:157:ARG:NH2	2.40	0.55
19:s:176:LYS:HE2	19:s:208:VAL:HG21	1.89	0.55
21:U:619:VAL:HG21	21:U:648:VAL:HA	1.89	0.55
22:V:323:GLY:HA3	31:e:24:ALA:HA	1.89	0.55
29:c:64:ASP:O	29:c:139:ARG:NH2	2.39	0.55
17:q:19:ARG:HH21	17:q:31:ASP:HB2	1.71	0.55
2:B:334:ILE:HA	2:B:337:LEU:HD23	1.88	0.54
12:L:34:ALA:HA	12:L:162:GLY:HA3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:1:THR:N	15:O:168:GLY:O	2.40	0.54
18:R:35:ILE:N	18:R:43:GLY:O	2.39	0.54
28:b:163:LYS:HD3	34:z:39:ASP:HA	1.89	0.54
30:d:234:ASP:OD2	30:d:236:THR:OG1	2.25	0.54
8:h:119:GLN:HG3	9:i:81:SER:HB2	1.89	0.54
10:j:143:ARG:NH2	10:j:145:TYR:OH	2.39	0.54
34:w:7:THR:HG22	34:w:69:LEU:HD23	1.89	0.54
2:B:429:LYS:HB3	3:C:314:LYS:HE3	1.89	0.54
4:D:391:ARG:NH1	4:D:393:ILE:O	2.41	0.54
6:F:49:ASP:O	28:b:27:GLN:NE2	2.40	0.54
9:I:118:LYS:NZ	9:I:132:VAL:O	2.40	0.54
12:L:192:LEU:HB3	12:L:236:LEU:HD22	1.89	0.54
20:T:188:GLN:HG2	20:T:201:GLY:HA3	1.89	0.54
24:X:414:LEU:HG	24:X:417:LYS:HE2	1.90	0.54
14:n:119:MET:HE3	20:t:58:ALA:HB2	1.89	0.54
17:q:7:ILE:O	17:q:14:LEU:N	2.32	0.54
1:A:23:ARG:HD2	1:A:25:LEU:H	1.71	0.54
2:B:107:MET:HB2	3:C:96:VAL:HB	1.90	0.54
5:E:247:THR:HG22	5:E:248:SER:H	1.71	0.54
6:F:184:GLN:HA	6:F:243:GLN:HE21	1.72	0.54
9:I:155:ASN:OD1	10:J:77:THR:OG1	2.26	0.54
10:J:209:ALA:HB1	10:J:217:LEU:HD11	1.89	0.54
13:M:40:ARG:HB2	13:M:148:LEU:HB2	1.90	0.54
13:M:97:ASN:OD1	13:M:101:ASN:ND2	2.40	0.54
27:a:168:ASN:OD1	27:a:171:SER:OG	2.24	0.54
32:f:607:LEU:HA	32:f:610:GLN:HG2	1.90	0.54
18:r:35:ILE:N	18:r:43:GLY:O	2.39	0.54
1:A:52:ILE:HD13	2:B:69:LYS:HA	1.89	0.54
2:B:90:GLU:OE1	2:B:93:GLU:N	2.40	0.54
8:H:77:SER:HB3	8:H:163:MET:HE2	1.88	0.54
19:S:79:ASN:HB3	19:S:81:LYS:HG2	1.90	0.54
23:W:313:GLU:HA	27:a:312:MET:HE1	1.88	0.54
20:t:211:ILE:HA	20:t:214:MET:HE3	1.89	0.54
1:A:177:VAL:HG22	1:A:224:LEU:HD13	1.89	0.54
16:P:143:ALA:HA	16:P:146:MET:HE2	1.88	0.54
26:Z:212:LEU:HA	26:Z:215:VAL:HG12	1.89	0.54
27:a:35:HIS:NE2	28:b:14:GLU:O	2.39	0.54
32:f:267:ARG:HG3	32:f:787:LEU:HD11	1.90	0.54
10:j:172:LEU:O	10:j:176:TYR:HB2	2.07	0.54
34:z:72:ARG:HH21	34:z:73:LEU:HA	1.73	0.54
1:A:347:ASP:O	1:A:351:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:195:GLY:N	35:C:501:ATP:O2A	2.39	0.54
6:F:206:MET:O	6:F:209:LYS:NZ	2.41	0.54
13:M:65:ARG:HH21	13:M:78:ALA:HA	1.72	0.54
32:f:568:GLY:N	32:f:598:CYS:O	2.35	0.54
7:g:141:ILE:HG22	7:g:151:VAL:HG22	1.90	0.54
7:g:180:GLU:HA	7:g:183:VAL:HG12	1.88	0.54
15:o:1:THR:O	15:o:129:SER:N	2.40	0.54
34:z:72:ARG:NH2	34:z:73:LEU:HA	2.23	0.54
27:a:77:VAL:HA	27:a:80:ILE:HG22	1.89	0.54
10:j:137:ASP:OD2	10:j:143:ARG:NH1	2.40	0.54
18:r:39:PRO:HA	18:r:184:TRP:HE1	1.72	0.54
3:C:337:ASN:HD21	25:Y:174:TRP:CG	2.26	0.54
6:F:225:MET:HB3	6:F:331:ALA:HA	1.90	0.54
19:S:192:ALA:HA	19:S:209:SER:HA	1.89	0.54
20:T:9:THR:O	20:T:41:ARG:NH1	2.41	0.54
24:X:35:ILE:HD12	24:X:46:LYS:HD2	1.90	0.54
9:I:36:GLY:HA2	9:I:45:LEU:HA	1.90	0.54
16:P:35:VAL:HG12	16:P:36:THR:HG23	1.89	0.54
19:s:125:ASP:OD1	19:s:129:SER:N	2.41	0.54
4:D:227:PHE:HA	4:D:261:ILE:HB	1.90	0.54
7:G:38:THR:O	7:G:52:THR:OG1	2.26	0.54
7:G:240:VAL:HA	23:W:94:ARG:HH12	1.71	0.54
21:U:266:GLN:O	21:U:270:THR:OG1	2.25	0.54
23:W:361:HIS:HA	23:W:364:ARG:HH21	1.73	0.54
27:a:34:TRP:HB3	27:a:71:VAL:HG22	1.90	0.54
16:p:62:THR:OG1	17:q:85:ARG:NH2	2.41	0.54
19:s:211:ARG:NH2	19:s:213:ASP:OD2	2.41	0.54
34:x:26:VAL:HG21	34:x:56:LEU:HD21	1.90	0.54
2:B:121:ALA:N	2:B:133:VAL:O	2.41	0.53
3:C:75:GLU:HA	3:C:113:ARG:HA	1.90	0.53
3:C:114:VAL:HG12	3:C:126:ILE:HA	1.90	0.53
3:C:325:ARG:HD3	3:C:354:ALA:H	1.73	0.53
8:H:204:THR:OG1	8:H:206:ASP:OD1	2.25	0.53
12:L:61:LYS:NZ	12:L:63:ILE:O	2.37	0.53
14:N:9:ASP:OD1	14:N:9:ASP:N	2.41	0.53
15:O:164:PHE:O	19:s:38:ARG:NH2	2.41	0.53
20:T:179:ARG:NH1	14:n:26:ILE:O	2.40	0.53
26:Z:235:ASN:ND2	27:a:349:MET:SD	2.81	0.53
8:h:11:THR:HB	8:h:19:LEU:HD22	1.90	0.53
14:n:109:GLY:O	14:n:122:ARG:NH2	2.41	0.53
7:G:10:ASP:O	7:G:24:GLN:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:154:HIS:HB3	11:K:59:MET:HE1	1.89	0.53
18:R:75:SER:HB2	18:R:107:ARG:HH22	1.73	0.53
22:V:321:ALA:HB1	22:V:324:PHE:HB3	1.90	0.53
15:o:22:GLU:HG2	15:o:27:ALA:HB2	1.90	0.53
8:H:71:HIS:HA	8:H:218:PHE:H	1.74	0.53
22:V:287:ARG:HH21	31:e:19:PHE:HA	1.74	0.53
25:Y:69:LEU:O	25:Y:73:MET:N	2.41	0.53
25:Y:217:LYS:HG2	25:Y:253:LEU:HD11	1.90	0.53
26:Z:133:LEU:H	26:Z:133:LEU:HD23	1.72	0.53
28:b:181:ASP:HA	28:b:184:ILE:HG12	1.90	0.53
30:d:167:ILE:HA	30:d:170:LEU:HB3	1.90	0.53
9:i:73:ALA:HB3	9:i:137:ILE:HD11	1.90	0.53
20:t:15:LYS:HG2	20:t:20:VAL:HG22	1.90	0.53
20:t:45:VAL:H	20:t:50:MET:HA	1.74	0.53
34:x:36:ILE:O	34:x:41:GLN:NE2	2.42	0.53
2:B:411:ARG:NH1	2:B:413:LYS:O	2.40	0.53
6:F:401:VAL:HG12	6:F:405:MET:HE1	1.91	0.53
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.91	0.53
21:U:743:ASN:HA	21:U:883:ARG:HD2	1.90	0.53
24:X:370:LEU:O	24:X:372:LYS:NZ	2.41	0.53
28:b:24:THR:HG22	28:b:26:LEU:H	1.74	0.53
18:r:179:VAL:HA	18:r:184:TRP:HA	1.90	0.53
1:A:386:ARG:NH1	35:A:501:ATP:O2'	2.42	0.53
8:H:74:LEU:HD12	8:H:134:LEU:HD12	1.90	0.53
8:H:222:THR:OG1	8:H:225:GLU:OE1	2.26	0.53
10:J:36:ARG:HA	10:J:41:VAL:HG12	1.91	0.53
21:U:251:ASP:O	21:U:255:SER:CB	2.56	0.53
26:Z:106:ILE:HG23	26:Z:153:LYS:HD2	1.90	0.53
18:r:115:ASP:OD1	18:r:119:ASN:N	2.41	0.53
7:G:155:ASP:OD1	7:G:159:TYR:N	2.42	0.53
15:O:21:THR:HG22	15:O:26:VAL:HA	1.91	0.53
21:U:219:CYS:O	21:U:223:LEU:N	2.42	0.53
27:a:343:LEU:O	27:a:345:GLN:N	2.41	0.53
10:j:71:MET:HE1	10:j:73:PHE:HB3	1.91	0.53
12:l:100:ASP:OD1	19:s:66:LYS:NZ	2.42	0.53
9:I:49:ARG:NH1	9:I:209:GLU:O	2.41	0.53
17:Q:5:ILE:HD11	17:Q:143:LEU:HD11	1.91	0.53
20:T:89:HIS:HE1	20:T:131:ALA:HB1	1.73	0.53
23:W:235:GLN:HG2	23:W:350:ARG:HH22	1.73	0.53
23:W:248:ARG:HH22	23:W:289:ARG:HG2	1.74	0.53
25:Y:231:LEU:HD21	25:Y:239:LYS:HZ1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:276:GLY:H	29:c:278:GLN:HE21	1.55	0.53
12:l:33:SER:OG	12:l:62:LYS:NZ	2.41	0.53
12:l:66:VAL:HG11	12:l:88:MET:HG3	1.90	0.53
1:A:218:PRO:HB2	2:B:343:ARG:HD3	1.90	0.53
6:F:358:ASN:O	6:F:362:ARG:NH1	2.42	0.53
9:I:53:HIS:CD2	9:I:55:LEU:HB2	2.44	0.53
12:L:103:LEU:HD23	12:L:108:LEU:HD12	1.90	0.53
22:V:218:TYR:HA	22:V:221:LEU:HB2	1.91	0.53
25:Y:239:LYS:HG3	25:Y:240:VAL:HG13	1.90	0.53
7:g:128:ASN:ND2	7:g:130:GLU:OE2	2.41	0.53
8:H:177:ARG:HD2	8:H:190:THR:HG23	1.91	0.53
9:I:119:GLN:HA	9:I:122:THR:HG22	1.90	0.53
16:P:173:ASN:HD21	19:s:157:ASN:HB2	1.74	0.53
17:Q:8:GLN:HA	17:Q:13:VAL:HA	1.90	0.53
1:A:375:ARG:HH22	11:K:175:GLU:HB2	1.74	0.53
3:C:70:GLY:O	3:C:118:ASN:ND2	2.42	0.53
16:P:54:ALA:O	16:P:106:GLU:N	2.39	0.53
19:S:55:SER:O	19:S:107:TYR:N	2.41	0.53
24:X:53:LEU:HD22	24:X:69:LEU:HD22	1.91	0.53
24:X:351:SER:HA	24:X:354:ILE:HG22	1.91	0.53
16:p:83:LYS:HD3	16:p:85:TYR:H	1.74	0.53
4:D:105:SER:OG	4:D:108:GLY:O	2.24	0.52
11:K:16:SER:OG	11:K:18:GLU:OE1	2.27	0.52
22:V:495:ARG:HD3	26:Z:278:ASN:HD21	1.74	0.52
26:Z:145:HIS:HB2	26:Z:151:THR:HA	1.91	0.52
29:c:167:MET:O	29:c:172:HIS:NE2	2.42	0.52
13:m:66:LEU:HD23	13:m:76:ALA:HB2	1.90	0.52
16:p:2:SER:N	16:p:5:SER:OG	2.42	0.52
34:w:18:GLU:HG3	34:w:20:SER:H	1.73	0.52
4:D:60:TYR:HB2	21:U:603:LEU:HD11	1.90	0.52
4:D:205:TYR:HD2	4:D:313:ARG:HH21	1.56	0.52
12:L:33:SER:OG	12:L:51:ARG:NE	2.40	0.52
13:M:38:GLY:HA3	13:M:136:MET:HE2	1.90	0.52
9:i:151:ASP:OD1	9:i:155:ASN:N	2.38	0.52
10:j:146:GLN:NE2	10:j:147:THR:O	2.42	0.52
19:s:12:ILE:O	19:s:138:GLY:N	2.39	0.52
2:B:227:PRO:O	2:B:230:THR:OG1	2.26	0.52
13:M:34:SER:OG	13:M:65:ARG:NH1	2.38	0.52
18:R:59:LEU:HD22	18:R:83:LEU:HB2	1.90	0.52
19:S:45:LYS:HA	19:S:51:VAL:HG22	1.90	0.52
21:U:529:ILE:HD13	21:U:555:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:287:ARG:NH2	31:e:17:ASP:OD2	2.42	0.52
22:V:397:ARG:HH21	30:d:116:HIS:HB3	1.75	0.52
9:i:153:SER:OG	9:i:155:ASN:ND2	2.42	0.52
11:k:157:ASP:OD2	11:k:159:SER:OG	2.27	0.52
34:w:5:VAL:HG22	34:w:67:LEU:HB2	1.91	0.52
1:A:71:GLY:HA2	2:B:162:VAL:HG12	1.92	0.52
3:C:89:VAL:HB	3:C:90:HIS:CE1	2.44	0.52
11:K:9:ASP:O	11:K:23:GLN:NE2	2.37	0.52
13:M:67:PHE:O	13:M:75:MET:N	2.41	0.52
27:a:69:HIS:O	27:a:70:ARG:HD2	2.09	0.52
10:j:88:ARG:HH11	17:q:70:ARG:HD3	1.74	0.52
34:z:73:LEU:O	34:z:74:ARG:HB2	2.09	0.52
2:B:227:PRO:O	2:B:232:LYS:NZ	2.41	0.52
6:F:92:ASN:N	6:F:125:LYS:O	2.42	0.52
7:G:32:ILE:HG12	7:G:136:CYS:HA	1.90	0.52
12:L:225:ASP:H	12:L:228:ASP:HB2	1.74	0.52
18:R:117:GLU:OE2	18:R:119:ASN:ND2	2.42	0.52
19:S:201:GLU:OE1	19:S:204:ARG:NH1	2.42	0.52
22:V:135:LEU:HD21	22:V:171:VAL:HG13	1.92	0.52
22:V:349:ARG:HH12	31:e:37:HIS:HE1	1.57	0.52
23:W:89:LEU:HA	23:W:92:LYS:HE3	1.91	0.52
25:Y:142:PHE:HE2	25:Y:176:ARG:HD2	1.75	0.52
30:d:18:LYS:HB3	30:d:61:TRP:HH2	1.74	0.52
8:h:143:ARG:NH1	8:h:145:TYR:OH	2.43	0.52
11:k:109:VAL:HG21	11:k:145:GLY:HA3	1.91	0.52
3:C:45:LEU:HB3	4:D:61:ILE:HG21	1.91	0.52
22:V:345:ARG:NH2	31:e:45:ASP:OD1	2.42	0.52
29:c:98:MET:HA	29:c:101:GLN:HG2	1.91	0.52
3:C:185:GLY:HA3	3:C:311:ILE:HA	1.90	0.52
3:C:406:LYS:O	9:I:78:GLY:N	2.41	0.52
7:G:10:ASP:HB3	7:G:23:TYR:HB2	1.92	0.52
18:R:9:ARG:HH22	18:R:146:ASP:HA	1.74	0.52
25:Y:121:LEU:HB3	25:Y:125:ARG:HH12	1.75	0.52
27:a:214:GLY:HA2	27:a:217:LEU:HD13	1.90	0.52
7:g:112:ASP:OD1	7:g:112:ASP:N	2.42	0.52
1:A:328:ASP:HB3	1:A:331:LEU:HD23	1.92	0.52
2:B:67:ARG:NH2	2:B:71:TYR:OH	2.36	0.52
12:L:7:ASP:OD1	12:L:21:GLN:NE2	2.43	0.52
18:R:191:ASN:HD21	16:p:203:ARG:HH12	1.56	0.52
23:W:219:THR:HG22	23:W:222:LEU:HD12	1.92	0.52
25:Y:51:ALA:HB2	25:Y:73:MET:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:134:LEU:HD21	25:Y:171:GLY:HA2	1.92	0.52
28:b:52:ILE:HD11	28:b:58:CYS:HB3	1.91	0.52
8:h:86:LEU:HD13	8:h:134:LEU:HD11	1.91	0.52
11:K:13:ASN:ND2	12:L:124:GLY:O	2.43	0.52
1:A:161:VAL:HG22	1:A:260:LEU:HD23	1.92	0.52
23:W:129:ARG:NH1	23:W:146:THR:OG1	2.43	0.52
30:d:139:LEU:HD21	30:d:170:LEU:HD21	1.92	0.52
32:f:188:VAL:HG21	32:f:211:ILE:HD12	1.91	0.52
32:f:574:GLU:HA	32:f:577:LEU:HB3	1.91	0.52
17:q:83:PHE:O	17:q:87:ASN:ND2	2.43	0.52
22:V:469:THR:O	22:V:470:ARG:NE	2.41	0.51
32:f:677:HIS:HA	32:f:680:ARG:HE	1.75	0.51
32:f:849:ALA:HB2	32:f:879:ARG:HB2	1.92	0.51
13:m:229:LYS:NZ	13:m:233:GLU:OE2	2.41	0.51
14:n:104:ASP:OD1	14:n:108:GLY:N	2.38	0.51
14:N:19:ARG:NH1	14:N:168:GLY:O	2.44	0.51
18:R:115:ASP:OD1	18:R:119:ASN:N	2.41	0.51
32:f:240:VAL:O	32:f:245:ASN:ND2	2.36	0.51
32:f:589:SER:HB3	32:f:649:HIS:CG	2.45	0.51
10:j:45:VAL:HG21	10:j:61:LYS:HD2	1.92	0.51
20:t:171:ARG:HG2	20:t:174:ARG:HH12	1.75	0.51
4:D:51:LEU:HA	4:D:54:LEU:HD23	1.93	0.51
5:E:83:CYS:HB2	5:E:89:LYS:HE2	1.92	0.51
5:E:289:LEU:HG	5:E:295:LEU:HG	1.92	0.51
25:Y:42:MET:HA	25:Y:45:VAL:HB	1.91	0.51
11:k:52:LYS:HE3	11:k:54:ILE:HD11	1.92	0.51
15:o:1:THR:N	15:o:168:GLY:O	2.41	0.51
4:D:230:VAL:O	4:D:265:ASP:N	2.39	0.51
6:F:236:LEU:HD13	6:F:354:PHE:HZ	1.76	0.51
12:L:22:ILE:HG13	12:L:26:MET:HE3	1.92	0.51
21:U:140:ARG:O	21:U:144:ASP:CB	2.58	0.51
23:W:304:ASP:O	23:W:308:LEU:N	2.43	0.51
26:Z:287:LYS:HG3	26:Z:288:LYS:HD3	1.93	0.51
8:h:45:VAL:HG23	8:h:212:ILE:HG22	1.91	0.51
11:k:206:MET:HG3	11:k:208:GLU:H	1.74	0.51
14:n:40:ARG:NH1	14:n:180:ALA:O	2.43	0.51
1:A:384:GLU:HB3	2:B:344:PRO:HG3	1.92	0.51
8:H:100:VAL:HG12	16:P:90:MET:HE1	1.92	0.51
8:H:120:GLU:OE1	8:H:123:GLN:NE2	2.40	0.51
15:O:138:PHE:O	15:O:142:PHE:CB	2.59	0.51
16:P:67:LEU:HD22	16:P:94:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:159:LEU:HA	17:Q:162:LYS:HE2	1.93	0.51
20:T:96:MET:HE1	20:T:106:LEU:HD12	1.92	0.51
21:U:251:ASP:O	21:U:255:SER:HB2	2.10	0.51
21:U:666:LYS:H	21:U:669:ILE:HD12	1.75	0.51
22:V:350:GLN:HB2	22:V:353:LEU:HB3	1.92	0.51
23:W:384:LEU:HD12	23:W:388:GLU:HG3	1.92	0.51
32:f:547:GLU:HA	32:f:550:LEU:HB2	1.92	0.51
32:f:559:PRO:HB2	32:f:594:LEU:HD23	1.91	0.51
7:g:119:ALA:HB3	8:h:84:ARG:HH12	1.76	0.51
10:j:88:ARG:HG2	17:q:69:MET:HE1	1.91	0.51
12:l:69:HIS:CE1	12:l:102:PRO:HB3	2.46	0.51
5:E:236:ASP:HB2	5:E:282:PRO:HD3	1.92	0.51
21:U:772:TRP:HB3	21:U:775:LEU:HG	1.91	0.51
32:f:704:LEU:HD23	32:f:707:LEU:HD21	1.93	0.51
20:t:126:ASP:OD1	20:t:130:VAL:N	2.44	0.51
2:B:337:LEU:HD12	2:B:341:LEU:HD11	1.91	0.51
4:D:194:ILE:HD12	4:D:196:ILE:HD11	1.91	0.51
9:I:47:ALA:HB3	9:I:212:GLU:HB2	1.93	0.51
15:O:19:ARG:NH1	15:O:167:LEU:O	2.42	0.51
28:b:163:LYS:HE2	34:z:52:ASP:CG	2.36	0.51
9:i:91:ARG:NH1	16:p:76:LEU:O	2.43	0.51
10:j:70:CYS:SG	10:j:71:MET:N	2.84	0.51
34:z:27:LYS:HE3	34:z:42:ARG:NH2	2.25	0.51
10:J:92:GLN:HG3	17:Q:62:LYS:HB3	1.93	0.51
21:U:613:ASP:OD1	21:U:616:ARG:NH2	2.39	0.51
28:b:133:LYS:O	34:z:40:GLN:HB3	2.11	0.51
30:d:8:GLU:O	30:d:13:SER:OG	2.28	0.51
11:k:129:ASP:N	11:k:129:ASP:OD1	2.44	0.51
1:A:398:ARG:NH1	2:B:195:GLN:OE1	2.44	0.51
7:G:31:ALA:HA	7:G:34:GLN:HG2	1.93	0.51
7:G:180:GLU:HA	7:G:183:VAL:HG12	1.93	0.51
10:J:80:ALA:HB2	10:J:129:ILE:HG21	1.93	0.51
12:L:134:ILE:HB	12:L:145:PHE:HB2	1.92	0.51
21:U:107:HIS:HA	21:U:110:LYS:HE3	1.93	0.51
23:W:112:VAL:HG22	23:W:124:LEU:HD13	1.93	0.51
23:W:227:TYR:HA	23:W:230:MET:HE3	1.92	0.51
25:Y:364:TRP:NE1	25:Y:368:GLU:OE2	2.44	0.51
29:c:100:LYS:HG2	29:c:105:PRO:HB3	1.92	0.51
11:k:121:LEU:HD11	12:l:126:ARG:HH21	1.76	0.51
17:q:143:LEU:O	17:q:147:TYR:CB	2.59	0.51
20:t:166:ARG:HH22	20:t:200:GLU:HG2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:205:VAL:HG13	7:G:206:LEU:HD12	1.93	0.51
8:H:100:VAL:O	16:P:89:SER:OG	2.29	0.51
12:L:39:LYS:HD2	12:L:142:PRO:HB2	1.91	0.51
14:N:104:ASP:OD1	14:N:108:GLY:N	2.42	0.51
16:P:83:LYS:NZ	16:P:113:ASP:OD1	2.44	0.51
22:V:419:LEU:HD12	22:V:456:GLY:HA2	1.92	0.51
23:W:446:ILE:HD13	26:Z:208:ILE:HG13	1.93	0.51
26:Z:81:MET:HE1	29:c:98:MET:HE1	1.92	0.51
26:Z:198:LEU:HA	26:Z:201:LEU:HD12	1.93	0.51
27:a:138:VAL:O	27:a:142:LEU:HB2	2.11	0.51
29:c:29:GLU:O	29:c:204:THR:OG1	2.28	0.51
12:l:72:ILE:HG22	12:l:134:ILE:HG12	1.91	0.51
12:l:155:ASP:HB3	13:m:62:SER:HB3	1.92	0.51
2:B:231:GLY:HA2	2:B:234:LEU:HD12	1.92	0.50
10:J:65:LEU:HD13	10:J:88:ARG:HG3	1.93	0.50
12:L:50:LYS:HE3	12:L:59:HIS:HB2	1.91	0.50
21:U:764:LEU:O	21:U:767:THR:OG1	2.30	0.50
10:j:229:VAL:O	10:j:233:GLU:HG2	2.11	0.50
1:A:308:GLY:O	6:F:238:ARG:NH2	2.45	0.50
2:B:219:PRO:O	2:B:326:LYS:NZ	2.43	0.50
3:C:368:MET:HA	3:C:371:LEU:HB3	1.92	0.50
12:L:13:TRP:HE1	13:M:129:ARG:HB2	1.76	0.50
16:P:34:MET:O	18:r:166:ARG:NH1	2.44	0.50
21:U:27:LEU:HD11	21:U:38:ILE:HG21	1.93	0.50
22:V:351:PRO:O	22:V:355:ARG:NH1	2.44	0.50
16:p:27:ARG:NH1	16:p:180:VAL:O	2.44	0.50
20:t:97:TYR:HA	20:t:100:ARG:HG2	1.93	0.50
11:K:93:ARG:O	11:K:96:THR:OG1	2.28	0.50
22:V:268:GLU:HA	22:V:271:VAL:HG22	1.92	0.50
27:a:290:GLN:O	27:a:330:ARG:NH2	2.44	0.50
28:b:95:LEU:O	28:b:99:HIS:ND1	2.40	0.50
12:l:126:ARG:NH1	12:l:127:PRO:O	2.45	0.50
12:l:189:LYS:NZ	12:l:234:GLU:O	2.37	0.50
1:A:89:SER:HA	1:A:93:LEU:HD23	1.92	0.50
3:C:191:PRO:O	3:C:196:LYS:NZ	2.34	0.50
4:D:335:LEU:HD22	4:D:371:SER:HA	1.94	0.50
13:M:145:GLY:O	13:M:147:GLN:NE2	2.45	0.50
17:Q:169:LYS:HD2	18:r:140:ASP:HB3	1.93	0.50
18:R:1:THR:O	18:R:130:SER:N	2.44	0.50
18:R:115:ASP:OD2	18:R:119:ASN:ND2	2.41	0.50
19:S:28:ARG:NH1	19:S:187:VAL:O	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:117:GLY:O	19:S:200:LYS:NZ	2.44	0.50
25:Y:247:LEU:HD12	25:Y:250:LEU:HD11	1.94	0.50
27:a:54:ASP:N	27:a:54:ASP:OD1	2.44	0.50
30:d:72:GLU:HA	30:d:75:MET:HG3	1.92	0.50
32:f:755:ASP:OD2	32:f:758:ASN:ND2	2.39	0.50
13:m:67:PHE:O	13:m:75:MET:N	2.37	0.50
2:B:343:ARG:HE	2:B:346:ARG:HE	1.60	0.50
2:B:365:PHE:O	2:B:369:THR:OG1	2.24	0.50
20:T:189:ILE:HG23	20:T:200:GLU:HB3	1.94	0.50
1:A:52:ILE:HG12	2:B:68:ILE:HG22	1.92	0.50
1:A:221:GLY:N	35:A:501:ATP:O2B	2.43	0.50
6:F:184:GLN:OE1	6:F:243:GLN:NE2	2.44	0.50
6:F:247:THR:HB	6:F:281:SER:HA	1.92	0.50
21:U:196:LYS:HA	21:U:199:ARG:HG2	1.92	0.50
21:U:245:ALA:HA	21:U:248:ILE:HG12	1.94	0.50
29:c:92:GLN:HE21	29:c:96:LEU:HG	1.77	0.50
30:d:109:GLN:OE1	30:d:111:ARG:NH1	2.36	0.50
32:f:367:SER:HA	32:f:370:MET:HE2	1.94	0.50
11:k:79:SER:N	11:k:140:ALA:O	2.41	0.50
15:o:46:ALA:HB3	15:o:97:ALA:HB3	1.92	0.50
15:o:163:ILE:HG12	15:o:170:GLY:HA2	1.93	0.50
16:p:2:SER:OG	16:p:3:ILE:N	2.44	0.50
34:w:39:ASP:N	34:w:39:ASP:OD1	2.43	0.50
3:C:406:LYS:HZ3	9:I:64:LYS:HA	1.77	0.50
12:L:125:ARG:HE	12:L:128:TYR:HE1	1.60	0.50
17:Q:47:VAL:HG23	17:Q:101:ASN:HB2	1.94	0.50
20:T:91:TRP:HE3	20:T:92:LEU:HD22	1.76	0.50
29:c:111:TRP:NE1	29:c:130:GLN:OE1	2.38	0.50
30:d:183:GLU:OE2	30:d:215:TRP:NE1	2.45	0.50
2:B:383:LEU:HD22	2:B:423:LYS:HD2	1.92	0.50
6:F:97:LEU:O	6:F:120:LYS:N	2.45	0.50
32:f:527:VAL:HG21	32:f:794:ALA:HB2	1.93	0.50
7:g:60:LEU:HD21	13:m:177:GLU:HG3	1.94	0.50
10:j:38:ARG:O	10:j:213:ARG:NH2	2.44	0.50
34:z:23:ILE:HG21	34:z:50:LEU:O	2.11	0.50
34:z:26:VAL:HG21	34:z:56:LEU:HD21	1.94	0.50
23:W:174:TYR:HB2	23:W:182:ARG:HH21	1.77	0.50
26:Z:96:HIS:ND1	26:Z:97:THR:O	2.43	0.50
30:d:9:TRP:HB2	30:d:57:ILE:HD11	1.94	0.50
8:h:74:LEU:HD21	8:h:87:VAL:HG22	1.93	0.50
10:j:64:ALA:HA	10:j:70:CYS:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:ARG:HA	2:B:283:PHE:HB3	1.94	0.49
3:C:320:PRO:O	3:C:325:ARG:NH1	2.45	0.49
5:E:56:ILE:N	5:E:100:LEU:O	2.40	0.49
8:H:100:VAL:HG13	16:P:93:ASN:HD22	1.77	0.49
14:N:20:THR:HB	14:N:28:ASN:HB3	1.94	0.49
22:V:311:ASN:OD1	22:V:314:ARG:NH2	2.45	0.49
24:X:122:ARG:HD2	24:X:125:LEU:HB2	1.93	0.49
26:Z:193:ASN:HA	26:Z:196:HIS:CE1	2.46	0.49
27:a:84:VAL:HA	27:a:87:MET:HG2	1.93	0.49
27:a:247:ARG:HA	27:a:250:THR:HG22	1.94	0.49
28:b:35:ILE:HD11	28:b:180:ALA:HB3	1.93	0.49
30:d:86:LYS:NZ	30:d:88:GLN:OE1	2.45	0.49
19:s:66:LYS:HE2	20:t:94:ARG:HD2	1.93	0.49
3:C:69:GLN:NE2	4:D:135:HIS:O	2.45	0.49
6:F:424:ILE:HG22	6:F:428:GLN:HE22	1.77	0.49
19:S:213:ASP:OD1	19:S:213:ASP:N	2.45	0.49
24:X:414:LEU:HD23	26:Z:276:ILE:HD13	1.94	0.49
7:g:211:LYS:HE3	7:g:212:PRO:HD2	1.93	0.49
9:i:216:LEU:HD12	9:i:225:ILE:HG12	1.94	0.49
12:l:51:ARG:O	12:l:59:HIS:ND1	2.44	0.49
34:w:44:ILE:HB	34:w:68:HIS:HB2	1.94	0.49
1:A:35:THR:O	1:A:39:SER:OG	2.30	0.49
2:B:174:MET:HE2	2:B:250:VAL:HA	1.94	0.49
4:D:315:ASP:OD1	4:D:315:ASP:N	2.44	0.49
4:D:380:GLN:HG2	5:E:164:ILE:HD11	1.94	0.49
4:D:381:GLU:HA	4:D:384:MET:HG3	1.93	0.49
6:F:410:ARG:NH1	6:F:419:ASP:OD1	2.42	0.49
13:M:34:SER:HG	13:M:65:ARG:HH12	1.59	0.49
20:T:50:MET:HB3	20:T:197:VAL:HG11	1.94	0.49
32:f:208:LEU:HA	32:f:211:ILE:HG22	1.94	0.49
10:J:41:VAL:HG23	10:J:211:MET:HB2	1.95	0.49
10:J:212:ARG:HB2	10:J:215:GLN:HB2	1.94	0.49
13:M:8:ASP:N	13:M:8:ASP:OD1	2.45	0.49
19:S:26:ASP:HB3	19:S:189:THR:HG23	1.94	0.49
24:X:421:LEU:HD11	26:Z:280:ILE:HG12	1.94	0.49
26:Z:77:ASN:O	26:Z:81:MET:HG2	2.13	0.49
27:a:113:LEU:HB2	27:a:154:ARG:HD3	1.94	0.49
28:b:125:VAL:HG12	28:b:129:LYS:HZ3	1.77	0.49
10:j:39:ASP:OD1	10:j:39:ASP:N	2.45	0.49
6:F:366:MET:HE1	6:F:384:LEU:HB2	1.94	0.49
7:G:54:LYS:N	7:G:214:GLU:O	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:166:ARG:HD3	16:p:34:MET:HB2	1.93	0.49
19:S:150:ASP:OD2	16:p:177:ARG:NH2	2.44	0.49
22:V:357:LEU:O	22:V:361:PHE:N	2.38	0.49
24:X:143:TYR:HD2	24:X:144:GLN:HG2	1.78	0.49
27:a:186:LYS:O	27:a:193:GLN:NE2	2.45	0.49
34:z:27:LYS:CE	34:z:42:ARG:HH21	2.24	0.49
34:z:37:PRO:HB2	34:z:40:GLN:CG	2.42	0.49
1:A:237:PHE:HD1	1:A:271:LEU:HB2	1.77	0.49
1:A:368:ILE:HD12	1:A:409:PHE:HE2	1.78	0.49
9:I:64:LYS:NZ	9:I:76:VAL:O	2.42	0.49
10:J:4:ASP:OD1	10:J:4:ASP:N	2.44	0.49
11:K:101:PHE:HB2	18:R:61:ARG:HD2	1.94	0.49
13:M:161:TRP:HB3	13:M:181:MET:HE1	1.94	0.49
14:N:3:ILE:O	14:N:128:GLY:N	2.46	0.49
23:W:154:GLU:HG2	23:W:159:VAL:HG12	1.94	0.49
23:W:407:ASP:OD2	24:X:344:ARG:NH2	2.46	0.49
24:X:145:GLU:HA	24:X:148:HIS:HB2	1.94	0.49
27:a:68:GLU:HG3	27:a:71:VAL:HG23	1.93	0.49
27:a:245:VAL:HG21	27:a:301:LYS:HG2	1.93	0.49
28:b:163:LYS:N	34:z:42:ARG:HH12	2.11	0.49
30:d:22:GLU:HA	30:d:25:ARG:HE	1.77	0.49
30:d:131:VAL:HA	30:d:134:LYS:HB3	1.93	0.49
32:f:389:LYS:HB2	32:f:392:THR:HB	1.94	0.49
32:f:675:PHE:O	32:f:679:LEU:N	2.46	0.49
32:f:894:LEU:HA	32:f:898:VAL:HG21	1.95	0.49
17:q:13:VAL:HG21	17:q:105:ALA:HB1	1.95	0.49
19:s:145:LEU:HD21	19:s:182:ALA:HB2	1.93	0.49
20:t:123:GLY:HA2	20:t:133:GLU:HG3	1.94	0.49
1:A:105:ASP:HB2	1:A:110:LYS:HB2	1.95	0.49
5:E:33:LEU:HD11	6:F:62:VAL:HA	1.94	0.49
21:U:399:TRP:CD1	29:c:176:GLN:HG2	2.48	0.49
21:U:637:VAL:HA	21:U:640:LEU:HD23	1.94	0.49
23:W:51:GLU:OE2	23:W:55:ARG:NH1	2.44	0.49
28:b:124:LEU:HB2	28:b:156:PHE:HD1	1.77	0.49
28:b:161:ASN:O	28:b:161:ASN:ND2	2.46	0.49
8:h:70:LYS:O	8:h:218:PHE:N	2.41	0.49
8:h:196:LYS:HA	8:h:203:MET:HE1	1.95	0.49
9:i:119:GLN:HG3	10:j:78:ALA:HB1	1.94	0.49
16:p:2:SER:N	16:p:5:SER:HG	2.10	0.49
34:w:2:GLN:H	34:w:63:LYS:HZ2	1.61	0.49
2:B:106:PRO:HB3	3:C:121:TYR:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:GLY:HA3	4:D:113:VAL:HG12	1.93	0.49
6:F:224:LEU:HD11	6:F:351:LYS:HD3	1.94	0.49
14:N:190:LEU:H	14:N:193:GLN:HB2	1.76	0.49
7:g:186:LYS:HG2	7:g:189:TRP:HE1	1.77	0.49
14:n:7:GLN:NE2	14:n:109:GLY:O	2.45	0.49
18:r:1:THR:O	18:r:130:SER:N	2.46	0.49
2:B:169:PRO:HB3	3:C:77:VAL:HG13	1.95	0.49
3:C:236:VAL:HG23	3:C:239:ARG:HH11	1.76	0.49
4:D:413:GLU:O	4:D:418:LYS:NZ	2.46	0.49
6:F:31:GLU:OE1	6:F:35:LYS:NZ	2.45	0.49
19:S:19:ASP:N	19:S:19:ASP:OD1	2.45	0.49
19:S:21:ALA:HB3	19:S:198:VAL:HB	1.95	0.49
24:X:208:ALA:HB2	24:X:238:GLY:HA3	1.94	0.49
27:a:323:SER:O	27:a:332:HIS:N	2.45	0.49
14:n:151:GLU:HA	14:n:154:GLN:HG2	1.94	0.49
34:w:3:ILE:HA	34:w:64:GLU:HA	1.94	0.49
1:A:38:GLN:OE1	1:A:40:THR:OG1	2.30	0.49
8:H:42:ASN:HD21	8:H:184:LEU:H	1.61	0.49
16:P:176:ASP:OD2	19:s:157:ASN:ND2	2.46	0.49
22:V:253:LEU:O	22:V:257:ASN:ND2	2.45	0.49
28:b:132:LYS:HE2	34:z:42:ARG:CD	2.42	0.49
29:c:197:ASN:O	29:c:198:ARG:C	2.56	0.49
32:f:572:ALA:O	32:f:574:GLU:N	2.46	0.49
18:r:41:LEU:HD23	18:r:103:GLY:HA3	1.95	0.49
34:z:37:PRO:O	34:z:41:GLN:HG2	2.12	0.49
7:G:217:VAL:HB	7:G:230:LEU:HB2	1.95	0.48
11:K:60:GLU:OE1	11:K:63:SER:N	2.46	0.48
12:L:35:THR:O	12:L:160:SER:OG	2.26	0.48
24:X:27:LEU:HB3	24:X:53:LEU:HD12	1.95	0.48
24:X:214:SER:O	24:X:218:HIS:ND1	2.43	0.48
25:Y:162:GLU:HA	25:Y:165:LYS:HB2	1.95	0.48
30:d:23:LEU:HG	30:d:27:LYS:HE2	1.95	0.48
32:f:571:GLU:O	32:f:573:ILE:N	2.46	0.48
7:g:53:GLN:HA	7:g:215:ILE:HG22	1.94	0.48
13:m:36:ALA:N	13:m:165:ILE:O	2.43	0.48
16:p:134:ASP:OD1	16:p:134:ASP:N	2.44	0.48
18:r:100:MET:HE1	18:r:113:TYR:HD1	1.78	0.48
34:x:43:LEU:HD13	34:x:67:LEU:HD21	1.95	0.48
3:C:88:LYS:HB3	3:C:94:LYS:HZ2	1.78	0.48
9:I:217:THR:O	9:I:224:VAL:N	2.36	0.48
14:N:12:VAL:HG21	14:N:101:ALA:HB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:41:ILE:HG12	15:O:102:GLY:HA3	1.95	0.48
18:R:46:ALA:O	18:R:98:GLY:N	2.46	0.48
21:U:157:THR:HG23	21:U:159:ARG:HB2	1.94	0.48
21:U:519:VAL:HG23	21:U:520:MET:SD	2.53	0.48
21:U:773:PHE:HB2	29:c:177:THR:HB	1.95	0.48
8:h:148:GLN:NE2	8:h:149:SER:O	2.46	0.48
13:m:141:SER:N	13:m:145:GLY:O	2.47	0.48
15:o:21:THR:HA	15:o:27:ALA:H	1.77	0.48
20:t:14:VAL:HA	20:t:136:SER:HA	1.94	0.48
35:A:501:ATP:O1G	2:B:343:ARG:NE	2.46	0.48
2:B:115:ILE:HD11	2:B:146:PRO:HD3	1.95	0.48
11:K:169:ALA:N	11:K:178:GLN:OE1	2.40	0.48
16:P:189:ILE:HB	16:P:196:THR:HB	1.95	0.48
22:V:216:ARG:HH21	22:V:220:PHE:HE2	1.61	0.48
23:W:406:VAL:HG23	23:W:413:ILE:HG22	1.95	0.48
27:a:131:THR:HA	27:a:134:THR:HG22	1.96	0.48
30:d:98:LEU:HA	30:d:101:LEU:HD12	1.94	0.48
32:f:208:LEU:HD21	32:f:217:LEU:HD12	1.94	0.48
32:f:253:LEU:HD21	32:f:281:ILE:HD11	1.96	0.48
11:k:98:ASN:OD1	18:r:61:ARG:NH2	2.47	0.48
16:p:30:ILE:HB	16:p:33:GLN:HG2	1.96	0.48
34:x:42:ARG:HB3	34:x:70:VAL:HB	1.94	0.48
1:A:212:VAL:HG22	1:A:339:ARG:HB3	1.95	0.48
2:B:140:ASP:OD1	2:B:140:ASP:N	2.46	0.48
5:E:61:LEU:HD11	5:E:72:LYS:HB2	1.94	0.48
17:Q:5:ILE:HG13	17:Q:131:ALA:HB2	1.95	0.48
17:Q:21:ALA:HB3	17:Q:29:LYS:HB3	1.95	0.48
18:R:3:THR:HG23	18:R:16:ALA:HB2	1.96	0.48
18:R:41:LEU:HD23	18:R:103:GLY:HA3	1.95	0.48
21:U:363:SER:OG	21:U:365:CYS:SG	2.64	0.48
25:Y:127:THR:O	25:Y:131:THR:OG1	2.24	0.48
27:a:111:VAL:HA	27:a:114:CYS:HB2	1.95	0.48
19:s:191:ASP:HA	19:s:212:LYS:HD3	1.95	0.48
20:t:122:LEU:HG	20:t:137:LEU:HD12	1.96	0.48
2:B:313:LEU:O	2:B:346:ARG:NH1	2.41	0.48
2:B:389:ASP:OD1	2:B:389:ASP:N	2.44	0.48
4:D:133:HIS:HB3	4:D:137:ASN:H	1.78	0.48
8:H:181:ASP:N	8:H:181:ASP:OD1	2.42	0.48
18:R:9:ARG:HH12	18:R:146:ASP:HA	1.78	0.48
24:X:317:PRO:O	24:X:318:ILE:HB	2.14	0.48
28:b:122:LYS:HB2	34:z:76:GLY:C	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:557:TRP:HA	32:f:560:LEU:HD12	1.94	0.48
15:o:106:THR:OG1	15:o:109:HIS:NE2	2.42	0.48
1:A:279:ALA:HB2	2:B:310:LEU:HD23	1.96	0.48
2:B:31:THR:HG23	2:B:32:ARG:HG2	1.94	0.48
4:D:175:GLN:NE2	4:D:179:GLU:OE2	2.46	0.48
6:F:86:LEU:O	6:F:87:PRO:C	2.56	0.48
21:U:602:LEU:HD11	21:U:621:SER:HB2	1.96	0.48
21:U:803:LYS:HB2	21:U:875:PHE:HA	1.96	0.48
23:W:316:ARG:NH1	23:W:380:GLN:O	2.38	0.48
26:Z:43:TRP:HB3	26:Z:90:ARG:HH21	1.79	0.48
29:c:29:GLU:HG3	29:c:65:TYR:HB2	1.95	0.48
32:f:285:CYS:O	32:f:291:GLN:NE2	2.46	0.48
18:r:21:THR:HA	18:r:27:ALA:H	1.77	0.48
4:D:349:THR:HA	4:D:352:MET:HB2	1.95	0.48
5:E:126:ASP:HB3	5:E:195:PHE:HB2	1.95	0.48
6:F:289:ASP:OD1	6:F:289:ASP:N	2.47	0.48
9:I:73:ALA:HB3	9:I:137:ILE:HD11	1.95	0.48
11:K:71:ASP:OD1	11:K:74:ILE:N	2.47	0.48
12:L:164:ARG:NH1	12:L:198:THR:O	2.46	0.48
22:V:278:GLU:HA	22:V:285:TRP:HZ2	1.79	0.48
28:b:123:ASP:HA	28:b:126:LYS:HZ3	1.77	0.48
29:c:197:ASN:O	29:c:199:HIS:N	2.47	0.48
14:n:1:THR:OG1	14:n:2:THR:N	2.47	0.48
1:A:390:THR:HG22	2:B:216:ILE:HG23	1.96	0.48
2:B:68:ILE:HD13	32:f:670:MET:HE1	1.96	0.48
3:C:100:ASP:H	3:C:103:ILE:HD11	1.78	0.48
4:D:325:GLY:N	4:D:328:ASP:OD1	2.41	0.48
21:U:73:ALA:HB1	21:U:76:GLU:HB2	1.96	0.48
22:V:177:ASN:O	22:V:179:LYS:NZ	2.47	0.48
24:X:187:ARG:HD3	24:X:194:ARG:HH22	1.79	0.48
24:X:317:PRO:HD2	24:X:319:ILE:HG13	1.95	0.48
25:Y:111:LEU:HD23	25:Y:114:ILE:HD11	1.96	0.48
27:a:257:GLN:HB3	27:a:261:LEU:HD22	1.96	0.48
28:b:163:LYS:HB2	34:z:52:ASP:HB2	1.95	0.48
30:d:201:ASN:C	30:d:203:PRO:HD2	2.38	0.48
32:f:679:LEU:HD21	32:f:694:LEU:HD11	1.96	0.48
7:g:206:LEU:HD12	7:g:210:PHE:HZ	1.79	0.48
3:C:236:VAL:HG23	3:C:239:ARG:HD3	1.96	0.48
5:E:124:HIS:ND1	5:E:125:GLU:O	2.47	0.48
5:E:254:GLN:HB3	5:E:258:MET:HE1	1.96	0.48
10:J:224:GLU:HA	10:J:227:LYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:113:ASP:OD2	16:P:116:THR:N	2.35	0.48
19:S:125:ASP:OD1	19:S:129:SER:N	2.47	0.48
25:Y:41:LEU:HD21	25:Y:57:LEU:HD11	1.95	0.48
25:Y:222:TYR:OH	25:Y:285:ASP:OD1	2.28	0.48
28:b:79:GLN:HG3	28:b:81:LYS:HG2	1.95	0.48
31:e:16:ASP:N	31:e:16:ASP:OD1	2.45	0.48
12:l:39:LYS:HE2	12:l:157:ARG:HA	1.95	0.48
20:t:99:ARG:HA	20:t:102:LYS:HE3	1.96	0.48
34:z:72:ARG:HG3	34:z:72:ARG:O	2.13	0.48
1:A:428:ARG:HH22	10:J:24:GLU:HG2	1.78	0.48
7:G:71:LYS:H	7:G:95:ARG:HH21	1.62	0.48
8:H:44:VAL:HG23	8:H:144:PRO:HB2	1.95	0.48
9:I:68:LEU:H	9:I:73:ALA:HA	1.79	0.48
18:R:69:ARG:O	18:R:71:LYS:NZ	2.40	0.48
21:U:181:LEU:HG	21:U:218:GLN:HE22	1.79	0.48
21:U:436:ALA:HB3	21:U:472:ILE:HD11	1.96	0.48
25:Y:112:CYS:HB2	25:Y:147:ILE:HD11	1.95	0.48
28:b:68:THR:HA	28:b:71:ILE:HD13	1.95	0.48
30:d:91:GLU:OE2	30:d:96:HIS:NE2	2.47	0.48
31:e:45:ASP:OD1	31:e:45:ASP:N	2.46	0.48
32:f:487:LEU:HA	32:f:524:MET:HE1	1.96	0.48
13:m:175:GLU:HB3	13:m:196:ILE:HG12	1.96	0.48
34:z:52:ASP:C	34:z:54:ARG:N	2.70	0.48
14:N:153:LEU:HD22	14:N:176:LEU:HD13	1.95	0.47
30:d:69:PRO:HA	30:d:72:GLU:HG2	1.96	0.47
32:f:278:VAL:HG12	32:f:305:LEU:HD11	1.96	0.47
18:r:18:SER:OG	18:r:173:ALA:N	2.44	0.47
20:t:153:VAL:HA	20:t:156:LYS:HG2	1.96	0.47
34:z:31:GLN:HB2	34:z:37:PRO:HA	1.96	0.47
3:C:365:GLU:HA	3:C:368:MET:HG3	1.95	0.47
17:Q:48:GLY:HA3	17:Q:100:VAL:HA	1.95	0.47
18:R:7:LYS:HD2	18:R:109:PRO:HB2	1.95	0.47
22:V:211:TYR:OH	22:V:234:ARG:NE	2.43	0.47
25:Y:157:ILE:O	25:Y:161:THR:N	2.47	0.47
27:a:226:ARG:HH12	27:a:233:LEU:HB3	1.79	0.47
29:c:46:ARG:HH21	29:c:147:PRO:HB2	1.78	0.47
12:l:41:LYS:O	12:l:217:LYS:NZ	2.43	0.47
18:r:182:ASP:OD1	18:r:182:ASP:N	2.43	0.47
19:s:52:ILE:HG13	19:s:110:ILE:HG12	1.96	0.47
20:t:89:HIS:HE1	20:t:131:ALA:HB1	1.80	0.47
1:A:357:ILE:HA	1:A:360:ARG:CZ	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:406:LYS:OXT	9:I:64:LYS:NZ	2.44	0.47
5:E:168:LYS:HD2	5:E:265:ASP:HB3	1.96	0.47
21:U:381:THR:HG22	21:U:412:HIS:HA	1.95	0.47
21:U:609:ASP:O	21:U:615:ARG:NH1	2.46	0.47
26:Z:228:TYR:HE2	27:a:340:VAL:HA	1.79	0.47
27:a:70:ARG:O	28:b:17:ARG:NH1	2.46	0.47
30:d:168:ASP:OD1	30:d:169:ILE:N	2.46	0.47
11:k:230:THR:HG23	11:k:233:GLU:H	1.80	0.47
3:C:266:ASP:HB3	3:C:269:VAL:HB	1.96	0.47
19:S:57:PHE:N	19:S:105:TYR:O	2.37	0.47
22:V:313:LEU:HD13	22:V:328:VAL:HG11	1.96	0.47
27:a:343:LEU:O	27:a:344:GLN:C	2.58	0.47
28:b:155:ALA:O	28:b:159:THR:OG1	2.25	0.47
30:d:190:LEU:HD22	30:d:192:THR:HG22	1.97	0.47
32:f:395:GLY:O	32:f:399:LEU:N	2.47	0.47
32:f:843:SER:HB2	32:f:845:ARG:HH12	1.80	0.47
14:n:119:MET:HB3	20:t:58:ALA:HB2	1.96	0.47
1:A:55:LEU:HA	1:A:58:LYS:HG2	1.96	0.47
6:F:304:ARG:O	6:F:308:ARG:NH1	2.47	0.47
9:I:90:LEU:HD21	9:I:114:LEU:HD12	1.96	0.47
10:J:196:LEU:HA	10:J:199:VAL:HG12	1.96	0.47
11:K:217:LEU:HB3	11:K:234:LEU:HD21	1.97	0.47
12:L:173:GLU:OE2	13:M:56:LYS:NZ	2.37	0.47
16:P:138:VAL:HG11	16:P:146:MET:HB3	1.97	0.47
23:W:405:LYS:HD3	24:X:343:SER:HB3	1.96	0.47
27:a:292:THR:HG23	27:a:295:GLU:H	1.79	0.47
29:c:54:MET:HE1	29:c:111:TRP:HE3	1.79	0.47
11:k:36:THR:HA	11:k:171:GLY:HA3	1.97	0.47
13:m:136:MET:SD	13:m:150:MET:HE1	2.55	0.47
20:t:8:GLY:N	20:t:55:GLY:O	2.46	0.47
3:C:269:VAL:HG12	3:C:273:MET:HE3	1.97	0.47
3:C:280:LEU:HD12	3:C:281:ASP:HB2	1.95	0.47
5:E:11:ASP:HA	5:E:14:LYS:HG2	1.96	0.47
8:H:177:ARG:NH1	24:X:202:CYS:SG	2.86	0.47
15:O:143:ARG:NH2	15:O:150:GLU:OE1	2.46	0.47
21:U:65:SER:O	21:U:77:SER:OG	2.30	0.47
21:U:510:GLU:HA	21:U:547:GLY:HA3	1.97	0.47
22:V:118:GLN:HG2	22:V:128:ARG:HH22	1.79	0.47
24:X:70:LEU:HD12	24:X:109:LEU:HD21	1.97	0.47
25:Y:142:PHE:HB3	25:Y:146:ARG:HH21	1.79	0.47
27:a:33:LEU:HA	28:b:18:ASN:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:r:64:ARG:NH1	18:r:64:ARG:O	2.48	0.47
20:t:40:SER:O	20:t:57:TYR:OH	2.32	0.47
1:A:351:ARG:NH1	1:A:378:PRO:O	2.47	0.47
1:A:394:MET:HE3	2:B:349:ARG:HH21	1.80	0.47
2:B:195:GLN:NE2	2:B:199:GLU:OE2	2.47	0.47
3:C:49:ARG:HD2	21:U:639:LEU:HD21	1.96	0.47
3:C:351:MET:HE2	3:C:354:ALA:HA	1.97	0.47
4:D:157:ASP:O	4:D:158:GLN:HB3	2.14	0.47
4:D:261:ILE:HG23	4:D:308:ILE:HD13	1.96	0.47
7:G:123:GLN:O	7:G:126:THR:OG1	2.26	0.47
8:H:171:LYS:NZ	8:H:175:GLU:OE2	2.47	0.47
13:M:192:GLU:O	13:M:196:ILE:HG12	2.15	0.47
14:N:46:SER:OG	14:N:97:GLY:O	2.28	0.47
16:P:22:ILE:HG23	16:P:188:HIS:HB2	1.97	0.47
19:S:57:PHE:HZ	20:T:128:LEU:HB3	1.79	0.47
23:W:374:THR:HA	23:W:412:ILE:HD12	1.97	0.47
29:c:281:LYS:HD3	29:c:281:LYS:HA	1.64	0.47
30:d:204:LYS:HA	30:d:204:LYS:HD2	1.66	0.47
32:f:222:ASP:HB3	32:f:225:ALA:HB3	1.95	0.47
32:f:699:VAL:HG23	32:f:731:MET:HG2	1.95	0.47
10:j:184:ASP:O	10:j:187:THR:OG1	2.25	0.47
12:l:120:THR:O	13:m:129:ARG:NH1	2.48	0.47
15:o:77:VAL:O	15:o:81:ARG:HG2	2.14	0.47
16:p:9:GLY:N	16:p:181:SER:OG	2.39	0.47
19:s:141:ALA:HA	19:s:144:MET:HE2	1.96	0.47
34:w:41:GLN:HA	34:w:71:LEU:HA	1.95	0.47
1:A:333:ARG:HE	1:A:336:ARG:NH1	2.13	0.47
2:B:67:ARG:NH2	32:f:664:GLU:OE2	2.48	0.47
2:B:220:LYS:HD3	2:B:326:LYS:HD3	1.97	0.47
6:F:202:ILE:HD11	6:F:223:VAL:HG21	1.97	0.47
9:I:123:GLN:HA	10:J:125:ARG:HE	1.80	0.47
10:J:30:SER:OG	10:J:48:LYS:NZ	2.41	0.47
15:O:173:ILE:HB	15:O:190:THR:HB	1.97	0.47
25:Y:104:MET:HE3	25:Y:127:THR:HA	1.96	0.47
28:b:122:LYS:HD2	28:b:126:LYS:HD3	1.96	0.47
32:f:862:ILE:HG12	32:f:879:ARG:HB3	1.97	0.47
8:h:213:CYS:HB2	8:h:218:PHE:HD1	1.79	0.47
13:m:72:HIS:NE2	13:m:105:ASN:OD1	2.48	0.47
14:n:3:ILE:O	14:n:128:GLY:N	2.48	0.47
18:r:22:ALA:N	18:r:25:TYR:O	2.41	0.47
1:A:308:GLY:HA2	6:F:234:THR:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:41:LYS:NZ	12:L:180:MET:O	2.43	0.47
15:O:143:ARG:H	15:O:146:MET:HE2	1.78	0.47
19:S:183:ALA:HB2	19:S:210:LEU:HD13	1.97	0.47
22:V:227:VAL:HG13	22:V:231:LEU:HD13	1.97	0.47
29:c:87:VAL:HG21	29:c:133:PHE:HZ	1.78	0.47
12:l:9:ASP:OD2	12:l:11:THR:OG1	2.32	0.47
12:l:14:SER:OG	12:l:16:GLN:OE1	2.33	0.47
12:l:134:ILE:HB	12:l:145:PHE:HB2	1.95	0.47
14:n:174:ILE:O	14:n:189:LEU:N	2.39	0.47
7:G:14:THR:HA	8:H:128:ARG:HB3	1.97	0.47
10:J:160:ALA:O	10:J:169:ARG:NH2	2.48	0.47
11:K:117:SER:HB2	12:L:82:ARG:HH12	1.79	0.47
15:O:11:GLY:HA2	15:O:108:PRO:HB3	1.96	0.47
19:S:145:LEU:HD22	19:S:178:VAL:HB	1.97	0.47
25:Y:134:LEU:HA	25:Y:137:ARG:CZ	2.45	0.47
26:Z:10:VAL:N	26:Z:48:LEU:O	2.48	0.47
27:a:314:ALA:HB1	27:a:319:LEU:HD11	1.97	0.47
13:m:197:ILE:HA	13:m:200:VAL:HG12	1.97	0.47
3:C:267:SER:O	3:C:271:ARG:NH1	2.49	0.46
4:D:57:GLN:O	4:D:61:ILE:HG12	2.15	0.46
5:E:178:THR:O	5:E:182:LEU:HB2	2.16	0.46
11:K:117:SER:OG	12:L:82:ARG:NH2	2.38	0.46
14:N:1:THR:N	14:N:169:SER:O	2.48	0.46
25:Y:98:SER:O	25:Y:102:ASP:N	2.48	0.46
30:d:42:LYS:HA	30:d:45:LYS:HB2	1.96	0.46
32:f:367:SER:O	32:f:371:ASN:ND2	2.49	0.46
12:l:39:LYS:HA	12:l:44:ALA:HA	1.97	0.46
14:n:192:ASP:N	14:n:192:ASP:OD1	2.46	0.46
17:q:19:ARG:HD3	17:q:177:THR:HG22	1.96	0.46
18:r:7:LYS:HD2	18:r:109:PRO:HB2	1.96	0.46
2:B:319:PHE:O	2:B:322:ARG:NH1	2.49	0.46
2:B:425:ASN:HA	2:B:428:TYR:HD2	1.80	0.46
3:C:186:VAL:HB	3:C:292:ILE:HA	1.97	0.46
9:I:239:LYS:O	9:I:242:GLU:HG3	2.15	0.46
10:J:157:LYS:HE2	11:K:58:LEU:HD12	1.96	0.46
22:V:301:GLU:HG2	22:V:304:GLU:HB2	1.96	0.46
30:d:66:LYS:HE3	30:d:165:PHE:HB2	1.97	0.46
34:z:36:ILE:O	34:z:41:GLN:NE2	2.48	0.46
1:A:103:ASN:HA	1:A:136:GLU:HG2	1.97	0.46
2:B:248:LEU:O	2:B:283:PHE:N	2.45	0.46
5:E:289:LEU:HD12	5:E:294:ARG:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:98:LEU:HB2	15:O:113:ILE:HB	1.97	0.46
16:P:83:LYS:HG3	16:P:85:TYR:H	1.80	0.46
32:f:534:VAL:HA	32:f:537:THR:HG22	1.97	0.46
32:f:658:ALA:HB3	32:f:696:LEU:HD23	1.98	0.46
15:o:112:SER:HB3	15:o:125:VAL:HG11	1.96	0.46
19:s:15:ILE:HD12	19:s:135:PHE:HB3	1.96	0.46
5:E:64:LEU:HG	5:E:65:THR:HG23	1.97	0.46
7:G:221:THR:HB	7:G:224:ASN:HB3	1.96	0.46
19:S:26:ASP:OD1	19:S:26:ASP:N	2.49	0.46
23:W:67:LEU:HB3	23:W:104:MET:SD	2.56	0.46
25:Y:365:GLN:NE2	25:Y:368:GLU:OE1	2.49	0.46
26:Z:261:TYR:HA	26:Z:265:LEU:HD13	1.98	0.46
32:f:323:ASN:HB3	32:f:326:LEU:HB2	1.97	0.46
9:i:151:ASP:OD2	9:i:153:SER:OG	2.30	0.46
10:j:90:GLU:HG3	10:j:110:TYR:CZ	2.50	0.46
12:l:225:ASP:H	12:l:228:ASP:HB2	1.80	0.46
17:q:6:GLY:N	17:q:130:ALA:O	2.39	0.46
17:q:31:ASP:N	17:q:31:ASP:OD1	2.47	0.46
17:q:106:GLY:O	17:q:114:ALA:N	2.46	0.46
22:V:212:TYR:HA	22:V:253:LEU:HD11	1.96	0.46
23:W:190:MET:HB2	23:W:202:THR:HG23	1.98	0.46
23:W:452:ILE:O	23:W:456:GLN:N	2.48	0.46
32:f:675:PHE:HA	32:f:678:LEU:HG	1.97	0.46
10:j:157:LYS:HD2	11:k:58:LEU:HD12	1.98	0.46
1:A:139:ARG:O	1:A:153:LEU:N	2.36	0.46
1:A:173:THR:HG22	1:A:175:SER:H	1.81	0.46
2:B:248:LEU:HB2	2:B:282:VAL:HG22	1.98	0.46
3:C:38:LYS:HG2	3:C:41:ASN:ND2	2.31	0.46
4:D:45:LYS:HG2	21:U:187:LEU:HB2	1.97	0.46
8:H:95:GLN:HG3	15:O:65:LEU:HD12	1.97	0.46
22:V:484:LEU:HG	26:Z:267:ARG:HH22	1.80	0.46
23:W:372:ARG:NH1	23:W:412:ILE:HG13	2.31	0.46
26:Z:15:VAL:HA	26:Z:18:SER:HB3	1.98	0.46
29:c:167:MET:HE3	29:c:170:LEU:HD23	1.97	0.46
15:o:113:ILE:HG12	15:o:119:THR:HG22	1.98	0.46
15:o:216:ILE:HD11	16:p:194:LYS:HD2	1.96	0.46
3:C:375:ARG:NH2	3:C:377:HIS:O	2.47	0.46
5:E:139:SER:HA	5:E:142:ILE:HD12	1.98	0.46
5:E:368:MET:HB3	5:E:372:ARG:NH1	2.30	0.46
12:L:105:VAL:HG21	12:L:136:GLY:HA3	1.97	0.46
15:O:45:GLY:HA2	15:O:98:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:48:ARG:NH2	16:P:192:LYS:O	2.48	0.46
16:P:85:TYR:HA	16:P:88:MET:HE2	1.98	0.46
21:U:27:LEU:HD11	21:U:38:ILE:HD13	1.98	0.46
21:U:819:VAL:HG22	21:U:821:LYS:H	1.81	0.46
23:W:446:ILE:HA	26:Z:227:ILE:HD11	1.98	0.46
34:w:22:THR:HG23	34:w:25:ASN:H	1.81	0.46
10:J:31:THR:OG1	10:J:163:ARG:O	2.33	0.46
11:K:235:GLU:HA	11:K:238:ILE:HB	1.98	0.46
13:M:120:HIS:O	13:M:123:THR:OG1	2.33	0.46
16:P:80:ARG:CZ	16:P:81:GLN:H	2.29	0.46
23:W:125:ILE:HG21	23:W:149:LEU:HD13	1.97	0.46
25:Y:77:ASN:O	25:Y:81:LEU:N	2.40	0.46
26:Z:70:LEU:HD12	26:Z:111:LEU:HD22	1.97	0.46
27:a:80:ILE:HG12	27:a:100:THR:HG21	1.97	0.46
29:c:226:MET:HE3	29:c:229:LEU:HD21	1.98	0.46
32:f:832:THR:HG23	32:f:870:THR:HG21	1.97	0.46
13:m:8:ASP:HB3	13:m:21:PHE:HD2	1.81	0.46
19:s:48:ASP:OD1	19:s:48:ASP:N	2.48	0.46
19:s:85:THR:HA	19:s:88:ILE:HD12	1.98	0.46
34:z:27:LYS:HD3	34:z:41:GLN:HG3	1.98	0.46
3:C:20:LEU:HD23	21:U:137:MET:HE3	1.98	0.46
6:F:35:LYS:HD2	6:F:38:THR:HB	1.98	0.46
9:I:70:GLU:O	9:I:223:THR:OG1	2.32	0.46
11:K:101:PHE:HA	18:R:57:ARG:HE	1.81	0.46
17:Q:35:MET:HG2	17:Q:181:ARG:HE	1.81	0.46
24:X:251:LEU:HA	24:X:254:MET:HG3	1.98	0.46
10:j:135:GLY:HA2	10:j:211:MET:HE1	1.98	0.46
1:A:102:ILE:HD12	1:A:112:ILE:HG22	1.97	0.46
1:A:414:ASN:HA	1:A:418:LYS:HB2	1.96	0.46
3:C:53:ASN:ND2	21:U:642:GLU:O	2.41	0.46
4:D:167:ILE:HG12	4:D:214:MET:HE2	1.98	0.46
7:G:96:TYR:O	7:G:100:ASN:ND2	2.49	0.46
13:M:102:PHE:HE1	14:N:82:LEU:HD21	1.81	0.46
14:N:7:GLN:NE2	14:N:109:GLY:O	2.49	0.46
23:W:128:LEU:O	23:W:132:THR:OG1	2.23	0.46
24:X:422:THR:OXT	26:Z:283:ARG:NE	2.49	0.46
27:a:276:CYS:HB2	27:a:280:MET:HE1	1.98	0.46
28:b:72:LEU:HA	28:b:75:LEU:HD12	1.97	0.46
28:b:121:GLU:OE1	28:b:152:LYS:HA	2.16	0.46
29:c:283:HIS:HD2	29:c:287:HIS:NE2	2.13	0.46
30:d:203:PRO:O	30:d:205:LYS:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:573:ILE:O	32:f:577:LEU:N	2.36	0.46
11:k:99:HIS:O	11:k:103:TYR:HB2	2.16	0.46
15:O:112:SER:HB3	15:O:125:VAL:HG21	1.97	0.45
22:V:259:LEU:HD11	22:V:294:ARG:HD3	1.97	0.45
29:c:269:GLN:HA	29:c:272:ILE:HG22	1.96	0.45
9:i:45:LEU:HD11	9:i:137:ILE:HG21	1.98	0.45
20:t:89:HIS:CE1	20:t:131:ALA:HB1	2.50	0.45
7:G:58:ASP:N	7:G:58:ASP:OD1	2.49	0.45
24:X:143:TYR:OH	25:Y:248:GLU:O	2.31	0.45
28:b:8:VAL:HA	28:b:110:ILE:HG13	1.98	0.45
28:b:84:ILE:HD12	28:b:115:SER:HB2	1.97	0.45
29:c:192:LEU:HB3	29:c:196:LEU:HG	1.99	0.45
32:f:304:PHE:HA	32:f:321:MET:HE2	1.98	0.45
9:i:140:ASP:OD1	9:i:144:GLY:N	2.50	0.45
1:A:100:LYS:HG3	1:A:137:GLY:HA2	1.97	0.45
6:F:402:GLU:HA	6:F:405:MET:HE2	1.97	0.45
10:J:39:ASP:OD1	10:J:39:ASP:N	2.49	0.45
12:L:70:ILE:HG12	12:L:105:VAL:HG22	1.98	0.45
12:L:72:ILE:HD12	12:L:132:LEU:HD11	1.98	0.45
21:U:585:THR:HA	21:U:588:MET:HG3	1.99	0.45
22:V:119:GLY:HA2	22:V:148:ARG:HD3	1.98	0.45
27:a:68:GLU:HG2	27:a:69:HIS:N	2.31	0.45
29:c:88:ASP:HB3	29:c:91:PHE:HB3	1.99	0.45
13:m:152:ASP:OD1	13:m:152:ASP:N	2.47	0.45
14:n:13:VAL:HG21	14:n:152:CYS:HB3	1.99	0.45
19:s:63:THR:HG23	20:t:94:ARG:HH12	1.81	0.45
1:A:124:ASP:HB2	6:F:86:LEU:HD22	1.99	0.45
3:C:188:LEU:HD12	3:C:294:ALA:HB2	1.98	0.45
3:C:215:SER:OG	3:C:218:GLU:OE1	2.23	0.45
10:J:137:ASP:OD2	10:J:143:ARG:NE	2.42	0.45
15:O:216:ILE:HG13	16:P:196:THR:HG23	1.98	0.45
20:T:1:THR:N	20:T:104:ASN:OD1	2.46	0.45
21:U:740:GLY:HA3	21:U:744:VAL:HG12	1.98	0.45
22:V:346:LEU:HD13	22:V:349:ARG:HD3	1.98	0.45
25:Y:104:MET:HE1	25:Y:130:LYS:HB2	1.98	0.45
28:b:124:LEU:HB2	28:b:156:PHE:CD1	2.51	0.45
32:f:585:GLU:CD	32:f:588:ARG:HH21	2.24	0.45
8:h:3:GLU:OE2	13:m:127:ALA:HB3	2.16	0.45
16:p:35:VAL:HG12	16:p:36:THR:HG23	1.98	0.45
19:s:19:ASP:N	19:s:19:ASP:OD1	2.50	0.45
34:w:27:LYS:HG2	34:w:41:GLN:HE22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:THR:HG21	2:B:353:PHE:HB3	1.97	0.45
2:B:305:ILE:O	2:B:309:MET:HG2	2.17	0.45
4:D:362:ASP:O	4:D:366:ARG:NE	2.50	0.45
5:E:171:LEU:HB2	5:E:295:LEU:HD22	1.98	0.45
5:E:263:GLN:HA	5:E:268:ASP:HB3	1.97	0.45
13:M:125:TYR:HB2	13:M:128:VAL:HG22	1.99	0.45
21:U:17:PRO:HB2	21:U:55:ARG:HH12	1.80	0.45
21:U:564:ASP:OD1	21:U:564:ASP:N	2.50	0.45
22:V:199:ASN:OD1	22:V:241:ARG:NH2	2.50	0.45
22:V:350:GLN:O	22:V:354:LYS:N	2.39	0.45
10:j:116:GLN:NE2	10:j:120:GLN:OE1	2.49	0.45
11:k:56:SER:HB3	11:k:59:MET:HE3	1.99	0.45
11:k:147:ASP:N	11:k:147:ASP:OD1	2.50	0.45
13:m:8:ASP:O	13:m:22:GLN:NE2	2.48	0.45
14:n:18:SER:OG	14:n:173:VAL:N	2.45	0.45
19:s:89:ALA:HA	19:s:124:PHE:HZ	1.82	0.45
34:w:61:ILE:HG23	34:w:65:SER:HB2	1.98	0.45
2:B:233:THR:HG22	2:B:237:LYS:HD2	1.99	0.45
2:B:234:LEU:HD11	35:B:501:ATP:H2'	1.99	0.45
3:C:305:LEU:HA	3:C:310:ARG:HG3	1.99	0.45
7:G:28:ALA:O	7:G:32:ILE:HG13	2.17	0.45
8:H:51:LYS:HB2	8:H:207:ASN:HB2	1.98	0.45
14:N:189:LEU:HD22	14:N:193:GLN:HB3	1.99	0.45
15:O:131:SER:O	15:O:135:MET:HB2	2.17	0.45
20:T:107:TRP:HA	20:T:127:MET:HE1	1.99	0.45
21:U:678:ASP:O	21:U:684:ARG:NH1	2.41	0.45
21:U:847:GLU:HA	21:U:850:GLU:HG2	1.98	0.45
21:U:886:PRO:HA	21:U:889:LEU:HG	1.99	0.45
22:V:123:SER:H	22:V:150:ARG:HH21	1.64	0.45
23:W:177:MET:HE3	23:W:182:ARG:NH2	2.32	0.45
17:q:7:ILE:N	17:q:14:LEU:O	2.43	0.45
1:A:372:LEU:HD21	11:K:205:VAL:HA	1.98	0.45
13:M:15:SER:OG	13:M:18:GLY:N	2.50	0.45
14:N:138:TYR:O	14:N:142:THR:OG1	2.28	0.45
18:R:95:LEU:HD23	19:S:100:ARG:HH21	1.81	0.45
21:U:854:MET:SD	21:U:855:GLU:N	2.89	0.45
23:W:429:SER:O	23:W:433:ASN:N	2.46	0.45
11:k:49:ALA:HB1	11:k:202:LEU:HD11	1.97	0.45
12:l:7:ASP:HA	12:l:20:HIS:HB2	1.98	0.45
17:q:11:ASP:N	17:q:11:ASP:OD1	2.49	0.45
19:s:51:VAL:HG23	19:s:203:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ASP:OD1	1:A:287:ASP:N	2.50	0.45
2:B:286:GLU:N	2:B:330:ALA:O	2.36	0.45
5:E:215:ILE:HG22	5:E:216:ARG:HD2	1.99	0.45
10:J:108:THR:HA	10:J:111:ILE:HG12	1.99	0.45
10:J:115:LYS:HZ3	10:J:147:THR:HB	1.81	0.45
12:L:43:HIS:HB3	12:L:214:ILE:HD11	1.99	0.45
13:M:80:LEU:H	13:M:133[A]:CYS:HB3	1.82	0.45
26:Z:269:VAL:HG12	26:Z:273:HIS:HE1	1.81	0.45
28:b:62:THR:HG21	28:b:71:ILE:HA	1.99	0.45
29:c:99:LEU:HD23	29:c:99:LEU:HA	1.84	0.45
32:f:282:PHE:HZ	32:f:317:LEU:HD21	1.80	0.45
32:f:420:TRP:NE1	32:f:453:SER:O	2.41	0.45
32:f:531:ASN:O	32:f:565:ASN:OD1	2.34	0.45
13:m:70:ASP:HB3	13:m:73:VAL:H	1.81	0.45
3:C:38:LYS:HG2	3:C:41:ASN:HD22	1.82	0.45
4:D:390:ASN:OD1	23:W:170:GLN:NE2	2.50	0.45
6:F:405:MET:O	6:F:409:ARG:HG2	2.16	0.45
12:L:80:ASP:OD2	12:L:129:GLY:N	2.49	0.45
15:O:22:GLU:HG2	15:O:27:ALA:HB2	1.99	0.45
17:Q:28:MET:HA	17:q:170:ARG:HH11	1.82	0.45
19:S:38:ARG:NH2	15:o:164:PHE:O	2.49	0.45
26:Z:11:VAL:O	26:Z:163:GLY:N	2.50	0.45
26:Z:82:PHE:HA	26:Z:85:VAL:HG12	1.98	0.45
28:b:7:MET:HB3	28:b:109:ILE:HG12	1.99	0.45
32:f:169:GLU:O	32:f:173:LEU:N	2.50	0.45
32:f:580:LEU:HD23	32:f:591:ALA:HB1	1.98	0.45
9:i:148:TYR:HE1	10:j:58:THR:HG21	1.82	0.45
9:i:214:ALA:HA	9:i:227:VAL:HA	1.98	0.45
16:p:14:MET:HG2	16:p:167:ILE:HD12	1.99	0.45
18:r:59:LEU:HD22	18:r:83:LEU:HB2	1.98	0.45
18:r:80:SER:HB3	18:r:101:ILE:HG21	1.97	0.45
20:t:43:MET:HE1	20:t:67:LEU:HD23	1.97	0.45
34:x:42:ARG:HE	34:x:72:ARG:HD2	1.82	0.45
1:A:347:ASP:OD1	1:A:347:ASP:N	2.47	0.45
1:A:391:GLU:HA	1:A:394:MET:HE2	1.98	0.45
3:C:164:VAL:HG23	3:C:165:ILE:HG23	1.97	0.45
4:D:342:ARG:NH1	24:X:234:GLU:OE2	2.49	0.45
11:K:4:THR:OG1	11:K:5:ARG:N	2.45	0.45
21:U:360:VAL:HG13	21:U:365:CYS:HB2	1.99	0.45
21:U:583:MET:HG3	21:U:584:TYR:N	2.32	0.45
26:Z:174:HIS:HA	26:Z:177:ARG:HE	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:121:GLU:O	28:b:123:ASP:N	2.50	0.45
32:f:478:ARG:HH12	32:f:509:LYS:HD2	1.81	0.45
7:g:54:LYS:N	7:g:214:GLU:O	2.40	0.45
10:j:199:VAL:HG12	10:j:202:GLY:H	1.81	0.45
16:p:27:ARG:HB2	16:p:183:MET:HB2	1.98	0.45
20:t:74:GLU:HG3	20:t:83:TYR:CE2	2.52	0.45
34:z:50:LEU:HD11	34:z:67:LEU:HD22	1.98	0.45
4:D:39:ASP:O	4:D:42:SER:OG	2.31	0.44
16:P:53:LEU:HB3	16:P:60:VAL:HG22	1.98	0.44
16:P:102:PRO:HG2	16:P:104:TYR:HE1	1.82	0.44
17:Q:95:ARG:NE	17:Q:95:ARG:O	2.50	0.44
25:Y:169:GLU:OE1	25:Y:169:GLU:N	2.43	0.44
30:d:51:ALA:HA	30:d:54:ILE:HG12	1.98	0.44
34:w:37:PRO:HD2	34:w:40:GLN:HE21	1.82	0.44
2:B:360:THR:O	2:B:364:ILE:HG12	2.16	0.44
4:D:353:ASN:HB3	5:E:162:VAL:HA	1.98	0.44
7:G:165:ALA:HB3	8:H:56:LEU:HD22	2.00	0.44
8:H:114:VAL:HA	8:H:117:VAL:HG12	2.00	0.44
15:O:120:ASP:OD1	15:O:121:LYS:N	2.50	0.44
23:W:314:LEU:HD23	23:W:362:ASN:HB3	1.98	0.44
24:X:144:GLN:HB3	24:X:148:HIS:CE1	2.53	0.44
32:f:783:SER:HB2	32:f:787:LEU:HD13	2.00	0.44
7:g:70:PHE:O	7:g:78:CYS:N	2.43	0.44
10:j:212:ARG:HB3	10:j:215:GLN:HG3	1.99	0.44
3:C:89:VAL:HG23	3:C:90:HIS:H	1.81	0.44
5:E:194:ASN:OD1	5:E:226:GLN:NE2	2.50	0.44
7:G:69:LEU:HD13	7:G:229:ILE:HG12	1.99	0.44
13:M:76:ALA:HB3	13:M:136:MET:HB3	1.99	0.44
13:M:108:LEU:HD12	13:M:111:LEU:HD11	1.99	0.44
23:W:230:MET:HG3	23:W:246:HIS:CD2	2.53	0.44
24:X:374:PHE:HZ	24:X:387:ILE:HG13	1.83	0.44
28:b:20:ASP:CG	28:b:25:ARG:HH21	2.25	0.44
8:h:93:LEU:HD11	8:h:117:VAL:HG21	1.99	0.44
15:o:190:THR:HG22	15:o:192:PRO:HD3	1.98	0.44
17:q:21:ALA:HB3	17:q:29:LYS:HB3	1.99	0.44
4:D:133:HIS:HB3	4:D:137:ASN:N	2.33	0.44
4:D:271:ALA:HB3	4:D:317:LEU:HD22	1.99	0.44
4:D:336:PRO:CG	4:D:369:LYS:HB3	2.48	0.44
5:E:194:ASN:C	5:E:196:LEU:H	2.24	0.44
7:G:41:ALA:N	7:G:166:THR:O	2.47	0.44
9:I:21:VAL:HG11	9:I:153:SER:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:23:GLN:HE22	10:J:150:SER:HB3	1.82	0.44
10:J:146:GLN:O	10:J:154:HIS:N	2.42	0.44
14:N:109:GLY:O	14:N:122:ARG:NH2	2.50	0.44
20:T:9:THR:OG1	20:T:10:SER:N	2.48	0.44
30:d:182:ILE:HA	30:d:186:TYR:HD2	1.83	0.44
32:f:809:ILE:HG23	32:f:814:SER:HB2	1.98	0.44
7:G:17:SER:N	7:G:21:ARG:O	2.45	0.44
7:G:238:HIS:O	7:G:242:LEU:HB2	2.17	0.44
10:J:152:THR:OG1	10:J:154:HIS:NE2	2.50	0.44
13:M:171:ALA:HA	13:M:174:THR:HG22	1.99	0.44
23:W:347:GLY:O	23:W:351:TRP:N	2.45	0.44
25:Y:334:LEU:HD22	25:Y:343:LEU:HD21	1.99	0.44
26:Z:21:ASP:OD1	26:Z:22:HIS:N	2.50	0.44
27:a:217:LEU:HD21	27:a:237:LEU:HB3	1.99	0.44
27:a:246:GLU:OE1	27:a:249:GLN:HB2	2.18	0.44
30:d:67:ASP:HB3	30:d:70:SER:HB2	1.99	0.44
14:n:95:MET:HA	14:n:116:MET:HE1	1.99	0.44
15:o:129:SER:OG	15:o:166:ASP:OD2	2.23	0.44
34:z:31:GLN:CG	34:z:37:PRO:HA	2.47	0.44
4:D:88:VAL:HG23	4:D:132:LEU:HB2	2.00	0.44
4:D:204:MET:HB2	4:D:310:ALA:HA	2.00	0.44
6:F:226:TYR:CZ	6:F:353:GLU:HB3	2.52	0.44
10:J:189:LYS:HA	10:J:232:ILE:HD11	2.00	0.44
12:L:72:ILE:HG22	12:L:134:ILE:HG13	1.99	0.44
12:L:117:GLN:O	12:L:120:THR:OG1	2.28	0.44
21:U:184:CYS:SG	21:U:194:ARG:NE	2.79	0.44
27:a:220:PRO:O	27:a:224:SER:OG	2.30	0.44
8:h:42:ASN:HD21	8:h:184:LEU:H	1.65	0.44
11:k:91:LYS:NZ	11:k:115:ALA:O	2.50	0.44
18:r:3:THR:HG23	18:r:16:ALA:HB2	1.99	0.44
19:s:198:VAL:HA	19:s:203:ILE:HG12	1.98	0.44
34:z:71:LEU:HD22	34:z:71:LEU:HA	1.78	0.44
2:B:352:GLU:OE2	2:B:353:PHE:N	2.51	0.44
3:C:365:GLU:OE2	4:D:329:ARG:NH1	2.50	0.44
4:D:159:LYS:HB3	4:D:160:PRO:HD3	2.00	0.44
7:G:70:PHE:N	7:G:78:CYS:O	2.41	0.44
14:N:160:LEU:O	14:N:164:MET:HG2	2.18	0.44
18:R:97:MET:N	18:R:116:SER:HB3	2.27	0.44
29:c:231:LEU:C	29:c:233:ASP:H	2.25	0.44
32:f:384:ALA:HA	32:f:419:LEU:HB3	1.99	0.44
32:f:413:SER:O	32:f:417:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:495:GLU:HA	32:f:498:LEU:HD23	2.00	0.44
3:C:267:SER:O	3:C:271:ARG:HG2	2.18	0.44
6:F:344:ARG:O	6:F:345:SER:HB3	2.18	0.44
8:H:72:ILE:HD13	8:H:110:LEU:HD12	1.99	0.44
9:I:54:LYS:HG3	9:I:55:LEU:HD12	1.98	0.44
10:J:11:SER:OG	10:J:15:HIS:N	2.51	0.44
11:K:52:LYS:HB3	11:K:54:ILE:HG12	1.98	0.44
11:K:240:ASP:OD1	11:K:240:ASP:N	2.42	0.44
17:Q:55:GLN:HG3	18:R:88:TYR:CZ	2.53	0.44
23:W:194:LEU:HG	23:W:202:THR:HG21	1.99	0.44
23:W:234:ASP:HA	23:W:237:GLU:HB2	1.98	0.44
26:Z:145:HIS:CD2	26:Z:152:SER:N	2.85	0.44
28:b:9:CYS:HB3	28:b:111:ALA:HA	2.00	0.44
28:b:125:VAL:O	28:b:129:LYS:HG3	2.18	0.44
32:f:143:ARG:NH2	32:f:149:GLU:O	2.51	0.44
9:i:136:TYR:HB2	9:i:148:TYR:HB2	2.00	0.44
17:q:32:HIS:HB3	17:q:34:LYS:HZ2	1.83	0.44
17:q:39:SER:HB3	17:q:42:ILE:HB	2.00	0.44
5:E:237:ALA:N	5:E:242:ARG:HH22	2.16	0.44
10:J:185:ASP:OD1	10:J:185:ASP:N	2.51	0.44
12:L:22:ILE:HD12	12:L:25:ALA:HB3	2.00	0.44
12:L:152:ASN:HD21	13:M:81:LEU:HD22	1.83	0.44
12:L:167:SER:HB3	12:L:197:GLU:HG3	1.99	0.44
15:O:122:LEU:HD12	15:O:125:VAL:HG12	2.00	0.44
17:Q:52:ASP:HB3	17:Q:56:PHE:CE2	2.53	0.44
15:o:143:ARG:H	15:o:146:MET:HE2	1.82	0.44
20:t:43:MET:HG3	20:t:64:LYS:HG3	1.98	0.44
2:B:64:LYS:O	2:B:68:ILE:HG12	2.18	0.43
3:C:25:LEU:HA	3:C:28:ILE:HG12	2.00	0.43
3:C:368:MET:HE1	3:C:372:ARG:HH21	1.82	0.43
5:E:272:ARG:O	5:E:274:LYS:NZ	2.51	0.43
6:F:381:TYR:HA	6:F:384:LEU:HD12	2.00	0.43
8:H:133:SER:H	8:H:163:MET:HE1	1.82	0.43
11:K:141:LEU:HB2	11:K:156:MET:HB3	1.99	0.43
12:L:69:HIS:CE1	12:L:102:PRO:HB3	2.53	0.43
18:R:178:HIS:HB3	18:R:185:ILE:HG13	2.00	0.43
20:T:2:GLN:NE2	20:T:103:MET:O	2.51	0.43
21:U:266:GLN:O	21:U:269:ARG:NH1	2.51	0.43
23:W:27:ARG:HG3	23:W:50:LEU:HD11	2.00	0.43
23:W:119:PRO:HA	23:W:122:LEU:HG	2.00	0.43
23:W:281:ASN:O	23:W:285:ASP:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:268:LEU:HD23	27:a:271:LYS:HD3	2.00	0.43
32:f:271:MET:HE3	32:f:787:LEU:HG	2.00	0.43
18:r:103:GLY:HA2	18:r:179:VAL:HG11	2.00	0.43
3:C:156:LYS:O	3:C:160:GLU:HG2	2.19	0.43
3:C:307:ARG:CZ	3:C:310:ARG:HE	2.31	0.43
4:D:163:MET:SD	4:D:166:ASP:N	2.91	0.43
7:G:112:ASP:N	7:G:112:ASP:OD1	2.51	0.43
8:H:196:LYS:HG3	8:H:203:MET:HE1	2.00	0.43
10:J:130:SER:OG	10:J:147:THR:O	2.33	0.43
11:K:93:ARG:NH1	18:R:68:LEU:O	2.51	0.43
13:M:109:LYS:NZ	14:N:70:LEU:HA	2.33	0.43
15:O:163:ILE:HG12	15:O:170:GLY:HA2	2.00	0.43
16:P:205:ASP:HB3	18:r:192:VAL:HG11	1.99	0.43
21:U:220:LEU:HG	21:U:229:VAL:HB	1.98	0.43
24:X:309:TYR:HB3	24:X:312:GLU:HB2	2.00	0.43
25:Y:84:LEU:HD13	25:Y:107:LYS:HA	2.00	0.43
27:a:344:GLN:H	27:a:344:GLN:CD	2.25	0.43
7:g:185:LYS:H	7:g:185:LYS:HG2	1.70	0.43
8:h:175:GLU:HG3	9:i:54:LYS:HD3	2.00	0.43
13:m:230:ASP:OD1	13:m:230:ASP:N	2.50	0.43
15:o:13:VAL:HG22	15:o:177:VAL:HG22	1.99	0.43
17:q:29:LYS:HD3	17:q:32:HIS:HD2	1.83	0.43
34:w:41:GLN:HB3	34:w:71:LEU:HG	2.00	0.43
5:E:148:VAL:HG13	5:E:149:ILE:HG13	2.00	0.43
6:F:221:LYS:NZ	6:F:317:LEU:O	2.40	0.43
8:H:222:THR:HG1	8:H:225:GLU:CD	2.23	0.43
17:Q:173:LEU:HD13	17:q:173:LEU:HD23	1.99	0.43
21:U:30:VAL:HG13	30:d:36:LEU:HD21	1.99	0.43
23:W:140:ILE:HG12	23:W:177:MET:HB2	2.01	0.43
28:b:125:VAL:HG13	28:b:159:THR:HG21	2.00	0.43
28:b:135:LYS:HB2	34:z:40:GLN:HE22	1.83	0.43
29:c:296:ILE:HG23	29:c:300:LEU:HD13	2.00	0.43
32:f:446:LEU:HD12	32:f:480:GLY:HA2	2.01	0.43
7:g:43:ARG:HH21	7:g:164:LYS:HA	1.83	0.43
18:r:131:GLY:HA2	18:r:134:TYR:HD2	1.83	0.43
20:t:70:MET:HE1	20:t:91:TRP:CZ2	2.53	0.43
2:B:293:LYS:NZ	2:B:335:GLU:O	2.41	0.43
4:D:391:ARG:HH12	4:D:395:LEU:N	2.17	0.43
10:J:111:ILE:HD11	10:J:147:THR:HG21	1.99	0.43
14:N:166:ARG:NH1	20:t:34:ALA:O	2.36	0.43
17:Q:171:PHE:CE2	17:Q:173:LEU:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:181:LEU:HG	21:U:218:GLN:NE2	2.34	0.43
23:W:84:ASN:O	23:W:88:MET:HG2	2.18	0.43
24:X:213:GLN:HA	24:X:216:ILE:HB	2.00	0.43
27:a:34:TRP:O	27:a:38:THR:OG1	2.31	0.43
28:b:109:ILE:HB	28:b:138:VAL:HG22	1.99	0.43
7:g:10:ASP:OD1	7:g:10:ASP:N	2.50	0.43
17:q:108:ASP:N	17:q:112:GLY:O	2.51	0.43
34:z:42:ARG:HA	34:z:42:ARG:NE	2.32	0.43
1:A:38:GLN:HG2	2:B:57:GLN:HB3	2.01	0.43
1:A:393:GLY:O	1:A:397:ILE:HG13	2.18	0.43
4:D:398:ASP:OD1	4:D:398:ASP:N	2.49	0.43
5:E:196:LEU:HB3	5:E:197:LYS:H	1.62	0.43
9:I:134:LEU:N	9:I:150:SER:OG	2.48	0.43
13:M:15:SER:OG	13:M:19:ARG:N	2.52	0.43
19:S:43:CYS:O	19:S:194:ARG:NH2	2.51	0.43
22:V:368:ARG:HH22	31:e:46:ASP:HB2	1.84	0.43
23:W:423:ASN:O	23:W:427:ASP:N	2.44	0.43
26:Z:269:VAL:HG12	26:Z:273:HIS:CE1	2.54	0.43
7:g:89:SER:HB3	13:m:117:MET:HE1	2.00	0.43
3:C:164:VAL:HG11	3:C:313:ARG:HG3	2.00	0.43
10:J:172:LEU:O	10:J:176:TYR:HB2	2.18	0.43
12:L:16:GLN:HG3	12:L:18:ARG:NE	2.34	0.43
18:R:140:ASP:OD1	17:q:170:ARG:NH2	2.50	0.43
20:T:5:MET:HE3	20:T:30:TYR:HE1	1.84	0.43
21:U:37:GLU:HG3	22:V:269:LYS:HD2	2.00	0.43
22:V:452:ASN:HB3	22:V:457:TYR:HB2	2.00	0.43
23:W:155:GLN:NE2	23:W:156:ASN:OD1	2.51	0.43
25:Y:23:ARG:O	25:Y:27:SER:N	2.51	0.43
25:Y:238:GLU:HA	25:Y:242:LYS:HB2	2.01	0.43
28:b:132:LYS:HE2	34:z:42:ARG:CB	2.32	0.43
29:c:278:GLN:O	29:c:282:ARG:HG3	2.18	0.43
13:m:37:ILE:HD11	13:m:193:VAL:HG13	2.00	0.43
18:r:4:LEU:HA	18:r:127:SER:HA	1.99	0.43
18:r:21:THR:HG22	18:r:26:ILE:HG12	1.99	0.43
19:s:199:THR:OG1	19:s:202:GLY:O	2.29	0.43
1:A:375:ARG:NE	11:K:173:ALA:HA	2.33	0.43
5:E:360:ASP:N	5:E:360:ASP:OD1	2.49	0.43
6:F:380:ASN:HB3	6:F:383:GLU:HB2	2.01	0.43
7:G:174:GLU:O	7:G:177:SER:OG	2.27	0.43
16:P:25:ASP:OD1	16:P:25:ASP:N	2.50	0.43
21:U:620:GLU:HG3	21:U:651:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:171:VAL:HG12	23:W:182:ARG:HG3	1.99	0.43
25:Y:223:THR:HA	25:Y:226:VAL:HG22	2.01	0.43
32:f:445:LEU:HG	32:f:466:LEU:HD13	2.01	0.43
32:f:564:LEU:C	32:f:566:HIS:H	2.27	0.43
1:A:113:ILE:HD11	1:A:149:ILE:HD11	1.99	0.43
1:A:169:LYS:HD3	1:A:169:LYS:HA	1.74	0.43
3:C:375:ARG:NE	3:C:377:HIS:HB2	2.34	0.43
4:D:318:ASP:HB3	4:D:321:LEU:HD23	2.01	0.43
5:E:98:VAL:HA	5:E:110:TYR:HA	2.00	0.43
6:F:87:PRO:HB3	6:F:155:LYS:HE2	2.01	0.43
6:F:92:ASN:HB2	6:F:125:LYS:HB3	2.01	0.43
18:R:63:CYS:O	18:R:67:GLU:HG2	2.19	0.43
19:S:113:LEU:HG	19:S:198:VAL:HG12	2.00	0.43
20:T:67:LEU:HA	20:T:70:MET:HE2	1.99	0.43
20:T:126:ASP:OD1	20:T:130:VAL:N	2.51	0.43
24:X:6:VAL:HG22	24:X:45:VAL:HG21	2.00	0.43
24:X:89:VAL:HG21	24:X:125:LEU:HD11	2.01	0.43
24:X:137:TYR:CG	24:X:142:ARG:HD2	2.54	0.43
27:a:343:LEU:C	27:a:345:GLN:N	2.77	0.43
32:f:372:LEU:HD13	32:f:406:GLY:HA2	1.99	0.43
32:f:600:TYR:CE2	32:f:608:LYS:HE3	2.54	0.43
7:g:10:ASP:CG	7:g:11:ARG:HE	2.27	0.43
11:k:13:ASN:HB2	12:l:126:ARG:HB3	2.01	0.43
17:q:107:TYR:HA	17:q:113:PRO:HA	2.00	0.43
18:r:87:VAL:HG11	18:r:97:MET:HE2	2.00	0.43
1:A:364:VAL:HA	1:A:404:ALA:H	1.84	0.43
4:D:204:MET:HE2	4:D:310:ALA:HB2	1.99	0.43
4:D:320:ALA:O	4:D:326:ARG:NH1	2.45	0.43
7:G:143:ILE:HA	7:G:149:PRO:HA	2.00	0.43
23:W:240:TYR:HA	23:W:243:ILE:HD12	2.00	0.43
25:Y:41:LEU:HD21	25:Y:57:LEU:HD21	2.00	0.43
27:a:370:GLN:HG2	30:d:244:LYS:HD2	2.01	0.43
29:c:37:ALA:O	29:c:41:MET:HG2	2.18	0.43
29:c:303:MET:O	29:c:306:THR:OG1	2.29	0.43
18:r:139:MET:HE2	18:r:143:TYR:HB2	2.00	0.43
3:C:175:PHE:HD1	3:C:178:LEU:HD12	1.84	0.43
4:D:129:SER:O	4:D:143:LEU:N	2.48	0.43
4:D:297:ASP:HB3	4:D:326:ARG:HH21	1.83	0.43
4:D:368:ASP:HB3	4:D:407:ILE:HD11	2.01	0.43
6:F:175:MET:HE2	6:F:251:LEU:HA	2.00	0.43
17:Q:11:ASP:N	17:Q:11:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:174:VAL:N	18:R:190:ASP:O	2.45	0.43
21:U:161:ASP:OD1	21:U:161:ASP:N	2.50	0.43
21:U:765:VAL:HG12	21:U:775:LEU:HB3	2.01	0.43
26:Z:198:LEU:HD21	27:a:360:VAL:HG13	2.01	0.43
30:d:61:TRP:CG	30:d:65:ARG:HH21	2.36	0.43
32:f:79:ARG:HH11	32:f:121:PHE:HE1	1.66	0.43
19:s:95:ILE:O	19:s:98:SER:OG	2.25	0.43
1:A:391:GLU:HG2	1:A:415:LYS:HG2	2.01	0.42
4:D:338:ARG:HH22	4:D:365:ALA:HA	1.84	0.42
6:F:376:SER:HB3	6:F:414:GLU:HG3	2.00	0.42
7:G:71:LYS:HE3	7:G:74:GLU:HA	2.01	0.42
9:I:239:LYS:O	9:I:242:GLU:N	2.50	0.42
13:M:99:ARG:NH2	13:M:105:ASN:OD1	2.49	0.42
20:T:179:ARG:HB3	14:n:25:TYR:HE1	1.84	0.42
25:Y:205:VAL:HA	25:Y:219:PHE:HE2	1.83	0.42
26:Z:62:ASP:OD1	26:Z:62:ASP:N	2.51	0.42
29:c:278:GLN:N	29:c:282:ARG:HE	2.17	0.42
32:f:85:SER:HB2	32:f:93:PRO:HB3	2.00	0.42
32:f:447:ALA:HA	32:f:450:ILE:HD12	2.01	0.42
32:f:842:VAL:O	32:f:870:THR:N	2.36	0.42
7:g:132:ARG:HB2	13:m:12:SER:HA	2.01	0.42
14:n:36:PRO:HA	14:n:42:PHE:CD1	2.54	0.42
16:p:112:LEU:HD23	16:p:119:PRO:HA	2.01	0.42
20:t:46:ASN:OD1	20:t:49:THR:N	2.52	0.42
5:E:172:LEU:HD12	5:E:278:ALA:HB2	2.01	0.42
10:J:2:SER:OG	10:J:3:TYR:N	2.52	0.42
10:J:121:SER:HB3	10:J:124:ARG:HD2	2.01	0.42
13:M:160:TYR:CG	13:M:163:CYS:HB2	2.54	0.42
20:T:174:ARG:NH1	20:T:206:GLU:O	2.52	0.42
21:U:358:ASP:N	21:U:358:ASP:OD1	2.51	0.42
21:U:803:LYS:HD2	21:U:875:PHE:CG	2.54	0.42
22:V:309:MET:HE1	22:V:328:VAL:HG22	2.00	0.42
24:X:310:ARG:HB3	24:X:314:ARG:HE	1.84	0.42
25:Y:98:SER:OG	25:Y:101:ARG:NH2	2.53	0.42
25:Y:240:VAL:HG23	25:Y:241:ILE:HG13	2.00	0.42
9:i:31:ALA:O	9:i:166:ASN:ND2	2.52	0.42
11:k:185:TYR:HA	11:k:189:MET:HE1	2.00	0.42
13:m:228:PRO:HD2	13:m:231:ILE:HD12	2.01	0.42
34:z:36:ILE:CG2	34:z:41:GLN:HB3	2.49	0.42
3:C:79:ALA:HA	3:C:85:VAL:HA	2.00	0.42
6:F:152:GLY:N	6:F:162:GLU:O	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:14:SER:OG	12:L:18:ARG:O	2.33	0.42
21:U:794:ASP:N	21:U:794:ASP:OD1	2.50	0.42
28:b:5:SER:HB3	28:b:64:LEU:HD21	2.01	0.42
30:d:135:HIS:NE2	30:d:157:ASN:O	2.52	0.42
32:f:490:ALA:HA	32:f:525:ILE:HA	2.02	0.42
10:j:160:ALA:O	10:j:169:ARG:NH2	2.52	0.42
13:m:68:ASN:HD21	13:m:224:HIS:CG	2.35	0.42
16:p:38:ASP:OD1	16:p:38:ASP:N	2.51	0.42
5:E:363:VAL:HG13	5:E:366:ASP:H	1.84	0.42
6:F:94:ILE:HD12	6:F:123:VAL:HG12	2.02	0.42
7:G:125:TYR:HA	7:G:128:ASN:HD21	1.84	0.42
8:H:118:MET:HB2	8:H:130:PHE:HZ	1.83	0.42
11:K:24:VAL:O	11:K:28:ILE:HG12	2.20	0.42
21:U:615:ARG:O	21:U:619:VAL:HG22	2.19	0.42
21:U:770:TRP:HZ3	29:c:183:HIS:HE1	1.67	0.42
23:W:166:LEU:HD23	23:W:189:GLN:HA	2.01	0.42
23:W:433:ASN:HA	23:W:436:MET:HE2	2.00	0.42
27:a:371:ALA:HB1	27:a:374:ILE:HD11	2.02	0.42
28:b:141:ILE:HA	28:b:171:VAL:HB	2.02	0.42
29:c:265:MET:SD	29:c:270:LEU:HD12	2.59	0.42
16:p:125:ASP:OD1	16:p:129:CYS:N	2.42	0.42
1:A:219:GLY:HA2	35:A:501:ATP:H5'1	2.02	0.42
3:C:307:ARG:HG3	3:C:309:GLY:H	1.85	0.42
5:E:198:VAL:HG21	5:E:232:MET:HG3	2.01	0.42
6:F:221:LYS:HA	6:F:327:LYS:HD3	2.02	0.42
9:I:215:THR:N	9:I:226:ARG:O	2.45	0.42
10:J:67:ASP:OD1	10:J:67:ASP:N	2.52	0.42
11:K:117:SER:HA	11:K:120:ALA:HB3	2.01	0.42
22:V:92:ARG:HD2	22:V:95:LEU:HD12	2.01	0.42
25:Y:74:LYS:HB3	25:Y:74:LYS:HE3	1.85	0.42
8:h:10:LEU:HD13	8:h:126:GLY:H	1.84	0.42
8:h:65:VAL:O	8:h:220:ARG:NH1	2.49	0.42
12:l:40:SER:N	12:l:43:HIS:O	2.46	0.42
15:o:138:PHE:O	15:o:142:PHE:CB	2.66	0.42
3:C:20:LEU:HD12	3:C:21:ARG:HG3	2.01	0.42
3:C:194:THR:HB	3:C:196:LYS:HZ2	1.84	0.42
4:D:230:VAL:HB	4:D:264:ILE:HG13	2.01	0.42
4:D:335:LEU:HD23	4:D:335:LEU:HA	1.78	0.42
5:E:124:HIS:O	5:E:196:LEU:HA	2.19	0.42
5:E:165:ILE:HG22	5:E:266:GLY:HA2	2.01	0.42
5:E:247:THR:O	5:E:249:ALA:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:153:SER:OG	9:I:155:ASN:ND2	2.52	0.42
19:S:46:LEU:HD23	19:S:72:LEU:HD11	2.01	0.42
22:V:95:LEU:HD11	25:Y:389:MET:HE3	2.01	0.42
22:V:465:ASP:OD1	22:V:466:ILE:N	2.47	0.42
26:Z:20:VAL:HG22	26:Z:126:VAL:HG23	2.02	0.42
26:Z:190:ARG:HG3	29:c:297:VAL:HG21	2.00	0.42
29:c:27:THR:HA	29:c:175:ARG:HA	2.01	0.42
29:c:54:MET:SD	29:c:113:HIS:HB3	2.60	0.42
31:e:57:ARG:HA	31:e:60:LEU:HG	1.99	0.42
13:m:163:CYS:SG	13:m:164:ALA:N	2.91	0.42
15:o:41:ILE:HG12	15:o:76:VAL:HG22	2.00	0.42
34:z:31:GLN:HB2	34:z:38:PRO:HD3	2.02	0.42
34:z:42:ARG:HE	34:z:42:ARG:CA	2.33	0.42
1:A:299:MET:HA	1:A:302:LEU:HD12	2.00	0.42
2:B:387:LYS:HD3	2:B:387:LYS:HA	1.86	0.42
4:D:202:VAL:HA	4:D:329:ARG:HB2	2.00	0.42
4:D:244:PRO:HD3	4:D:288:ILE:HG12	2.00	0.42
5:E:252:GLU:HA	5:E:255:ARG:HH21	1.85	0.42
21:U:558:GLY:HA2	21:U:560:MET:HE3	2.01	0.42
23:W:120:ILE:HG23	23:W:123:ARG:HH21	1.84	0.42
24:X:74:ARG:HH21	24:X:116:TRP:HD1	1.67	0.42
24:X:148:HIS:HA	25:Y:2:PRO:HB3	2.00	0.42
25:Y:155:ASP:OD1	25:Y:155:ASP:N	2.51	0.42
26:Z:239:ASP:OD1	26:Z:239:ASP:N	2.53	0.42
29:c:232:GLN:NE2	29:c:236:GLU:HB2	2.35	0.42
15:o:202:TYR:OH	16:p:153:LEU:O	2.35	0.42
16:p:29:GLY:HA2	16:p:35:VAL:HG23	2.02	0.42
34:w:15:LEU:HG	34:w:17:VAL:HG13	2.00	0.42
2:B:198:LYS:HB2	2:B:198:LYS:HE2	1.76	0.42
35:B:501:ATP:O3B	3:C:307:ARG:NH1	2.53	0.42
3:C:377:HIS:CD2	25:Y:174:TRP:HH2	2.37	0.42
4:D:335:LEU:HB2	4:D:336:PRO:HD3	2.00	0.42
4:D:414:HIS:O	4:D:416:PHE:N	2.46	0.42
7:G:212:PRO:HB2	7:G:232:GLU:HG2	2.01	0.42
11:K:236:GLU:HA	11:K:239:LYS:HE3	1.99	0.42
16:P:28:PHE:HB2	16:P:39:PHE:HB2	2.02	0.42
19:S:71:ARG:HA	19:S:74:MET:HG3	2.02	0.42
21:U:367:THR:HA	21:U:370:VAL:HG22	2.01	0.42
28:b:122:LYS:HG3	28:b:123:ASP:N	2.34	0.42
32:f:239:TYR:CE1	32:f:666:ILE:HD12	2.55	0.42
32:f:572:ALA:O	32:f:573:ILE:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:28:ALA:O	7:g:32:ILE:HG13	2.19	0.42
11:k:209:LYS:NZ	11:k:210:LEU:O	2.53	0.42
34:w:27:LYS:HB3	34:w:38:PRO:HB3	2.01	0.42
4:D:210:CYS:SG	4:D:333:PHE:HB3	2.59	0.42
5:E:256:THR:HG22	5:E:260:LEU:HD23	2.02	0.42
9:I:136:TYR:HB2	9:I:148:TYR:HB2	2.02	0.42
14:N:36:PRO:HA	14:N:42:PHE:CD1	2.55	0.42
17:Q:9:GLY:HA3	17:Q:12:TYR:CZ	2.55	0.42
21:U:21:GLU:OE2	21:U:56:SER:OG	2.37	0.42
21:U:103:LYS:HB2	21:U:103:LYS:HE3	1.82	0.42
21:U:406:ALA:HA	21:U:445:ALA:HB2	2.02	0.42
23:W:362:ASN:HA	23:W:365:ILE:HG12	2.01	0.42
7:g:144:ASP:O	7:g:148:GLY:N	2.53	0.42
8:h:34:PRO:O	8:h:48:THR:OG1	2.32	0.42
8:h:40:ALA:N	8:h:43:GLY:O	2.51	0.42
18:r:42:LEU:HB2	18:r:102:CYS:HB2	2.01	0.42
19:s:148:LEU:HD23	19:s:178:VAL:HG12	2.00	0.42
34:w:37:PRO:HD2	34:w:40:GLN:NE2	2.35	0.42
4:D:292:LEU:O	4:D:296:MET:HG3	2.20	0.42
10:J:110:TYR:O	10:J:113:SER:OG	2.33	0.42
16:P:183:MET:HG3	16:P:204:MET:HA	2.00	0.42
21:U:423:MET:HE2	21:U:442:GLY:HA3	2.01	0.42
25:Y:237:ARG:HA	25:Y:241:ILE:HD12	2.02	0.42
25:Y:288:PHE:CE1	25:Y:292:TYR:HB2	2.55	0.42
28:b:126:LYS:HD2	34:z:72:ARG:HD2	2.01	0.42
8:h:166:ASN:ND2	8:h:169:ASN:OD1	2.48	0.42
9:i:241:GLU:HA	9:i:244:GLU:HG3	2.01	0.42
12:l:45:VAL:HG22	12:l:214:ILE:HG12	2.01	0.42
17:q:101:ASN:OD1	17:q:120:TYR:N	2.53	0.42
19:s:16:ALA:HB2	19:s:121:VAL:HG23	2.02	0.42
20:t:26:MET:HE1	20:t:186:ARG:HG2	2.01	0.42
1:A:140:VAL:HB	1:A:149:ILE:HG23	2.01	0.41
3:C:347:ILE:HA	3:C:350:LEU:HD12	2.00	0.41
5:E:188:ALA:HB2	5:E:195:PHE:CZ	2.55	0.41
7:G:137:CYS:SG	7:G:138:MET:N	2.93	0.41
8:H:118:MET:HE1	8:H:151:PRO:HA	2.02	0.41
15:O:20:ALA:HB3	15:O:28:ASP:HB3	2.02	0.41
21:U:65:SER:OG	21:U:77:SER:O	2.38	0.41
21:U:212:ASP:H	21:U:215:ASN:HD21	1.67	0.41
21:U:320:ASP:HB3	21:U:321:GLN:H	1.67	0.41
21:U:397:THR:OG1	21:U:398:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:563:ALA:O	21:U:567:ILE:HG12	2.19	0.41
22:V:61:GLU:OE1	22:V:65:ARG:NH2	2.52	0.41
23:W:24:VAL:O	23:W:28:LEU:HG	2.20	0.41
23:W:251:TYR:CZ	23:W:267:LEU:HD13	2.54	0.41
23:W:357:ARG:HD3	23:W:357:ARG:HA	1.73	0.41
25:Y:312:ARG:HA	25:Y:356:THR:HG22	2.01	0.41
27:a:127:ASP:HA	27:a:131:THR:HG21	2.01	0.41
27:a:138:VAL:HA	27:a:141:MET:HE2	2.02	0.41
32:f:298:LEU:O	32:f:302:GLY:N	2.52	0.41
9:i:82:ASP:HB3	9:i:130:PHE:HD1	1.85	0.41
10:j:49:SER:O	10:j:51:ALA:N	2.53	0.41
1:A:194:PRO:HB3	1:A:201:PHE:HE2	1.85	0.41
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.90	0.41
4:D:60:TYR:HB2	21:U:603:LEU:HD21	2.03	0.41
5:E:135:ILE:HG22	5:E:182:LEU:HD23	2.02	0.41
8:H:3:GLU:HB3	8:H:4:ARG:H	1.59	0.41
12:L:234:GLU:OE1	12:L:234:GLU:N	2.49	0.41
13:M:77:VAL:HG11	13:M:84:ALA:HB1	2.02	0.41
13:M:164:ALA:HB3	13:M:173:LYS:HG3	2.03	0.41
15:O:14:LEU:O	15:O:176:CYS:N	2.49	0.41
18:R:81:LYS:HE2	18:R:120:ARG:CZ	2.49	0.41
20:T:13:GLY:N	20:T:137:LEU:O	2.53	0.41
21:U:226:PRO:HG3	21:U:263:SER:HB2	2.02	0.41
21:U:791:LEU:HD23	21:U:911:ILE:HD11	2.01	0.41
23:W:188:GLU:OE2	23:W:225:LYS:NZ	2.38	0.41
24:X:258:LYS:HD3	24:X:266:ASP:HB3	2.03	0.41
24:X:270:LEU:HD23	24:X:270:LEU:HA	1.94	0.41
24:X:400:ALA:O	24:X:403:THR:OG1	2.34	0.41
25:Y:367:GLN:HA	25:Y:370:ILE:HG12	2.02	0.41
8:h:203:MET:HA	8:h:207:ASN:HD21	1.84	0.41
14:n:167:ASP:HB3	14:n:170:SER:HB2	2.01	0.41
16:p:53:LEU:HB3	16:p:60:VAL:HG22	2.02	0.41
16:p:159:ASP:OD1	16:p:159:ASP:N	2.53	0.41
17:q:164:LEU:HD23	17:q:167:LEU:HD12	2.02	0.41
1:A:53:GLN:HG3	1:A:57:LYS:HZ3	1.85	0.41
4:D:268:ASP:OD1	4:D:268:ASP:N	2.51	0.41
5:E:238:ILE:HD13	5:E:253:ILE:HD11	2.00	0.41
6:F:70:LYS:O	6:F:74:LYS:NZ	2.44	0.41
6:F:88:TYR:O	6:F:89:LEU:C	2.62	0.41
21:U:757:MET:SD	21:U:757:MET:N	2.93	0.41
23:W:55:ARG:NH1	23:W:96:GLN:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:377:ILE:HG12	25:Y:312:ARG:HB3	2.03	0.41
25:Y:189:VAL:HG13	25:Y:194:PHE:HE1	1.84	0.41
29:c:137:SER:OG	29:c:138:GLU:N	2.53	0.41
7:g:128:ASN:HB3	7:g:131:MET:HE1	2.02	0.41
10:j:80:ALA:HB2	10:j:129:ILE:HG21	2.01	0.41
11:k:40:ILE:HD12	11:k:198:SER:HB2	2.01	0.41
12:l:226:ASP:OD1	12:l:226:ASP:N	2.50	0.41
19:s:71:ARG:HA	19:s:74:MET:HG3	2.02	0.41
2:B:106:PRO:O	2:B:154:HIS:ND1	2.48	0.41
2:B:224:LEU:HB2	2:B:330:ALA:HA	2.01	0.41
2:B:288:ASP:OD1	2:B:288:ASP:N	2.51	0.41
4:D:404:LYS:HA	4:D:407:ILE:HG22	2.02	0.41
14:N:7:GLN:HB2	14:N:111:VAL:HG23	2.03	0.41
15:O:143:ARG:NH1	15:O:144:PRO:O	2.53	0.41
16:P:7:ASN:O	16:P:27:ARG:NH1	2.53	0.41
16:P:103:TYR:HA	17:Q:93:ARG:HH22	1.85	0.41
17:Q:13:VAL:HG11	17:Q:105:ALA:HB1	2.02	0.41
19:S:99:ARG:NE	19:S:102:PHE:O	2.34	0.41
22:V:192:MET:HA	22:V:195:ILE:HG12	2.03	0.41
22:V:224:LEU:HA	22:V:227:VAL:HB	2.02	0.41
22:V:408:ARG:NH1	22:V:446:VAL:O	2.53	0.41
26:Z:39:LEU:H	26:Z:94:TRP:HA	1.84	0.41
27:a:286:ALA:HA	27:a:289:ARG:HB3	2.03	0.41
28:b:63:THR:N	28:b:70:ARG:HH12	2.18	0.41
29:c:161:ARG:HB3	29:c:201:TYR:CZ	2.55	0.41
29:c:284:LEU:HD13	29:c:284:LEU:HA	1.79	0.41
30:d:202:THR:O	30:d:203:PRO:C	2.62	0.41
32:f:59:LEU:HA	32:f:62:ARG:HG2	2.01	0.41
32:f:793:VAL:HA	32:f:796:LEU:HG	2.02	0.41
13:m:215:TRP:CE3	13:m:227:VAL:HG22	2.56	0.41
2:B:41:LYS:HB2	2:B:278:ALA:HB2	2.02	0.41
5:E:198:VAL:HB	5:E:232:MET:HA	2.01	0.41
7:G:167:ALA:HB3	7:G:176:THR:HG23	2.03	0.41
10:J:86:ARG:HG2	10:J:114:LEU:HD11	2.03	0.41
11:K:99:HIS:ND1	11:K:107:MET:HE2	2.35	0.41
13:M:80:LEU:H	13:M:133[B]:CYS:HB2	1.85	0.41
14:N:192:ASP:OD1	14:N:192:ASP:N	2.53	0.41
17:Q:37:LYS:HA	17:Q:43:LEU:HD23	2.03	0.41
21:U:327:LYS:O	21:U:330:SER:OG	2.28	0.41
21:U:445:ALA:HA	21:U:448:LEU:HD12	2.02	0.41
21:U:925:VAL:HG22	21:U:927:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:420:ASP:N	23:W:420:ASP:OD1	2.52	0.41
25:Y:38:ARG:HG2	25:Y:42:MET:HE1	2.02	0.41
28:b:142:ASN:HB2	28:b:172:THR:HA	2.02	0.41
11:k:71:ASP:N	11:k:74:ILE:O	2.38	0.41
34:z:42:ARG:HB3	34:z:70:VAL:CG1	2.50	0.41
1:A:164:MET:HE3	1:A:240:VAL:HA	2.02	0.41
7:G:43:ARG:HH21	7:G:164:LYS:HG2	1.85	0.41
9:I:42:GLY:HA3	9:I:186:LEU:HD21	2.03	0.41
12:L:70:ILE:HD13	12:L:108:LEU:HD13	2.02	0.41
15:O:3:ILE:HD12	15:O:99:VAL:HG23	2.01	0.41
16:P:183:MET:HE2	16:P:183:MET:HB2	1.99	0.41
17:Q:172:ILE:HG23	17:Q:173:LEU:HD22	2.02	0.41
21:U:445:ALA:HA	21:U:448:LEU:HB2	2.03	0.41
22:V:309:MET:HE3	22:V:328:VAL:HG13	2.01	0.41
24:X:310:ARG:O	24:X:314:ARG:NE	2.53	0.41
24:X:351:SER:O	24:X:355:LYS:N	2.53	0.41
25:Y:191:ILE:HA	31:e:39:TRP:HE1	1.86	0.41
28:b:123:ASP:O	28:b:126:LYS:HB2	2.20	0.41
32:f:452:ASN:ND2	32:f:461:PRO:HD2	2.35	0.41
7:g:103:TYR:HB2	14:n:61:TYR:CD1	2.56	0.41
7:g:132:ARG:HA	7:g:133:PRO:HD3	1.82	0.41
10:j:132:LEU:HD21	10:j:159:ASN:HD22	1.85	0.41
1:A:124:ASP:OD1	1:A:125:LEU:N	2.53	0.41
8:H:59:GLU:HG3	8:H:206:ASP:HB2	2.03	0.41
12:L:16:GLN:HG3	12:L:18:ARG:HE	1.85	0.41
19:S:19:ASP:HA	19:S:118:LYS:HA	2.02	0.41
21:U:160:LEU:HD12	21:U:200:VAL:HG21	2.03	0.41
21:U:247:GLN:HB2	21:U:913:ILE:HD13	2.01	0.41
21:U:873:PRO:HB2	21:U:875:PHE:H	1.85	0.41
23:W:399:ASN:HB3	23:W:401:THR:HG22	2.02	0.41
32:f:83:ARG:O	32:f:87:THR:OG1	2.24	0.41
7:g:49:VAL:HG22	7:g:219:VAL:HG23	2.01	0.41
8:h:192:ILE:HG21	8:h:233:ILE:HG21	2.03	0.41
9:i:90:LEU:HG	9:i:114:LEU:HD13	2.01	0.41
12:l:80:ASP:CG	12:l:126:ARG:HH22	2.29	0.41
19:s:58:HIS:HB3	20:t:130:VAL:HG13	2.03	0.41
19:s:213:ASP:OD1	19:s:213:ASP:N	2.53	0.41
1:A:339:ARG:NH1	6:F:426:GLU:OE2	2.54	0.41
1:A:429:TYR:OH	11:K:33:LEU:O	2.36	0.41
2:B:383:LEU:HD11	2:B:419:PHE:HB3	2.01	0.41
6:F:380:ASN:HD22	6:F:383:GLU:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:42:ASN:N	8:H:42:ASN:OD1	2.53	0.41
8:H:123:GLN:HA	9:I:128:ARG:HH21	1.85	0.41
9:I:44:LEU:HD23	9:I:186:LEU:HD13	2.02	0.41
12:L:44:ALA:HB2	12:L:142:PRO:HB3	2.02	0.41
15:O:219:LEU:HD13	16:P:194:LYS:HA	2.03	0.41
20:T:56:ASP:HB2	20:T:107:TRP:HB3	2.01	0.41
21:U:485:ALA:HB3	21:U:519:VAL:HG12	2.03	0.41
21:U:486:MET:HE1	21:U:518:LEU:HD22	2.01	0.41
22:V:320:THR:HB	31:e:18:GLU:HG2	2.03	0.41
23:W:108:CYS:O	23:W:112:VAL:HG23	2.20	0.41
23:W:314:LEU:HD13	23:W:381:LEU:HD11	2.01	0.41
24:X:1:MET:HE1	24:X:35:ILE:HA	2.03	0.41
27:a:148:VAL:HG12	27:a:150:SER:H	1.86	0.41
34:z:52:ASP:O	34:z:54:ARG:N	2.53	0.41
1:A:289:ALA:HB1	6:F:296:PHE:HB3	2.03	0.41
2:B:192:ASN:O	2:B:196:GLU:HG2	2.21	0.41
3:C:193:GLY:H	35:C:501:ATP:PB	2.44	0.41
5:E:168:LYS:HB3	5:E:275:MET:HE2	2.02	0.41
5:E:355:ILE:HD11	6:F:217:ILE:HD11	2.02	0.41
9:I:39:ALA:HA	9:I:184:MET:HG2	2.03	0.41
10:J:104:VAL:HA	10:J:107:ILE:HG22	2.02	0.41
11:K:76:CYS:SG	11:K:141:LEU:HD12	2.61	0.41
14:N:82:LEU:HD23	14:N:82:LEU:HA	1.94	0.41
14:N:110:GLN:HG2	14:N:122:ARG:CZ	2.51	0.41
15:O:29:LYS:NZ	19:s:184:GLU:OE2	2.47	0.41
16:P:145:GLN:O	16:P:149:MET:HG3	2.21	0.41
19:S:149:LEU:HD21	19:S:178:VAL:HG11	2.03	0.41
21:U:384:GLN:HA	21:U:387:ARG:HB2	2.03	0.41
22:V:309:MET:HE2	22:V:331:LEU:HD23	2.02	0.41
23:W:199:TYR:HE2	23:W:236:HIS:CG	2.39	0.41
24:X:99:MET:SD	24:X:100:GLU:N	2.94	0.41
24:X:363:ARG:O	24:X:366:SER:OG	2.36	0.41
26:Z:40:LEU:HD21	26:Z:54:PHE:HE1	1.86	0.41
28:b:163:LYS:CB	34:z:52:ASP:H	2.33	0.41
30:d:195:THR:HG21	30:d:201:ASN:HB3	2.03	0.41
32:f:196:MET:HE2	32:f:196:MET:HB3	1.90	0.41
7:g:51:VAL:HG23	7:g:217:VAL:HG22	2.03	0.41
7:g:137:CYS:SG	7:g:138:MET:N	2.94	0.41
7:g:170:VAL:HG13	7:g:171:LYS:HG2	2.02	0.41
8:h:101:TYR:HE1	16:p:90:MET:HE2	1.85	0.41
9:i:71:ASP:HB3	9:i:72:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:116:GLN:HG3	11:k:83:ALA:HB1	2.02	0.41
11:k:166:ASP:HB2	12:l:56:LEU:HB3	2.02	0.41
14:n:33:LYS:HB3	14:n:45:ARG:HB2	2.03	0.41
15:o:45:GLY:HA2	15:o:98:LEU:HD23	2.02	0.41
17:q:36:PHE:HB2	17:q:44:LEU:HB3	2.03	0.41
18:r:19:ARG:NH1	18:r:168:ALA:O	2.54	0.41
34:z:37:PRO:HD2	34:z:40:GLN:HB2	2.02	0.41
2:B:143:LEU:HD11	2:B:162:VAL:HG11	2.03	0.41
4:D:92:PHE:HB3	4:D:128:ALA:N	2.35	0.41
4:D:206:GLY:HA2	4:D:313:ARG:HH22	1.86	0.41
5:E:196:LEU:HA	5:E:196:LEU:HD22	1.81	0.41
5:E:261:LEU:HD13	5:E:294:ARG:HD3	2.03	0.41
6:F:413:THR:OG1	6:F:414:GLU:OE1	2.30	0.41
7:G:18:PRO:O	7:G:19:GLU:CB	2.66	0.41
8:H:55:ILE:HD12	8:H:55:ILE:H	1.86	0.41
8:H:113:ARG:O	8:H:116:SER:OG	2.32	0.41
8:H:116:SER:O	8:H:119:GLN:HG3	2.21	0.41
9:I:14:PRO:HA	10:J:21:TYR:CG	2.56	0.41
10:J:116:GLN:HA	10:J:119:THR:HG22	2.03	0.41
10:J:158:ALA:HB3	11:K:58:LEU:HD21	2.02	0.41
12:L:156:CYS:HA	13:M:58:TYR:HA	2.02	0.41
13:M:69:VAL:HA	13:M:92:ARG:NE	2.36	0.41
19:S:33:PHE:HD1	15:o:167:LEU:HB2	1.86	0.41
21:U:162:VAL:HG23	21:U:165:LYS:HE3	2.02	0.41
22:V:80:LYS:HE3	22:V:80:LYS:HB3	1.87	0.41
26:Z:124:ILE:HA	26:Z:135:THR:HG22	2.02	0.41
28:b:142:ASN:N	28:b:171:VAL:O	2.43	0.41
32:f:447:ALA:O	32:f:451:VAL:HG23	2.20	0.41
7:g:122:SER:OG	7:g:156:PRO:O	2.39	0.41
16:p:22:ILE:HG23	16:p:188:HIS:HB2	2.03	0.41
16:p:26:ARG:HE	16:p:184:GLY:C	2.29	0.41
1:A:49:GLU:HB3	2:B:65:LEU:HD21	2.03	0.40
1:A:52:ILE:HD12	1:A:55:LEU:HB3	2.02	0.40
3:C:88:LYS:HB2	3:C:94:LYS:HD2	2.03	0.40
3:C:187:LEU:HD23	3:C:314:LYS:HG3	2.03	0.40
5:E:195:PHE:O	5:E:196:LEU:C	2.63	0.40
8:H:118:MET:HE2	8:H:130:PHE:HZ	1.86	0.40
8:H:148:GLN:OE1	8:H:158:TRP:NE1	2.54	0.40
20:T:151:ARG:HA	20:T:154:LEU:HG	2.04	0.40
21:U:807:LYS:HA	21:U:808:PRO:HD3	1.97	0.40
23:W:245:LYS:NZ	23:W:286:LEU:HD21	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:73:VAL:O	24:X:77:LEU:N	2.54	0.40
24:X:90:ARG:HH22	24:X:132:ARG:HG2	1.85	0.40
26:Z:284:ASP:HA	26:Z:287:LYS:HG2	2.03	0.40
29:c:245:VAL:HG13	29:c:248:MET:HE3	2.02	0.40
29:c:251:LEU:HD21	29:c:284:LEU:HD13	2.03	0.40
10:j:94:HIS:ND1	10:j:102:VAL:HG12	2.36	0.40
14:n:12:VAL:HG21	14:n:101:ALA:HB1	2.03	0.40
19:s:26:ASP:OD1	19:s:26:ASP:N	2.45	0.40
19:s:27:THR:HB	19:s:40:SER:H	1.86	0.40
20:t:186:ARG:HE	20:t:202:PRO:HB2	1.86	0.40
34:z:8:LEU:H	34:z:71:LEU:CB	2.33	0.40
2:B:48:LYS:HE2	2:B:48:LYS:HB2	1.93	0.40
2:B:188:GLY:HA3	2:B:364:ILE:HD13	2.04	0.40
3:C:80:MET:N	3:C:84:LYS:O	2.54	0.40
3:C:399:MET:SD	9:I:53:HIS:HE1	2.44	0.40
4:D:56:VAL:HG11	21:U:599:ILE:HG23	2.03	0.40
4:D:308:ILE:O	4:D:309:MET:HE2	2.21	0.40
5:E:166:PRO:O	5:E:293:GLY:HA2	2.21	0.40
5:E:321:THR:OG1	5:E:360:ASP:O	2.24	0.40
17:Q:171:PHE:HE2	17:Q:173:LEU:HB2	1.84	0.40
18:R:1:THR:N	18:R:169:TYR:O	2.54	0.40
19:S:57:PHE:HB2	19:S:105:TYR:HB3	2.02	0.40
21:U:133:ILE:HG13	21:U:136:LYS:HE3	2.03	0.40
21:U:338:HIS:CD2	21:U:785:PRO:HB3	2.56	0.40
23:W:174:TYR:O	23:W:182:ARG:NH2	2.54	0.40
24:X:421:LEU:HB2	26:Z:283:ARG:HH21	1.84	0.40
26:Z:187:LEU:HG	29:c:293:THR:HG22	2.04	0.40
32:f:270:LEU:HD21	32:f:298:LEU:HD21	2.03	0.40
11:k:157:ASP:OD1	11:k:157:ASP:N	2.54	0.40
12:l:31:GLN:O	12:l:51:ARG:NH2	2.55	0.40
1:A:254:ALA:O	1:A:258:ARG:HG3	2.22	0.40
1:A:375:ARG:NH2	11:K:176:GLY:H	2.17	0.40
4:D:87:LEU:HD22	4:D:133:HIS:HA	2.02	0.40
5:E:95:GLY:O	5:E:113:ARG:NH2	2.36	0.40
8:H:38:ILE:HG12	8:H:160:ALA:HB1	2.03	0.40
8:H:118:MET:HB2	8:H:130:PHE:CZ	2.56	0.40
10:J:155:ALA:HB3	11:K:63:SER:HB2	2.03	0.40
13:M:69:VAL:HA	13:M:92:ARG:HE	1.85	0.40
22:V:305:ALA:O	22:V:309:MET:HB3	2.21	0.40
24:X:201:TYR:C	24:X:202:CYS:SG	3.05	0.40
26:Z:108:ILE:HG12	26:Z:112:MET:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:81:LEU:HA	27:a:84:VAL:HG12	2.04	0.40
30:d:49:ILE:HD12	30:d:52:ARG:HH21	1.85	0.40
32:f:581:GLU:HA	32:f:588:ARG:HD2	2.04	0.40
8:h:3:GLU:HG2	13:m:127:ALA:HB3	2.03	0.40
9:i:230:GLN:HA	9:i:233:VAL:HB	2.02	0.40
12:l:4:ASN:HD21	12:l:20:HIS:CE1	2.39	0.40
12:l:32:GLY:C	12:l:51:ARG:HH21	2.30	0.40
16:p:11:VAL:O	16:p:12:MET:HE2	2.21	0.40
1:A:115:VAL:HG21	1:A:118:PHE:HB3	2.03	0.40
3:C:343:ASN:HB3	3:C:346:LYS:HD3	2.02	0.40
4:D:271:ALA:HB3	4:D:317:LEU:HD13	2.04	0.40
8:H:67:PRO:HA	8:H:73:GLY:HA2	2.02	0.40
9:I:172:VAL:O	9:I:176:LYS:HG3	2.22	0.40
11:K:41:GLN:NE2	11:K:151:PRO:O	2.55	0.40
11:K:157:ASP:OD1	11:K:161:THR:N	2.54	0.40
14:N:18:SER:OG	14:N:29:ARG:O	2.36	0.40
28:b:58:CYS:HB3	28:b:92:VAL:HG11	2.04	0.40
30:d:142:TYR:CD1	30:d:150:LYS:HE2	2.56	0.40
32:f:350:LYS:HD3	32:f:353:LEU:HD21	2.02	0.40
15:o:19:ARG:O	15:o:33:LYS:NZ	2.45	0.40
16:p:189:ILE:HB	16:p:196:THR:HB	2.03	0.40
19:s:29:LEU:O	19:s:36:HIS:N	2.54	0.40
1:A:375:ARG:NH1	11:K:172:SER:O	2.55	0.40
3:C:165:ILE:HG13	3:C:166:GLU:HG3	2.04	0.40
5:E:56:ILE:HB	5:E:100:LEU:HB2	2.03	0.40
6:F:87:PRO:HB3	6:F:155:LYS:HG3	2.03	0.40
8:H:189:HIS:HB3	8:H:233:ILE:HD11	2.03	0.40
13:M:236:GLU:HB3	13:M:240:LYS:HZ1	1.86	0.40
23:W:239:SER:O	23:W:242:SER:OG	2.33	0.40
25:Y:28:LEU:O	25:Y:32:ARG:N	2.55	0.40
26:Z:74:TYR:O	26:Z:78:MET:HG2	2.21	0.40
27:a:55:GLY:HA2	27:a:58:LYS:HG2	2.04	0.40
27:a:277:LEU:HD11	27:a:310:LEU:HD23	2.02	0.40
29:c:186:LYS:HA	29:c:187:PRO:HD3	1.96	0.40
29:c:280:PRO:HG2	29:c:282:ARG:NH2	2.36	0.40
30:d:44:THR:OG1	30:d:47:GLN:NE2	2.54	0.40
30:d:218:GLY:HA3	30:d:223:TYR:HE2	1.87	0.40
7:g:58:ASP:OD1	7:g:58:ASP:N	2.55	0.40
10:j:98:VAL:HG12	10:j:100:ASP:HB2	2.04	0.40
11:k:127:ASP:N	11:k:127:ASP:OD1	2.54	0.40
12:l:93:LEU:HD21	19:s:73:LYS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:200:PRO:HD2	12:l:203:GLN:HB2	2.04	0.40
14:n:100:ILE:N	14:n:112:TYR:O	2.43	0.40
20:t:9:THR:OG1	20:t:10:SER:N	2.44	0.40
20:t:74:GLU:HG3	20:t:83:TYR:HE2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/433 (95%)	373 (91%)	38 (9%)	0	100	100
2	B	409/440 (93%)	359 (88%)	50 (12%)	0	100	100
3	C	394/398 (99%)	353 (90%)	37 (9%)	4 (1%)	12	48
4	D	378/418 (90%)	322 (85%)	50 (13%)	6 (2%)	7	38
5	E	387/403 (96%)	328 (85%)	59 (15%)	0	100	100
6	F	391/439 (89%)	354 (90%)	33 (8%)	4 (1%)	12	48
7	G	238/246 (97%)	218 (92%)	19 (8%)	1 (0%)	30	67
7	g	242/246 (98%)	230 (95%)	12 (5%)	0	100	100
8	H	230/234 (98%)	218 (95%)	12 (5%)	0	100	100
8	h	230/234 (98%)	219 (95%)	10 (4%)	1 (0%)	30	67
9	I	246/261 (94%)	236 (96%)	10 (4%)	0	100	100
9	i	248/261 (95%)	240 (97%)	8 (3%)	0	100	100
10	J	237/248 (96%)	227 (96%)	10 (4%)	0	100	100
10	j	237/248 (96%)	220 (93%)	16 (7%)	1 (0%)	30	67
11	K	236/241 (98%)	224 (95%)	12 (5%)	0	100	100
11	k	232/241 (96%)	222 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	238/263 (90%)	226 (95%)	12 (5%)	0	100	100
12	l	236/263 (90%)	229 (97%)	7 (3%)	0	100	100
13	M	241/255 (94%)	232 (96%)	9 (4%)	0	100	100
13	m	238/255 (93%)	233 (98%)	5 (2%)	0	100	100
14	N	201/239 (84%)	194 (96%)	7 (4%)	0	100	100
14	n	200/239 (84%)	194 (97%)	6 (3%)	0	100	100
15	O	218/277 (79%)	209 (96%)	9 (4%)	0	100	100
15	o	218/277 (79%)	209 (96%)	9 (4%)	0	100	100
16	P	202/205 (98%)	191 (95%)	11 (5%)	0	100	100
16	p	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
17	Q	198/201 (98%)	190 (96%)	8 (4%)	0	100	100
17	q	197/201 (98%)	189 (96%)	8 (4%)	0	100	100
18	R	199/263 (76%)	192 (96%)	7 (4%)	0	100	100
18	r	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
19	S	211/241 (88%)	200 (95%)	11 (5%)	0	100	100
19	s	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
20	T	214/264 (81%)	208 (97%)	6 (3%)	0	100	100
20	t	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
21	U	874/953 (92%)	808 (92%)	66 (8%)	0	100	100
22	V	442/534 (83%)	423 (96%)	19 (4%)	0	100	100
23	W	439/456 (96%)	429 (98%)	10 (2%)	0	100	100
24	X	420/422 (100%)	401 (96%)	17 (4%)	2 (0%)	24	63
25	Y	387/389 (100%)	365 (94%)	22 (6%)	0	100	100
26	Z	284/324 (88%)	247 (87%)	34 (12%)	3 (1%)	11	46
27	a	371/376 (99%)	342 (92%)	27 (7%)	2 (0%)	24	63
28	b	189/377 (50%)	163 (86%)	24 (13%)	2 (1%)	11	46
29	c	285/310 (92%)	242 (85%)	39 (14%)	4 (1%)	9	40
30	d	255/350 (73%)	215 (84%)	38 (15%)	2 (1%)	16	54
31	e	48/70 (69%)	42 (88%)	6 (12%)	0	100	100
32	f	840/908 (92%)	807 (96%)	31 (4%)	2 (0%)	43	78
34	w	74/76 (97%)	72 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	x	74/76 (97%)	74 (100%)	0	0	100	100
34	z	74/76 (97%)	60 (81%)	9 (12%)	5 (7%)	1	11
All	All	13639/15104 (90%)	12723 (93%)	877 (6%)	39 (0%)	37	72

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	159	LYS
4	D	336	PRO
6	F	344	ARG
6	F	345	SER
24	X	318	ILE
27	a	343	LEU
28	b	121	GLU
28	b	122	LYS
29	c	196	LEU
29	c	197	ASN
29	c	280	PRO
30	d	202	THR
32	f	572	ALA
34	z	73	LEU
3	C	90	HIS
3	C	252	ASP
26	Z	145	HIS
27	a	344	GLN
29	c	198	ARG
32	f	573	ILE
10	j	50	VAL
4	D	157	ASP
4	D	335	LEU
6	F	87	PRO
6	F	326	VAL
7	G	19	GLU
24	X	106	GLU
8	h	4	ARG
26	Z	134	PRO
26	Z	136	GLU
30	d	204	LYS
34	z	72	ARG
3	C	91	PRO
4	D	160	PRO

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Mol	Chain	Res	Type
4	D	162	VAL
34	z	38	PRO
34	z	53	GLY
3	C	89	VAL
34	z	35	GLY

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	348/372 (94%)	346 (99%)	2 (1%)	78	83
2	B	357/385 (93%)	356 (100%)	1 (0%)	86	86
3	C	340/346 (98%)	334 (98%)	6 (2%)	51	68
4	D	333/366 (91%)	329 (99%)	4 (1%)	63	75
5	E	341/353 (97%)	340 (100%)	1 (0%)	86	86
6	F	340/379 (90%)	336 (99%)	4 (1%)	63	75
7	G	202/210 (96%)	201 (100%)	1 (0%)	81	83
7	g	201/210 (96%)	200 (100%)	1 (0%)	81	83
8	H	187/191 (98%)	187 (100%)	0	100	100
8	h	188/191 (98%)	187 (100%)	1 (0%)	81	83
9	I	202/221 (91%)	202 (100%)	0	100	100
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	197/211 (93%)	197 (100%)	0	100	100
10	j	196/211 (93%)	196 (100%)	0	100	100
11	K	197/203 (97%)	197 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/224 (90%)	202 (100%)	0	100	100
12	l	201/224 (90%)	201 (100%)	0	100	100
13	M	199/212 (94%)	198 (100%)	1 (0%)	81	83
13	m	198/212 (93%)	198 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	158/181 (87%)	158 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	178/228 (78%)	178 (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	169/171 (99%)	169 (100%)	0	100	100
17	q	166/171 (97%)	166 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	154/202 (76%)	154 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	177/199 (89%)	177 (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	752/816 (92%)	751 (100%)	1 (0%)	88	89
22	V	390/460 (85%)	390 (100%)	0	100	100
23	W	406/416 (98%)	406 (100%)	0	100	100
24	X	362/362 (100%)	360 (99%)	2 (1%)	78	83
25	Y	344/344 (100%)	344 (100%)	0	100	100
26	Z	257/295 (87%)	257 (100%)	0	100	100
27	a	333/336 (99%)	332 (100%)	1 (0%)	86	86
28	b	167/312 (54%)	161 (96%)	6 (4%)	31	52
29	c	252/268 (94%)	246 (98%)	6 (2%)	43	64
30	d	231/294 (79%)	230 (100%)	1 (0%)	84	84
31	e	44/63 (70%)	43 (98%)	1 (2%)	44	64
32	f	711/763 (93%)	709 (100%)	2 (0%)	86	86
34	w	68/68 (100%)	68 (100%)	0	100	100
34	x	68/68 (100%)	68 (100%)	0	100	100
34	z	68/68 (100%)	61 (90%)	7 (10%)	7	23
All	All	11655/12818 (91%)	11606 (100%)	49 (0%)	81	84

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	360	ARG
1	A	403	ILE
2	B	125	THR
3	C	41	ASN
3	C	89	VAL
3	C	90	HIS
3	C	109	THR
3	C	210	THR
3	C	252	ASP
4	D	157	ASP
4	D	159	LYS
4	D	161	ASP
4	D	337	ASP
5	E	196	LEU
6	F	86	LEU
6	F	326	VAL
6	F	344	ARG
6	F	416	THR
7	G	21	ARG
13	M	152	ASP
21	U	583	MET
24	X	106	GLU
24	X	318	ILE
27	a	343	LEU
28	b	120	ASN
28	b	121	GLU
28	b	122	LYS
28	b	123	ASP
28	b	124	LEU
28	b	161	ASN
29	c	196	LEU
29	c	198	ARG
29	c	278	GLN
29	c	280	PRO
29	c	281	LYS
29	c	284	LEU
30	d	201	ASN
31	e	54	ASN
32	f	573	ILE
32	f	619	HIS
7	g	11	ARG
8	h	3	GLU
34	z	36	ILE

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Mol	Chain	Res	Type
34	z	40	GLN
34	z	51	GLU
34	z	71	LEU
34	z	72	ARG
34	z	73	LEU
34	z	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	53	GLN
1	A	54	GLN
1	A	197	HIS
1	A	203	ASN
1	A	247	GLN
2	B	82	GLN
2	B	84	GLN
2	B	306	GLN
2	B	314	ASN
3	C	41	ASN
3	C	50	ASN
3	C	67	GLN
3	C	278	ASN
3	C	337	ASN
4	D	135	HIS
4	D	257	ASN
4	D	278	GLN
5	E	155	ASN
5	E	262	ASN
5	E	359	HIS
6	F	243	GLN
6	F	316	GLN
6	F	323	ASN
6	F	428	GLN
7	G	68	HIS
7	G	127	GLN
7	G	147	GLN
8	H	88	HIS
8	H	102	GLN
9	I	40	ASN
9	I	53	HIS

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Mol	Chain	Res	Type
9	I	95	GLN
9	I	142	HIS
9	I	146	GLN
9	I	155	ASN
10	J	94	HIS
10	J	116	GLN
11	K	41	GLN
11	K	224	GLN
12	L	31	GLN
12	L	90	GLN
12	L	166	GLN
13	M	147	GLN
13	M	170	GLN
14	N	7	GLN
15	O	62	ASN
15	O	91	GLN
15	O	116	HIS
15	O	181	ASN
16	P	93	ASN
16	P	169	GLN
16	P	173	ASN
17	Q	63	ASN
17	Q	82	ASN
17	Q	110	HIS
19	S	157	ASN
21	U	189	GLN
21	U	338	HIS
21	U	355	ASN
21	U	527	GLN
21	U	734	GLN
21	U	743	ASN
21	U	801	GLN
21	U	874	ASN
21	U	888	GLN
22	V	109	ASN
22	V	488	ASN
23	W	86	ASN
24	X	44	GLN
24	X	105	GLN
24	X	178	HIS
24	X	182	ASN
24	X	213	GLN

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Mol	Chain	Res	Type
24	X	296	ASN
24	X	334	ASN
24	X	416	ASN
25	Y	48	ASN
25	Y	154	ASN
25	Y	178	ASN
25	Y	306	GLN
26	Z	22	HIS
26	Z	77	ASN
26	Z	189	GLN
26	Z	193	ASN
26	Z	196	HIS
26	Z	235	ASN
26	Z	243	GLN
26	Z	278	ASN
27	a	46	GLN
27	a	193	GLN
27	a	288	HIS
28	b	79	GLN
29	c	274	ASN
29	c	278	GLN
29	c	283	HIS
30	d	15	ASN
30	d	252	GLN
31	e	37	HIS
32	f	737	ASN
7	g	75	ASN
8	h	21	GLN
8	h	63	HIS
8	h	102	GLN
8	h	189	HIS
9	i	146	GLN
10	j	116	GLN
10	j	175	ASN
10	j	215	GLN
11	k	182	GLN
12	l	53	GLN
12	l	86	ASN
12	l	146	GLN
13	m	63	ASN
13	m	110	HIS
14	n	7	GLN

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Mol	Chain	Res	Type
14	n	158	ASN
15	o	91	GLN
15	o	153	ASN
16	p	93	ASN
17	q	82	ASN
18	r	29	GLN
18	r	62	GLN
19	s	79	ASN
19	s	159	GLN
34	w	40	GLN
34	w	41	GLN
34	x	25	ASN
34	x	41	GLN
34	z	40	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	ADP	D	501	36	27,29,29	1.38	4 (14%)	42,45,45	2.05	9 (21%)
35	ATP	C	501	36	29,33,33	0.31	0	44,52,52	0.50	0
35	ATP	F	501	36	29,33,33	0.30	0	44,52,52	0.46	0
35	ATP	B	501	36	29,33,33	0.30	0	44,52,52	0.54	0
35	ATP	A	501	36	29,33,33	0.32	0	44,52,52	0.58	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
37	ADP	D	501	36	-	3/16/32/32	0/3/3/3
35	ATP	C	501	36	-	6/22/38/38	0/3/3/3
35	ATP	F	501	36	-	2/22/38/38	0/3/3/3
35	ATP	B	501	36	-	2/22/38/38	0/3/3/3
35	ATP	A	501	36	-	3/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D	501	ADP	C5-C4	4.68	1.47	1.39
37	D	501	ADP	C5-C6	2.75	1.48	1.41
37	D	501	ADP	C8-N7	2.32	1.36	1.31
37	D	501	ADP	C5-N7	-2.19	1.34	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D	501	ADP	C5-C4-N3	-6.85	117.82	126.75
37	D	501	ADP	N3-C4-N9	5.44	136.05	127.08
37	D	501	ADP	C2-N3-C4	4.07	121.36	111.75
37	D	501	ADP	PA-O3A-PB	-3.52	120.76	132.83
37	D	501	ADP	C4-C5-N7	-3.27	106.63	110.62
37	D	501	ADP	N3-C2-N1	-3.05	123.83	128.60
37	D	501	ADP	C5-N7-C8	2.81	107.50	103.51
37	D	501	ADP	C3'-C2'-C1'	2.77	106.69	101.43
37	D	501	ADP	C4-N9-C8	2.37	108.30	105.73

There are no chirality outliers.

All (16) torsion outliers are listed below:

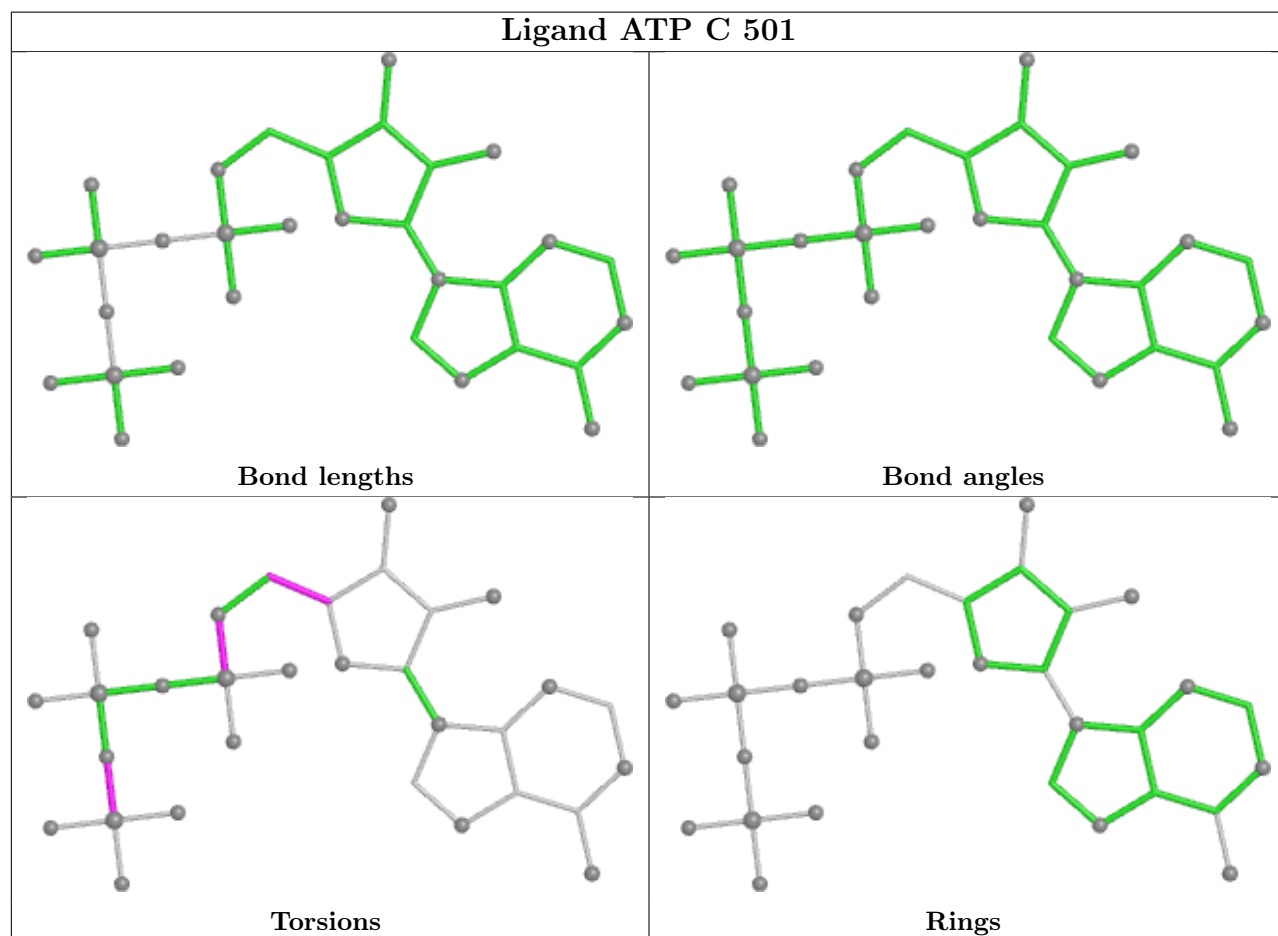
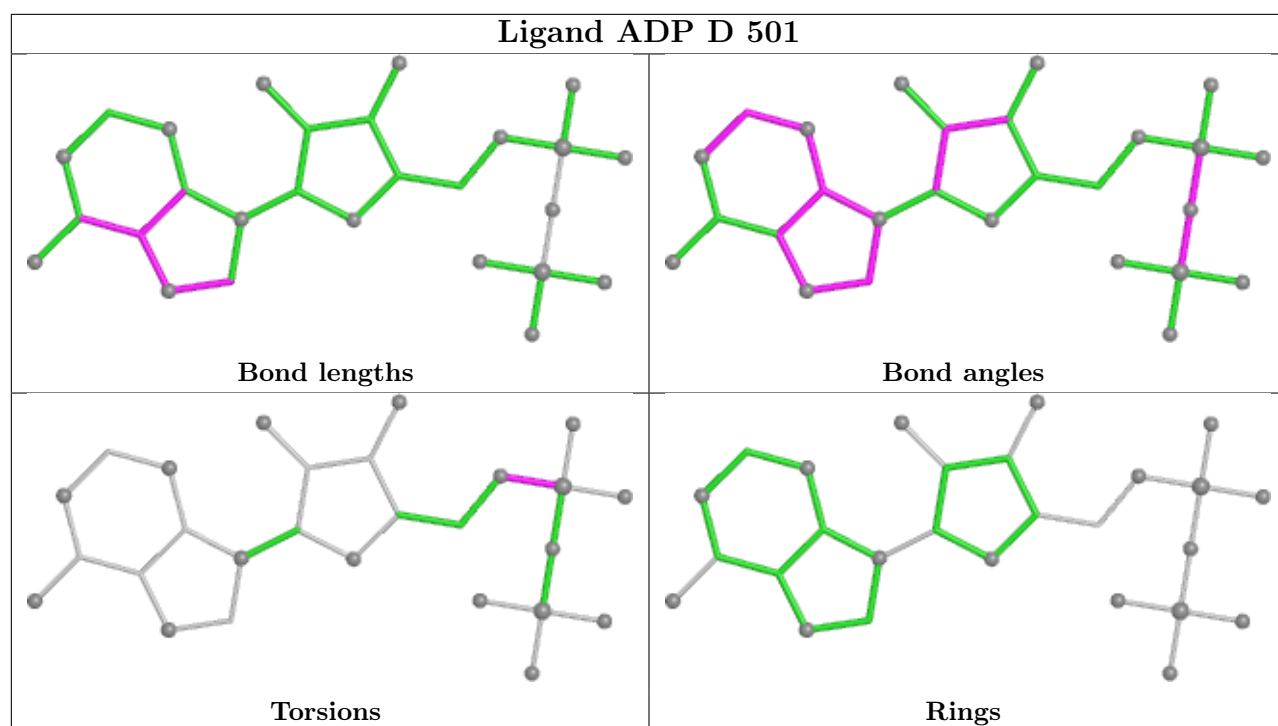
Mol	Chain	Res	Type	Atoms
35	A	501	ATP	C5'-O5'-PA-O1A
35	C	501	ATP	PB-O3B-PG-O3G
35	C	501	ATP	C5'-O5'-PA-O1A
35	C	501	ATP	C5'-O5'-PA-O2A
35	C	501	ATP	C5'-O5'-PA-O3A
35	F	501	ATP	O4'-C4'-C5'-O5'
37	D	501	ADP	C5'-O5'-PA-O2A
35	F	501	ATP	C3'-C4'-C5'-O5'
35	C	501	ATP	C3'-C4'-C5'-O5'
35	C	501	ATP	O4'-C4'-C5'-O5'
35	A	501	ATP	PB-O3B-PG-O1G
37	D	501	ADP	C5'-O5'-PA-O3A
35	B	501	ATP	C5'-O5'-PA-O3A
35	A	501	ATP	PG-O3B-PB-O2B
35	B	501	ATP	C5'-O5'-PA-O2A
37	D	501	ADP	C5'-O5'-PA-O1A

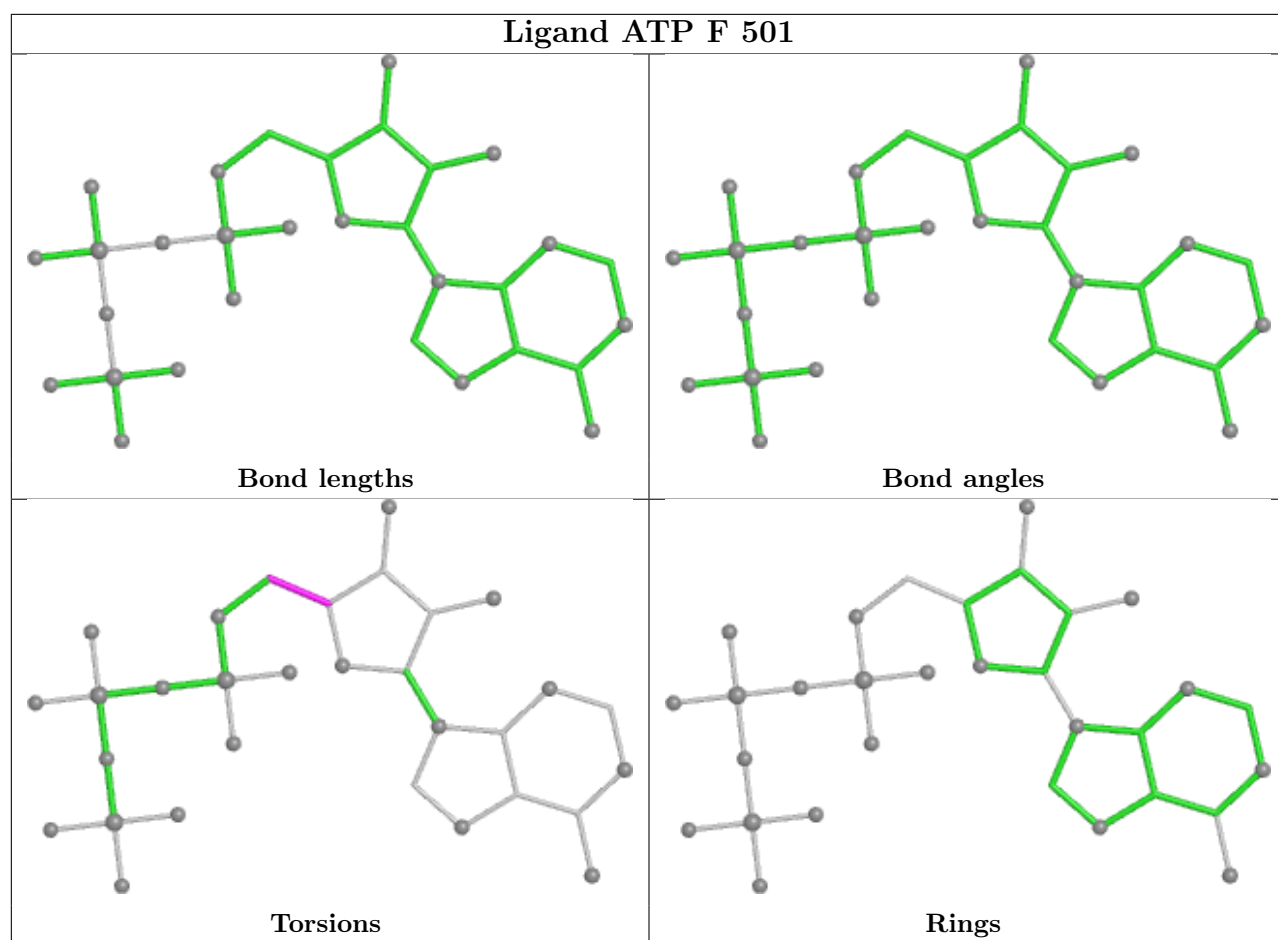
There are no ring outliers.

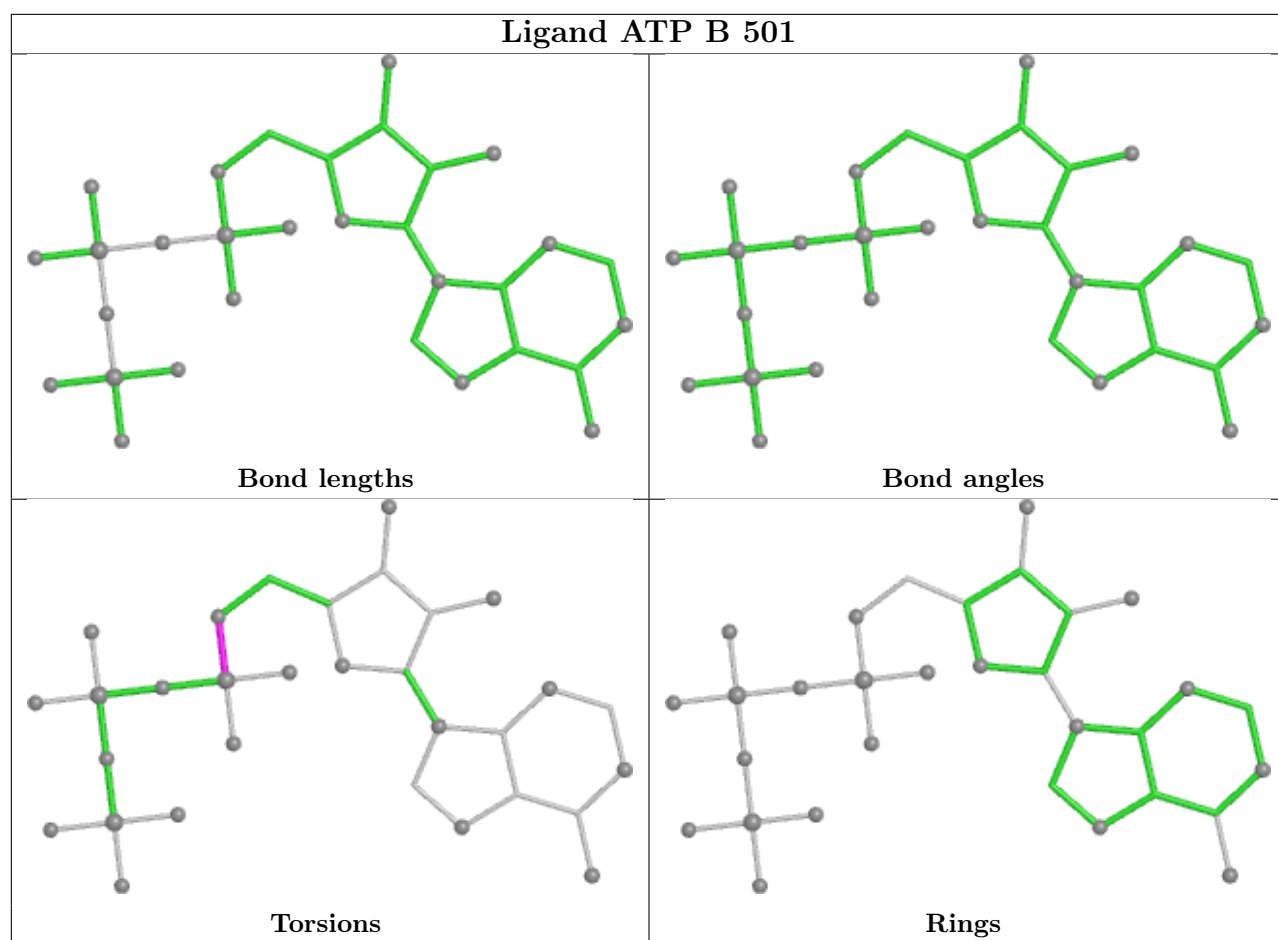
3 monomers are involved in 11 short contacts:

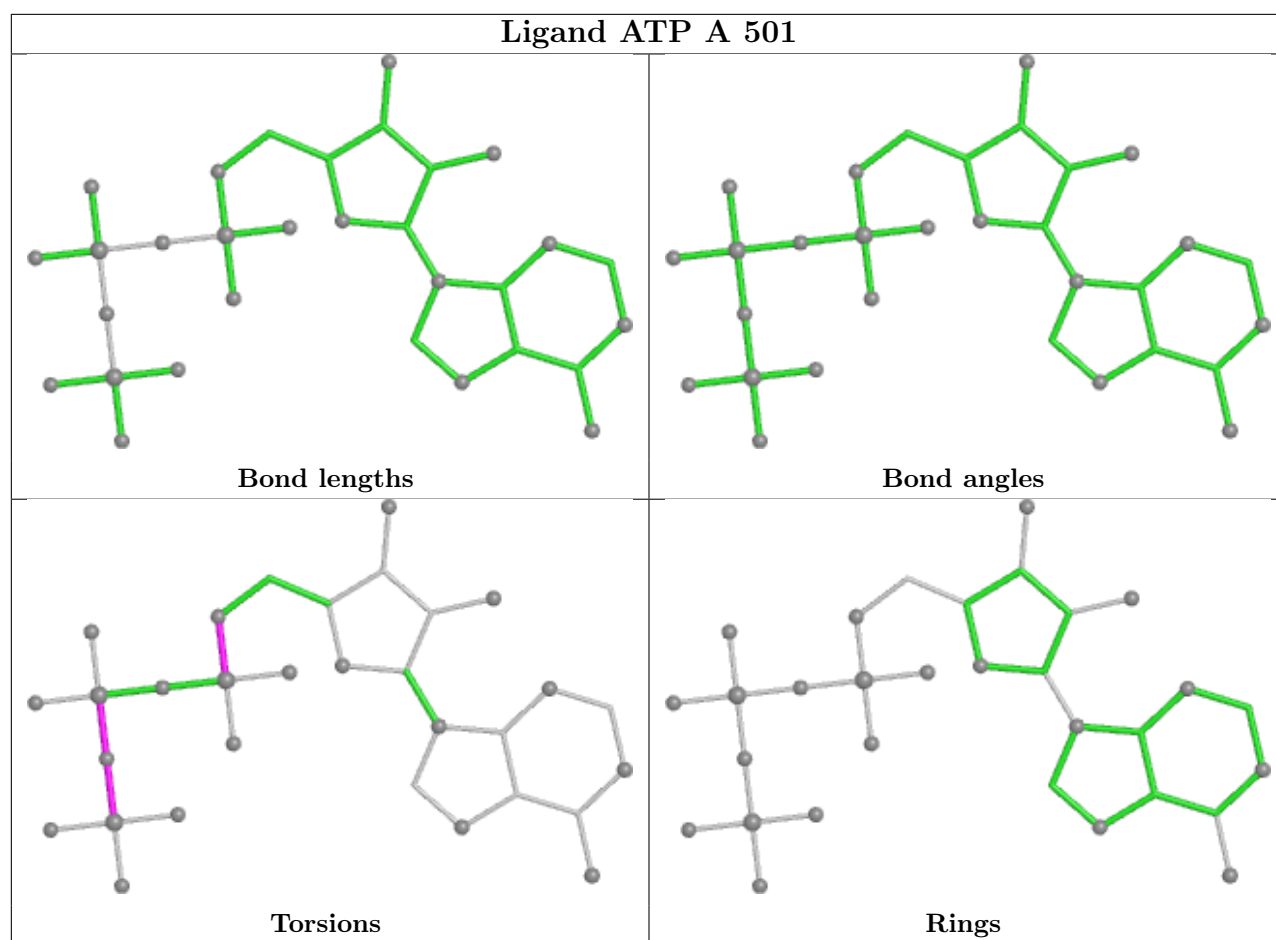
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	C	501	ATP	3	0
35	B	501	ATP	2	0
35	A	501	ATP	6	0

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.

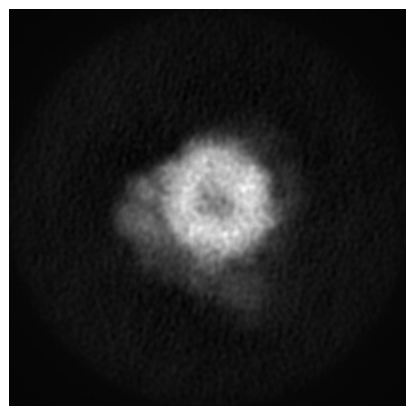
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62081. These allow visual inspection of the internal detail of the map and identification of artifacts.

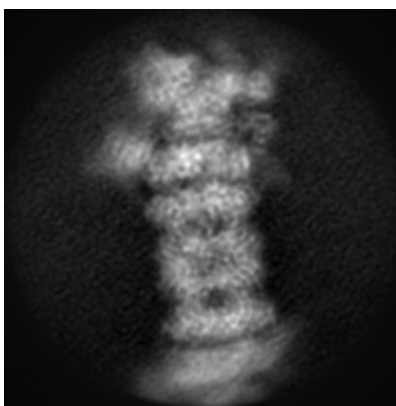
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

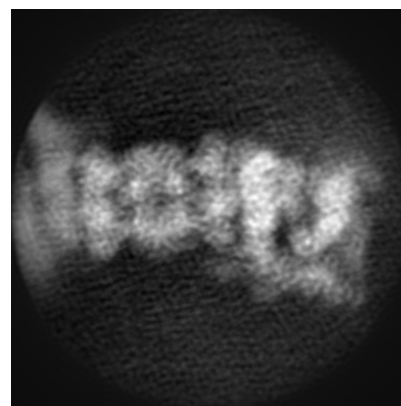
6.1.1 Primary map



X

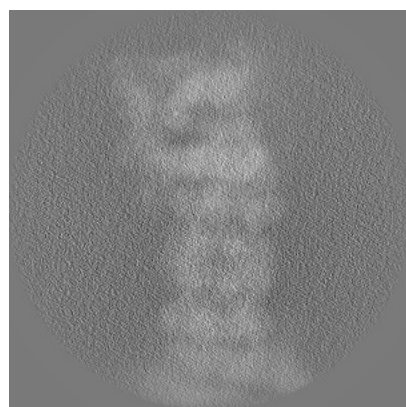


Y

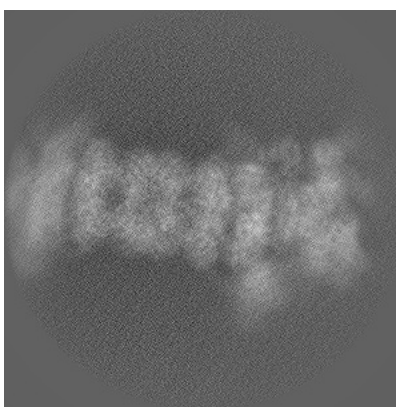


Z

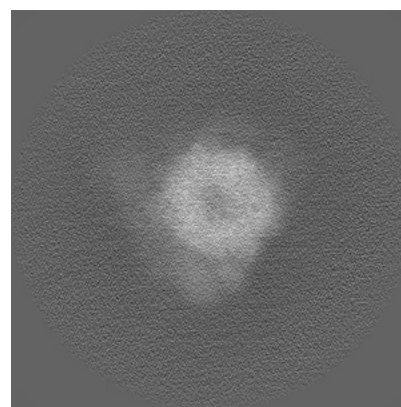
6.1.2 Raw map



X



Y

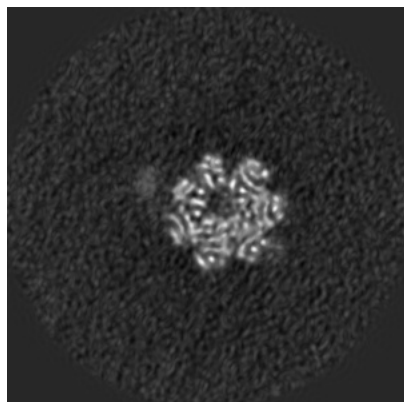


Z

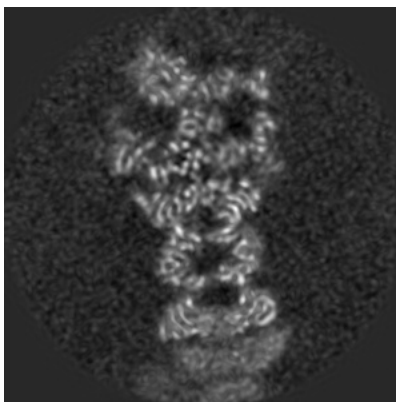
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

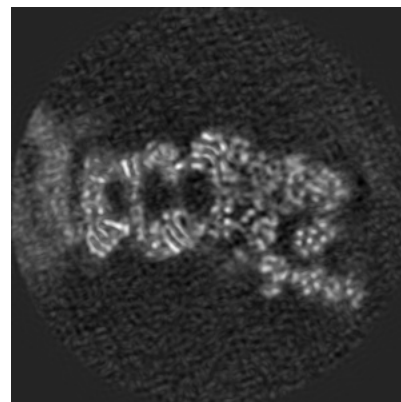
6.2.1 Primary map



X Index: 300

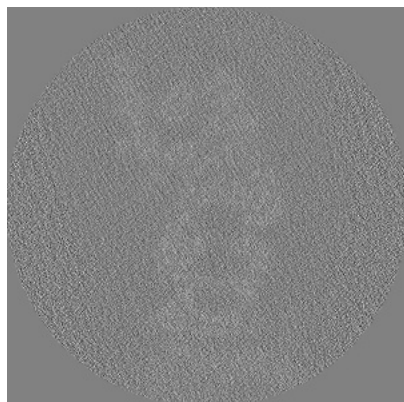


Y Index: 300

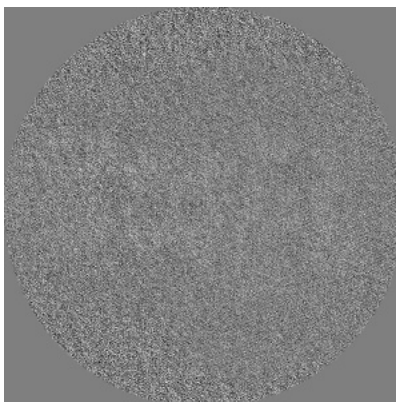


Z Index: 300

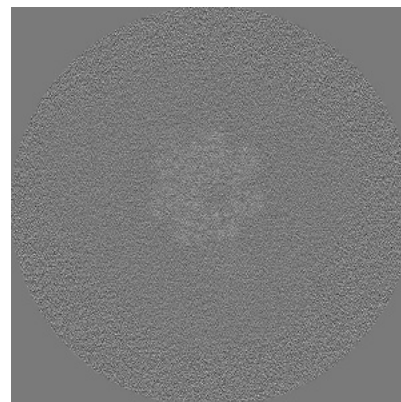
6.2.2 Raw map



X Index: 300



Y Index: 300

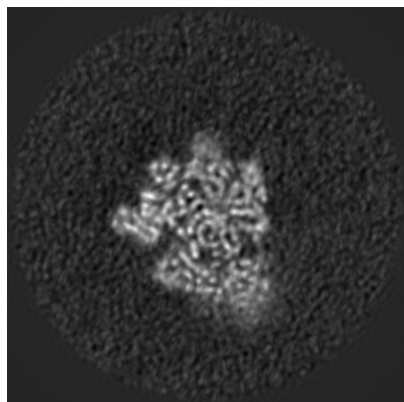


Z Index: 300

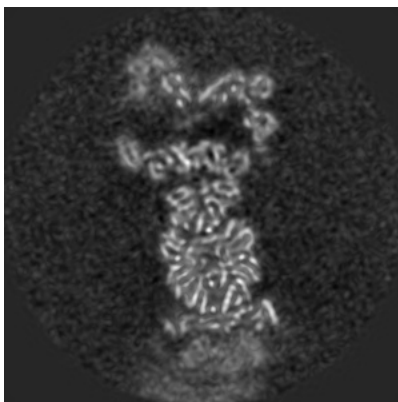
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

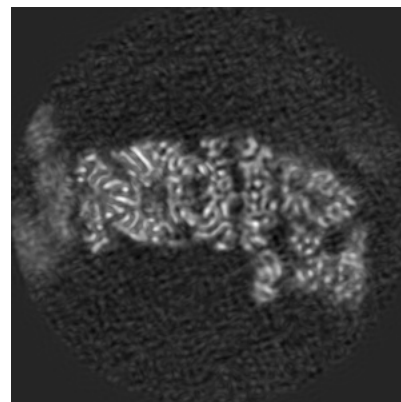
6.3.1 Primary map



X Index: 378

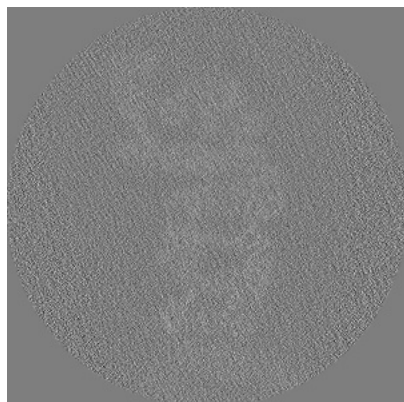


Y Index: 274

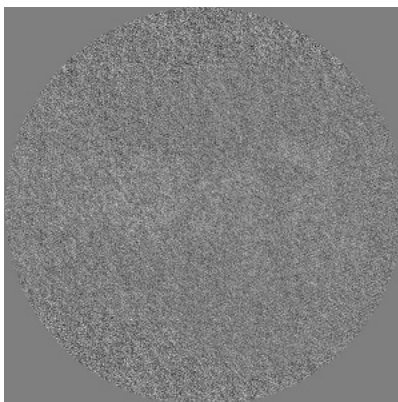


Z Index: 274

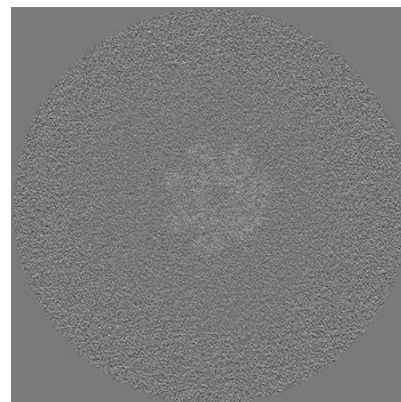
6.3.2 Raw map



X Index: 288



Y Index: 266

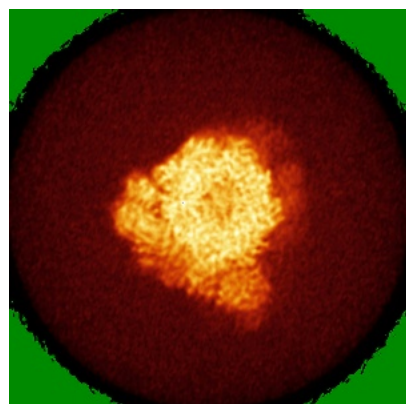


Z Index: 247

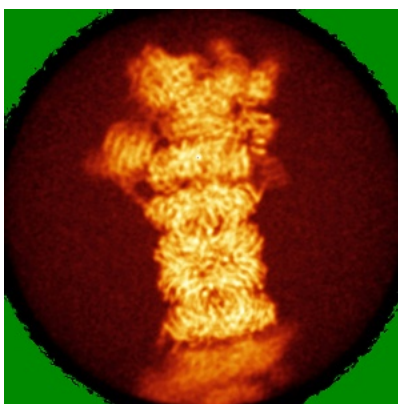
The images above show the largest variance slices of the map in three orthogonal directions.

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

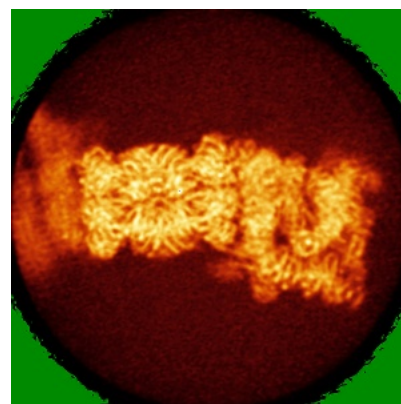
6.4.1 Primary map



X

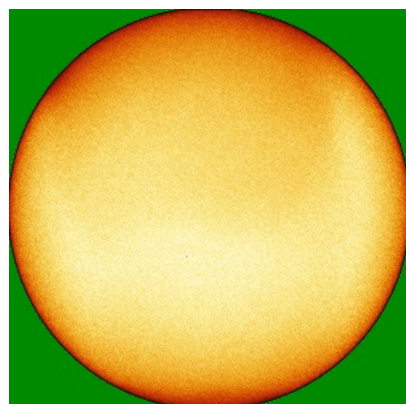


Y

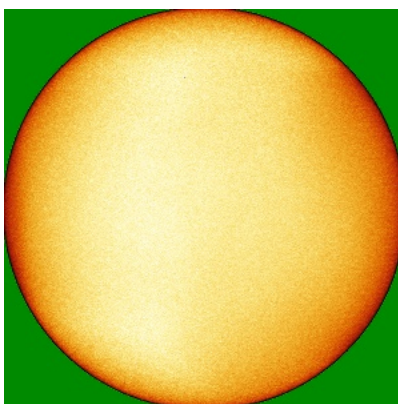


Z

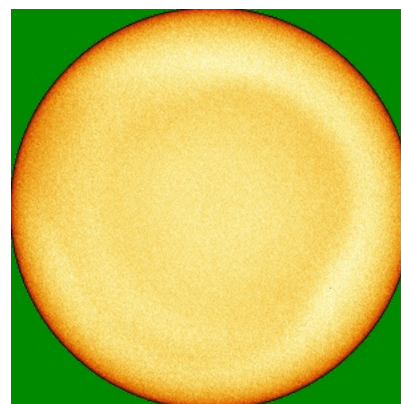
6.4.2 Raw map



X



Y

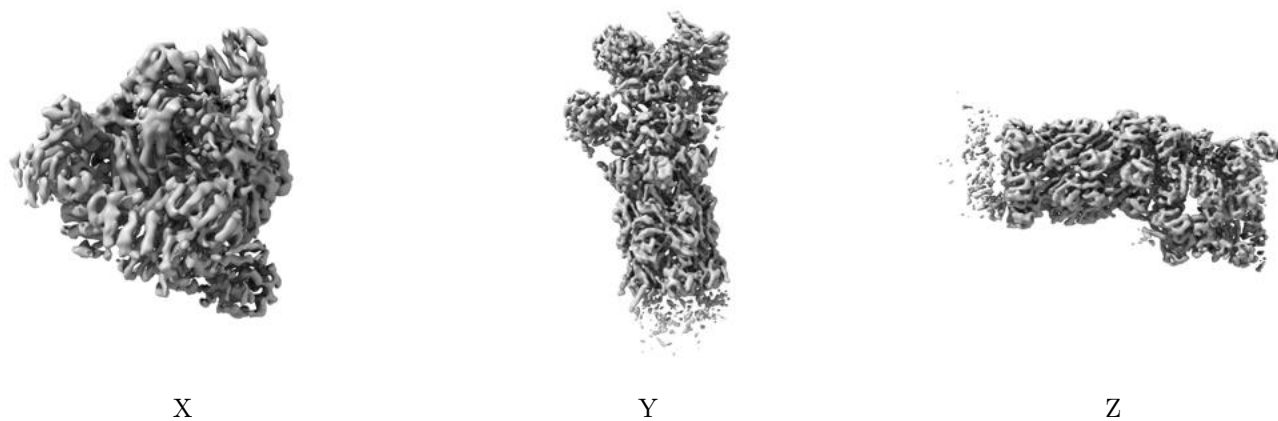


Z

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

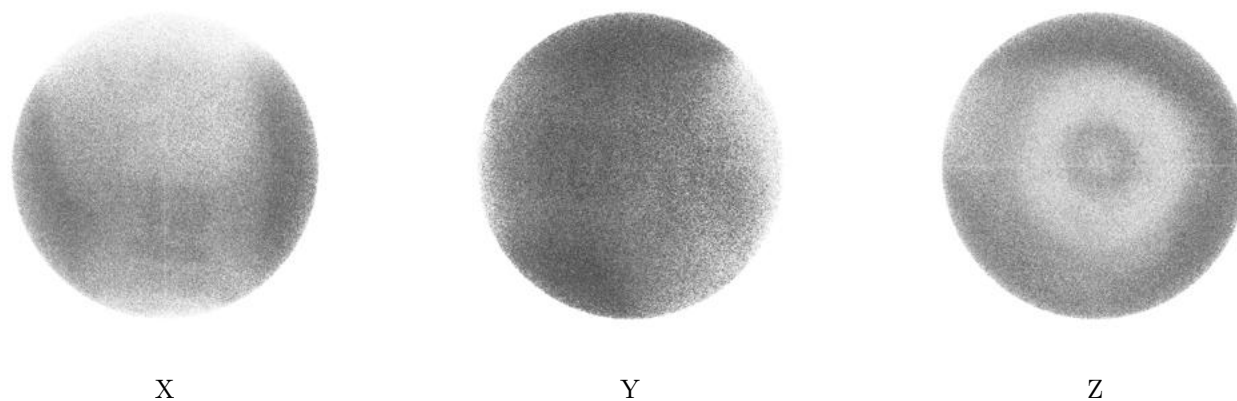
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00578. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

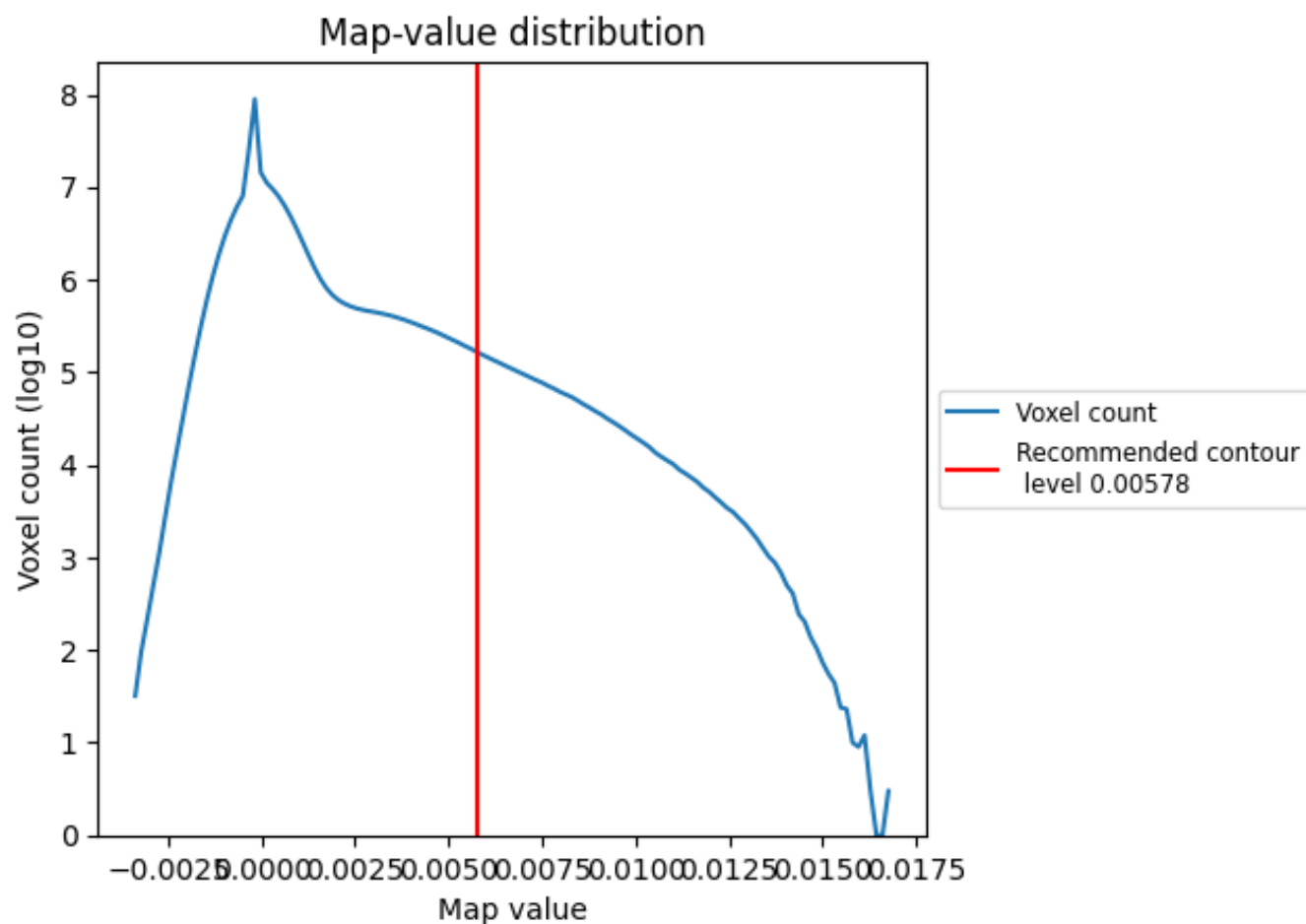
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

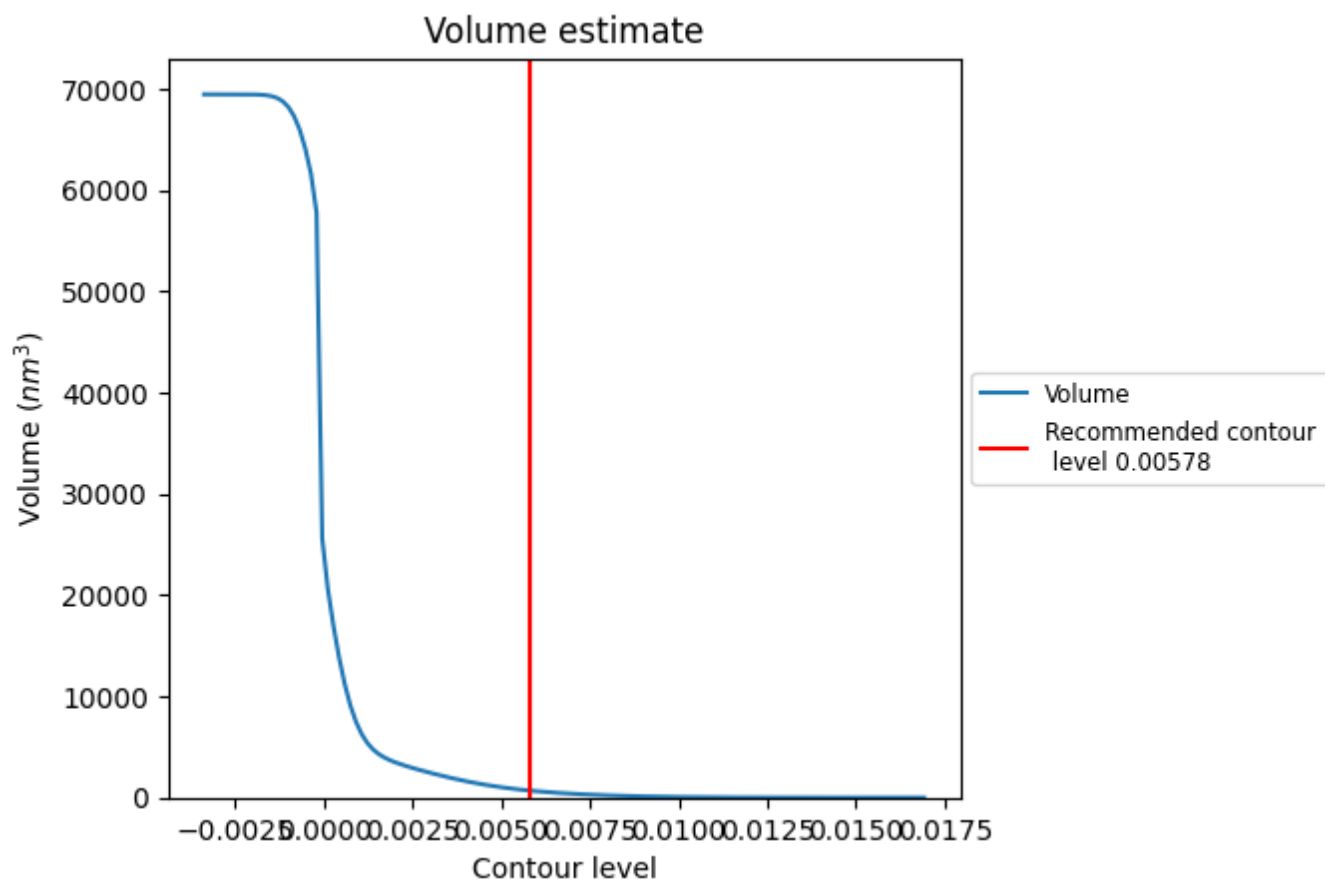
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

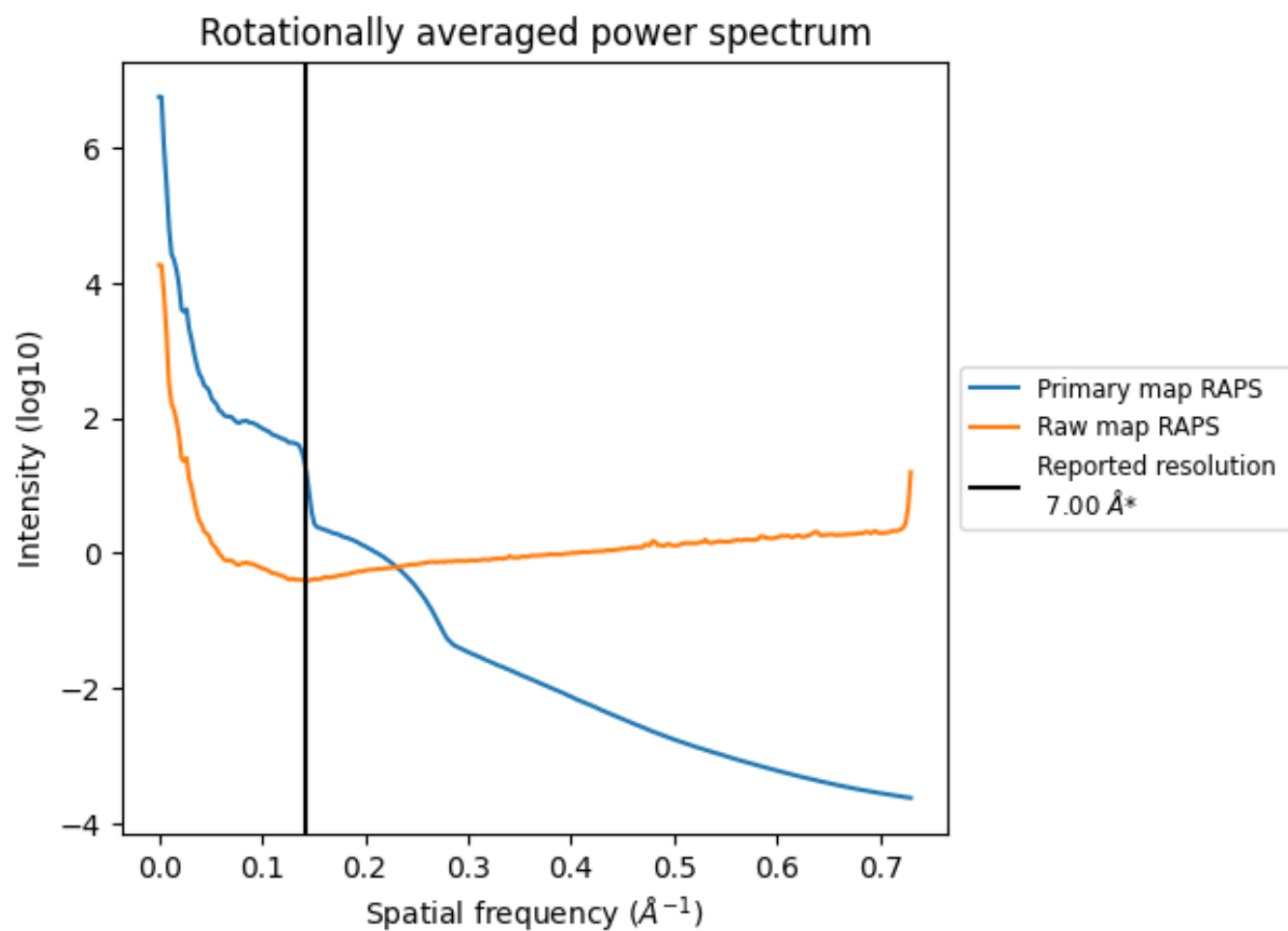
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 697 nm³; this corresponds to an approximate mass of 630 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 ⓘ

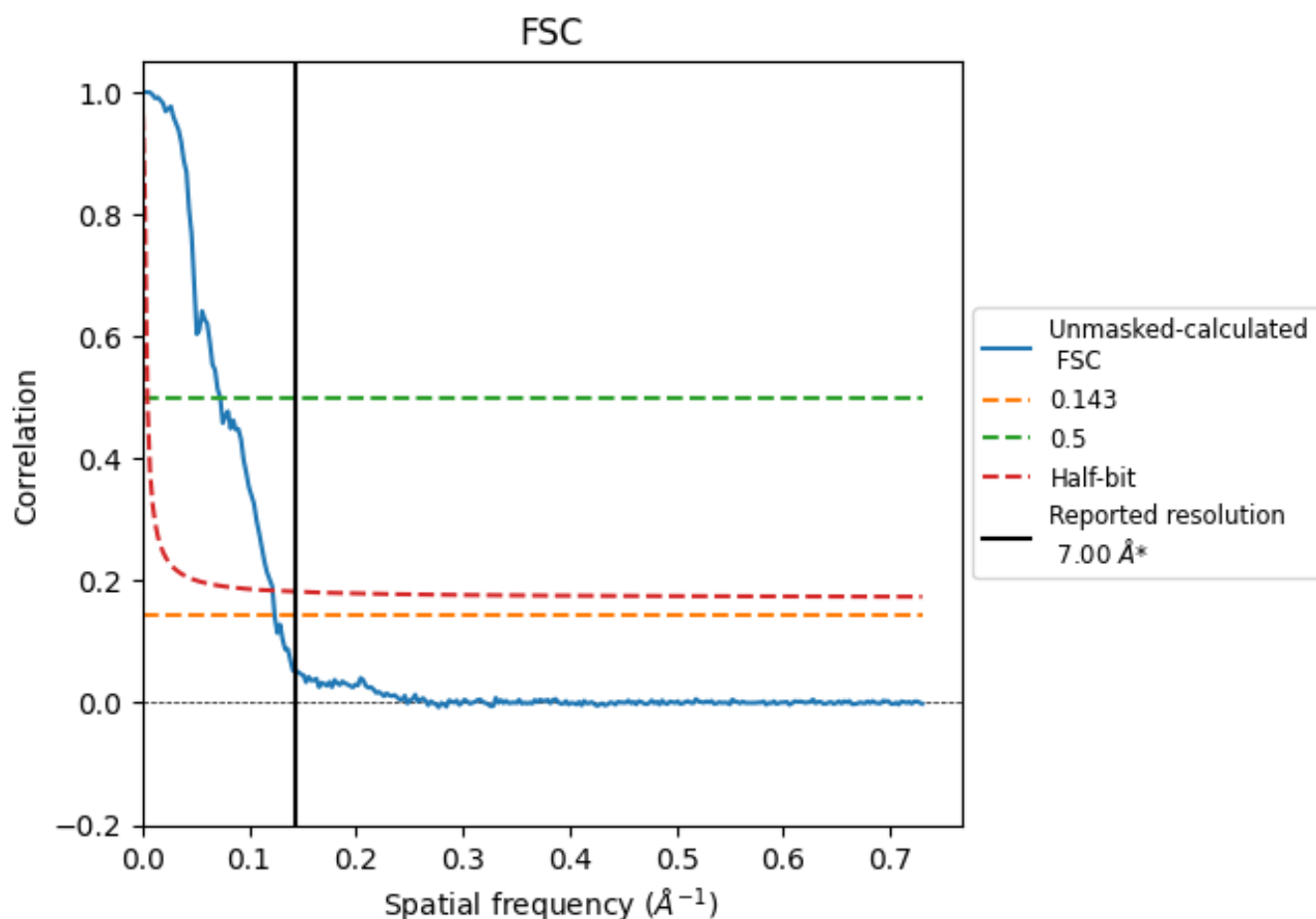


*Reported resolution corresponds to spatial frequency of 0.143 Å⁻¹

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 0.143 \AA^{-1}

8.2 Resolution estimates [i](#)

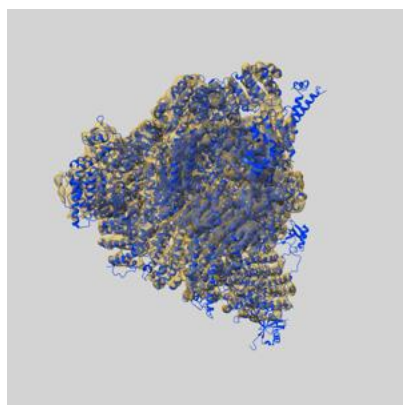
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.07	13.70	8.20

*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 8.07 differs from the reported value 7.0 by more than 10 %

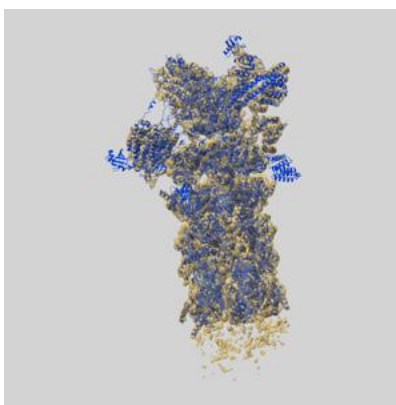
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62081 and PDB model 9K55. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

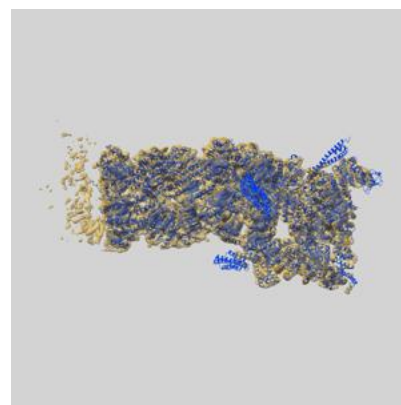
9.1 Map-model overlay [i](#)



X



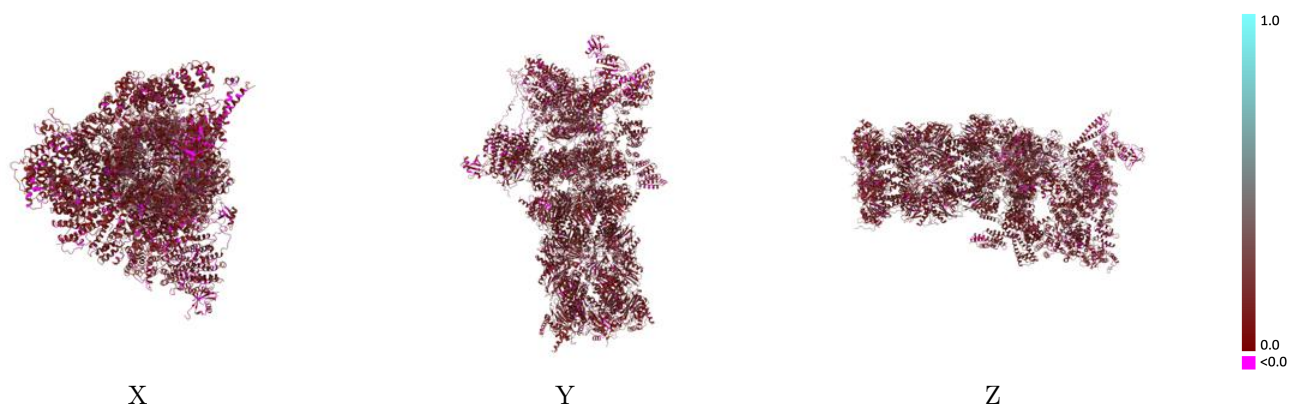
Y



Z

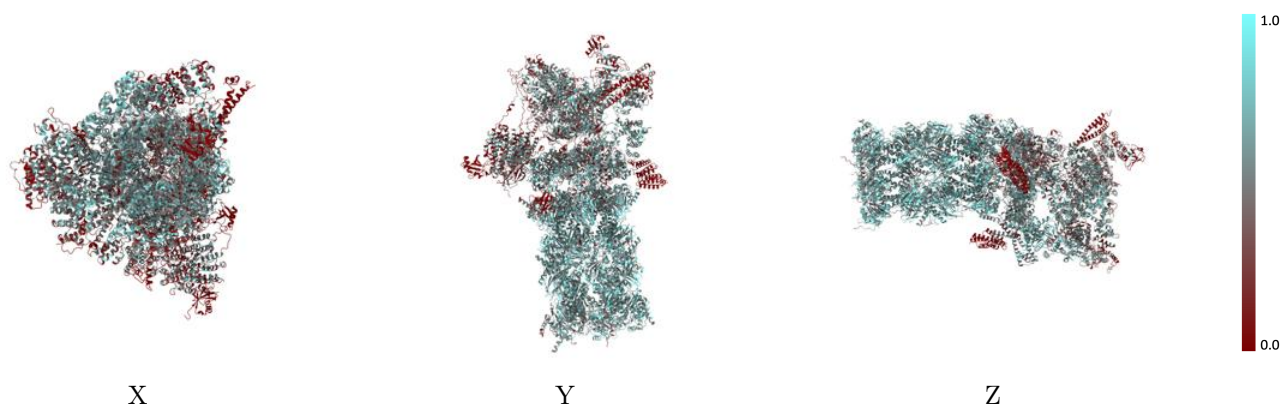
The images above show the 3D surface view of the map at the recommended contour level 0.00578 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



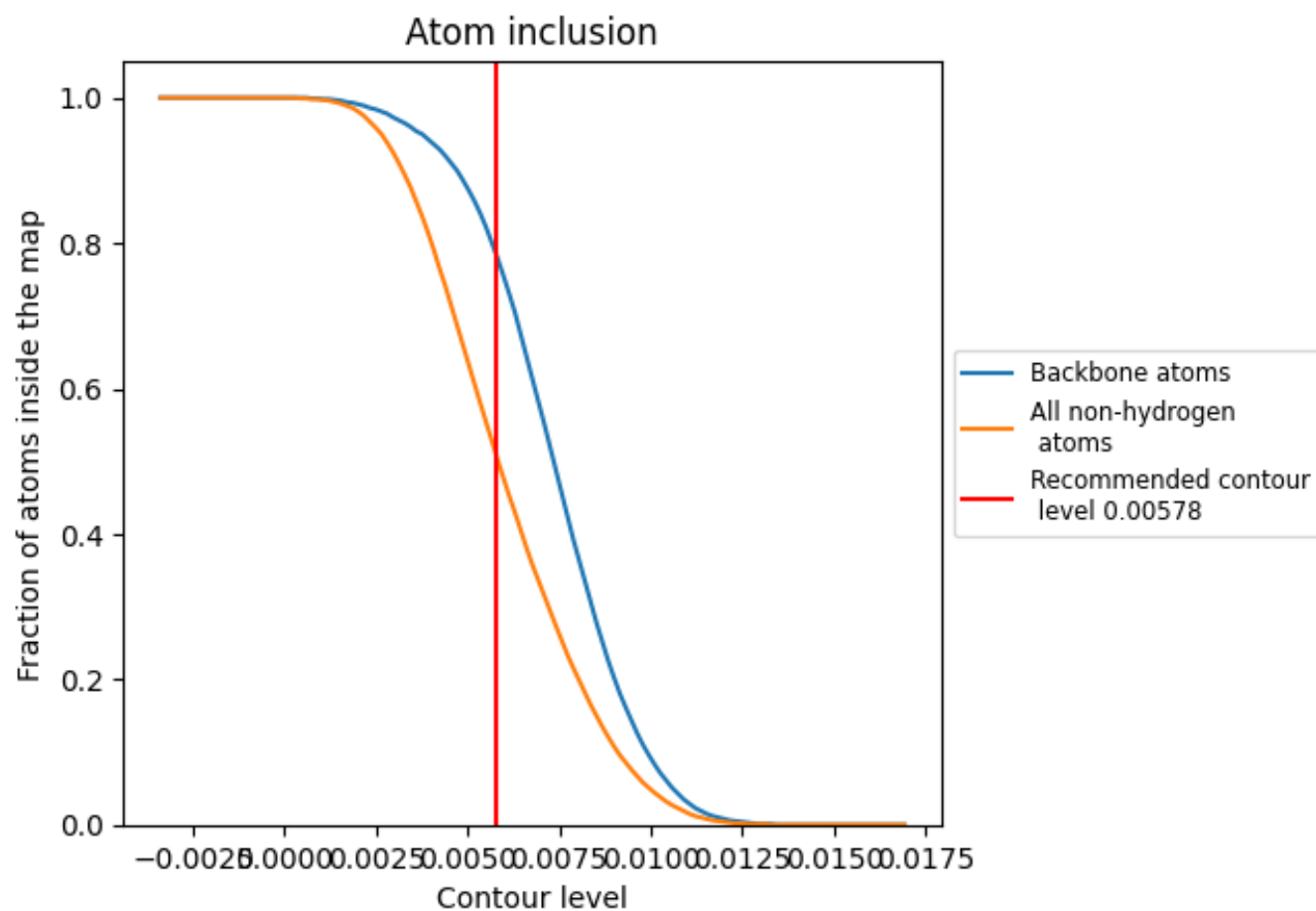
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00578).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 51% 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 (0.00578) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5090	 0.1700
A	 0.4630	 0.1890
B	 0.4610	 0.1820
C	 0.5000	 0.1840
D	 0.5180	 0.1850
E	 0.3310	 0.1530
F	 0.4180	 0.1720
G	 0.6040	 0.1890
H	 0.6370	 0.1970
I	 0.5920	 0.1910
J	 0.5990	 0.1940
K	 0.5880	 0.1890
L	 0.6340	 0.1930
M	 0.6190	 0.1820
N	 0.6410	 0.1860
O	 0.6750	 0.1950
P	 0.6440	 0.1800
Q	 0.6610	 0.1860
R	 0.6590	 0.1820
S	 0.6360	 0.1790
T	 0.6180	 0.1940
U	 0.4360	 0.1440
V	 0.4530	 0.1590
W	 0.3630	 0.1660
X	 0.4150	 0.1640
Y	 0.6010	 0.1590
Z	 0.4460	 0.1480
a	 0.4940	 0.1530
b	 0.3780	 0.1460
c	 0.4640	 0.1620
d	 0.3400	 0.1510
e	 0.4200	 0.1870
f	 0.3480	 0.1550
g	 0.5840	 0.1710
h	 0.5910	 0.1750



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Chain	Atom inclusion	Q-score
i	 0.5580	 0.1860
j	 0.5280	 0.1710
k	 0.5720	 0.1760
l	 0.6280	 0.1790
m	 0.5930	 0.1730
n	 0.6410	 0.1810
o	 0.6490	 0.1810
p	 0.6220	 0.1650
q	 0.6130	 0.1730
r	 0.6620	 0.1790
s	 0.6360	 0.1740
t	 0.6550	 0.1800
v	 0.1390	 0.2120
w	 0.0000	 0.0720
x	 0.0000	 0.1060
z	 0.0980	 0.0490