



## Full wwPDB EM Validation Report ⓘ

Apr 21, 2026 – 02:12 PM JST

PDB ID : 9K4O / pdb\_00009k4o  
EMDB ID : EMD-62065  
Title : Structure of substrate-engaged human 26S proteasome RP-CP subcomplex in state EA2.2  
Authors : Wu, Z.; Chen, E.; Mao, Y.  
Deposited on : 2024-10-21  
Resolution : 6.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

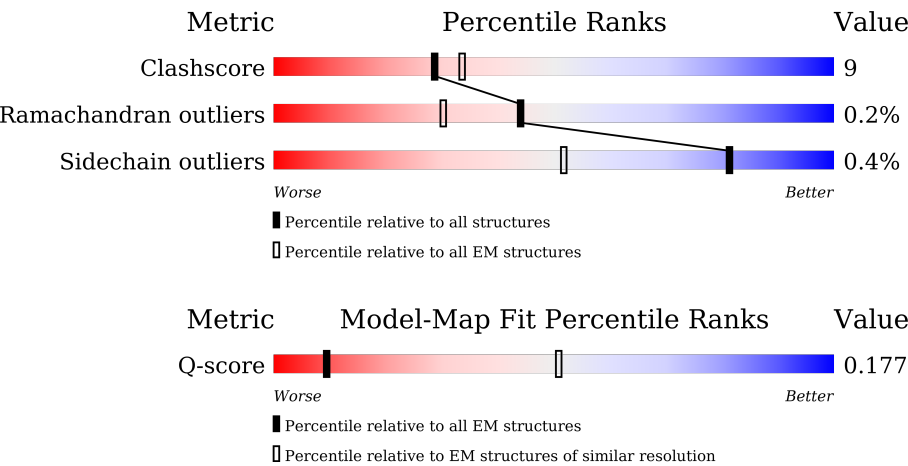
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.00 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	525 ( 5.50 - 6.50 )

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

Mol	Chain	Length	Quality of chain
1	A	433	<div><div>34%</div><div>65%</div><div>26%</div><div>9%</div></div>
2	B	440	<div><div>34%</div><div>62%</div><div>25%</div><div>13%</div></div>
3	C	398	<div><div>39%</div><div>66%</div><div>24%</div><div>9%</div></div>
4	D	418	<div><div>28%</div><div>67%</div><div>23%</div><div>9%</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	u	76	
33	x	76	
33	y	76	
34	v	10	

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 107132 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	394	Total	C	N	O	S	0	0
			3096	1951	543	584	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	384	Total	C	N	O	S	0	0
			3018	1901	515	587	15		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	380	Total	C	N	O	S	0	0
			3039	1923	524	579	13		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	250	Total	C	N	O	S	1	0
			1958	1236	336	376	10		
9	i	250	Total	C	N	O	S	0	0
			1955	1234	336	375	10		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1880	1179	333	363	5		
10	j	239	Total	C	N	O	S	0	0
			1861	1168	332	356	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	234	Total	C	N	O	S	0	0
			1777	1117	295	354	11		
11	k	234	Total	C	N	O	S	0	0
			1782	1119	295	357	11		

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	238	Total	C	N	O	S	0	0
			1866	1169	336	350	11		
12	l	238	Total	C	N	O	S	0	0
			1861	1165	335	350	11		

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1876	1191	321	353	11		
13	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

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

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

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

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

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

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

- Molecule 17 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
18	r	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	818	Total	C	N	O	S	0	0
			6373	4047	1084	1197	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	444	Total	C	N	O	S	0	0
			3612	2301	645	653	13		

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



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

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

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

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

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

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
31	e	50	Total	C	N	O	0	0
			425	260	65	100		

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

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

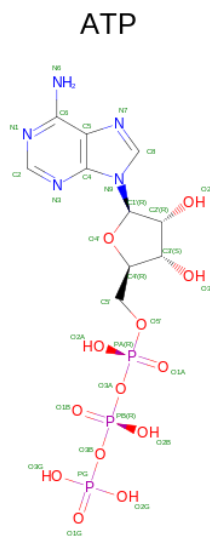
- Molecule 33 is a protein called Ubiquitin.

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

- Molecule 34 is a protein called Substrate.

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

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).

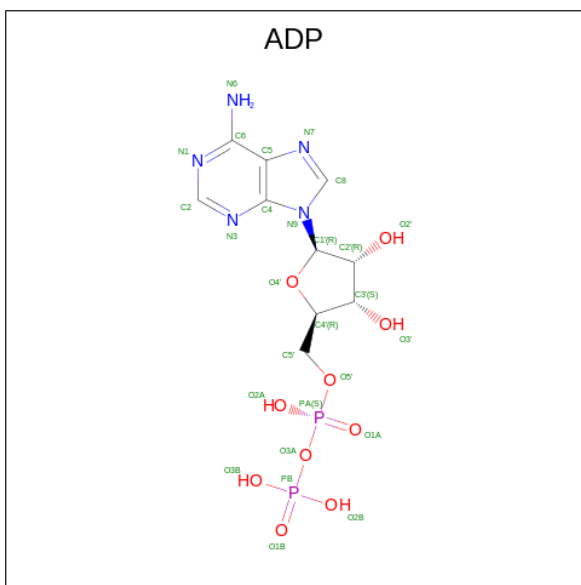


Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total 31	C 10	N 5	O 13	P 3	0
35	B	1	Total 31	C 10	N 5	O 13	P 3	0
35	D	1	Total 31	C 10	N 5	O 13	P 3	0
35	E	1	Total 31	C 10	N 5	O 13	P 3	0

- 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 1 1	0
36	B	1	Total Mg 1 1	0
36	D	1	Total Mg 1 1	0
36	E	1	Total Mg 1 1	0
36	F	1	Total Mg 1 1	0

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).

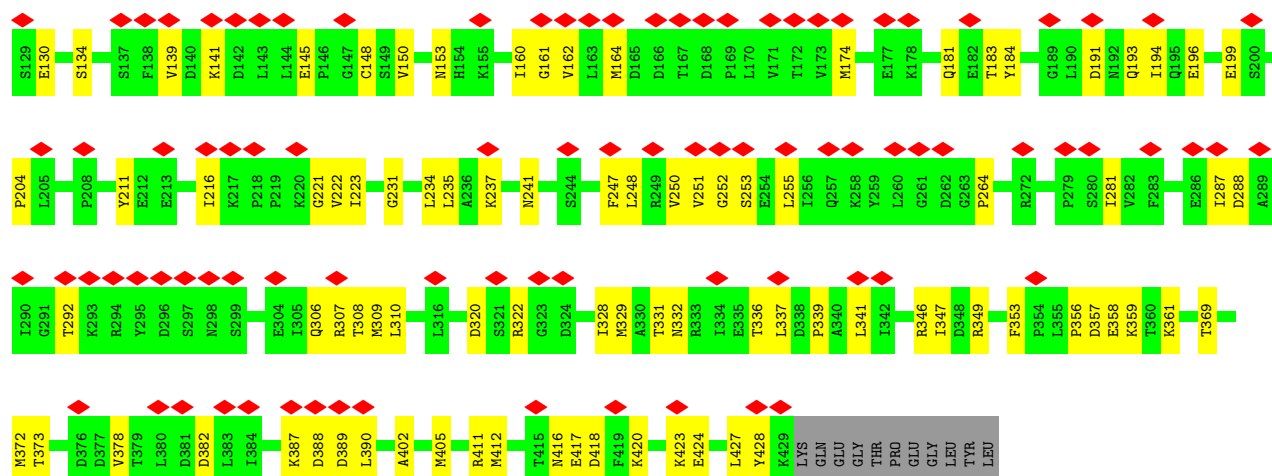


Mol	Chain	Residues	Atoms					AltConf
37	C	1	Total 27	C 10	N 5	O 10	P 2	0
37	F	1	Total 27	C 10	N 5	O 10	P 2	0

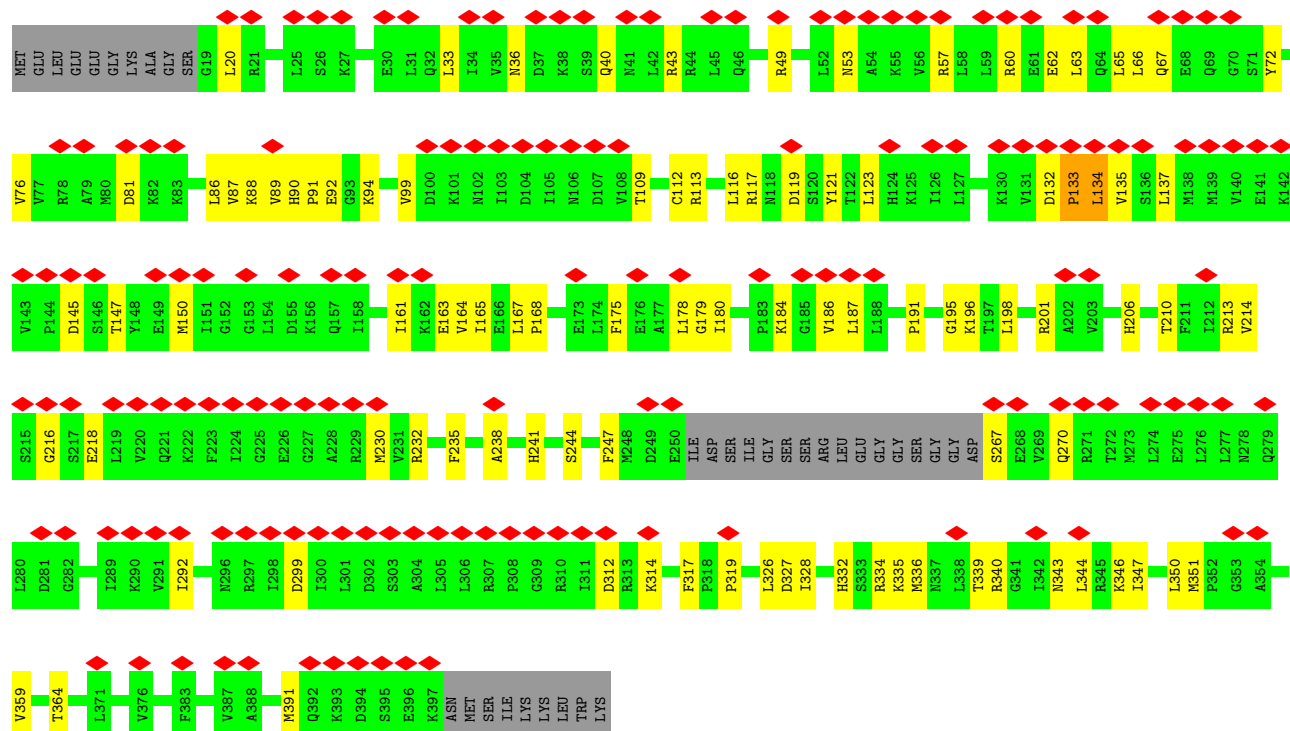
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

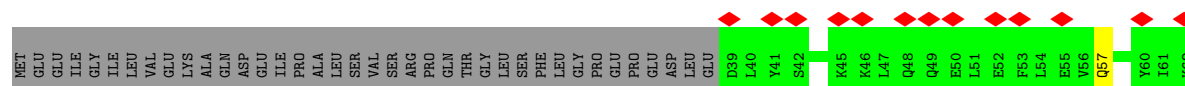


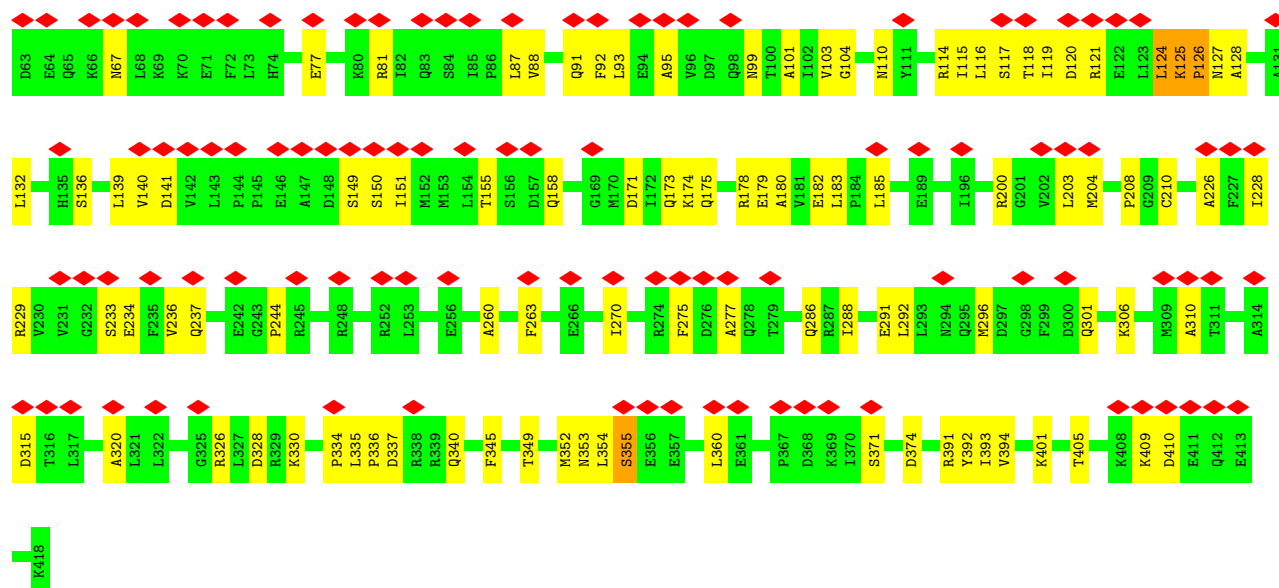


• Molecule 3: 26S proteasome regulatory subunit 8

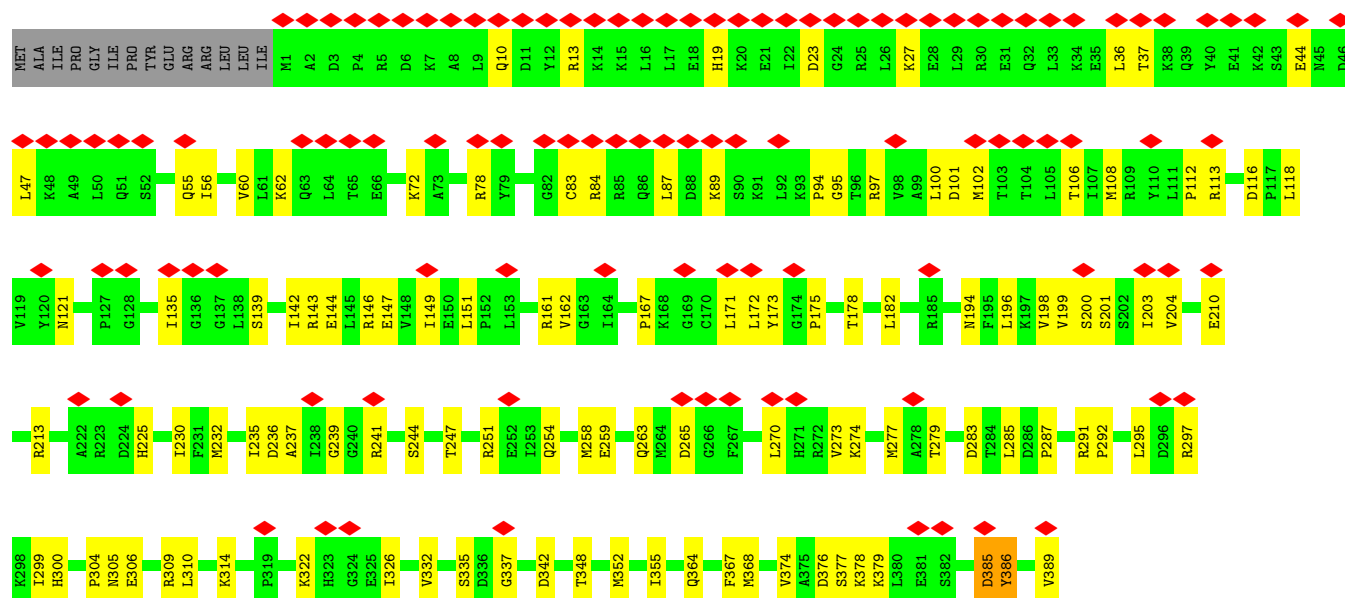


• Molecule 4: 26S proteasome regulatory subunit 6B

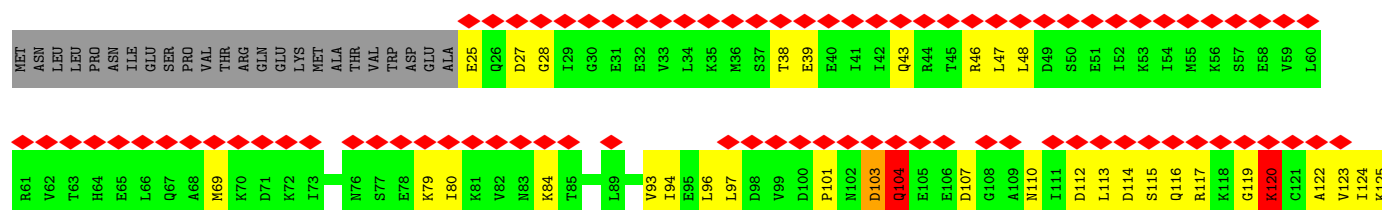


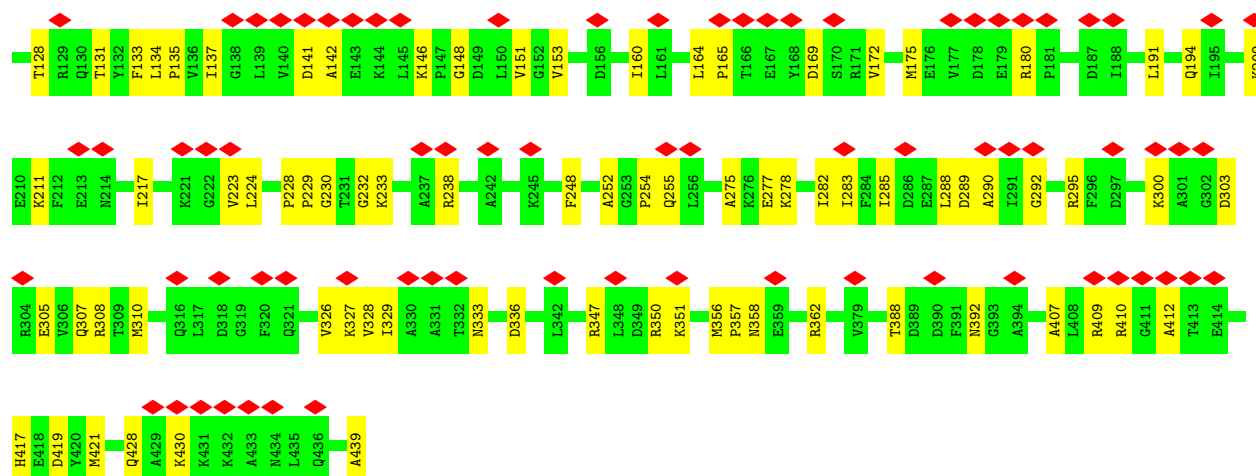


• Molecule 5: Proteasome 26S subunit, ATPase 6

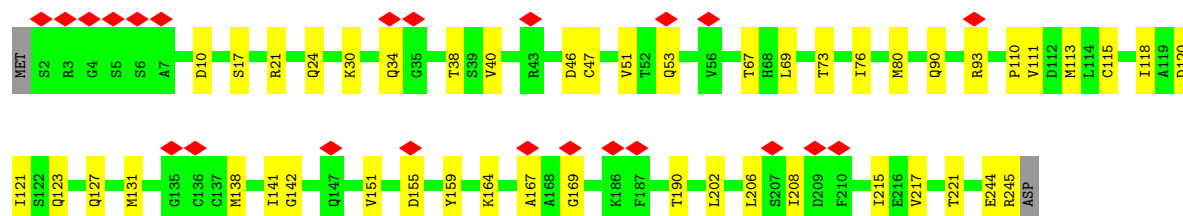
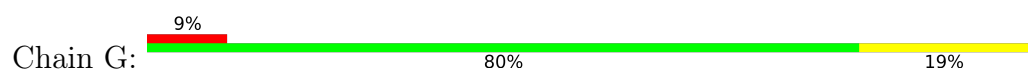


• Molecule 6: 26S proteasome regulatory subunit 6A

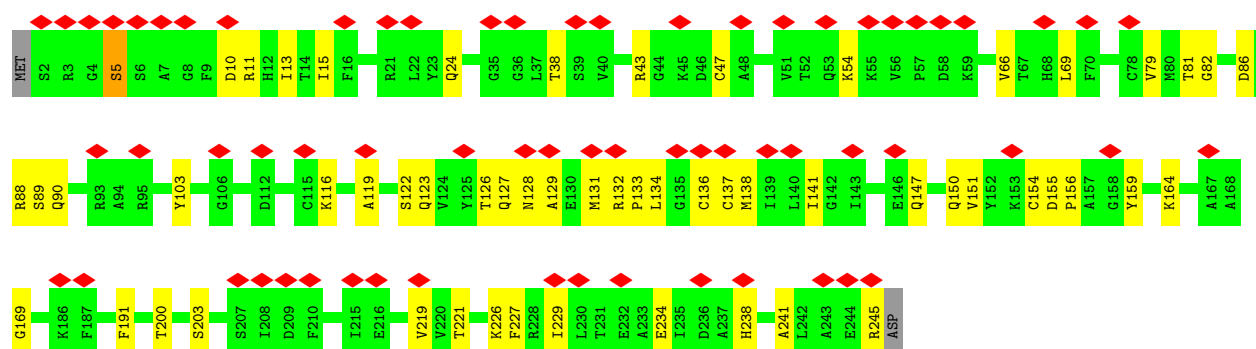
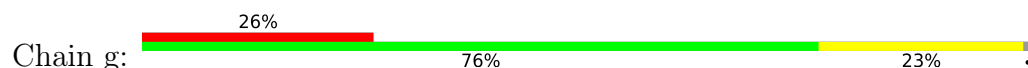




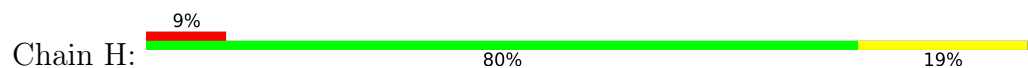
• Molecule 7: Proteasome subunit alpha type-6



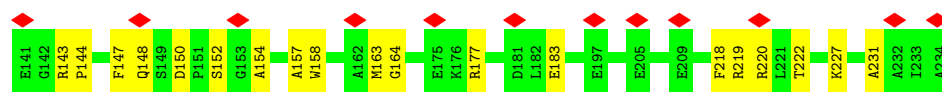
• Molecule 7: Proteasome subunit alpha type-6



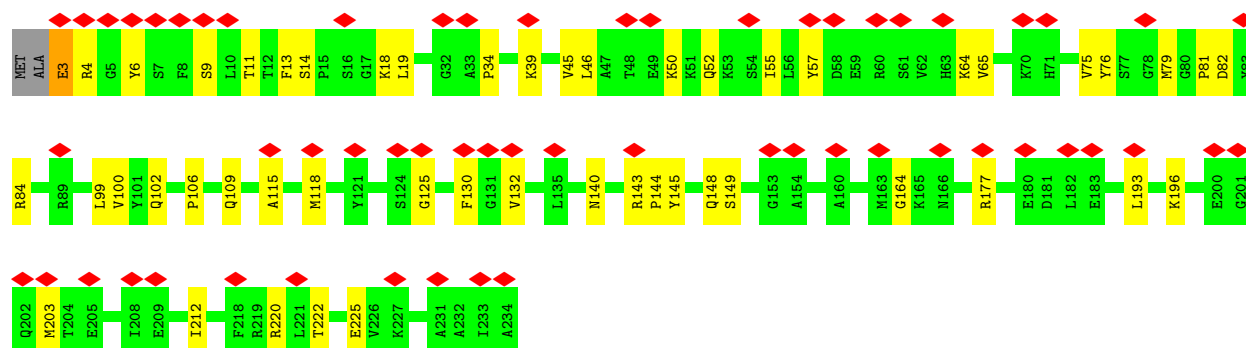
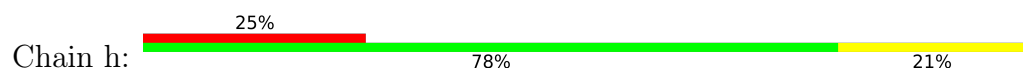
• Molecule 8: Proteasome subunit alpha type-2



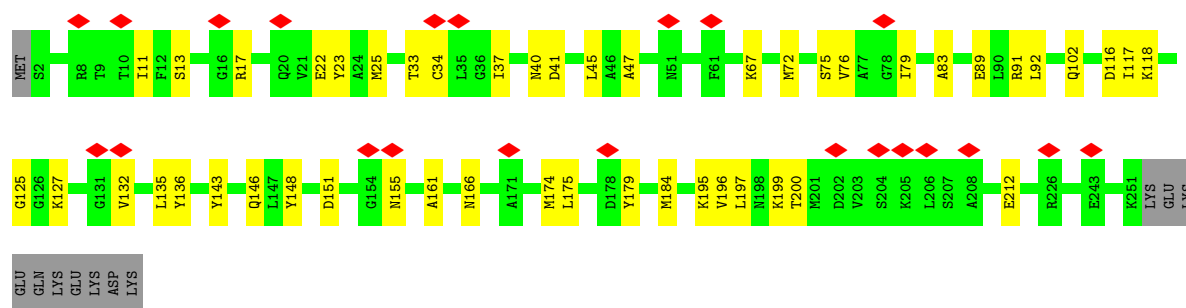
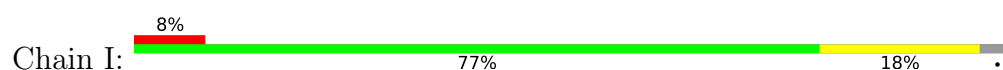




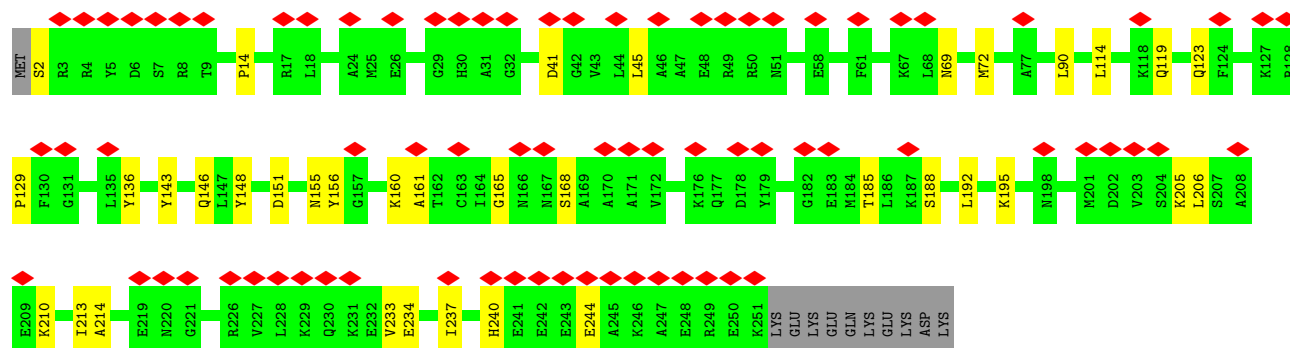
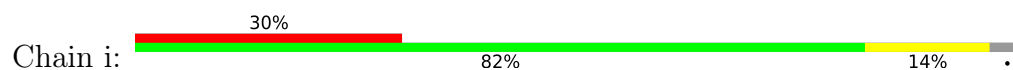
• Molecule 8: Proteasome subunit alpha type-2



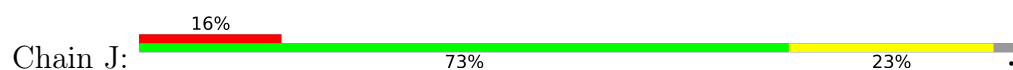
• Molecule 9: Proteasome subunit alpha type-4

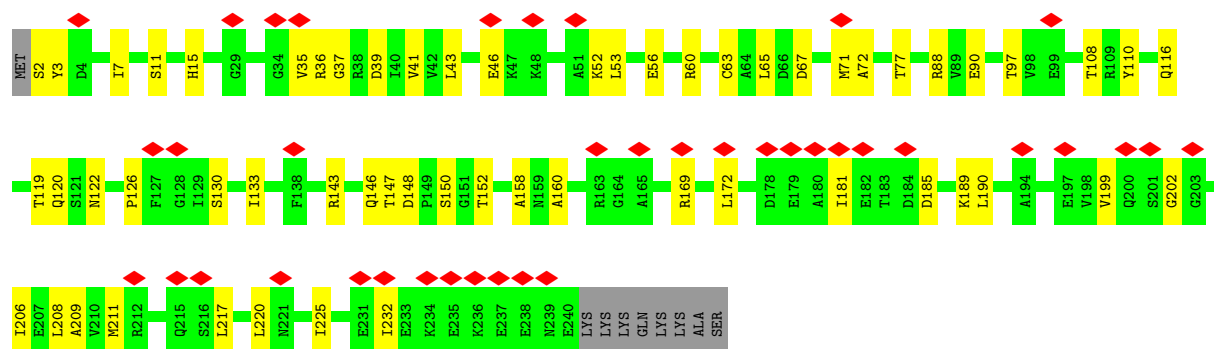


• Molecule 9: Proteasome subunit alpha type-4

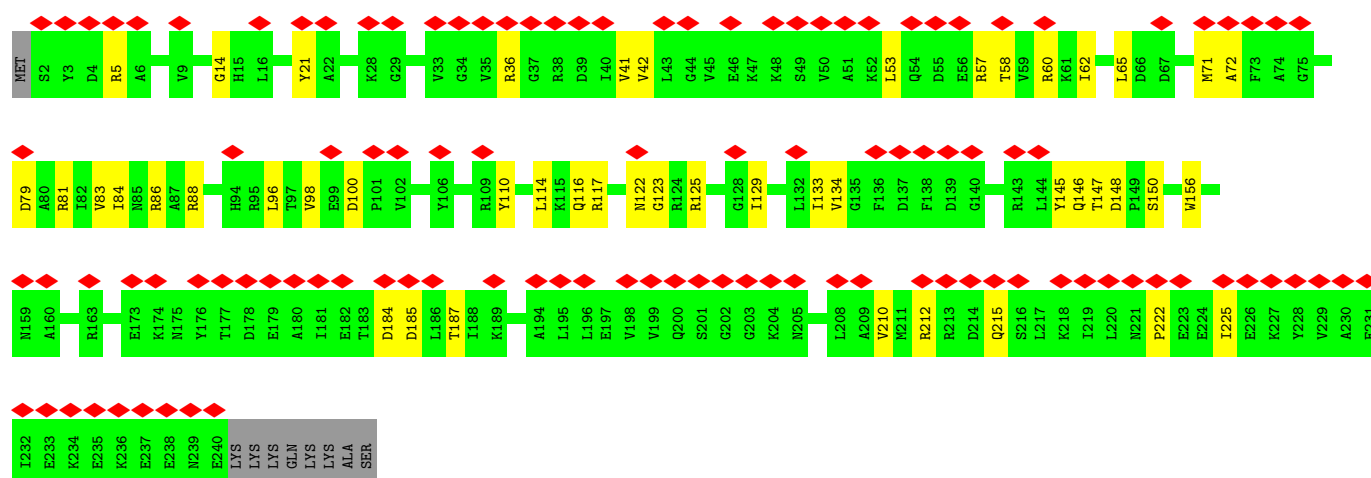
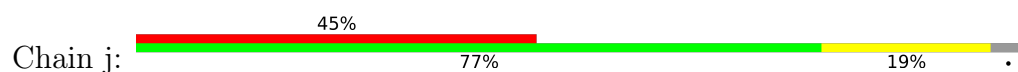


• Molecule 10: Proteasome subunit alpha type-7

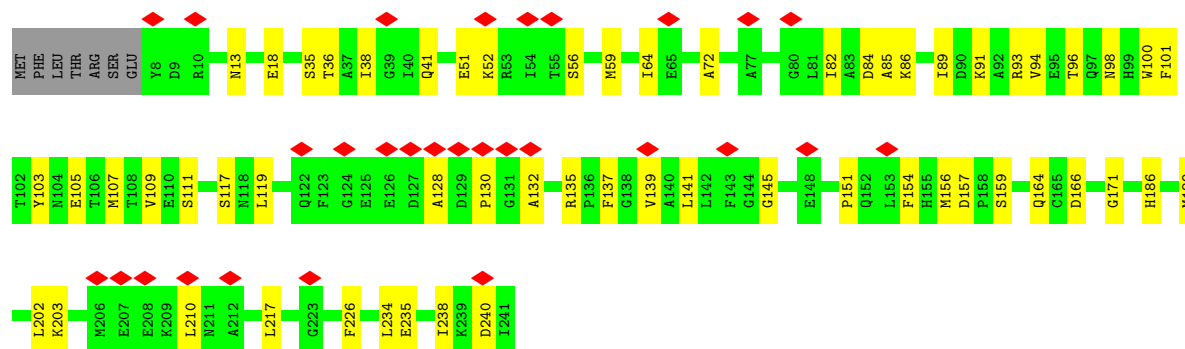
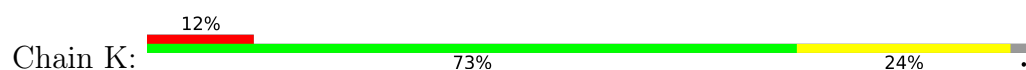




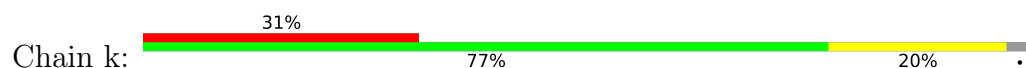
• Molecule 10: Proteasome subunit alpha type-7

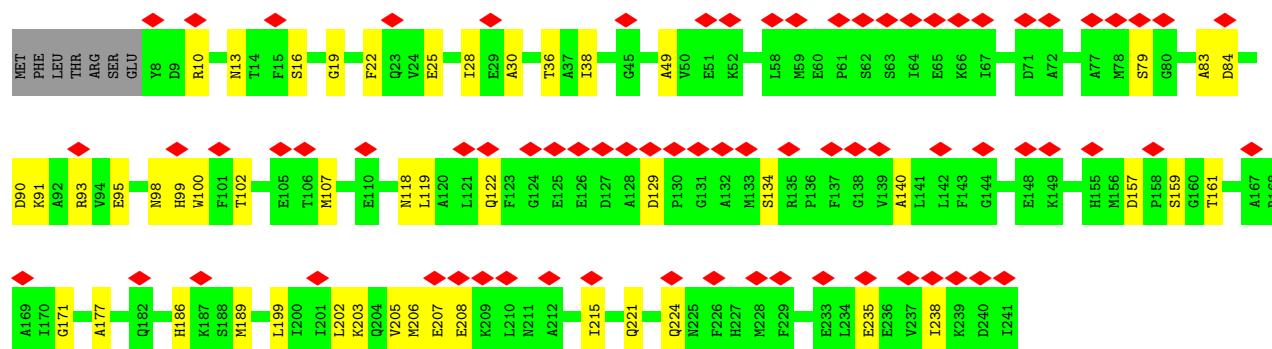


• Molecule 11: Proteasome subunit alpha type-5

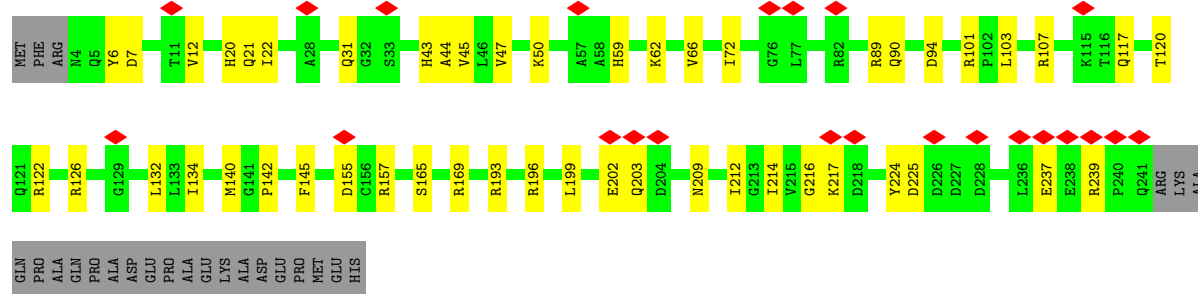


• Molecule 11: Proteasome subunit alpha type-5

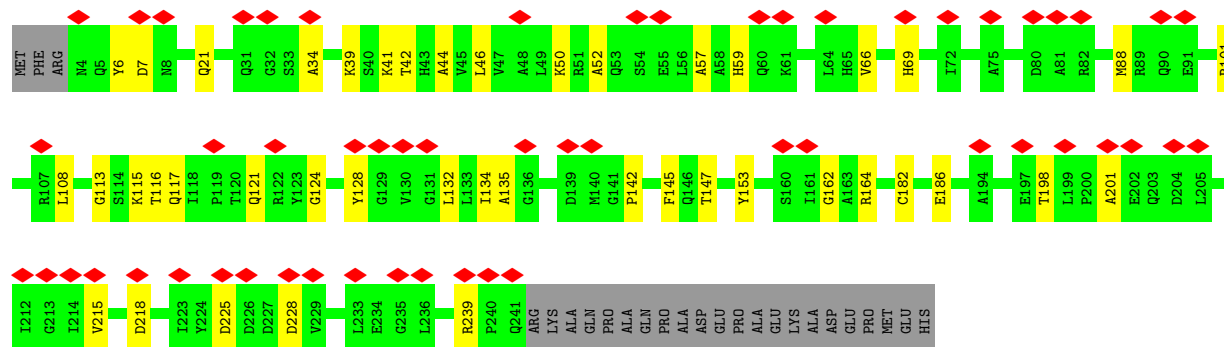
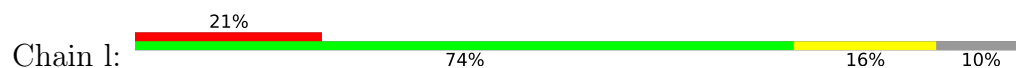




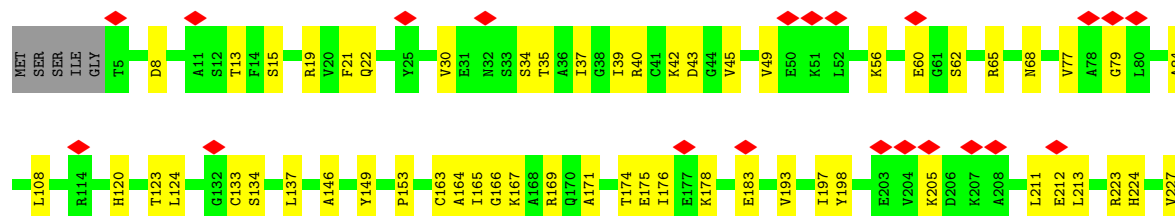
• Molecule 12: Proteasome subunit alpha type-1

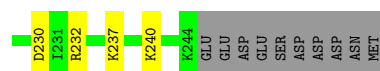


• Molecule 12: Proteasome subunit alpha type-1

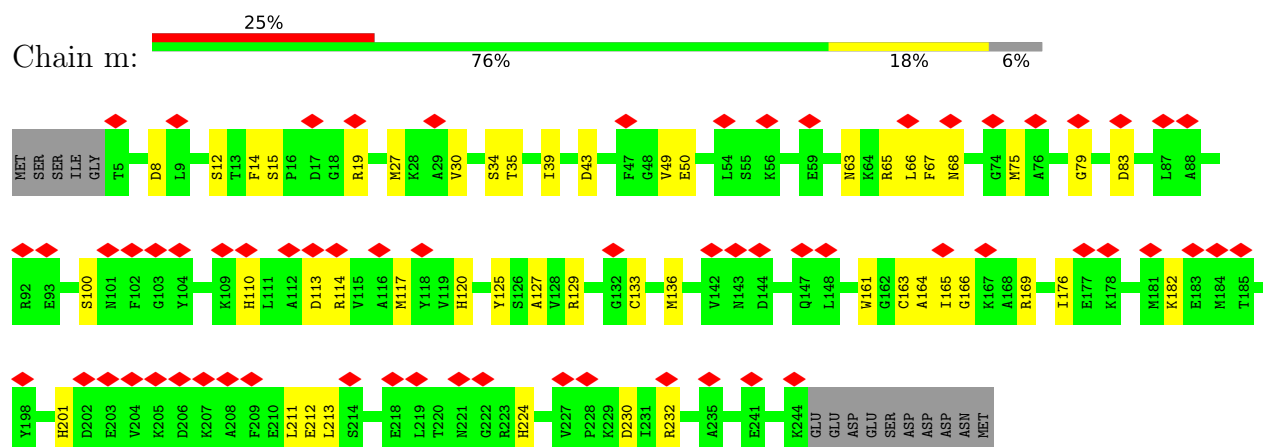


• Molecule 13: Proteasome subunit alpha type-3

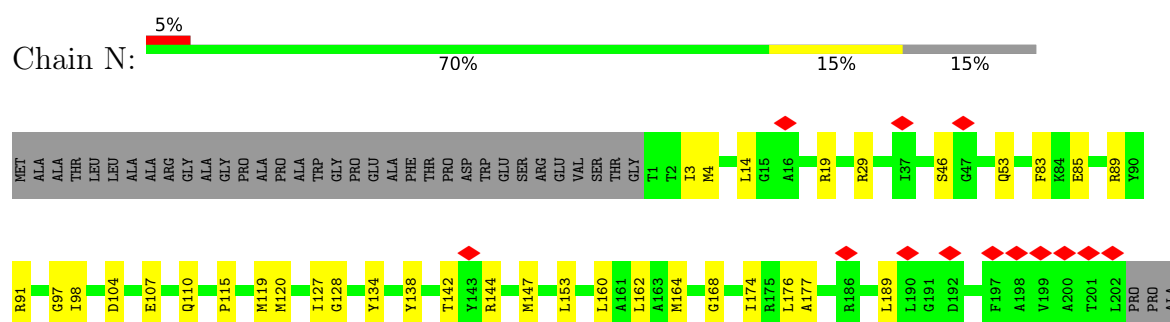




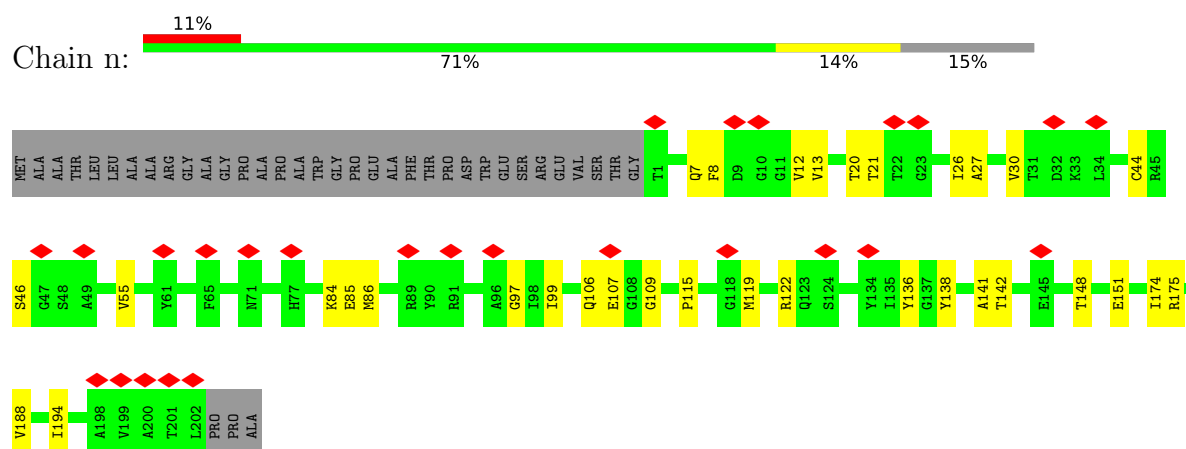
• Molecule 13: Proteasome subunit alpha type-3



• Molecule 14: Proteasome subunit beta type-6

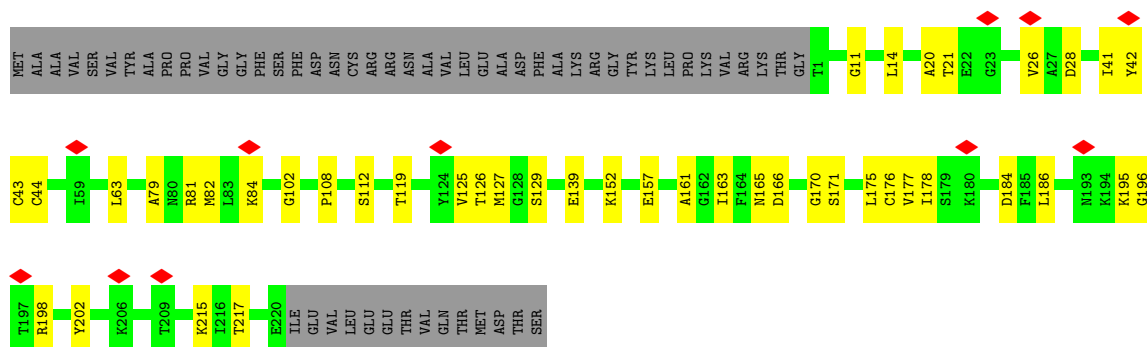


• Molecule 14: Proteasome subunit beta type-6

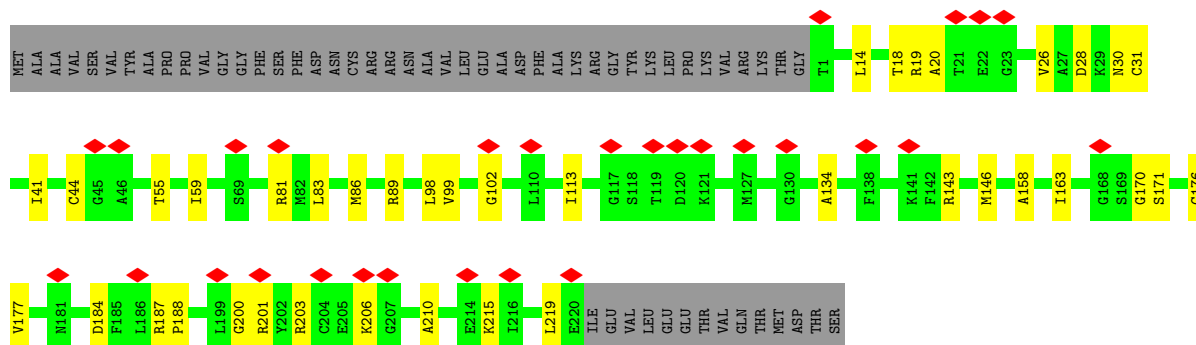


• Molecule 15: Proteasome subunit beta type-7

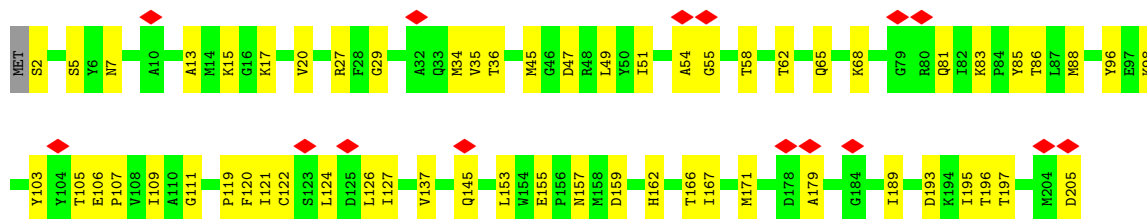




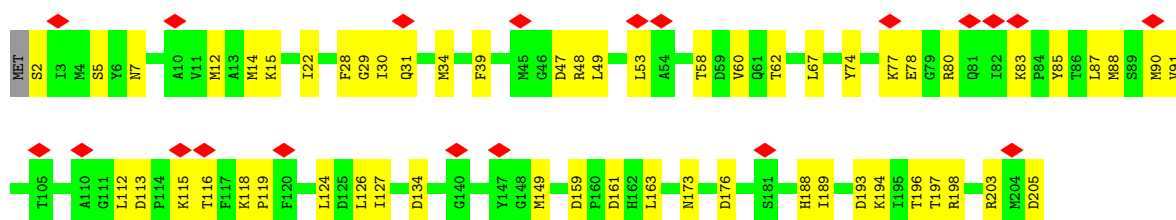
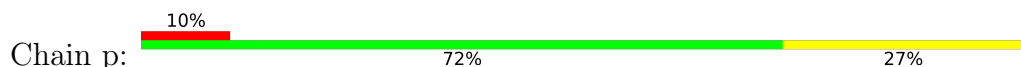
• Molecule 15: Proteasome subunit beta type-7



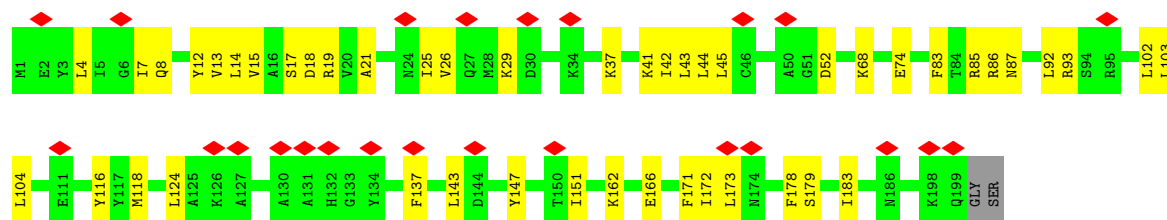
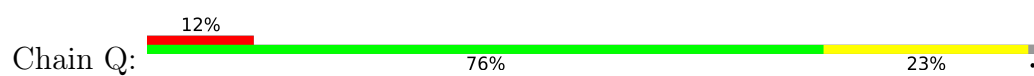
• Molecule 16: Proteasome subunit beta type-3



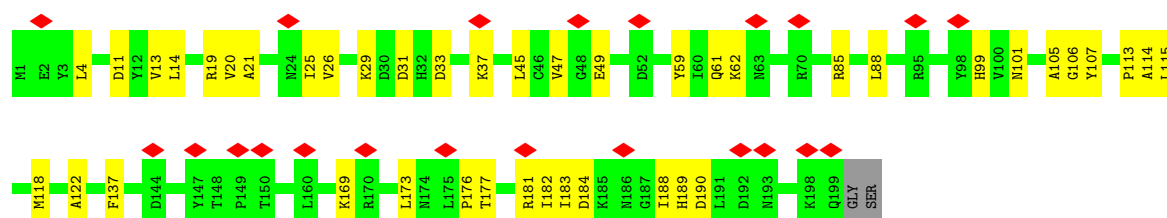
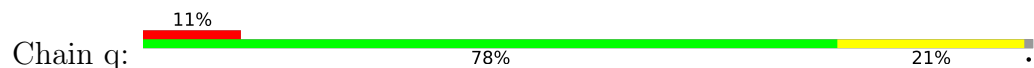
• Molecule 16: Proteasome subunit beta type-3



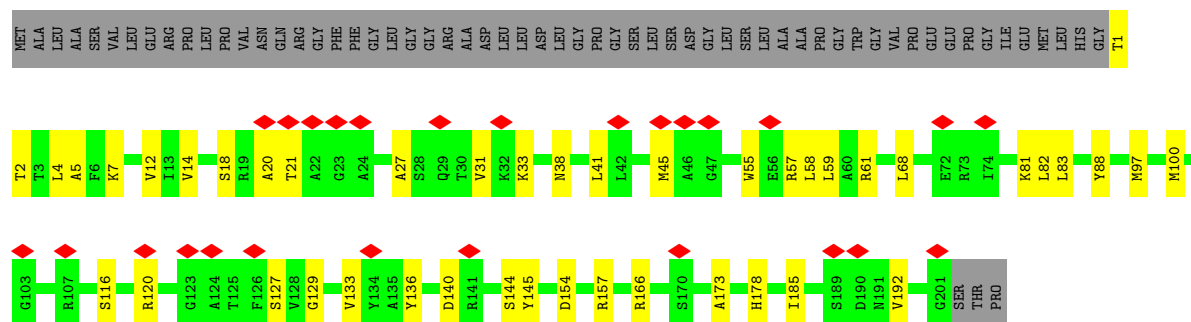
• Molecule 17: Proteasome subunit beta type-2



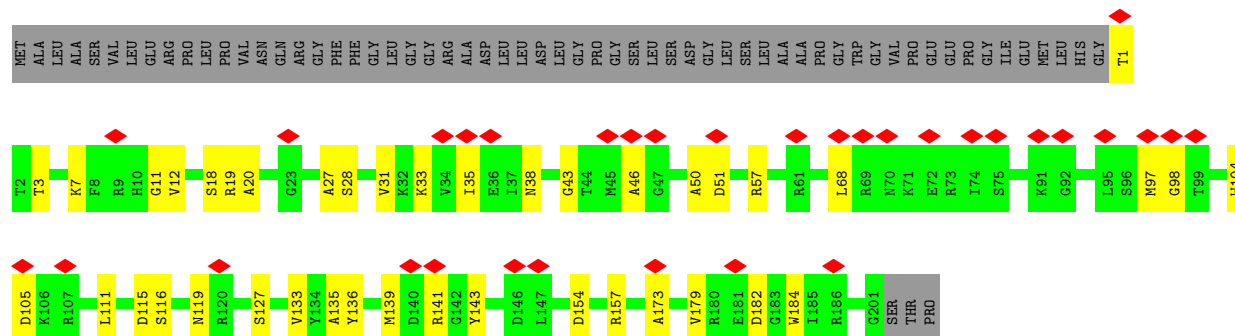
• Molecule 17: Proteasome subunit beta type-2



• Molecule 18: Proteasome subunit beta type-5

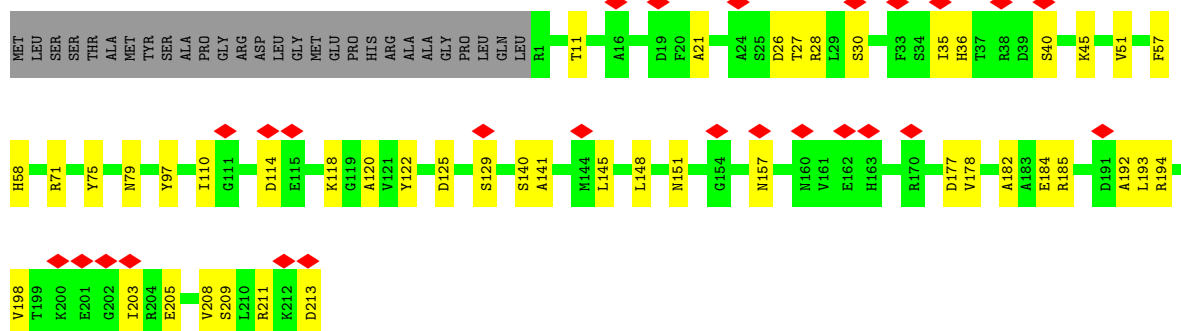


• Molecule 18: Proteasome subunit beta type-5



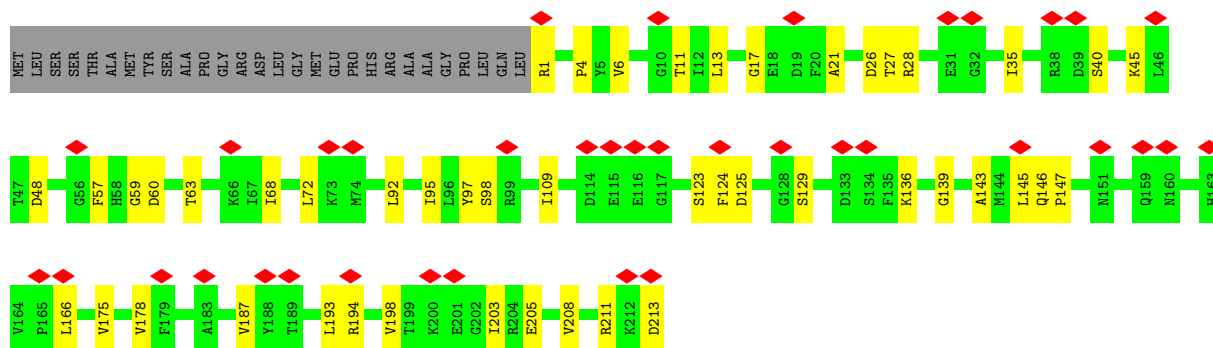
• Molecule 19: Proteasome subunit beta type-1

Chain S: 



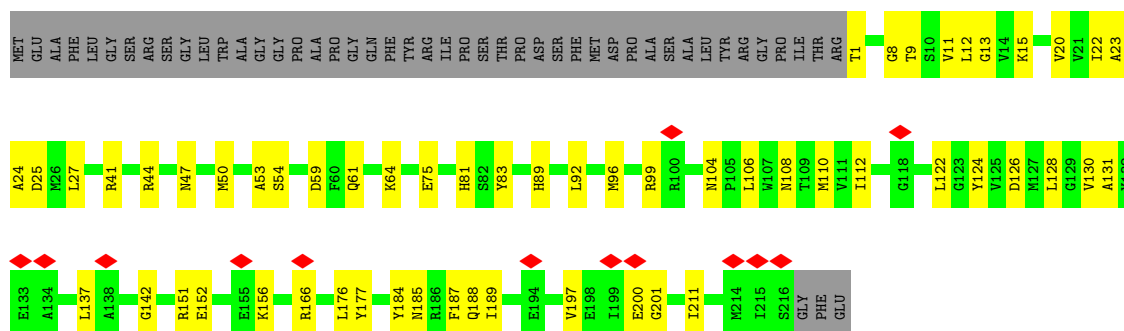
• Molecule 19: Proteasome subunit beta type-1

Chain s: 



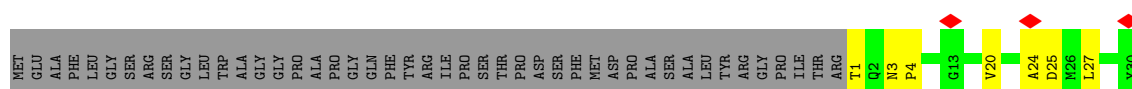
• Molecule 20: Proteasome subunit beta type-4

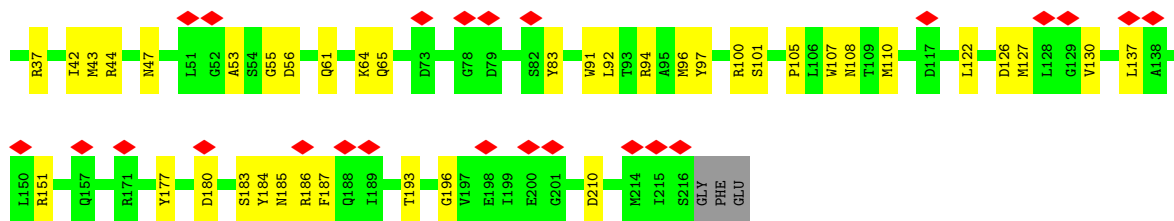
Chain T: 



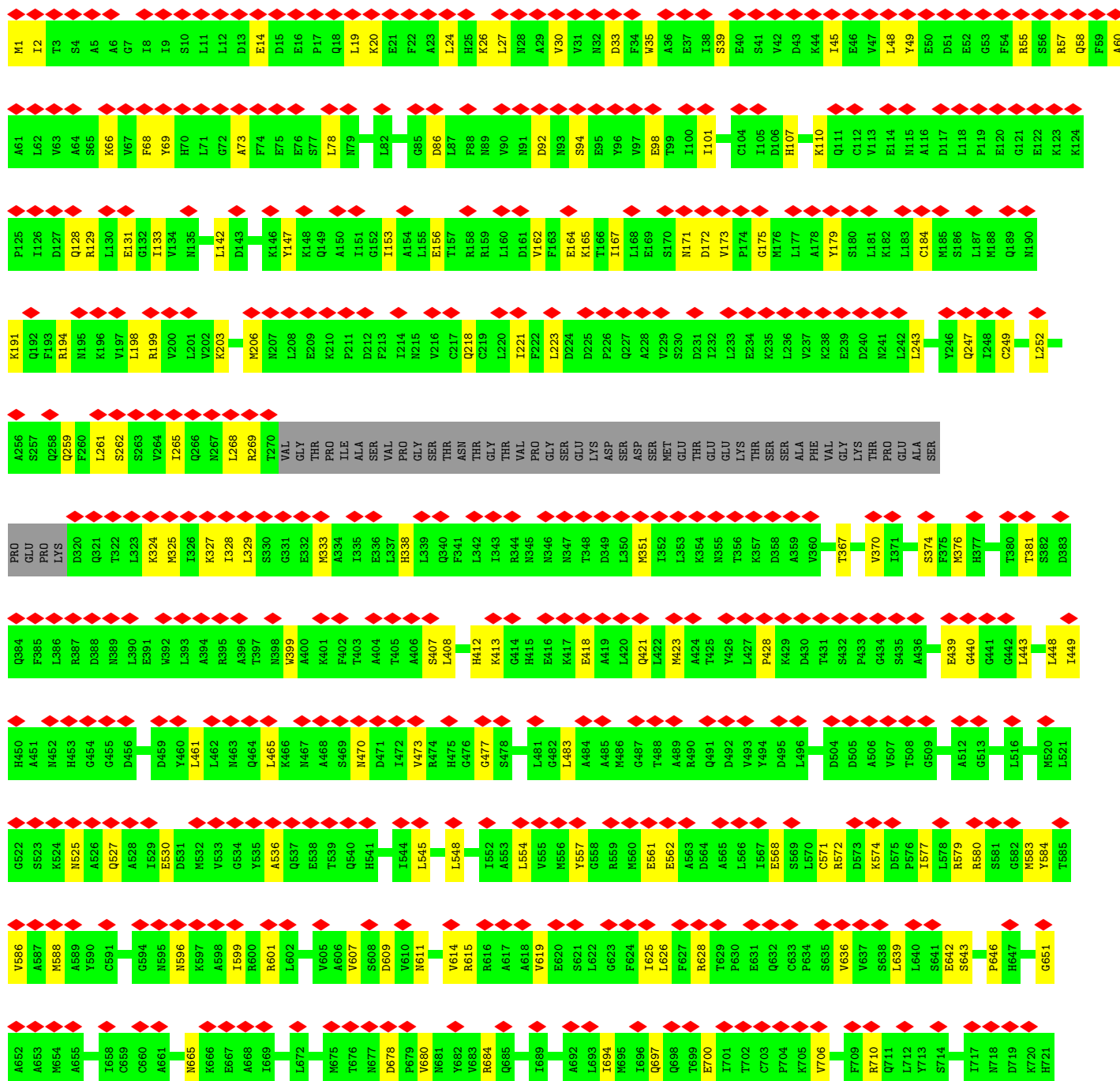
• Molecule 20: Proteasome subunit beta type-4

Chain t: 





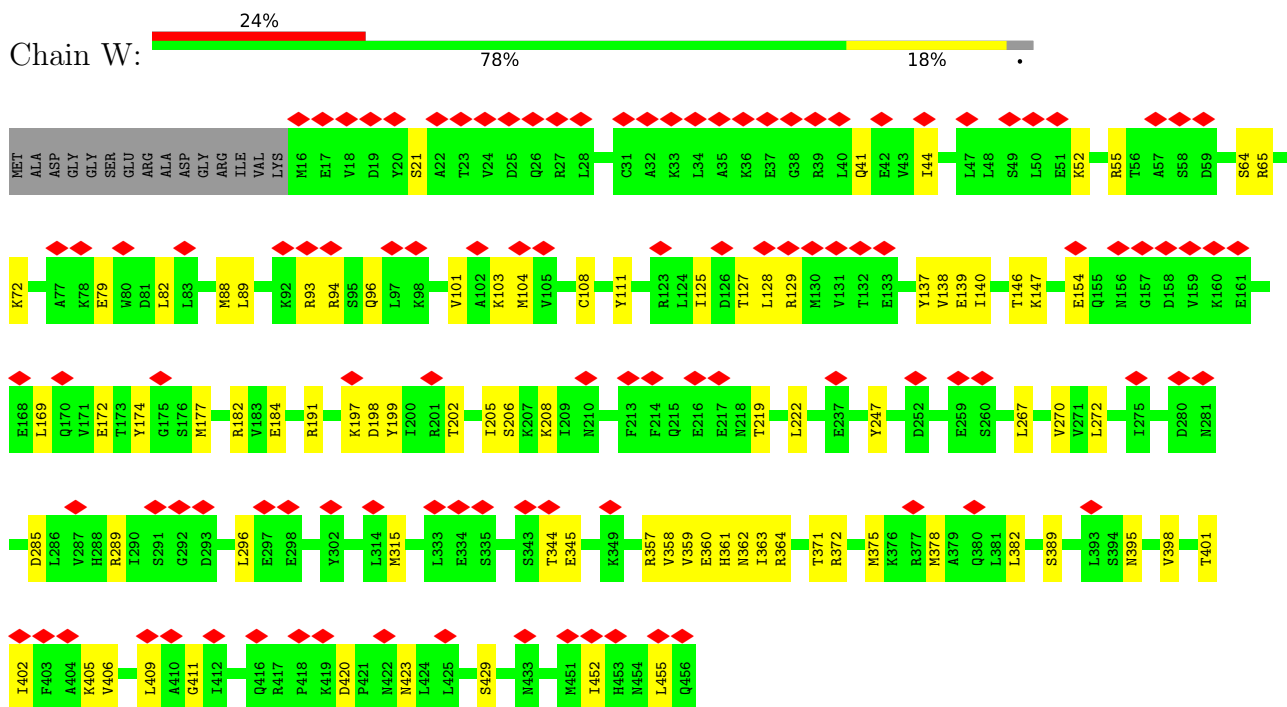
• Molecule 21: 26S proteasome non-ATPase regulatory subunit 1



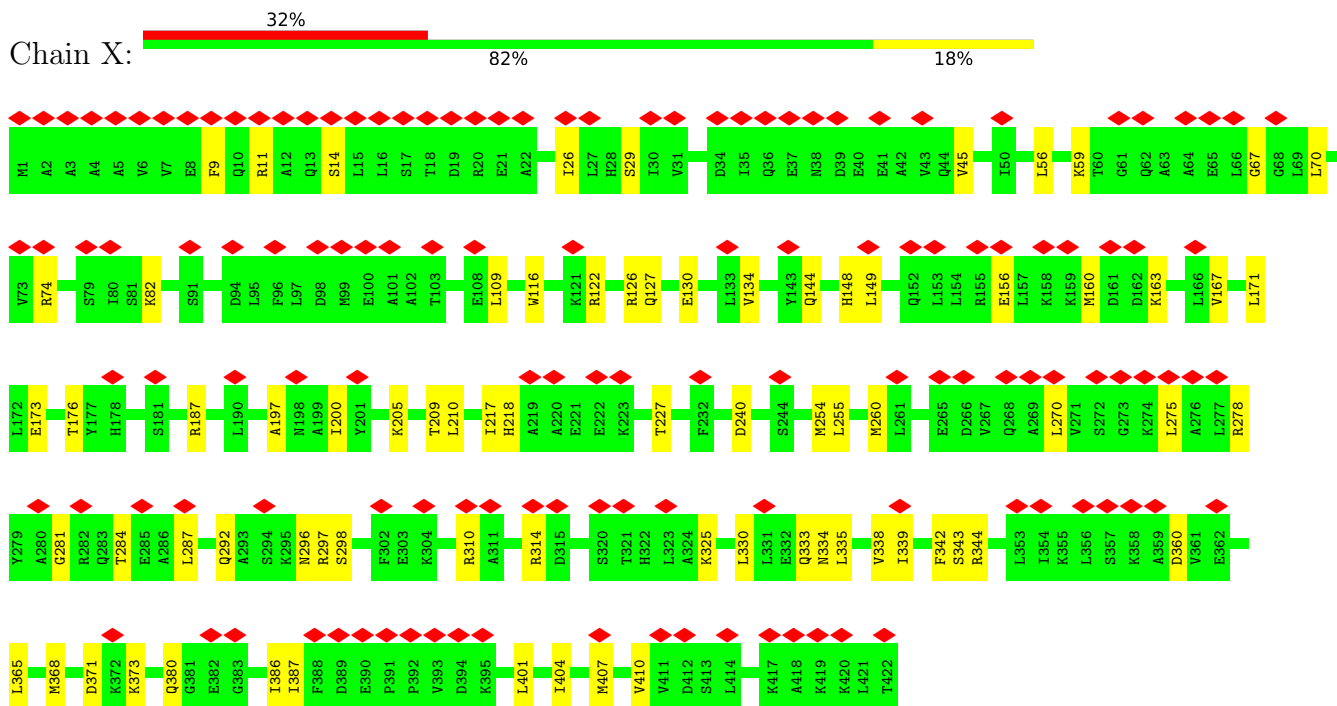




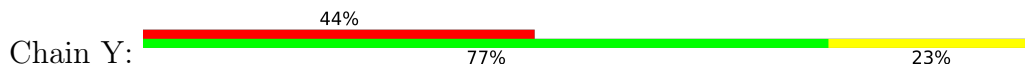
- Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

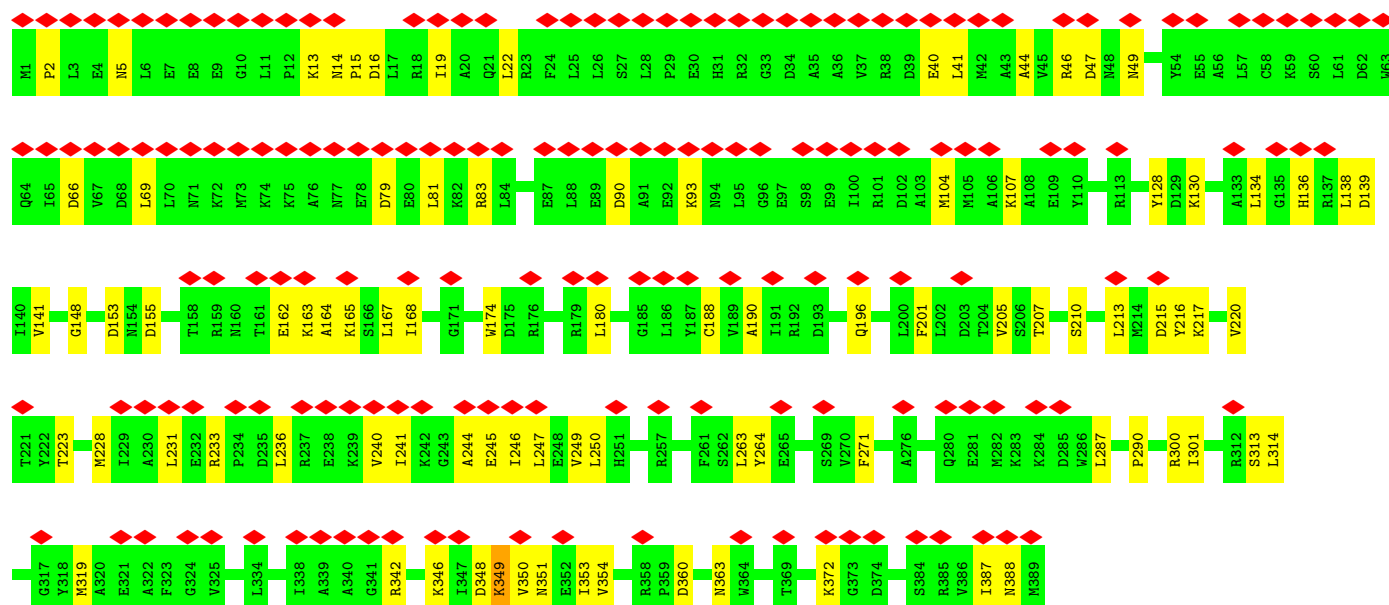


- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11



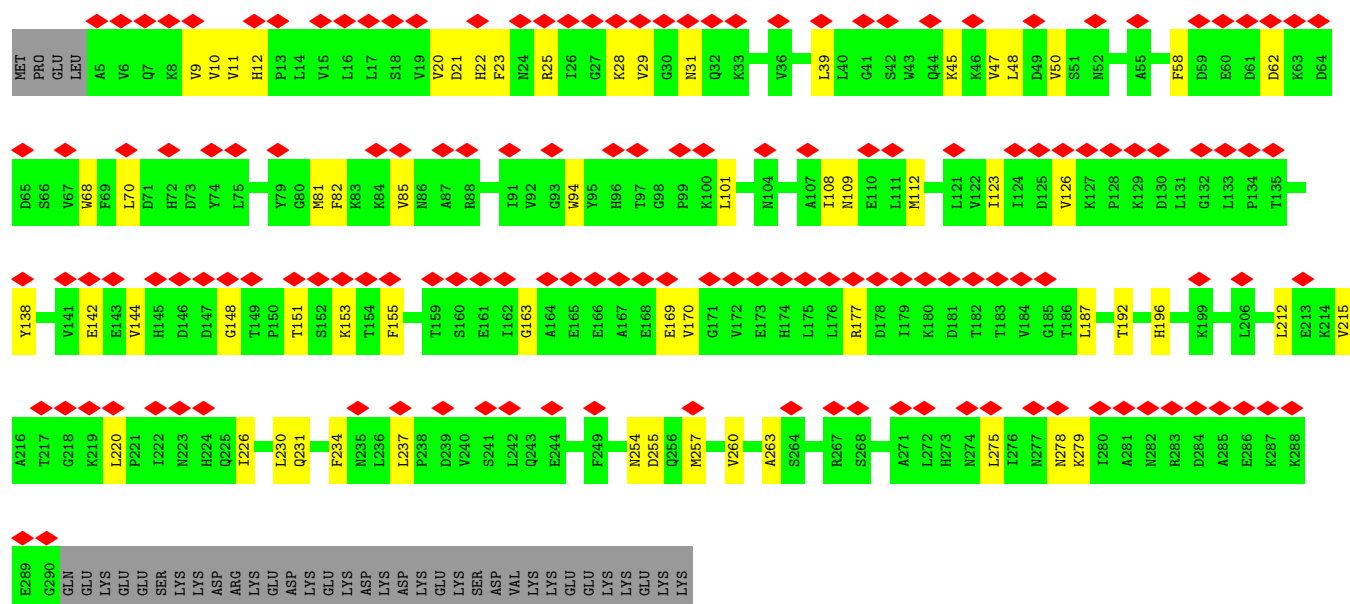
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6





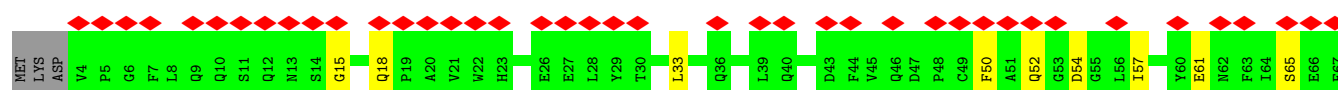
• Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

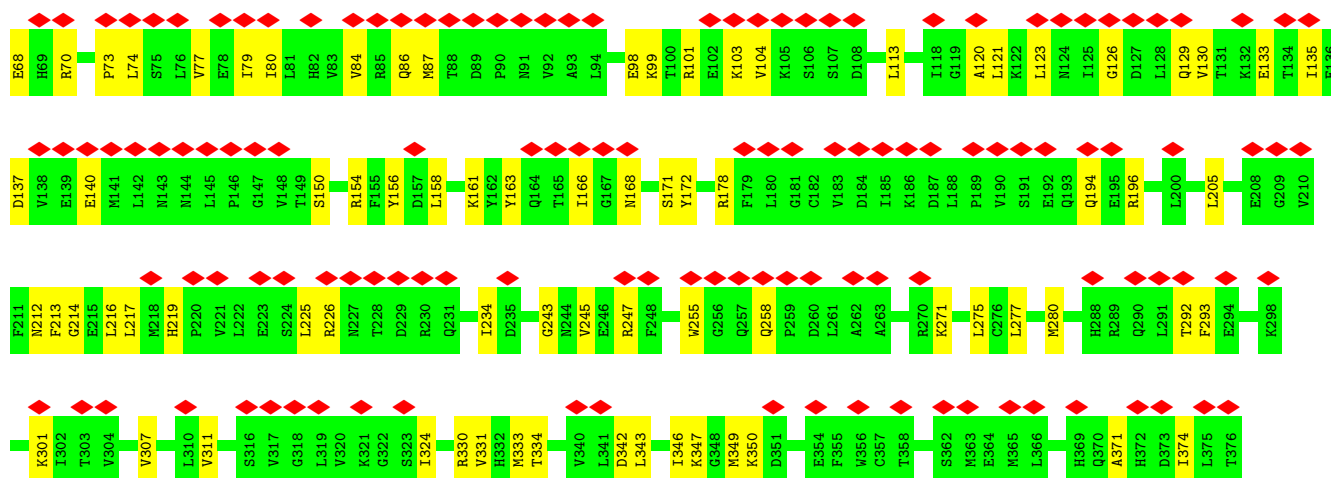
Chain Z:



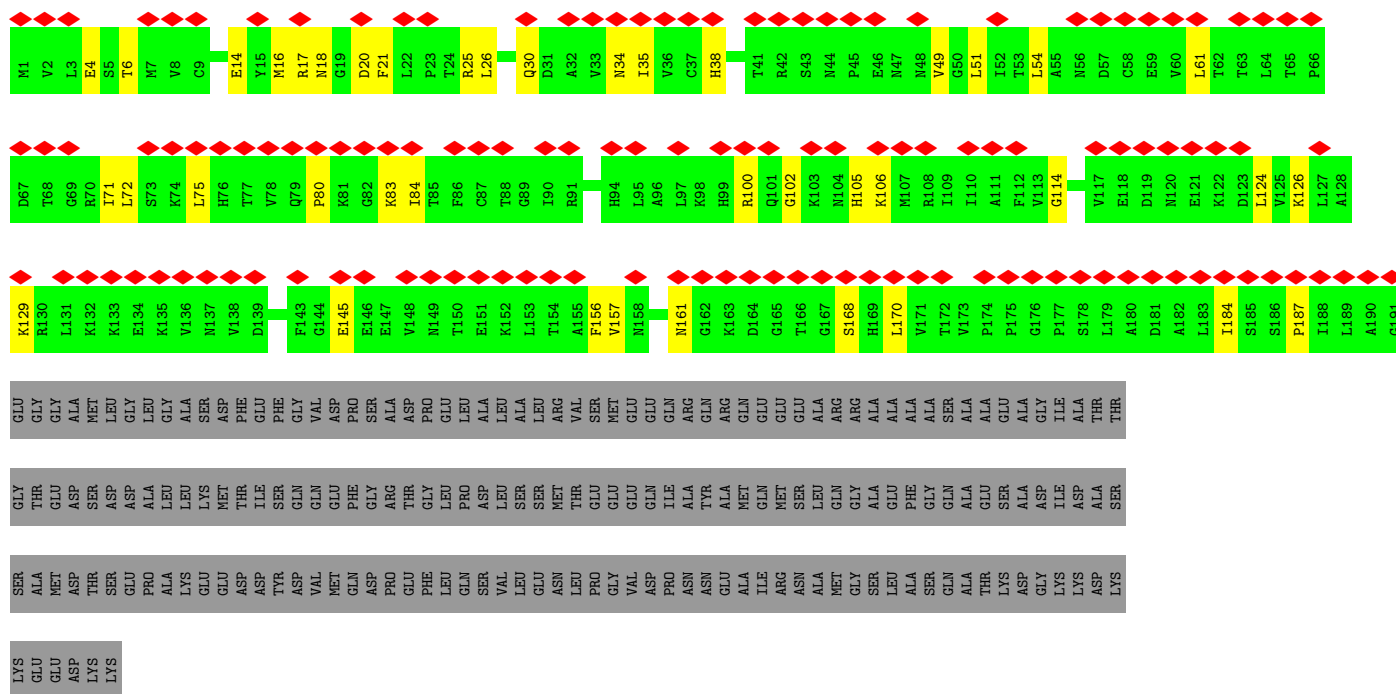
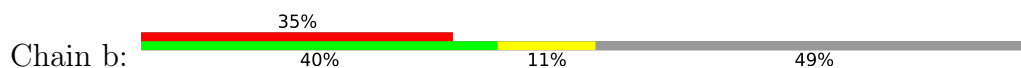
• Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

Chain a:

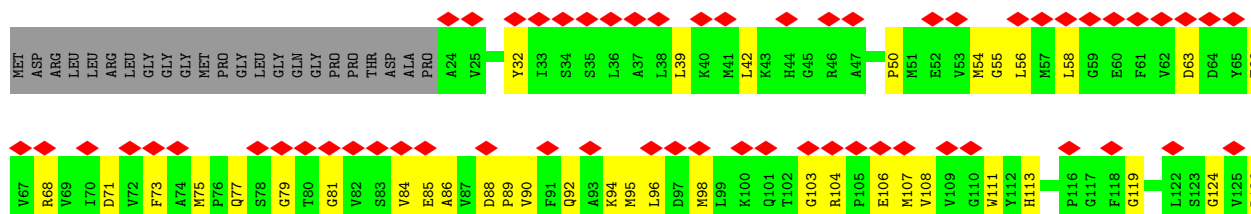


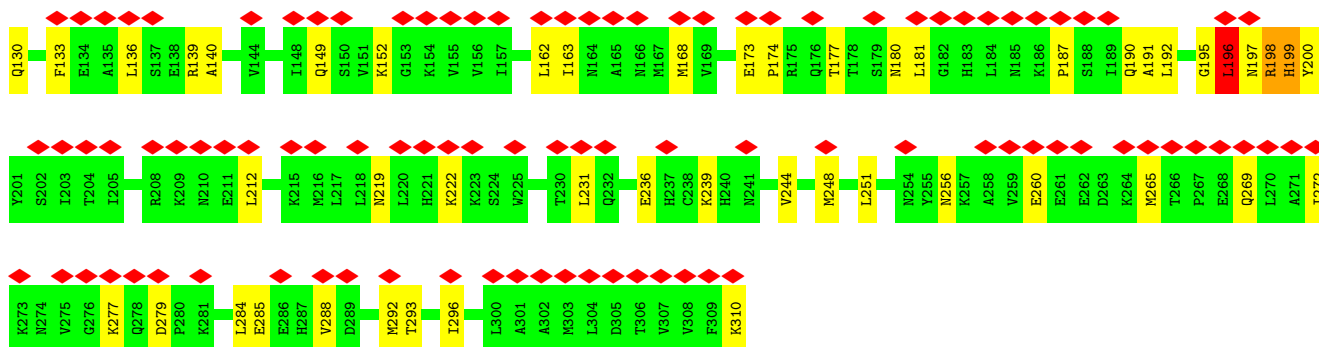


• Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

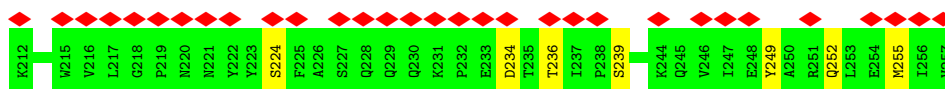
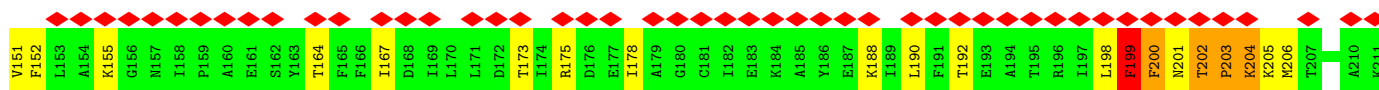
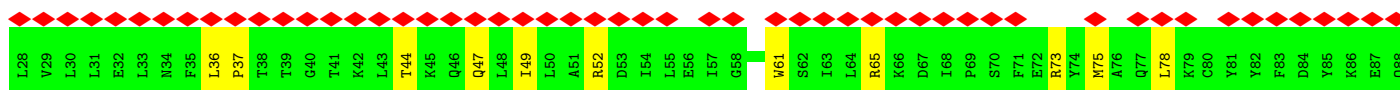
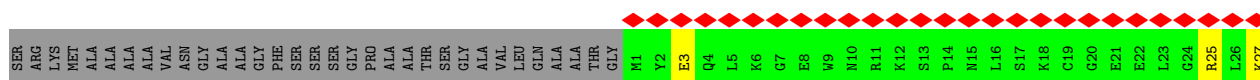


• Molecule 29: 26S proteasome non-ATPase regulatory subunit 14

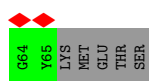
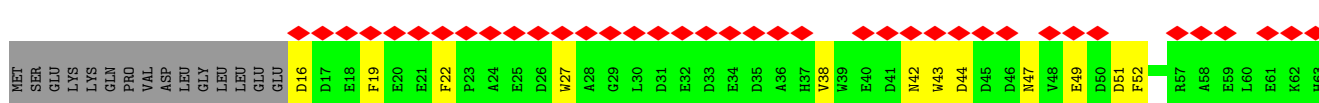




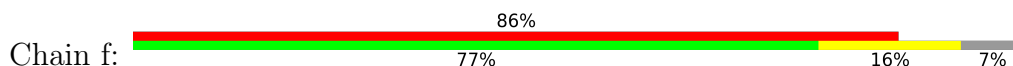
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 8



• Molecule 31: 26S proteasome complex subunit SEM1



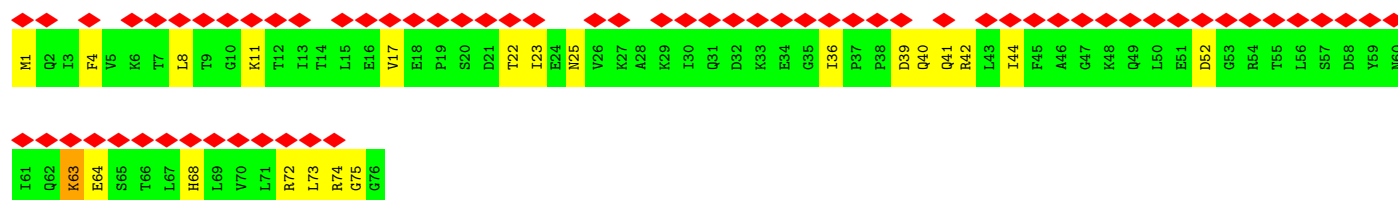
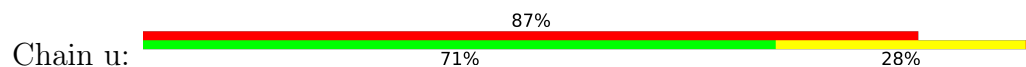
• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2



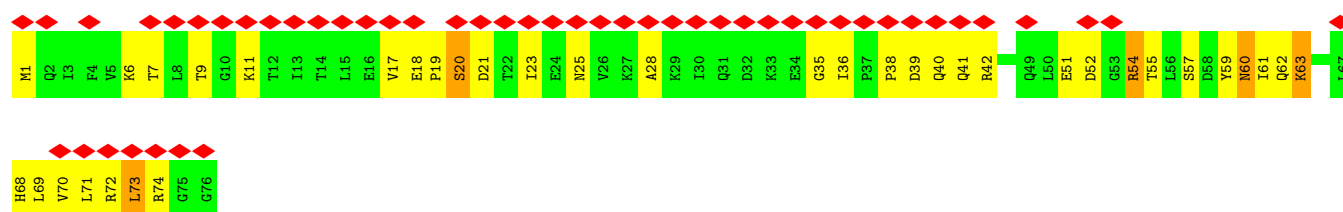
L787	F727	I666	V606	S546	L485	G425	V365	L305	P241	R181	F121	E61	MET
M788	A728	G667	L607	E647	G486	L426	D366	E306	E242	E182	A122	R62	GLU
S789	M729	A668	K608	T648	L487	T427	S367	L307	P243	P183	A123	L63	GLY
Q790	G730	E669	V609	E649	A488	Q428	A368	S308	E244	L184	D124	G64	GLY
V791	M731	M670	Q610	E509	A489	I429	R369	E309	N245	L185	I125	E65	ARG
A792	V732	A671	Q611	K651	A490	D430	M370	D310	S246	T186	I126	K66	ASP
V793	G733	L672	L612	D552	G491	K431	N371	V311	A247	L187	S127	D67	LYS
A794	S734	T673	L613	T653	S492	Y432	L372	E312	L248	V188	L128	T68	ALA
L796	G735	T674	H614	Y554	N493	L433	A373	E313	L249	K189	L129	S69	PRO
L797	T736	F675	I615	A555	R494	L434	S374	E314	R250	E190	A130	L70	VAL
L798	N737	G676	C616	R556	E495	S435	S375	E315	C251	I191	M131	Y71	GLN
V799	N738	H677	S617	W557	D496	S436	F376	D316	C252	V192	T132	R72	GLN
L800	A739	L678	E618	L558	V497	E437	V377	D317	A253	F193	M133	F73	SER
V801	R740	L679	H619	P559	L498	E438	N378	T318	L253	Y194	S134	A74	PRO
S802	L741	R680	F620	G561	T499	Y439	G379	E319	K257	H195	G135	L75	ALA
F803	A743	G681	D621	L562	L500	I440	F380	I320	K258	M196	E136	E76	ALA
L804	M744	G683	LYS	G563	L501	K441	V381	M321	P262	A197	R137	E77	PRO
D805	L745	L564	GLY	N382	L502	S442	N382	S322	P263	H198	E138	L78	GLY
V806	P746	N565	LYS	G564	P503	G443	A383	N323	E264	M199	C139	R79	THR
R807	R746	H566	GLY	M505	V504	A444	F385	V324	A265	A200	L140	R80	ASP
N808	Q747	G568	GLU	G506	L446	L445	G386	L326	L266	E201	K141	R80	GLU
I809	L748	K569	ASP	D507	L447	A447	Q387	N327	R267	H202	Y142	Q81	LYS
V810	A749	G570	LYS	S508	C448	G449	D388	S328	L268	E203	R143	R83	SER
L811	Q750	E571	LYS	K509	G449	G454	K389	N329	A269	C205	L144	S84	GLY
G812	Y751	A572	GLY	S510	I450	V451	L390	F330	L270	D206	V145	R85	LYS
K813	H752	I573	LYS	S511	V451	G455	L391	F330	M271	L207	G146	T86	ARG
A814	A753	E574	ASP	M512	N452	V455	T392	A332	L272	L207	S147	T87	ARG
H815	K754	A575	LYS	E513	S453	G454	D393	L333	Q148	L208	Q148	S88	ASP
Y816	P756	I576	ASP	V514	G454	V455	D394	A334	E149	M209	E149	R89	ALA
V817	N757	L577	LYS	A515	R456	V455	K395	R335	E276	E210	L151	T90	GLY
L818	Q758	A578	GLY	V517	N457	V455	N396	E336	L277	I211	A152	S91	ASP
Y819	L759	A579	ALA	T518	E458	V455	K397	L337	V278	E212	S153	V92	LYS
G820	M760	L580	PRO	A519	C459	V455	W398	D338	E279	V214	W154	P93	GLU
L821	V762	E581		L520	D460	L465	L399	I339	D280	D215	G155	K94	Q43
V822	R763	V582	D645	A521	P461	L465	Y400	M340	I281	K216	G156	P95	E44
A823	L764	S584	M646	C522	A462	L465	K401	E341	F282	L217	H156	L96	L45
G824	A765	E585	G648	G523	L463	L465	N402	P342	T283	E218	E157	K97	S46
M825	Q766	P586	H649	M524	A464	L465	K403	K343	T283	K219	Y158	F98	E47
Q826	G767	F587	Q650	I525	L465	L466	D404	V344	C285	D220	V159	L99	E48
P827	L707	F587	A526	V527	L466	S467	H405	P344	K286	R100	R160	P100	D49
R828	D708	R588	V527	G528	S467	D468	G406	D346	D287	P101	H161	P101	K50
M829	T709	S589	G528	S529	D468	L408	M407	D347	V288	L162	H161	P102	Q51
L830	H710	F590	C530	C530	Y469	L408	L408	I348	V289	E223	A163	Y103	L52
V831	S711	A591	N531	N531	S409	Y349	S409	I348	V290	G164	G164	Y104	Q53
T832	G712	N592	G532	G532	V470	L471	A410	K350	Q291	A225	E165	K105	D54
F833	F713	T593	D532	D532	L471	L471	A411	T351	Q291	Y226	V166	L106	E55
D834	S714	L594	D533	D533	H472	L472	A412	H352	A227	K227	A167	K107	L56
E835	H715	V595	G532	G532	M473	S474	A413	L353	Q293	K168	E167	E108	E57
E836	D716	D596	T537	T537	S474	N475	S413	E354	A295	E169	E169	Y109	M58
L837	A717	V597	I660	I660	N475	L476	L414	N355	F296	W170	W170	Y110	L59
R838	D718	C598	I638	I638	T476	M416	G415	N356	M297	Q171	E172	E111	
P839	P719	L539	L539	L539	M416	M416	M416	R357	L298	E172	E172	M112	
L840	Q600	Q640	Q640	Q640	L478	L478	I417	F358	G299	L173	L173	M113	
P841	T541	T541	T541	T541	L479	L479	L418	R300	R300	D174	D174	A114	
V842	I542	I542	I542	I542	G480	G480	L419	H301	D175	D175	D175	P115	
S843	G602	G602	G602	G602	A481	A481	W420	G302	E176	G116	G116	E117	
V844	M543	M543	M543	M543	I482	I482	D421	V303	E177	N238	N238	L178	
R845	E544	E544	E544	E544	F483	F483	V422	F304	V179	V179	V179	K119	
V846	K545	K545	K545	K545	G484	G484	D423	G424	Q180	Q180	Q180	R120	



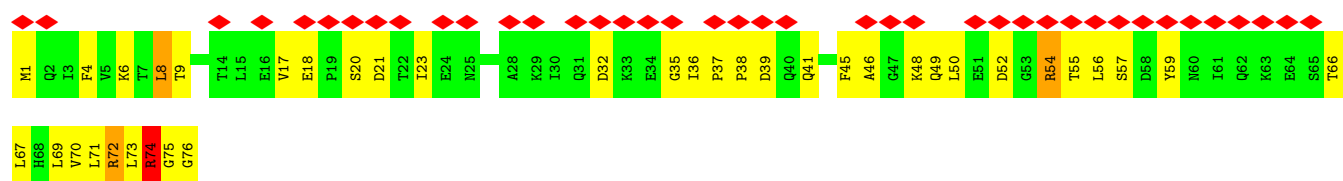
• Molecule 33: Ubiquitin



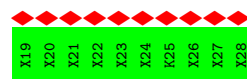
• Molecule 33: Ubiquitin



• Molecule 33: Ubiquitin



• Molecule 34: Substrate



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.012	Depositor
Minimum map value	-0.004	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0044	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: ATP, ADP, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.20	0/3148	0.55	0/4250
2	B	0.19	0/3061	0.53	0/4129
3	C	0.20	0/2902	0.50	0/3904
4	D	0.23	0/3089	0.52	0/4168
5	E	0.19	0/3145	0.47	0/4233
6	F	0.21	0/3292	0.46	0/4435
7	G	0.19	0/1923	0.46	0/2601
7	g	0.18	0/1914	0.43	0/2590
8	H	0.16	0/1844	0.44	0/2499
8	h	0.16	0/1844	0.43	0/2497
9	I	0.16	0/1991	0.43	0/2685
9	i	0.15	0/1985	0.40	0/2677
10	J	0.18	0/1906	0.42	0/2573
10	j	0.15	0/1887	0.42	0/2549
11	K	0.18	0/1804	0.42	0/2436
11	k	0.17	0/1809	0.47	0/2444
12	L	0.15	0/1901	0.37	0/2570
12	l	0.15	0/1896	0.40	0/2565
13	M	0.16	0/1911	0.42	0/2573
13	m	0.13	0/1916	0.36	0/2580
14	N	0.15	0/1540	0.38	0/2085
14	n	0.16	0/1536	0.39	0/2080
15	O	0.16	0/1676	0.41	1/2271 (0.0%)
15	o	0.14	0/1686	0.44	0/2282
16	P	0.19	0/1616	0.53	2/2180 (0.1%)
16	p	0.16	0/1620	0.44	0/2184
17	Q	0.14	0/1621	0.36	0/2194
17	q	0.14	0/1621	0.37	0/2194
18	R	0.15	0/1590	0.41	0/2147
18	r	0.15	0/1590	0.41	0/2147
19	S	0.15	0/1671	0.39	0/2252
19	s	0.16	0/1684	0.43	0/2268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
20	T	0.15	0/1716	0.39	0/2323
20	t	0.15	0/1720	0.41	0/2328
21	U	0.18	0/6488	0.49	0/8782
22	V	0.16	0/3681	0.42	0/4969
23	W	0.16	0/3644	0.44	0/4901
24	X	0.17	0/3381	0.47	0/4558
25	Y	0.19	0/3261	0.50	0/4393
26	Z	0.19	0/2324	0.55	0/3150
27	a	0.18	0/3053	0.51	0/4133
28	b	0.20	0/1478	0.52	0/2001
29	c	0.26	0/2302	0.58	0/3110
30	d	0.25	0/2162	0.58	2/2919 (0.1%)
31	e	0.20	0/437	0.60	1/595 (0.2%)
32	f	0.20	0/6640	0.51	1/8988 (0.0%)
33	u	0.27	0/607	0.66	2/816 (0.2%)
33	x	0.60	0/607	1.01	0/816
33	y	0.51	0/607	0.98	0/816
34	v	0.03	0/8	0.06	0/8
All	All	0.19	0/108735	0.48	9/146848 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	115	PRO	CA-N-CD	-9.51	98.69	112.00
33	u	75	GLY	CA-C-N	-8.36	106.64	121.70
33	u	75	GLY	C-N-CA	-8.36	106.64	121.70
31	e	38	VAL	N-CA-C	-6.17	106.73	112.83
30	d	204	LYS	N-CA-C	-5.99	105.63	113.17
16	P	96	TYR	CA-C-N	-5.17	111.61	121.94
16	P	96	TYR	C-N-CA	-5.17	111.61	121.94
15	O	157	GLU	N-CA-CB	5.12	118.19	110.30
30	d	199	PHE	CA-C-O	-5.10	113.21	120.51

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	3096	0	3139	84	0
2	B	3018	0	3081	78	0
3	C	2864	0	2971	63	0
4	D	3039	0	3075	77	0
5	E	3097	0	3173	83	0
6	F	3251	0	3318	87	0
7	G	1889	0	1885	32	0
7	g	1880	0	1875	39	0
8	H	1805	0	1784	31	0
8	h	1805	0	1798	36	0
9	I	1958	0	1960	31	0
9	i	1955	0	1955	25	0
10	J	1880	0	1892	41	0
10	j	1861	0	1865	34	0
11	K	1777	0	1762	39	0
11	k	1782	0	1766	32	0
12	L	1866	0	1852	35	0
12	l	1861	0	1839	28	0
13	M	1876	0	1861	40	0
13	m	1881	0	1868	34	0
14	N	1514	0	1487	21	0
14	n	1510	0	1483	21	0
15	O	1649	0	1659	28	0
15	o	1659	0	1681	27	0
16	P	1587	0	1598	39	0
16	p	1591	0	1609	41	0
17	Q	1588	0	1584	35	0
17	q	1588	0	1584	31	0
18	R	1559	0	1523	29	0
18	r	1559	0	1523	31	0
19	S	1641	0	1639	36	0
19	s	1654	0	1656	36	0
20	T	1683	0	1662	39	0
20	t	1687	0	1666	32	0
21	U	6373	0	6411	129	0
22	V	3612	0	3682	69	0
23	W	3596	0	3713	50	0
24	X	3335	0	3435	57	0
25	Y	3202	0	3204	55	0
26	Z	2281	0	2312	51	0
27	a	2995	0	3012	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	b	1458	0	1505	25	0
29	c	2260	0	2276	79	0
30	d	2116	0	2146	45	0
31	e	425	0	328	14	0
32	f	6529	0	6541	90	0
33	u	601	0	627	31	0
33	x	601	0	627	90	0
33	y	601	0	629	114	0
34	v	53	0	21	0	0
35	A	31	0	12	3	0
35	B	31	0	12	2	0
35	D	31	0	12	2	0
35	E	31	0	12	1	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	D	1	0	0	0	0
36	E	1	0	0	0	0
36	F	1	0	0	0	0
37	C	27	0	12	1	0
37	F	27	0	12	3	0
38	c	1	0	0	0	0
All	All	107132	0	107614	2026	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 9.

All (2026) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:x:63:LYS:NZ	33:y:76:GLY:C	1.67	1.53
33:u:4:PHE:CE2	33:u:64:GLU:HG2	1.58	1.37
33:x:60:ASN:HA	33:y:8:LEU:CD1	1.54	1.37
33:x:60:ASN:HB3	33:y:8:LEU:CB	1.56	1.34
33:x:60:ASN:CA	33:y:8:LEU:HD12	1.55	1.34
33:x:60:ASN:CB	33:y:8:LEU:HB2	1.67	1.24
33:x:57:SER:CB	33:y:73:LEU:HD12	1.65	1.23
33:x:20:SER:HA	33:y:73:LEU:HD21	1.20	1.19
33:u:4:PHE:HE2	33:u:64:GLU:CG	1.58	1.17
33:x:63:LYS:HZ2	33:y:76:GLY:C	1.33	1.15
33:y:6:LYS:CD	33:y:66:THR:HG21	1.80	1.12
33:y:48:LYS:HG3	33:y:49:GLN:H	0.96	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:y:6:LYS:CE	33:y:66:THR:HG21	1.80	1.10
33:u:63:LYS:HE3	33:u:64:GLU:HB2	1.37	1.06
33:u:63:LYS:HE3	33:u:64:GLU:CB	1.85	1.05
33:x:20:SER:HA	33:y:73:LEU:CD2	1.87	1.05
33:x:57:SER:HB2	33:y:73:LEU:HD12	1.05	1.02
33:y:48:LYS:HG3	33:y:49:GLN:N	1.73	1.02
33:u:63:LYS:CE	33:u:64:GLU:HB3	1.90	1.01
33:x:60:ASN:CB	33:y:8:LEU:CD1	2.38	1.01
33:x:20:SER:CA	33:y:73:LEU:HD21	1.91	1.00
33:y:6:LYS:HD2	33:y:66:THR:HG21	1.43	0.99
33:u:63:LYS:HE2	33:u:64:GLU:HB3	1.45	0.97
33:x:57:SER:HB2	33:y:73:LEU:CD1	1.94	0.97
33:u:64:GLU:O	33:u:64:GLU:CD	2.08	0.96
33:x:57:SER:CB	33:y:73:LEU:CD1	2.44	0.95
33:y:48:LYS:CG	33:y:49:GLN:H	1.78	0.95
33:x:57:SER:OG	33:y:73:LEU:HA	1.65	0.95
33:x:60:ASN:HB3	33:y:8:LEU:CD1	1.94	0.95
33:y:73:LEU:O	33:y:74:ARG:HB2	1.68	0.94
33:x:60:ASN:CA	33:y:8:LEU:CD1	2.25	0.93
4:D:93:LEU:O	4:D:125:LYS:HE2	1.68	0.93
33:x:57:SER:CB	33:y:73:LEU:HA	1.99	0.93
33:u:4:PHE:HE2	33:u:64:GLU:HG2	0.76	0.93
33:x:19:PRO:C	33:y:73:LEU:HD11	1.93	0.93
33:x:63:LYS:CE	33:y:76:GLY:C	2.43	0.92
33:x:19:PRO:HB2	33:y:74:ARG:H	1.34	0.92
33:y:6:LYS:CD	33:y:66:THR:CG2	2.47	0.91
33:u:63:LYS:CE	33:u:64:GLU:CB	2.47	0.91
33:x:60:ASN:CB	33:y:8:LEU:HD12	2.00	0.91
33:x:60:ASN:HA	33:y:8:LEU:HD12	0.91	0.90
33:y:6:LYS:HE3	33:y:66:THR:HG21	1.52	0.90
33:x:19:PRO:HG2	33:y:74:ARG:HA	1.51	0.90
33:x:19:PRO:O	33:y:73:LEU:HD11	1.73	0.89
33:y:6:LYS:HE3	33:y:66:THR:CG2	2.04	0.88
33:y:23:ILE:HG12	33:y:54:ARG:O	1.73	0.86
4:D:91:GLN:HG3	4:D:128:ALA:O	1.75	0.85
33:x:20:SER:HA	33:y:73:LEU:HD11	1.58	0.85
33:x:73:LEU:H	33:x:73:LEU:HD23	1.39	0.84
33:y:6:LYS:HD2	33:y:66:THR:CG2	2.07	0.84
33:y:8:LEU:CD2	33:y:70:VAL:HA	2.06	0.84
33:x:60:ASN:HB3	33:y:8:LEU:CG	2.08	0.84
33:x:63:LYS:CE	33:x:63:LYS:H	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:96:LEU:HD12	33:u:8:LEU:HD22	1.61	0.83
33:x:60:ASN:HB3	33:y:8:LEU:HB2	0.84	0.81
29:c:136:LEU:HD11	33:u:11:LYS:HD3	1.63	0.80
33:x:57:SER:HB3	33:y:73:LEU:CD1	2.11	0.80
33:x:63:LYS:H	33:x:63:LYS:HE3	1.48	0.79
33:x:20:SER:CA	33:y:73:LEU:HD11	2.12	0.79
33:x:20:SER:HA	33:y:73:LEU:CG	2.12	0.78
29:c:191:ALA:HB1	29:c:196:LEU:HD23	1.64	0.78
33:x:20:SER:HA	33:y:73:LEU:CD1	2.13	0.78
4:D:121:ARG:HA	4:D:124:LEU:CD1	2.14	0.78
33:x:60:ASN:CB	33:y:8:LEU:HD13	2.15	0.76
24:X:310:ARG:HD2	24:X:314:ARG:HE	1.51	0.76
33:u:64:GLU:O	33:u:64:GLU:OE1	2.03	0.76
4:D:92:PHE:HE2	4:D:125:LYS:HD2	1.50	0.75
29:c:187:PRO:HB3	29:c:196:LEU:HG	1.68	0.75
33:x:59:TYR:C	33:x:60:ASN:OD1	2.30	0.75
4:D:125:LYS:N	4:D:126:PRO:HD3	2.03	0.74
33:x:62:GLN:HB3	33:y:9:THR:HA	1.69	0.74
29:c:198:ARG:C	29:c:200:TYR:H	1.95	0.73
33:x:19:PRO:HB2	33:y:74:ARG:N	2.03	0.73
3:C:230:MET:HG3	3:C:232:ARG:H	1.53	0.73
30:d:199:PHE:O	30:d:200:PHE:HB2	1.87	0.72
27:a:333:MET:HE3	27:a:334:THR:H	1.55	0.72
21:U:194:ARG:O	21:U:198:LEU:HB2	1.90	0.72
8:h:6:TYR:HH	9:i:2:SER:N	1.87	0.72
33:x:1:MET:SD	33:y:76:GLY:O	2.48	0.72
33:y:8:LEU:HD22	33:y:70:VAL:HA	1.71	0.72
22:V:416:ARG:HB3	25:Y:348:ASP:OD1	1.90	0.72
4:D:121:ARG:HA	4:D:124:LEU:HD11	1.72	0.71
29:c:58:LEU:HB3	29:c:71:ASP:HB3	1.73	0.71
33:y:6:LYS:HG3	33:y:66:THR:HG23	1.71	0.71
4:D:126:PRO:HB3	29:c:277:LYS:NZ	2.06	0.70
6:F:97:LEU:O	6:F:120:LYS:HA	1.92	0.70
10:j:114:LEU:HA	10:j:117:ARG:HE	1.56	0.70
32:f:502:LEU:HA	32:f:505:MET:HE2	1.74	0.69
33:y:6:LYS:HG3	33:y:66:THR:CG2	2.22	0.69
1:A:173:THR:HG22	1:A:175:SER:H	1.57	0.69
5:E:44:GLU:HG3	5:E:47:LEU:HD12	1.74	0.69
21:U:418:GLU:HG3	21:U:421:GLN:HE21	1.54	0.69
33:y:73:LEU:O	33:y:74:ARG:CB	2.40	0.69
8:h:50:LYS:HG2	8:h:64:LYS:HZ2	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:y:71:LEU:HD12	33:y:71:LEU:N	2.06	0.69
11:K:36:THR:HA	11:K:171:GLY:HA3	1.75	0.68
16:p:88:MET:HG2	16:p:124:LEU:HD11	1.74	0.68
1:A:113:ILE:HG22	1:A:121:PHE:H	1.57	0.68
10:J:211:MET:HE1	10:J:217:LEU:HB2	1.75	0.68
10:j:133:ILE:HD11	10:j:147:THR:HG23	1.75	0.68
21:U:328:ILE:HG13	21:U:329:LEU:HG	1.76	0.67
9:i:119:GLN:NE2	10:j:79:ASP:OD1	2.28	0.67
9:I:79:ILE:H	9:I:132:VAL:HG22	1.60	0.67
22:V:85:ALA:HB2	22:V:93:PHE:HB2	1.77	0.67
21:U:78:LEU:O	21:U:129:ARG:NH2	2.28	0.67
21:U:101:ILE:HG22	21:U:133:ILE:HD11	1.77	0.67
25:Y:240:VAL:HG23	25:Y:241:ILE:HG13	1.77	0.66
12:l:121:GLN:HG3	13:m:129:ARG:HG2	1.76	0.66
33:x:38:PRO:C	33:x:40:GLN:H	2.03	0.66
33:x:60:ASN:OD1	33:x:60:ASN:N	2.27	0.66
33:u:72:ARG:HD3	33:u:74:ARG:HD2	1.78	0.66
32:f:738:ASN:HB3	32:f:741:LEU:HD12	1.78	0.66
6:F:229:PRO:HB3	6:F:333:ASN:HD22	1.60	0.66
29:c:92:GLN:HA	29:c:95:MET:HE2	1.78	0.66
12:L:72:ILE:HB	12:L:132:LEU:HD11	1.78	0.66
29:c:256:ASN:O	29:c:260:GLU:HB2	1.96	0.66
33:x:20:SER:N	33:y:73:LEU:HD11	2.09	0.66
30:d:200:PHE:HB3	30:d:203:PRO:HG3	1.77	0.65
17:q:183:ILE:HG12	17:q:188:ILE:HG12	1.78	0.65
12:L:134:ILE:HB	12:L:145:PHE:HB2	1.78	0.65
33:x:20:SER:CB	33:y:73:LEU:HD21	2.26	0.65
7:G:80:MET:SD	7:G:90:GLN:NE2	2.69	0.65
26:Z:70:LEU:HD11	26:Z:108:ILE:HG23	1.78	0.65
15:O:215:LYS:HB3	16:P:197:THR:HB	1.79	0.65
23:W:401:THR:HG23	23:W:402:ILE:HD12	1.79	0.65
13:M:35:THR:HA	13:M:166:GLY:HA3	1.79	0.65
9:i:192:LEU:HD12	9:i:195:LYS:HE3	1.78	0.65
5:E:144:GLU:O	5:E:297:ARG:NH2	2.26	0.65
16:P:15:LYS:HE3	16:P:121:ILE:HG12	1.79	0.65
21:U:724:VAL:HB	29:c:181:LEU:HD21	1.77	0.65
24:X:407:MET:HA	24:X:410:VAL:HG22	1.78	0.64
24:X:260:MET:SD	24:X:325:LYS:NZ	2.70	0.64
7:g:141:ILE:HG22	7:g:151:VAL:HG12	1.79	0.64
9:I:47:ALA:HB3	9:I:212:GLU:HB3	1.77	0.64
21:U:530:GLU:HG2	33:y:4:PHE:CD1	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:VAL:HG12	1:A:404:ALA:HB3	1.80	0.64
4:D:126:PRO:HB3	29:c:277:LYS:HZ3	1.63	0.64
6:F:356:MET:HE3	6:F:357:PRO:HD2	1.78	0.64
24:X:254:MET:HE1	24:X:270:LEU:HD13	1.78	0.64
33:x:60:ASN:CA	33:y:8:LEU:HD13	2.22	0.64
33:y:6:LYS:CG	33:y:66:THR:CG2	2.75	0.64
13:M:108:LEU:HD11	13:M:137:LEU:HB3	1.78	0.64
27:a:73:PRO:HG3	27:a:104:VAL:HG11	1.80	0.64
24:X:82:LYS:HB3	24:X:122:ARG:HH22	1.62	0.64
27:a:98:GLU:HG2	27:a:101:ARG:HH21	1.62	0.64
3:C:213:ARG:HB3	3:C:247:PHE:HB3	1.80	0.63
19:s:21:ALA:HB3	19:s:198:VAL:HB	1.79	0.63
33:x:60:ASN:HD22	33:y:8:LEU:HB3	1.62	0.63
8:h:14:SER:HB3	8:h:18:LYS:H	1.63	0.63
33:x:63:LYS:HE2	33:y:76:GLY:C	2.23	0.63
5:E:352:MET:HE2	6:F:350:ARG:HH12	1.63	0.63
15:O:14:LEU:HB2	15:O:176:CYS:HB3	1.80	0.63
17:q:25:ILE:HG22	17:q:26:VAL:HG13	1.80	0.63
21:U:1:MET:HG3	21:U:2:ILE:HG13	1.80	0.63
21:U:571:CYS:HB3	21:U:601:ARG:HH22	1.64	0.63
25:Y:46:ARG:HH12	25:Y:49:ASN:HA	1.64	0.63
21:U:758:PRO:HB2	21:U:781:LEU:HB3	1.80	0.63
33:x:19:PRO:CG	33:y:74:ARG:HA	2.27	0.63
21:U:243:LEU:HG	21:U:913:ILE:HG23	1.81	0.63
4:D:91:GLN:NE2	4:D:127:ASN:OD1	2.31	0.63
4:D:182:GLU:HA	4:D:185:LEU:HB2	1.79	0.63
6:F:120:LYS:HG3	6:F:142:ALA:HB1	1.80	0.63
11:k:221:GLN:HB2	11:k:224:GLN:HG2	1.81	0.63
5:E:36:LEU:HB3	6:F:69:MET:HE1	1.81	0.62
5:E:101:ASP:HB2	5:E:108:MET:HE3	1.81	0.62
18:R:2:THR:HA	18:R:129:GLY:HA3	1.80	0.62
32:f:684:PRO:HB2	32:f:688:ARG:HH21	1.63	0.62
1:A:425:ALA:HA	2:B:339:PRO:HB2	1.81	0.62
5:E:84:ARG:HG2	29:c:50:PRO:HG3	1.81	0.62
9:I:197:LEU:HA	9:I:200:THR:HG22	1.81	0.62
17:Q:172:ILE:HG13	17:q:173:LEU:HD22	1.82	0.62
19:S:151:ASN:HD21	16:p:149:MET:HE3	1.64	0.62
20:T:25:ASP:HA	20:T:187:PHE:HA	1.80	0.62
32:f:822:VAL:HA	32:f:825:MET:HE3	1.80	0.62
28:b:14:GLU:HB2	28:b:17:ARG:HH21	1.64	0.62
6:F:175:MET:SD	6:F:255:GLN:NE2	2.72	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:203:LYS:HA	11:k:206:MET:HE3	1.81	0.62
18:r:97:MET:H	18:r:116:SER:HB3	1.65	0.62
33:u:23:ILE:HB	33:u:52:ASP:HA	1.81	0.62
4:D:116:LEU:HD23	4:D:118:THR:H	1.65	0.62
4:D:352:MET:HE2	4:D:394:VAL:HG23	1.81	0.62
8:H:74:LEU:HD22	8:H:134:LEU:HD12	1.80	0.62
17:Q:21:ALA:HB3	17:Q:29:LYS:HB3	1.81	0.62
28:b:6:THR:HB	28:b:49:VAL:HG22	1.80	0.62
14:n:44:CYS:HB2	14:n:99:ILE:HB	1.81	0.62
4:D:244:PRO:HB3	4:D:291:GLU:HG3	1.82	0.62
10:J:208:LEU:HD12	10:J:225:ILE:HG12	1.81	0.62
27:a:150:SER:OG	27:a:154:ARG:NH1	2.33	0.62
30:d:175:ARG:NH2	30:d:199:PHE:HB2	2.15	0.62
10:j:133:ILE:HB	10:j:145:TYR:HB2	1.81	0.62
13:m:136:MET:HE3	13:m:165:ILE:HG12	1.81	0.62
1:A:277:ILE:HG12	1:A:321:THR:HB	1.81	0.61
13:m:211:LEU:O	13:m:232:ARG:NH1	2.33	0.61
5:E:355:ILE:HD11	6:F:211:LYS:HG2	1.81	0.61
10:J:71:MET:HE1	10:J:133:ILE:HG23	1.82	0.61
7:g:147:GLN:OE1	7:g:150:GLN:NE2	2.33	0.61
15:O:175:LEU:HD23	15:O:186:LEU:HD12	1.80	0.61
15:o:177:VAL:HB	15:o:184:ASP:HB2	1.82	0.61
8:H:143:ARG:NH1	8:H:144:PRO:O	2.34	0.61
11:K:18:GLU:O	12:L:31:GLN:NE2	2.34	0.61
21:U:798:PRO:O	21:U:880:ASN:ND2	2.31	0.61
22:V:99:ARG:O	31:e:16:ASP:N	2.33	0.61
25:Y:388:ASN:HD21	26:Z:275:LEU:HD22	1.64	0.61
18:r:7:LYS:HG3	18:r:111:LEU:HD22	1.83	0.61
2:B:112:LEU:HD12	2:B:148:CYS:HB3	1.83	0.61
5:E:265:ASP:OD2	5:E:291:ARG:NH2	2.33	0.61
6:F:357:PRO:O	6:F:362:ARG:NH1	2.34	0.61
21:U:247:GLN:HG3	21:U:904:LYS:HD2	1.82	0.61
23:W:55:ARG:NH1	23:W:94:ARG:O	2.34	0.61
4:D:67:ASN:ND2	21:U:607:VAL:O	2.34	0.61
5:E:241:ARG:NH2	5:E:283:ASP:O	2.34	0.61
20:t:122:LEU:HG	20:t:137:LEU:HD12	1.81	0.61
6:F:282:ILE:HG22	6:F:327:LYS:HB2	1.81	0.61
15:O:163:ILE:HG12	15:O:170:GLY:HA2	1.81	0.61
17:Q:83:PHE:O	17:Q:87:ASN:ND2	2.34	0.61
21:U:49:TYR:HA	21:U:57:ARG:HB2	1.81	0.61
1:A:98:CYS:HA	1:A:141:GLY:HA2	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:117:SER:HA	4:D:121:ARG:HH22	1.65	0.61
6:F:113:LEU:HD13	29:c:81:GLY:H	1.65	0.61
5:E:237:ALA:HB1	6:F:308:ARG:HG3	1.82	0.61
6:F:358:ASN:HD21	13:M:205:LYS:HE3	1.66	0.61
13:M:223:ARG:NH2	20:T:75:GLU:OE2	2.34	0.61
10:j:116:GLN:NE2	11:k:84:ASP:OD1	2.33	0.61
7:G:155:ASP:OD1	7:G:159:TYR:N	2.34	0.61
22:V:490:SER:HA	26:Z:275:LEU:HD21	1.83	0.61
23:W:174:TYR:O	23:W:182:ARG:NH2	2.33	0.61
26:Z:187:LEU:HB3	29:c:293:THR:HG22	1.81	0.61
33:y:72:ARG:HH11	33:y:72:ARG:CG	2.14	0.61
1:A:324:PRO:HA	1:A:327:LEU:HD23	1.82	0.60
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.82	0.60
11:K:103:TYR:OH	19:S:71:ARG:NH2	2.33	0.60
17:Q:45:LEU:HB2	17:Q:103:LEU:HB2	1.83	0.60
19:S:110:ILE:HB	19:S:122:TYR:HB2	1.82	0.60
22:V:311:ASN:OD1	22:V:314:ARG:NH1	2.34	0.60
14:n:106:GLN:HG3	14:n:107:GLU:HG2	1.81	0.60
8:H:219:ARG:HH12	8:H:222:THR:HG23	1.66	0.60
22:V:351:PRO:O	22:V:355:ARG:NH1	2.34	0.60
33:x:63:LYS:HE2	33:y:76:GLY:O	2.01	0.60
1:A:210:LYS:NZ	1:A:313:GLY:O	2.34	0.60
1:A:426:THR:N	1:A:427:PRO:HD2	2.16	0.60
9:I:143:TYR:HB2	9:I:146:GLN:HE21	1.66	0.60
26:Z:263:ALA:HB1	29:c:288:VAL:HG13	1.83	0.60
33:x:57:SER:HB3	33:y:73:LEU:HD12	1.65	0.60
27:a:255:TRP:O	27:a:258:GLN:NE2	2.34	0.60
30:d:49:ILE:HD12	30:d:52:ARG:HH21	1.66	0.60
11:k:36:THR:HA	11:k:171:GLY:HA3	1.83	0.60
13:m:35:THR:HA	13:m:166:GLY:HA3	1.82	0.60
33:x:19:PRO:HG2	33:y:74:ARG:CA	2.28	0.60
2:B:145:GLU:HG2	2:B:148:CYS:HB2	1.83	0.60
4:D:77:GLU:OE2	26:Z:177:ARG:NH2	2.34	0.60
6:F:117:ARG:NH2	6:F:135:PRO:O	2.35	0.60
13:M:165:ILE:HA	13:M:169:ARG:HE	1.67	0.60
14:N:14:LEU:HB3	14:N:177:ALA:HB3	1.83	0.60
11:k:90:ASP:OD1	11:k:93:ARG:NH2	2.34	0.60
33:u:4:PHE:CE2	33:u:64:GLU:CG	2.49	0.60
33:y:45:PHE:CG	33:y:46:ALA:N	2.70	0.60
1:A:300:LEU:HD13	6:F:290:ALA:HB2	1.84	0.60
19:S:45:LYS:HA	19:S:51:VAL:HG22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:231:LEU:HG	25:Y:236:LEU:HD12	1.84	0.60
7:g:103:TYR:O	15:o:81:ARG:NH2	2.34	0.60
16:p:194:LYS:NZ	16:p:196:THR:OG1	2.35	0.60
22:V:228:ARG:HH22	22:V:261:TYR:HB2	1.66	0.60
10:j:65:LEU:HD21	10:j:84:ILE:HG23	1.84	0.60
16:p:2:SER:N	16:p:5:SER:HG	1.99	0.60
10:J:209:ALA:HB1	10:J:217:LEU:HD11	1.84	0.60
15:o:14:LEU:HB2	15:o:176:CYS:HB3	1.84	0.60
4:D:336:PRO:HB3	4:D:340:GLN:HB2	1.82	0.60
21:U:609:ASP:O	21:U:615:ARG:NH1	2.35	0.60
27:a:50:PHE:O	27:a:86:GLN:NE2	2.35	0.60
29:c:119:GLY:HA3	29:c:190:GLN:HG3	1.83	0.60
32:f:350:LYS:HE3	32:f:746:ARG:HH11	1.66	0.60
33:x:19:PRO:CG	33:y:74:ARG:C	2.75	0.60
4:D:320:ALA:O	4:D:326:ARG:NH1	2.35	0.59
16:P:58:THR:O	17:Q:85:ARG:NH2	2.34	0.59
17:Q:85:ARG:HD2	17:Q:124:LEU:HD23	1.83	0.59
19:S:194:ARG:NH1	19:S:205:GLU:OE1	2.34	0.59
7:G:244:GLU:HG2	7:G:245:ARG:HG2	1.83	0.59
15:O:21:THR:HG22	15:O:26:VAL:HA	1.84	0.59
22:V:122:THR:HG21	22:V:155:ALA:HB1	1.84	0.59
29:c:244:VAL:HG12	29:c:248:MET:HE1	1.84	0.59
13:m:50:GLU:OE2	13:m:201:HIS:ND1	2.35	0.59
19:s:145:LEU:HD22	19:s:178:VAL:HB	1.84	0.59
6:F:153:VAL:HG22	6:F:160:ILE:HG22	1.85	0.59
7:G:123:GLN:NE2	8:H:82:ASP:OD1	2.35	0.59
21:U:625:ILE:HG13	21:U:626:LEU:HG	1.83	0.59
22:V:266:GLN:HA	22:V:269:LYS:HD2	1.84	0.59
19:s:63:THR:HG22	20:t:94:ARG:HH12	1.67	0.59
18:R:166:ARG:NH1	16:p:34:MET:O	2.36	0.59
21:U:68:PHE:HB3	21:U:73:ALA:HB3	1.84	0.59
32:f:531:ASN:O	32:f:565:ASN:ND2	2.35	0.59
32:f:654:VAL:HA	32:f:657:ILE:HD12	1.84	0.59
1:A:268:LYS:HB2	32:f:352:HIS:HD2	1.67	0.59
11:K:109:VAL:HG21	11:K:145:GLY:HA3	1.83	0.59
12:L:196:ARG:NH1	12:L:237:GLU:O	2.33	0.59
7:g:123:GLN:NE2	8:h:82:ASP:OD1	2.36	0.59
12:l:225:ASP:H	12:l:228:ASP:HB3	1.67	0.59
3:C:175:PHE:O	3:C:179:GLY:N	2.35	0.59
11:K:186:HIS:H	11:K:189:MET:HE3	1.67	0.59
17:Q:41:LYS:HG3	17:Q:42:ILE:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:52:LYS:HZ1	23:W:93:ARG:HH11	1.51	0.59
3:C:235:PHE:HA	3:C:238:ALA:HB3	1.84	0.59
7:G:110:PRO:HG2	7:G:113:MET:HB2	1.85	0.59
18:R:7:LYS:HG2	18:R:12:VAL:HG22	1.84	0.59
30:d:122:LEU:HB3	30:d:125:LYS:HB2	1.85	0.59
9:i:205:LYS:O	9:i:210:LYS:NZ	2.35	0.59
5:E:55:GLN:N	6:F:133:PHE:O	2.34	0.59
9:I:174:MET:HG2	9:I:199:LYS:HE3	1.85	0.59
21:U:678:ASP:O	21:U:684:ARG:NH1	2.36	0.59
12:l:39:LYS:HE3	12:l:142:PRO:HB2	1.85	0.59
13:m:100:SER:HA	20:t:65:GLN:HE21	1.67	0.59
33:x:57:SER:HB3	33:y:73:LEU:HD13	1.85	0.59
3:C:332:HIS:O	3:C:335:LYS:NZ	2.36	0.59
24:X:187:ARG:NH2	24:X:217:ILE:O	2.36	0.59
33:x:19:PRO:C	33:y:73:LEU:CD1	2.73	0.59
6:F:43:GLN:HG2	6:F:47:LEU:HD23	1.85	0.58
24:X:275:LEU:HD11	24:X:278:ARG:HH21	1.68	0.58
32:f:512:MET:HE1	32:f:552:ASP:HB3	1.85	0.58
9:i:123:GLN:NE2	10:j:125:ARG:O	2.36	0.58
33:y:8:LEU:HD23	33:y:69:LEU:O	2.02	0.58
3:C:163:GLU:HA	3:C:167:LEU:HD13	1.85	0.58
4:D:353:ASN:ND2	4:D:392:TYR:O	2.37	0.58
7:G:111:VAL:HG21	7:G:142:GLY:HA3	1.85	0.58
10:J:116:GLN:NE2	11:K:84:ASP:OD1	2.36	0.58
11:K:105:GLU:OE2	19:S:75:TYR:OH	2.21	0.58
15:O:41:ILE:HG12	15:O:102:GLY:HA3	1.85	0.58
30:d:3:GLU:O	30:d:25:ARG:NH1	2.37	0.58
8:h:65:VAL:O	8:h:220:ARG:NH1	2.35	0.58
2:B:382:ASP:OD2	2:B:423:LYS:NZ	2.36	0.58
5:E:259:GLU:OE2	5:E:263:GLN:NE2	2.37	0.58
12:L:203:GLN:O	12:L:239:ARG:NH2	2.36	0.58
23:W:101:VAL:HA	23:W:104:MET:HE3	1.85	0.58
33:u:63:LYS:CE	33:u:64:GLU:HB2	2.20	0.58
33:y:8:LEU:HD21	33:y:70:VAL:HA	1.85	0.58
5:E:56:ILE:HB	5:E:100:LEU:HB2	1.86	0.58
25:Y:360:ASP:HB2	25:Y:363:ASN:HB2	1.86	0.58
26:Z:169:GLU:HG3	29:c:152:LYS:HE3	1.83	0.58
29:c:198:ARG:C	29:c:200:TYR:N	2.61	0.58
22:V:228:ARG:HH21	22:V:258:TYR:HA	1.67	0.58
23:W:267:LEU:HD21	23:W:296:LEU:HA	1.84	0.58
33:u:4:PHE:CD2	33:u:64:GLU:HG2	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:103:ASP:O	6:F:104:GLN:C	2.46	0.58
15:O:177:VAL:HB	15:O:184:ASP:HB2	1.84	0.58
3:C:40:GLN:OE1	3:C:43:ARG:NH2	2.36	0.58
21:U:269:ARG:HB3	21:U:325:MET:HE1	1.86	0.58
32:f:490:ALA:HA	32:f:525:ILE:HA	1.85	0.58
10:J:37:GLY:HA2	10:J:181:ILE:HB	1.86	0.58
11:K:41:GLN:NE2	11:K:151:PRO:O	2.36	0.58
19:S:194:ARG:HD2	19:S:205:GLU:HB3	1.86	0.58
23:W:79:GLU:HB3	23:W:82:LEU:HB2	1.84	0.58
16:p:58:THR:O	17:q:85:ARG:NH2	2.37	0.58
2:B:222:VAL:HG22	2:B:349:ARG:HB2	1.84	0.58
9:I:40:ASN:ND2	9:I:184:MET:O	2.37	0.58
13:M:227:VAL:O	13:M:232:ARG:NH1	2.37	0.58
14:N:91:ARG:NH1	20:T:59:ASP:OD1	2.37	0.58
23:W:172:GLU:HA	23:W:182:ARG:HD3	1.86	0.58
12:l:69:HIS:HA	12:l:215:VAL:HG21	1.85	0.58
15:o:163:ILE:HG12	15:o:170:GLY:HA2	1.86	0.58
4:D:92:PHE:CE2	4:D:125:LYS:HD2	2.35	0.58
6:F:153:VAL:HA	6:F:160:ILE:HA	1.86	0.58
21:U:697:GLN:NE2	21:U:744:VAL:O	2.36	0.58
26:Z:138:TYR:HB3	26:Z:155:PHE:HB3	1.85	0.58
19:s:4:PRO:O	20:t:100:ARG:NH2	2.36	0.58
24:X:368:MET:HB2	24:X:373:LYS:HB2	1.85	0.57
19:S:21:ALA:HB3	19:S:198:VAL:HB	1.85	0.57
7:g:234:GLU:O	7:g:238:HIS:ND1	2.32	0.57
1:A:399:ALA:O	1:A:400:ARG:NE	2.37	0.57
3:C:133:PRO:O	3:C:135:VAL:N	2.37	0.57
21:U:665:ASN:HB3	21:U:694:ILE:HD11	1.86	0.57
19:s:57:PHE:HB3	19:s:60:ASP:HB2	1.85	0.57
10:J:65:LEU:HD12	10:J:88:ARG:HG3	1.85	0.57
13:M:213:LEU:O	13:M:232:ARG:NH2	2.38	0.57
22:V:474:LEU:O	22:V:478:GLN:NE2	2.37	0.57
23:W:64:SER:HB3	23:W:103:LYS:HG3	1.85	0.57
23:W:140:ILE:HG12	23:W:177:MET:HB3	1.86	0.57
25:Y:210:SER:HB3	25:Y:213:LEU:HD23	1.86	0.57
26:Z:11:VAL:O	26:Z:163:GLY:N	2.36	0.57
7:g:81:THR:OG1	7:g:137:CYS:SG	2.61	0.57
2:B:320:ASP:O	2:B:322:ARG:NH1	2.36	0.57
3:C:117:ARG:NH2	3:C:123:LEU:O	2.36	0.57
5:E:167:PRO:O	5:E:274:LYS:NZ	2.35	0.57
5:E:337:GLY:O	5:E:378:LYS:NZ	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:146:GLN:NE2	10:J:147:THR:O	2.37	0.57
22:V:355:ARG:HB2	31:e:27:TRP:HB2	1.85	0.57
27:a:292:THR:HA	27:a:330:ARG:HA	1.87	0.57
8:h:196:LYS:HG3	8:h:203:MET:HE3	1.85	0.57
6:F:252:ALA:HB3	6:F:255:GLN:HB2	1.86	0.57
10:J:97:THR:HG23	18:R:82:LEU:HD21	1.87	0.57
14:N:19:ARG:NH1	14:N:168:GLY:O	2.37	0.57
16:P:29:GLY:HA3	16:P:34:MET:HA	1.87	0.57
11:k:207:GLU:HG2	11:k:208:GLU:HG2	1.87	0.57
2:B:174:MET:HE1	2:B:250:VAL:HB	1.87	0.57
20:T:61:GLN:HA	20:T:64:LYS:HZ3	1.69	0.57
21:U:381:THR:HG22	21:U:412:HIS:HA	1.86	0.57
22:V:150:ARG:NH1	22:V:157:THR:O	2.38	0.57
24:X:371:ASP:OD1	25:Y:233:ARG:NH1	2.38	0.57
7:g:38:THR:HA	7:g:169:GLY:HA3	1.86	0.57
12:l:134:ILE:HB	12:l:145:PHE:HB2	1.86	0.57
20:T:27:LEU:HD22	20:T:184:TYR:HB2	1.86	0.57
25:Y:314:LEU:O	25:Y:354:VAL:N	2.38	0.57
29:c:54:MET:HE2	29:c:84:VAL:HG22	1.86	0.57
13:m:34:SER:OG	13:m:65:ARG:NH1	2.37	0.57
20:t:55:GLY:HA3	20:t:108:ASN:HA	1.86	0.57
1:A:69:ASP:HB2	1:A:72:LEU:H	1.70	0.57
17:q:47:VAL:O	17:q:101:ASN:N	2.38	0.57
3:C:63:LEU:O	3:C:67:GLN:NE2	2.34	0.57
20:T:54:SER:O	20:T:108:ASN:ND2	2.30	0.57
21:U:94:SER:HA	21:U:98:GLU:HG3	1.86	0.57
22:V:177:ASN:O	22:V:179:LYS:NZ	2.38	0.57
25:Y:188:CYS:SG	25:Y:196:GLN:NE2	2.78	0.57
9:I:11:ILE:HG22	10:J:7:ILE:HG23	1.87	0.56
11:K:13:ASN:HB3	12:L:126:ARG:HB3	1.85	0.56
14:N:115:PRO:HD2	14:N:119:MET:HB3	1.87	0.56
15:O:112:SER:HB2	15:O:125:VAL:HG21	1.86	0.56
30:d:149:ASN:HB3	30:d:199:PHE:CZ	2.40	0.56
12:l:39:LYS:HA	12:l:44:ALA:HA	1.87	0.56
1:A:79:ASP:OD2	2:B:91:LYS:NZ	2.38	0.56
5:E:244:SER:HB2	6:F:300:LYS:HD3	1.87	0.56
19:S:157:ASN:ND2	16:p:176:ASP:OD2	2.38	0.56
13:m:39:ILE:HD11	13:m:176:ILE:HG12	1.86	0.56
2:B:139:VAL:HG23	2:B:161:GLY:HA2	1.85	0.56
6:F:107:ASP:HA	6:F:110:ASN:HB2	1.87	0.56
8:H:77:SER:HB3	8:H:163:MET:HE1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:35:VAL:HG12	16:P:36:THR:HG23	1.88	0.56
26:Z:20:VAL:HG13	29:c:212:LEU:HD23	1.86	0.56
27:a:226:ARG:HB3	27:a:234:ILE:HD11	1.87	0.56
28:b:124:LEU:HD13	28:b:156:PHE:HB2	1.87	0.56
29:c:96:LEU:CD1	33:u:8:LEU:HD22	2.32	0.56
32:f:123:ALA:HA	32:f:126:ILE:HD12	1.86	0.56
32:f:791:VAL:HG12	32:f:823:ALA:HB1	1.87	0.56
32:f:851:ASP:O	32:f:855:GLN:NE2	2.38	0.56
10:j:62:ILE:HG12	10:j:72:ALA:HB2	1.87	0.56
20:t:24:ALA:HB3	20:t:42:ILE:HD11	1.86	0.56
20:t:25:ASP:HA	20:t:187:PHE:HA	1.85	0.56
33:y:18:GLU:H	33:y:21:ASP:CG	2.14	0.56
11:K:52:LYS:NZ	11:K:64:ILE:O	2.38	0.56
13:M:34:SER:OG	13:M:65:ARG:NH1	2.38	0.56
18:R:55:TRP:NE1	19:S:97:TYR:OH	2.38	0.56
19:S:28:ARG:NH2	19:S:213:ASP:OXT	2.38	0.56
21:U:164:GLU:HA	21:U:167:ILE:HG12	1.87	0.56
20:t:27:LEU:HD22	20:t:184:TYR:HB2	1.86	0.56
17:Q:104:LEU:HB3	17:Q:116:TYR:HB2	1.87	0.56
2:B:74:MET:HA	2:B:77:GLU:HG2	1.88	0.56
10:J:199:VAL:HG22	10:J:202:GLY:H	1.70	0.56
20:T:44:ARG:NH2	20:T:47:ASN:OD1	2.39	0.56
18:r:27:ALA:O	19:s:136:LYS:NZ	2.38	0.56
33:y:71:LEU:N	33:y:71:LEU:CD1	2.68	0.56
5:E:83:CYS:HB2	5:E:89:LYS:HE2	1.87	0.56
10:J:120:GLN:NE2	11:K:135:ARG:O	2.33	0.56
29:c:89:PRO:HG2	33:u:44:ILE:HD11	1.86	0.56
5:E:13:ARG:NH2	6:F:25:GLU:OE2	2.38	0.56
21:U:243:LEU:HD13	21:U:903:PHE:HB3	1.88	0.56
32:f:271:MET:HE3	32:f:787:LEU:HA	1.87	0.56
8:h:222:THR:HG23	8:h:225:GLU:H	1.71	0.56
10:j:57:ARG:O	10:j:60:ARG:NH2	2.39	0.56
33:x:60:ASN:CB	33:y:8:LEU:CB	2.48	0.56
4:D:275:PHE:HB3	4:D:286:GLN:HE21	1.71	0.56
23:W:154:GLU:OE2	23:W:191:ARG:NH1	2.39	0.56
3:C:343:ASN:HB3	3:C:346:LYS:HB3	1.87	0.56
16:P:98:LYS:HE3	16:P:103:TYR:HE2	1.70	0.56
23:W:360:GLU:HG2	23:W:364:ARG:HE	1.70	0.56
25:Y:360:ASP:OD2	25:Y:363:ASN:ND2	2.40	0.56
9:i:136:TYR:HB2	9:i:148:TYR:HB2	1.88	0.56
16:p:7:ASN:ND2	16:p:29:GLY:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:r:115:ASP:OD1	18:r:119:ASN:N	2.39	0.56
19:s:125:ASP:OD1	19:s:129:SER:N	2.39	0.56
4:D:200:ARG:HH12	4:D:301:GLN:HA	1.71	0.55
22:V:343:PRO:O	31:e:43:TRP:NE1	2.39	0.55
27:a:371:ALA:HA	27:a:374:ILE:HD13	1.87	0.55
33:x:20:SER:HB3	33:y:73:LEU:HD21	1.86	0.55
1:A:415:LYS:O	1:A:419:SER:HB3	2.05	0.55
3:C:347:ILE:HD12	3:C:350:LEU:HD12	1.87	0.55
6:F:38:THR:HG22	6:F:39:GLU:HG2	1.87	0.55
11:K:235:GLU:HA	11:K:238:ILE:HB	1.88	0.55
12:L:193:ARG:HG2	12:L:196:ARG:HH21	1.72	0.55
16:P:55:GLY:HA3	16:P:105:THR:HA	1.88	0.55
30:d:75:MET:HA	30:d:78:LEU:HB2	1.87	0.55
13:m:213:LEU:HD12	13:m:232:ARG:HG3	1.88	0.55
6:F:191:LEU:HG	6:F:194:GLN:HB2	1.87	0.55
22:V:355:ARG:HD2	31:e:27:TRP:HD1	1.71	0.55
17:q:33:ASP:OD2	17:q:181:ARG:NH2	2.40	0.55
11:K:96:THR:HA	11:K:107:MET:HE1	1.88	0.55
15:O:198:ARG:NH1	16:P:155:GLU:OE2	2.39	0.55
19:S:192:ALA:HA	19:S:209:SER:HA	1.87	0.55
21:U:443:LEU:HD13	21:U:461:LEU:HG	1.87	0.55
14:n:7:GLN:NE2	14:n:109:GLY:O	2.40	0.55
20:t:126:ASP:OD1	20:t:130:VAL:N	2.39	0.55
2:B:58:CYS:SG	2:B:59:ARG:N	2.80	0.55
13:M:163:CYS:SG	13:M:164:ALA:N	2.80	0.55
21:U:554:LEU:HD12	21:U:764:LEU:HD11	1.88	0.55
21:U:700:GLU:H	21:U:706:VAL:HG21	1.70	0.55
12:l:41:LYS:HG3	12:l:42:THR:HG23	1.88	0.55
1:A:309:PHE:H	6:F:238:ARG:HD3	1.72	0.55
21:U:243:LEU:HD22	21:U:903:PHE:HD2	1.71	0.55
23:W:452:ILE:HD13	26:Z:101:LEU:HG	1.87	0.55
32:f:62:ARG:HE	32:f:74:ALA:HB2	1.72	0.55
20:t:1:THR:N	20:t:105:PRO:O	2.39	0.55
9:I:22:GLU:HA	9:I:25:MET:HG3	1.89	0.55
12:L:44:ALA:HB2	12:L:142:PRO:HB3	1.87	0.55
19:S:27:THR:HB	19:S:40:SER:H	1.72	0.55
18:r:154:ASP:OD1	18:r:157:ARG:NH1	2.40	0.55
1:A:327:LEU:HB3	1:A:331:LEU:HD11	1.89	0.55
9:I:13:SER:OG	9:I:17:ARG:N	2.37	0.55
12:L:157:ARG:NH1	13:M:56:LYS:O	2.40	0.55
15:O:175:LEU:HB3	15:O:186:LEU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:409:LEU:HD21	24:X:344:ARG:HG2	1.89	0.55
27:a:15:GLY:O	27:a:18:GLN:NE2	2.34	0.55
31:e:44:ASP:OD1	31:e:47:ASN:ND2	2.40	0.55
32:f:668:ALA:HA	32:f:697:ILE:HD11	1.88	0.55
33:x:63:LYS:CE	33:y:76:GLY:O	2.54	0.55
33:y:8:LEU:HD23	33:y:8:LEU:H	1.72	0.55
5:E:309:ARG:NH1	5:E:335:SER:O	2.40	0.55
16:P:7:ASN:ND2	16:P:29:GLY:O	2.36	0.55
17:Q:104:LEU:O	17:Q:116:TYR:N	2.38	0.55
17:Q:171:PHE:HA	17:q:26:VAL:HG12	1.89	0.55
19:S:148:LEU:HA	19:S:151:ASN:HD22	1.70	0.55
21:U:33:ASP:OD1	22:V:236:ARG:NH1	2.40	0.55
21:U:733:ALA:O	21:U:737:LEU:HB2	2.07	0.55
30:d:110:ASN:OD1	30:d:173:THR:OG1	2.23	0.55
13:m:49:VAL:HB	13:m:212:GLU:HB3	1.89	0.55
4:D:180:ALA:O	4:D:306:LYS:NZ	2.40	0.55
13:M:37:ILE:HD11	13:M:193:VAL:HG13	1.89	0.55
21:U:265:ILE:O	21:U:269:ARG:NH1	2.40	0.55
24:X:335:LEU:HA	24:X:338:VAL:HG22	1.87	0.55
1:A:332:MET:HA	1:A:337:LEU:HD12	1.90	0.54
1:A:417:ILE:O	1:A:421:ALA:HB2	2.07	0.54
4:D:81:ARG:NH2	29:c:149:GLN:OE1	2.39	0.54
5:E:247:THR:O	5:E:251:ARG:NH1	2.40	0.54
6:F:232:GLY:HA2	37:F:501:ADP:H5'2	1.90	0.54
15:O:81:ARG:HD2	15:O:84:LYS:HD3	1.89	0.54
16:P:153:LEU:HB3	16:P:166:THR:HG23	1.89	0.54
17:Q:162:LYS:O	18:r:141:ARG:NH2	2.40	0.54
21:U:574:LYS:O	21:U:579:ARG:NH2	2.39	0.54
29:c:168:MET:HE2	29:c:198:ARG:HH21	1.71	0.54
30:d:3:GLU:HB2	30:d:25:ARG:HD2	1.89	0.54
30:d:200:PHE:O	30:d:203:PRO:HD3	2.06	0.54
33:x:57:SER:HB3	33:y:73:LEU:HA	1.88	0.54
1:A:250:VAL:HA	1:A:294:GLU:HG3	1.89	0.54
35:A:501:ATP:O2G	2:B:346:ARG:NH1	2.37	0.54
7:G:53:GLN:HA	7:G:215:ILE:HA	1.89	0.54
23:W:359:VAL:HG23	23:W:382:LEU:HD22	1.90	0.54
28:b:54:LEU:HD13	28:b:84:ILE:HG13	1.89	0.54
10:j:96:LEU:HD21	17:q:62:LYS:HG2	1.89	0.54
33:x:60:ASN:CG	33:y:8:LEU:HD13	2.32	0.54
13:M:134:SER:HB2	13:M:153:PRO:HD3	1.90	0.54
22:V:467:TYR:O	26:Z:254:ASN:ND2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:11:THR:HA	19:s:139:GLY:HA3	1.89	0.54
33:x:23:ILE:HG12	33:x:54:ARG:O	2.07	0.54
33:y:1:MET:N	33:y:17:VAL:O	2.40	0.54
3:C:53:ASN:ND2	21:U:642:GLU:O	2.40	0.54
5:E:385:ASP:O	5:E:386:TYR:HB2	2.07	0.54
8:H:79:MET:HE3	8:H:81:PRO:HD2	1.89	0.54
11:K:98:ASN:OD1	18:R:61:ARG:NH2	2.41	0.54
19:S:35:ILE:O	20:T:151:ARG:NH2	2.39	0.54
21:U:367:THR:HA	21:U:370:VAL:HG22	1.89	0.54
24:X:343:SER:HA	24:X:387:ILE:HB	1.89	0.54
26:Z:9:VAL:HG12	26:Z:48:LEU:HB3	1.88	0.54
26:Z:142:GLU:OE2	26:Z:153:LYS:NZ	2.40	0.54
32:f:46:SER:HB3	32:f:49:ASP:HB2	1.89	0.54
11:k:98:ASN:O	11:k:102:THR:OG1	2.22	0.54
11:k:118:ASN:O	11:k:122:GLN:NE2	2.40	0.54
2:B:181:GLN:O	2:B:241:ASN:ND2	2.41	0.54
11:K:203:LYS:HB2	11:K:210:LEU:HD22	1.90	0.54
15:O:171:SER:OG	19:s:211:ARG:NH2	2.41	0.54
17:Q:25:ILE:HG22	17:Q:26:VAL:HG13	1.90	0.54
22:V:345:ARG:NE	31:e:42:ASN:O	2.41	0.54
29:c:236:GLU:HA	29:c:239:LYS:HG2	1.89	0.54
29:c:265:MET:HG2	29:c:269:GLN:HB3	1.89	0.54
17:q:181:ARG:HG2	17:q:190:ASP:HA	1.90	0.54
4:D:233:SER:OG	5:E:259:GLU:OE1	2.25	0.54
16:p:126:LEU:HG	16:p:127:ILE:HG23	1.89	0.54
17:q:19:ARG:HD3	17:q:177:THR:HG22	1.89	0.54
1:A:236:CYS:H	32:f:352:HIS:HE1	1.55	0.54
4:D:117:SER:O	4:D:121:ARG:NH1	2.38	0.54
25:Y:81:LEU:HD22	25:Y:107:LYS:HE3	1.89	0.54
30:d:52:ARG:HH22	30:d:92:SER:HB3	1.72	0.54
32:f:367:SER:O	32:f:371:ASN:ND2	2.40	0.54
10:j:71:MET:HG3	10:j:133:ILE:HA	1.90	0.54
19:s:28:ARG:NH1	19:s:187:VAL:O	2.41	0.54
3:C:328:ILE:HG22	3:C:359:VAL:HG11	1.89	0.54
4:D:208:PRO:HB2	5:E:291:ARG:HD3	1.90	0.54
7:G:30:LYS:NZ	7:G:34:GLN:OE1	2.41	0.54
17:Q:12:TYR:OH	17:Q:151:ILE:O	2.26	0.54
25:Y:155:ASP:OD1	25:Y:155:ASP:N	2.40	0.54
27:a:216:LEU:HA	27:a:219:HIS:HB2	1.90	0.54
32:f:422:VAL:HG12	32:f:455:VAL:HG11	1.89	0.54
35:A:501:ATP:O3G	2:B:346:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:MET:HE1	3:C:198:LEU:HD22	1.90	0.54
7:G:38:THR:HA	7:G:169:GLY:HA3	1.89	0.54
9:I:41:ASP:OD1	9:I:41:ASP:N	2.40	0.54
9:I:75:SER:HB3	9:I:135:LEU:HB2	1.90	0.54
17:Q:52:ASP:OD1	18:R:88:TYR:OH	2.23	0.54
23:W:146:THR:HG21	23:W:169:LEU:HD21	1.89	0.54
26:Z:192:THR:O	26:Z:196:HIS:ND1	2.32	0.54
30:d:164:THR:HA	30:d:167:ILE:HG12	1.89	0.54
32:f:845:ARG:HB3	32:f:865:PHE:HB2	1.89	0.54
7:g:43:ARG:HH21	7:g:164:LYS:HG2	1.73	0.54
14:n:148:THR:H	14:n:151:GLU:HB2	1.72	0.54
5:E:62:LYS:HA	5:E:94:PRO:HB3	1.88	0.53
5:E:291:ARG:O	5:E:295:LEU:N	2.39	0.53
21:U:413:LYS:HA	21:U:449:ILE:HA	1.90	0.53
29:c:130:GLN:NE2	29:c:140:ALA:O	2.41	0.53
4:D:104:GLY:HA2	4:D:110:ASN:HA	1.90	0.53
19:S:213:ASP:OD2	15:o:19:ARG:NH2	2.39	0.53
29:c:173:GLU:OE1	29:c:180:ASN:ND2	2.41	0.53
8:H:42:ASN:ND2	8:H:183:GLU:OE1	2.41	0.53
8:H:150:ASP:OD1	8:H:154:ALA:N	2.42	0.53
32:f:615:ILE:O	32:f:650:GLN:NE2	2.35	0.53
7:g:241:ALA:O	7:g:245:ARG:NH1	2.40	0.53
11:k:202:LEU:HA	11:k:205:VAL:HG22	1.88	0.53
21:U:440:GLY:HA2	21:U:473:VAL:HG13	1.90	0.53
17:q:107:TYR:HA	17:q:113:PRO:HA	1.90	0.53
13:M:49:VAL:HB	13:M:212:GLU:HG3	1.91	0.53
24:X:380:GLN:HB2	25:Y:314:LEU:HA	1.90	0.53
25:Y:148:GLY:HA2	25:Y:153:ASP:HB3	1.91	0.53
8:h:3:GLU:N	13:m:125:TYR:HB3	2.22	0.53
9:i:156:TYR:OH	10:j:81:ARG:NH1	2.41	0.53
14:n:7:GLN:HE22	14:n:122:ARG:HH21	1.55	0.53
4:D:119:ILE:O	4:D:121:ARG:NH1	2.41	0.53
5:E:198:VAL:HG12	5:E:200:SER:H	1.74	0.53
22:V:175:MET:HE3	22:V:184:ALA:HA	1.90	0.53
15:o:86:MET:HA	15:o:89:ARG:HE	1.74	0.53
33:x:19:PRO:O	33:y:73:LEU:CD1	2.51	0.53
1:A:158:ASP:HB3	1:A:161:VAL:HG12	1.90	0.53
4:D:229:ARG:HG3	4:D:263:PHE:HD2	1.73	0.53
4:D:234:GLU:O	4:D:237:GLN:NE2	2.41	0.53
13:M:40:ARG:HG3	13:M:45:VAL:HG22	1.90	0.53
21:U:584:TYR:OH	21:U:768:GLN:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:287:LEU:HD23	25:Y:290:PRO:HB2	1.91	0.53
26:Z:215:VAL:HA	26:Z:220:LEU:HB2	1.89	0.53
7:g:89:SER:HA	13:m:117:MET:HE2	1.90	0.53
11:k:13:ASN:ND2	12:l:124:GLY:O	2.40	0.53
1:A:347:ASP:O	1:A:351:ARG:NH2	2.40	0.53
11:K:82:ILE:HG22	11:K:86:LYS:HZ1	1.73	0.53
21:U:725:MET:HG3	29:c:181:LEU:HD22	1.91	0.53
8:h:34:PRO:HA	8:h:164:GLY:HA3	1.91	0.53
12:l:164:ARG:NE	12:l:198:THR:O	2.34	0.53
18:r:20:ALA:HB2	18:r:31:VAL:HG21	1.89	0.53
33:y:36:ILE:O	33:y:41:GLN:NE2	2.41	0.53
1:A:267:LYS:HD3	32:f:357:ARG:HH12	1.74	0.53
2:B:221:GLY:HA3	2:B:347:ILE:HA	1.91	0.53
6:F:43:GLN:HA	6:F:46:ARG:HG2	1.91	0.53
17:Q:68:LYS:HD3	17:Q:74:GLU:HG2	1.91	0.53
21:U:536:ALA:HB2	21:U:548:LEU:HD22	1.91	0.53
24:X:67:GLY:HA2	24:X:109:LEU:HD21	1.91	0.53
2:B:193:GLN:HG3	2:B:353:PHE:HE1	1.74	0.53
8:H:14:SER:OG	8:H:18:LYS:N	2.40	0.53
13:M:68:ASN:OD1	13:M:224:HIS:ND1	2.39	0.53
24:X:74:ARG:HH22	24:X:116:TRP:HB2	1.73	0.53
29:c:85:GLU:HG2	33:u:74:ARG:HB3	1.91	0.53
12:l:34:ALA:HA	12:l:162:GLY:HA3	1.91	0.53
17:q:118:MET:HE2	17:q:122:ALA:HA	1.91	0.53
20:t:91:TRP:HE3	20:t:92:LEU:HD22	1.73	0.53
6:F:410:ARG:NH2	6:F:419:ASP:OD2	2.42	0.52
22:V:287:ARG:HH21	31:e:19:PHE:HA	1.74	0.52
24:X:218:HIS:NE2	24:X:227:THR:OG1	2.43	0.52
26:Z:21:ASP:O	26:Z:25:ARG:CB	2.57	0.52
27:a:74:LEU:HD22	27:a:113:LEU:HD21	1.91	0.52
28:b:20:ASP:OD1	28:b:20:ASP:N	2.40	0.52
28:b:35:ILE:HD12	28:b:184:ILE:HD13	1.91	0.52
33:u:44:ILE:HB	33:u:68:HIS:HB2	1.91	0.52
3:C:334:ARG:HB2	25:Y:174:TRP:H	1.73	0.52
8:H:103:GLU:OE1	16:P:86:THR:OG1	2.25	0.52
21:U:107:HIS:HA	21:U:110:LYS:HE3	1.91	0.52
16:p:62:THR:OG1	17:q:85:ARG:NH2	2.41	0.52
33:x:19:PRO:CG	33:y:74:ARG:CA	2.86	0.52
33:y:72:ARG:NH1	33:y:72:ARG:HG2	2.23	0.52
3:C:164:VAL:HG12	3:C:165:ILE:HG13	1.91	0.52
7:G:202:LEU:O	7:G:206:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:119:GLN:O	8:H:122:THR:OG1	2.27	0.52
12:L:50:LYS:HB3	12:L:59:HIS:HB3	1.90	0.52
16:P:51:ILE:HG13	16:P:109:ILE:HG12	1.91	0.52
32:f:151:LEU:HB3	32:f:159:VAL:HG22	1.90	0.52
8:h:82:ASP:HB3	8:h:130:PHE:HD1	1.74	0.52
33:x:18:GLU:N	33:x:21:ASP:OD2	2.41	0.52
5:E:322:LYS:HD3	5:E:326:ILE:HG13	1.90	0.52
10:J:119:THR:HG22	10:J:126:PRO:HB3	1.91	0.52
21:U:628:ARG:NH1	21:U:749:GLN:OE1	2.42	0.52
22:V:327:THR:HA	22:V:330:LYS:HD2	1.91	0.52
27:a:133:GLU:O	27:a:137:ASP:N	2.42	0.52
10:j:36:ARG:HA	10:j:41:VAL:HG12	1.90	0.52
12:l:52:ALA:HB1	12:l:57:ALA:HB3	1.90	0.52
17:q:4:LEU:HD22	17:q:45:LEU:HD23	1.90	0.52
9:I:125:GLY:O	9:I:127:LYS:NZ	2.36	0.52
12:L:66:VAL:HG23	12:L:89:ARG:HG3	1.91	0.52
23:W:108:CYS:HB3	23:W:128:LEU:HD11	1.91	0.52
24:X:380:GLN:N	25:Y:313:SER:O	2.43	0.52
26:Z:25:ARG:HD3	29:c:103:GLY:HA3	1.91	0.52
30:d:202:THR:HA	30:d:206:MET:SD	2.50	0.52
17:q:49:GLU:HB2	17:q:99:HIS:HB3	1.92	0.52
19:s:136:LYS:HA	19:s:146:GLN:HE22	1.75	0.52
2:B:204:PRO:HG3	2:B:211:TYR:HE2	1.75	0.52
14:N:3:ILE:O	14:N:128:GLY:N	2.40	0.52
16:P:17:LYS:HB2	16:P:157:ASN:HA	1.91	0.52
19:S:145:LEU:HD21	19:S:182:ALA:HB2	1.90	0.52
21:U:530:GLU:HG2	33:y:4:PHE:CE1	2.45	0.52
24:X:404:ILE:HG21	25:Y:372:LYS:HB3	1.91	0.52
29:c:269:GLN:HA	29:c:272:ILE:HG22	1.91	0.52
32:f:99:LEU:HD22	32:f:106:LEU:HD11	1.91	0.52
7:g:133:PRO:HD2	13:m:14:PHE:HE2	1.75	0.52
19:s:45:LYS:HE3	19:s:203:ILE:HD12	1.92	0.52
33:x:62:GLN:H	33:x:62:GLN:CD	2.15	0.52
22:V:338:LEU:HG	22:V:398:LEU:HD12	1.91	0.52
22:V:452:ASN:HB3	22:V:457:TYR:HB2	1.92	0.52
25:Y:2:PRO:HG2	25:Y:5:ASN:HB2	1.92	0.52
29:c:96:LEU:CD1	33:u:8:LEU:HB3	2.40	0.52
20:t:37:ARG:O	20:t:186:ARG:NH1	2.40	0.52
3:C:145:ASP:HA	3:C:201:ARG:HG2	1.92	0.52
14:N:29:ARG:NH2	15:O:139:GLU:OE1	2.43	0.52
22:V:76:LYS:HA	22:V:120:PHE:HZ	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:321:ALA:HB1	22:V:324:PHE:HB3	1.92	0.52
30:d:201:ASN:O	30:d:202:THR:C	2.52	0.52
16:p:22:ILE:HG23	16:p:188:HIS:HB2	1.90	0.52
18:r:19:ARG:H	18:r:33:LYS:HZ2	1.55	0.52
19:s:1:ARG:NH2	20:t:3:ASN:OD1	2.39	0.52
1:A:252:GLU:HG3	1:A:256:MET:HE3	1.91	0.52
1:A:295:VAL:HG11	2:B:307:ARG:HH21	1.74	0.52
16:P:62:THR:OG1	17:Q:85:ARG:NH2	2.43	0.52
23:W:197:LYS:NZ	23:W:199:TYR:OH	2.39	0.52
29:c:55:GLY:HA2	29:c:75:MET:HE1	1.92	0.52
32:f:338:ASP:HA	32:f:340:MET:HE1	1.92	0.52
32:f:425:GLY:HA3	32:f:451:VAL:HG21	1.90	0.52
13:m:27:MET:HA	13:m:30:VAL:HG12	1.91	0.52
33:y:55:THR:OG1	33:y:57:SER:OG	2.28	0.52
2:B:48:LYS:HE3	32:f:673:ARG:HD3	1.91	0.52
4:D:114:ARG:NH2	4:D:136:SER:OG	2.43	0.52
4:D:349:THR:HG21	4:D:360:LEU:HD21	1.92	0.52
24:X:127:GLN:NE2	24:X:156:GLU:OE1	2.42	0.52
30:d:106:LEU:HG	30:d:111:ARG:HB2	1.92	0.52
30:d:131:VAL:HA	30:d:134:LYS:HB3	1.91	0.52
32:f:94:LYS:HA	32:f:97:LYS:HD3	1.91	0.52
32:f:151:LEU:HA	32:f:154:TRP:HD1	1.74	0.52
7:g:11:ARG:O	7:g:24:GLN:NE2	2.43	0.52
33:x:41:GLN:HG2	33:x:69:LEU:HD11	1.91	0.52
8:H:148:GLN:OE1	8:H:158:TRP:NE1	2.43	0.51
24:X:187:ARG:HE	24:X:217:ILE:HG22	1.74	0.51
25:Y:104:MET:HE3	25:Y:130:LYS:HD3	1.92	0.51
26:Z:21:ASP:O	26:Z:25:ARG:HB2	2.10	0.51
29:c:75:MET:SD	29:c:77:GLN:NE2	2.74	0.51
10:j:148:ASP:OD2	10:j:150:SER:OG	2.28	0.51
16:p:159:ASP:N	16:p:159:ASP:OD1	2.41	0.51
33:x:38:PRO:C	33:x:40:GLN:N	2.66	0.51
4:D:345:PHE:HB3	4:D:360:LEU:HD23	1.92	0.51
5:E:199:VAL:HG23	5:E:201:SER:H	1.75	0.51
17:Q:15:VAL:HG21	17:Q:45:LEU:HD11	1.91	0.51
21:U:1:MET:HE1	30:d:37:PRO:HB3	1.91	0.51
21:U:351:MET:HG3	21:U:818:GLU:HA	1.92	0.51
12:l:117:GLN:NE2	13:m:83:ASP:OD1	2.43	0.51
18:r:38:ASN:O	18:r:184:TRP:NE1	2.32	0.51
7:G:138:MET:N	7:G:138:MET:SD	2.83	0.51
10:J:43:LEU:HD21	10:J:72:ALA:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:599:ILE:HD13	21:U:625:ILE:HD11	1.92	0.51
24:X:292:GLN:O	24:X:296:ASN:ND2	2.43	0.51
25:Y:13:LYS:HG3	25:Y:16:ASP:HA	1.93	0.51
27:a:194:GLN:HA	27:a:225:LEU:HB3	1.92	0.51
29:c:39:LEU:HD23	29:c:42:LEU:HD21	1.91	0.51
32:f:140:LEU:HD12	32:f:143:ARG:HB3	1.92	0.51
7:g:69:LEU:HD11	7:g:229:ILE:HD13	1.91	0.51
11:k:157:ASP:OD2	11:k:159:SER:OG	2.27	0.51
1:A:44:GLN:OE1	1:A:47:GLN:NE2	2.39	0.51
4:D:171:ASP:HA	4:D:174:LYS:HB2	1.93	0.51
5:E:60:VAL:HG13	5:E:95:GLY:H	1.76	0.51
5:E:173:TYR:CZ	5:E:300:HIS:HB2	2.45	0.51
5:E:241:ARG:HH22	5:E:389:VAL:HG21	1.74	0.51
15:O:161:ALA:O	15:O:165:ASN:ND2	2.38	0.51
21:U:98:GLU:HA	21:U:101:ILE:HG12	1.92	0.51
27:a:342:ASP:N	27:a:342:ASP:OD1	2.43	0.51
28:b:26:LEU:HD21	28:b:80:PRO:HG3	1.91	0.51
15:o:20:ALA:HB3	15:o:28:ASP:HB3	1.91	0.51
16:p:189:ILE:HB	16:p:196:THR:HB	1.93	0.51
1:A:142:VAL:HG22	1:A:149:ILE:HA	1.93	0.51
3:C:267:SER:OG	3:C:270:GLN:NE2	2.36	0.51
4:D:328:ASP:OD1	4:D:328:ASP:N	2.41	0.51
5:E:143:ARG:NH1	5:E:144:GLU:OE1	2.44	0.51
6:F:223:VAL:HG12	6:F:350:ARG:HB2	1.92	0.51
23:W:89:LEU:O	23:W:93:ARG:HG2	2.11	0.51
29:c:77:GLN:HA	29:c:86:ALA:HA	1.92	0.51
8:h:79:MET:HE3	8:h:81:PRO:HD2	1.91	0.51
8:h:115:ALA:HA	8:h:118:MET:HE2	1.93	0.51
9:i:160:LYS:HD2	10:j:53:LEU:HA	1.91	0.51
16:p:83:LYS:HD3	16:p:85:TYR:H	1.75	0.51
33:x:19:PRO:HG3	33:y:74:ARG:C	2.36	0.51
33:x:62:GLN:HB2	33:x:63:LYS:HE3	1.93	0.51
1:A:210:LYS:HZ1	1:A:315:ILE:H	1.59	0.51
6:F:428:GLN:HB3	6:F:430:LYS:HD3	1.93	0.51
21:U:66:LYS:HD2	21:U:69:TYR:HE1	1.76	0.51
7:g:122:SER:OG	7:g:156:PRO:O	2.29	0.51
18:r:51:ASP:HA	19:s:97:TYR:HE1	1.76	0.51
33:x:19:PRO:HB2	33:y:74:ARG:CA	2.40	0.51
33:y:72:ARG:CG	33:y:72:ARG:NH1	2.73	0.51
4:D:335:LEU:HD11	4:D:371:SER:HA	1.92	0.51
12:L:47:VAL:HG22	12:L:212:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:19:ARG:NH1	17:Q:179:SER:OG	2.43	0.51
21:U:898:CYS:O	21:U:901:GLN:NE2	2.43	0.51
23:W:88:MET:HE3	23:W:127:THR:HG23	1.93	0.51
27:a:205:LEU:O	27:a:271:LYS:NZ	2.38	0.51
14:n:55:VAL:HG22	14:n:86:MET:HE3	1.92	0.51
2:B:357:ASP:OD2	2:B:359:LYS:NZ	2.43	0.51
3:C:214:VAL:HG22	3:C:216:GLY:H	1.76	0.51
4:D:391:ARG:HG2	4:D:393:ILE:H	1.76	0.51
15:O:20:ALA:HB3	15:O:28:ASP:HB3	1.93	0.51
19:S:184:GLU:HA	19:S:211:ARG:HH11	1.75	0.51
8:h:177:ARG:HH12	8:h:193:LEU:HD13	1.75	0.51
18:r:3:THR:O	18:r:127:SER:OG	2.25	0.51
18:r:46:ALA:HB3	18:r:98:GLY:HA3	1.93	0.51
20:t:43:MET:HE1	20:t:64:LYS:HG3	1.93	0.51
33:y:6:LYS:HE3	33:y:66:THR:HG23	1.91	0.51
9:I:34:CYS:SG	9:I:75:SER:OG	2.63	0.51
10:J:11:SER:OG	10:J:15:HIS:N	2.41	0.51
15:O:152:LYS:HG2	15:O:175:LEU:HD21	1.93	0.51
20:T:211:ILE:HG23	14:n:30:VAL:HG11	1.92	0.51
21:U:175:GLY:O	21:U:179:TYR:N	2.43	0.51
22:V:440:LYS:NZ	30:d:148:TYR:OH	2.35	0.51
25:Y:300:ARG:HH21	31:e:52:PHE:HD1	1.58	0.51
27:a:343:LEU:HA	27:a:346:ILE:HD12	1.93	0.51
7:g:69:LEU:HA	7:g:79:VAL:HA	1.91	0.51
7:g:123:GLN:NE2	7:g:127:GLN:OE1	2.44	0.51
12:l:7:ASP:O	12:l:21:GLN:NE2	2.42	0.51
33:x:63:LYS:H	33:x:63:LYS:HE2	1.73	0.51
2:B:106:PRO:HB3	3:C:121:TYR:HB2	1.93	0.51
2:B:356:PRO:O	2:B:361:LYS:NZ	2.42	0.51
3:C:351:MET:HA	3:C:391:MET:HE1	1.93	0.51
4:D:115:ILE:HB	4:D:139:LEU:HD22	1.92	0.51
4:D:236:VAL:O	4:D:237:GLN:NE2	2.44	0.51
9:I:136:TYR:HB2	9:I:148:TYR:HB2	1.92	0.51
11:K:38:ILE:HD12	11:K:202:LEU:HG	1.93	0.51
21:U:199:ARG:HH21	21:U:223:LEU:HD11	1.76	0.51
21:U:568:GLU:OE2	21:U:572:ARG:NE	2.41	0.51
29:c:96:LEU:HD12	33:u:8:LEU:HD13	1.92	0.51
8:h:81:PRO:HA	8:h:84:ARG:HE	1.76	0.51
19:s:17:GLY:HA2	19:s:166:LEU:HD11	1.92	0.51
20:t:44:ARG:NH2	20:t:47:ASN:OD1	2.45	0.51
13:M:175:GLU:HG3	13:M:178:LYS:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:92:ASP:OD1	21:U:92:ASP:N	2.44	0.50
21:U:184:CYS:SG	21:U:218:GLN:NE2	2.84	0.50
27:a:212:ASN:OD1	27:a:213:PHE:N	2.44	0.50
8:h:45:VAL:HG12	8:h:212:ILE:HG22	1.93	0.50
14:n:7:GLN:HA	14:n:12:VAL:HG12	1.92	0.50
3:C:339:THR:O	3:C:340:ARG:NE	2.45	0.50
3:C:344:LEU:HA	3:C:347:ILE:HG22	1.93	0.50
14:N:144:ARG:H	14:N:147:MET:HE3	1.76	0.50
21:U:39:SER:OG	22:V:273:LYS:NZ	2.43	0.50
23:W:371:THR:HG22	23:W:372:ARG:HG3	1.92	0.50
32:f:143:ARG:NH2	32:f:147:SER:O	2.44	0.50
32:f:902:LYS:NZ	32:f:903:ASN:O	2.43	0.50
1:A:413:VAL:HG13	1:A:417:ILE:HD13	1.92	0.50
2:B:234:LEU:HD22	35:B:501:ATP:H2'	1.93	0.50
5:E:84:ARG:HB2	5:E:87:LEU:HD23	1.93	0.50
5:E:376:ASP:HA	5:E:379:LYS:HD3	1.92	0.50
21:U:55:ARG:O	21:U:58:GLN:NE2	2.44	0.50
21:U:583:MET:HA	21:U:586:VAL:HG12	1.93	0.50
27:a:347:LYS:HD3	27:a:350:LYS:HZ1	1.77	0.50
32:f:96:LEU:HD13	32:f:129:LEU:HD13	1.93	0.50
32:f:478:ARG:HH12	32:f:509:LYS:HD2	1.76	0.50
33:u:40:GLN:HA	33:u:72:ARG:HB2	1.94	0.50
2:B:181:GLN:HG2	2:B:237:LYS:HD3	1.93	0.50
2:B:292:THR:HG23	2:B:336:THR:HG21	1.93	0.50
6:F:93:VAL:HA	6:F:124:ILE:HG22	1.93	0.50
6:F:123:VAL:HG22	6:F:133:PHE:HA	1.94	0.50
12:L:90:GLN:NE2	12:L:94:ASP:OD1	2.45	0.50
18:R:1:THR:HA	18:R:33:LYS:HZ3	1.77	0.50
21:U:194:ARG:HH21	21:U:218:GLN:HE21	1.60	0.50
23:W:375:MET:HE1	23:W:411:GLY:HA2	1.92	0.50
24:X:70:LEU:HD13	24:X:109:LEU:HD23	1.93	0.50
28:b:51:LEU:HD23	28:b:71:ILE:HG23	1.94	0.50
17:q:21:ALA:HB3	17:q:29:LYS:HB3	1.93	0.50
33:x:6:LYS:O	33:x:68:HIS:HA	2.10	0.50
2:B:387:LYS:HE2	2:B:427:LEU:HD13	1.92	0.50
3:C:62:GLU:HA	3:C:65:LEU:HB3	1.93	0.50
4:D:171:ASP:OD1	4:D:171:ASP:N	2.43	0.50
6:F:289:ASP:OD1	6:F:289:ASP:N	2.43	0.50
17:Q:8:GLN:HA	17:Q:13:VAL:HA	1.94	0.50
18:R:97:MET:HB3	18:R:116:SER:HB3	1.93	0.50
21:U:710:ARG:NH2	21:U:738:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:100:ARG:NH1	28:b:102:GLY:O	2.45	0.50
9:i:151:ASP:OD1	9:i:155:ASN:N	2.44	0.50
6:F:120:LYS:O	6:F:137:ILE:HD11	2.11	0.50
6:F:336:ASP:OD1	6:F:336:ASP:N	2.44	0.50
25:Y:216:TYR:OH	25:Y:245:GLU:OE2	2.29	0.50
32:f:403:LYS:HG3	32:f:406:GLY:H	1.76	0.50
15:o:134:ALA:HB1	15:o:158:ALA:HB1	1.93	0.50
19:s:13:LEU:HD23	19:s:175:VAL:HG23	1.94	0.50
1:A:258:ARG:HH12	6:F:255:GLN:HA	1.76	0.50
2:B:337:LEU:HD12	2:B:341:LEU:HD23	1.94	0.50
5:E:101:ASP:HB3	5:E:106:THR:H	1.76	0.50
9:I:155:ASN:OD1	10:J:77:THR:OG1	2.30	0.50
12:L:107:ARG:HH12	20:T:83:TYR:HE1	1.60	0.50
15:O:175:LEU:O	15:O:186:LEU:N	2.45	0.50
20:T:1:THR:N	20:T:104:ASN:OD1	2.45	0.50
32:f:175:ASP:N	32:f:175:ASP:OD1	2.44	0.50
33:u:39:ASP:O	33:u:42:ARG:NH2	2.44	0.50
4:D:126:PRO:HD2	4:D:128:ALA:HB2	1.94	0.50
11:K:91:LYS:HG2	11:K:119:LEU:HD11	1.94	0.50
12:L:7:ASP:O	12:L:21:GLN:NE2	2.42	0.50
23:W:147:LYS:NZ	23:W:184:GLU:OE1	2.37	0.50
26:Z:212:LEU:HD21	27:a:349:MET:HG2	1.94	0.50
27:a:65:SER:HA	27:a:68:GLU:HB3	1.94	0.50
32:f:298:LEU:O	32:f:302:GLY:N	2.40	0.50
15:o:206:LYS:HD3	16:p:161:ASP:HB3	1.94	0.50
33:y:6:LYS:CE	33:y:66:THR:CG2	2.59	0.50
11:K:100:TRP:O	18:R:57:ARG:NH2	2.40	0.50
16:P:205:ASP:O	18:r:19:ARG:NH1	2.39	0.50
25:Y:244:ALA:HA	25:Y:247:LEU:HB2	1.94	0.50
26:Z:109:ASN:HD22	26:Z:155:PHE:HE1	1.59	0.50
32:f:66:LYS:HE3	32:f:67:ASP:H	1.75	0.50
32:f:894:LEU:HA	32:f:898:VAL:HG21	1.94	0.50
7:g:138:MET:HB2	7:g:154:CYS:HB3	1.93	0.50
11:k:10:ARG:HH11	11:k:22:PHE:HZ	1.58	0.50
15:o:143:ARG:H	15:o:146:MET:HE2	1.76	0.50
1:A:174:TYR:OH	1:A:192:GLU:OE2	2.30	0.49
3:C:57:ARG:HA	3:C:60:ARG:HG2	1.93	0.49
4:D:374:ASP:HB3	5:E:292:PRO:HG2	1.92	0.49
8:H:8:PHE:HB3	10:J:3:TYR:HE1	1.77	0.49
10:J:2:SER:OG	10:J:3:TYR:N	2.39	0.49
21:U:465:LEU:HD11	21:U:477:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:741:LEU:HA	32:f:744:MET:SD	2.52	0.49
32:f:755:ASP:OD2	32:f:758:ASN:ND2	2.44	0.49
18:r:127:SER:HB3	18:r:136:TYR:CE1	2.47	0.49
6:F:224:LEU:N	6:F:350:ARG:O	2.40	0.49
17:Q:4:LEU:HD22	17:Q:45:LEU:HD23	1.94	0.49
22:V:398:LEU:HA	22:V:401:ASN:HB2	1.94	0.49
26:Z:170:VAL:HG22	29:c:152:LYS:HA	1.94	0.49
9:i:165:GLY:O	9:i:168:SER:OG	2.30	0.49
13:m:164:ALA:O	13:m:169:ARG:NH2	2.42	0.49
15:o:215:LYS:HB2	16:p:197:THR:HB	1.94	0.49
19:s:27:THR:HB	19:s:40:SER:H	1.77	0.49
1:A:269:ALA:O	32:f:352:HIS:NE2	2.45	0.49
2:B:287:ILE:HG12	2:B:329:MET:HE2	1.94	0.49
7:G:47:CYS:HB3	7:G:221:THR:HG23	1.95	0.49
13:M:197:ILE:HG21	13:M:211:LEU:HD13	1.94	0.49
22:V:225:ASP:OD1	22:V:228:ARG:NH1	2.45	0.49
23:W:205:ILE:HA	23:W:208:LYS:HE3	1.95	0.49
32:f:216:MET:HA	32:f:219:LYS:HE2	1.93	0.49
8:h:143:ARG:NH2	8:h:145:TYR:OH	2.45	0.49
11:k:91:LYS:NZ	11:k:95:GLU:OE2	2.43	0.49
2:B:373:THR:OG1	2:B:412:MET:O	2.30	0.49
13:M:8:ASP:HB3	13:M:21:PHE:HD2	1.78	0.49
7:g:155:ASP:OD1	7:g:159:TYR:N	2.45	0.49
12:l:153:TYR:O	13:m:63:ASN:ND2	2.38	0.49
16:p:203:ARG:NH2	16:p:205:ASP:OD2	2.44	0.49
2:B:235:LEU:HD13	2:B:353:PHE:HZ	1.77	0.49
3:C:86:LEU:HD21	3:C:94:LYS:HD3	1.94	0.49
7:G:120:ASP:OD1	8:H:84:ARG:NH1	2.45	0.49
10:J:56:GLU:O	10:J:60:ARG:NH1	2.44	0.49
20:T:122:LEU:HG	20:T:137:LEU:HD12	1.93	0.49
24:X:9:PHE:CZ	24:X:45:VAL:HG13	2.47	0.49
28:b:25:ARG:NH2	28:b:145:GLU:OE1	2.46	0.49
29:c:96:LEU:HD12	33:u:8:LEU:CD2	2.39	0.49
4:D:121:ARG:HA	4:D:124:LEU:HD12	1.92	0.49
5:E:236:ASP:OD2	5:E:279:THR:OG1	2.30	0.49
6:F:228:PRO:O	6:F:233:LYS:NZ	2.46	0.49
11:K:72:ALA:O	11:K:226:PHE:N	2.46	0.49
12:L:212:ILE:HB	12:L:224:TYR:HB2	1.95	0.49
16:P:47:ASP:OD2	16:P:81:GLN:NE2	2.40	0.49
16:p:78:GLU:HB3	16:p:80:ARG:HG2	1.95	0.49
5:E:210:GLU:OE1	5:E:213:ARG:NE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:71:HIS:HA	8:H:218:PHE:H	1.77	0.49
10:J:46:GLU:HA	10:J:206:ILE:HG22	1.95	0.49
14:N:85:GLU:OE2	14:N:89:ARG:NH2	2.46	0.49
14:N:138:TYR:O	14:N:142:THR:OG1	2.23	0.49
22:V:122:THR:OG1	22:V:148:ARG:NH2	2.46	0.49
24:X:360:ASP:N	24:X:360:ASP:OD1	2.46	0.49
7:g:13:ILE:HB	7:g:129:ALA:HB1	1.94	0.49
7:g:47:CYS:HA	7:g:221:THR:HA	1.94	0.49
7:g:164:LYS:NZ	8:h:55:ILE:O	2.35	0.49
8:h:3:GLU:OE2	13:m:127:ALA:HB3	2.13	0.49
10:j:86:ARG:NH2	10:j:110:TYR:OH	2.43	0.49
16:p:30:ILE:HG22	16:p:31:GLN:H	1.77	0.49
10:J:67:ASP:OD1	10:J:67:ASP:N	2.44	0.49
11:K:154:PHE:HD1	11:K:164:GLN:HA	1.78	0.49
21:U:57:ARG:NH1	21:U:58:GLN:OE1	2.46	0.49
29:c:219:ASN:HB2	29:c:222:LYS:HD3	1.95	0.49
30:d:129:THR:OG1	30:d:130:ASN:N	2.46	0.49
7:g:116:LYS:HG3	8:h:84:ARG:HH11	1.77	0.49
1:A:272:ILE:O	1:A:318:LEU:N	2.44	0.49
5:E:374:VAL:O	5:E:377:SER:OG	2.29	0.49
22:V:419:LEU:HA	22:V:422:ILE:HG22	1.94	0.49
7:g:69:LEU:HB3	7:g:79:VAL:HG23	1.95	0.49
2:B:378:VAL:HG12	2:B:416:ASN:HA	1.95	0.49
4:D:352:MET:HE1	5:E:162:VAL:HG13	1.95	0.49
13:M:43:ASP:OD1	13:M:43:ASP:N	2.46	0.49
17:Q:102:LEU:HB3	17:Q:118:MET:HE2	1.95	0.49
19:S:185:ARG:NH1	15:o:26:VAL:O	2.44	0.49
19:S:211:ARG:NH2	15:o:171:SER:OG	2.45	0.49
22:V:132:LEU:HD23	22:V:135:LEU:HD21	1.95	0.49
25:Y:215:ASP:OD2	25:Y:217:LYS:NZ	2.34	0.49
32:f:343:LYS:HZ2	32:f:773:LYS:HE2	1.78	0.49
32:f:360:GLY:HA3	32:f:365:VAL:HG21	1.94	0.49
8:h:46:LEU:HD13	8:h:75:VAL:HG13	1.93	0.49
33:x:7:THR:C	33:x:9:THR:H	2.21	0.49
1:A:41:TYR:HB2	2:B:57:GLN:HB3	1.94	0.48
1:A:171:ASP:OD1	1:A:171:ASP:N	2.43	0.48
21:U:580:ARG:NH2	21:U:768:GLN:OE1	2.45	0.48
25:Y:246:ILE:HG22	25:Y:250:LEU:HD23	1.95	0.48
27:a:277:LEU:HA	27:a:280:MET:HG2	1.94	0.48
29:c:279:ASP:OD1	29:c:279:ASP:N	2.46	0.48
33:x:20:SER:O	33:x:21:ASP:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:PHE:HA	1:A:318:LEU:HB2	1.94	0.48
2:B:424:GLU:HA	2:B:428:TYR:HD2	1.76	0.48
5:E:121:ASN:OD1	6:F:146:LYS:NZ	2.46	0.48
6:F:439:ALA:HB1	12:L:62:LYS:HE3	1.94	0.48
16:P:107:PRO:HG2	16:P:124:LEU:HB2	1.93	0.48
21:U:26:LYS:HD3	30:d:36:LEU:HD22	1.96	0.48
21:U:749:GLN:NE2	21:U:750:SER:O	2.38	0.48
22:V:477:HIS:ND1	30:d:249:TYR:OH	2.33	0.48
23:W:378:MET:HE1	23:W:389:SER:HB3	1.93	0.48
25:Y:205:VAL:HG22	25:Y:223:THR:HG21	1.93	0.48
26:Z:231:GLN:HA	26:Z:234:PHE:HB2	1.95	0.48
14:n:84:LYS:NZ	14:n:85:GLU:OE2	2.44	0.48
20:t:56:ASP:N	20:t:107:TRP:O	2.41	0.48
5:E:194:ASN:OD1	5:E:225:HIS:ND1	2.45	0.48
22:V:345:ARG:HH21	31:e:43:TRP:HA	1.79	0.48
23:W:357:ARG:NH1	23:W:360:GLU:OE1	2.46	0.48
32:f:566:HIS:HA	32:f:569:LYS:HZ3	1.77	0.48
9:i:185:THR:N	9:i:188:SER:OG	2.46	0.48
1:A:189:GLU:HG3	1:A:190:VAL:HG13	1.95	0.48
3:C:186:VAL:HB	3:C:292:ILE:HG12	1.95	0.48
8:H:177:ARG:HD3	24:X:160:MET:HE3	1.95	0.48
10:J:158:ALA:HB1	10:J:172:LEU:HD23	1.95	0.48
13:M:42:LYS:HE3	13:M:183:GLU:HA	1.95	0.48
21:U:19:LEU:HG	30:d:27:LYS:HE2	1.95	0.48
10:j:185:ASP:OD1	10:j:185:ASP:N	2.45	0.48
13:m:15:SER:OG	13:m:19:ARG:N	2.46	0.48
16:p:134:ASP:OD1	16:p:134:ASP:N	2.45	0.48
18:r:105:ASP:OD1	18:r:105:ASP:N	2.45	0.48
33:x:60:ASN:ND2	33:y:8:LEU:HB3	2.27	0.48
3:C:184:LYS:N	3:C:312:ASP:OD2	2.37	0.48
12:L:140:MET:HE1	20:T:81:HIS:CE1	2.49	0.48
20:T:126:ASP:OD1	20:T:130:VAL:N	2.45	0.48
29:c:133:PHE:HZ	33:u:73:LEU:HD13	1.78	0.48
32:f:276:GLU:HG2	32:f:277:LEU:HD12	1.95	0.48
10:j:116:GLN:HG3	11:k:83:ALA:HB1	1.94	0.48
11:k:100:TRP:O	18:r:57:ARG:NH2	2.47	0.48
19:s:59:GLY:H	20:t:130:VAL:HG22	1.78	0.48
33:u:1:MET:N	33:u:17:VAL:O	2.36	0.48
33:x:1:MET:N	33:x:17:VAL:O	2.42	0.48
1:A:139:ARG:NH2	2:B:130:GLU:OE2	2.47	0.48
2:B:248:LEU:N	2:B:281:ILE:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:102:MET:N	5:E:102:MET:SD	2.87	0.48
10:J:35:VAL:HG11	10:J:190:LEU:HD23	1.94	0.48
10:J:148:ASP:OD2	10:J:150:SER:OG	2.31	0.48
21:U:399:TRP:HD1	29:c:174:PRO:HB2	1.79	0.48
21:U:619:VAL:HG23	21:U:651:GLY:HA3	1.95	0.48
24:X:298:SER:HA	24:X:334:ASN:HD21	1.79	0.48
8:h:106:PRO:HB2	8:h:109:GLN:HG2	1.96	0.48
10:j:98:VAL:HG12	10:j:100:ASP:HB2	1.95	0.48
2:B:183:THR:OG1	2:B:184:TYR:N	2.43	0.48
6:F:80:ILE:O	6:F:84:LYS:N	2.47	0.48
7:G:51:VAL:HG23	7:G:217:VAL:HG22	1.95	0.48
21:U:269:ARG:NH2	21:U:325:MET:SD	2.87	0.48
27:a:50:PHE:HD2	27:a:52:GLN:HB3	1.78	0.48
3:C:119:ASP:N	3:C:119:ASP:OD1	2.45	0.48
4:D:155:THR:H	4:D:158:GLN:HB2	1.77	0.48
4:D:203:LEU:HD11	4:D:330:LYS:HG3	1.96	0.48
6:F:169:ASP:HB2	6:F:172:VAL:HG23	1.95	0.48
9:I:118:LYS:NZ	9:I:151:ASP:O	2.47	0.48
10:J:122:ASN:ND2	11:K:132:ALA:O	2.47	0.48
21:U:545:LEU:HB3	21:U:577:ILE:HG21	1.96	0.48
21:U:751:ARG:NH2	21:U:907:SER:O	2.47	0.48
23:W:363:ILE:HD11	23:W:382:LEU:HD11	1.95	0.48
24:X:368:MET:HA	24:X:373:LYS:HD3	1.95	0.48
1:A:185:GLU:OE1	1:A:188:ARG:NH2	2.40	0.48
7:G:76:ILE:HG12	7:G:111:VAL:HG22	1.95	0.48
14:N:53:GLN:HE22	15:O:119:THR:H	1.60	0.48
14:N:120:MET:H	20:T:61:GLN:HE22	1.62	0.48
17:Q:18:ASP:OD1	17:Q:18:ASP:N	2.46	0.48
20:T:53:ALA:HB2	20:T:110:MET:HG3	1.95	0.48
21:U:376:MET:HA	21:U:740:GLY:H	1.79	0.48
24:X:401:LEU:HA	24:X:404:ILE:HD12	1.96	0.48
27:a:70:ARG:NH1	27:a:70:ARG:O	2.47	0.48
7:g:128:ASN:HB2	7:g:131:MET:HE1	1.96	0.48
10:j:65:LEU:HD22	10:j:88:ARG:HG3	1.96	0.48
15:o:44:CYS:HB2	15:o:99:VAL:HB	1.94	0.48
17:q:105:ALA:HB2	17:q:115:LEU:HD13	1.96	0.48
3:C:89:VAL:HB	3:C:92:GLU:HB3	1.94	0.48
3:C:191:PRO:HG2	3:C:319:PRO:HG3	1.94	0.48
5:E:23:ASP:OD2	5:E:27:LYS:NZ	2.45	0.48
5:E:171:LEU:HD22	5:E:295:LEU:HD13	1.94	0.48
7:G:164:LYS:N	8:H:56:LEU:O	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:43:HIS:CD2	12:L:216:GLY:HA3	2.49	0.48
12:L:157:ARG:NH2	13:M:60:GLU:OE1	2.46	0.48
18:R:178:HIS:HB3	18:R:185:ILE:HG13	1.95	0.48
21:U:770:TRP:O	29:c:177:THR:OG1	2.32	0.48
29:c:90:VAL:O	29:c:94:LYS:HB2	2.13	0.48
9:i:148:TYR:HE1	10:j:58:THR:HG21	1.78	0.48
11:k:99:HIS:CE1	11:k:107:MET:HB2	2.49	0.48
13:m:66:LEU:HD12	13:m:212:GLU:HG2	1.95	0.48
14:n:8:PHE:HE1	14:n:13:VAL:HG23	1.79	0.48
20:t:4:PRO:HB3	20:t:107:TRP:CD1	2.49	0.48
4:D:173:GLN:HE22	4:D:334:PRO:HD2	1.79	0.47
6:F:277:GLU:OE1	6:F:278:LYS:NZ	2.40	0.47
11:K:101:PHE:HB2	18:R:61:ARG:HD2	1.96	0.47
19:S:58:HIS:HB3	20:T:130:VAL:HG22	1.95	0.47
19:S:177:ASP:OD2	15:o:200:GLY:N	2.46	0.47
21:U:191:LYS:HA	21:U:194:ARG:HB3	1.95	0.47
23:W:405:LYS:HD2	24:X:343:SER:HB3	1.96	0.47
24:X:187:ARG:HH21	24:X:217:ILE:HG22	1.79	0.47
26:Z:94:TRP:HB3	26:Z:112:MET:HE3	1.96	0.47
27:a:99:LYS:O	27:a:103:LYS:HB3	2.14	0.47
28:b:30:GLN:HG3	28:b:75:LEU:HD13	1.95	0.47
29:c:79:GLY:HA2	29:c:84:VAL:HA	1.94	0.47
4:D:409:LYS:NZ	4:D:410:ASP:O	2.41	0.47
5:E:97:ARG:NH2	5:E:112:PRO:O	2.41	0.47
7:G:127:GLN:HG3	8:H:128:ARG:H	1.78	0.47
10:J:130:SER:OG	10:J:147:THR:O	2.29	0.47
12:L:50:LYS:HB2	12:L:209:ASN:HA	1.95	0.47
1:A:390:THR:HA	2:B:216:ILE:HD11	1.95	0.47
4:D:95:ALA:HA	4:D:101:ALA:HA	1.97	0.47
5:E:47:LEU:HD22	6:F:79:LYS:HD2	1.96	0.47
5:E:173:TYR:O	5:E:300:HIS:ND1	2.44	0.47
5:E:348:THR:HA	6:F:217:ILE:HD11	1.94	0.47
6:F:151:VAL:HA	6:F:164:LEU:H	1.78	0.47
6:F:417:HIS:CE1	6:F:421:MET:HE3	2.49	0.47
12:L:6:TYR:O	12:L:20:HIS:ND1	2.48	0.47
28:b:25:ARG:NH1	28:b:114:GLY:O	2.47	0.47
29:c:32:TYR:HB2	29:c:68:ARG:HA	1.95	0.47
7:g:88:ARG:NH2	13:m:113:ASP:OD1	2.47	0.47
10:j:36:ARG:NH2	10:j:156:TRP:O	2.47	0.47
10:j:41:VAL:HG21	10:j:134:VAL:HB	1.96	0.47
14:n:20:THR:HG22	14:n:27:ALA:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:ASP:OD1	2:B:118:ASP:N	2.41	0.47
2:B:388:ASP:OD1	2:B:388:ASP:N	2.47	0.47
10:J:63:CYS:HB3	10:J:88:ARG:HH22	1.80	0.47
19:S:125:ASP:OD1	19:S:129:SER:N	2.47	0.47
32:f:318:THR:O	32:f:322:SER:N	2.45	0.47
1:A:394:MET:HA	1:A:397:ILE:HD12	1.96	0.47
4:D:57:GLN:HE21	21:U:636:VAL:HG12	1.78	0.47
18:R:18:SER:OG	18:R:173:ALA:N	2.47	0.47
20:T:166:ARG:NH1	20:T:200:GLU:OE1	2.46	0.47
27:a:243:GLY:HA2	27:a:275:LEU:HG	1.96	0.47
32:f:473:ASN:HA	32:f:478:ARG:HH21	1.79	0.47
1:A:325:ASP:OD1	1:A:325:ASP:N	2.47	0.47
3:C:57:ARG:NH2	21:U:643:SER:O	2.46	0.47
4:D:88:VAL:HG23	4:D:132:LEU:HB2	1.95	0.47
4:D:126:PRO:HB3	29:c:277:LYS:HZ1	1.80	0.47
5:E:232:MET:HG3	5:E:235:ILE:HD12	1.97	0.47
6:F:407:ALA:HB1	6:F:412:ALA:HB3	1.97	0.47
17:Q:44:LEU:HD11	17:Q:102:LEU:HD12	1.96	0.47
21:U:45:ILE:HG23	21:U:60:ALA:HB1	1.97	0.47
22:V:276:PHE:HZ	22:V:284:GLU:HG3	1.80	0.47
25:Y:66:ASP:HB3	25:Y:69:LEU:HB3	1.96	0.47
27:a:156:TYR:HE2	27:a:196:ARG:HH21	1.63	0.47
32:f:807:ARG:HA	32:f:811:LEU:HD12	1.97	0.47
4:D:296:MET:HE1	4:D:326:ARG:HA	1.97	0.47
8:H:219:ARG:NH1	8:H:220:ARG:O	2.47	0.47
9:I:161:ALA:HB1	9:I:175:LEU:HD13	1.97	0.47
10:J:189:LYS:HA	10:J:232:ILE:HD11	1.96	0.47
13:M:137:LEU:N	13:M:149:TYR:O	2.41	0.47
14:N:153:LEU:HD22	14:N:176:LEU:HD13	1.97	0.47
19:S:145:LEU:HD22	19:S:178:VAL:HB	1.95	0.47
19:S:193:LEU:N	19:S:208:VAL:O	2.48	0.47
23:W:219:THR:HA	23:W:222:LEU:HD13	1.96	0.47
25:Y:41:LEU:HD12	25:Y:44:ALA:HB3	1.96	0.47
26:Z:29:VAL:HG12	26:Z:31:ASN:H	1.80	0.47
30:d:203:PRO:HD2	30:d:206:MET:SD	2.55	0.47
10:j:146:GLN:OE1	10:j:156:TRP:NE1	2.47	0.47
11:k:199:LEU:HA	11:k:202:LEU:HG	1.96	0.47
12:l:66:VAL:HG11	12:l:88:MET:HE1	1.95	0.47
1:A:274:PHE:N	1:A:318:LEU:O	2.38	0.47
3:C:43:ARG:HH12	22:V:495:ARG:HH22	1.63	0.47
4:D:114:ARG:HH22	4:D:136:SER:HG	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:277:MET:HE1	5:E:279:THR:HB	1.97	0.47
12:L:202:GLU:OE2	12:L:203:GLN:NE2	2.43	0.47
13:M:79:GLY:HA3	13:M:133:CYS:HA	1.97	0.47
18:R:5:ALA:HB2	18:R:14:VAL:HG13	1.97	0.47
21:U:153:ILE:HA	21:U:156:GLU:HB2	1.97	0.47
22:V:417:ILE:HB	22:V:458:VAL:HB	1.96	0.47
26:Z:144:VAL:HG22	26:Z:151:THR:HA	1.96	0.47
26:Z:148:GLY:HA2	27:a:178:ARG:HA	1.96	0.47
27:a:214:GLY:HA2	27:a:217:LEU:HD13	1.95	0.47
29:c:104:ARG:NH1	29:c:106:GLU:HB2	2.30	0.47
29:c:198:ARG:O	29:c:200:TYR:N	2.48	0.47
11:k:129:ASP:N	11:k:129:ASP:OD1	2.46	0.47
11:k:186:HIS:H	11:k:189:MET:HE2	1.79	0.47
12:l:88:MET:HB2	12:l:108:LEU:HD11	1.97	0.47
12:l:218:ASP:OD1	12:l:218:ASP:N	2.47	0.47
6:F:120:LYS:H	6:F:120:LYS:HG2	1.43	0.47
7:G:127:GLN:HA	8:H:128:ARG:HG2	1.96	0.47
12:L:101:ARG:HH22	12:L:103:LEU:HD12	1.80	0.47
17:Q:37:LYS:HA	17:Q:43:LEU:HD23	1.97	0.47
13:m:163:CYS:SG	13:m:164:ALA:N	2.87	0.47
1:A:238:ILE:HB	1:A:272:ILE:HG13	1.97	0.47
10:J:39:ASP:N	10:J:39:ASP:OD1	2.48	0.47
11:K:107:MET:N	11:K:107:MET:SD	2.88	0.47
11:K:117:SER:HB3	11:K:156:MET:HE1	1.95	0.47
21:U:895:PRO:HG2	21:U:902:PRO:HD3	1.97	0.47
22:V:212:TYR:HD1	22:V:253:LEU:HD21	1.80	0.47
25:Y:233:ARG:NH2	25:Y:264:TYR:O	2.47	0.47
32:f:196:MET:HG3	32:f:201:GLU:HG3	1.96	0.47
15:o:201:ARG:HH12	15:o:203:ARG:HE	1.63	0.47
20:t:180:ASP:HB3	20:t:183:SER:HB3	1.97	0.47
2:B:387:LYS:HB3	2:B:390:LEU:HB3	1.97	0.46
12:L:12:VAL:HG13	13:M:22:GLN:HE22	1.80	0.46
21:U:86:ASP:N	21:U:86:ASP:OD1	2.47	0.46
22:V:461:LYS:HA	22:V:461:LYS:HD2	1.76	0.46
27:a:374:ILE:HG23	30:d:255:MET:HE1	1.96	0.46
7:g:132:ARG:HB2	13:m:12:SER:HA	1.97	0.46
10:j:212:ARG:HB2	10:j:215:GLN:HB2	1.98	0.46
12:l:132:LEU:HB2	12:l:134:ILE:HD11	1.97	0.46
15:o:219:LEU:N	16:p:193:ASP:O	2.40	0.46
33:x:63:LYS:HE2	33:x:63:LYS:HB3	1.54	0.46
1:A:143:ASP:HB3	1:A:150:HIS:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:ALA:HA	2:B:405:MET:SD	2.55	0.46
5:E:175:PRO:HD2	5:E:178:THR:HG21	1.96	0.46
8:H:17:GLY:HA2	9:I:23:TYR:HB3	1.98	0.46
11:K:240:ASP:N	11:K:240:ASP:OD1	2.48	0.46
20:T:15:LYS:HG2	20:T:20:VAL:HG22	1.96	0.46
23:W:198:ASP:O	23:W:202:THR:OG1	2.23	0.46
25:Y:90:ASP:HA	25:Y:93:LYS:HD2	1.97	0.46
25:Y:314:LEU:HD21	25:Y:319:MET:HE3	1.97	0.46
30:d:139:LEU:HD11	30:d:151:VAL:HG13	1.96	0.46
11:k:93:ARG:NH1	18:r:68:LEU:O	2.48	0.46
7:G:93:ARG:HH21	7:G:121:ILE:HD12	1.79	0.46
27:a:137:ASP:HA	27:a:140:GLU:HB2	1.97	0.46
27:a:168:ASN:ND2	27:a:171:SER:OG	2.47	0.46
11:k:157:ASP:OD1	11:k:161:THR:N	2.48	0.46
16:p:14:MET:HG3	16:p:163:LEU:HD11	1.97	0.46
33:x:73:LEU:HD23	33:x:73:LEU:N	2.18	0.46
4:D:175:GLN:HG2	4:D:178:ARG:HH11	1.79	0.46
35:E:401:ATP:O2G	6:F:347:ARG:NH1	2.38	0.46
15:O:129:SER:OG	15:O:166:ASP:OD2	2.33	0.46
21:U:324:LYS:HA	21:U:327:LYS:HE3	1.97	0.46
21:U:327:LYS:HA	21:U:333:MET:HE1	1.97	0.46
21:U:611:ASN:HB3	21:U:614:VAL:HG12	1.97	0.46
24:X:240:ASP:OD1	24:X:278:ARG:NH2	2.49	0.46
32:f:320:ILE:HA	32:f:325:GLN:HE22	1.81	0.46
32:f:658:ALA:HB2	32:f:693:ALA:HB1	1.97	0.46
17:q:14:LEU:HA	17:q:182:ILE:HG12	1.97	0.46
20:t:97:TYR:O	20:t:101:SER:OG	2.27	0.46
33:x:62:GLN:OE1	33:x:62:GLN:N	2.32	0.46
1:A:424:SER:O	1:A:426:THR:HG22	2.15	0.46
8:H:50:LYS:HB3	8:H:64:LYS:HD3	1.98	0.46
11:K:157:ASP:OD2	11:K:159:SER:OG	2.31	0.46
13:M:34:SER:HA	13:M:167:LYS:HE2	1.97	0.46
20:T:188:GLN:HG2	20:T:201:GLY:HA3	1.97	0.46
22:V:461:LYS:HG3	22:V:463:MET:HE1	1.97	0.46
32:f:478:ARG:HD2	32:f:514:VAL:HG11	1.98	0.46
2:B:153:ASN:HA	2:B:160:ILE:HD11	1.98	0.46
3:C:178:LEU:HD23	3:C:180:ILE:HD13	1.98	0.46
19:S:26:ASP:OD1	19:S:26:ASP:N	2.43	0.46
21:U:742:HIS:CD2	21:U:814:PRO:HG3	2.51	0.46
23:W:125:ILE:HG23	23:W:129:ARG:HH21	1.80	0.46
24:X:205:LYS:O	24:X:209:THR:OG1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:255:LEU:HD12	24:X:287:LEU:HD13	1.98	0.46
25:Y:19:ILE:HG23	25:Y:41:LEU:HD11	1.98	0.46
11:k:177:ALA:HB2	11:k:205:VAL:HG11	1.98	0.46
16:p:48:ARG:HB3	16:p:112:LEU:HB2	1.97	0.46
6:F:112:ASP:HA	6:F:116:GLN:HG2	1.98	0.46
6:F:305:GLU:HA	6:F:308:ARG:HD3	1.97	0.46
14:N:104:ASP:OD1	14:N:110:GLN:NE2	2.42	0.46
16:P:120:PHE:HE2	16:P:122:CYS:HB3	1.80	0.46
20:T:96:MET:HE1	20:T:106:LEU:HD12	1.98	0.46
20:T:189:ILE:O	20:T:200:GLU:N	2.43	0.46
21:U:172:ASP:OD1	21:U:172:ASP:N	2.48	0.46
25:Y:387:ILE:HG23	26:Z:279:LYS:HD2	1.98	0.46
26:Z:126:VAL:HB	29:c:212:LEU:HD11	1.98	0.46
28:b:126:LYS:HA	28:b:129:LYS:HG2	1.98	0.46
30:d:44:THR:O	30:d:47:GLN:NE2	2.48	0.46
8:h:11:THR:HG22	8:h:19:LEU:HD12	1.98	0.46
13:m:79:GLY:HA3	13:m:133:CYS:HA	1.97	0.46
3:C:66:LEU:O	4:D:114:ARG:NH2	2.41	0.46
6:F:362:ARG:NE	6:F:388:THR:O	2.49	0.46
13:M:237:LYS:HA	13:M:240:LYS:HE3	1.96	0.46
28:b:51:LEU:HD11	28:b:61:LEU:HB2	1.98	0.46
29:c:63:ASP:O	29:c:139:ARG:NH1	2.49	0.46
32:f:343:LYS:NZ	32:f:381:VAL:O	2.48	0.46
1:A:63:THR:OG1	32:f:680:ARG:NH1	2.48	0.46
5:E:306:GLU:HA	5:E:309:ARG:HE	1.81	0.46
7:G:40:VAL:HA	7:G:167:ALA:HA	1.98	0.46
9:I:33:THR:OG1	9:I:166:ASN:O	2.32	0.46
16:P:49:LEU:HA	16:P:111:GLY:HA3	1.97	0.46
22:V:461:LYS:NZ	22:V:462:GLU:O	2.48	0.46
32:f:66:LYS:HE3	32:f:66:LYS:HB2	1.41	0.46
16:p:74:TYR:HH	16:p:80:ARG:HH21	1.63	0.46
33:x:38:PRO:O	33:x:40:GLN:N	2.48	0.46
1:A:222:LYS:HA	1:A:343:PHE:HE2	1.81	0.46
2:B:417:GLU:HA	2:B:420:LYS:HB2	1.98	0.46
5:E:37:THR:HG23	6:F:69:MET:HE2	1.98	0.46
5:E:304:PRO:HB2	5:E:309:ARG:HG2	1.98	0.46
12:L:45:VAL:HG12	12:L:214:ILE:HG12	1.97	0.46
22:V:98:LEU:HD13	22:V:209:LYS:HE2	1.97	0.46
29:c:89:PRO:HA	29:c:92:GLN:HG2	1.98	0.46
13:m:110:HIS:CE1	13:m:114:ARG:HH11	2.34	0.46
15:o:206:LYS:HA	15:o:206:LYS:HD2	1.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:211:ARG:NH2	19:s:213:ASP:OD2	2.48	0.46
35:D:501:ATP:H5'1	5:E:291:ARG:HH12	1.81	0.45
9:I:37:ILE:HG23	9:I:179:TYR:HE1	1.80	0.45
20:T:9:THR:O	20:T:41:ARG:NH1	2.47	0.45
28:b:16:MET:HE3	28:b:25:ARG:HB3	1.98	0.45
30:d:78:LEU:HD13	30:d:98:LEU:HD21	1.98	0.45
32:f:271:MET:HE1	32:f:788:MET:H	1.81	0.45
7:g:82:GLY:HA3	7:g:136:CYS:HA	1.99	0.45
7:g:86:ASP:OD1	13:m:120:HIS:NE2	2.40	0.45
2:B:306:GLN:HA	2:B:309:MET:HE3	1.98	0.45
3:C:134:LEU:O	3:C:137:LEU:N	2.49	0.45
3:C:299:ASP:OD1	3:C:299:ASP:N	2.41	0.45
5:E:146:ARG:HA	5:E:149:ILE:HG12	1.98	0.45
11:K:56:SER:HB3	11:K:59:MET:HG2	1.98	0.45
11:K:93:ARG:HD3	18:R:68:LEU:HB3	1.97	0.45
20:T:8:GLY:O	20:T:54:SER:OG	2.34	0.45
21:U:203:LYS:HA	21:U:206:MET:HE3	1.98	0.45
23:W:129:ARG:NH1	23:W:146:THR:OG1	2.49	0.45
24:X:297:ARG:NH1	24:X:333:GLN:O	2.47	0.45
26:Z:45:LYS:HE3	26:Z:47:VAL:HG12	1.98	0.45
29:c:133:PHE:CZ	33:u:73:LEU:HD13	2.51	0.45
32:f:63:LEU:HD21	32:f:75:LEU:HG	1.98	0.45
32:f:93:PRO:HG2	32:f:96:LEU:HB2	1.98	0.45
8:h:106:PRO:HA	8:h:140:ASN:HD21	1.81	0.45
15:o:210:ALA:O	16:p:198:ARG:NH2	2.43	0.45
17:q:31:ASP:OD1	17:q:31:ASP:N	2.49	0.45
33:y:8:LEU:CD2	33:y:69:LEU:O	2.65	0.45
1:A:222:LYS:NZ	1:A:321:THR:O	2.36	0.45
3:C:20:LEU:HD13	21:U:101:ILE:HD12	1.98	0.45
4:D:92:PHE:HA	4:D:103:VAL:HG12	1.97	0.45
4:D:141:ASP:N	4:D:141:ASP:OD1	2.50	0.45
5:E:254:GLN:O	5:E:258:MET:HG2	2.17	0.45
7:G:24:GLN:HE22	13:M:13:THR:HG23	1.81	0.45
13:M:40:ARG:HA	13:M:45:VAL:HA	1.97	0.45
15:O:217:THR:HB	16:P:195:ILE:HB	1.98	0.45
17:Q:7:ILE:O	17:Q:14:LEU:N	2.44	0.45
19:S:11:THR:HG21	19:S:141:ALA:HB3	1.98	0.45
20:T:152:GLU:O	20:T:156:LYS:NZ	2.48	0.45
21:U:376:MET:HA	21:U:739:ALA:HA	1.99	0.45
27:a:70:ARG:HA	27:a:70:ARG:HD2	1.83	0.45
32:f:694:LEU:HA	32:f:697:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:13:ILE:HG13	7:g:15:ILE:HG12	1.98	0.45
2:B:114:GLU:OE2	2:B:122:ILE:N	2.50	0.45
3:C:76:VAL:HG22	3:C:87:VAL:HG22	1.98	0.45
4:D:315:ASP:OD1	4:D:315:ASP:N	2.49	0.45
7:G:115:CYS:HA	7:G:118:ILE:HG22	1.97	0.45
10:J:90:GLU:HG3	10:J:110:TYR:CZ	2.52	0.45
18:R:4:LEU:HA	18:R:100:MET:HE1	1.98	0.45
27:a:33:LEU:HA	28:b:18:ASN:HB2	1.98	0.45
27:a:324:ILE:HG13	27:a:331:VAL:HG13	1.97	0.45
28:b:184:ILE:HA	28:b:187:PRO:HD2	1.99	0.45
32:f:120:ARG:CZ	32:f:146:GLY:HA2	2.47	0.45
14:n:174:ILE:HD12	14:n:194:ILE:HG12	1.99	0.45
18:r:18:SER:OG	18:r:173:ALA:N	2.49	0.45
4:D:150:SER:OG	4:D:228:ILE:HG23	2.16	0.45
6:F:101:PRO:HA	6:F:115:SER:HB2	1.98	0.45
8:H:150:ASP:OD2	8:H:152:SER:OG	2.33	0.45
29:c:124:GLY:HA2	29:c:127:ILE:HG22	1.99	0.45
32:f:192:VAL:HG13	32:f:204:ALA:HB1	1.99	0.45
10:j:14:GLY:HA3	11:k:30:ALA:HB2	1.97	0.45
11:k:235:GLU:HA	11:k:238:ILE:HG22	1.98	0.45
12:l:50:LYS:HB3	12:l:59:HIS:HB3	1.98	0.45
33:u:36:ILE:HB	33:u:41:GLN:HE21	1.82	0.45
33:x:55:THR:OG1	33:y:73:LEU:HD13	2.17	0.45
33:x:57:SER:OG	33:y:73:LEU:CA	2.53	0.45
2:B:196:GLU:OE1	2:B:349:ARG:NH1	2.49	0.45
8:H:34:PRO:O	8:H:48:THR:OG1	2.32	0.45
10:J:52:LYS:HG3	10:J:53:LEU:HD12	1.99	0.45
11:K:111:SER:OG	19:S:79:ASN:ND2	2.48	0.45
19:S:114:ASP:OD1	19:S:118:LYS:N	2.49	0.45
29:c:285:GLU:OE1	29:c:285:GLU:N	2.49	0.45
8:h:13:PHE:HE2	9:i:129:PRO:HD2	1.82	0.45
14:n:21:THR:HG22	14:n:26:ILE:HA	1.97	0.45
17:q:11:ASP:N	17:q:11:ASP:OD1	2.49	0.45
33:x:19:PRO:HG3	33:y:75:GLY:N	2.31	0.45
33:y:17:VAL:HG21	33:y:56:LEU:CD1	2.47	0.45
1:A:306:LEU:O	1:A:312:ARG:NH1	2.48	0.45
7:G:10:ASP:OD1	7:G:10:ASP:N	2.50	0.45
7:G:46:ASP:OD1	7:G:46:ASP:N	2.48	0.45
11:K:217:LEU:HB3	11:K:234:LEU:HD11	1.99	0.45
16:P:2:SER:N	16:P:5:SER:OG	2.49	0.45
17:Q:166:GLU:HB2	18:r:141:ARG:HH21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:173:LEU:HD23	17:q:173:LEU:HD23	1.99	0.45
23:W:285:ASP:HB3	23:W:289:ARG:HH22	1.81	0.45
17:q:47:VAL:HG23	17:q:101:ASN:HB2	1.98	0.45
19:s:95:ILE:O	19:s:98:SER:OG	2.30	0.45
19:s:193:LEU:HB3	19:s:208:VAL:HB	1.99	0.45
33:y:48:LYS:CG	33:y:49:GLN:N	2.47	0.45
1:A:85:GLN:O	1:A:89:SER:OG	2.28	0.45
1:A:307:ASP:HB2	1:A:336:ARG:NH2	2.32	0.45
2:B:120:HIS:HA	2:B:134:SER:HA	1.98	0.45
3:C:336:MET:N	3:C:336:MET:SD	2.90	0.45
6:F:114:ASP:OD1	6:F:114:ASP:N	2.46	0.45
7:G:127:GLN:NE2	8:H:128:ARG:O	2.50	0.45
10:J:185:ASP:OD1	10:J:185:ASP:N	2.48	0.45
24:X:11:ARG:NH1	24:X:14:SER:OG	2.49	0.45
16:p:12:MET:HE2	16:p:14:MET:HE2	1.97	0.45
1:A:141:GLY:N	1:A:151:ILE:O	2.47	0.45
2:B:231:GLY:N	35:B:501:ATP:O2B	2.49	0.45
2:B:358:GLU:HA	2:B:361:LYS:HD3	1.98	0.45
4:D:226:ALA:HB3	4:D:260:ALA:HA	1.99	0.45
8:H:3:GLU:OE2	12:L:122:ARG:NH1	2.49	0.45
20:T:12:LEU:HB2	20:T:23:ALA:HB3	1.99	0.45
20:T:124:TYR:HB2	20:T:137:LEU:HD13	1.99	0.45
21:U:259:GLN:HA	21:U:262:SER:HB2	1.99	0.45
22:V:192:MET:HE3	22:V:196:SER:HB3	1.98	0.45
25:Y:349:LYS:HD2	25:Y:349:LYS:HA	1.74	0.45
27:a:61:GLU:HG3	27:a:79:ILE:HD13	1.98	0.45
8:h:148:GLN:NE2	8:h:149:SER:O	2.50	0.45
11:k:79:SER:HB3	11:k:140:ALA:HB3	1.99	0.45
33:y:70:VAL:C	33:y:71:LEU:HD12	2.42	0.45
3:C:72:TYR:N	3:C:116:LEU:O	2.50	0.45
15:O:11:GLY:HA2	15:O:108:PRO:HB3	2.00	0.45
21:U:408:LEU:HD23	21:U:423:MET:HE1	1.98	0.45
21:U:725:MET:HA	21:U:728:PHE:HB3	1.99	0.45
24:X:126:ARG:NH2	24:X:130:GLU:OE2	2.50	0.45
25:Y:228:MET:HE1	25:Y:236:LEU:HD21	1.98	0.45
28:b:72:LEU:HA	28:b:75:LEU:HD12	1.99	0.45
16:p:113:ASP:HB2	16:p:118:LYS:HG2	1.98	0.45
18:r:35:ILE:HD12	18:r:43:GLY:HA3	1.99	0.45
1:A:84:LYS:O	1:A:88:GLN:N	2.51	0.44
1:A:426:THR:H	1:A:427:PRO:HD2	1.80	0.44
2:B:222:VAL:O	2:B:329:MET:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:147:GLU:HG3	5:E:151:LEU:HD12	2.00	0.44
6:F:230:GLY:HA3	6:F:392:ASN:ND2	2.31	0.44
9:I:195:LYS:HG2	9:I:199:LYS:HZ2	1.81	0.44
10:J:148:ASP:OD1	10:J:152:THR:N	2.48	0.44
15:O:43:CYS:SG	15:O:44:CYS:N	2.90	0.44
18:R:59:LEU:HD22	18:R:83:LEU:HD22	1.98	0.44
21:U:14:GLU:HG2	30:d:73:ARG:HH11	1.81	0.44
21:U:554:LEU:HD11	21:U:761:VAL:HG13	1.97	0.44
26:Z:11:VAL:HA	26:Z:50:VAL:HB	1.97	0.44
26:Z:81:MET:HE1	29:c:98:MET:HE1	1.99	0.44
29:c:163:ILE:HG22	29:c:199:HIS:C	2.42	0.44
31:e:49:GLU:HG3	31:e:51:ASP:H	1.81	0.44
32:f:324:VAL:HG13	32:f:422:VAL:HG11	1.99	0.44
9:i:14:PRO:HA	10:j:21:TYR:CZ	2.52	0.44
3:C:133:PRO:O	3:C:134:LEU:C	2.60	0.44
4:D:354:LEU:O	4:D:355:SER:C	2.60	0.44
6:F:248:PHE:HD1	6:F:282:ILE:HG13	1.81	0.44
6:F:295:ARG:HG2	6:F:307:GLN:HG3	1.99	0.44
18:R:192:VAL:HG11	16:p:205:ASP:HB3	1.99	0.44
21:U:20:LYS:HD3	21:U:48:LEU:HD21	1.99	0.44
21:U:268:LEU:HD23	21:U:325:MET:HB3	1.98	0.44
24:X:330:LEU:HA	24:X:333:GLN:HB2	1.98	0.44
27:a:84:VAL:HA	27:a:87:MET:HG2	2.00	0.44
27:a:126:GLY:HA3	27:a:129:GLN:HE22	1.82	0.44
7:g:131:MET:N	7:g:131:MET:SD	2.91	0.44
33:y:38:PRO:O	33:y:39:ASP:C	2.61	0.44
1:A:321:THR:OG1	1:A:322:ASN:N	2.50	0.44
6:F:94:ILE:HD12	6:F:123:VAL:HG12	2.00	0.44
7:G:73:THR:HB	7:G:76:ILE:HB	2.00	0.44
10:J:211:MET:SD	10:J:217:LEU:HD13	2.57	0.44
15:O:63:LEU:HD11	15:O:79:ALA:HB2	1.98	0.44
24:X:134:VAL:HG21	24:X:149:LEU:HB2	1.98	0.44
24:X:410:VAL:HG12	29:c:256:ASN:HA	2.00	0.44
26:Z:10:VAL:N	26:Z:48:LEU:O	2.51	0.44
32:f:466:LEU:HB3	32:f:485:LEU:HD23	1.99	0.44
14:n:138:TYR:O	14:n:142:THR:OG1	2.26	0.44
20:t:210:ASP:OD1	20:t:210:ASP:N	2.50	0.44
33:x:25:ASN:O	33:x:28:ALA:HB3	2.17	0.44
6:F:288:LEU:O	6:F:292:GLY:N	2.50	0.44
11:K:93:ARG:O	11:K:96:THR:OG1	2.29	0.44
12:L:117:GLN:O	12:L:120:THR:OG1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:140:MET:SD	12:L:140:MET:N	2.90	0.44
16:P:54:ALA:O	16:P:106:GLU:N	2.46	0.44
18:R:21:THR:HA	18:R:27:ALA:H	1.81	0.44
21:U:740:GLY:HA3	21:U:744:VAL:HG22	1.99	0.44
22:V:212:TYR:HA	22:V:253:LEU:HD11	1.98	0.44
22:V:467:TYR:OH	26:Z:255:ASP:OD1	2.24	0.44
22:V:487:HIS:O	22:V:490:SER:OG	2.27	0.44
25:Y:47:ASP:N	25:Y:47:ASP:OD1	2.50	0.44
32:f:735:GLY:O	32:f:828:ARG:NH1	2.50	0.44
7:g:191:PHE:HE1	7:g:219:VAL:HG21	1.81	0.44
9:i:45:LEU:N	9:i:214:ALA:O	2.41	0.44
14:n:30:VAL:O	14:n:175:ARG:NH2	2.50	0.44
18:r:179:VAL:HA	18:r:184:TRP:HA	1.99	0.44
1:A:215:PHE:CD2	1:A:324:PRO:HG3	2.53	0.44
5:E:305:ASN:O	5:E:309:ARG:HG3	2.17	0.44
7:G:206:LEU:HB3	7:G:208:ILE:HG13	2.00	0.44
12:L:196:ARG:HA	12:L:199:LEU:HD13	1.99	0.44
20:T:13:GLY:HA2	20:T:22:ILE:HA	2.00	0.44
21:U:448:LEU:HA	21:U:483:LEU:HD23	2.00	0.44
23:W:395:ASN:HA	23:W:398:VAL:HG22	1.98	0.44
24:X:281:GLY:H	24:X:284:THR:HG22	1.82	0.44
25:Y:351:ASN:O	25:Y:353:ILE:HG13	2.18	0.44
29:c:113:HIS:NE2	29:c:126:ASP:OD2	2.50	0.44
32:f:783:SER:HB2	32:f:787:LEU:HD13	1.98	0.44
12:l:201:ALA:O	12:l:239:ARG:NH1	2.50	0.44
6:F:94:ILE:HD11	6:F:125:LYS:HB2	1.99	0.44
18:R:133:VAL:HG21	17:q:137:PHE:HB3	1.99	0.44
22:V:131:LEU:HD22	22:V:171:VAL:HG11	2.00	0.44
22:V:176:MET:HE1	22:V:217:VAL:HA	2.00	0.44
32:f:230:CYS:HA	32:f:233:LEU:HD12	1.98	0.44
19:s:92:LEU:HD23	19:s:124:PHE:CE2	2.53	0.44
1:A:356:LYS:O	1:A:360:ARG:HG2	2.17	0.44
2:B:288:ASP:OD1	2:B:288:ASP:N	2.50	0.44
3:C:81:ASP:OD1	3:C:81:ASP:N	2.48	0.44
5:E:95:GLY:O	5:E:113:ARG:NH1	2.39	0.44
5:E:116:ASP:O	5:E:118:LEU:N	2.51	0.44
19:S:151:ASN:OD1	16:p:173:ASN:ND2	2.50	0.44
23:W:52:LYS:HZ1	23:W:93:ARG:NH1	2.13	0.44
23:W:420:ASP:HB3	23:W:423:ASN:HB2	1.99	0.44
24:X:330:LEU:HD12	24:X:333:GLN:HB2	2.00	0.44
3:C:195:GLY:N	37:C:501:ADP:O2A	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:125:LYS:HA	6:F:131:THR:HA	2.00	0.44
14:N:83:PHE:CE2	14:N:98:ILE:HG21	2.53	0.44
19:S:57:PHE:HZ	20:T:128:LEU:HB3	1.81	0.44
26:Z:260:VAL:HG13	29:c:292:MET:HE1	1.99	0.44
30:d:61:TRP:HB3	30:d:65:ARG:HH21	1.83	0.44
32:f:438:ASP:N	32:f:438:ASP:OD1	2.48	0.44
32:f:482:ILE:HD12	32:f:518:THR:HG23	1.99	0.44
9:i:240:HIS:NE2	9:i:244:GLU:OE2	2.50	0.44
12:l:182:CYS:HB3	12:l:186:GLU:HB3	1.98	0.44
16:p:67:LEU:HD21	16:p:87:LEU:HD11	2.00	0.44
19:s:48:ASP:OD1	19:s:48:ASP:N	2.47	0.44
2:B:251:VAL:HG12	2:B:253:SER:H	1.83	0.44
3:C:195:GLY:HA2	3:C:198:LEU:HG	2.00	0.44
12:L:165:SER:OG	12:L:169:ARG:NH1	2.50	0.44
13:M:39:ILE:HD11	13:M:176:ILE:HG12	2.00	0.44
13:M:198:TYR:HE2	13:M:240:LYS:HB3	1.83	0.44
17:Q:92:LEU:HG	17:Q:93:ARG:HD2	1.98	0.44
23:W:315:MET:HE1	23:W:361:HIS:ND1	2.33	0.44
24:X:26:ILE:O	24:X:29:SER:OG	2.30	0.44
26:Z:101:LEU:HB3	26:Z:123:ILE:HD11	1.99	0.44
30:d:203:PRO:HG2	30:d:205:LYS:H	1.82	0.44
9:i:69:ASN:OD1	9:i:72:MET:N	2.49	0.44
33:y:50:LEU:CD2	33:y:59:TYR:CD2	3.00	0.44
33:y:67:LEU:N	33:y:67:LEU:HD12	2.33	0.44
4:D:210:CYS:N	35:D:501:ATP:O1B	2.51	0.43
18:R:127:SER:HB3	18:R:136:TYR:CE1	2.53	0.43
21:U:470:ASN:OD1	21:U:470:ASN:N	2.51	0.43
25:Y:141:VAL:HG11	25:Y:164:ALA:HB2	2.00	0.43
14:n:175:ARG:HG2	14:n:188:VAL:HG22	2.00	0.43
15:o:86:MET:HB2	15:o:89:ARG:HH21	1.82	0.43
15:o:187:ARG:HA	15:o:188:PRO:HA	1.85	0.43
16:p:115:LYS:HG3	16:p:116:THR:HG23	1.99	0.43
33:x:42:ARG:HB3	33:x:70:VAL:HB	1.99	0.43
1:A:177:VAL:HG22	1:A:224:LEU:HD23	2.01	0.43
1:A:300:LEU:HD22	6:F:254:PRO:HD3	2.01	0.43
2:B:67:ARG:HB3	32:f:670:MET:HE1	2.00	0.43
3:C:33:LEU:HA	3:C:36:ASN:HD22	1.83	0.43
7:G:67:THR:HG22	7:G:69:LEU:H	1.83	0.43
16:P:193:ASP:OD1	16:P:193:ASP:N	2.49	0.43
20:T:44:ARG:HG3	20:T:197:VAL:HB	2.00	0.43
23:W:247:TYR:HB3	23:W:270:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:34:ASN:O	28:b:38:HIS:ND1	2.33	0.43
28:b:157:VAL:HG21	28:b:170:LEU:HB2	1.99	0.43
32:f:62:ARG:NE	32:f:74:ALA:HB2	2.34	0.43
8:h:9:SER:HA	8:h:125:GLY:HA2	2.00	0.43
8:h:193:LEU:HD23	8:h:196:LYS:HD3	2.01	0.43
9:i:161:ALA:HB3	10:j:53:LEU:HD23	2.00	0.43
12:l:46:LEU:HD11	12:l:135:ALA:HB3	2.00	0.43
19:s:109:ILE:HG12	19:s:123:SER:HA	2.01	0.43
20:t:20:VAL:HG11	20:t:122:LEU:HD13	1.99	0.43
16:P:189:ILE:HB	16:P:196:THR:HB	2.01	0.43
17:Q:137:PHE:HB3	18:r:133:VAL:HG11	1.99	0.43
23:W:72:LYS:HD2	23:W:111:TYR:OH	2.18	0.43
10:j:122:ASN:HD21	11:k:134:SER:HB2	1.83	0.43
15:o:55:THR:O	15:o:59:ILE:HG12	2.19	0.43
4:D:270:ILE:HD12	4:D:288:ILE:HG21	1.99	0.43
15:O:198:ARG:HD3	15:O:202:TYR:HE2	1.84	0.43
16:P:88:MET:HE1	16:P:120:PHE:CE2	2.54	0.43
20:T:142:GLY:HA2	20:T:176:LEU:HD11	2.00	0.43
21:U:2:ILE:HD13	21:U:30:VAL:HG13	1.99	0.43
29:c:56:LEU:HA	29:c:111:TRP:HA	2.01	0.43
30:d:200:PHE:O	30:d:201:ASN:C	2.62	0.43
10:j:184:ASP:O	10:j:187:THR:OG1	2.29	0.43
16:p:53:LEU:HD22	16:p:60:VAL:HG13	2.00	0.43
1:A:189:GLU:O	1:A:193:THR:OG1	2.36	0.43
5:E:203:ILE:HG13	5:E:204:VAL:HG13	2.01	0.43
10:J:208:LEU:HB2	10:J:220:LEU:HB2	2.00	0.43
13:M:171:ALA:HA	13:M:174:THR:HG22	2.00	0.43
14:N:46:SER:OG	14:N:97:GLY:O	2.28	0.43
17:Q:17:SER:O	17:Q:179:SER:N	2.37	0.43
20:T:99:ARG:NE	20:T:104:ASN:O	2.43	0.43
22:V:82:LEU:HD23	22:V:94:VAL:HG22	2.00	0.43
7:g:123:GLN:O	7:g:126:THR:OG1	2.29	0.43
9:i:41:ASP:OD1	9:i:41:ASP:N	2.46	0.43
10:j:42:VAL:HG22	10:j:210:VAL:HG22	2.01	0.43
18:r:7:LYS:HG2	18:r:12:VAL:HB	2.00	0.43
19:s:6:VAL:HG12	19:s:57:PHE:HE1	1.83	0.43
33:y:45:PHE:O	33:y:46:ALA:C	2.61	0.43
2:B:76:GLU:HA	2:B:79:ILE:HG22	1.99	0.43
5:E:376:ASP:OD1	5:E:376:ASP:N	2.49	0.43
6:F:180:ARG:HH22	6:F:248:PHE:H	1.67	0.43
8:H:147:PHE:HA	8:H:157:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:160:ALA:O	10:J:169:ARG:NH2	2.52	0.43
21:U:333:MET:SD	21:U:333:MET:N	2.92	0.43
24:X:365:LEU:HA	24:X:368:MET:HG2	2.00	0.43
30:d:114:GLU:HA	30:d:117:THR:HG22	2.00	0.43
11:k:202:LEU:HD13	11:k:215:ILE:HG12	2.00	0.43
18:r:20:ALA:HB3	18:r:28:SER:H	1.83	0.43
20:t:97:TYR:HA	20:t:100:ARG:HG2	2.01	0.43
33:y:36:ILE:HA	33:y:37:PRO:HD2	1.90	0.43
1:A:143:ASP:OD1	1:A:143:ASP:N	2.52	0.43
2:B:223:ILE:HA	2:B:329:MET:HB3	1.99	0.43
3:C:332:HIS:HE1	3:C:364:THR:HG23	1.84	0.43
4:D:87:LEU:HD22	4:D:140:VAL:HG21	1.99	0.43
21:U:249:CYS:HB3	21:U:328:ILE:HB	2.01	0.43
25:Y:201:PHE:O	25:Y:205:VAL:N	2.50	0.43
26:Z:39:LEU:H	26:Z:94:TRP:HA	1.83	0.43
26:Z:62:ASP:N	26:Z:62:ASP:OD1	2.51	0.43
9:i:90:LEU:HD21	9:i:114:LEU:HD22	2.00	0.43
10:j:83:VAL:HG21	10:j:129:ILE:HD11	2.01	0.43
12:l:101:ARG:HH21	20:t:83:TYR:HE1	1.66	0.43
13:m:43:ASP:OD1	13:m:43:ASP:N	2.49	0.43
13:m:230:ASP:OD1	13:m:230:ASP:N	2.50	0.43
17:q:37:LYS:O	17:q:61:GLN:NE2	2.52	0.43
2:B:64:LYS:HG2	32:f:666:ILE:HD13	2.00	0.43
3:C:53:ASN:HD21	21:U:643:SER:HA	1.84	0.43
4:D:277:ALA:HB2	4:D:286:GLN:HE22	1.84	0.43
5:E:241:ARG:NH1	5:E:285:LEU:O	2.51	0.43
6:F:230:GLY:HA3	6:F:392:ASN:HD22	1.84	0.43
17:Q:104:LEU:HB2	17:Q:118:MET:HE1	2.01	0.43
19:S:45:LYS:HE3	19:S:203:ILE:HD12	2.00	0.43
21:U:24:LEU:HD23	21:U:27:LEU:HD11	2.00	0.43
21:U:261:LEU:HD23	21:U:329:LEU:HA	2.00	0.43
21:U:748:LEU:HD11	21:U:763:VAL:HG11	2.01	0.43
29:c:66:THR:O	29:c:139:ARG:NH1	2.49	0.43
30:d:114:GLU:O	30:d:118:GLU:HB2	2.19	0.43
32:f:907:ASP:OD1	32:f:907:ASP:N	2.52	0.43
8:h:39:LYS:HG3	8:h:144:PRO:HB2	2.00	0.43
8:h:100:VAL:HG12	16:p:90:MET:HE1	2.01	0.43
19:s:213:ASP:N	19:s:213:ASP:OD1	2.52	0.43
5:E:196:LEU:HD12	5:E:230:ILE:HG22	2.01	0.43
16:P:45:MET:HB2	16:P:49:LEU:HG	2.00	0.43
17:Q:18:ASP:HA	17:Q:178:PHE:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:120:ALA:HB1	19:S:122:TYR:HE1	1.83	0.43
22:V:159:LEU:HD23	22:V:159:LEU:HA	1.90	0.43
27:a:77:VAL:HA	27:a:80:ILE:HG22	2.01	0.43
28:b:21:PHE:HD2	28:b:25:ARG:HG2	1.83	0.43
2:B:199:GLU:O	2:B:211:TYR:OH	2.37	0.43
3:C:88:LYS:HA	3:C:94:LYS:HA	2.00	0.43
9:I:116:ASP:OD1	9:I:117:ILE:N	2.52	0.43
14:N:160:LEU:O	14:N:164:MET:HG2	2.18	0.43
23:W:202:THR:O	23:W:206:SER:HB3	2.19	0.43
24:X:56:LEU:HA	24:X:59:LYS:HG2	2.01	0.43
24:X:144:GLN:O	24:X:148:HIS:N	2.51	0.43
26:Z:226:ILE:HG22	26:Z:230:LEU:HB2	2.01	0.43
27:a:163:TYR:CG	27:a:172:TYR:HB2	2.54	0.43
29:c:248:MET:HA	29:c:251:LEU:HB2	2.00	0.43
7:g:10:ASP:OD1	7:g:10:ASP:N	2.51	0.43
13:m:100:SER:HA	20:t:65:GLN:NE2	2.32	0.43
16:p:49:LEU:HD21	16:p:87:LEU:HD22	2.01	0.43
16:p:91:VAL:HG12	16:p:124:LEU:HD22	2.00	0.43
3:C:327:ASP:N	3:C:327:ASP:OD1	2.52	0.42
5:E:200:SER:O	5:E:200:SER:OG	2.37	0.42
5:E:310:LEU:HD11	5:E:314:LYS:HE3	2.00	0.42
6:F:275:ALA:HB1	6:F:326:VAL:HG11	2.00	0.42
10:J:208:LEU:C	10:J:220:LEU:HG	2.44	0.42
14:N:134:TYR:HB3	14:n:136:TYR:HB2	2.00	0.42
16:P:13:ALA:HB3	16:P:137:VAL:HG23	2.01	0.42
24:X:171:LEU:HD11	24:X:210:LEU:HA	2.00	0.42
24:X:310:ARG:HD2	24:X:314:ARG:NE	2.28	0.42
26:Z:20:VAL:HA	26:Z:23:PHE:HD2	1.84	0.42
19:s:35:ILE:HB	20:t:151:ARG:HH12	1.83	0.42
33:u:22:THR:OG1	33:u:25:ASN:ND2	2.52	0.42
1:A:100:LYS:O	1:A:114:ASN:N	2.53	0.42
2:B:77:GLU:HB3	2:B:80:ARG:HH21	1.84	0.42
2:B:331:THR:OG1	2:B:332:ASN:N	2.51	0.42
4:D:349:THR:HB	4:D:354:LEU:HD11	2.01	0.42
9:I:195:LYS:HG2	9:I:199:LYS:NZ	2.34	0.42
10:J:108:THR:HG23	10:J:133:ILE:HD12	1.99	0.42
16:P:167:ILE:O	16:P:171:MET:HG2	2.19	0.42
21:U:338:HIS:CG	21:U:785:PRO:HG3	2.53	0.42
23:W:429:SER:HB2	29:c:231:LEU:HB2	2.01	0.42
30:d:141:GLN:HA	30:d:144:MET:HE3	2.00	0.42
19:s:57:PHE:HD2	19:s:60:ASP:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:x:9:THR:C	33:x:11:LYS:H	2.27	0.42
33:y:4:PHE:O	33:y:67:LEU:HD12	2.19	0.42
2:B:411:ARG:NH2	2:B:418:ASP:OD2	2.52	0.42
3:C:196:LYS:HA	3:C:317:PHE:HE2	1.84	0.42
6:F:96:LEU:HD21	6:F:120:LYS:HB3	2.02	0.42
13:M:15:SER:HB3	13:M:19:ARG:H	1.84	0.42
15:O:195:LYS:NZ	15:O:196:GLY:O	2.45	0.42
16:P:2:SER:N	16:P:5:SER:HG	2.17	0.42
25:Y:162:GLU:HA	25:Y:165:LYS:HG2	2.01	0.42
25:Y:263:LEU:HB2	25:Y:271:PHE:CE1	2.54	0.42
27:a:245:VAL:HG11	27:a:301:LYS:HD3	2.00	0.42
15:o:83:LEU:HD11	15:o:113:ILE:HG12	2.00	0.42
20:t:92:LEU:HB3	20:t:96:MET:HE2	2.01	0.42
1:A:279:ALA:HB2	2:B:310:LEU:HG	2.00	0.42
2:B:164:MET:SD	2:B:164:MET:N	2.89	0.42
2:B:191:ASP:H	2:B:194:ILE:HD12	1.85	0.42
3:C:49:ARG:NH1	21:U:639:LEU:O	2.53	0.42
5:E:232:MET:HB2	5:E:277:MET:HB3	2.01	0.42
16:P:145:GLN:HG3	19:s:147:PRO:HG2	2.00	0.42
21:U:571:CYS:HA	21:U:579:ARG:HG2	2.00	0.42
22:V:287:ARG:HG2	31:e:22:PHE:HE2	1.84	0.42
26:Z:170:VAL:HA	29:c:152:LYS:HD2	2.01	0.42
32:f:62:ARG:HD3	32:f:70:LEU:HG	2.01	0.42
8:h:50:LYS:HD3	8:h:64:LYS:HD3	2.02	0.42
8:h:99:LEU:O	8:h:102:GLN:NE2	2.52	0.42
12:l:6:TYR:OH	13:m:8:ASP:OD2	2.31	0.42
16:p:15:LYS:HE2	16:p:119:PRO:HB2	2.00	0.42
2:B:77:GLU:HA	2:B:80:ARG:HE	1.84	0.42
5:E:19:HIS:CE1	6:F:48:LEU:HD22	2.55	0.42
8:H:227:LYS:O	8:H:231:ALA:N	2.53	0.42
9:I:45:LEU:HD13	9:I:75:SER:HB2	2.02	0.42
14:N:107:GLU:HB3	14:N:110:GLN:NE2	2.34	0.42
17:Q:43:LEU:HD12	17:Q:183:ILE:HD11	2.02	0.42
20:T:92:LEU:HD12	20:T:112:ILE:HD11	2.01	0.42
21:U:167:ILE:O	21:U:171:ASN:ND2	2.42	0.42
25:Y:14:ASN:HA	25:Y:15:PRO:HA	1.93	0.42
27:a:129:GLN:HG2	27:a:130:VAL:HG13	2.01	0.42
32:f:56:LEU:HD11	32:f:99:LEU:HD21	2.01	0.42
32:f:803:PHE:CE1	32:f:810:ILE:HG13	2.54	0.42
16:p:205:ASP:OD1	16:p:205:ASP:N	2.46	0.42
1:A:166:VAL:HG11	1:A:237:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PHE:HD1	1:A:271:LEU:HD23	1.84	0.42
1:A:238:ILE:N	1:A:271:LEU:O	2.45	0.42
3:C:187:LEU:HD23	3:C:314:LYS:HG3	2.02	0.42
3:C:218:GLU:HG2	4:D:275:PHE:H	1.84	0.42
11:K:137:PHE:HB3	11:K:139:VAL:HG22	2.01	0.42
13:M:8:ASP:O	13:M:22:GLN:NE2	2.37	0.42
14:N:174:ILE:HB	14:N:189:LEU:HB2	2.00	0.42
18:R:140:ASP:OD1	17:q:169:LYS:NZ	2.43	0.42
22:V:175:MET:HE1	22:V:187:ILE:HD12	2.02	0.42
22:V:278:GLU:HA	22:V:285:TRP:HZ2	1.84	0.42
23:W:21:SER:HA	23:W:65:ARG:HH21	1.83	0.42
24:X:167:VAL:HG21	24:X:197:ALA:HB2	2.01	0.42
26:Z:12:HIS:ND1	26:Z:50:VAL:O	2.34	0.42
26:Z:25:ARG:HG3	29:c:104:ARG:HD2	2.00	0.42
28:b:100:ARG:NH1	28:b:105:HIS:O	2.52	0.42
29:c:251:LEU:HB3	29:c:284:LEU:HD12	2.00	0.42
7:g:226:LYS:HE2	7:g:226:LYS:HB2	1.91	0.42
8:h:64:LYS:HB2	8:h:76:TYR:HE1	1.84	0.42
9:i:213:ILE:HD12	9:i:233:VAL:HG22	2.02	0.42
33:x:60:ASN:HB3	33:y:8:LEU:HD12	1.73	0.42
2:B:387:LYS:HG3	2:B:389:ASP:H	1.84	0.42
3:C:168:PRO:HG3	3:C:175:PHE:CZ	2.55	0.42
16:P:27:ARG:NH1	16:P:179:ALA:O	2.52	0.42
16:P:126:LEU:HG	16:P:127:ILE:HG23	2.01	0.42
18:R:33:LYS:HG2	18:R:45:MET:HE3	2.02	0.42
22:V:412:LEU:O	25:Y:346:LYS:NZ	2.43	0.42
23:W:55:ARG:HD2	23:W:96:GLN:HA	2.02	0.42
23:W:344:THR:OG1	23:W:345:GLU:N	2.52	0.42
28:b:4:GLU:HA	28:b:106:LYS:N	2.35	0.42
29:c:58:LEU:HD23	29:c:104:ARG:HH22	1.85	0.42
29:c:73:PHE:HE2	29:c:95:MET:HE3	1.85	0.42
7:g:54:LYS:HE3	7:g:66:VAL:HG23	2.02	0.42
19:s:175:VAL:HA	19:s:178:VAL:HG22	2.02	0.42
20:t:105:PRO:HB2	20:t:127:MET:HE2	2.01	0.42
3:C:241:HIS:O	3:C:244:SER:OG	2.30	0.42
5:E:135:ILE:HD13	5:E:182:LEU:HD23	2.02	0.42
6:F:224:LEU:HD12	6:F:351:LYS:HG2	2.02	0.42
12:L:225:ASP:OD1	12:L:225:ASP:N	2.53	0.42
16:P:65:GLN:OE1	17:Q:86:ARG:NH2	2.53	0.42
16:P:159:ASP:HB3	16:P:162:HIS:HD2	1.84	0.42
19:S:57:PHE:CZ	20:T:128:LEU:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:128:GLN:HB3	21:U:131:GLU:HG2	2.02	0.42
21:U:374:SER:HB3	21:U:407:SER:HB3	2.02	0.42
21:U:580:ARG:HB3	21:U:614:VAL:HG23	2.01	0.42
27:a:293:PHE:HB2	27:a:307:VAL:HG21	2.01	0.42
7:g:69:LEU:HD13	7:g:227:PHE:HZ	1.84	0.42
8:h:50:LYS:HG2	8:h:64:LYS:NZ	2.33	0.42
8:h:130:PHE:HB3	8:h:132:VAL:HG22	2.01	0.42
9:i:206:LEU:HA	9:i:210:LYS:HD2	2.01	0.42
17:q:184:ASP:HB2	17:q:189:HIS:CE1	2.54	0.42
1:A:241:ILE:HA	1:A:275:ASP:HB3	2.02	0.42
2:B:196:GLU:CD	2:B:349:ARG:HH11	2.28	0.42
2:B:320:ASP:HB2	2:B:322:ARG:HH22	1.84	0.42
3:C:90:HIS:HB3	3:C:91:PRO:HD3	2.01	0.42
5:E:72:LYS:HA	5:E:78:ARG:HA	2.01	0.42
9:I:143:TYR:HB2	9:I:146:GLN:NE2	2.34	0.42
21:U:173:VAL:HG22	21:U:175:GLY:H	1.84	0.42
24:X:163:LYS:HZ2	24:X:200:ILE:HA	1.84	0.42
25:Y:301:ILE:HG13	25:Y:342:ARG:HD3	2.02	0.42
27:a:166:ILE:H	27:a:166:ILE:HD12	1.84	0.42
30:d:203:PRO:O	30:d:206:MET:HE1	2.20	0.42
32:f:282:PHE:HE2	32:f:311:VAL:HG21	1.83	0.42
10:j:5:ARG:O	10:j:123:GLY:N	2.53	0.42
13:m:113:ASP:OD2	13:m:114:ARG:NH2	2.52	0.42
15:o:18:THR:O	15:o:31:CYS:N	2.47	0.42
33:y:50:LEU:HD23	33:y:59:TYR:CE2	2.54	0.42
1:A:333:ARG:NH1	37:F:501:ADP:O3'	2.53	0.42
6:F:285:ILE:N	6:F:329:ILE:O	2.50	0.42
22:V:435:GLU:HA	22:V:438:VAL:HG22	2.01	0.42
22:V:495:ARG:H	26:Z:278:ASN:ND2	2.17	0.42
24:X:163:LYS:NZ	24:X:200:ILE:HA	2.33	0.42
29:c:196:LEU:C	29:c:198:ARG:N	2.78	0.42
30:d:104:LEU:HD12	30:d:104:LEU:HA	1.92	0.42
32:f:304:PHE:HA	32:f:321:MET:HE2	2.02	0.42
11:k:16:SER:OG	11:k:19:GLY:N	2.52	0.42
16:p:30:ILE:HD12	16:p:30:ILE:HG23	1.86	0.42
1:A:224:LEU:N	35:A:501:ATP:O2A	2.44	0.41
2:B:264:PRO:HG3	2:B:308:THR:HA	2.01	0.41
6:F:122:ALA:HB3	6:F:134:LEU:HD11	2.02	0.41
9:I:102:GLN:HE22	16:P:68:LYS:HE3	1.84	0.41
9:I:196:VAL:HA	9:I:199:LYS:HE2	2.02	0.41
11:K:35:SER:HB3	11:K:51:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:772:TRP:HB3	21:U:775:LEU:HB2	2.02	0.41
22:V:355:ARG:HD2	31:e:27:TRP:CD1	2.53	0.41
24:X:173:GLU:HA	24:X:176:THR:HG22	2.01	0.41
26:Z:237:LEU:HD12	29:c:310:LYS:HE2	2.01	0.41
2:B:247:PHE:HA	2:B:281:ILE:HB	2.02	0.41
11:K:141:LEU:H	11:K:156:MET:HB2	1.85	0.41
15:O:126:THR:O	15:O:127:MET:HE2	2.19	0.41
21:U:525:ASN:ND2	21:U:527:GLN:HE21	2.18	0.41
22:V:114:TYR:HD1	22:V:135:LEU:HD11	1.84	0.41
25:Y:22:LEU:HD11	25:Y:40:GLU:HG2	2.02	0.41
26:Z:275:LEU:HD23	26:Z:275:LEU:HA	1.85	0.41
27:a:346:ILE:HA	27:a:349:MET:SD	2.61	0.41
9:i:234:GLU:HA	9:i:237:ILE:HG12	2.02	0.41
17:q:88:LEU:HD12	17:q:88:LEU:HA	1.90	0.41
19:s:194:ARG:NH1	19:s:205:GLU:OE1	2.53	0.41
33:x:36:ILE:HD12	33:x:69:LEU:HD21	2.01	0.41
2:B:119:ASN:HA	2:B:141:LYS:HZ3	1.84	0.41
10:J:36:ARG:HH11	10:J:143:ARG:HA	1.85	0.41
11:K:85:ALA:O	11:K:89:ILE:HG12	2.21	0.41
19:S:11:THR:OG1	19:S:140:SER:OG	2.34	0.41
20:T:177:TYR:CZ	20:T:185:ASN:HB2	2.55	0.41
21:U:557:TYR:HB2	21:U:588:MET:HE2	2.02	0.41
21:U:748:LEU:HD21	21:U:763:VAL:HG11	2.02	0.41
23:W:406:VAL:HG23	24:X:342:PHE:HB3	2.02	0.41
29:c:63:ASP:N	29:c:63:ASP:OD1	2.54	0.41
30:d:190:LEU:HD22	30:d:192:THR:HG22	2.02	0.41
32:f:667:GLY:HA2	32:f:670:MET:HB2	2.02	0.41
10:j:222:PRO:HA	10:j:225:ILE:HG22	2.02	0.41
11:k:38:ILE:HB	11:k:49:ALA:HB3	2.01	0.41
12:l:147:THR:HG22	12:l:153:TYR:HB3	2.02	0.41
1:A:306:LEU:HB3	1:A:336:ARG:HG2	2.01	0.41
4:D:345:PHE:O	4:D:349:THR:OG1	2.28	0.41
5:E:161:ARG:NH2	23:W:139:GLU:OE2	2.53	0.41
5:E:364:GLN:HE22	5:E:368:MET:HE3	1.86	0.41
7:G:244:GLU:O	7:G:245:ARG:NE	2.51	0.41
12:L:43:HIS:CE1	12:L:217:LYS:HE2	2.56	0.41
13:M:230:ASP:OD1	13:M:230:ASP:N	2.53	0.41
15:O:42:TYR:HB2	15:O:178:ILE:HD11	2.01	0.41
18:R:20:ALA:HB3	18:R:31:VAL:HG21	2.01	0.41
18:R:38:ASN:OD1	18:R:41:LEU:N	2.53	0.41
18:R:81:LYS:HE2	18:R:120:ARG:HE	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:106:LEU:O	20:T:108:ASN:N	2.53	0.41
22:V:78:HIS:NE2	22:V:100:MET:SD	2.94	0.41
25:Y:79:ASP:HB3	25:Y:83:ARG:HH21	1.86	0.41
26:Z:58:PHE:HE1	26:Z:68:TRP:HB2	1.86	0.41
32:f:727:PHE:CE2	32:f:803:PHE:HE2	2.39	0.41
12:l:115:LYS:HE3	12:l:128:TYR:HE2	1.86	0.41
18:r:1:THR:HA	18:r:33:LYS:HZ3	1.85	0.41
18:r:139:MET:O	18:r:143:TYR:N	2.53	0.41
20:t:53:ALA:HA	20:t:110:MET:HA	2.01	0.41
20:t:193:THR:N	20:t:196:GLY:O	2.50	0.41
33:y:32:ASP:OD1	33:y:32:ASP:C	2.62	0.41
4:D:270:ILE:HG21	4:D:292:LEU:HD21	2.03	0.41
5:E:270:LEU:HD21	5:E:273:VAL:HB	2.01	0.41
6:F:283:ILE:HG23	6:F:328:VAL:HA	2.03	0.41
6:F:307:GLN:HA	6:F:310:MET:HG3	2.03	0.41
8:H:58:ASP:HB3	8:H:61:SER:HB2	2.02	0.41
13:M:40:ARG:HE	13:M:146:ALA:HB3	1.85	0.41
18:R:154:ASP:OD1	18:R:157:ARG:NH2	2.38	0.41
23:W:358:VAL:O	23:W:362:ASN:ND2	2.53	0.41
24:X:339:ILE:HA	24:X:342:PHE:CZ	2.54	0.41
24:X:344:ARG:HG3	24:X:386:ILE:HG12	2.01	0.41
25:Y:138:LEU:HD21	25:Y:167:LEU:HB2	2.02	0.41
26:Z:257:MET:HE1	29:c:296:ILE:HD13	2.03	0.41
29:c:88:ASP:N	29:c:88:ASP:OD1	2.53	0.41
7:g:119:ALA:HB1	8:h:84:ARG:HH22	1.85	0.41
8:h:52:GLN:HB3	8:h:57:TYR:HD2	1.86	0.41
19:s:193:LEU:N	19:s:208:VAL:O	2.53	0.41
2:B:389:ASP:OD1	2:B:389:ASP:N	2.53	0.41
4:D:179:GLU:HA	4:D:183:LEU:HB3	2.03	0.41
7:G:131:MET:HE3	13:M:124:LEU:HD13	2.01	0.41
8:H:35:SER:N	8:H:163:MET:O	2.49	0.41
10:J:208:LEU:HD23	10:J:208:LEU:HA	1.91	0.41
11:K:91:LYS:HA	11:K:94:VAL:HG12	2.02	0.41
13:M:30:VAL:HG21	13:M:153:PRO:HG2	2.02	0.41
20:T:50:MET:HE2	20:T:197:VAL:HG13	2.02	0.41
21:U:428:PRO:HA	21:U:439:GLU:HB2	2.02	0.41
27:a:120:ALA:HA	27:a:123:LEU:HD13	2.02	0.41
30:d:249:TYR:O	30:d:252:GLN:NE2	2.53	0.41
32:f:370:MET:HE1	32:f:759:LEU:HD23	2.02	0.41
32:f:472:HIS:CE1	32:f:477:MET:HG3	2.55	0.41
13:m:67:PHE:HB2	13:m:75:MET:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ILE:HD12	1:A:112:ILE:HG22	2.03	0.41
2:B:61:LYS:HA	2:B:64:LYS:HD2	2.02	0.41
5:E:241:ARG:HG3	5:E:287:PRO:HD3	2.02	0.41
5:E:309:ARG:HH21	5:E:332:VAL:HG22	1.85	0.41
7:G:17:SER:OG	7:G:21:ARG:N	2.48	0.41
13:M:77:VAL:HG11	13:M:84:ALA:HB1	2.03	0.41
15:O:79:ALA:HA	15:O:82:MET:HG2	2.02	0.41
21:U:35:TRP:O	21:U:39:SER:N	2.46	0.41
21:U:646:PRO:HG3	21:U:680:VAL:HG21	2.03	0.41
21:U:787:CYS:HA	21:U:884:VAL:HG12	2.01	0.41
23:W:137:TYR:HD1	23:W:138:VAL:HG13	1.85	0.41
23:W:272:LEU:HD23	23:W:272:LEU:HA	1.86	0.41
28:b:161:ASN:HD22	28:b:168:SER:HB2	1.86	0.41
30:d:175:ARG:HD3	30:d:178:ILE:HD12	2.03	0.41
32:f:695:ALA:HB2	32:f:728:ALA:HA	2.03	0.41
16:p:47:ASP:OD1	16:p:47:ASP:N	2.54	0.41
2:B:387:LYS:H	2:B:390:LEU:HD23	1.86	0.41
5:E:10:GLN:HA	5:E:13:ARG:HB2	2.02	0.41
14:N:162:LEU:HD11	14:n:141:ALA:HB2	2.03	0.41
16:P:145:GLN:HE22	19:s:143:ALA:HB1	1.86	0.41
18:R:58:LEU:HA	18:R:61:ARG:HG2	2.02	0.41
22:V:76:LYS:HB2	22:V:147:PHE:HZ	1.85	0.41
25:Y:134:LEU:HD11	25:Y:167:LEU:HB3	2.03	0.41
27:a:54:ASP:HA	27:a:57:ILE:HG22	2.02	0.41
31:e:47:ASN:OD1	31:e:47:ASN:N	2.53	0.41
32:f:111:GLU:HG2	32:f:112:ASN:H	1.85	0.41
16:p:28:PHE:HB2	16:p:39:PHE:HB2	2.02	0.41
17:q:13:VAL:HG13	17:q:113:PRO:HB2	2.03	0.41
18:r:1:THR:HG21	18:r:46:ALA:HA	2.01	0.41
1:A:181:LYS:HA	1:A:184:ILE:HD12	2.03	0.41
1:A:247:GLN:HG3	1:A:252:GLU:HB3	2.02	0.41
2:B:369:THR:HA	2:B:372:MET:HE2	2.03	0.41
3:C:147:THR:OG1	3:C:206:HIS:NE2	2.39	0.41
3:C:326:LEU:HD12	3:C:344:LEU:HG	2.03	0.41
4:D:99:ASN:ND2	4:D:117:SER:OG	2.53	0.41
4:D:204:MET:HB3	4:D:310:ALA:HA	2.02	0.41
4:D:337:ASP:OD1	4:D:337:ASP:N	2.43	0.41
5:E:139:SER:HA	5:E:142:ILE:HD12	2.02	0.41
6:F:96:LEU:CD2	6:F:120:LYS:HB3	2.51	0.41
6:F:209:LYS:HE2	6:F:209:LYS:HB2	1.88	0.41
6:F:303:ASP:N	6:F:303:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:83:LYS:NZ	16:P:85:TYR:HB3	2.36	0.41
21:U:162:VAL:HA	21:U:165:LYS:HE3	2.03	0.41
21:U:878:LEU:HD23	21:U:878:LEU:HA	1.97	0.41
22:V:386:PHE:HB2	22:V:392:TYR:HD1	1.86	0.41
24:X:335:LEU:HD22	24:X:339:ILE:HD11	2.03	0.41
25:Y:168:ILE:HD12	25:Y:180:LEU:HD22	2.03	0.41
25:Y:190:ALA:HA	25:Y:287:LEU:HD21	2.01	0.41
26:Z:82:PHE:HA	26:Z:85:VAL:HG12	2.02	0.41
27:a:123:LEU:HD21	27:a:161:LYS:HG3	2.01	0.41
28:b:14:GLU:OE2	28:b:83:LYS:NZ	2.44	0.41
29:c:162:LEU:HD12	29:c:199:HIS:O	2.21	0.41
30:d:152:PHE:HA	30:d:155:LYS:HB2	2.02	0.41
32:f:573:ILE:HG21	32:f:599:ALA:HB2	2.02	0.41
11:k:91:LYS:HE3	11:k:119:LEU:HD11	2.03	0.41
12:l:50:LYS:O	12:l:59:HIS:ND1	2.49	0.41
14:n:115:PRO:HD2	14:n:119:MET:HB3	2.02	0.41
15:o:30:ASN:OD1	15:o:187:ARG:NH2	2.54	0.41
15:o:41:ILE:HG12	15:o:102:GLY:HA3	2.03	0.41
18:r:50:ALA:HB2	19:s:129:SER:N	2.36	0.41
19:s:68:ILE:O	19:s:72:LEU:HG	2.20	0.41
33:x:19:PRO:CB	33:y:74:ARG:CA	2.99	0.41
33:x:21:ASP:OD1	33:x:21:ASP:N	2.54	0.41
33:x:51:GLU:HB2	33:x:54:ARG:NE	2.36	0.41
33:y:18:GLU:O	33:y:21:ASP:N	2.49	0.41
1:A:119:ALA:HB2	6:F:128:THR:HG23	2.02	0.41
1:A:258:ARG:NH2	1:A:301:GLU:OE1	2.54	0.41
3:C:99:VAL:HG12	3:C:123:LEU:HD22	2.01	0.41
9:I:72:MET:HA	9:I:72:MET:HE3	2.03	0.41
9:I:76:VAL:HG11	9:I:83:ALA:HB1	2.03	0.41
21:U:191:LYS:HD2	21:U:194:ARG:HB3	2.03	0.41
21:U:561:GLU:HG2	21:U:562:GLU:HG3	2.03	0.41
21:U:596:ASN:HA	21:U:599:ILE:HG22	2.03	0.41
22:V:91:PRO:HD2	22:V:92:ARG:NH1	2.36	0.41
22:V:289:LEU:HB3	22:V:312:ALA:HB2	2.02	0.41
23:W:41:GLN:HA	23:W:44:ILE:HB	2.02	0.41
27:a:311:VAL:HG21	27:a:324:ILE:HG12	2.02	0.41
30:d:188:LYS:HD3	30:d:224:SER:H	1.86	0.41
30:d:236:THR:O	30:d:239:SER:OG	2.27	0.41
11:k:157:ASP:OD1	11:k:157:ASP:N	2.54	0.41
13:m:161:TRP:CD2	13:m:182:LYS:HE2	2.56	0.41
16:p:74:TYR:HA	16:p:77:LYS:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ILE:HD12	1:A:134:ILE:HG23	1.86	0.40
6:F:27:ASP:OD1	6:F:28:GLY:N	2.54	0.40
11:K:164:GLN:NE2	11:K:166:ASP:OD1	2.53	0.40
11:K:202:LEU:HD23	11:K:202:LEU:HA	1.96	0.40
16:P:20:VAL:HG13	16:P:119:PRO:HB3	2.02	0.40
25:Y:136:HIS:HA	25:Y:139:ASP:HB2	2.03	0.40
27:a:84:VAL:HG21	27:a:121:LEU:HD21	2.02	0.40
27:a:245:VAL:HG12	27:a:247:ARG:HE	1.85	0.40
7:g:90:GLN:HE21	7:g:134:LEU:HD22	1.86	0.40
11:k:25:GLU:HA	11:k:28:ILE:HB	2.03	0.40
13:m:68:ASN:OD1	13:m:224:HIS:ND1	2.35	0.40
15:o:98:LEU:HB2	15:o:113:ILE:HB	2.04	0.40
18:r:135:ALA:O	18:r:139:MET:HG3	2.21	0.40
33:y:18:GLU:C	33:y:20:SER:N	2.78	0.40
3:C:161:ILE:HD12	3:C:161:ILE:HA	1.94	0.40
5:E:364:GLN:HA	5:E:367:PHE:HD2	1.87	0.40
6:F:93:VAL:O	6:F:148:GLY:N	2.37	0.40
6:F:164:LEU:HA	6:F:165:PRO:HD3	1.95	0.40
16:P:205:ASP:N	16:P:205:ASP:OD1	2.53	0.40
17:Q:143:LEU:O	17:Q:147:TYR:N	2.54	0.40
26:Z:28:LYS:HD2	26:Z:29:VAL:HG23	2.02	0.40
27:a:135:ILE:HG23	27:a:158:LEU:HD13	2.02	0.40
29:c:192:LEU:HA	29:c:195:GLY:O	2.21	0.40
32:f:386:GLY:HA2	32:f:418:LEU:HG	2.03	0.40
32:f:560:LEU:O	32:f:564:LEU:N	2.54	0.40
9:i:143:TYR:HB2	9:i:146:GLN:HE21	1.86	0.40
12:l:113:GLY:HA2	12:l:116:THR:HG22	2.03	0.40
14:n:119:MET:SD	20:t:61:GLN:NE2	2.94	0.40
33:y:18:GLU:O	33:y:20:SER:N	2.55	0.40
33:y:71:LEU:O	33:y:72:ARG:C	2.64	0.40
1:A:189:GLU:OE2	6:F:409:ARG:NH2	2.53	0.40
1:A:252:GLU:OE2	1:A:255:ARG:NH2	2.41	0.40
1:A:279:ALA:O	2:B:307:ARG:NE	2.55	0.40
1:A:312:ARG:HB2	1:A:315:ILE:HD12	2.03	0.40
2:B:150:VAL:HG12	2:B:162:VAL:HG23	2.03	0.40
2:B:252:GLY:HA2	2:B:255:LEU:HD23	2.03	0.40
4:D:401:LYS:O	4:D:405:THR:OG1	2.28	0.40
5:E:235:ILE:O	5:E:239:GLY:N	2.44	0.40
6:F:141:ASP:OD1	6:F:141:ASP:N	2.53	0.40
6:F:233:LYS:H	37:F:501:ADP:PA	2.45	0.40
12:L:155:ASP:HB3	13:M:62:SER:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:76:LYS:HE3	22:V:149:PRO:HB3	2.02	0.40
22:V:131:LEU:HD13	22:V:171:VAL:HG21	2.02	0.40
24:X:56:LEU:HA	24:X:56:LEU:HD23	1.95	0.40
25:Y:220:VAL:HG21	25:Y:249:VAL:HG21	2.03	0.40
26:Z:22:HIS:HA	26:Z:25:ARG:HB3	2.01	0.40
9:i:72:MET:HE1	9:i:136:TYR:HB3	2.03	0.40
1:A:103:ASN:HA	1:A:136:GLU:HB3	2.04	0.40
1:A:426:THR:N	1:A:427:PRO:CD	2.83	0.40
2:B:222:VAL:HB	2:B:328:ILE:HG22	2.03	0.40
4:D:120:ASP:OD1	4:D:120:ASP:N	2.52	0.40
5:E:342:ASP:OD1	5:E:342:ASP:N	2.53	0.40
9:I:89:GLU:HA	9:I:92:LEU:HD12	2.04	0.40
10:J:36:ARG:HA	10:J:41:VAL:HG12	2.03	0.40
12:L:22:ILE:HD12	12:L:22:ILE:HA	1.93	0.40
20:T:11:VAL:HG13	20:T:24:ALA:HB2	2.03	0.40
20:T:89:HIS:CE1	20:T:131:ALA:HB1	2.57	0.40
21:U:142:LEU:HD23	21:U:147:TYR:HE1	1.85	0.40
21:U:221:ILE:HD11	21:U:252:LEU:HD22	2.02	0.40
22:V:281:ASN:OD1	22:V:282:ASN:N	2.54	0.40
22:V:333:ILE:HG23	22:V:343:PRO:HG3	2.04	0.40
24:X:56:LEU:HA	24:X:59:LYS:HZ2	1.86	0.40
30:d:198:LEU:O	30:d:199:PHE:CB	2.69	0.40
32:f:75:LEU:HD23	32:f:75:LEU:HA	1.94	0.40
17:q:59:TYR:O	17:q:62:LYS:HG3	2.22	0.40
17:q:106:GLY:O	17:q:114:ALA:N	2.50	0.40
20:t:177:TYR:CZ	20:t:185:ASN:HB2	2.56	0.40
3:C:112:CYS:SG	3:C:113:ARG:N	2.95	0.40
5:E:172:LEU:HD23	5:E:299:ILE:HB	2.04	0.40
6:F:39:GLU:HB3	6:F:43:GLN:HB2	2.03	0.40
8:H:34:PRO:HA	8:H:164:GLY:HA3	2.03	0.40
9:I:67:LYS:O	9:I:91:ARG:NH2	2.54	0.40
13:M:120:HIS:O	13:M:123:THR:OG1	2.39	0.40
14:N:4:MET:HA	14:N:127:ILE:HA	2.03	0.40
18:R:144:SER:OG	18:R:145:TYR:N	2.54	0.40
19:S:30:SER:HA	19:S:36:HIS:H	1.86	0.40
21:U:19:LEU:HA	21:U:19:LEU:HD23	1.88	0.40
22:V:435:GLU:HG2	22:V:453:HIS:CD2	2.56	0.40
25:Y:128:TYR:CE1	25:Y:163:LYS:HD3	2.56	0.40
30:d:234:ASP:OD2	30:d:236:THR:OG1	2.26	0.40
31:e:16:ASP:N	31:e:16:ASP:OD1	2.54	0.40
7:g:200:THR:HA	7:g:203:SER:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:46:SER:OG	14:n:97:GLY:O	2.32	0.40
17:q:20:VAL:HG21	17:q:176:PRO:HD2	2.03	0.40
18:r:11:GLY:HA2	18:r:104:TRP:HZ3	1.87	0.40
18:r:182:ASP:OD1	18:r:182:ASP:N	2.53	0.40
19:s:26:ASP:OD1	19:s:26:ASP:N	2.50	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/433 (90%)	347 (88%)	43 (11%)	2 (0%)	24	63
2	B	382/440 (87%)	346 (91%)	36 (9%)	0	100	100
3	C	359/398 (90%)	333 (93%)	24 (7%)	2 (1%)	21	59
4	D	378/418 (90%)	338 (89%)	38 (10%)	2 (0%)	24	63
5	E	387/403 (96%)	351 (91%)	35 (9%)	1 (0%)	36	72
6	F	413/439 (94%)	376 (91%)	34 (8%)	3 (1%)	18	56
7	G	242/246 (98%)	230 (95%)	11 (4%)	1 (0%)	30	67
7	g	242/246 (98%)	223 (92%)	18 (7%)	1 (0%)	30	67
8	H	230/234 (98%)	222 (96%)	8 (4%)	0	100	100
8	h	230/234 (98%)	218 (95%)	12 (5%)	0	100	100
9	I	249/261 (95%)	241 (97%)	8 (3%)	0	100	100
9	i	248/261 (95%)	244 (98%)	4 (2%)	0	100	100
10	J	237/248 (96%)	224 (94%)	13 (6%)	0	100	100
10	j	237/248 (96%)	225 (95%)	12 (5%)	0	100	100
11	K	232/241 (96%)	218 (94%)	12 (5%)	2 (1%)	14	50
11	k	232/241 (96%)	225 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	236/263 (90%)	231 (98%)	5 (2%)	0	100	100
12	l	236/263 (90%)	226 (96%)	10 (4%)	0	100	100
13	M	238/255 (93%)	231 (97%)	7 (3%)	0	100	100
13	m	238/255 (93%)	232 (98%)	6 (2%)	0	100	100
14	N	200/239 (84%)	194 (97%)	6 (3%)	0	100	100
14	n	200/239 (84%)	192 (96%)	8 (4%)	0	100	100
15	O	218/277 (79%)	210 (96%)	8 (4%)	0	100	100
15	o	218/277 (79%)	212 (97%)	6 (3%)	0	100	100
16	P	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
16	p	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
17	Q	197/201 (98%)	189 (96%)	8 (4%)	0	100	100
17	q	197/201 (98%)	190 (96%)	7 (4%)	0	100	100
18	R	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
18	r	199/263 (76%)	192 (96%)	7 (4%)	0	100	100
19	S	211/241 (88%)	200 (95%)	11 (5%)	0	100	100
19	s	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
20	T	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
20	t	214/264 (81%)	201 (94%)	13 (6%)	0	100	100
21	U	812/953 (85%)	756 (93%)	56 (7%)	0	100	100
22	V	442/534 (83%)	428 (97%)	13 (3%)	1 (0%)	43	77
23	W	439/456 (96%)	430 (98%)	9 (2%)	0	100	100
24	X	420/422 (100%)	399 (95%)	21 (5%)	0	100	100
25	Y	387/389 (100%)	362 (94%)	24 (6%)	1 (0%)	36	72
26	Z	284/324 (88%)	254 (89%)	30 (11%)	0	100	100
27	a	371/376 (99%)	347 (94%)	24 (6%)	0	100	100
28	b	189/377 (50%)	172 (91%)	17 (9%)	0	100	100
29	c	285/310 (92%)	258 (90%)	25 (9%)	2 (1%)	18	56
30	d	255/350 (73%)	218 (86%)	33 (13%)	4 (2%)	7	37
31	e	48/70 (69%)	43 (90%)	5 (10%)	0	100	100
32	f	840/908 (92%)	804 (96%)	35 (4%)	1 (0%)	48	83
33	u	74/76 (97%)	70 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	x	74/76 (97%)	59 (80%)	12 (16%)	3 (4%)	2	17
33	y	74/76 (97%)	57 (77%)	15 (20%)	2 (3%)	4	25
34	v	1/10 (10%)	0	1 (100%)	0	100	100
All	All	13515/15114 (89%)	12708 (94%)	779 (6%)	28 (0%)	44	77

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	134	LEU
4	D	126	PRO
30	d	199	PHE
30	d	200	PHE
30	d	203	PRO
32	f	66	LYS
7	g	5	SER
1	A	428	ARG
5	E	386	TYR
6	F	104	GLN
6	F	119	GLY
33	x	39	ASP
33	y	74	ARG
6	F	120	LYS
11	K	130	PRO
22	V	496	PHE
33	x	61	ILE
3	C	133	PRO
4	D	355	SER
29	c	196	LEU
29	c	199	HIS
33	y	35	GLY
1	A	427	PRO
11	K	128	ALA
7	G	190	THR
30	d	202	THR
33	x	35	GLY
25	Y	350	VAL

### 5.3.2 Protein sidechains ⓘ

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



entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	337/372 (91%)	335 (99%)	2 (1%)	78	82
2	B	339/385 (88%)	338 (100%)	1 (0%)	86	85
3	C	314/346 (91%)	311 (99%)	3 (1%)	68	78
4	D	333/366 (91%)	329 (99%)	4 (1%)	63	75
5	E	341/353 (97%)	340 (100%)	1 (0%)	86	85
6	F	357/379 (94%)	354 (99%)	3 (1%)	73	80
7	G	205/210 (98%)	205 (100%)	0	100	100
7	g	202/210 (96%)	201 (100%)	1 (0%)	81	83
8	H	188/191 (98%)	188 (100%)	0	100	100
8	h	188/191 (98%)	186 (99%)	2 (1%)	65	76
9	I	207/221 (94%)	207 (100%)	0	100	100
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	201/211 (95%)	201 (100%)	0	100	100
10	j	196/211 (93%)	196 (100%)	0	100	100
11	K	193/203 (95%)	193 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/224 (90%)	202 (100%)	0	100	100
12	l	201/224 (90%)	201 (100%)	0	100	100
13	M	196/212 (92%)	196 (100%)	0	100	100
13	m	198/212 (93%)	198 (100%)	0	100	100
14	N	157/181 (87%)	157 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	179/228 (78%)	179 (100%)	0	100	100
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	172 (100%)	0	100	100
16	p	173/174 (99%)	173 (100%)	0	100	100
17	Q	168/171 (98%)	168 (100%)	0	100	100
17	q	168/171 (98%)	168 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	r	156/202 (77%)	156 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	178/199 (89%)	178 (100%)	0	100	100
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	179 (100%)	0	100	100
21	U	696/816 (85%)	696 (100%)	0	100	100
22	V	390/460 (85%)	390 (100%)	0	100	100
23	W	406/416 (98%)	405 (100%)	1 (0%)	87	86
24	X	362/362 (100%)	362 (100%)	0	100	100
25	Y	344/344 (100%)	342 (99%)	2 (1%)	78	82
26	Z	257/295 (87%)	257 (100%)	0	100	100
27	a	333/336 (99%)	333 (100%)	0	100	100
28	b	167/312 (54%)	167 (100%)	0	100	100
29	c	252/268 (94%)	247 (98%)	5 (2%)	48	66
30	d	231/294 (79%)	230 (100%)	1 (0%)	84	84
31	e	44/63 (70%)	44 (100%)	0	100	100
32	f	711/763 (93%)	709 (100%)	2 (0%)	86	85
33	u	68/68 (100%)	67 (98%)	1 (2%)	57	72
33	x	68/68 (100%)	59 (87%)	9 (13%)	4	15
33	y	68/68 (100%)	63 (93%)	5 (7%)	13	33
34	v	1/1 (100%)	1 (100%)	0	100	100
All	All	11573/12819 (90%)	11530 (100%)	43 (0%)	81	84

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	403	ILE
1	A	426	THR
2	B	125	THR
3	C	109	THR
3	C	132	ASP
3	C	210	THR
4	D	124	LEU
4	D	125	LYS
4	D	149	SER

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Mol	Chain	Res	Type
4	D	151	ILE
5	E	385	ASP
6	F	103	ASP
6	F	104	GLN
6	F	120	LYS
23	W	455	LEU
25	Y	207	THR
25	Y	349	LYS
29	c	107	MET
29	c	108	VAL
29	c	196	LEU
29	c	197	ASN
29	c	198	ARG
30	d	204	LYS
32	f	66	LYS
32	f	67	ASP
7	g	5	SER
8	h	3	GLU
8	h	4	ARG
33	u	63	LYS
33	x	20	SER
33	x	52	ASP
33	x	54	ARG
33	x	60	ASN
33	x	63	LYS
33	x	71	LEU
33	x	72	ARG
33	x	73	LEU
33	x	74	ARG
33	y	8	LEU
33	y	52	ASP
33	y	54	ARG
33	y	72	ARG
33	y	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	183	GLN
1	A	293	ASN
2	B	57	GLN

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Mol	Chain	Res	Type
3	C	53	ASN
3	C	90	HIS
3	C	171	HIS
3	C	343	ASN
3	C	380	GLN
4	D	49	GLN
4	D	57	GLN
4	D	91	GLN
4	D	99	ASN
4	D	110	ASN
4	D	135	HIS
4	D	286	GLN
4	D	340	GLN
5	E	51	GLN
5	E	75	ASN
5	E	86	GLN
5	E	155	ASN
5	E	263	GLN
5	E	339	ASN
6	F	83	ASN
6	F	208	HIS
6	F	243	GLN
6	F	255	GLN
6	F	258	GLN
6	F	321	GLN
6	F	325	GLN
7	G	24	GLN
7	G	150	GLN
8	H	189	HIS
9	I	95	GLN
10	J	146	GLN
10	J	154	HIS
10	J	221	ASN
11	K	97	GLN
12	L	5	GLN
12	L	8	ASN
12	L	86	ASN
13	M	180	GLN
13	M	221	ASN
14	N	158	ASN
15	O	91	GLN
16	P	33	GLN

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Mol	Chain	Res	Type
17	Q	27	GLN
17	Q	63	ASN
17	Q	168	GLN
18	R	85	ASN
18	R	89	GLN
19	S	79	ASN
19	S	80	ASN
19	S	151	ASN
21	U	111	GLN
21	U	218	GLN
21	U	258	GLN
21	U	267	ASN
21	U	362	ASN
21	U	421	GLN
21	U	491	GLN
21	U	525	ASN
21	U	595	ASN
21	U	718	ASN
21	U	742	HIS
21	U	768	GLN
21	U	805	ASN
22	V	257	ASN
22	V	350	GLN
22	V	473	GLN
22	V	487	HIS
23	W	53	GLN
23	W	86	ASN
24	X	44	GLN
24	X	148	HIS
24	X	152	GLN
24	X	292	GLN
24	X	296	ASN
24	X	380	GLN
25	Y	136	HIS
25	Y	160	ASN
25	Y	365	GLN
25	Y	388	ASN
26	Z	31	ASN
26	Z	278	ASN
27	a	168	ASN
27	a	288	HIS
27	a	369	HIS

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Mol	Chain	Res	Type
29	c	199	HIS
29	c	214	GLN
32	f	238	ASN
32	f	323	ASN
32	f	472	HIS
32	f	614	HIS
32	f	855	GLN
7	g	68	HIS
9	i	102	GLN
10	j	23	GLN
10	j	92	GLN
10	j	122	ASN
10	j	154	HIS
10	j	175	ASN
12	l	60	GLN
12	l	203	GLN
13	m	32	ASN
14	n	7	GLN
15	o	35	HIS
15	o	62	ASN
15	o	91	GLN
15	o	116	HIS
15	o	153	ASN
16	p	173	ASN
16	p	188	HIS
17	q	61	GLN
17	q	82	ASN
17	q	189	HIS
18	r	162	GLN
19	s	152	GLN
20	t	65	GLN
33	u	25	ASN
33	u	41	GLN
33	y	25	ASN
33	y	31	GLN
33	y	68	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
35	ATP	A	501	36	29,33,33	0.31	0	44,52,52	0.50	1 (2%)
37	ADP	C	501	-	27,29,29	1.36	4 (14%)	42,45,45	2.05	9 (21%)
35	ATP	D	501	36	29,33,33	0.31	0	44,52,52	0.49	1 (2%)
35	ATP	E	401	36	29,33,33	0.29	0	44,52,52	0.45	1 (2%)
37	ADP	F	501	36	27,29,29	1.36	4 (14%)	42,45,45	1.94	10 (23%)
35	ATP	B	501	36	29,33,33	0.29	0	44,52,52	0.45	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	A	501	36	-	2/22/38/38	0/3/3/3
37	ADP	C	501	-	-	2/16/32/32	0/3/3/3
35	ATP	D	501	36	-	4/22/38/38	0/3/3/3
35	ATP	E	401	36	-	2/22/38/38	0/3/3/3
37	ADP	F	501	36	-	6/16/32/32	0/3/3/3
35	ATP	B	501	36	-	5/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C	501	ADP	C5-C4	4.56	1.47	1.39
37	F	501	ADP	C5-C4	4.54	1.47	1.39
37	F	501	ADP	C5-C6	2.63	1.48	1.41
37	C	501	ADP	C5-C6	2.54	1.48	1.41
37	C	501	ADP	C5-N7	-2.40	1.34	1.39
37	F	501	ADP	C8-N7	2.35	1.36	1.31
37	F	501	ADP	C5-N7	-2.29	1.34	1.39
37	C	501	ADP	C8-N7	2.18	1.35	1.31

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	501	ADP	C5-C4-N3	-6.73	117.97	126.75
37	F	501	ADP	C5-C4-N3	-6.25	118.59	126.75
37	C	501	ADP	N3-C4-N9	5.47	136.10	127.08
37	F	501	ADP	N3-C4-N9	4.86	135.09	127.08
37	C	501	ADP	C2-N3-C4	3.99	121.18	111.75
37	F	501	ADP	C2-N3-C4	3.75	120.60	111.75
37	C	501	ADP	PA-O3A-PB	-3.50	120.82	132.83
37	F	501	ADP	PA-O3A-PB	-3.38	121.24	132.83
37	F	501	ADP	C4-C5-N7	-3.29	106.62	110.62
37	C	501	ADP	N3-C2-N1	-3.03	123.86	128.60
37	C	501	ADP	C4-C5-N7	-3.01	106.95	110.62
37	F	501	ADP	N3-C2-N1	-2.95	123.99	128.60
37	C	501	ADP	C3'-C2'-C1'	2.90	106.94	101.43
37	F	501	ADP	C5-N7-C8	2.79	107.47	103.51
37	C	501	ADP	C5-N7-C8	2.56	107.14	103.51
37	F	501	ADP	C4-N9-C8	2.40	108.32	105.73
37	C	501	ADP	C4-N9-C8	2.35	108.27	105.73
37	F	501	ADP	C3'-C2'-C1'	2.10	105.42	101.43
37	F	501	ADP	C6-C5-N7	2.04	135.82	132.02
35	B	501	ATP	PB-O3B-PG	2.04	139.81	132.83
35	A	501	ATP	PB-O3B-PG	2.03	139.80	132.83
35	E	401	ATP	PB-O3B-PG	2.01	139.72	132.83
35	D	501	ATP	PB-O3B-PG	2.00	139.70	132.83

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	B	501	ATP	PB-O3B-PG-O3G

*Continued on next page...*



*Continued from previous page...*

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

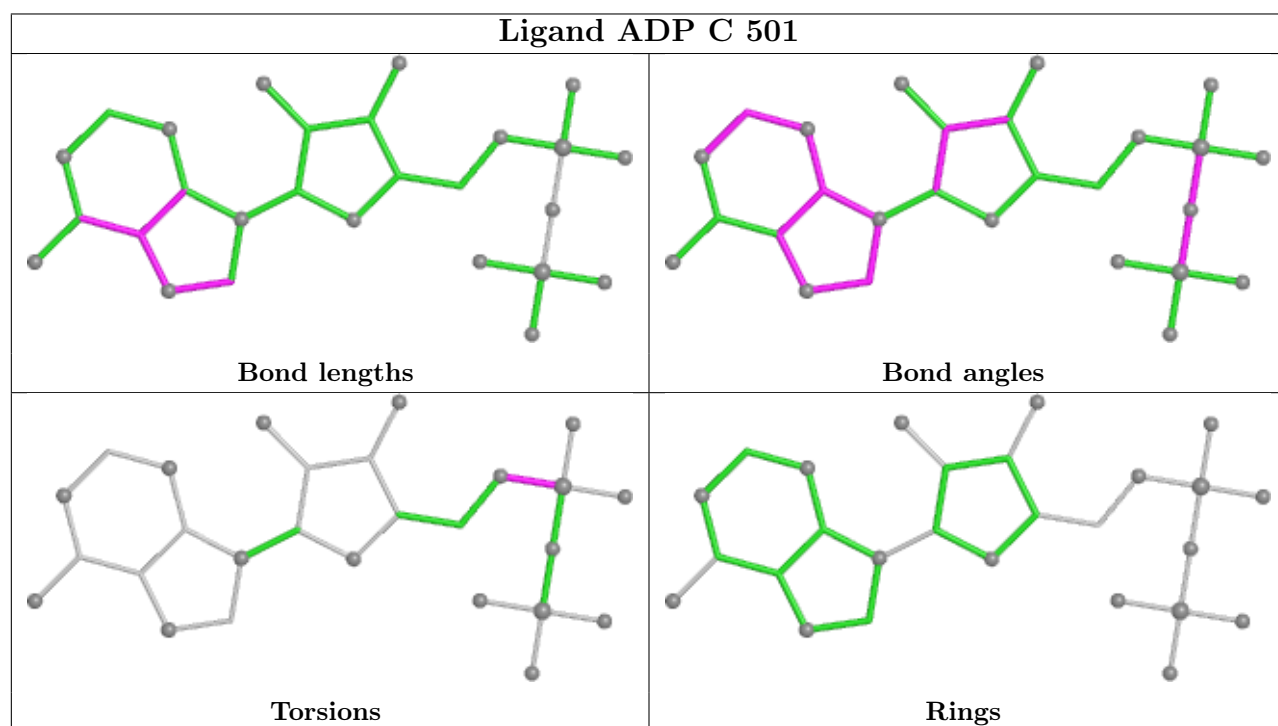
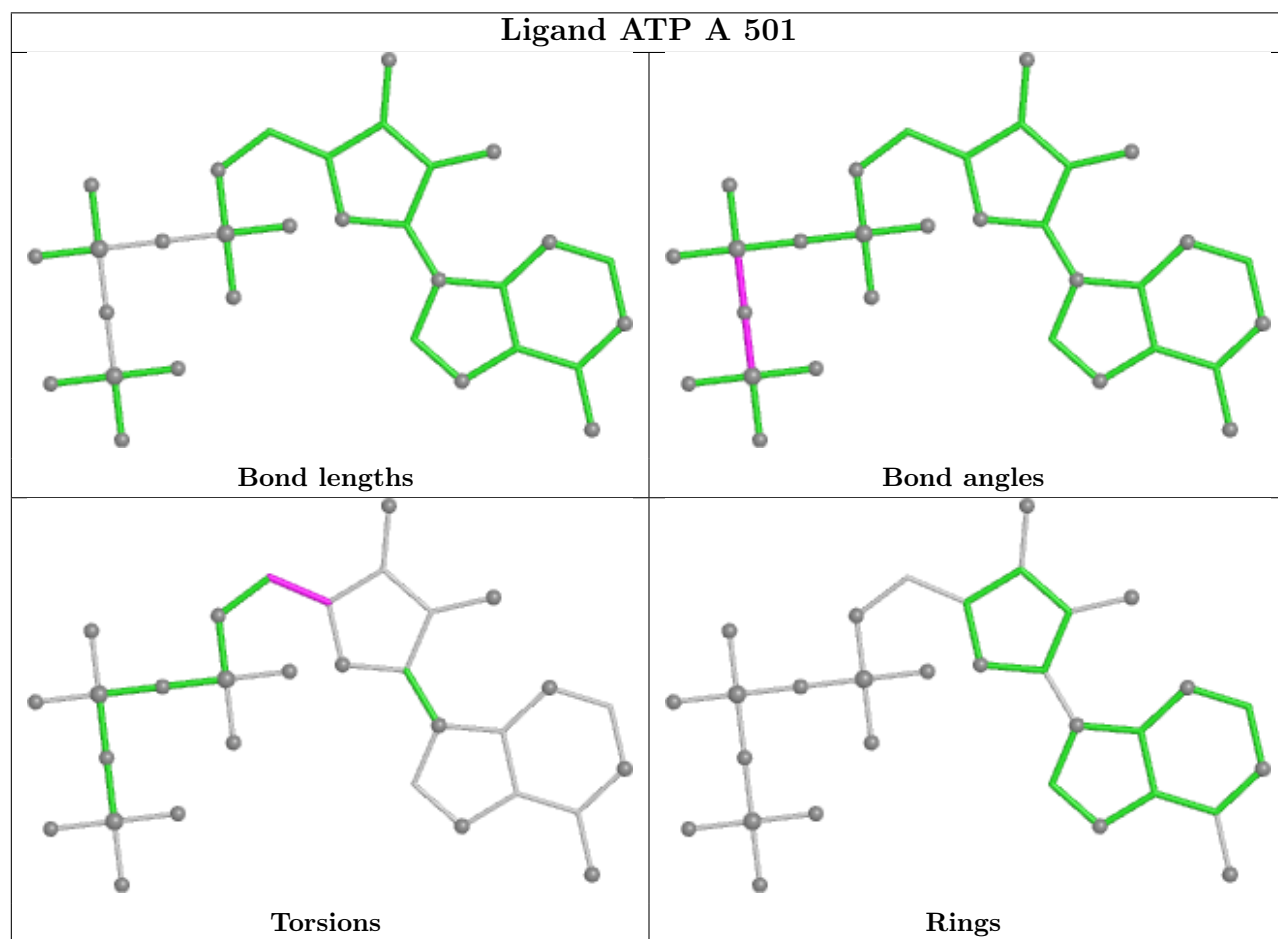
There are no ring outliers.

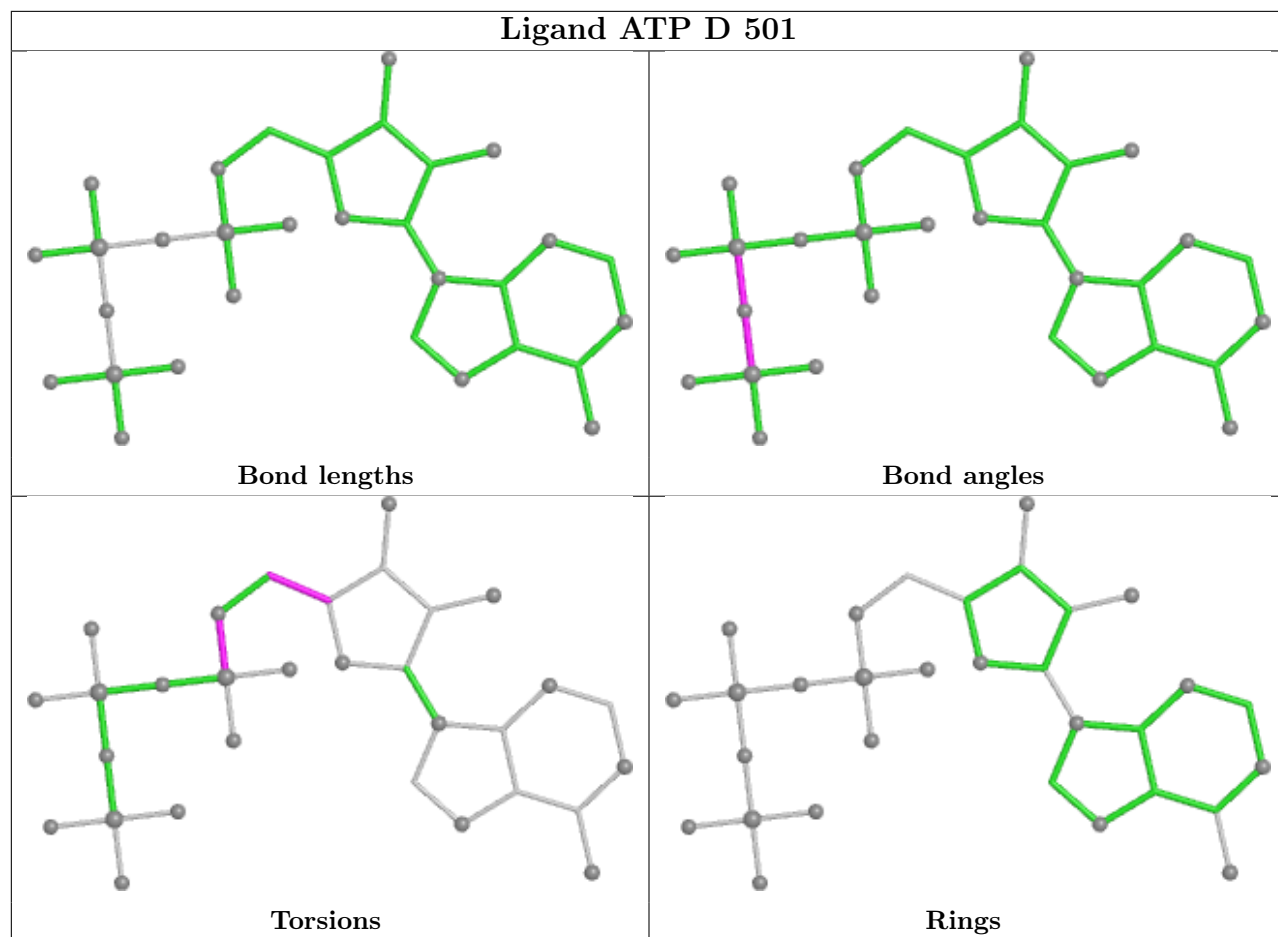
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	501	ATP	3	0
37	C	501	ADP	1	0
35	D	501	ATP	2	0
35	E	401	ATP	1	0
37	F	501	ADP	3	0
35	B	501	ATP	2	0

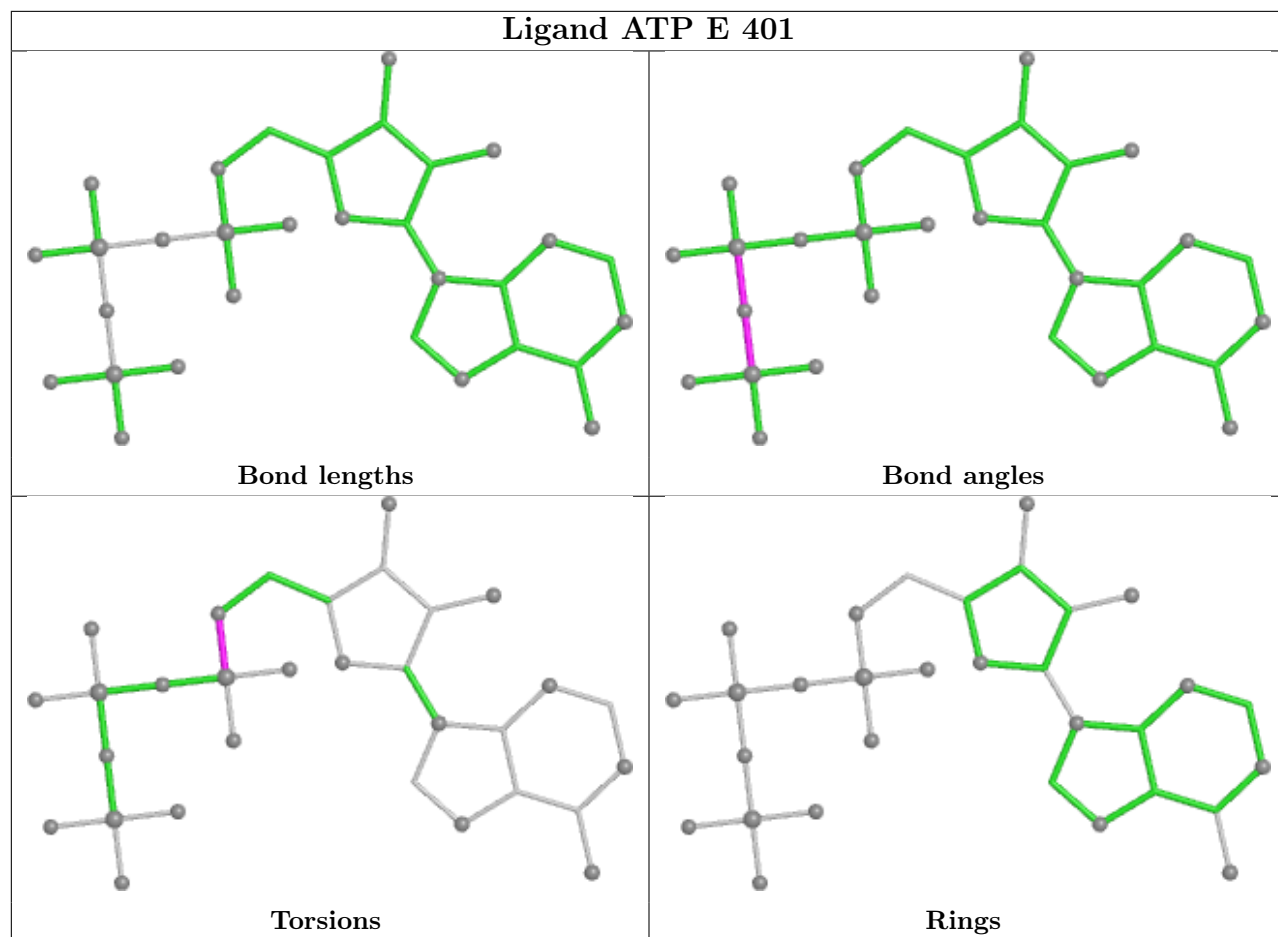
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

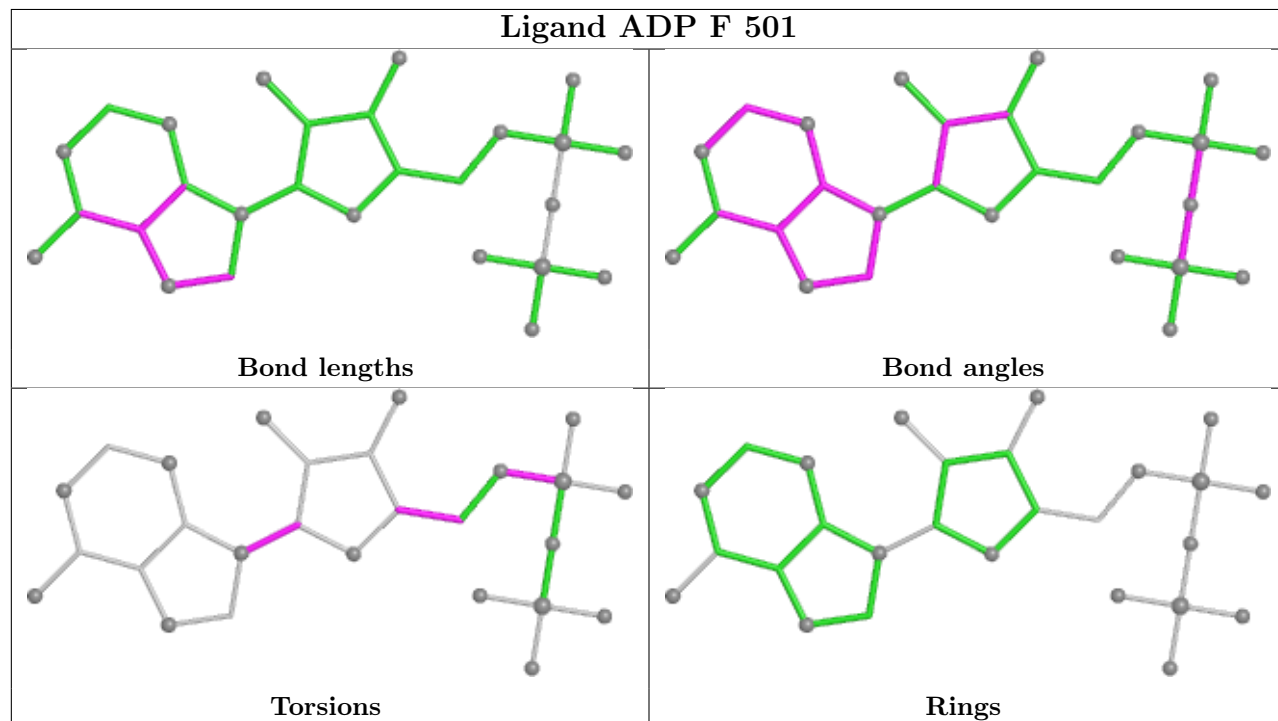


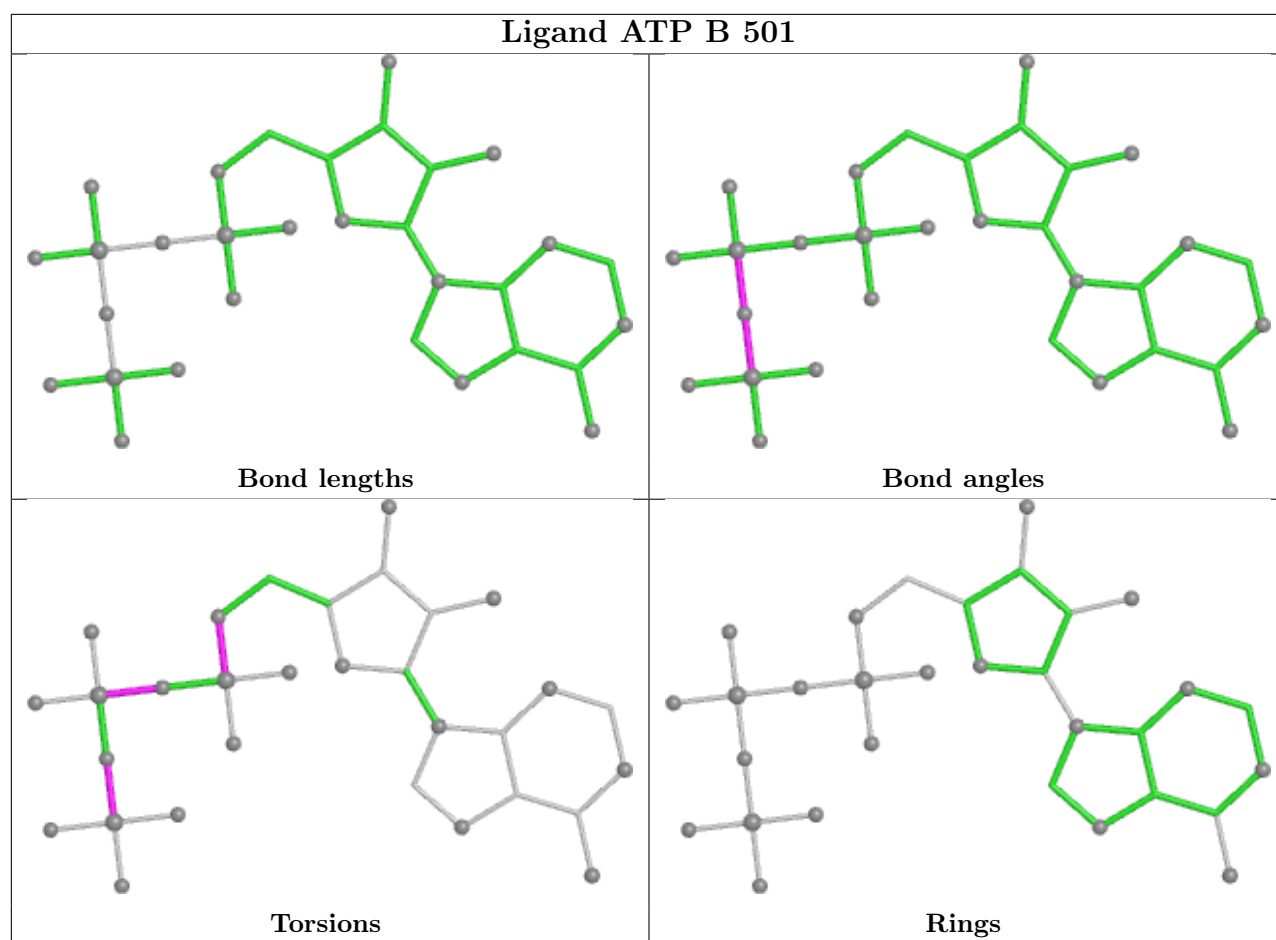


## Ligand ATP E 401



## Ligand ADP F 501





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

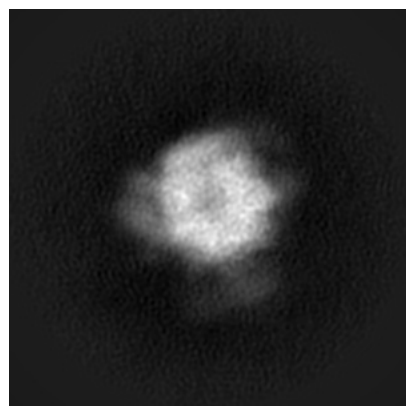
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62065. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

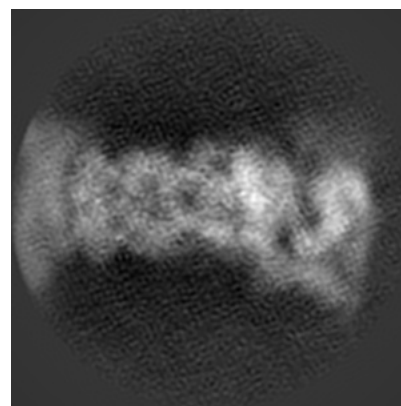
#### 6.1.1 Primary map



X

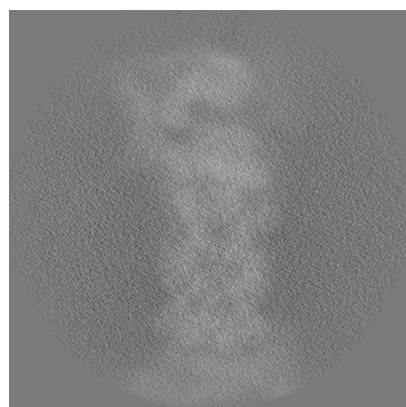


Y

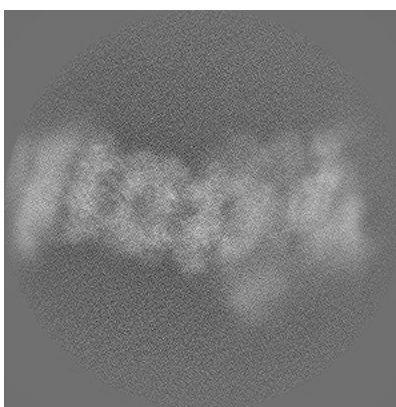


Z

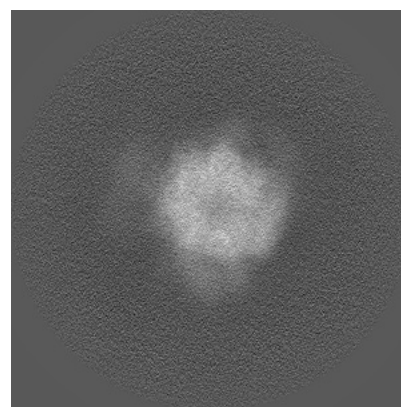
#### 6.1.2 Raw map



X



Y

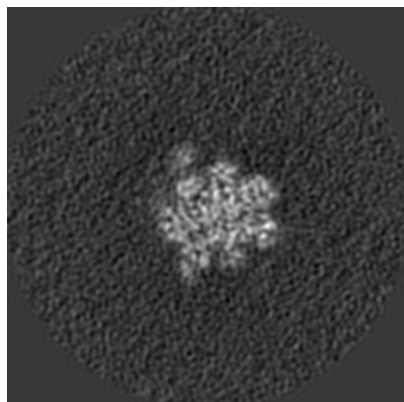


Z

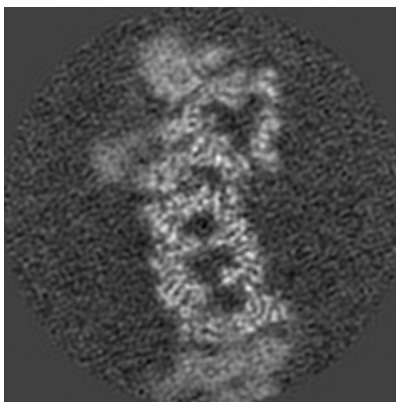
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

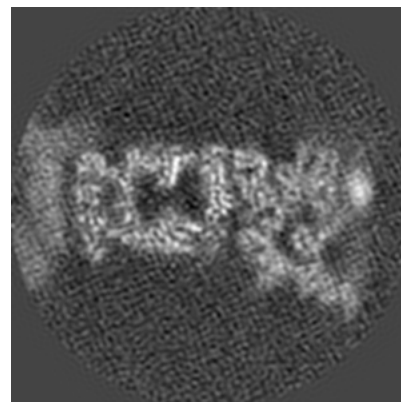
### 6.2.1 Primary map



X Index: 300

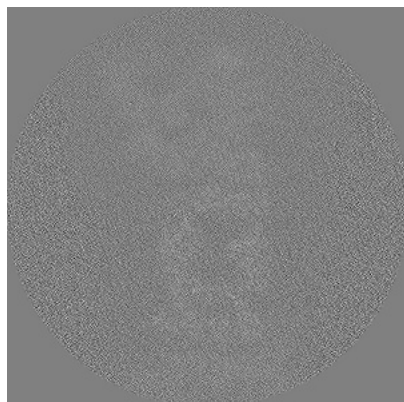


Y Index: 300

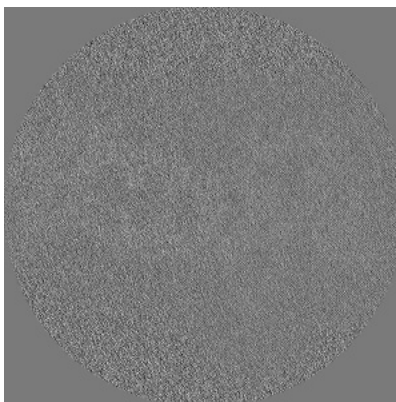


Z Index: 300

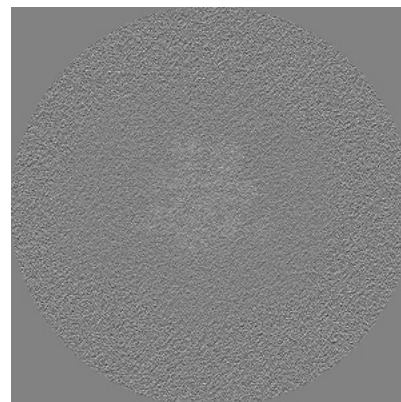
### 6.2.2 Raw map



X Index: 300



Y Index: 300



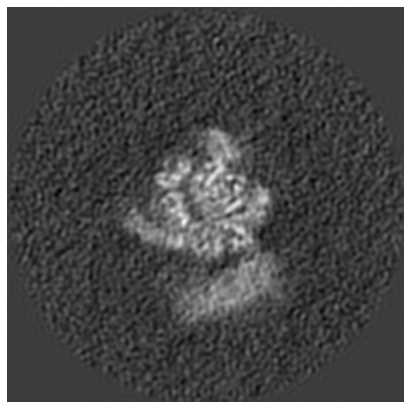
Z Index: 300

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

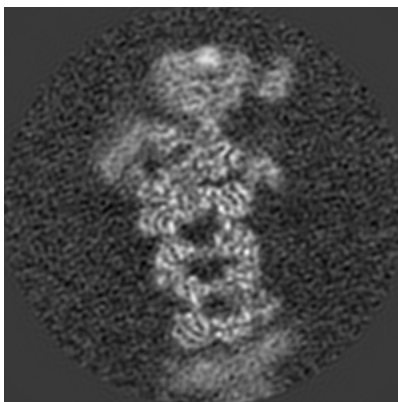


## 6.3 Largest variance slices [i](#)

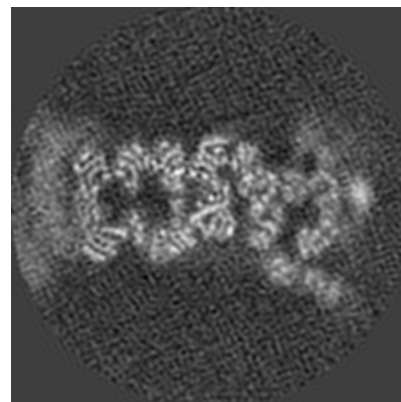
### 6.3.1 Primary map



X Index: 364

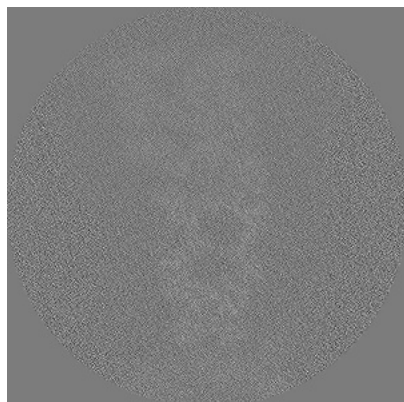


Y Index: 329

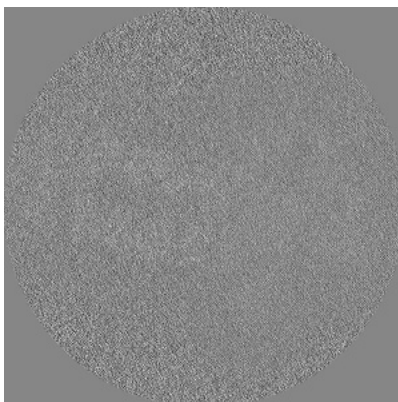


Z Index: 319

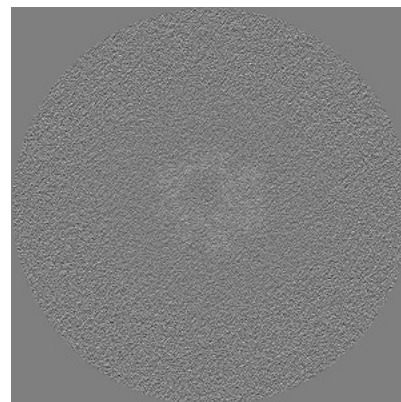
### 6.3.2 Raw map



X Index: 287



Y Index: 308



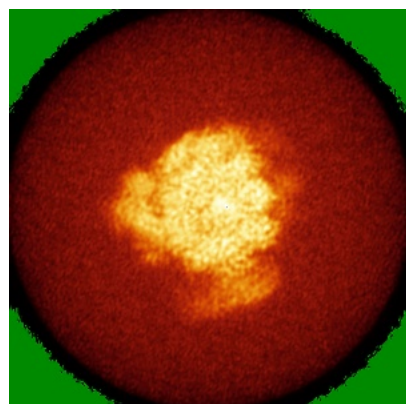
Z Index: 256

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

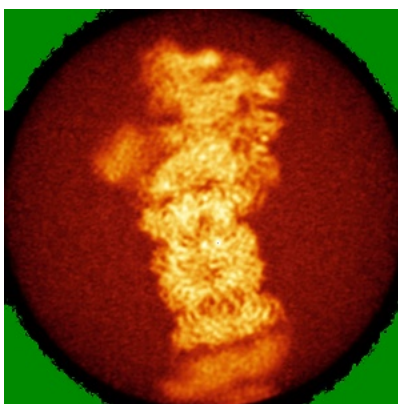


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

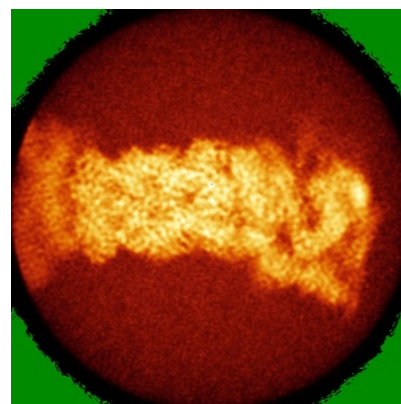
### 6.4.1 Primary map



X

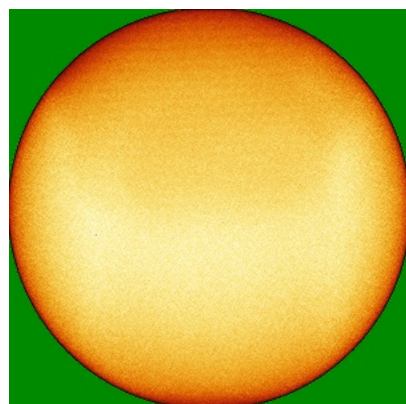


Y

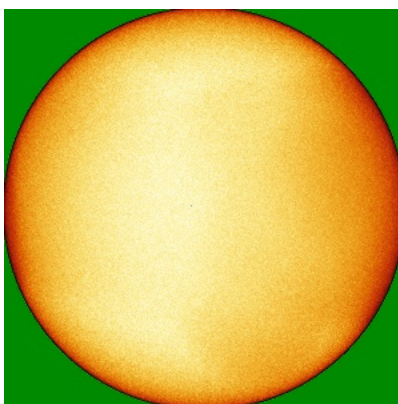


Z

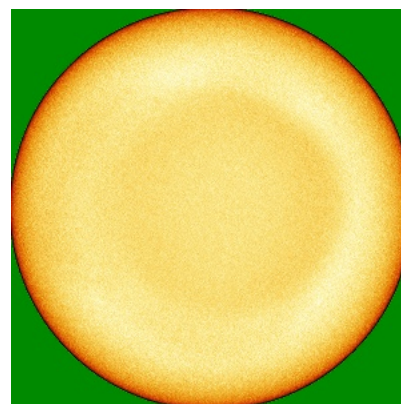
### 6.4.2 Raw map



X



Y

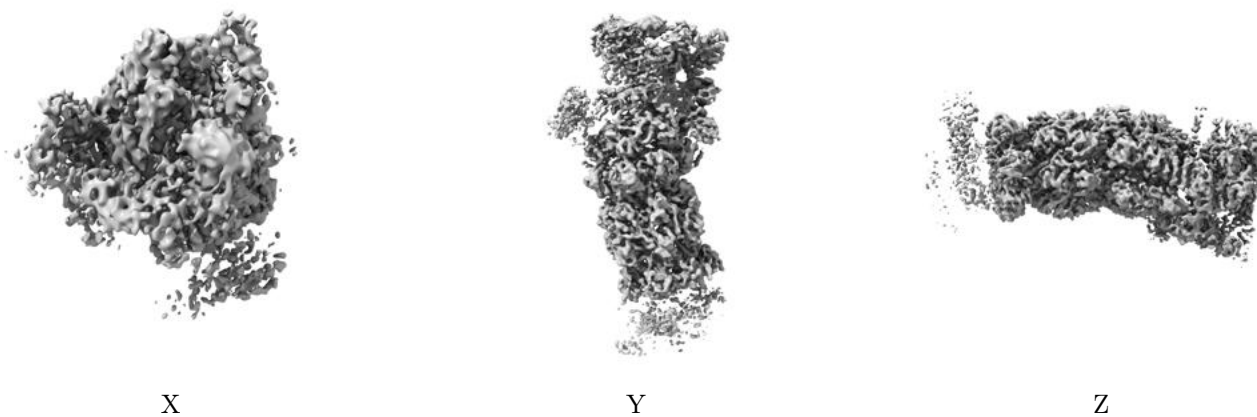


Z

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.

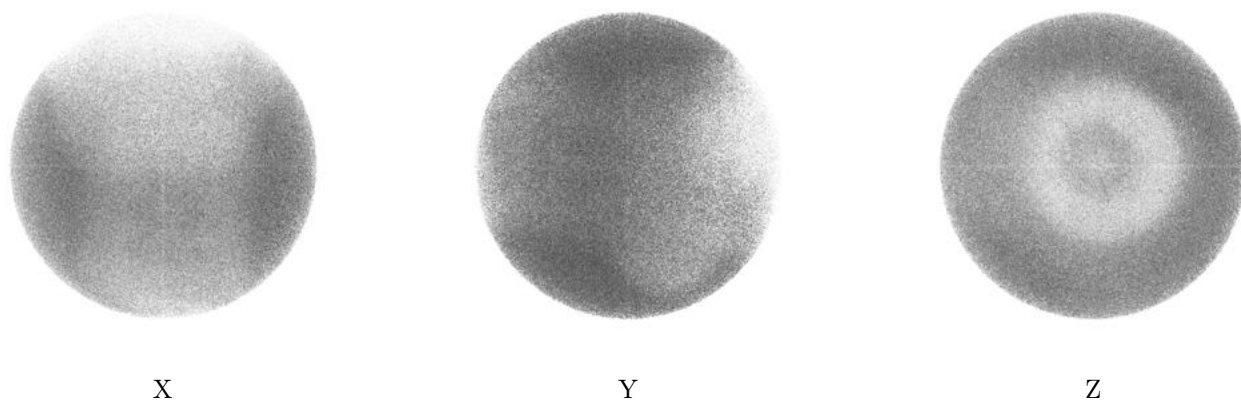
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0044. 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.

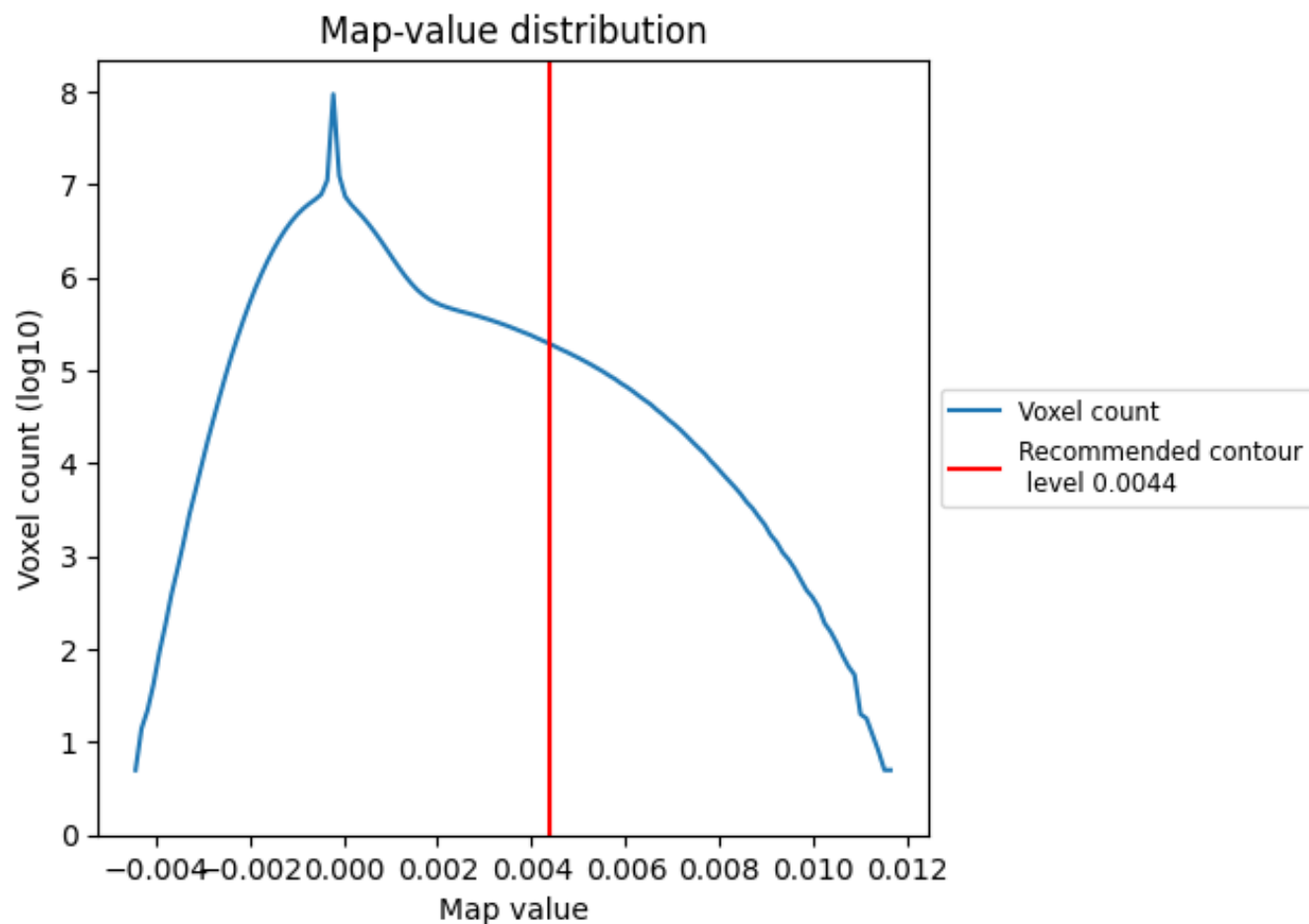
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

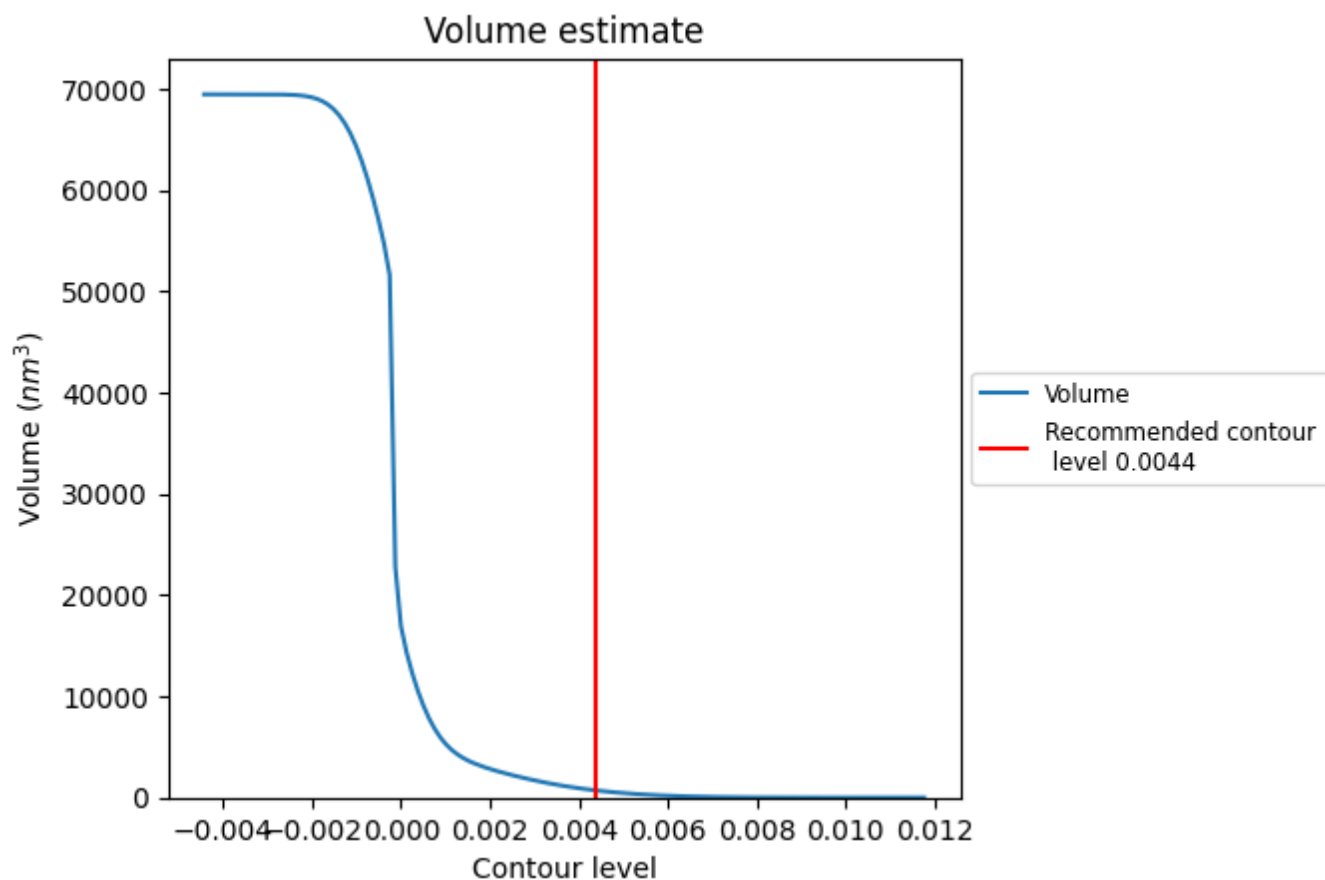
This section contains the results of statistical analysis of the map.

### 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.

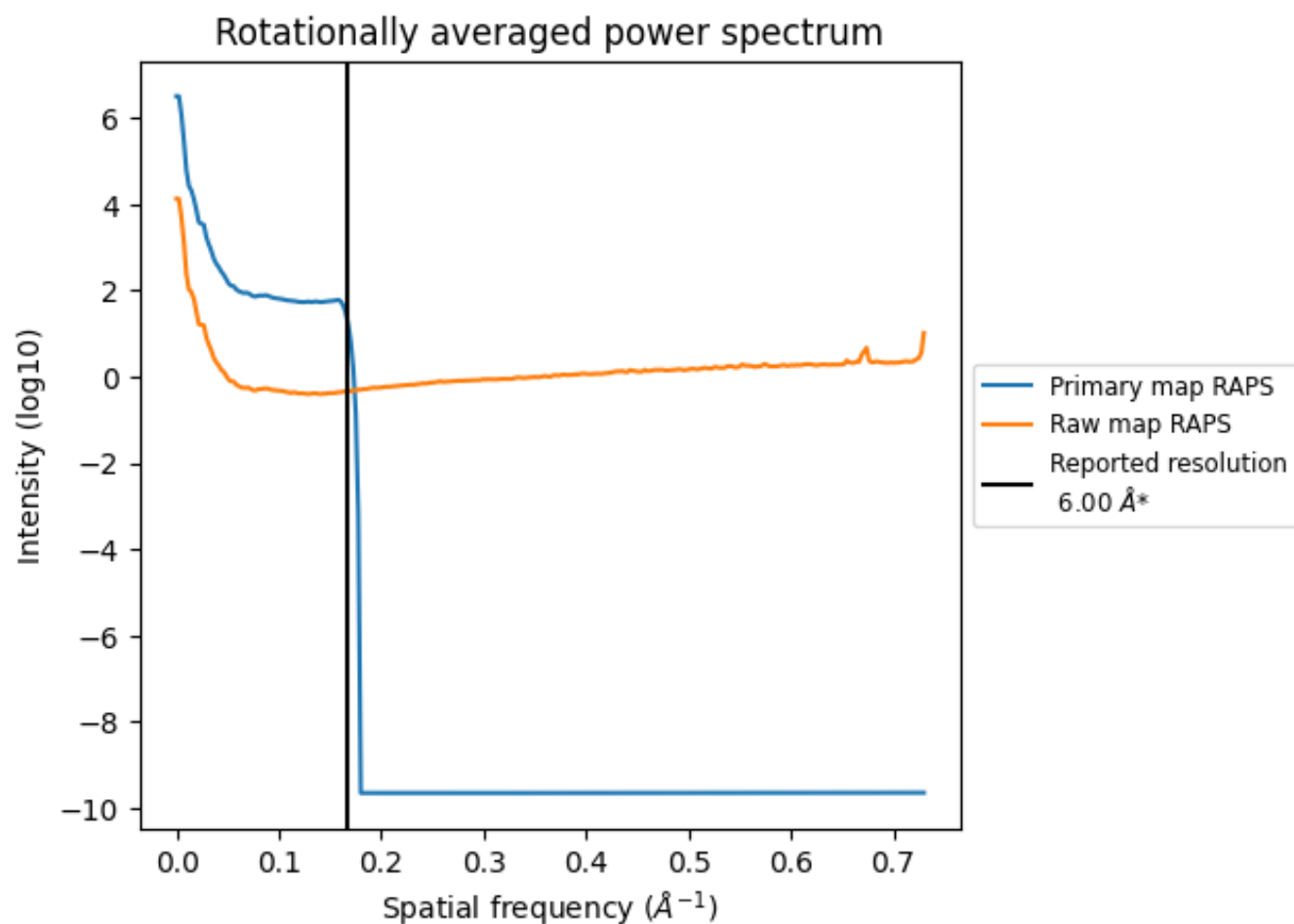
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 699 nm<sup>3</sup>; this corresponds to an approximate mass of 631 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 ⓘ

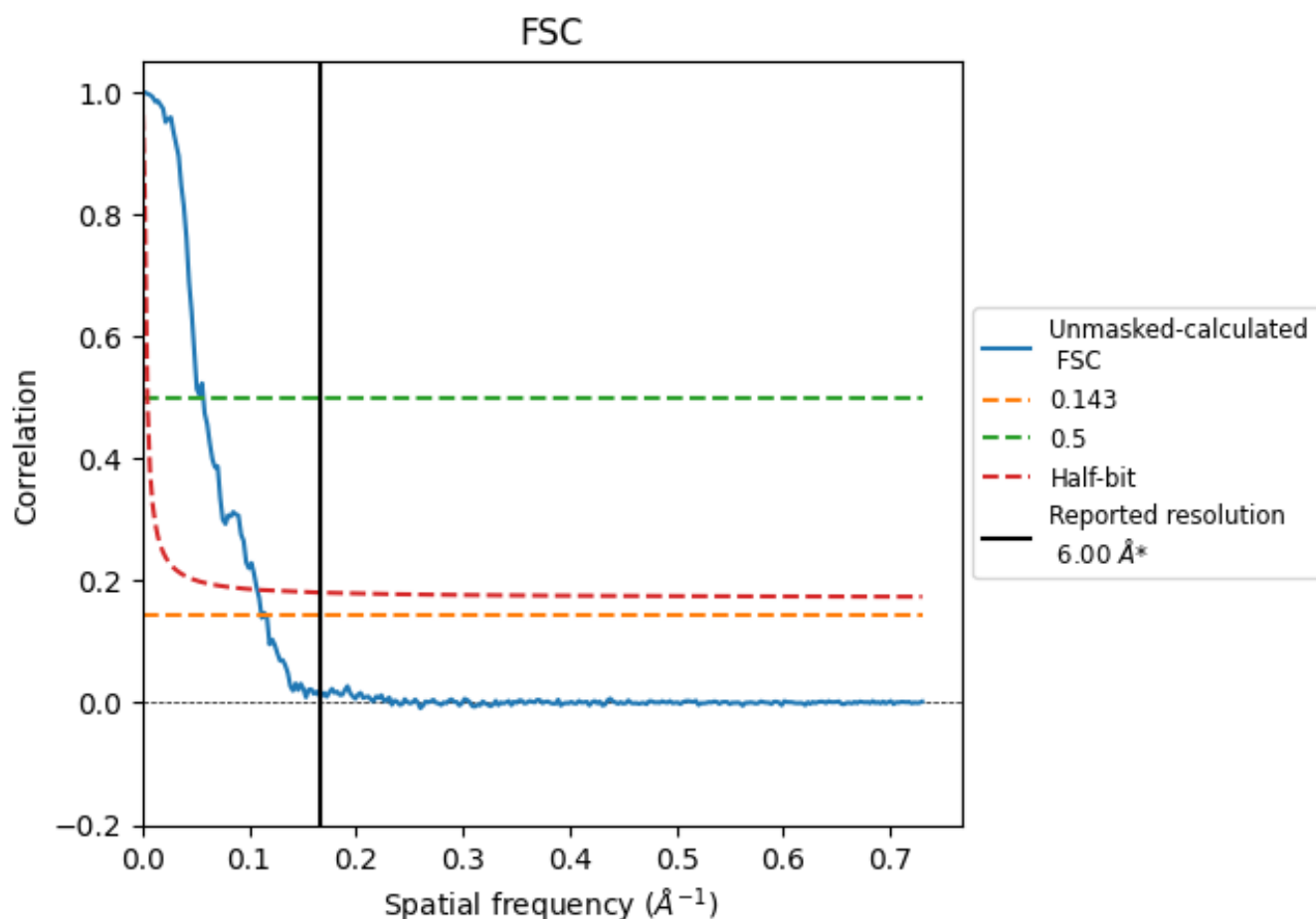


\*Reported resolution corresponds to spatial frequency of 0.167 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.167 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

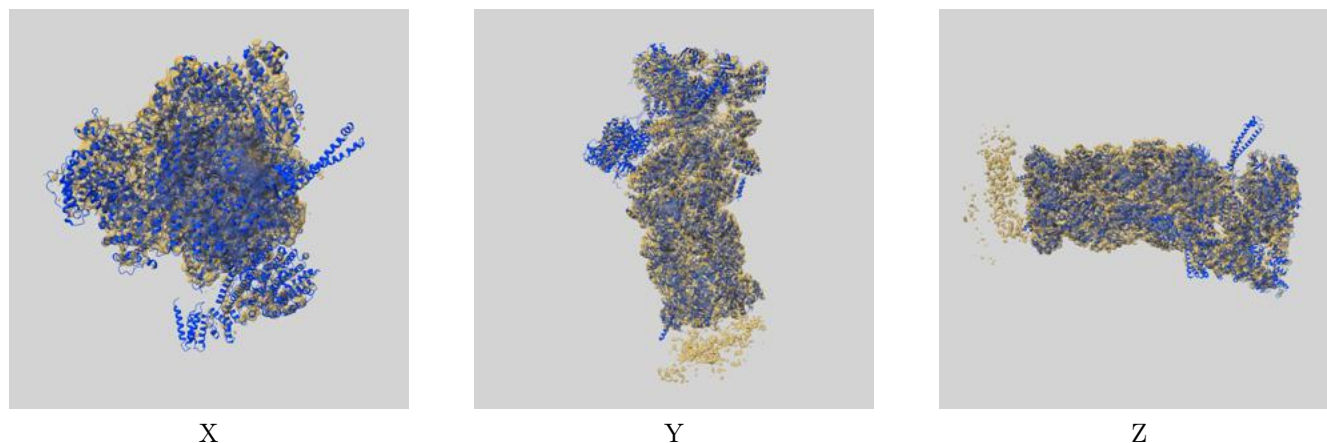
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.96	17.51	9.30

\*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 8.96 differs from the reported value 6.0 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-62065 and PDB model 9K4O. Per-residue inclusion information can be found in section 3 on page 13.

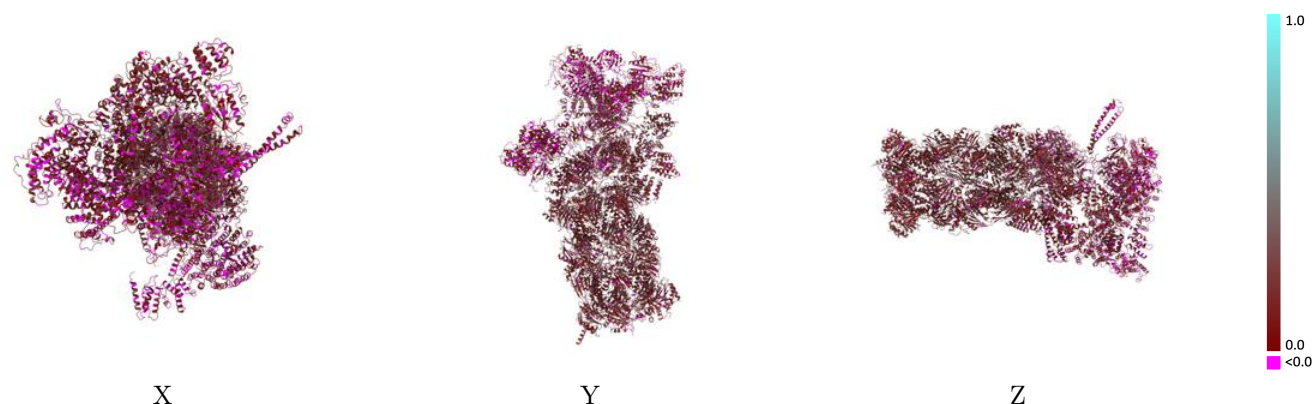
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0044 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

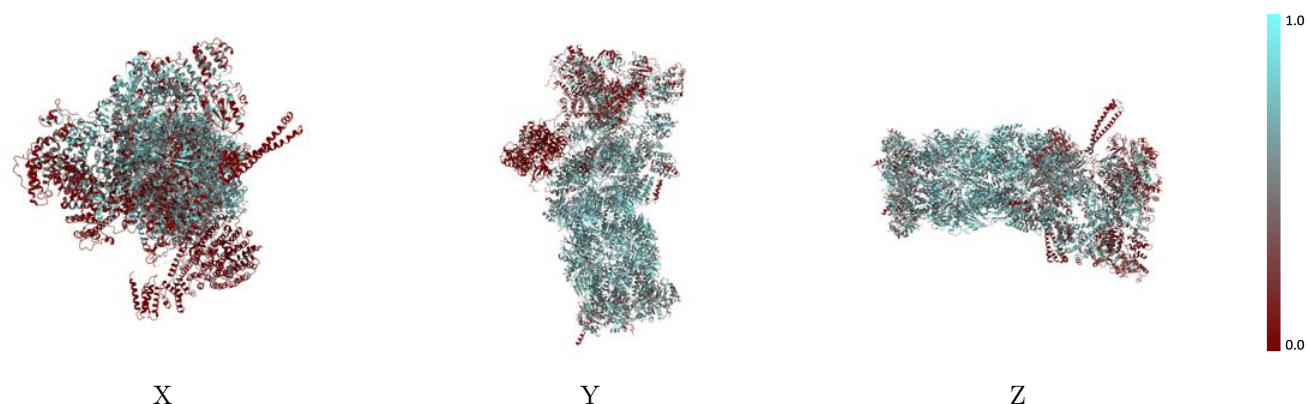


## 9.2 Q-score mapped to coordinate model [i](#)



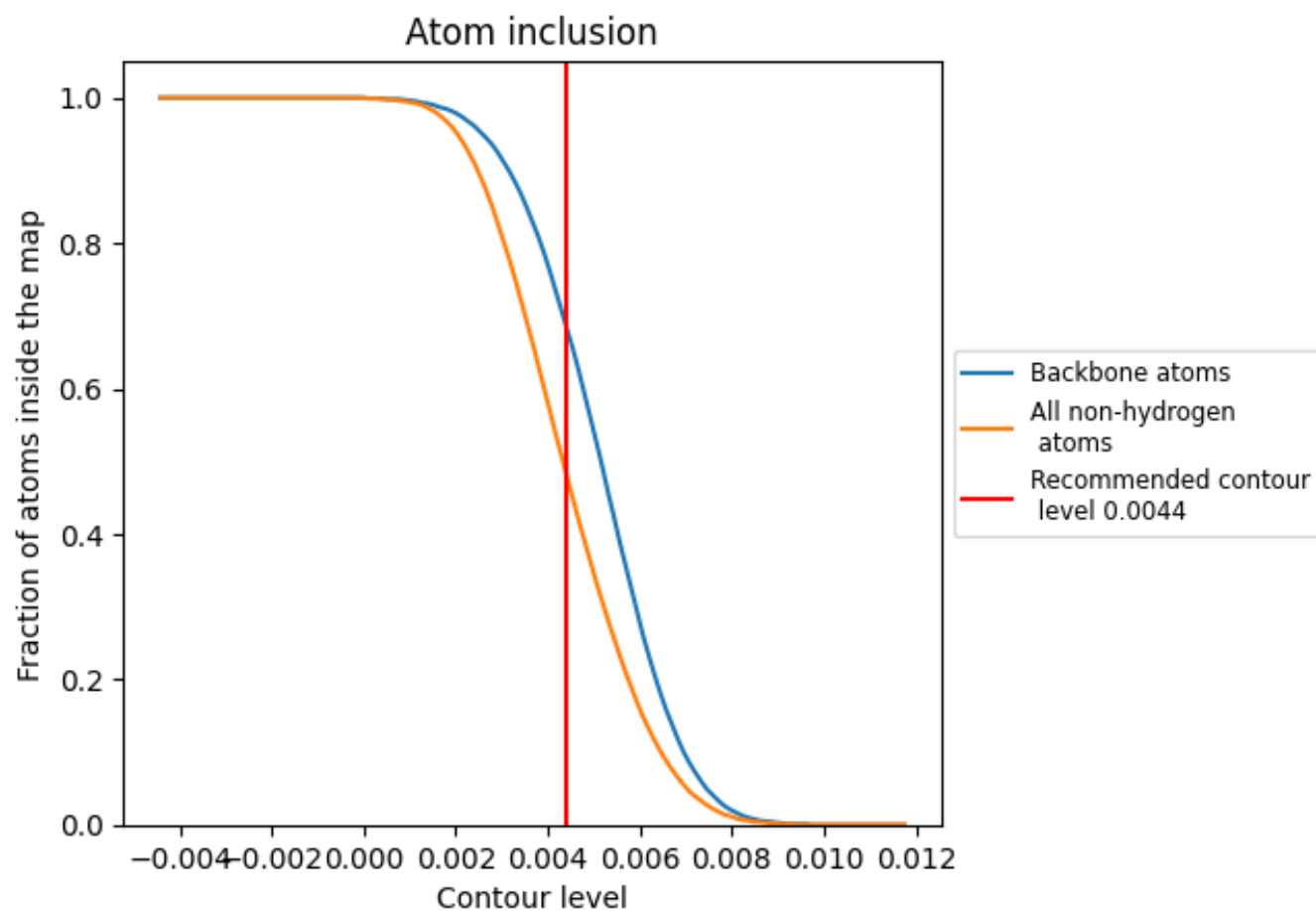
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0044).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 48% 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 (0.0044) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4840	 0.1770
A	 0.4780	 0.1810
B	 0.4770	 0.1800
C	 0.4700	 0.1770
D	 0.5060	 0.1740
E	 0.5160	 0.1840
F	 0.4660	 0.1780
G	 0.6570	 0.2190
H	 0.6730	 0.2180
I	 0.6590	 0.2180
J	 0.5980	 0.2010
K	 0.6370	 0.2200
L	 0.6840	 0.2200
M	 0.6560	 0.2110
N	 0.6940	 0.2200
O	 0.6870	 0.2330
P	 0.6870	 0.2130
Q	 0.6340	 0.2140
R	 0.6500	 0.2150
S	 0.6430	 0.2110
T	 0.6940	 0.2250
U	 0.3070	 0.1060
V	 0.2820	 0.1470
W	 0.5430	 0.1770
X	 0.5100	 0.1680
Y	 0.4620	 0.1330
Z	 0.3970	 0.1460
a	 0.4500	 0.1520
b	 0.3060	 0.1300
c	 0.3970	 0.1440
d	 0.2160	 0.1150
e	 0.1770	 0.1180
f	 0.0790	 0.0970
g	 0.4980	 0.2060
h	 0.5190	 0.2070



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Chain	Atom inclusion	Q-score
i	 0.4870	 0.2160
j	 0.4240	 0.2000
k	 0.4850	 0.2140
l	 0.5470	 0.2180
m	 0.5210	 0.1990
n	 0.6180	 0.2160
o	 0.6130	 0.2240
p	 0.6270	 0.2070
q	 0.6290	 0.2180
r	 0.6390	 0.2140
s	 0.6020	 0.2260
t	 0.6380	 0.2230
u	 0.1640	 0.1100
v	 0.0570	 0.0500
x	 0.3380	 0.0200
y	 0.4460	 0.0340