



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:16 PM UTC

PDB ID : 7QXU / pdb_00007qxu
EMDB ID : EMD-14203
Title : Proteasome-ZFAND5 Complex Z+C state
Authors : Zhu, Y.; Lu, Y.
Deposited on : 2022-01-27
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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

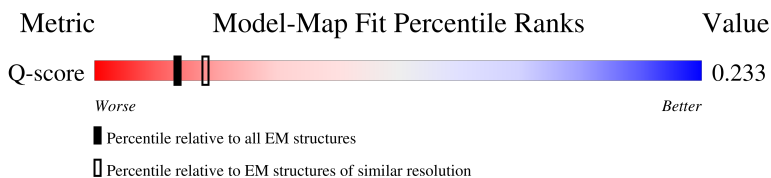
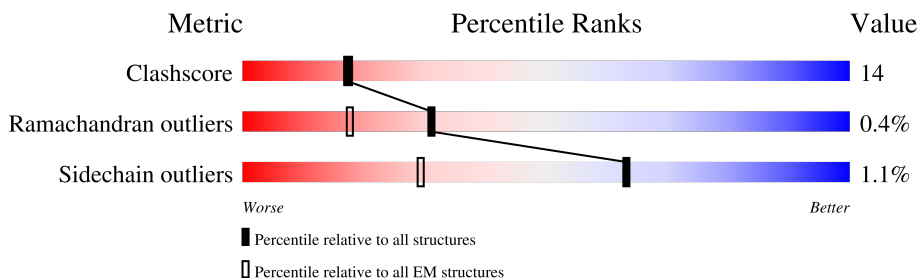
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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	4585 (3.80 - 4.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	U	953	50% 61% 24% 15%
2	V	533	56% 67% 27% 5%
3	W	456	15% 61% 36%
4	X	422	14% 76% 14% 10%

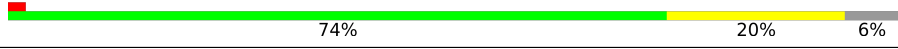
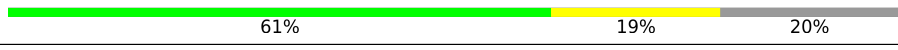
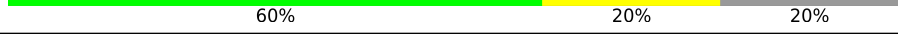
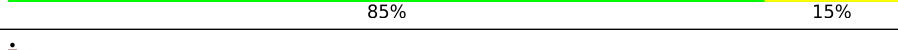
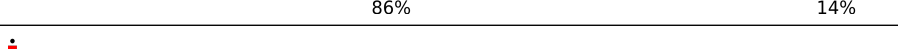
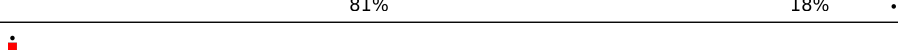
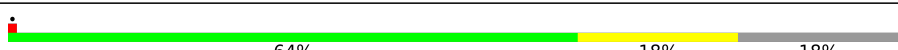
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Mol	Chain	Length	Quality of chain
5	Y	389	
6	Z	324	
7	a	376	
8	b	377	
9	c	309	
10	d	349	
11	e	70	
12	f	908	
13	A	433	
14	B	429	
15	C	389	
16	D	418	
17	E	403	
18	F	439	
19	G	245	
19	g	245	
20	H	233	
20	h	233	
21	I	260	
21	i	260	
22	J	247	
22	j	247	
23	K	240	
23	k	240	
24	L	268	

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Mol	Chain	Length	Quality of chain
24	l	268	
25	M	254	
25	m	254	
26	N	238	
26	n	238	
27	O	276	
27	o	276	
28	P	204	
28	p	204	
29	Q	201	
29	q	201	
30	R	262	
30	r	262	
31	S	240	
31	s	240	
32	T	263	
32	t	263	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	ATP	E	401	-	-	X	-
36	ADP	C	501	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103719 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 non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	812	Total	C	N	O	S	0	0
			6334	4023	1078	1189	44		

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	508	Total	C	N	O	S	0	0
			3994	2530	712	738	14		

- Molecule 3 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	380	Total	C	N	O	S	0	0
			3009	1918	509	570	12		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 11 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	889	Total	C	N	O	S	0	0
			6860	4309	1174	1331	46		

- Molecule 13 is a protein called 26S protease regulatory subunit 7.

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

- Molecule 14 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	384	Total	C	N	O	S	0	0
			3011	1895	515	586	15		

- Molecule 15 is a protein called 26S proteasome regulatory subunit 8.

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

- Molecule 16 is a protein called 26S protease regulatory subunit 6B.

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

- Molecule 17 is a protein called 26S proteasome regulatory subunit 10B.

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

- Molecule 18 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	376	Total	C	N	O	S	0	0
			2858	1802	496	545	15		

- Molecule 19 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		
19	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 20 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	H	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		
20	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 21 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		
21	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 22 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	J	239	Total	C	N	O	S	0	0
			1713	1062	311	335	5		
22	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 23 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	K	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		
23	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 24 is a protein called Isoform Long of Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		
24	l	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 25 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		
25	m	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 26 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
26	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 27 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
27	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 28 is a protein called Proteasome subunit beta type-3.

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

- Molecule 29 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
29	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 30 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
30	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 31 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
31	s	213	Total	C	N	O	S	0	0
			1644	1039	282	313	10		

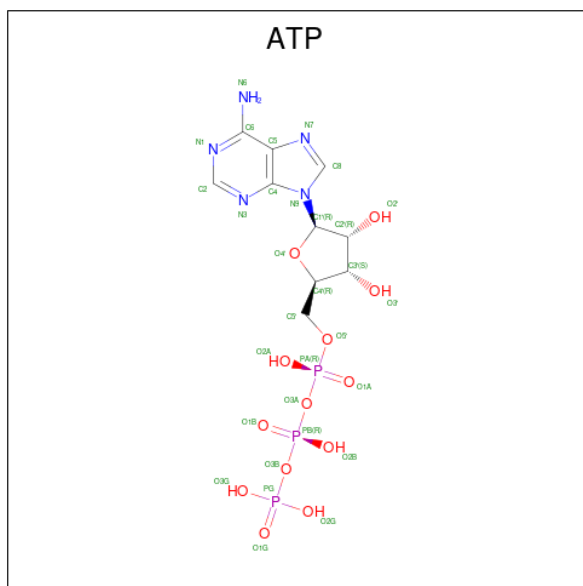
- Molecule 32 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
32	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

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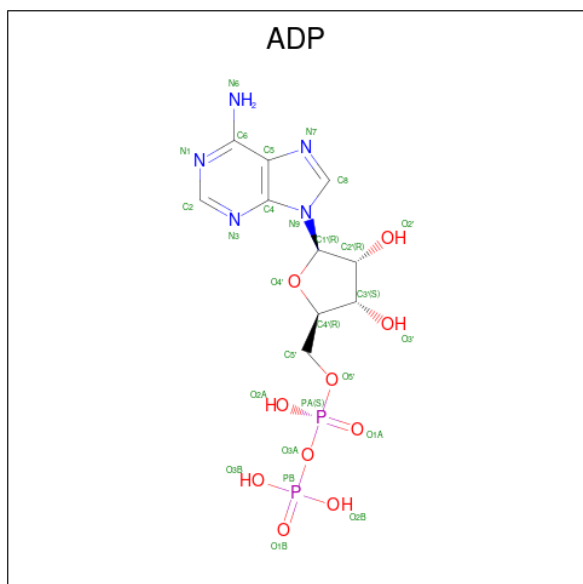
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Mol	Chain	Residues	Atoms					AltConf
34	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

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

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

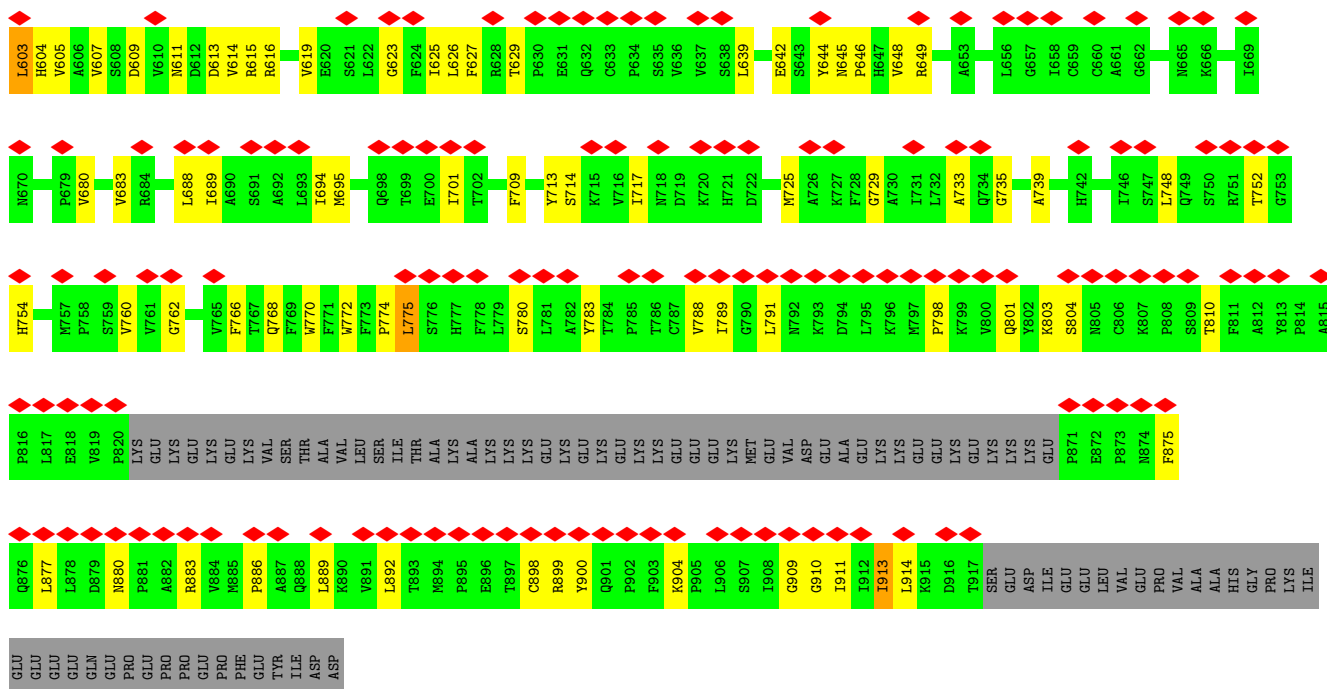


Mol	Chain	Residues	Atoms					AltConf
36	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

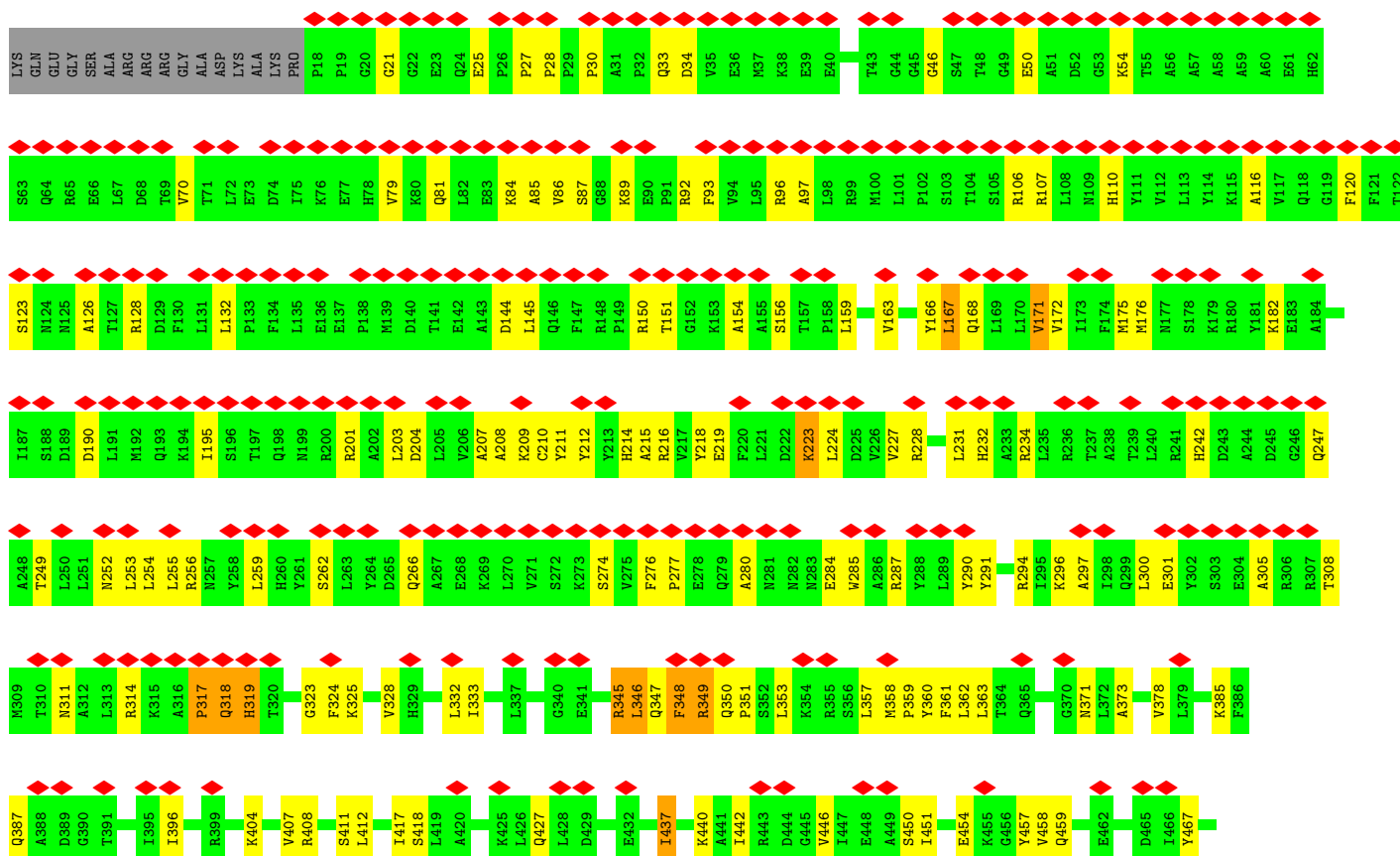
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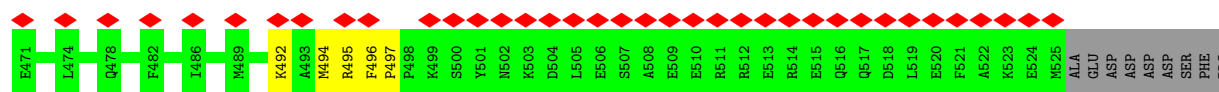
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
36	F	1	27	10	5	10	2	0

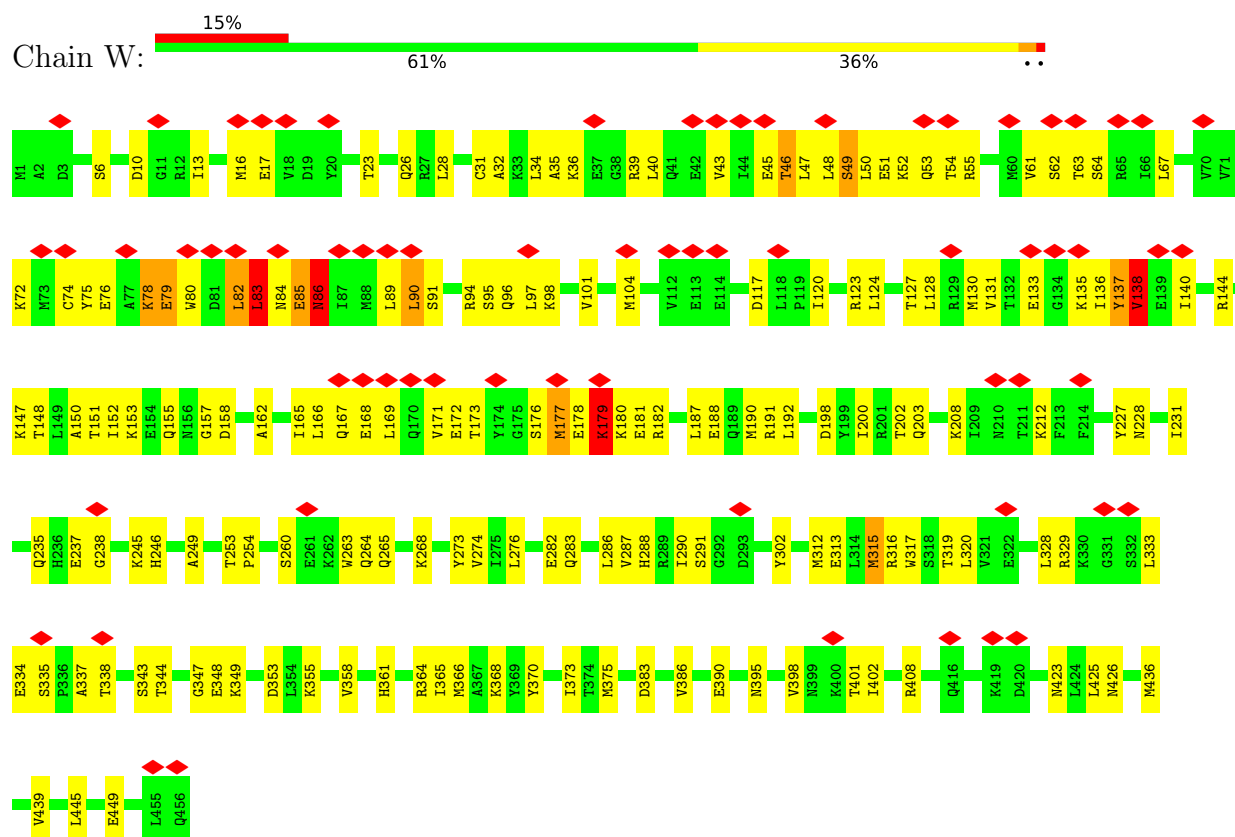


- Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

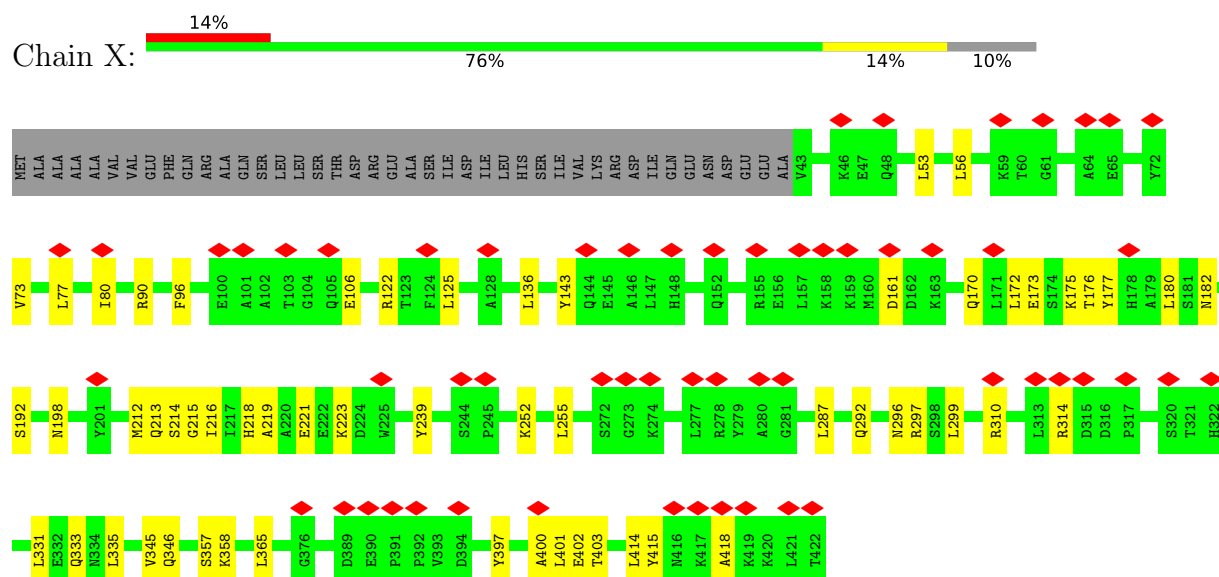




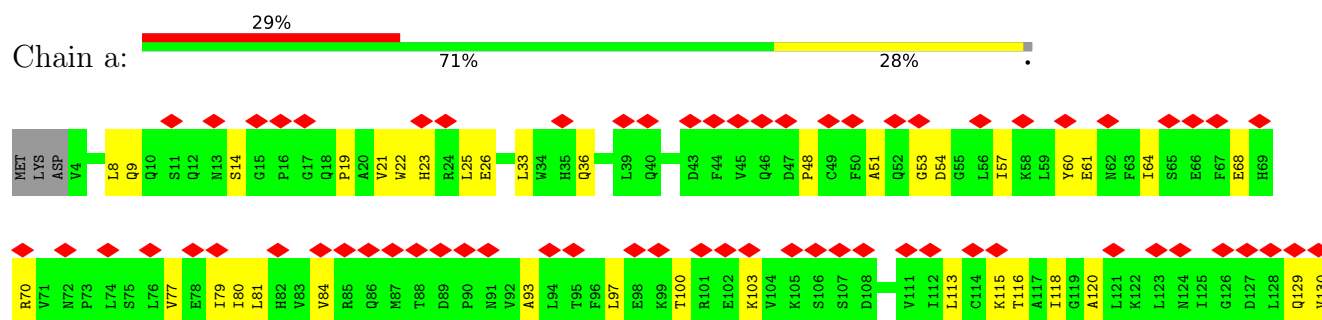
- Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

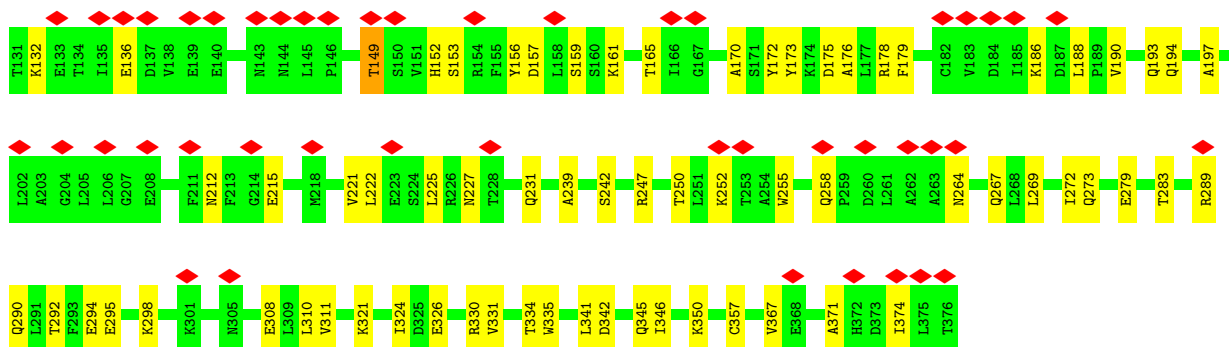


- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

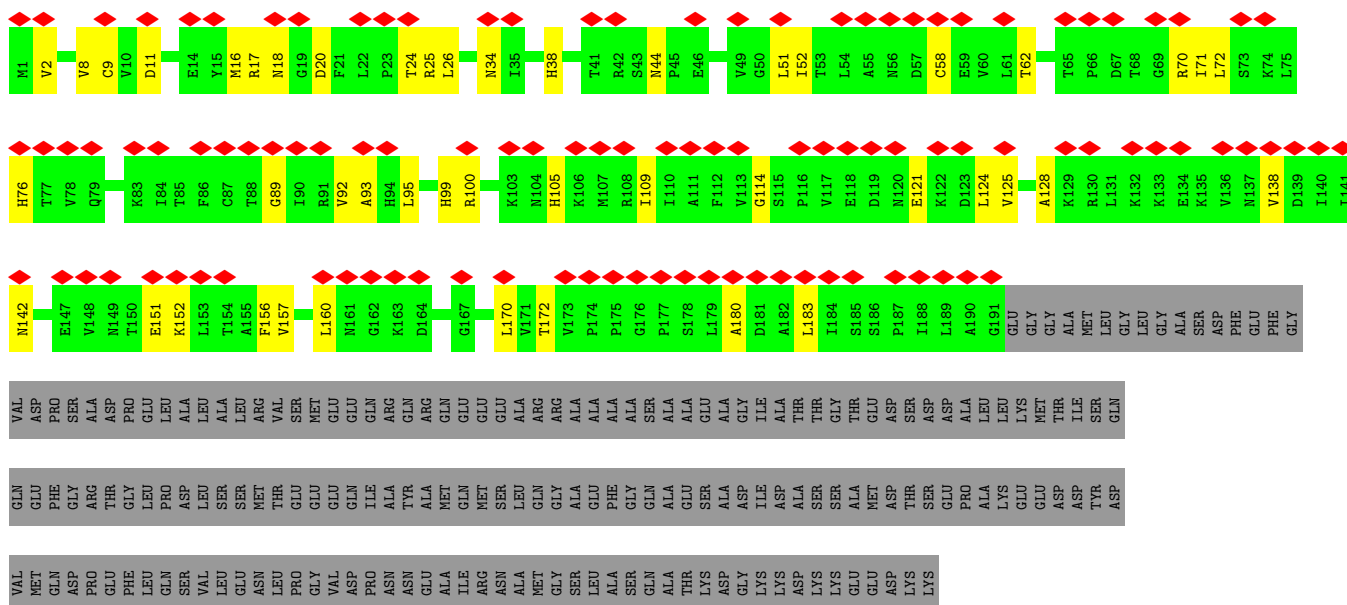
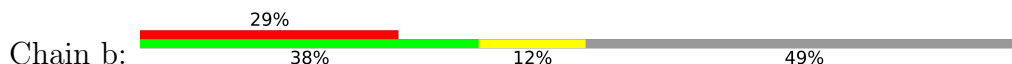


- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

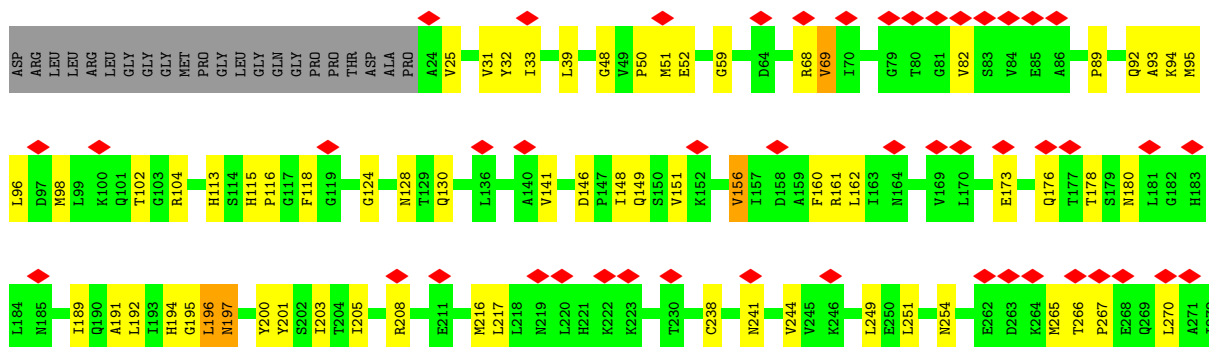


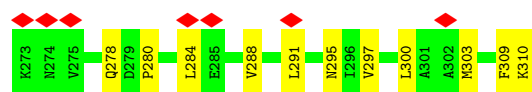


- Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

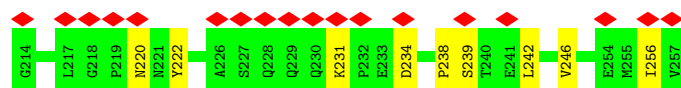
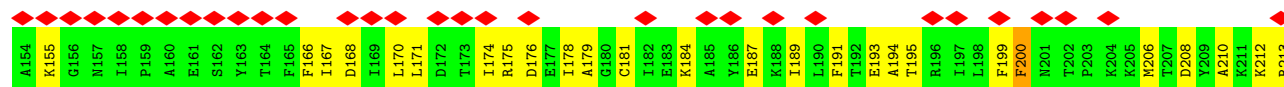
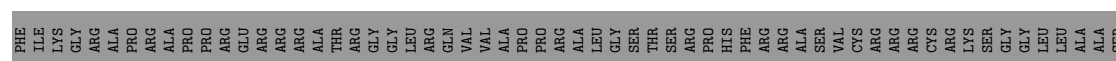


- Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

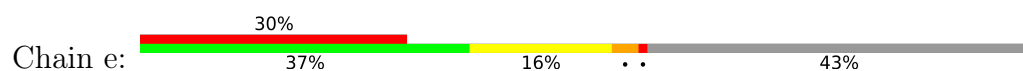




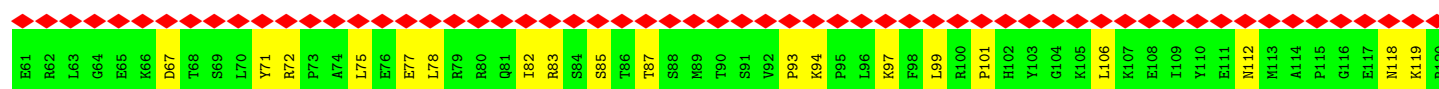
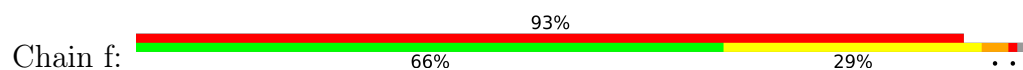
- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8



- Molecule 11: 26S proteasome complex subunit SEM1

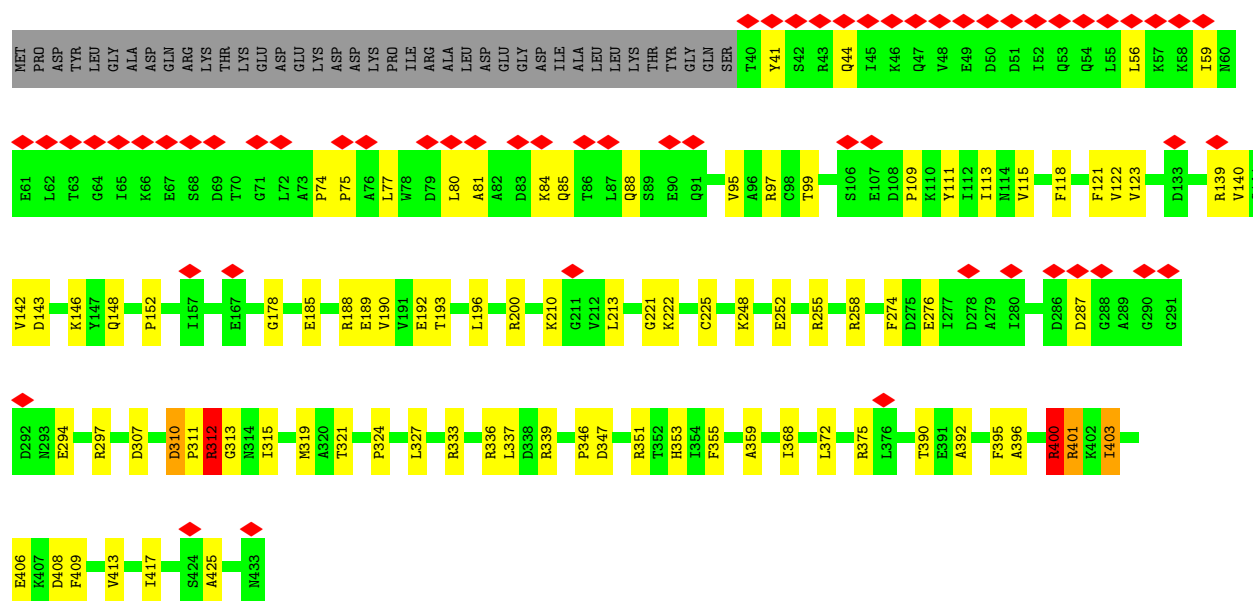
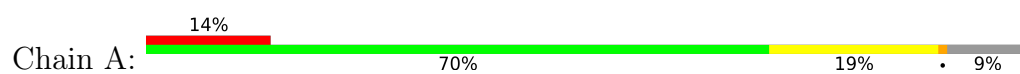


- Molecule 12: 26S proteasome non-ATPase regulatory subunit 2

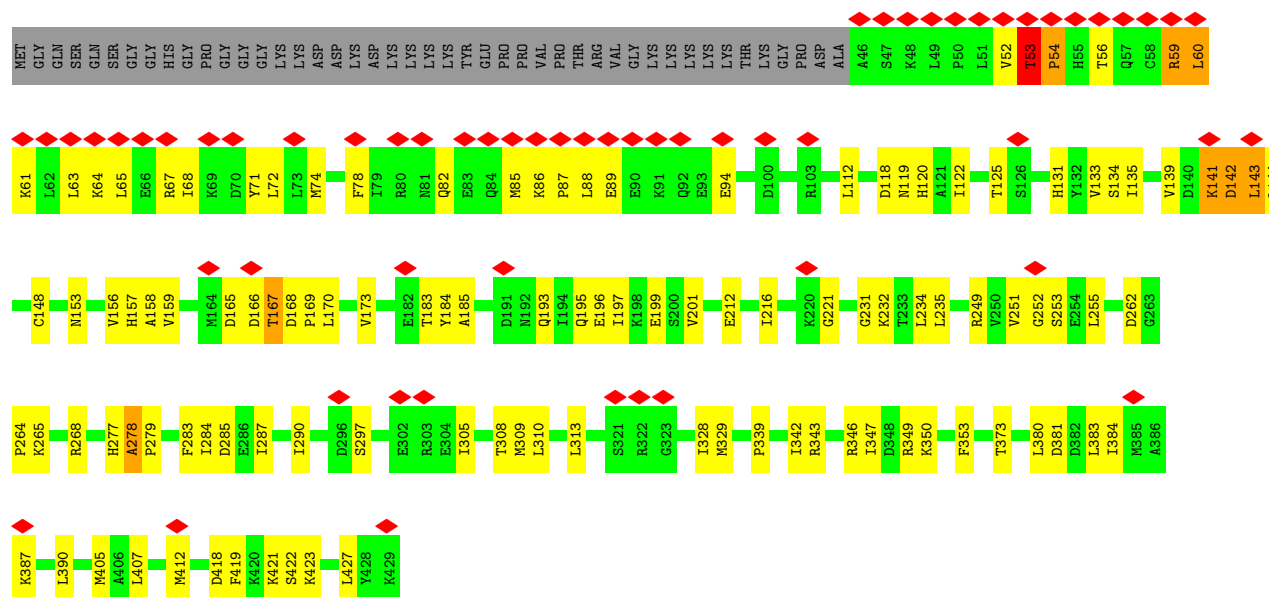


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TTR	V846	Q786	T726	H605	K545	G484	V422	G362	G302	E242	E182	A122
ASP	G847	L787	F727	V606	S546	L485	D423	S363	V303	P243	P183	A123
LEU	Q848	K788	A728	L607	E547	G486	G424	Q364	F304	E244	L184	D124
	A849	S789	M729	K608	T548	L487	G425	V365	L305	N245	L185	I125
	V850	Q790	G730	V609	E549	A488	L426	D366	L306	S246	T186	I126
	V852	V791	M731	Q610	L550	Y489	T427	S367	L307	A247	L187	S127
	V853	L792	V732	Q611	K551	S492	Q428	A368	S308	L248	V188	V128
	G854	A793	G733	H614	D552	N493	L429	R369	E309	L249	K189	L129
	G855	F675	S734	L615	T553	R494	D430	M370	D310	R250	E190	A130
	A856	G676	G735	L616	Y554	E495	K431	N371	V311	C251	I191	M131
	G857	H677	T736	S617	A555	D496	Y432	L372	E312	A252	V192	T132
	K858	L678	M737	E618	R556	V497	L433	A373	E313	L253	P193	M133
	P859	L679	M738	H619	N557	L498	Y434	S374	Y314	G254	P194	S134
	L860	R680	A739	F620	L558	T499	S435	S375	E315	V255	N195	G135
	V861	Y801	R740	D621	P559	L500	S436	F376	D316	F256	M196	E136
	L862	G682	L741	D622	L560	L501	E437	V377	L317	R257	A197	R137
	F863	E683	A742	K623	G561	L502	D438	N378	T318	K258	H198	E138
	L864	P684	A743	E624	L562	L503	Y439	G379	E319	F259	N199	C139
	D865	T685	M744	K625	G563	V504	L440	F380	I320	S260	A200	L140
	V866	L686	L745	E626	H565	M505	K441	V381	M321	R261	E201	K141
	R867	R687	Q747	F627	H566	G506	S442	N382	S322	F262	H202	Y142
	H868	A689	L748	D628	G568	D507	G443	A383	N323	P263	E203	R143
	L869	V690	A749	K629	K569	S508	A444	A384	Q324	E264	A204	L144
	T870	P691	Q750	K631	G570	K509	L445	F385	Q325	A265	C205	V145
	P871	L692	Y751	E632	E571	S510	A447	G386	L326	L266	D206	G146
	V872	A693	H752	K633	A572	S511	C448	Q387	N327	R267	L207	S147
	L873	L694	K753	K634	I573	M512	G449	D388	S328	L268	L208	Q148
	L874	L695	A754	K635	I574	E513	I450	K389	N329	A269	E149	E149
	A875	L696	D755	D636	E574	V514	V451	L391	F330	L270	E210	E150
	H876	L697	F756	K637	L576	A515	G455	T392	L331	M271	I211	L151
	G877	S698	N757	K638	L577	G516	V455	D393	A332	L272	E212	A152
	E878	V699	N758	K640	A578	T518	K456	D394	L333	N273	Q213	S153
	R879	S700	L759	F641	A579	A519	M457	G395	R335	M275	D215	W154
	A880	G820	F760	E642	L580	L520	E458	N396	E336	E276	M216	G155
	E881	N701	M761	A642	E581	A521	C459	K397	L337	L277	E157	H156
	L882	P702	V762	A644	E582	C522	D460	K398	D338	L278	E218	E157
	A883	L704	R763	D645	V583	N524	A462	L399	I339	E279	E219	V159
	T884	N705	L764	K646	S584	I525	A463	Y400	M340	D280	D220	R160
	S885	M706	A765	A648	E585	A526	A464	K401	I281	D282	I221	H161
	P886	L707	Q766	G647	P586	V527	L465	M402	P342	F282	D222	L162
	F887	D708	G767	K649	F587	G528	L466	K403	K343	T283	E223	A163
	L888	T709	L768	Q650	H588	S529	L466	D404	V344	S284	N224	G164
	V889	L710	T769	Y652	S589	C530	D468	H405	P345	C285	A225	E165
	VAL	F590	F770	A653	F590	N531	Y469	G406	D347	K286	Y226	V166
THR	L830	K711	L771	V654	G532	G532	V470	M407	D347	D287	A227	A167
PRO	V831	K712	G772	V654	A591	G533	L471	L408	I348	V288	K228	K168
ILE	T832	F713	G773	L655	N592	D533	L471	S409	V349	V289	V229	E169
GLU	D834	S714	G774	T593	T593	E534	H472	A410	K350	V290	C230	W170
GLY	E835	H715	T775	L657	L594	T535	M473	A419	T351	Q291	L231	Q171
PHE	E836	D716	L776	A658	V595	S536	S474	A412	H352	K292	Y232	E172
VAL	L837	A717	T777	L659	D596	T537	M475	A413	L353	Q293	L233	L173
ILE	L837	D718	L778	T660	V597	I538	T476	S413	E354	M294	T234	D174
LEU	R838	P719	L778	A661	C598	L539	M477	L414	N355	A295	S235	D175
ARG	P839	E720	G779	M662	A599	Q540	R478	G415	N356	F296	C236	A176
LYS	L840	V721	T780	G663	V600	T541	L479	M416	R357	M297	V237	E177
ASN	P841	S722	Y781	E664	A601	I542	G480	L418	F358	N297	N238	K178
PRO	V842	Y723	H782	E664	G602	M543	S481	L419	G359	G299	Y239	V179
	S843	W724	S783	E664	S603	M543	L482	W420	G360	R300	V240	Q180

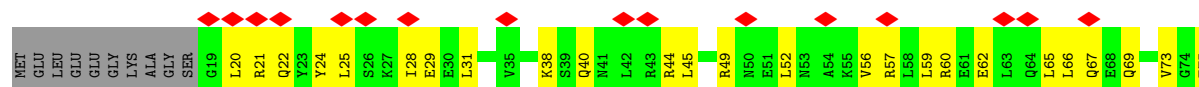
- Molecule 13: 26S protease regulatory subunit 7

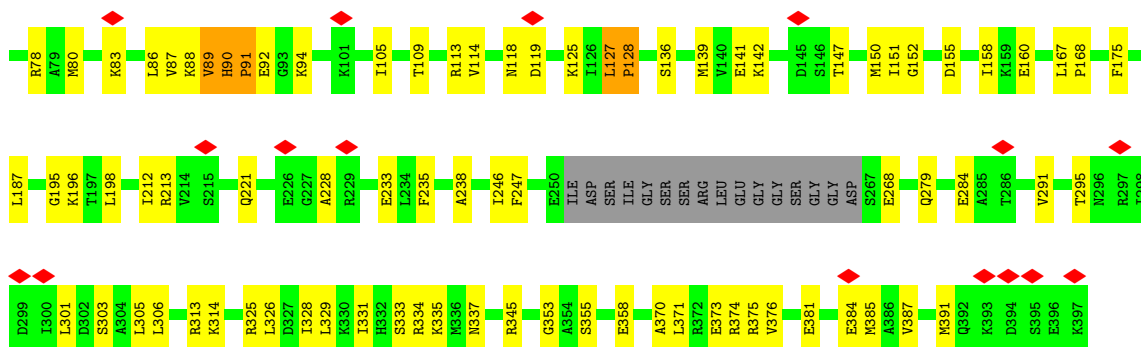


• Molecule 14: 26S proteasome regulatory subunit 4

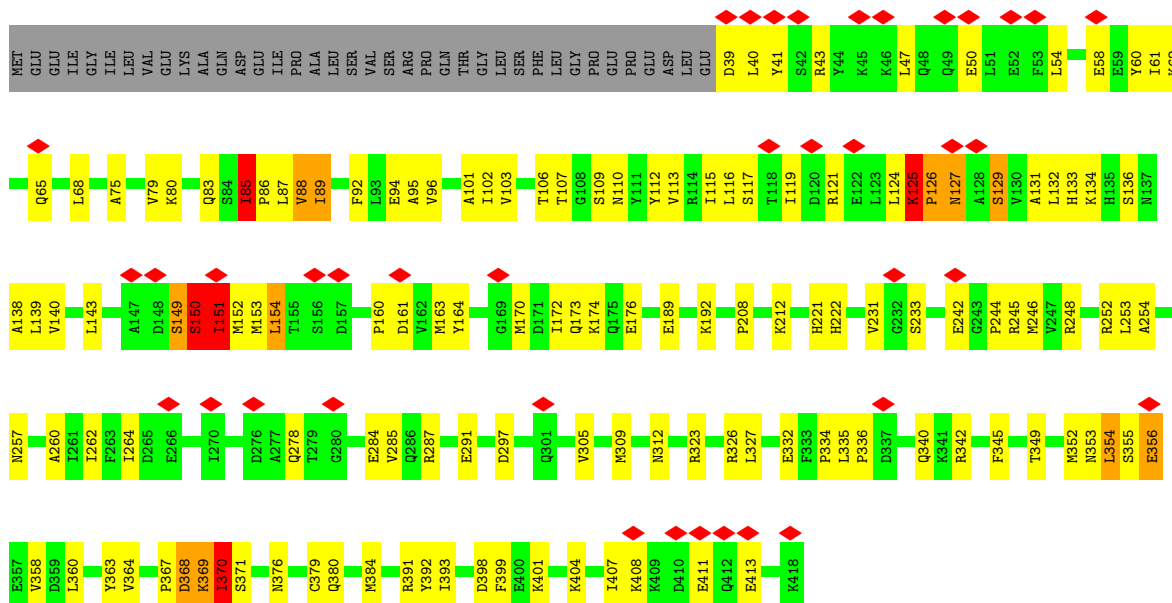


• Molecule 15: 26S proteasome regulatory subunit 8

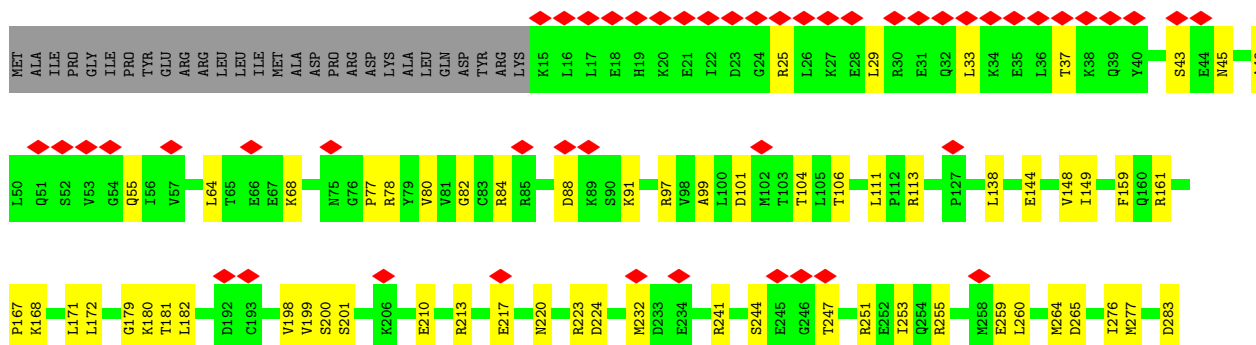


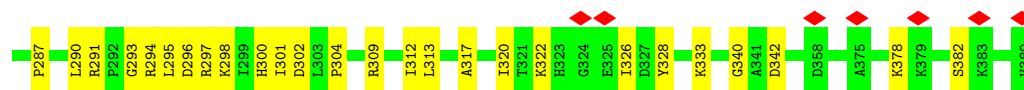


• Molecule 16: 26S protease regulatory subunit 6B

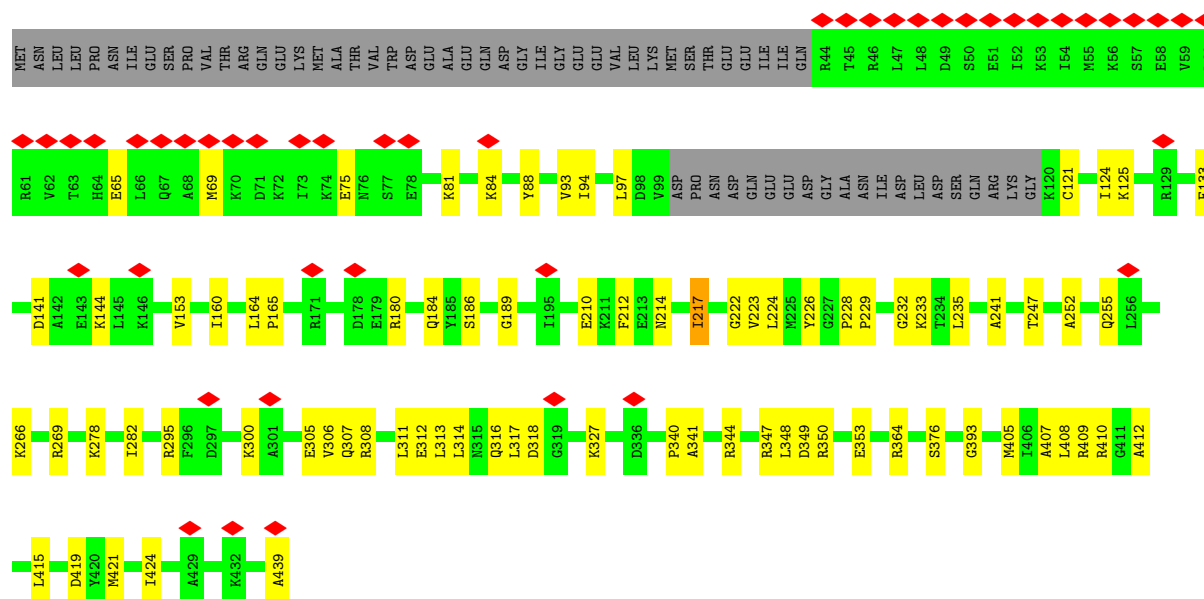


• Molecule 17: 26S proteasome regulatory subunit 10B

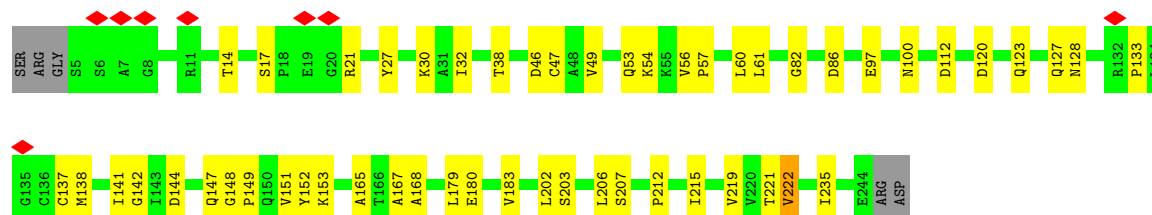
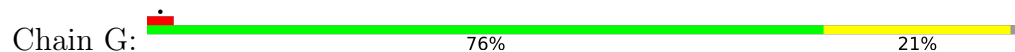




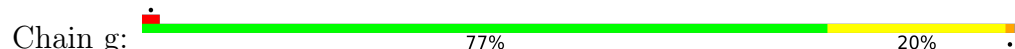
• Molecule 18: 26S protease regulatory subunit 6A



• Molecule 19: Proteasome subunit alpha type-6

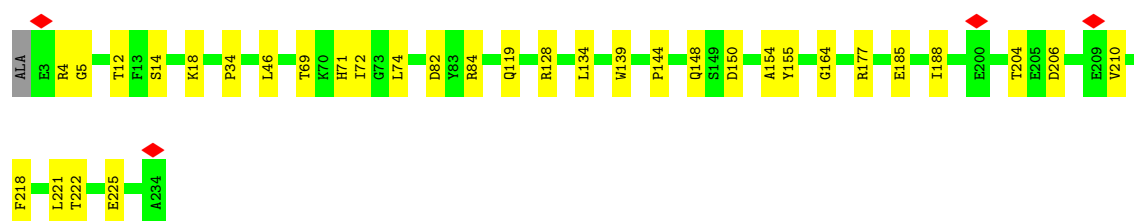


• Molecule 19: Proteasome subunit alpha type-6



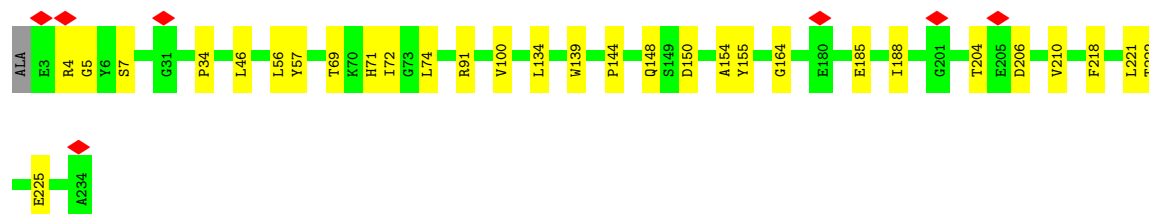
• Molecule 20: Proteasome subunit alpha type-2

Chain H:  85% 14%



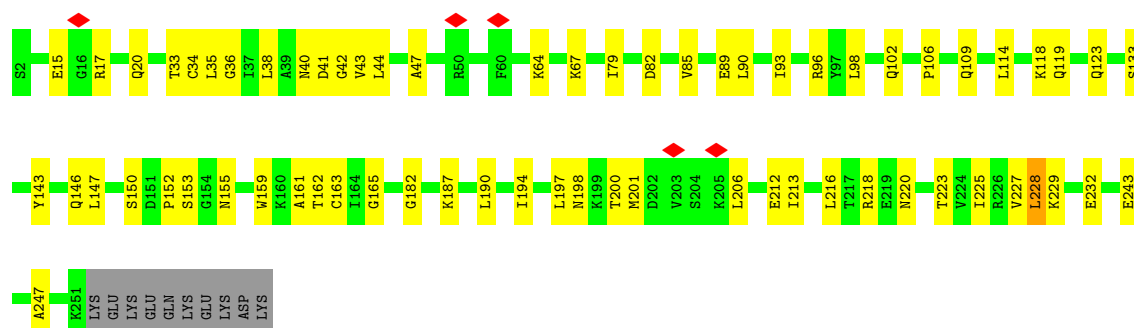
- Molecule 20: Proteasome subunit alpha type-2

Chain h:  87% 13%



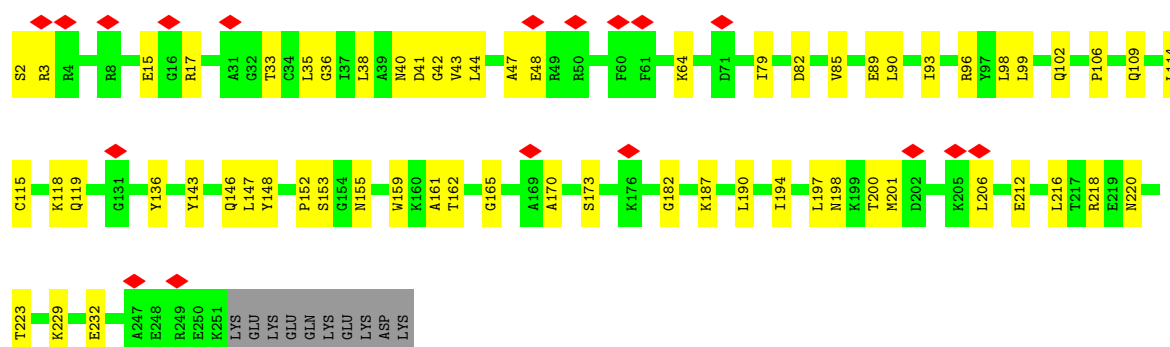
- Molecule 21: Proteasome subunit alpha type-4

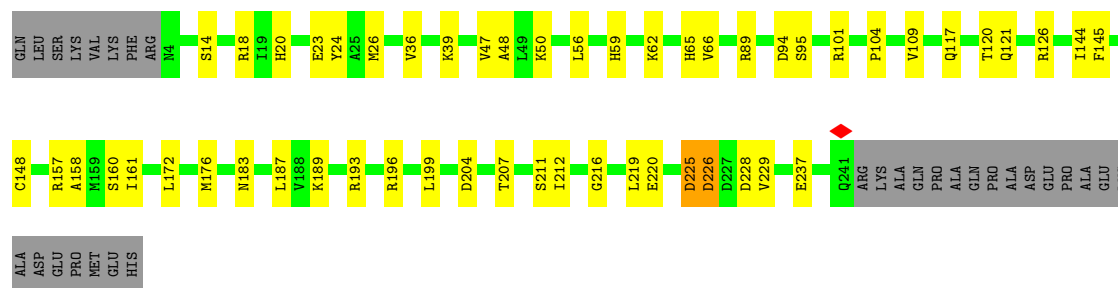
Chain I:  71% 25%



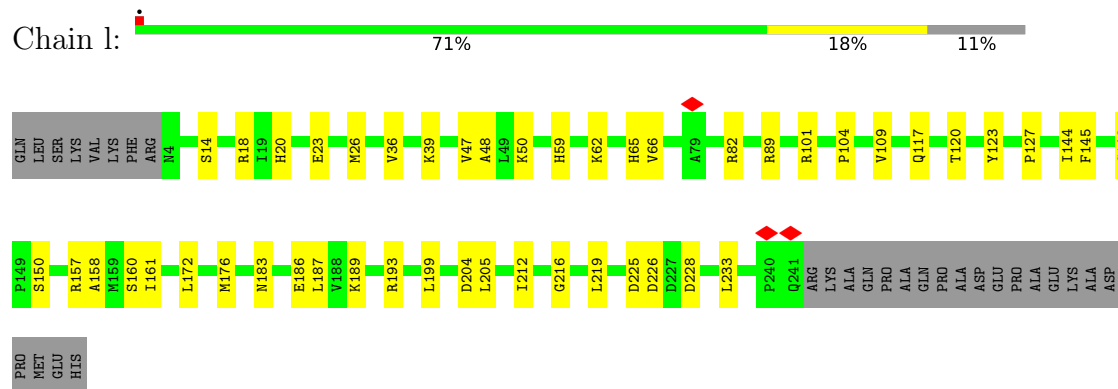
- Molecule 21: Proteasome subunit alpha type-4

Chain i:  72% 24%

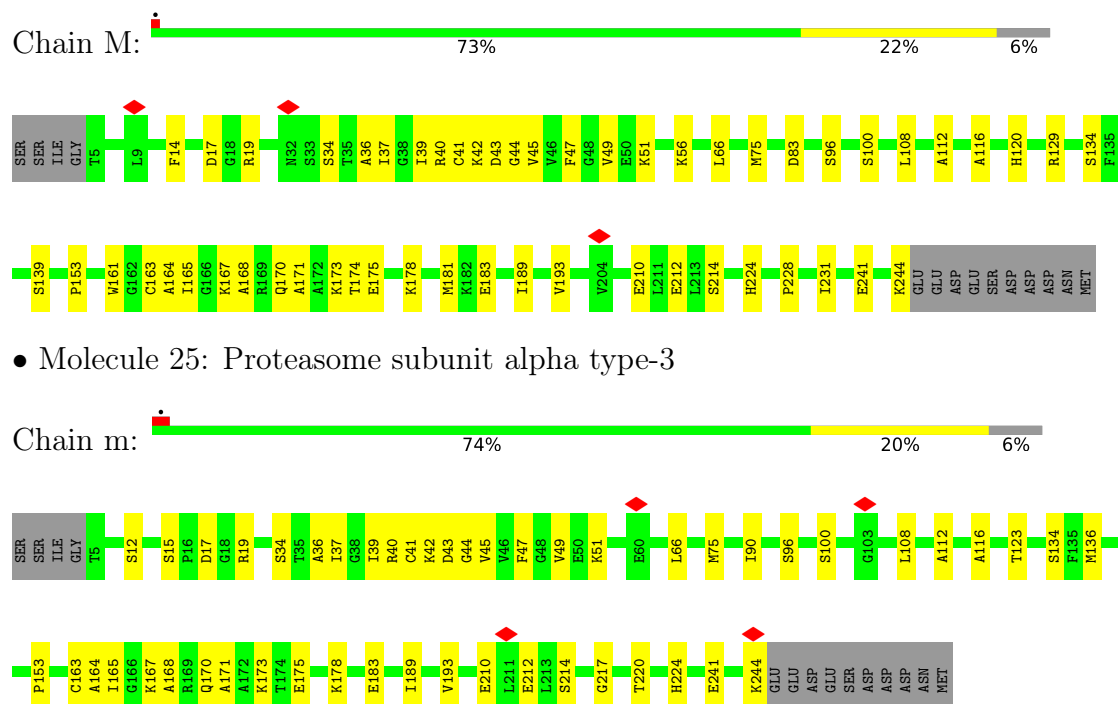




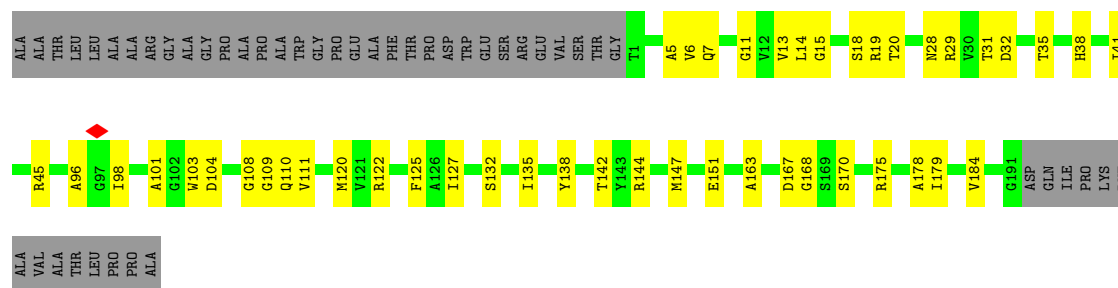
- Molecule 24: Isoform Long of Proteasome subunit alpha type-1



- Molecule 25: Proteasome subunit alpha type-3

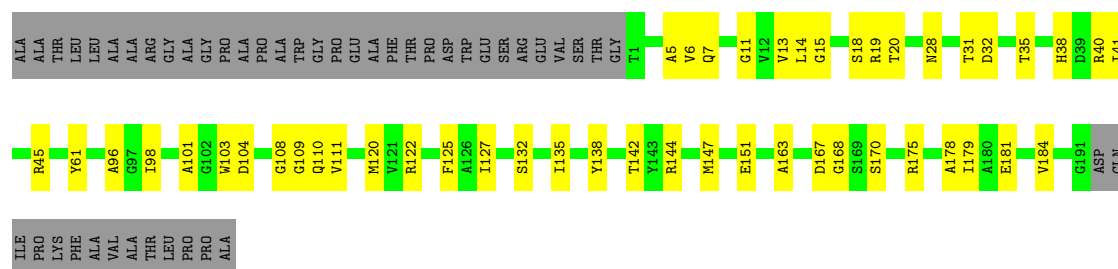


- Molecule 26: Proteasome subunit beta type-6



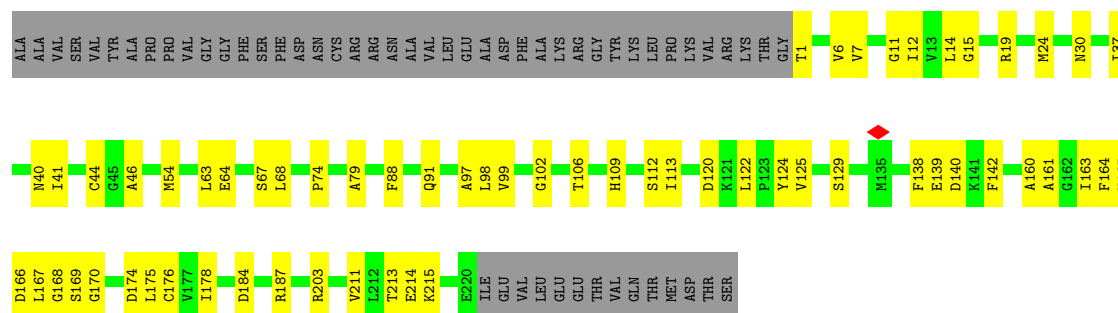
• Molecule 26: Proteasome subunit beta type-6

Chain n: 60% 20% 20%



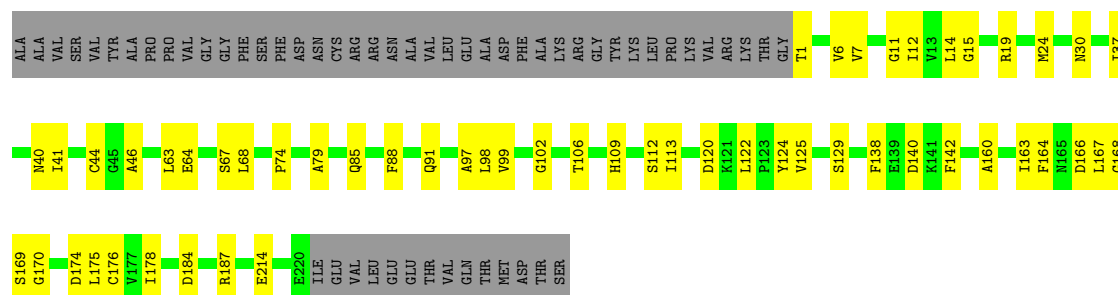
• Molecule 27: Proteasome subunit beta type-7

Chain O: 57% 22% 20%



• Molecule 27: Proteasome subunit beta type-7

Chain o: 60% 20% 20%



• Molecule 28: Proteasome subunit beta type-3

Chain P:  85% 15%



- Molecule 28: Proteasome subunit beta type-3

Chain p:  86% 14%



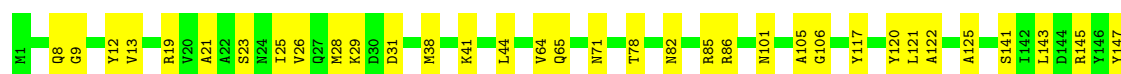
- Molecule 29: Proteasome subunit beta type-2

Chain Q:  81% 18%



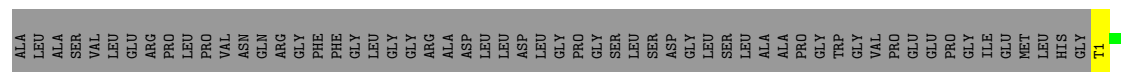
- Molecule 29: Proteasome subunit beta type-2

Chain q:  79% 20%



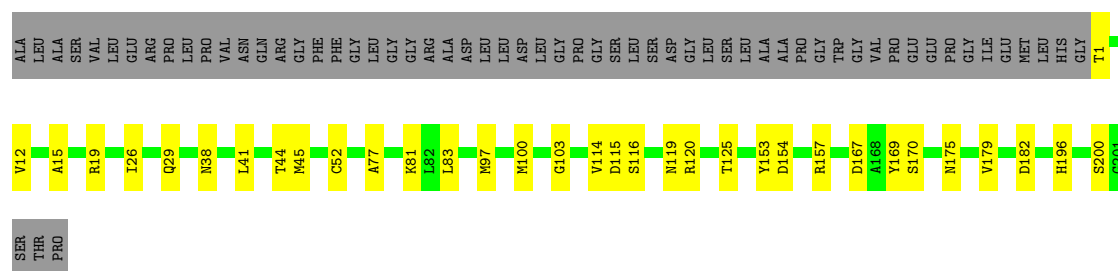
- Molecule 30: Proteasome subunit beta type-5

Chain R:  61% 16% 23%



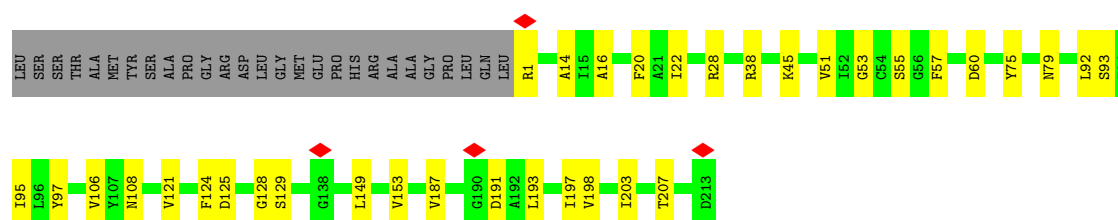
- Molecule 30: Proteasome subunit beta type-5

Chain r:  64% 13% 23%



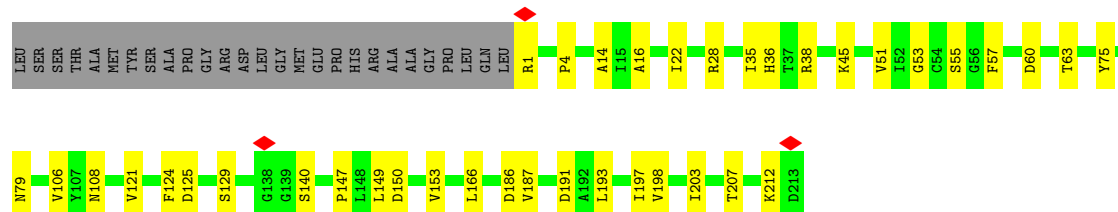
• Molecule 31: Proteasome subunit beta type-1

Chain S:  74% 15% 11%



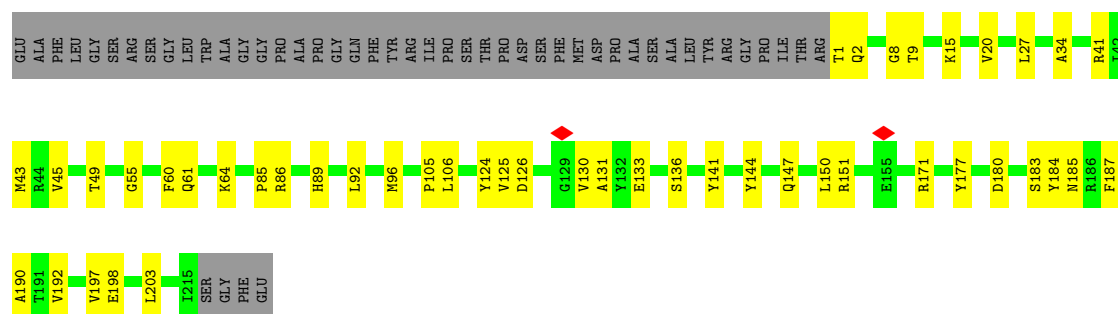
• Molecule 31: Proteasome subunit beta type-1

Chain s:  72% 16% 11%



• Molecule 32: Proteasome subunit beta type-4

Chain T:  64% 18% 18%



• Molecule 32: Proteasome subunit beta type-4

Chain t:  63% 19% 18%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29419	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 ($e^-/\text{\AA}^2$)	46.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0332	Depositor
Map size (Å)	438.4, 438.4, 438.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	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, ZN, ADP, MG

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	U	0.24	0/6449	0.63	2/8729 (0.0%)
2	V	0.33	1/4072 (0.0%)	0.78	5/5510 (0.1%)
3	W	0.30	0/3751	0.77	2/5042 (0.0%)
4	X	0.24	0/3053	0.56	0/4115
5	Y	0.26	0/3173	0.63	0/4273
6	Z	0.25	0/2324	0.67	2/3150 (0.1%)
7	a	0.23	0/3053	0.63	2/4133 (0.0%)
8	b	0.22	0/1478	0.63	0/2001
9	c	0.27	0/2302	0.70	2/3110 (0.1%)
10	d	0.26	0/2162	0.69	2/2919 (0.1%)
11	e	0.28	0/338	0.79	0/450
12	f	0.30	0/6973	0.83	16/9424 (0.2%)
13	A	0.27	0/3148	0.68	2/4250 (0.0%)
14	B	0.28	0/3053	0.74	6/4118 (0.1%)
15	C	0.25	0/2902	0.66	2/3904 (0.1%)
16	D	0.28	0/3089	0.67	4/4168 (0.1%)
17	E	0.26	0/2904	0.62	0/3924
18	F	0.25	0/2896	0.57	0/3912
19	G	0.24	0/1859	0.53	0/2523
19	g	0.24	0/1859	0.53	0/2523
20	H	0.24	0/1743	0.50	0/2372
20	h	0.24	0/1743	0.50	0/2372
21	I	0.24	0/1942	0.57	0/2628
21	i	0.24	0/1942	0.56	0/2628
22	J	0.23	0/1737	0.56	0/2369
22	j	0.23	0/1728	0.56	0/2358
23	K	0.24	0/1747	0.51	0/2364
23	k	0.24	0/1747	0.51	0/2364
24	L	0.26	0/1885	0.59	1/2552 (0.0%)
24	l	0.25	0/1885	0.60	2/2552 (0.1%)
25	M	0.24	0/1891	0.52	0/2552
25	m	0.24	0/1891	0.52	0/2552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	N	0.22	0/1454	0.50	0/1967
26	n	0.22	0/1454	0.50	0/1967
27	O	0.23	0/1670	0.49	0/2265
27	o	0.23	0/1670	0.49	0/2265
28	P	0.24	0/1620	0.48	0/2184
28	p	0.24	0/1620	0.48	0/2184
29	Q	0.26	0/1603	0.52	0/2174
29	q	0.26	0/1603	0.53	0/2174
30	R	0.25	0/1579	0.46	0/2134
30	r	0.25	0/1579	0.46	0/2134
31	S	0.24	0/1671	0.49	0/2253
31	s	0.24	0/1674	0.49	0/2257
32	T	0.24	0/1700	0.51	0/2305
32	t	0.24	0/1700	0.51	0/2305
All	All	0.26	1/105316 (0.0%)	0.62	50/142409 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	132	LEU	C-N	5.32	1.38	1.33

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	53	THR	CA-C-N	13.59	136.82	119.84
14	B	53	THR	C-N-CA	13.59	136.82	119.84
12	f	651	GLY	N-CA-C	-10.85	99.36	112.49
6	Z	245	PHE	N-CA-C	-10.61	99.72	111.28
12	f	755	ASP	CA-C-N	10.47	132.93	119.84
12	f	755	ASP	C-N-CA	10.47	132.93	119.84
13	A	310	ASP	CA-C-N	9.67	131.93	119.84
13	A	310	ASP	C-N-CA	9.67	131.93	119.84
12	f	755	ASP	N-CA-C	-8.64	100.42	112.17
15	C	127	LEU	CA-C-N	8.61	130.61	119.84
15	C	127	LEU	C-N-CA	8.61	130.61	119.84
12	f	810	ILE	N-CA-C	8.30	120.92	109.46
16	D	150	SER	N-CA-C	-8.10	93.78	107.80
16	D	125	LYS	N-CA-C	8.00	127.50	109.81
2	V	171	VAL	N-CA-C	-7.89	105.50	113.47
1	U	473	VAL	N-CA-C	-7.75	105.21	112.96
12	f	713	PHE	N-CA-C	-7.43	103.12	111.07
1	U	178	ALA	N-CA-C	-7.40	102.59	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	f	679	LEU	N-CA-C	7.21	118.69	108.74
14	B	60	LEU	N-CA-C	-6.98	103.60	111.14
12	f	774	GLY	N-CA-C	-6.78	106.64	115.59
12	f	808	ASN	N-CA-C	6.69	119.83	108.67
12	f	787	LEU	N-CA-C	6.36	120.61	112.86
12	f	680	ARG	N-CA-C	-6.27	97.44	110.80
3	W	86	ASN	N-CA-C	5.95	117.69	107.28
12	f	379	GLY	N-CA-C	5.93	119.67	112.49
14	B	167	THR	CB-CA-C	-5.79	108.90	115.79
12	f	772	GLY	O-C-N	5.77	130.20	122.70
2	V	223	LYS	N-CA-C	5.76	118.22	111.02
9	c	48	GLY	CA-C-N	5.64	123.80	120.24
9	c	48	GLY	C-N-CA	5.64	123.80	120.24
12	f	809	ILE	N-CA-C	5.64	121.07	109.34
2	V	266	GLN	N-CA-C	-5.58	106.41	113.43
2	V	28	PRO	N-CA-C	5.54	117.45	110.70
6	Z	244	GLU	N-CA-C	-5.47	106.68	113.19
12	f	788	MET	N-CA-C	5.44	117.12	108.79
24	L	225	ASP	N-CA-C	5.37	117.16	108.41
3	W	46	THR	CB-CA-C	-5.36	104.79	111.43
10	d	231	LYS	N-CA-C	5.34	120.94	113.57
24	l	225	ASP	CA-C-N	5.29	131.63	121.54
24	l	225	ASP	C-N-CA	5.29	131.63	121.54
7	a	186	LYS	CA-C-N	5.22	131.51	121.54
7	a	186	LYS	C-N-CA	5.22	131.51	121.54
16	D	160	PRO	CA-C-N	5.14	129.71	122.46
16	D	160	PRO	C-N-CA	5.14	129.71	122.46
14	B	118	ASP	CA-C-N	5.09	131.27	121.54
14	B	118	ASP	C-N-CA	5.09	131.27	121.54
10	d	174	ILE	N-CA-C	-5.06	107.50	113.42
2	V	27	PRO	N-CA-C	5.05	116.86	110.70
12	f	639	LYS	N-CA-C	-5.03	107.09	113.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	6334	0	6365	203	0
2	V	3994	0	3960	203	0
3	W	3703	0	3822	227	0
4	X	3009	0	3113	37	0
5	Y	3115	0	3120	75	0
6	Z	2281	0	2310	74	0
7	a	2995	0	3011	67	0
8	b	1458	0	1505	33	0
9	c	2260	0	2275	107	0
10	d	2116	0	2146	71	0
11	e	334	0	294	47	0
12	f	6860	0	6859	372	0
13	A	3096	0	3138	76	0
14	B	3011	0	3075	143	0
15	C	2864	0	2969	228	0
16	D	3039	0	3075	234	0
17	E	2860	0	2826	98	0
18	F	2858	0	2852	61	0
19	G	1826	0	1796	41	0
19	g	1826	0	1796	47	0
20	H	1708	0	1594	22	0
20	h	1708	0	1594	18	0
21	I	1912	0	1851	53	0
21	i	1912	0	1851	44	0
22	J	1713	0	1537	30	0
22	j	1704	0	1517	27	0
23	K	1722	0	1673	35	0
23	k	1722	0	1673	33	0
24	L	1850	0	1822	39	0
24	l	1850	0	1822	30	0
25	M	1856	0	1814	35	0
25	m	1856	0	1814	32	0
26	N	1430	0	1398	28	0
26	n	1430	0	1398	29	0
27	O	1643	0	1644	43	0
27	o	1643	0	1644	38	0
28	P	1591	0	1609	24	0
28	p	1591	0	1609	21	0
29	Q	1570	0	1547	26	0
29	q	1570	0	1547	30	0
30	R	1548	0	1499	30	0
30	r	1548	0	1499	23	0
31	S	1641	0	1616	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	s	1644	0	1625	30	0
32	T	1667	0	1628	30	0
32	t	1667	0	1628	36	0
33	c	1	0	0	0	0
34	A	31	0	12	0	0
34	B	31	0	12	8	0
34	D	31	0	12	2	0
34	E	31	0	10	35	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	D	1	0	0	0	0
35	E	1	0	0	0	0
35	F	1	0	0	0	0
36	C	27	0	12	13	0
36	F	27	0	12	8	0
All	All	103719	0	102830	2825	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 14.

All (2825) 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)
3:W:137:TYR:CE1	16:D:392:TYR:CD1	1.78	1.68
3:W:137:TYR:CZ	16:D:392:TYR:CD1	1.79	1.62
12:f:222:ASP:CB	14:B:60:LEU:CD2	1.76	1.62
15:C:90:HIS:HE1	16:D:109:SER:CB	1.03	1.61
3:W:97:LEU:HD21	3:W:138:VAL:CG2	1.23	1.60
16:D:87:LEU:CD1	16:D:140:VAL:HG11	1.31	1.59
3:W:97:LEU:CD2	3:W:138:VAL:HG21	1.31	1.57
1:U:171:ASN:CG	1:U:176:MET:HE1	1.15	1.56
9:c:196:LEU:HA	9:c:200:TYR:CZ	1.38	1.54
16:D:87:LEU:CD2	16:D:131:ALA:HB1	1.29	1.54
3:W:48:LEU:CD2	3:W:95:SER:HB2	1.34	1.54
16:D:335:LEU:CD2	16:D:369:LYS:CG	1.83	1.53
16:D:335:LEU:HD23	16:D:369:LYS:CG	1.37	1.51
1:U:171:ASN:ND2	1:U:176:MET:CE	1.71	1.51
12:f:222:ASP:CG	14:B:60:LEU:CD2	1.78	1.50
15:C:24:TYR:CE2	16:D:40:LEU:HG	1.47	1.49
9:c:196:LEU:HA	9:c:200:TYR:CE2	1.45	1.49
3:W:137:TYR:CE1	16:D:392:TYR:CE1	1.96	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:87:LEU:HD11	16:D:140:VAL:CB	1.40	1.49
15:C:90:HIS:CE1	16:D:109:SER:CB	1.95	1.49
12:f:250:ARG:CZ	12:f:281:ILE:HD12	1.39	1.48
1:U:171:ASN:ND2	1:U:176:MET:HE1	1.15	1.48
15:C:24:TYR:CD2	16:D:40:LEU:HG	1.47	1.48
3:W:48:LEU:HD21	3:W:95:SER:CB	1.40	1.47
12:f:708:ASP:CB	12:f:787:LEU:CD2	1.92	1.46
16:D:87:LEU:HD21	16:D:131:ALA:CB	1.42	1.46
12:f:708:ASP:CB	12:f:787:LEU:HD23	1.45	1.45
12:f:838:ARG:CD	12:f:839:PRO:HD3	1.44	1.45
15:C:90:HIS:CG	15:C:91:PRO:HD3	1.50	1.44
15:C:152:GLY:H	36:C:501:ADP:N6	1.16	1.43
9:c:191:ALA:O	9:c:196:LEU:CD2	1.65	1.43
15:C:152:GLY:N	36:C:501:ADP:HN62	1.11	1.41
3:W:178:GLU:OE1	3:W:181:GLU:CB	1.67	1.40
16:D:335:LEU:CD2	16:D:369:LYS:HG3	1.41	1.38
10:d:195:THR:O	10:d:200:PHE:CE1	1.74	1.38
17:E:340:GLY:HA3	34:E:401:ATP:N7	1.38	1.37
12:f:658:ALA:HB3	14:B:78:PHE:CE2	1.58	1.37
16:D:87:LEU:HD11	16:D:140:VAL:CG1	1.52	1.37
12:f:759:LEU:CD2	12:f:806:VAL:HG11	1.56	1.36
3:W:137:TYR:CZ	16:D:392:TYR:HD1	1.23	1.36
9:c:196:LEU:CA	9:c:200:TYR:CZ	2.09	1.36
12:f:755:ASP:CB	12:f:756:PRO:HD3	1.50	1.35
16:D:85:ILE:HG23	16:D:86:PRO:CD	1.56	1.35
19:g:46:ASP:CB	19:g:222:VAL:CG2	2.06	1.34
2:V:195:ILE:HG21	15:C:25:LEU:CD1	1.57	1.34
16:D:87:LEU:CD1	16:D:140:VAL:CG1	2.04	1.33
19:g:46:ASP:CB	19:g:222:VAL:HG21	1.55	1.33
2:V:345:ARG:HH21	2:V:361:PHE:N	1.26	1.31
16:D:87:LEU:CD2	16:D:131:ALA:CB	2.03	1.31
17:E:180:LYS:N	34:E:401:ATP:O2A	1.61	1.31
1:U:567:ILE:CG2	1:U:601:ARG:HH22	1.42	1.31
3:W:48:LEU:CD2	3:W:95:SER:CB	1.99	1.29
17:E:179:GLY:CA	34:E:401:ATP:O2A	1.80	1.29
15:C:90:HIS:CD2	15:C:91:PRO:HD2	1.69	1.28
2:V:195:ILE:HG13	15:C:25:LEU:CD2	1.62	1.28
12:f:673:ARG:NE	12:f:712:LYS:HG2	1.46	1.27
3:W:137:TYR:CZ	16:D:392:TYR:CE1	2.16	1.27
10:d:155:LYS:NZ	10:d:171:LEU:HG	1.48	1.27
12:f:766:GLN:HG3	12:f:807:ARG:NH2	1.50	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:222:ASP:CB	14:B:60:LEU:HD21	1.47	1.25
12:f:838:ARG:HD2	12:f:839:PRO:CD	1.67	1.25
12:f:222:ASP:OD2	14:B:60:LEU:HD23	1.31	1.25
12:f:222:ASP:CG	14:B:60:LEU:HD22	1.38	1.24
3:W:178:GLU:OE1	3:W:181:GLU:HB3	1.05	1.23
14:B:53:THR:HG23	14:B:54:PRO:CD	1.66	1.23
17:E:182:LEU:HD22	34:E:401:ATP:O2'	1.07	1.23
12:f:250:ARG:CZ	12:f:281:ILE:CD1	2.17	1.22
15:C:90:HIS:CD2	15:C:91:PRO:CD	2.22	1.21
3:W:137:TYR:HB3	3:W:144:ARG:NH2	1.55	1.21
15:C:90:HIS:CE1	16:D:109:SER:HB3	1.68	1.21
1:U:171:ASN:CG	1:U:176:MET:CE	2.07	1.20
12:f:340:MET:SD	12:f:757:ASN:ND2	2.13	1.20
3:W:316:ARG:HD2	3:W:383:ASP:OD2	1.40	1.20
17:E:179:GLY:N	34:E:401:ATP:O2A	1.74	1.20
1:U:151:ILE:HD11	1:U:177:LEU:CD2	1.70	1.19
17:E:179:GLY:C	34:E:401:ATP:O2A	1.84	1.19
9:c:195:GLY:O	9:c:200:TYR:CD1	1.96	1.19
9:c:196:LEU:CA	9:c:200:TYR:CE2	2.24	1.19
1:U:644:TYR:O	15:C:60:ARG:NH1	1.75	1.18
3:W:178:GLU:CD	3:W:181:GLU:H	1.52	1.17
2:V:195:ILE:HG13	15:C:25:LEU:CG	1.73	1.17
12:f:222:ASP:HB3	14:B:60:LEU:CD2	1.69	1.17
12:f:838:ARG:HB3	12:f:839:PRO:CD	1.70	1.17
14:B:278:ALA:HB1	14:B:279:PRO:CD	1.75	1.17
11:e:56:LEU:HD11	11:e:59:GLU:HB3	1.17	1.16
12:f:650:GLN:OE1	14:B:72:LEU:HD13	1.46	1.16
15:C:31:LEU:HD21	16:D:47:LEU:HD12	1.25	1.16
12:f:810:ILE:HD13	12:f:853:VAL:O	1.42	1.16
2:V:345:ARG:NH2	2:V:361:PHE:N	1.95	1.15
19:g:47:CYS:HB3	19:g:221:THR:HG22	1.23	1.15
1:U:583:MET:HE1	1:U:602:LEU:HD23	1.18	1.15
15:C:90:HIS:CG	15:C:91:PRO:CD	2.29	1.14
3:W:137:TYR:OH	16:D:392:TYR:HD1	0.81	1.14
12:f:708:ASP:HB3	12:f:787:LEU:CD2	1.63	1.13
12:f:755:ASP:OD1	12:f:756:PRO:HD2	1.46	1.13
3:W:137:TYR:HB3	3:W:144:ARG:CZ	1.76	1.13
12:f:759:LEU:CD2	12:f:806:VAL:CG1	2.26	1.13
9:c:196:LEU:HA	9:c:200:TYR:CE1	1.84	1.12
11:e:56:LEU:HD11	11:e:59:GLU:CB	1.77	1.12
3:W:48:LEU:HD23	3:W:95:SER:N	1.63	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:567:ILE:HG22	1:U:601:ARG:NH2	1.64	1.12
14:B:278:ALA:HB1	14:B:279:PRO:HD3	1.19	1.12
19:G:46:ASP:CB	19:G:222:VAL:HG21	1.79	1.12
9:c:195:GLY:C	9:c:200:TYR:CE1	2.27	1.11
3:W:90:LEU:CD2	3:W:96:GLN:HG3	1.80	1.11
9:c:191:ALA:C	9:c:196:LEU:HD21	1.74	1.11
12:f:708:ASP:HB3	12:f:787:LEU:HD21	1.28	1.11
15:C:73:VAL:HG23	15:C:127:LEU:HD11	1.26	1.11
12:f:783:SER:O	12:f:786:GLN:NE2	1.81	1.11
1:U:151:ILE:HD11	1:U:177:LEU:HD21	1.13	1.10
12:f:556:ARG:HD3	12:f:786:GLN:HG2	1.14	1.10
3:W:48:LEU:HD21	3:W:95:SER:HB3	1.28	1.10
12:f:250:ARG:NH2	12:f:281:ILE:HD12	1.65	1.10
15:C:24:TYR:CE2	16:D:40:LEU:CG	2.33	1.10
14:B:56:THR:O	14:B:61:LYS:NZ	1.84	1.10
15:C:90:HIS:HE1	16:D:109:SER:HB3	0.93	1.10
16:D:85:ILE:HG23	16:D:86:PRO:HD3	1.10	1.10
19:G:46:ASP:CB	19:G:222:VAL:CG2	2.30	1.10
15:C:113:ARG:HB3	15:C:127:LEU:HD12	1.34	1.09
2:V:195:ILE:HG21	15:C:25:LEU:CG	1.81	1.09
12:f:673:ARG:HH21	12:f:712:LYS:HG3	1.13	1.09
3:W:178:GLU:OE1	3:W:181:GLU:CA	2.00	1.08
15:C:90:HIS:CE1	16:D:109:SER:HB2	1.70	1.08
15:C:90:HIS:CB	15:C:91:PRO:HD3	1.81	1.08
16:D:88:VAL:O	16:D:132:LEU:N	1.84	1.08
2:V:195:ILE:HG21	15:C:25:LEU:HD11	1.23	1.08
16:D:87:LEU:HD11	16:D:140:VAL:HB	1.26	1.08
12:f:556:ARG:HD3	12:f:786:GLN:CG	1.83	1.08
2:V:195:ILE:HB	15:C:25:LEU:HD21	1.32	1.08
12:f:838:ARG:HB3	12:f:839:PRO:HD2	1.12	1.08
12:f:708:ASP:CG	12:f:787:LEU:CD2	2.26	1.07
1:U:567:ILE:HG22	1:U:601:ARG:HH22	0.95	1.07
9:c:191:ALA:O	9:c:196:LEU:HD21	0.91	1.07
12:f:673:ARG:HE	12:f:712:LYS:CG	1.67	1.07
12:f:222:ASP:CG	14:B:60:LEU:HD23	1.58	1.07
15:C:198:LEU:HD23	36:C:501:ADP:H5'2	1.31	1.07
12:f:658:ALA:CB	14:B:78:PHE:CD2	2.38	1.07
12:f:708:ASP:HB2	12:f:787:LEU:HD23	1.09	1.07
16:D:87:LEU:CG	16:D:131:ALA:HB1	1.84	1.07
3:W:178:GLU:CD	3:W:181:GLU:CB	2.27	1.06
12:f:250:ARG:NH1	12:f:281:ILE:HD12	1.68	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:178:GLU:CD	3:W:181:GLU:HB3	1.80	1.06
12:f:222:ASP:HB3	14:B:60:LEU:HD21	1.21	1.06
12:f:755:ASP:CG	12:f:756:PRO:HD3	1.79	1.06
12:f:755:ASP:HB2	12:f:756:PRO:HD3	1.11	1.06
2:V:195:ILE:HG13	15:C:25:LEU:HG	1.38	1.05
3:W:90:LEU:HD21	3:W:96:GLN:HG3	1.15	1.05
16:D:150:SER:OG	16:D:153:MET:HE1	1.56	1.05
12:f:222:ASP:HB2	14:B:60:LEU:HD21	1.30	1.05
9:c:196:LEU:HA	9:c:200:TYR:CD2	1.92	1.05
12:f:759:LEU:HD23	12:f:806:VAL:HG11	1.11	1.05
14:B:278:ALA:CB	14:B:279:PRO:CD	2.34	1.05
15:C:152:GLY:CA	36:C:501:ADP:HN62	1.67	1.05
2:V:195:ILE:CG1	15:C:25:LEU:HG	1.87	1.05
12:f:708:ASP:CG	12:f:787:LEU:HD23	1.81	1.04
16:D:370:ILE:H	16:D:370:ILE:HD12	1.22	1.04
2:V:195:ILE:CG1	15:C:25:LEU:CD2	2.34	1.04
12:f:222:ASP:HB2	14:B:60:LEU:CD2	1.77	1.04
12:f:766:GLN:CG	12:f:807:ARG:HH22	1.69	1.04
15:C:24:TYR:CD2	16:D:40:LEU:CG	2.40	1.04
17:E:182:LEU:CD2	34:E:401:ATP:O2'	2.03	1.04
2:V:166:TYR:O	2:V:175:MET:HE1	1.56	1.04
17:E:312:ILE:HG12	34:E:401:ATP:N1	1.39	1.04
16:D:87:LEU:CD1	16:D:140:VAL:CB	2.34	1.04
6:Z:223:ASN:CG	6:Z:227:ILE:CG1	2.31	1.04
16:D:335:LEU:HD21	16:D:369:LYS:HG2	1.06	1.04
17:E:312:ILE:CG1	34:E:401:ATP:N1	2.15	1.04
12:f:759:LEU:HD21	12:f:806:VAL:CG1	1.86	1.03
24:L:211:SER:OG	24:L:225:ASP:OD1	1.74	1.03
12:f:755:ASP:CB	12:f:756:PRO:CD	2.36	1.03
9:c:195:GLY:O	9:c:200:TYR:CE1	2.12	1.03
12:f:673:ARG:NE	12:f:712:LYS:CG	2.21	1.03
12:f:222:ASP:OD2	14:B:60:LEU:HA	1.59	1.02
15:C:73:VAL:HG23	15:C:127:LEU:CD1	1.89	1.02
2:V:317:PRO:HG2	11:e:4:LYS:CG	1.89	1.02
2:V:496:PHE:CE1	15:C:40:GLN:NE2	2.27	1.02
12:f:250:ARG:NH2	12:f:281:ILE:CD1	2.22	1.02
1:U:583:MET:CE	1:U:602:LEU:HD23	1.90	1.02
2:V:195:ILE:HG13	15:C:25:LEU:HD23	1.33	1.02
2:V:496:PHE:CD1	15:C:40:GLN:NE2	2.28	1.02
3:W:48:LEU:HD23	3:W:95:SER:CB	1.89	1.01
12:f:755:ASP:OD1	12:f:756:PRO:CD	2.07	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:182:LEU:HD22	34:E:401:ATP:C2'	1.90	1.01
17:E:312:ILE:HG23	34:E:401:ATP:C2	1.94	1.01
12:f:556:ARG:CD	12:f:786:GLN:HG2	1.89	1.01
12:f:658:ALA:CB	14:B:78:PHE:CE2	2.42	1.01
2:V:345:ARG:NH2	2:V:361:PHE:H	1.52	1.01
2:V:346:LEU:HD12	11:e:46:ASP:OD2	1.60	1.01
16:D:335:LEU:HD21	16:D:369:LYS:CG	1.64	1.00
12:f:810:ILE:CD1	12:f:853:VAL:O	2.10	1.00
3:W:137:TYR:HB2	3:W:144:ARG:NH1	1.76	1.00
14:B:53:THR:CG2	14:B:54:PRO:HD3	1.90	0.99
15:C:31:LEU:CD2	16:D:47:LEU:HD12	1.91	0.99
16:D:335:LEU:HD23	16:D:369:LYS:CD	1.91	0.99
13:A:401:ARG:NH1	13:A:408:ASP:OD2	1.95	0.99
2:V:317:PRO:HG2	11:e:4:LYS:HG3	1.39	0.99
16:D:87:LEU:HD23	16:D:131:ALA:HB1	1.44	0.99
17:E:180:LYS:HB2	34:E:401:ATP:O2B	1.63	0.98
1:U:567:ILE:CG2	1:U:601:ARG:NH2	2.24	0.98
15:C:52:LEU:HG	16:D:68:LEU:HD13	1.44	0.98
15:C:90:HIS:HE1	16:D:109:SER:HB2	1.07	0.98
12:f:766:GLN:HG3	12:f:807:ARG:HH22	0.82	0.98
12:f:838:ARG:CB	12:f:839:PRO:CD	2.41	0.98
12:f:647:GLY:O	14:B:71:TYR:CB	2.11	0.98
3:W:137:TYR:CB	3:W:144:ARG:NH1	2.26	0.97
11:e:56:LEU:CD1	11:e:59:GLU:HB3	1.93	0.97
16:D:85:ILE:HG23	16:D:86:PRO:HD2	1.42	0.97
3:W:178:GLU:OE1	3:W:181:GLU:N	1.96	0.97
12:f:673:ARG:NH2	12:f:712:LYS:HB3	1.79	0.96
9:c:191:ALA:O	9:c:196:LEU:CG	2.12	0.96
2:V:495:ARG:H	15:C:44:ARG:NH1	1.61	0.96
7:a:64:ILE:O	7:a:68:GLU:HB2	1.66	0.96
3:W:46:THR:HG22	3:W:50:LEU:CD1	1.95	0.96
3:W:55:ARG:NH1	3:W:78:LYS:HD2	1.81	0.96
16:D:85:ILE:CG2	16:D:86:PRO:CD	2.43	0.95
2:V:195:ILE:CB	15:C:25:LEU:HD21	1.96	0.95
2:V:319:HIS:NE2	11:e:4:LYS:HG3	1.81	0.95
12:f:556:ARG:HG2	12:f:786:GLN:HE21	1.32	0.95
16:D:87:LEU:HD21	16:D:131:ALA:HB3	1.45	0.95
24:L:207:THR:O	24:L:226:ASP:HB2	1.67	0.95
2:V:496:PHE:HE1	15:C:40:GLN:CG	1.79	0.95
3:W:315:MET:O	3:W:319:THR:OG1	1.84	0.95
3:W:137:TYR:CB	3:W:144:ARG:CZ	2.44	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:146:ASP:HB3	9:c:156:VAL:HB	1.49	0.95
15:C:90:HIS:CE1	16:D:109:SER:CA	2.50	0.95
19:G:46:ASP:O	19:G:222:VAL:HG23	1.65	0.95
14:B:53:THR:HG23	14:B:54:PRO:HD3	0.95	0.94
2:V:195:ILE:CG2	15:C:25:LEU:HD11	1.96	0.94
12:f:712:LYS:HD3	12:f:715:HIS:HB2	1.45	0.94
12:f:213:GLN:O	12:f:217:LEU:HB2	1.67	0.94
12:f:673:ARG:HE	12:f:712:LYS:HG2	1.01	0.94
14:B:53:THR:CG2	14:B:54:PRO:CD	2.45	0.93
2:V:494:MET:H	15:C:44:ARG:HH12	1.12	0.93
9:c:196:LEU:H	9:c:196:LEU:HD22	1.34	0.93
21:i:36:GLY:O	21:i:161:ALA:HA	1.69	0.93
17:E:312:ILE:HG23	34:E:401:ATP:N1	1.83	0.93
12:f:708:ASP:CB	12:f:787:LEU:HD21	1.82	0.93
12:f:673:ARG:NH2	12:f:712:LYS:HG3	1.83	0.93
16:D:335:LEU:CD2	16:D:369:LYS:HG2	1.69	0.93
17:E:340:GLY:CA	34:E:401:ATP:N7	2.29	0.93
13:A:401:ARG:CD	13:A:403:ILE:O	2.17	0.92
21:I:36:GLY:O	21:I:161:ALA:HA	1.69	0.92
10:d:155:LYS:HZ2	10:d:171:LEU:HG	1.18	0.92
3:W:48:LEU:CG	3:W:95:SER:HB2	2.00	0.92
6:Z:223:ASN:OD1	6:Z:227:ILE:HG13	1.67	0.92
12:f:395:GLY:O	12:f:399:LEU:HB2	1.68	0.92
9:c:196:LEU:CB	9:c:200:TYR:CE2	2.53	0.92
10:d:195:THR:O	10:d:200:PHE:CD1	2.21	0.92
12:f:673:ARG:NH2	12:f:712:LYS:CG	2.33	0.92
12:f:678:LEU:HG	12:f:679:LEU:HG	1.51	0.92
19:g:47:CYS:CB	19:g:221:THR:HG22	2.00	0.92
16:D:151:ILE:HD12	16:D:151:ILE:H	1.34	0.91
12:f:838:ARG:CD	12:f:839:PRO:CD	2.36	0.91
2:V:46:GLY:O	2:V:50:GLU:HB2	1.70	0.91
9:c:196:LEU:HB3	9:c:200:TYR:CE2	2.05	0.91
16:D:87:LEU:HD13	16:D:140:VAL:HG11	0.92	0.91
12:f:755:ASP:HB2	12:f:756:PRO:CD	1.99	0.91
3:W:178:GLU:CD	3:W:181:GLU:N	2.29	0.91
11:e:57:ARG:HG2	11:e:57:ARG:HH11	1.34	0.91
15:C:31:LEU:HD21	16:D:47:LEU:CD1	2.01	0.91
11:e:56:LEU:HD11	11:e:59:GLU:CA	2.01	0.91
15:C:52:LEU:HD23	16:D:68:LEU:HD12	1.52	0.91
2:V:167:LEU:HD21	2:V:171:VAL:HG11	1.52	0.91
3:W:48:LEU:HD23	3:W:95:SER:CA	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:759:LEU:CD1	12:f:808:ASN:HA	2.01	0.91
3:W:90:LEU:HD21	3:W:96:GLN:CG	2.00	0.90
12:f:658:ALA:HB3	14:B:78:PHE:CD2	2.03	0.90
10:d:195:THR:O	10:d:200:PHE:HE1	1.48	0.90
1:U:567:ILE:CB	1:U:601:ARG:HH22	1.84	0.90
16:D:85:ILE:CG2	16:D:86:PRO:HD3	2.01	0.90
1:U:642:GLU:OE1	15:C:57:ARG:NH2	2.05	0.90
1:U:171:ASN:ND2	1:U:176:MET:HE2	1.84	0.89
3:W:48:LEU:HD23	3:W:95:SER:HB2	1.48	0.89
12:f:281:ILE:HG22	12:f:282:PHE:HB2	1.52	0.89
6:Z:223:ASN:CG	6:Z:227:ILE:HG12	1.82	0.89
19:G:202:LEU:O	19:G:206:LEU:HB2	1.73	0.89
12:f:755:ASP:CG	12:f:756:PRO:CD	2.45	0.89
10:d:155:LYS:HZ1	10:d:171:LEU:HG	1.30	0.89
6:Z:146:ASP:O	7:a:178:ARG:NH1	1.96	0.88
2:V:195:ILE:HG21	15:C:25:LEU:HG	1.54	0.88
12:f:712:LYS:O	12:f:715:HIS:CB	2.22	0.88
3:W:55:ARG:HH12	3:W:78:LYS:NZ	1.71	0.88
19:g:202:LEU:O	19:g:206:LEU:HB2	1.73	0.88
2:V:242:HIS:CE1	15:C:29:GLU:HB2	2.09	0.88
9:c:196:LEU:CA	9:c:200:TYR:CE1	2.51	0.88
12:f:758:ASN:HB2	12:f:809:ILE:HG21	1.55	0.87
16:D:50:GLU:O	16:D:54:LEU:HB2	1.73	0.87
12:f:712:LYS:O	12:f:715:HIS:HB2	1.73	0.87
27:O:37:ILE:HB	27:O:41:ILE:O	1.75	0.87
3:W:137:TYR:HE1	16:D:392:TYR:CD1	1.61	0.87
12:f:222:ASP:CB	14:B:60:LEU:HD23	1.89	0.87
12:f:705:ASN:HA	12:f:787:LEU:HD22	1.55	0.87
15:C:24:TYR:HD2	16:D:40:LEU:HG	1.31	0.87
3:W:90:LEU:CD2	3:W:96:GLN:CG	2.53	0.87
12:f:658:ALA:HB3	14:B:78:PHE:CZ	2.09	0.87
13:A:400:ARG:HG2	13:A:400:ARG:HH11	1.40	0.87
2:V:242:HIS:CE1	15:C:29:GLU:CB	2.58	0.87
12:f:673:ARG:CZ	12:f:712:LYS:CG	2.52	0.87
17:E:312:ILE:CG2	34:E:401:ATP:N1	2.38	0.87
16:D:87:LEU:HD11	16:D:140:VAL:CG2	2.03	0.86
2:V:345:ARG:NH1	2:V:357:LEU:HA	1.89	0.86
3:W:46:THR:HG22	3:W:50:LEU:HD13	1.55	0.86
3:W:55:ARG:HH12	3:W:78:LYS:CE	1.87	0.86
3:W:75:TYR:HA	3:W:78:LYS:HE3	1.56	0.86
12:f:838:ARG:CB	12:f:839:PRO:HD2	2.00	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:238:PRO:O	10:d:242:LEU:HB2	1.76	0.86
15:C:31:LEU:CD2	16:D:47:LEU:HB3	2.06	0.86
16:D:125:LYS:O	16:D:125:LYS:NZ	2.08	0.86
9:c:196:LEU:N	9:c:200:TYR:CE1	2.44	0.86
10:d:168:ASP:HA	10:d:171:LEU:HD12	1.58	0.86
16:D:87:LEU:HD13	16:D:140:VAL:CG1	1.86	0.86
15:C:152:GLY:N	36:C:501:ADP:N6	1.89	0.86
7:a:93:ALA:O	7:a:97:LEU:HB2	1.75	0.85
9:c:191:ALA:O	9:c:196:LEU:HD11	1.76	0.85
2:V:495:ARG:HB2	15:C:44:ARG:CZ	2.06	0.85
3:W:137:TYR:CD1	16:D:392:TYR:CE1	2.64	0.85
5:Y:101:ARG:O	5:Y:105:MET:HB3	1.76	0.85
15:C:24:TYR:HE2	16:D:40:LEU:HG	1.30	0.85
2:V:242:HIS:CD2	15:C:29:GLU:OE1	2.28	0.85
12:f:673:ARG:HH21	12:f:712:LYS:CG	1.87	0.85
14:B:53:THR:N	14:B:54:PRO:HD2	1.91	0.85
9:c:191:ALA:O	9:c:196:LEU:CD1	2.25	0.85
27:o:37:ILE:HB	27:o:41:ILE:O	1.75	0.85
1:U:644:TYR:HD2	15:C:60:ARG:NH2	1.72	0.85
19:G:46:ASP:O	19:G:222:VAL:CG2	2.23	0.85
3:W:344:THR:O	3:W:348:GLU:HB2	1.78	0.84
9:c:280:PRO:O	9:c:284:LEU:HB2	1.77	0.84
12:f:222:ASP:OD2	14:B:60:LEU:CD2	2.05	0.84
3:W:55:ARG:NH1	3:W:78:LYS:CE	2.40	0.84
12:f:680:ARG:NH2	12:f:715:HIS:NE2	2.08	0.84
3:W:316:ARG:CD	3:W:383:ASP:OD2	2.25	0.84
21:i:42:GLY:HA2	21:i:216:LEU:O	1.76	0.84
3:W:82:LEU:O	3:W:82:LEU:HD22	1.78	0.83
3:W:231:ILE:O	3:W:235:GLN:HB2	1.78	0.83
21:I:42:GLY:HA2	21:I:216:LEU:O	1.76	0.83
12:f:649:HIS:NE2	14:B:68:ILE:HG12	1.94	0.83
12:f:673:ARG:NH2	12:f:712:LYS:CB	2.41	0.83
16:D:376:ASN:O	16:D:380:GLN:HB2	1.79	0.83
2:V:195:ILE:CG2	15:C:25:LEU:HG	2.07	0.83
1:U:567:ILE:HG21	1:U:601:ARG:HH12	1.43	0.83
12:f:646:MET:HG2	14:B:64:LYS:HG2	1.60	0.83
14:B:54:PRO:HB3	14:B:61:LYS:HD2	1.60	0.83
10:d:155:LYS:NZ	10:d:170:LEU:HD22	1.94	0.83
16:D:85:ILE:CG2	16:D:86:PRO:HD2	2.08	0.82
16:D:335:LEU:CD2	16:D:369:LYS:CD	2.53	0.82
23:K:73:HIS:O	23:K:145:GLY:HA2	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:k:73:HIS:O	23:k:145:GLY:HA2	1.79	0.82
2:V:345:ARG:HH12	2:V:357:LEU:HA	1.45	0.82
2:V:495:ARG:H	15:C:44:ARG:CZ	1.91	0.82
17:E:340:GLY:HA3	34:E:401:ATP:C8	2.14	0.82
12:f:838:ARG:HD2	12:f:839:PRO:HD3	0.82	0.82
16:D:87:LEU:HD12	16:D:140:VAL:HG21	1.61	0.82
1:U:171:ASN:OD1	1:U:176:MET:HE1	1.79	0.81
16:D:89:ILE:HD11	17:E:80:VAL:HG23	1.61	0.81
2:V:195:ILE:CG2	15:C:25:LEU:CG	2.58	0.81
15:C:90:HIS:CE1	16:D:109:SER:HA	2.14	0.81
15:C:24:TYR:HE2	16:D:40:LEU:CG	1.87	0.81
19:g:46:ASP:O	19:g:222:VAL:CG2	2.28	0.81
2:V:319:HIS:CE1	11:e:4:LYS:HB2	2.16	0.81
12:f:759:LEU:HG	12:f:808:ASN:HA	1.63	0.81
9:c:197:ASN:HA	9:c:200:TYR:O	1.79	0.81
13:A:401:ARG:HD2	13:A:403:ILE:O	1.79	0.81
1:U:642:GLU:HA	15:C:57:ARG:HH12	1.45	0.80
15:C:198:LEU:CD2	36:C:501:ADP:H5'2	2.11	0.80
5:Y:233:ARG:NH1	5:Y:264:TYR:O	2.14	0.80
10:d:155:LYS:HZ2	10:d:171:LEU:CG	1.94	0.80
10:d:200:PHE:HE2	10:d:206:MET:HB3	1.46	0.80
16:D:253:LEU:O	16:D:257:ASN:HB2	1.81	0.80
12:f:647:GLY:HA3	14:B:67:ARG:O	1.82	0.80
12:f:708:ASP:CG	12:f:787:LEU:HD21	2.00	0.80
3:W:55:ARG:NH1	3:W:78:LYS:CD	2.45	0.80
16:D:87:LEU:CD1	16:D:140:VAL:HG21	2.10	0.80
21:i:2:SER:N	24:l:123:TYR:HH	1.80	0.80
1:U:171:ASN:ND2	1:U:176:MET:SD	2.54	0.80
12:f:145:VAL:O	12:f:149:GLU:HB3	1.82	0.80
17:E:181:THR:CB	34:E:401:ATP:O1B	2.18	0.80
12:f:780:PRO:O	12:f:784:ASP:HB2	1.81	0.80
18:F:393:GLY:HA3	36:F:501:ADP:N3	1.96	0.80
14:B:142:ASP:O	14:B:144:LEU:N	2.13	0.80
1:U:644:TYR:C	15:C:60:ARG:HH12	1.89	0.79
12:f:651:GLY:O	12:f:655:LEU:HD12	1.82	0.79
19:G:46:ASP:CB	19:G:222:VAL:HG23	2.12	0.79
2:V:318:GLN:HA	2:V:318:GLN:NE2	1.97	0.79
16:D:87:LEU:HD23	16:D:131:ALA:CB	2.02	0.79
21:I:213:ILE:HG22	21:I:228:LEU:HD21	1.64	0.79
15:C:152:GLY:CA	36:C:501:ADP:N6	2.41	0.79
3:W:316:ARG:HD2	3:W:383:ASP:CG	2.06	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:335:LEU:HD23	16:D:369:LYS:HG3	0.80	0.79
18:F:232:GLY:HA2	36:F:501:ADP:H5'2	1.64	0.79
2:V:242:HIS:CE1	15:C:29:GLU:OE1	2.36	0.79
9:c:196:LEU:N	9:c:200:TYR:CZ	2.50	0.79
2:V:495:ARG:HB2	15:C:44:ARG:NE	1.98	0.79
14:B:234:LEU:HG	34:B:501:ATP:H2'	1.63	0.79
2:V:346:LEU:CD1	11:e:46:ASP:OD2	2.30	0.78
15:C:90:HIS:ND1	16:D:109:SER:HA	1.97	0.78
16:D:129:SER:O	16:D:143:LEU:HB2	1.82	0.78
17:E:179:GLY:H	34:E:401:ATP:PA	2.06	0.78
2:V:195:ILE:CB	15:C:25:LEU:CD2	2.58	0.78
3:W:48:LEU:HD23	3:W:95:SER:H	1.45	0.78
9:c:32:TYR:O	9:c:68:ARG:HA	1.83	0.78
10:d:155:LYS:HD3	10:d:171:LEU:HD21	1.64	0.78
12:f:766:GLN:CG	12:f:807:ARG:NH2	2.36	0.78
16:D:88:VAL:C	16:D:132:LEU:H	1.90	0.78
3:W:36:LYS:HA	3:W:85:GLU:HA	1.66	0.78
3:W:48:LEU:HD21	3:W:95:SER:HB2	0.98	0.78
3:W:137:TYR:OH	16:D:392:TYR:CD1	1.72	0.78
9:c:196:LEU:CB	9:c:200:TYR:CZ	2.65	0.78
3:W:282:GLU:O	3:W:286:LEU:HB2	1.83	0.78
12:f:764:LEU:HD21	12:f:774:GLY:O	1.84	0.78
15:C:113:ARG:HB3	15:C:127:LEU:CD1	2.12	0.78
10:d:155:LYS:NZ	10:d:171:LEU:CG	2.41	0.78
31:s:149:LEU:O	31:s:153:VAL:HB	1.83	0.78
3:W:97:LEU:CG	3:W:138:VAL:HG21	2.13	0.78
12:f:759:LEU:HD12	12:f:808:ASN:HA	1.65	0.78
14:B:232:LYS:NZ	34:B:501:ATP:O2B	2.17	0.78
15:C:24:TYR:CE1	16:D:41:TYR:HA	2.19	0.77
15:C:52:LEU:CG	16:D:68:LEU:HD13	2.14	0.77
31:S:149:LEU:O	31:S:153:VAL:HB	1.83	0.77
2:V:345:ARG:HH21	2:V:361:PHE:H	1.05	0.77
3:W:137:TYR:CE1	16:D:392:TYR:CG	2.70	0.77
10:d:170:LEU:O	10:d:170:LEU:HD23	1.84	0.77
14:B:278:ALA:CB	14:B:279:PRO:HD2	2.14	0.77
19:g:203:SER:O	19:g:207:SER:HA	1.85	0.77
12:f:759:LEU:CG	12:f:808:ASN:HA	2.13	0.77
3:W:137:TYR:HH	16:D:392:TYR:H	1.30	0.77
12:f:764:LEU:HD11	12:f:773:LYS:O	1.85	0.77
19:G:203:SER:O	19:G:207:SER:HA	1.85	0.77
2:V:21:GLY:O	2:V:25:GLU:HB2	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:137:TYR:HB3	3:W:144:ARG:HH22	1.48	0.77
12:f:759:LEU:HA	12:f:808:ASN:O	1.85	0.77
12:f:223:GLU:HA	14:B:63:LEU:CD1	2.14	0.77
2:V:242:HIS:ND1	15:C:29:GLU:HB2	1.97	0.77
12:f:712:LYS:HE3	12:f:782:HIS:NE2	1.99	0.77
2:V:496:PHE:HD1	15:C:40:GLN:NE2	1.80	0.76
6:Z:25:ARG:HH11	9:c:104:ARG:H	1.33	0.76
16:D:87:LEU:CD1	16:D:140:VAL:CG2	2.63	0.76
31:S:55:SER:O	31:S:106:VAL:HA	1.85	0.76
2:V:195:ILE:CG1	15:C:25:LEU:HD23	2.07	0.76
12:f:646:MET:CG	14:B:64:LYS:HG2	2.16	0.76
12:f:708:ASP:HB2	12:f:787:LEU:CD2	1.83	0.76
12:f:838:ARG:HD3	12:f:839:PRO:HD3	1.61	0.76
15:C:73:VAL:CG2	15:C:127:LEU:CD1	2.64	0.76
19:g:47:CYS:HB3	19:g:221:THR:CG2	2.11	0.76
31:s:55:SER:O	31:s:106:VAL:HA	1.85	0.76
12:f:835:GLU:HA	12:f:840:LEU:HD23	1.67	0.76
16:D:369:LYS:N	16:D:369:LYS:HE3	1.99	0.76
10:d:155:LYS:HZ3	10:d:170:LEU:HD22	1.49	0.76
3:W:137:TYR:HE1	16:D:392:TYR:CG	2.03	0.76
16:D:133:HIS:HD2	16:D:136:SER:H	1.32	0.76
1:U:644:TYR:C	15:C:60:ARG:NH1	2.44	0.76
12:f:222:ASP:CB	14:B:60:LEU:HD22	1.76	0.75
1:U:149:GLN:OE1	16:D:39:ASP:OD1	2.04	0.75
9:c:92:GLN:O	9:c:96:LEU:HB2	1.86	0.75
16:D:87:LEU:HG	16:D:131:ALA:HB1	1.69	0.75
13:A:400:ARG:HG2	13:A:400:ARG:NH1	1.98	0.75
14:B:53:THR:H	14:B:54:PRO:HD2	1.50	0.75
2:V:166:TYR:O	2:V:175:MET:CE	2.32	0.75
2:V:319:HIS:NE2	11:e:4:LYS:CG	2.49	0.75
16:D:369:LYS:O	16:D:369:LYS:NZ	2.20	0.75
19:g:46:ASP:CB	19:g:222:VAL:HG23	2.12	0.75
2:V:317:PRO:HD3	11:e:4:LYS:HE2	1.69	0.75
3:W:55:ARG:CZ	3:W:78:LYS:HD2	2.17	0.75
12:f:658:ALA:HB2	14:B:78:PHE:CD2	2.22	0.75
21:I:85:VAL:O	21:I:89:GLU:HB2	1.87	0.75
23:k:157:ASP:HB2	23:k:161:THR:O	1.87	0.75
2:V:496:PHE:HE1	15:C:40:GLN:HG3	1.51	0.75
21:i:85:VAL:O	21:i:89:GLU:HB2	1.87	0.75
6:Z:223:ASN:CG	6:Z:226:ILE:HG22	2.12	0.74
2:V:328:VAL:O	2:V:332:LEU:HB2	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:e:48:VAL:O	11:e:52:PHE:HB3	1.86	0.74
3:W:137:TYR:CZ	16:D:392:TYR:HE1	2.02	0.74
10:d:171:LEU:O	10:d:175:ARG:HG2	1.87	0.74
12:f:556:ARG:CG	12:f:786:GLN:HE21	2.01	0.74
15:C:31:LEU:CD1	16:D:47:LEU:HB3	2.18	0.74
2:V:496:PHE:HE1	15:C:40:GLN:NE2	1.80	0.74
7:a:367:VAL:O	7:a:371:ALA:HB3	1.88	0.74
14:B:168:ASP:CG	14:B:169:PRO:HD2	2.12	0.74
12:f:712:LYS:HD3	12:f:712:LYS:O	1.87	0.74
15:C:38:LYS:HB3	16:D:54:LEU:HD11	1.69	0.74
15:C:31:LEU:HD21	16:D:47:LEU:HB3	1.68	0.73
27:o:138:PHE:O	27:o:142:PHE:HB2	1.89	0.73
9:c:191:ALA:HB1	9:c:196:LEU:HG	1.71	0.73
3:W:178:GLU:OE2	3:W:181:GLU:N	2.22	0.73
12:f:712:LYS:HE3	12:f:715:HIS:CD2	2.23	0.73
2:V:317:PRO:CG	11:e:4:LYS:HG3	2.15	0.73
14:B:54:PRO:CB	14:B:61:LYS:HD2	2.18	0.73
21:I:213:ILE:CG2	21:I:228:LEU:HD21	2.19	0.73
1:U:151:ILE:CD1	1:U:177:LEU:CD2	2.61	0.73
17:E:179:GLY:CA	34:E:401:ATP:PA	2.77	0.73
3:W:97:LEU:HD21	3:W:138:VAL:HG22	1.61	0.73
9:c:196:LEU:HA	9:c:200:TYR:CD1	2.23	0.73
1:U:457:ILE:O	1:U:461:LEU:HB2	1.89	0.72
2:V:317:PRO:CG	11:e:4:LYS:CG	2.67	0.72
2:V:496:PHE:CD2	15:C:44:ARG:NH2	2.57	0.72
27:O:138:PHE:O	27:O:142:PHE:HB2	1.89	0.72
15:C:24:TYR:CZ	16:D:41:TYR:HA	2.24	0.72
23:K:157:ASP:HB2	23:K:161:THR:O	1.87	0.72
3:W:178:GLU:CD	3:W:181:GLU:HB2	2.12	0.72
12:f:665:GLU:O	12:f:669:GLU:HB2	1.90	0.72
13:A:401:ARG:HD3	13:A:403:ILE:O	1.87	0.72
16:D:85:ILE:CD1	17:E:82:GLY:H	2.03	0.72
2:V:496:PHE:HE1	15:C:40:GLN:CD	1.96	0.72
25:M:47:PHE:HB2	25:M:214:SER:HB3	1.71	0.72
2:V:195:ILE:CG1	15:C:25:LEU:CG	2.49	0.72
2:V:242:HIS:CE1	15:C:29:GLU:HB3	2.23	0.72
10:d:170:LEU:HD23	10:d:170:LEU:C	2.14	0.72
16:D:88:VAL:CG1	16:D:133:HIS:O	2.38	0.72
19:g:46:ASP:O	19:g:222:VAL:HG22	1.90	0.72
3:W:179:LYS:HD2	3:W:180:LYS:HG3	1.72	0.72
5:Y:122:THR:O	5:Y:126:LYS:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:583:MET:HE1	1:U:602:LEU:CD2	2.10	0.71
2:V:242:HIS:CG	15:C:29:GLU:OE1	2.43	0.71
5:Y:233:ARG:NH2	5:Y:306:GLN:HE22	1.87	0.71
16:D:88:VAL:HG13	16:D:133:HIS:C	2.13	0.71
12:f:222:ASP:OD1	14:B:60:LEU:HD22	1.86	0.71
16:D:85:ILE:HD11	17:E:82:GLY:H	1.55	0.71
12:f:610:GLN:O	12:f:614:HIS:HB2	1.89	0.71
15:C:90:HIS:HB2	15:C:91:PRO:HD3	1.72	0.71
14:B:142:ASP:C	14:B:144:LEU:H	1.97	0.71
2:V:214:HIS:O	2:V:218:TYR:HB3	1.90	0.71
12:f:759:LEU:HD21	12:f:806:VAL:CB	2.20	0.71
16:D:79:VAL:HG22	16:D:116:LEU:HD21	1.72	0.71
2:V:242:HIS:NE2	15:C:29:GLU:OE1	2.23	0.71
2:V:348:PHE:O	2:V:350:GLN:N	2.22	0.71
29:q:143:LEU:O	29:q:147:TYR:HB2	1.91	0.71
16:D:356:GLU:HA	16:D:356:GLU:OE2	1.89	0.71
17:E:340:GLY:HA3	34:E:401:ATP:C5	2.24	0.71
1:U:171:ASN:OD1	1:U:176:MET:CE	2.37	0.71
1:U:177:LEU:HD23	1:U:180:SER:CB	2.20	0.71
8:b:9:CYS:HA	8:b:52:ILE:O	1.91	0.71
15:C:90:HIS:HD2	15:C:91:PRO:HD2	1.51	0.71
16:D:151:ILE:HD12	16:D:151:ILE:N	2.06	0.71
19:g:46:ASP:O	19:g:222:VAL:HG23	1.89	0.71
25:m:47:PHE:HB2	25:m:214:SER:HB3	1.71	0.71
2:V:495:ARG:H	15:C:44:ARG:HH12	1.38	0.70
22:J:200:GLN:HE21	22:J:200:GLN:C	1.99	0.70
29:Q:143:LEU:O	29:Q:147:TYR:HB2	1.91	0.70
12:f:652:VAL:HG21	12:f:685:THR:HB	1.74	0.70
15:C:31:LEU:CD2	16:D:47:LEU:CD1	2.65	0.70
12:f:759:LEU:HD23	12:f:806:VAL:CG1	2.03	0.70
12:f:712:LYS:CE	12:f:715:HIS:CD2	2.74	0.70
1:U:219:CYS:O	1:U:223:LEU:HB2	1.92	0.70
15:C:198:LEU:HD23	36:C:501:ADP:C5'	2.16	0.70
2:V:219:GLU:HG3	2:V:256:ARG:HH12	1.55	0.70
2:V:496:PHE:CE1	15:C:40:GLN:CG	2.70	0.70
2:V:345:ARG:NH2	2:V:357:LEU:O	2.24	0.69
3:W:97:LEU:CD2	3:W:138:VAL:CG2	2.15	0.69
15:C:90:HIS:CD2	15:C:90:HIS:H	2.08	0.69
3:W:51:GLU:OE1	3:W:51:GLU:N	2.24	0.69
12:f:680:ARG:HH21	12:f:715:HIS:CD2	2.10	0.69
12:f:712:LYS:NZ	12:f:715:HIS:HD2	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:79:VAL:CG2	16:D:116:LEU:HD21	2.21	0.69
10:d:167:ILE:HA	10:d:170:LEU:HB3	1.75	0.69
11:e:56:LEU:HD21	11:e:59:GLU:HB3	1.73	0.69
12:f:222:ASP:OD2	14:B:60:LEU:CA	2.37	0.69
3:W:46:THR:CG2	3:W:50:LEU:HD13	2.22	0.69
12:f:223:GLU:HA	14:B:63:LEU:HD11	1.73	0.69
12:f:764:LEU:HD11	12:f:774:GLY:HA3	1.74	0.69
29:Q:41:LYS:O	29:Q:106:GLY:HA2	1.93	0.69
2:V:345:ARG:HH21	2:V:361:PHE:CA	2.06	0.69
10:d:67:ASP:O	10:d:71:PHE:HB2	1.93	0.69
14:B:418:ASP:O	14:B:422:SER:HB2	1.93	0.69
10:d:200:PHE:HD1	10:d:200:PHE:H	1.39	0.69
4:X:175:LYS:HG2	4:X:213:GLN:HE22	1.56	0.68
12:f:250:ARG:NH2	12:f:281:ILE:HD13	2.08	0.68
2:V:167:LEU:CD2	2:V:171:VAL:HG11	2.22	0.68
27:O:176:CYS:HA	27:O:184:ASP:O	1.94	0.68
29:Q:78:THR:O	29:Q:82:ASN:HB2	1.93	0.68
24:l:14:SER:HB3	24:l:18:ARG:H	1.58	0.68
29:q:41:LYS:O	29:q:106:GLY:HA2	1.93	0.68
5:Y:336:ARG:O	5:Y:340:ALA:HB2	1.93	0.68
24:L:66:VAL:HA	24:L:89:ARG:HE	1.58	0.68
2:V:345:ARG:CZ	2:V:357:LEU:HB2	2.23	0.68
10:d:167:ILE:O	10:d:171:LEU:HD12	1.93	0.68
24:L:14:SER:HB3	24:L:18:ARG:H	1.58	0.68
1:U:229:VAL:O	1:U:233:LEU:HB2	1.93	0.68
10:d:122:LEU:HB2	10:d:125:LYS:HB2	1.76	0.68
12:f:708:ASP:OD2	12:f:787:LEU:HD21	1.93	0.68
29:Q:183:ILE:HA	29:Q:187:GLY:O	1.94	0.68
24:l:66:VAL:HA	24:l:89:ARG:HE	1.58	0.68
29:q:78:THR:O	29:q:82:ASN:HB2	1.93	0.68
9:c:196:LEU:HA	9:c:200:TYR:CG	2.28	0.68
21:I:67:LYS:NZ	21:I:225:ILE:HD12	2.08	0.68
16:D:150:SER:CB	16:D:153:MET:HE1	2.24	0.68
11:e:56:LEU:HD11	11:e:59:GLU:N	2.09	0.68
12:f:337:LEU:HD23	12:f:341:GLU:OE1	1.94	0.68
5:Y:346:LYS:O	5:Y:355:GLU:HB3	1.94	0.67
12:f:425:GLY:HA3	12:f:451:VAL:HG11	1.76	0.67
15:C:73:VAL:CG2	15:C:127:LEU:HD11	2.16	0.67
2:V:358:MET:O	2:V:362:LEU:HB2	1.94	0.67
3:W:46:THR:HG22	3:W:50:LEU:HD11	1.75	0.67
27:o:176:CYS:HA	27:o:184:ASP:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:556:ARG:HG2	12:f:786:GLN:NE2	2.08	0.67
3:W:137:TYR:CB	3:W:144:ARG:HH12	2.07	0.67
12:f:198:HIS:O	12:f:202:HIS:HB2	1.94	0.67
12:f:764:LEU:HD11	12:f:774:GLY:CA	2.25	0.67
15:C:31:LEU:CD2	16:D:47:LEU:CG	2.73	0.67
29:q:183:ILE:HA	29:q:187:GLY:O	1.94	0.67
16:D:96:VAL:HG23	16:D:102:ILE:HD11	1.77	0.67
18:F:224:LEU:HB2	18:F:348:LEU:HD23	1.77	0.67
5:Y:168:ILE:HG23	5:Y:173:ASP:HB2	1.77	0.67
16:D:115:ILE:HA	16:D:139:LEU:HB2	1.77	0.66
3:W:49:SER:H	3:W:94:ARG:HD3	1.59	0.66
6:Z:193:ASN:O	6:Z:197:GLY:HA3	1.95	0.66
2:V:440:LYS:HD3	10:d:146:GLY:HA2	1.78	0.66
28:p:62:THR:OG1	29:q:85:ARG:NH2	2.28	0.66
1:U:98:GLU:HB3	15:C:22:GLN:HG3	1.78	0.66
12:f:658:ALA:CB	14:B:78:PHE:CG	2.79	0.66
34:E:401:ATP:O1A	34:E:401:ATP:H3'	1.96	0.66
3:W:43:VAL:HA	3:W:94:ARG:HH11	1.60	0.66
3:W:135:LYS:HB2	3:W:144:ARG:HH21	1.59	0.66
3:W:97:LEU:HD11	3:W:138:VAL:HG23	1.76	0.66
15:C:31:LEU:HD22	16:D:47:LEU:HG	1.78	0.66
16:D:369:LYS:HE3	16:D:369:LYS:H	1.60	0.66
21:i:143:TYR:HB2	21:i:146:GLN:HE21	1.60	0.66
1:U:583:MET:CE	1:U:602:LEU:CD2	2.71	0.66
10:d:181:CYS:HB2	10:d:184:LYS:HE2	1.78	0.66
12:f:328:SER:OG	12:f:808:ASN:ND2	2.21	0.66
12:f:785:ARG:C	12:f:787:LEU:H	2.04	0.66
12:f:838:ARG:CG	12:f:839:PRO:HD3	2.25	0.66
16:D:88:VAL:HG13	16:D:133:HIS:O	1.96	0.66
16:D:125:LYS:HD2	16:D:125:LYS:C	2.20	0.66
26:N:120:MET:H	32:T:61:GLN:HE22	1.44	0.66
2:V:84:LYS:HG2	2:V:123:SER:HB2	1.76	0.65
10:d:195:THR:C	10:d:200:PHE:CE1	2.68	0.65
14:B:53:THR:CG2	14:B:54:PRO:HD2	2.24	0.65
7:a:188:LEU:HD11	7:a:193:GLN:HE21	1.61	0.65
9:c:59:GLY:HA3	9:c:69:VAL:HA	1.79	0.65
19:g:47:CYS:CB	19:g:221:THR:CG2	2.72	0.65
1:U:540:GLN:HB2	9:c:68:ARG:HH22	1.62	0.65
5:Y:233:ARG:N	5:Y:234:PRO:HD2	2.11	0.65
12:f:786:GLN:OE1	12:f:786:GLN:HA	1.96	0.65
7:a:129:GLN:HG3	7:a:130:VAL:HG23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:226:TYR:O	18:F:353:GLU:HA	1.95	0.65
24:L:207:THR:O	24:L:226:ASP:CB	2.42	0.65
11:e:56:LEU:CD1	11:e:59:GLU:N	2.60	0.65
3:W:48:LEU:CD2	3:W:95:SER:N	2.52	0.65
6:Z:123:ILE:HB	6:Z:136:GLU:HB3	1.79	0.65
18:F:93:VAL:HA	18:F:124:ILE:HG22	1.79	0.65
6:Z:223:ASN:OD1	6:Z:226:ILE:HG22	1.96	0.65
12:f:67:ASP:O	12:f:71:TYR:HB2	1.97	0.65
17:E:182:LEU:CD2	34:E:401:ATP:C2'	2.73	0.65
21:I:143:TYR:HB2	21:I:146:GLN:HE21	1.60	0.64
2:V:319:HIS:CE1	11:e:4:LYS:CB	2.79	0.64
9:c:146:ASP:HB3	9:c:156:VAL:CB	2.26	0.64
12:f:764:LEU:CD1	12:f:774:GLY:HA3	2.26	0.64
12:f:828:ARG:O	12:f:860:LYS:HA	1.95	0.64
27:O:163:ILE:HG12	27:O:170:GLY:HA2	1.78	0.64
13:A:221:GLY:O	13:A:225:CYS:HB2	1.97	0.64
12:f:652:VAL:HG21	12:f:685:THR:CB	2.27	0.64
14:B:278:ALA:HB3	14:B:279:PRO:HD2	1.79	0.64
16:D:354:LEU:HD23	16:D:358:VAL:HB	1.79	0.64
14:B:231:GLY:CA	34:B:501:ATP:O1A	2.46	0.64
15:C:195:GLY:N	36:C:501:ADP:O1A	2.24	0.64
6:Z:9:VAL:HA	6:Z:48:LEU:HB3	1.80	0.64
12:f:697:ILE:HG12	12:f:737:ASN:HD21	1.62	0.64
13:A:41:TYR:HB2	13:A:44:GLN:HB3	1.78	0.64
13:A:210:LYS:HB2	13:A:312:ARG:NH2	2.12	0.64
31:S:197:ILE:O	31:S:203:ILE:HA	1.98	0.64
3:W:78:LYS:HB2	3:W:82:LEU:HD12	1.80	0.64
5:Y:319:MET:O	5:Y:323:PHE:HB3	1.98	0.64
15:C:59:LEU:CD1	16:D:75:ALA:HB1	2.27	0.64
1:U:567:ILE:CB	1:U:601:ARG:NH2	2.58	0.64
23:K:100:TRP:O	30:R:57:ARG:NH2	2.30	0.64
7:a:341:LEU:HB2	7:a:345:GLN:HE21	1.61	0.64
5:Y:301:ILE:HG13	5:Y:343:LEU:HD12	1.80	0.63
27:o:163:ILE:HG12	27:o:170:GLY:HA2	1.78	0.63
12:f:712:LYS:O	12:f:715:HIS:HB3	1.97	0.63
16:D:151:ILE:H	16:D:151:ILE:CD1	2.00	0.63
24:L:211:SER:CB	24:L:225:ASP:OD1	2.47	0.63
5:Y:101:ARG:NH2	5:Y:126:LYS:O	2.30	0.63
7:a:19:PRO:HA	7:a:22:TRP:HD1	1.62	0.63
15:C:31:LEU:CD2	16:D:47:LEU:CB	2.77	0.63
1:U:169:GLU:HG3	1:U:171:ASN:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:646:MET:HB3	14:B:67:ARG:HD2	1.80	0.63
31:s:197:ILE:O	31:s:203:ILE:HA	1.98	0.63
11:e:57:ARG:HG2	11:e:57:ARG:NH1	2.05	0.63
12:f:759:LEU:HA	12:f:808:ASN:C	2.24	0.63
1:U:108:TYR:OH	1:U:159:ARG:NH1	2.31	0.63
8:b:34:ASN:O	8:b:38:HIS:ND1	2.31	0.63
10:d:200:PHE:CE2	10:d:206:MET:HB3	2.32	0.63
17:E:179:GLY:N	34:E:401:ATP:PA	2.69	0.63
25:m:108:LEU:HD21	25:m:139:SER:HB3	1.81	0.63
2:V:195:ILE:CB	15:C:25:LEU:HG	2.29	0.63
7:a:8:LEU:HD11	7:a:26:GLU:HB3	1.80	0.63
9:c:191:ALA:C	9:c:196:LEU:CD2	2.51	0.63
17:E:179:GLY:HA2	34:E:401:ATP:PA	2.39	0.63
21:I:67:LYS:HZ3	21:I:225:ILE:HD12	1.63	0.63
2:V:247:GLN:HE21	2:V:274:SER:HA	1.63	0.63
2:V:496:PHE:CE1	15:C:40:GLN:HG3	2.31	0.63
6:Z:25:ARG:HB2	9:c:104:ARG:HG2	1.79	0.63
12:f:759:LEU:HD21	12:f:806:VAL:HB	1.81	0.63
1:U:151:ILE:CD1	1:U:177:LEU:HD21	2.08	0.62
25:M:108:LEU:HD21	25:M:139:SER:HB3	1.81	0.62
1:U:642:GLU:CA	15:C:57:ARG:HH12	2.12	0.62
2:V:144:ASP:H	2:V:150:ARG:HH22	1.46	0.62
2:V:349:ARG:HA	2:V:353:LEU:HB2	1.81	0.62
9:c:196:LEU:N	9:c:196:LEU:HD13	2.15	0.62
12:f:657:ILE:N	12:f:657:ILE:HD12	2.15	0.62
12:f:673:ARG:CZ	12:f:712:LYS:CB	2.77	0.62
2:V:296:LYS:HE2	2:V:305:ALA:HB2	1.82	0.62
2:V:345:ARG:HH22	2:V:360:TYR:HB3	1.65	0.62
3:W:55:ARG:NH1	3:W:78:LYS:HE3	2.14	0.62
6:Z:10:VAL:HG13	6:Z:163:GLY:HA3	1.81	0.62
7:a:227:ASN:O	7:a:231:GLN:NE2	2.32	0.62
15:C:31:LEU:HD22	16:D:47:LEU:CG	2.29	0.62
15:C:38:LYS:CB	16:D:54:LEU:HD11	2.30	0.62
26:N:18:SER:HB2	26:N:31:THR:H	1.64	0.62
1:U:559:ARG:HB3	1:U:562:GLU:HB2	1.82	0.62
3:W:167:GLN:HG3	3:W:168:GLU:HG3	1.81	0.62
27:O:15:GLY:HA2	27:O:174:ASP:O	1.99	0.62
3:W:50:LEU:H	3:W:50:LEU:HD12	1.64	0.62
11:e:56:LEU:CG	11:e:59:GLU:HB3	2.30	0.62
12:f:609:VAL:HG11	14:B:74:MET:HG2	1.81	0.62
26:n:120:MET:H	32:t:61:GLN:HE22	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:98:GLU:HB2	15:C:22:GLN:O	1.99	0.62
5:Y:29:PRO:HB2	5:Y:32:ARG:HB3	1.81	0.62
16:D:85:ILE:H	16:D:86:PRO:HD2	1.63	0.62
16:D:88:VAL:O	16:D:131:ALA:HA	1.99	0.62
2:V:195:ILE:CB	15:C:25:LEU:CG	2.78	0.62
3:W:155:GLN:HG2	3:W:157:GLY:H	1.65	0.62
9:c:196:LEU:HB3	9:c:200:TYR:HE2	1.64	0.62
20:H:119:GLN:NE2	21:I:82:ASP:OD1	2.33	0.62
1:U:177:LEU:CD2	1:U:180:SER:HB3	2.29	0.62
12:f:712:LYS:NZ	12:f:715:HIS:CD2	2.68	0.62
15:C:196:LYS:NZ	15:C:295:THR:O	2.33	0.62
21:I:213:ILE:CB	21:I:228:LEU:HD21	2.30	0.62
7:a:264:ASN:HB3	7:a:267:GLN:HE21	1.65	0.62
17:E:312:ILE:CG2	34:E:401:ATP:C6	2.83	0.62
28:P:58:THR:O	29:Q:85:ARG:NH2	2.32	0.62
3:W:48:LEU:HB3	3:W:94:ARG:HD2	1.82	0.61
16:D:89:ILE:HD11	17:E:80:VAL:CG2	2.30	0.61
18:F:439:ALA:HB1	24:L:62:LYS:HD3	1.82	0.61
21:I:123:GLN:HG3	22:J:125:ARG:HE	1.64	0.61
1:U:402:PHE:HB2	1:U:437:TYR:HB3	1.81	0.61
12:f:764:LEU:CD1	12:f:773:LYS:O	2.48	0.61
14:B:231:GLY:C	34:B:501:ATP:O1A	2.42	0.61
26:n:35:THR:OG1	26:n:45:ARG:NH2	2.34	0.61
16:D:345:PHE:HB3	16:D:360:LEU:HD23	1.80	0.61
27:o:15:GLY:HA2	27:o:174:ASP:O	1.99	0.61
3:W:48:LEU:CD2	3:W:95:SER:H	2.13	0.61
7:a:321:LYS:HB2	7:a:335:TRP:HB3	1.81	0.61
12:f:223:GLU:HA	14:B:63:LEU:HD12	1.81	0.61
12:f:276:GLU:O	12:f:286:LYS:NZ	2.34	0.61
15:C:24:TYR:OH	16:D:41:TYR:CA	2.48	0.61
16:D:349:THR:HB	16:D:354:LEU:CD1	2.29	0.61
16:D:353:ASN:ND2	16:D:392:TYR:O	2.33	0.61
18:F:252:ALA:HB3	18:F:255:GLN:HB2	1.81	0.61
3:W:90:LEU:HD22	3:W:96:GLN:HG3	1.79	0.61
9:c:52:GLU:H	9:c:82:VAL:HG13	1.64	0.61
9:c:196:LEU:CA	9:c:200:TYR:CD2	2.73	0.61
24:L:183:ASN:O	24:L:187:LEU:HB2	2.01	0.61
26:N:35:THR:OG1	26:N:45:ARG:NH2	2.34	0.61
24:l:183:ASN:O	24:l:187:LEU:HB2	2.01	0.61
1:U:126:ILE:HG23	1:U:130:LEU:HB3	1.81	0.61
1:U:151:ILE:HD11	1:U:177:LEU:CG	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:i:47:ALA:HB1	21:i:64:LYS:HE3	1.83	0.61
3:W:315:MET:O	3:W:315:MET:HE2	2.00	0.61
12:f:773:LYS:HD2	12:f:776:LEU:HD13	1.81	0.61
18:F:312:GLU:O	18:F:316:GLN:HB3	1.99	0.61
12:f:790:GLN:HG2	12:f:794:ALA:HB3	1.82	0.61
12:f:840:LEU:H	12:f:840:LEU:HD12	1.65	0.61
27:o:11:GLY:HA3	27:o:178:ILE:O	2.01	0.61
21:I:47:ALA:HB1	21:I:64:LYS:HE3	1.83	0.61
26:N:15:GLY:HA2	26:N:175:ARG:O	2.01	0.61
26:n:18:SER:HB2	26:n:31:THR:H	1.64	0.61
2:V:495:ARG:N	15:C:44:ARG:NH1	2.42	0.60
7:a:54:ASP:HA	7:a:57:ILE:HG22	1.82	0.60
1:U:191:LYS:HD2	1:U:194:ARG:HH11	1.66	0.60
3:W:55:ARG:HH12	3:W:78:LYS:HZ1	1.47	0.60
6:Z:172:VAL:HG13	9:c:217:LEU:HD21	1.82	0.60
8:b:124:LEU:O	8:b:128:ALA:HB2	2.00	0.60
9:c:115:HIS:HB3	9:c:118:PHE:HB2	1.81	0.60
12:f:99:LEU:HG	12:f:101:PRO:HD2	1.83	0.60
13:A:297:ARG:HH22	18:F:306:VAL:HG21	1.67	0.60
29:Q:21:ALA:HB3	29:Q:29:LYS:HB3	1.83	0.60
10:d:208:ASP:O	10:d:212:LYS:HB2	2.01	0.60
12:f:640:LYS:HG2	12:f:678:LEU:HD13	1.82	0.60
13:A:400:ARG:HH11	13:A:400:ARG:CG	2.13	0.60
22:J:38:ARG:NH1	22:J:181:ILE:O	2.34	0.60
27:O:7:VAL:HG22	27:O:12:ILE:HG12	1.82	0.60
27:O:11:GLY:HA3	27:O:178:ILE:O	2.01	0.60
2:V:92:ARG:HG2	2:V:96:ARG:HH22	1.66	0.60
15:C:31:LEU:HD11	16:D:47:LEU:HB3	1.83	0.60
27:O:214:GLU:HA	28:P:198:ARG:HG2	1.83	0.60
2:V:494:MET:N	15:C:44:ARG:HH12	1.93	0.60
15:C:221:GLN:HE22	15:C:228:ALA:HB3	1.66	0.60
16:D:260:ALA:O	16:D:305:VAL:HA	2.01	0.60
19:g:46:ASP:CA	19:g:222:VAL:CG2	2.80	0.60
29:q:21:ALA:HB3	29:q:29:LYS:HB3	1.83	0.60
1:U:598:ALA:O	1:U:602:LEU:HB2	2.02	0.60
1:U:639:LEU:HD12	15:C:49:ARG:HH12	1.66	0.60
2:V:79:VAL:HG13	2:V:81:GLN:H	1.66	0.60
3:W:343:SER:O	3:W:347:GLY:HA3	2.00	0.60
6:Z:263:ALA:HB1	9:c:288:VAL:HG13	1.83	0.60
13:A:396:ALA:HB1	13:A:401:ARG:HG2	1.83	0.60
24:L:117:GLN:NE2	25:M:83:ASP:OD1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:j:38:ARG:NH1	22:j:181:ILE:O	2.34	0.60
26:n:15:GLY:HA2	26:n:175:ARG:O	2.01	0.60
27:o:7:VAL:HG22	27:o:12:ILE:HG12	1.82	0.60
1:U:639:LEU:CD1	15:C:49:ARG:HH12	2.14	0.60
1:U:567:ILE:HG21	1:U:601:ARG:NH1	2.15	0.60
12:f:125:ILE:HD11	12:f:128:VAL:HB	1.82	0.60
15:C:56:VAL:HG21	16:D:68:LEU:HD22	1.84	0.60
21:i:35:LEU:HA	21:i:162:THR:O	2.01	0.60
2:V:418:SER:HA	2:V:457:TYR:HA	1.83	0.60
2:V:450:SER:HB3	2:V:459:GLN:HE21	1.66	0.60
13:A:121:PHE:HA	18:F:88:TYR:O	2.02	0.60
3:W:171:VAL:HG12	17:E:161:ARG:HH21	1.67	0.59
4:X:198:ASN:ND2	15:C:385:MET:O	2.35	0.59
6:Z:244:GLU:OE1	6:Z:244:GLU:N	2.36	0.59
7:a:342:ASP:OD1	7:a:345:GLN:NE2	2.35	0.59
12:f:586:PRO:HA	12:f:589:SER:HB2	1.83	0.59
12:f:838:ARG:CG	12:f:839:PRO:CD	2.80	0.59
16:D:119:ILE:O	16:D:121:ARG:NH1	2.35	0.59
21:I:227:VAL:HG12	21:I:227:VAL:O	2.01	0.59
28:P:205:ASP:OD2	30:r:19:ARG:NH2	2.34	0.59
2:V:345:ARG:NH2	2:V:360:TYR:C	2.59	0.59
3:W:46:THR:CB	3:W:50:LEU:HD13	2.32	0.59
4:X:214:SER:O	4:X:218:HIS:ND1	2.35	0.59
17:E:342:ASP:OD2	17:E:378:LYS:NZ	2.35	0.59
21:I:35:LEU:HA	21:I:162:THR:O	2.01	0.59
6:Z:135:THR:HG21	6:Z:162:ILE:HD11	1.84	0.59
9:c:31:VAL:HB	9:c:205:ILE:HG22	1.84	0.59
12:f:634:LYS:HD2	12:f:637:LYS:HD2	1.84	0.59
21:I:213:ILE:HG22	21:I:228:LEU:CD2	2.31	0.59
21:I:225:ILE:O	21:I:225:ILE:HG22	2.02	0.59
12:f:759:LEU:HG	12:f:806:VAL:HG12	1.84	0.59
12:f:222:ASP:HB3	14:B:60:LEU:HD23	1.62	0.59
29:Q:141:SER:O	29:Q:145:ARG:HB2	2.03	0.59
2:V:359:PRO:HG2	2:V:385:LYS:HG2	1.85	0.59
12:f:646:MET:HE3	14:B:64:LYS:NZ	2.17	0.59
2:V:227:VAL:O	2:V:231:LEU:HB2	2.03	0.59
2:V:347:GLN:OE1	2:V:347:GLN:HA	2.03	0.59
3:W:375:MET:HE2	3:W:386:VAL:HB	1.84	0.59
14:B:284:ILE:HG21	14:B:287:ILE:HD12	1.84	0.59
23:K:77:ALA:HB3	23:K:142:LEU:HB2	1.84	0.59
1:U:362:ASN:HB2	9:c:173:GLU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:317:PRO:HG2	11:e:4:LYS:HG2	1.80	0.59
5:Y:173:ASP:HA	15:C:334:ARG:HG3	1.84	0.59
18:F:222:GLY:O	18:F:349:ASP:N	2.36	0.59
15:C:69:GLN:NE2	15:C:119:ASP:OD2	2.35	0.59
3:W:79:GLU:HA	3:W:83:LEU:HB2	1.83	0.58
7:a:132:LYS:O	7:a:136:GLU:HB2	2.02	0.58
9:c:267:PRO:HA	9:c:270:LEU:HB2	1.85	0.58
12:f:679:LEU:HB2	12:f:681:TYR:H	1.68	0.58
7:a:255:TRP:O	7:a:258:GLN:NE2	2.36	0.58
10:d:2:TYR:O	10:d:25:ARG:NH2	2.35	0.58
17:E:148:VAL:HG13	17:E:149:ILE:HG23	1.84	0.58
5:Y:192:ARG:NH1	11:e:40:GLU:OE1	2.36	0.58
13:A:324:PRO:HA	13:A:327:LEU:HD13	1.84	0.58
14:B:231:GLY:HA2	34:B:501:ATP:O1A	2.01	0.58
19:G:46:ASP:CA	19:G:222:VAL:CG2	2.82	0.58
2:V:195:ILE:CG2	15:C:25:LEU:CD1	2.51	0.58
2:V:290:TYR:OH	2:V:294:ARG:NH2	2.36	0.58
4:X:299:LEU:HD21	4:X:331:LEU:HA	1.86	0.58
13:A:111:TYR:O	13:A:122:VAL:HA	2.02	0.58
15:C:89:VAL:HB	15:C:92:GLU:HB3	1.85	0.58
19:g:144:ASP:HB3	19:g:147:GLN:HB2	1.85	0.58
3:W:169:LEU:O	3:W:182:ARG:NH1	2.37	0.58
13:A:210:LYS:NZ	13:A:313:GLY:O	2.31	0.58
15:C:52:LEU:HD23	16:D:68:LEU:CD1	2.28	0.58
15:C:151:ILE:HG21	15:C:158:ILE:HD11	1.84	0.58
18:F:228:PRO:O	18:F:233:LYS:NZ	2.37	0.58
23:K:209:LYS:O	23:K:214:ASN:ND2	2.37	0.58
29:Q:8:GLN:NE2	29:Q:9:GLY:O	2.36	0.58
2:V:300:LEU:HD13	10:d:113:ALA:HA	1.84	0.58
11:e:56:LEU:CD2	11:e:59:GLU:HB3	2.32	0.58
12:f:575:ALA:O	12:f:579:ALA:HB3	2.04	0.58
20:H:71:HIS:HA	20:H:218:PHE:H	1.69	0.58
30:R:44:THR:HG21	30:R:100:MET:HE3	1.86	0.58
23:k:50:VAL:HG11	23:k:66:LYS:HB2	1.86	0.58
25:m:214:SER:OG	25:m:224:HIS:NE2	2.30	0.58
2:V:228:ARG:O	2:V:232:HIS:ND1	2.37	0.58
3:W:329:ARG:NH1	3:W:334:GLU:OE1	2.37	0.58
12:f:228:LYS:HB3	12:f:231:LEU:HD13	1.86	0.58
16:D:87:LEU:CD2	16:D:131:ALA:HB2	2.21	0.58
16:D:150:SER:OG	16:D:153:MET:CE	2.44	0.58
16:D:264:ILE:HB	16:D:309:MET:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:241:ARG:NH2	17:E:283:ASP:O	2.37	0.58
34:E:401:ATP:PA	34:E:401:ATP:H3'	2.44	0.58
26:N:29:ARG:NH1	27:O:139:GLU:OE2	2.37	0.58
23:k:209:LYS:O	23:k:214:ASN:ND2	2.37	0.58
2:V:204:ASP:OD1	2:V:234:ARG:NH2	2.37	0.58
10:d:195:THR:HA	10:d:200:PHE:CZ	2.39	0.58
12:f:139:CYS:O	12:f:143:ARG:NH1	2.37	0.58
12:f:378:ASN:O	12:f:382:ASN:ND2	2.37	0.58
14:B:53:THR:HG23	14:B:54:PRO:HD2	1.76	0.58
23:K:50:VAL:HG11	23:K:66:LYS:HB2	1.86	0.58
2:V:116:ALA:O	2:V:120:PHE:HB2	2.02	0.58
3:W:34:LEU:HA	3:W:39:ARG:HB2	1.86	0.58
3:W:90:LEU:HD22	3:W:96:GLN:CG	2.31	0.58
14:B:173:VAL:HG21	15:C:233:GLU:HG3	1.85	0.58
16:D:297:ASP:OD2	16:D:326:ARG:NH2	2.36	0.58
29:q:141:SER:O	29:q:145:ARG:HB2	2.03	0.58
16:D:85:ILE:CD1	17:E:82:GLY:N	2.67	0.58
16:D:208:PRO:HB2	17:E:291:ARG:HD3	1.84	0.58
17:E:220:ASN:OD1	17:E:223:ARG:NH2	2.37	0.58
13:A:85:GLN:HA	13:A:88:GLN:HB3	1.86	0.57
17:E:247:THR:O	17:E:251:ARG:NH2	2.38	0.57
19:g:137:CYS:SG	19:g:138:MET:N	2.76	0.57
23:k:77:ALA:HB3	23:k:142:LEU:HB2	1.84	0.57
1:U:540:GLN:O	9:c:68:ARG:NH1	2.34	0.57
3:W:366:MET:O	3:W:370:TYR:HB2	2.04	0.57
31:S:38:ARG:HH12	32:T:151:ARG:HD3	1.69	0.57
25:m:168:ALA:HB1	25:m:171:ALA:HB3	1.85	0.57
32:t:27:LEU:HD11	32:t:34:ALA:HB1	1.86	0.57
3:W:48:LEU:CB	3:W:94:ARG:HD2	2.34	0.57
12:f:438:ASP:HA	12:f:477:MET:HE2	1.85	0.57
15:C:78:ARG:HH12	15:C:80:MET:HE3	1.69	0.57
18:F:393:GLY:HA3	36:F:501:ADP:C2	2.39	0.57
32:T:27:LEU:HD11	32:T:34:ALA:HB1	1.86	0.57
2:V:128:ARG:HG2	2:V:167:LEU:HD13	1.86	0.57
2:V:319:HIS:NE2	11:e:4:LYS:CB	2.67	0.57
8:b:100:ARG:HH12	8:b:105:HIS:HB2	1.69	0.57
13:A:192:GLU:HB2	13:A:196:LEU:HD13	1.86	0.57
15:C:59:LEU:HD12	16:D:75:ALA:HB1	1.86	0.57
15:C:212:ILE:O	15:C:246:ILE:HA	2.04	0.57
19:G:144:ASP:HB3	19:G:147:GLN:HB2	1.85	0.57
1:U:694:ILE:HG23	1:U:695:MET:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:O:6:VAL:HG23	27:O:124:TYR:HB3	1.87	0.57
27:O:213:THR:O	28:P:198:ARG:HA	2.05	0.57
30:r:44:THR:HG21	30:r:100:MET:HE3	1.86	0.57
1:U:593:SER:OG	1:U:595:ASN:ND2	2.38	0.57
1:U:729:GLY:O	1:U:733:ALA:HB2	2.04	0.57
3:W:96:GLN:NE2	3:W:135:LYS:O	2.38	0.57
9:c:192:LEU:HA	9:c:196:LEU:CD2	2.35	0.57
29:q:8:GLN:NE2	29:q:9:GLY:O	2.36	0.57
1:U:416:GLU:OE1	1:U:450:HIS:NE2	2.37	0.57
16:D:163:MET:HA	16:D:222:HIS:HE1	1.70	0.57
17:E:97:ARG:O	17:E:111:LEU:HB2	2.04	0.57
2:V:249:THR:O	2:V:253:LEU:HB2	2.04	0.57
12:f:556:ARG:CG	12:f:786:GLN:HG2	2.35	0.57
12:f:665:GLU:HG2	12:f:669:GLU:HG3	1.87	0.57
15:C:24:TYR:OH	16:D:41:TYR:C	2.48	0.57
21:I:213:ILE:O	21:I:228:LEU:CD2	2.53	0.57
29:Q:27:GLN:NE2	29:q:169:LYS:O	2.28	0.57
20:h:71:HIS:HA	20:h:218:PHE:H	1.69	0.57
1:U:9:ILE:HG12	1:U:38:ILE:HB	1.87	0.57
2:V:323:GLY:HA2	11:e:9:ASP:H	1.69	0.57
18:F:223:VAL:HG12	18:F:350:ARG:HB2	1.87	0.57
19:G:32:ILE:HA	19:G:82:GLY:HA2	1.86	0.57
25:M:168:ALA:HB1	25:M:171:ALA:HB3	1.85	0.57
32:T:192:VAL:HG12	32:T:197:VAL:HG22	1.87	0.57
3:W:86:ASN:OD1	3:W:89:LEU:C	2.48	0.57
3:W:178:GLU:OE2	3:W:181:GLU:HB2	2.04	0.57
6:Z:14:LEU:HG	9:c:39:LEU:HB3	1.87	0.57
15:C:90:HIS:CD2	15:C:90:HIS:N	2.73	0.57
15:C:387:VAL:O	15:C:391:MET:HB2	2.04	0.57
32:T:171:ARG:NH2	27:o:140:ASP:OD2	2.38	0.57
20:h:7:SER:HG	22:j:2:SER:N	2.03	0.57
25:m:214:SER:HG	25:m:224:HIS:HE2	1.52	0.57
27:o:6:VAL:HG23	27:o:124:TYR:HB3	1.87	0.57
12:f:712:LYS:HD3	12:f:715:HIS:CB	2.26	0.56
16:D:88:VAL:HG11	16:D:133:HIS:O	2.04	0.56
26:N:144:ARG:NH2	26:N:151:GLU:OE1	2.38	0.56
19:g:132:ARG:HB2	25:m:12:SER:HA	1.86	0.56
29:q:19:ARG:HH21	29:q:31:ASP:HB2	1.71	0.56
32:t:192:VAL:HG12	32:t:197:VAL:HG22	1.87	0.56
1:U:184:CYS:HA	1:U:187:LEU:HG	1.88	0.56
5:Y:233:ARG:O	5:Y:237:ARG:N	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:e:51:ASP:O	11:e:55:GLN:OE1	2.22	0.56
12:f:337:LEU:HD23	12:f:341:GLU:CD	2.29	0.56
13:A:248:LYS:NZ	16:D:278:GLN:OE1	2.35	0.56
15:C:59:LEU:HD12	16:D:75:ALA:CB	2.35	0.56
15:C:141:GLU:O	16:D:323:ARG:NH1	2.38	0.56
2:V:195:ILE:CD1	15:C:25:LEU:HG	2.34	0.56
2:V:297:ALA:HA	2:V:301:GLU:HG2	1.87	0.56
2:V:325:LYS:HA	2:V:328:VAL:HG12	1.86	0.56
3:W:124:LEU:HA	3:W:127:THR:HG22	1.86	0.56
7:a:190:VAL:HB	7:a:225:LEU:HD11	1.87	0.56
9:c:194:HIS:HB2	9:c:196:LEU:HD11	1.87	0.56
12:f:240:VAL:HA	12:f:257:ARG:HH21	1.71	0.56
12:f:759:LEU:H	12:f:809:ILE:CG2	2.18	0.56
12:f:773:LYS:C	12:f:775:THR:H	2.14	0.56
13:A:372:LEU:HD23	13:A:375:ARG:HH21	1.70	0.56
13:A:390:THR:HA	14:B:216:ILE:HD11	1.87	0.56
15:C:125:LYS:NZ	16:D:112:TYR:OH	2.38	0.56
26:N:19:ARG:NH1	26:N:168:GLY:O	2.39	0.56
26:N:179:ILE:HG12	26:N:184:VAL:HG22	1.88	0.56
31:S:28:ARG:NH2	31:S:191:ASP:OD1	2.38	0.56
21:i:99:LEU:O	29:q:86:ARG:NH2	2.38	0.56
26:n:19:ARG:NH1	26:n:168:GLY:O	2.39	0.56
26:n:179:ILE:HG12	26:n:184:VAL:HG22	1.88	0.56
2:V:495:ARG:N	15:C:44:ARG:CZ	2.66	0.56
3:W:268:LYS:NZ	3:W:302:TYR:OH	2.39	0.56
6:Z:15:VAL:HA	6:Z:18:SER:HB3	1.86	0.56
13:A:294:GLU:HA	13:A:297:ARG:HH11	1.70	0.56
19:g:32:ILE:HA	19:g:82:GLY:HA2	1.86	0.56
1:U:567:ILE:HB	1:U:601:ARG:NH2	2.20	0.56
7:a:290:GLN:O	7:a:330:ARG:NH2	2.38	0.56
12:f:189:LYS:HG2	12:f:190:GLU:HG2	1.87	0.56
12:f:469:TYR:OH	12:f:478:ARG:NH1	2.39	0.56
13:A:339:ARG:NH2	18:F:405:MET:SD	2.78	0.56
15:C:31:LEU:HD21	16:D:47:LEU:CB	2.33	0.56
26:n:127:ILE:HG12	26:n:132:SER:HB2	1.88	0.56
5:Y:69:LEU:HA	5:Y:72:LYS:HE3	1.88	0.56
7:a:170:ALA:HA	7:a:173:TYR:HB3	1.88	0.56
14:B:52:VAL:O	14:B:52:VAL:HG13	2.05	0.56
16:D:127:ASN:HB3	16:D:252:ARG:HD3	1.87	0.56
25:m:175:GLU:HA	25:m:178:LYS:HD3	1.88	0.56
1:U:177:LEU:CD2	1:U:180:SER:CB	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:492:LYS:O	15:C:44:ARG:NH1	2.38	0.56
10:d:155:LYS:NZ	10:d:167:ILE:O	2.39	0.56
10:d:167:ILE:O	10:d:171:LEU:CD1	2.53	0.56
18:F:141:ASP:OD1	18:F:144:LYS:NZ	2.35	0.56
18:F:311:LEU:HD23	18:F:314:LEU:HD12	1.87	0.56
24:L:121:GLN:HG3	25:M:129:ARG:HG2	1.88	0.56
25:m:51:LYS:HB3	25:m:210:GLU:HB3	1.87	0.56
6:Z:256:GLN:NE2	9:c:295:ASN:O	2.38	0.56
8:b:124:LEU:HD21	8:b:152:LYS:HB3	1.87	0.56
12:f:41:LYS:O	12:f:45:LEU:HB2	2.05	0.56
12:f:222:ASP:HB2	14:B:60:LEU:HD22	1.62	0.56
19:g:46:ASP:CB	19:g:222:VAL:HG22	2.25	0.56
24:l:50:LYS:HB3	24:l:59:HIS:HB3	1.88	0.56
28:p:2:SER:N	28:p:5:SER:HG	2.03	0.56
1:U:646:PRO:HA	1:U:649:ARG:HB2	1.87	0.56
2:V:211:TYR:HD2	2:V:253:LEU:HD13	1.70	0.56
5:Y:233:ARG:NH2	5:Y:306:GLN:NE2	2.54	0.56
12:f:243:PRO:HA	12:f:247:ALA:HB3	1.88	0.56
12:f:487:LEU:HD11	12:f:804:LEU:HD12	1.87	0.56
12:f:658:ALA:HB2	14:B:78:PHE:O	2.06	0.56
24:L:50:LYS:HB3	24:L:59:HIS:HB3	1.88	0.56
31:S:193:LEU:O	31:S:207:THR:HA	2.06	0.56
30:r:77:ALA:O	30:r:120:ARG:NH2	2.39	0.56
31:s:193:LEU:O	31:s:207:THR:HA	2.06	0.56
1:U:465:LEU:HD11	1:U:477:GLY:HA3	1.88	0.56
3:W:49:SER:N	3:W:94:ARG:HD3	2.21	0.56
3:W:74:CYS:O	3:W:78:LYS:HB3	2.06	0.56
6:Z:138:TYR:HA	6:Z:157:HIS:HA	1.87	0.56
9:c:51:MET:HA	9:c:82:VAL:HG22	1.88	0.56
2:V:328:VAL:O	2:V:332:LEU:CB	2.54	0.55
3:W:133:GLU:HG2	16:D:391:ARG:HD3	1.88	0.55
3:W:288:HIS:HA	3:W:291:SER:HB3	1.87	0.55
6:Z:78:MET:HE3	9:c:95:MET:HE1	1.87	0.55
6:Z:109:ASN:ND2	6:Z:140:SER:OG	2.39	0.55
9:c:50:PRO:HG3	17:E:84:ARG:HG2	1.86	0.55
28:P:2:SER:N	28:P:5:SER:HG	2.03	0.55
31:S:38:ARG:NH2	27:o:164:PHE:O	2.39	0.55
24:l:26:MET:HE1	24:l:148:CYS:HB2	1.87	0.55
29:q:117:TYR:HB3	29:q:125:ALA:HB3	1.87	0.55
5:Y:104:MET:O	5:Y:108:ALA:CB	2.54	0.55
12:f:465:LEU:O	12:f:481:SER:OG	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:196:GLU:OE2	14:B:349:ARG:NH1	2.35	0.55
14:B:387:LYS:HB3	14:B:390:LEU:HB3	1.88	0.55
27:o:41:ILE:HG12	27:o:102:GLY:HA3	1.88	0.55
2:V:348:PHE:CD1	2:V:348:PHE:N	2.73	0.55
2:V:497:PRO:HB3	6:Z:282:ASN:HB2	1.87	0.55
3:W:128:LEU:HD13	3:W:131:VAL:HG21	1.88	0.55
3:W:172:GLU:H	3:W:172:GLU:CD	2.14	0.55
8:b:157:VAL:HG21	8:b:170:LEU:HB2	1.88	0.55
9:c:94:LYS:O	9:c:98:MET:HB2	2.06	0.55
10:d:155:LYS:CD	10:d:171:LEU:HD21	2.35	0.55
12:f:658:ALA:HB1	14:B:78:PHE:CG	2.42	0.55
15:C:24:TYR:CE2	16:D:40:LEU:CB	2.89	0.55
16:D:85:ILE:HD12	17:E:82:GLY:N	2.22	0.55
16:D:87:LEU:HD21	16:D:131:ALA:HB1	1.07	0.55
16:D:212:LYS:NZ	34:D:501:ATP:O1G	2.39	0.55
19:G:46:ASP:O	19:G:222:VAL:HG22	2.05	0.55
19:g:223:GLU:O	19:g:225:PRO:HD3	2.07	0.55
26:n:144:ARG:NH2	26:n:151:GLU:OE1	2.38	0.55
2:V:210:CYS:O	2:V:214:HIS:HB2	2.06	0.55
3:W:32:ALA:HA	3:W:35:ALA:HB3	1.87	0.55
3:W:97:LEU:HD11	3:W:138:VAL:CG2	2.37	0.55
3:W:334:GLU:O	3:W:338:THR:OG1	2.22	0.55
15:C:113:ARG:CB	15:C:127:LEU:HB2	2.37	0.55
17:E:312:ILE:CB	34:E:401:ATP:N1	2.69	0.55
21:I:213:ILE:HB	21:I:228:LEU:HD21	1.87	0.55
25:M:51:LYS:HB3	25:M:210:GLU:HB3	1.87	0.55
25:M:175:GLU:HA	25:M:178:LYS:HD3	1.88	0.55
27:O:41:ILE:HG12	27:O:102:GLY:HA3	1.88	0.55
1:U:177:LEU:HD23	1:U:180:SER:HB3	1.86	0.55
1:U:602:LEU:C	1:U:602:LEU:HD22	2.32	0.55
2:V:218:TYR:OH	2:V:223:LYS:NZ	2.40	0.55
3:W:82:LEU:HD22	3:W:82:LEU:C	2.31	0.55
4:X:106:GLU:HB3	4:X:136:LEU:HD21	1.88	0.55
12:f:335:ARG:HB3	12:f:853:VAL:HG21	1.88	0.55
15:C:113:ARG:HB2	15:C:127:LEU:HB2	1.89	0.55
30:R:19:ARG:NH2	28:p:205:ASP:OD2	2.40	0.55
3:W:28:LEU:O	3:W:32:ALA:HB2	2.07	0.55
12:f:796:LEU:HA	12:f:799:VAL:HG12	1.89	0.55
15:C:52:LEU:CD2	16:D:68:LEU:HD12	2.32	0.55
20:H:4:ARG:NH1	20:H:5:GLY:O	2.39	0.55
24:L:26:MET:HE1	24:L:148:CYS:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Q:117:TYR:HB3	29:Q:125:ALA:HB3	1.88	0.55
31:s:28:ARG:NH2	31:s:191:ASP:OD1	2.38	0.55
9:c:146:ASP:OD2	9:c:149:GLN:NE2	2.40	0.55
12:f:712:LYS:HD3	12:f:712:LYS:C	2.31	0.55
16:D:124:LEU:C	16:D:126:PRO:HD3	2.32	0.55
26:N:127:ILE:HG12	26:N:132:SER:HB2	1.88	0.55
32:T:27:LEU:HD22	32:T:184:TYR:HB2	1.88	0.55
27:o:88:PHE:O	27:o:91:GLN:NE2	2.40	0.55
5:Y:297:ARG:HH22	11:e:51:ASP:HB3	1.70	0.55
9:c:191:ALA:C	9:c:196:LEU:CG	2.78	0.55
17:E:182:LEU:HD22	34:E:401:ATP:H2'	1.85	0.55
29:Q:19:ARG:HH21	29:Q:31:ASP:HB2	1.71	0.55
20:h:4:ARG:NH1	20:h:5:GLY:O	2.39	0.55
21:i:3:ARG:HB2	22:j:5:ARG:HH12	1.71	0.55
12:f:559:PRO:HB2	12:f:594:LEU:HG	1.88	0.55
13:A:213:LEU:HD22	13:A:337:LEU:HD23	1.87	0.55
14:B:89:GLU:HB2	14:B:94:GLU:HG2	1.89	0.55
17:E:144:GLU:OE2	17:E:297:ARG:NH1	2.40	0.55
25:m:17:ASP:OD2	25:m:19:ARG:NH2	2.40	0.55
1:U:613:ASP:OD1	1:U:616:ARG:NH2	2.36	0.55
2:V:280:ALA:HB3	2:V:285:TRP:HB2	1.88	0.55
12:f:556:ARG:CD	12:f:786:GLN:HE21	2.20	0.55
12:f:663:GLY:O	14:B:86:LYS:NZ	2.34	0.55
17:E:244:SER:H	18:F:300:LYS:HA	1.72	0.55
20:H:222:THR:OG1	20:H:225:GLU:OE1	2.24	0.55
21:I:85:VAL:O	21:I:89:GLU:CB	2.55	0.55
1:U:217:CYS:HB2	1:U:248:ILE:HD12	1.89	0.54
2:V:277:PRO:HD2	2:V:285:TRP:HZ3	1.71	0.54
3:W:52:LYS:HD3	3:W:55:ARG:HD3	1.89	0.54
4:X:402:GLU:HB2	9:c:249:LEU:HD11	1.89	0.54
12:f:718:ASP:HB2	12:f:760:PHE:CD2	2.43	0.54
27:O:1:THR:N	27:O:168:GLY:O	2.40	0.54
12:f:556:ARG:HD3	12:f:786:GLN:CB	2.38	0.54
14:B:232:LYS:HE2	34:B:501:ATP:O1G	2.07	0.54
14:B:251:VAL:HG12	14:B:253:SER:H	1.72	0.54
23:K:97:GLN:HB3	30:R:61:ARG:HG3	1.90	0.54
25:M:17:ASP:OD2	25:M:19:ARG:NH2	2.40	0.54
27:o:30:ASN:OD1	27:o:187:ARG:NH2	2.40	0.54
30:r:196:HIS:O	30:r:200:SER:HB3	2.08	0.54
5:Y:141:VAL:HG13	5:Y:160:ASN:HB2	1.88	0.54
12:f:219:LYS:HE3	14:B:59:ARG:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:222:ASP:CG	14:B:60:LEU:HA	2.30	0.54
12:f:291:GLN:HE22	12:f:324:VAL:HG11	1.71	0.54
18:F:233:LYS:N	36:F:501:ADP:O1A	2.33	0.54
32:T:45:VAL:HB	32:T:49:THR:O	2.08	0.54
21:i:85:VAL:O	21:i:89:GLU:CB	2.55	0.54
27:o:1:THR:N	27:o:168:GLY:O	2.40	0.54
32:t:27:LEU:HD22	32:t:184:TYR:HB2	1.88	0.54
2:V:345:ARG:CZ	2:V:357:LEU:CB	2.86	0.54
11:e:56:LEU:CD1	11:e:59:GLU:CB	2.66	0.54
12:f:296:PHE:O	12:f:807:ARG:NH2	2.40	0.54
14:B:262:ASP:OD1	14:B:265:LYS:NZ	2.40	0.54
16:D:40:LEU:HD12	16:D:43:ARG:HG3	1.89	0.54
18:F:94:ILE:HD11	18:F:125:LYS:HB2	1.89	0.54
19:G:141:ILE:HG22	19:G:151:VAL:HG22	1.88	0.54
30:R:77:ALA:O	30:R:120:ARG:NH2	2.39	0.54
19:g:141:ILE:HG22	19:g:151:VAL:HG22	1.88	0.54
30:r:12:VAL:HB	30:r:179:VAL:HB	1.90	0.54
1:U:607:VAL:O	1:U:615:ARG:NH1	2.38	0.54
1:U:639:LEU:HD12	15:C:49:ARG:NH1	2.23	0.54
5:Y:57:LEU:HD11	5:Y:63:TRP:HB2	1.88	0.54
6:Z:250:TYR:O	6:Z:254:ASN:HB2	2.08	0.54
12:f:150:GLU:O	12:f:156:HIS:ND1	2.40	0.54
12:f:414:LEU:HD23	12:f:417:ILE:HD12	1.90	0.54
27:O:140:ASP:OD2	32:t:171:ARG:NH2	2.40	0.54
30:R:196:HIS:O	30:R:200:SER:CB	2.56	0.54
1:U:768:GLN:HB2	1:U:775:LEU:HD12	1.90	0.54
31:S:75:TYR:O	31:S:79:ASN:HB2	2.08	0.54
1:U:456:ASP:O	1:U:460:TYR:HB3	2.08	0.54
1:U:471:ASP:HA	1:U:474:ARG:HB2	1.90	0.54
6:Z:66:SER:OG	6:Z:103:LYS:NZ	2.40	0.54
25:M:214:SER:OG	25:M:224:HIS:NE2	2.30	0.54
2:V:210:CYS:O	2:V:214:HIS:CB	2.55	0.54
5:Y:104:MET:O	5:Y:108:ALA:HB2	2.07	0.54
8:b:11:ASP:HB3	8:b:16:MET:HE2	1.90	0.54
15:C:24:TYR:HD2	16:D:40:LEU:CG	1.99	0.54
16:D:117:SER:HA	16:D:121:ARG:HH22	1.72	0.54
17:E:171:LEU:HD21	17:E:298:LYS:HG2	1.90	0.54
28:P:15:LYS:HA	28:P:20:VAL:HG23	1.90	0.54
21:i:198:ASN:HA	21:i:206:LEU:HD21	1.90	0.54
30:r:154:ASP:OD1	30:r:157:ARG:NH1	2.40	0.54
1:U:603:LEU:HD21	16:D:60:TYR:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:136:ILE:HG22	3:W:140:ILE:HB	1.90	0.54
9:c:191:ALA:CB	9:c:196:LEU:HG	2.38	0.54
9:c:196:LEU:HD22	9:c:196:LEU:N	2.15	0.54
13:A:189:GLU:OE2	18:F:409:ARG:NH2	2.41	0.54
15:C:152:GLY:N	36:C:501:ADP:C6	2.59	0.54
16:D:355:SER:OG	16:D:358:VAL:HG23	2.08	0.54
17:E:171:LEU:HD22	17:E:295:LEU:HD13	1.90	0.54
17:E:312:ILE:HG21	34:E:401:ATP:C6	2.43	0.54
30:R:154:ASP:OD1	30:R:157:ARG:NH1	2.40	0.54
26:n:11:GLY:HA3	26:n:179:ILE:O	2.08	0.54
32:t:45:VAL:HB	32:t:49:THR:O	2.08	0.54
1:U:77:SER:O	1:U:81:ALA:HB2	2.08	0.54
1:U:770:TRP:HA	9:c:180:ASN:HB3	1.90	0.54
7:a:197:ALA:HB2	7:a:222:LEU:HD22	1.89	0.54
12:f:373:ALA:HB2	12:f:744:MET:HA	1.89	0.54
15:C:69:GLN:OE1	15:C:69:GLN:N	2.39	0.54
16:D:125:LYS:N	16:D:126:PRO:HD3	2.23	0.54
19:G:127:GLN:HA	20:H:128:ARG:HH21	1.72	0.54
24:L:157:ARG:NH2	25:M:56:LYS:O	2.41	0.54
1:U:510:GLU:OE2	1:U:546:ARG:NH2	2.39	0.53
1:U:602:LEU:HD22	1:U:602:LEU:O	2.08	0.53
2:V:345:ARG:NH2	2:V:360:TYR:HB3	2.22	0.53
8:b:2:VAL:O	8:b:44:ASN:ND2	2.41	0.53
8:b:72:LEU:O	8:b:76:HIS:ND1	2.33	0.53
9:c:192:LEU:CA	9:c:196:LEU:HD21	2.38	0.53
12:f:591:ALA:HA	12:f:594:LEU:HD23	1.90	0.53
13:A:190:VAL:HG21	13:A:339:ARG:HG3	1.90	0.53
14:B:249:ARG:HG3	14:B:283:PHE:HD2	1.71	0.53
16:D:332:GLU:HG3	16:D:334:PRO:HD3	1.89	0.53
27:O:30:ASN:OD1	27:O:187:ARG:NH2	2.41	0.53
26:n:144:ARG:H	26:n:147:MET:HE3	1.72	0.53
28:p:15:LYS:HA	28:p:20:VAL:HG23	1.90	0.53
2:V:495:ARG:H	15:C:44:ARG:NH2	2.06	0.53
3:W:46:THR:HA	3:W:50:LEU:CD1	2.38	0.53
15:C:75:GLU:H	15:C:87:VAL:HG13	1.73	0.53
16:D:152:MET:HE3	16:D:154:LEU:HD13	1.90	0.53
22:J:119:THR:HG22	22:J:126:PRO:HB3	1.90	0.53
28:P:48:ARG:HH12	28:P:114:PRO:HA	1.73	0.53
30:R:196:HIS:O	30:R:200:SER:HB3	2.08	0.53
30:r:196:HIS:O	30:r:200:SER:CB	2.56	0.53
3:W:48:LEU:HG	3:W:95:SER:HB2	1.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:124:LEU:HD13	8:b:156:PHE:HB2	1.89	0.53
10:d:47:GLN:HG2	10:d:48:LEU:HG	1.89	0.53
19:G:120:ASP:OD1	20:H:84:ARG:NH1	2.40	0.53
27:O:88:PHE:O	27:O:91:GLN:NE2	2.40	0.53
28:p:48:ARG:HH12	28:p:114:PRO:HA	1.73	0.53
31:s:14:ALA:HA	31:s:22:ILE:O	2.08	0.53
2:V:259:LEU:HD11	2:V:294:ARG:HD2	1.90	0.53
3:W:390:GLU:HG3	3:W:408:ARG:HH21	1.73	0.53
15:C:52:LEU:CD2	16:D:68:LEU:CD1	2.86	0.53
17:E:232:MET:HB3	17:E:277:MET:HG2	1.90	0.53
26:N:144:ARG:H	26:N:147:MET:HE3	1.72	0.53
31:S:14:ALA:HA	31:S:22:ILE:O	2.08	0.53
23:k:41:GLN:HA	23:k:46:VAL:HG22	1.91	0.53
31:s:75:TYR:O	31:s:79:ASN:HB2	2.08	0.53
1:U:218:GLN:NE2	1:U:752:THR:O	2.42	0.53
2:V:495:ARG:O	15:C:44:ARG:HG3	2.08	0.53
3:W:344:THR:O	3:W:348:GLU:CB	2.54	0.53
3:W:425:LEU:HD13	6:Z:245:PHE:CE1	2.43	0.53
12:f:250:ARG:NH1	12:f:285:CYS:SG	2.81	0.53
15:C:371:LEU:O	15:C:374:ARG:NH1	2.40	0.53
24:L:48:ALA:HB1	24:L:62:LYS:HE3	1.89	0.53
19:g:164:LYS:NZ	20:h:57:TYR:O	2.41	0.53
21:i:118:LYS:HD3	21:i:152:PRO:HA	1.91	0.53
2:V:319:HIS:NE2	11:e:4:LYS:HB2	2.23	0.53
5:Y:168:ILE:HG21	5:Y:177:ARG:HB2	1.90	0.53
12:f:694:LEU:HD12	12:f:729:MET:HE1	1.90	0.53
12:f:828:ARG:HH22	12:f:842:VAL:HG23	1.72	0.53
17:E:304:PRO:O	17:E:309:ARG:NH1	2.42	0.53
17:E:340:GLY:CA	34:E:401:ATP:C5	2.88	0.53
30:R:12:VAL:HB	30:R:179:VAL:HB	1.90	0.53
21:i:218:ARG:NH1	21:i:223:THR:OG1	2.41	0.53
22:j:200:GLN:OE1	22:j:202:GLY:N	2.41	0.53
28:p:169:GLN:O	28:p:173:ASN:ND2	2.42	0.53
1:U:64:ALA:HA	1:U:67:VAL:HG12	1.90	0.53
2:V:70:VAL:HG21	2:V:209:LYS:HD3	1.90	0.53
2:V:211:TYR:O	2:V:215:ALA:CB	2.57	0.53
9:c:280:PRO:O	9:c:284:LEU:CB	2.54	0.53
12:f:813:LYS:HD3	12:f:815:HIS:HE1	1.73	0.53
16:D:233:SER:OG	17:E:259:GLU:OE1	2.26	0.53
17:E:101:ASP:HB3	17:E:106:THR:H	1.74	0.53
19:G:153:LYS:NZ	19:G:167:ALA:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:I:118:LYS:HD3	21:I:152:PRO:HA	1.91	0.53
21:I:198:ASN:HA	21:I:206:LEU:HD21	1.90	0.53
25:M:241:GLU:O	25:M:244:LYS:NZ	2.37	0.53
26:N:11:GLY:HA3	26:N:179:ILE:O	2.08	0.53
27:O:112:SER:OG	27:O:120:ASP:OD1	2.26	0.53
19:g:153:LYS:NZ	19:g:167:ALA:O	2.42	0.53
1:U:17:PRO:O	1:U:55:ARG:NH1	2.41	0.53
1:U:639:LEU:CD1	15:C:49:ARG:NH1	2.72	0.53
7:a:33:LEU:HA	8:b:18:ASN:HD22	1.73	0.53
8:b:121:GLU:HA	8:b:124:LEU:HG	1.91	0.53
8:b:121:GLU:HB3	8:b:152:LYS:HG2	1.90	0.53
19:G:137:CYS:SG	19:G:138:MET:N	2.76	0.53
32:T:180:ASP:HB3	32:T:183:SER:HB3	1.91	0.53
20:h:222:THR:OG1	20:h:225:GLU:OE1	2.24	0.53
23:k:117:SER:HB2	24:l:82:ARG:HH12	1.73	0.53
24:l:48:ALA:HB1	24:l:62:LYS:HE3	1.89	0.53
1:U:490:ARG:HB2	1:U:493:VAL:HG12	1.90	0.53
2:V:190:ASP:OD1	2:V:234:ARG:NH1	2.39	0.53
2:V:345:ARG:NH1	2:V:357:LEU:CA	2.69	0.53
3:W:86:ASN:OD1	3:W:91:SER:N	2.37	0.53
12:f:642:ALA:N	12:f:643:PRO:HD2	2.23	0.53
12:f:650:GLN:HE21	13:A:56:LEU:HD12	1.74	0.53
15:C:86:LEU:HD11	15:C:94:LYS:HD3	1.91	0.53
32:T:89:HIS:NE2	32:T:124:TYR:O	2.41	0.53
22:j:119:THR:HG22	22:j:126:PRO:HB3	1.89	0.53
1:U:772:TRP:HB3	1:U:775:LEU:HB2	1.90	0.53
2:V:387:GLN:NE2	10:d:128:GLN:OE1	2.41	0.53
15:C:114:VAL:C	15:C:127:LEU:HG	2.34	0.53
16:D:86:PRO:HB2	16:D:134:LYS:HD2	1.90	0.53
17:E:333:LYS:HE3	19:G:57:PRO:HA	1.90	0.53
22:J:200:GLN:HA	22:J:200:GLN:NE2	2.24	0.53
23:K:79:SER:HB2	23:K:140:ALA:HB3	1.91	0.53
1:U:241:ASN:HD22	1:U:244:MET:HE3	1.74	0.52
7:a:324:ILE:HA	7:a:331:VAL:HG12	1.90	0.52
12:f:296:PHE:HA	12:f:807:ARG:HD2	1.91	0.52
14:B:405:MET:HE2	14:B:421:LYS:HD2	1.91	0.52
3:W:162:ALA:HB1	3:W:192:LEU:HD13	1.90	0.52
13:A:346:PRO:O	13:A:351:ARG:NH1	2.42	0.52
17:E:340:GLY:CA	34:E:401:ATP:C8	2.88	0.52
34:E:401:ATP:O3G	18:F:347:ARG:NH2	2.42	0.52
18:F:229:PRO:O	36:F:501:ADP:O2B	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:O:211:VAL:HG11	28:P:198:ARG:HD3	1.90	0.52
28:P:169:GLN:O	28:P:173:ASN:ND2	2.42	0.52
32:t:9:THR:O	32:t:41:ARG:NH2	2.42	0.52
3:W:274:VAL:HG21	3:W:290:ILE:HD13	1.90	0.52
12:f:219:LYS:HE3	14:B:59:ARG:HB2	1.90	0.52
12:f:593:THR:O	12:f:635:LYS:NZ	2.40	0.52
12:f:679:LEU:HD11	12:f:686:LEU:HD11	1.92	0.52
14:B:153:ASN:HD22	14:B:156:VAL:HG22	1.74	0.52
24:L:65:HIS:O	24:L:89:ARG:NH2	2.39	0.52
23:k:99:HIS:HB2	23:k:107:MET:HE3	1.91	0.52
29:q:38:MET:O	29:q:65:GLN:NE2	2.43	0.52
2:V:227:VAL:O	2:V:231:LEU:CB	2.57	0.52
4:X:177:TYR:HB3	4:X:182:ASN:HB3	1.92	0.52
5:Y:367:GLN:HE21	5:Y:371:LYS:HE2	1.74	0.52
8:b:8:VAL:O	8:b:51:LEU:HA	2.09	0.52
12:f:684:PRO:HA	12:f:687:ARG:HB3	1.90	0.52
23:k:79:SER:HB2	23:k:140:ALA:HB3	1.91	0.52
24:l:101:ARG:HH12	24:l:104:PRO:HD3	1.75	0.52
26:n:28:ASN:HD21	27:o:122:LEU:HD21	1.75	0.52
27:o:64:GLU:O	27:o:68:LEU:HB2	2.09	0.52
2:V:357:LEU:O	2:V:360:TYR:N	2.39	0.52
3:W:273:TYR:HA	3:W:276:LEU:HB2	1.91	0.52
5:Y:42:MET:SD	5:Y:46:ARG:NH2	2.81	0.52
12:f:219:LYS:HE2	12:f:223:GLU:OE2	2.09	0.52
12:f:723:TYR:O	12:f:727:PHE:HB3	2.09	0.52
16:D:87:LEU:CD1	16:D:140:VAL:HB	2.18	0.52
16:D:363:TYR:HE2	16:D:399:PHE:HB3	1.75	0.52
32:T:9:THR:O	32:T:41:ARG:NH2	2.42	0.52
30:r:115:ASP:HB2	30:r:119:ASN:HB2	1.92	0.52
31:s:1:ARG:HE	32:t:2:GLN:HE22	1.57	0.52
32:t:180:ASP:HB3	32:t:183:SER:HB3	1.91	0.52
2:V:106:ARG:O	2:V:110:HIS:ND1	2.43	0.52
2:V:496:PHE:N	15:C:44:ARG:NH2	2.56	0.52
17:E:182:LEU:CD2	34:E:401:ATP:H2'	2.40	0.52
21:I:106:PRO:HB2	21:I:109:GLN:HG2	1.92	0.52
23:K:36:THR:HA	23:K:171:GLY:HA3	1.92	0.52
27:O:98:LEU:HB2	27:O:113:ILE:HB	1.92	0.52
23:k:36:THR:HA	23:k:171:GLY:HA3	1.92	0.52
6:Z:22:HIS:HA	6:Z:25:ARG:HG2	1.91	0.52
7:a:19:PRO:HA	7:a:22:TRP:CD1	2.44	0.52
22:J:11:SER:OG	22:J:15:HIS:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:156:SER:HA	2:V:159:LEU:HB2	1.91	0.52
2:V:167:LEU:CG	2:V:171:VAL:HG11	2.37	0.52
3:W:48:LEU:HB2	3:W:94:ARG:HH21	1.74	0.52
3:W:287:VAL:O	3:W:291:SER:HB2	2.10	0.52
16:D:284:GLU:OE1	16:D:287:ARG:NH1	2.43	0.52
23:K:41:GLN:HA	23:K:46:VAL:HG22	1.91	0.52
21:i:106:PRO:HB2	21:i:109:GLN:HG2	1.92	0.52
1:U:599:ILE:HD13	1:U:625:ILE:HD11	1.92	0.52
6:Z:249:PHE:HZ	9:c:303:MET:HG2	1.75	0.52
12:f:650:GLN:OE1	14:B:72:LEU:CD1	2.39	0.52
14:B:112:LEU:HD12	14:B:148:CYS:HB3	1.92	0.52
15:C:370:ALA:HB1	15:C:375:ARG:HB2	1.92	0.52
16:D:164:TYR:O	16:D:174:LYS:NZ	2.38	0.52
16:D:335:LEU:HD23	16:D:369:LYS:HD3	1.84	0.52
24:L:101:ARG:HH12	24:L:104:PRO:HD3	1.75	0.52
28:P:15:LYS:HE3	28:P:121:ILE:HG12	1.92	0.52
31:S:28:ARG:NH1	31:S:187:VAL:O	2.43	0.52
19:g:165:ALA:HB3	20:h:56:LEU:HD22	1.91	0.52
6:Z:109:ASN:HD22	6:Z:155:PHE:HE1	1.58	0.52
6:Z:184:VAL:HG13	6:Z:188:SER:HB3	1.92	0.52
9:c:141:VAL:HG22	9:c:161:ARG:HH11	1.75	0.52
12:f:680:ARG:HB2	12:f:763:ARG:HE	1.74	0.52
12:f:712:LYS:HZ1	12:f:715:HIS:HD2	1.58	0.52
12:f:759:LEU:CD2	12:f:806:VAL:HG12	2.31	0.52
13:A:113:ILE:HD12	13:A:123:VAL:HG21	1.92	0.52
16:D:89:ILE:HB	17:E:78:ARG:O	2.10	0.52
17:E:113:ARG:NH1	17:E:224:ASP:OD1	2.43	0.52
23:K:167:ALA:H	24:L:56:LEU:HD13	1.75	0.52
20:h:148:GLN:O	20:h:155:TYR:HA	2.10	0.52
1:U:791:LEU:HD22	1:U:911:ILE:HD11	1.92	0.51
2:V:317:PRO:CD	11:e:4:LYS:HE2	2.38	0.51
4:X:122:ARG:HH21	20:H:185:GLU:HG3	1.73	0.51
15:C:24:TYR:CZ	16:D:41:TYR:CA	2.92	0.51
21:I:218:ARG:NH1	21:I:223:THR:OG1	2.41	0.51
30:R:115:ASP:HB2	30:R:119:ASN:HB2	1.91	0.51
19:g:123:GLN:O	19:g:127:GLN:HB2	2.10	0.51
2:V:451:ILE:HG23	2:V:458:VAL:HG22	1.91	0.51
2:V:467:TYR:O	6:Z:254:ASN:ND2	2.42	0.51
6:Z:223:ASN:CG	6:Z:227:ILE:HG13	2.09	0.51
9:c:191:ALA:HB1	9:c:196:LEU:CG	2.39	0.51
12:f:94:LYS:HA	12:f:97:LYS:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:168:LYS:HD3	12:f:204:ALA:HB1	1.92	0.51
18:F:318:ASP:OD2	18:F:344:ARG:NH2	2.44	0.51
21:I:40:ASN:ND2	21:I:182:GLY:O	2.43	0.51
23:K:41:GLN:NE2	23:K:151:PRO:O	2.43	0.51
27:O:64:GLU:O	27:O:68:LEU:HB2	2.10	0.51
21:i:33:THR:HA	21:i:165:GLY:HA2	1.91	0.51
31:s:28:ARG:NH1	31:s:187:VAL:O	2.43	0.51
32:t:49:THR:HB	32:t:85:PRO:HG3	1.92	0.51
1:U:268:LEU:HD22	1:U:329:LEU:HD11	1.91	0.51
9:c:254:ASN:OD1	9:c:278:GLN:NE2	2.44	0.51
12:f:823:ALA:HB1	12:f:825:MET:HG3	1.92	0.51
16:D:58:GLU:O	16:D:62:LYS:HB2	2.11	0.51
18:F:341:ALA:O	18:F:347:ARG:NH1	2.42	0.51
1:U:242:LEU:HA	1:U:245:ALA:HB3	1.91	0.51
5:Y:231:LEU:HB2	5:Y:235:ASP:HB2	1.92	0.51
6:Z:250:TYR:OH	10:d:234:ASP:O	2.29	0.51
7:a:57:ILE:HG13	7:a:61:GLU:HG2	1.92	0.51
15:C:24:TYR:HE2	16:D:40:LEU:CD1	2.23	0.51
22:J:200:GLN:NE2	22:J:200:GLN:CA	2.73	0.51
23:k:41:GLN:NE2	23:k:151:PRO:O	2.43	0.51
28:p:15:LYS:HE3	28:p:121:ILE:HG12	1.92	0.51
1:U:219:CYS:SG	1:U:220:LEU:N	2.84	0.51
1:U:780:SER:HA	1:U:783:TYR:HD2	1.75	0.51
12:f:708:ASP:OD2	12:f:787:LEU:CD2	2.56	0.51
13:A:185:GLU:OE1	13:A:188:ARG:NH2	2.43	0.51
15:C:31:LEU:HD21	16:D:47:LEU:CG	2.37	0.51
15:C:65:LEU:C	15:C:67:GLN:H	2.19	0.51
16:D:92:PHE:HA	16:D:103:VAL:HG12	1.93	0.51
18:F:318:ASP:HB3	18:F:347:ARG:HG2	1.92	0.51
20:H:148:GLN:O	20:H:155:TYR:HA	2.10	0.51
32:T:49:THR:HB	32:T:85:PRO:HG3	1.92	0.51
1:U:373:ASN:HA	1:U:376:MET:HG2	1.92	0.51
1:U:376:MET:HA	1:U:739:ALA:HA	1.92	0.51
7:a:371:ALA:HA	7:a:374:ILE:HD13	1.91	0.51
12:f:773:LYS:C	12:f:775:THR:N	2.69	0.51
13:A:312:ARG:HB2	13:A:315:ILE:HB	1.91	0.51
21:I:33:THR:HA	21:I:165:GLY:HA2	1.91	0.51
28:P:26:ARG:HH21	28:P:38:ASP:HA	1.76	0.51
31:s:4:PRO:O	32:t:100:ARG:NH2	2.39	0.51
1:U:714:SER:HA	1:U:717:ILE:HG22	1.92	0.51
1:U:798:PRO:O	1:U:880:ASN:ND2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:293:ARG:NH2	11:e:52:PHE:O	2.43	0.51
6:Z:283:ARG:NH1	6:Z:284:ASP:OD1	2.44	0.51
14:B:142:ASP:C	14:B:144:LEU:N	2.60	0.51
16:D:369:LYS:HE3	16:D:369:LYS:CA	2.30	0.51
23:K:99:HIS:HB2	23:K:107:MET:HE3	1.91	0.51
21:i:197:LEU:O	21:i:201:MET:CB	2.59	0.51
27:o:112:SER:OG	27:o:120:ASP:OD1	2.26	0.51
5:Y:315:THR:HA	5:Y:353:ILE:HA	1.92	0.51
7:a:57:ILE:HD12	7:a:60:TYR:HB3	1.93	0.51
15:C:88:LYS:HB3	15:C:94:LYS:HG2	1.93	0.51
24:L:117:GLN:O	24:L:120:THR:OG1	2.29	0.51
29:Q:38:MET:O	29:Q:65:GLN:NE2	2.43	0.51
31:S:45:LYS:HA	31:S:51:VAL:HG22	1.93	0.51
31:s:45:LYS:HA	31:s:51:VAL:HG22	1.93	0.51
32:t:89:HIS:NE2	32:t:124:TYR:O	2.41	0.51
2:V:437:ILE:HA	10:d:146:GLY:HA3	1.91	0.51
6:Z:189:GLN:HA	6:Z:192:THR:HG22	1.93	0.51
9:c:25:VAL:O	9:c:176:GLN:NE2	2.42	0.51
17:E:181:THR:HB	34:E:401:ATP:O1B	2.00	0.51
23:k:146:VAL:HG11	23:k:222:PRO:HA	1.93	0.51
27:o:98:LEU:HB2	27:o:113:ILE:HB	1.92	0.51
28:p:58:THR:OG1	29:q:121:LEU:O	2.23	0.51
1:U:27:LEU:HD13	1:U:63:VAL:HG21	1.92	0.51
1:U:47:VAL:O	1:U:51:ASP:HB2	2.10	0.51
3:W:80:TRP:CG	3:W:130:MET:HE2	2.45	0.51
3:W:158:ASP:O	3:W:162:ALA:CB	2.59	0.51
9:c:196:LEU:O	9:c:200:TYR:CD2	2.64	0.51
17:E:25:ARG:O	17:E:29:LEU:CB	2.59	0.51
20:H:185:GLU:HA	20:H:188:ILE:HD12	1.93	0.51
19:g:46:ASP:CA	19:g:222:VAL:HG22	2.41	0.51
28:p:2:SER:OG	28:p:3:ILE:N	2.44	0.51
1:U:62:LEU:HD12	1:U:84:ALA:HB1	1.93	0.50
3:W:373:ILE:HA	7:a:326:GLU:HB3	1.94	0.50
3:W:408:ARG:HB3	4:X:345:VAL:HG23	1.93	0.50
9:c:192:LEU:HA	9:c:196:LEU:HD21	1.93	0.50
12:f:218:GLU:HA	12:f:221:ILE:HG22	1.92	0.50
20:H:204:THR:OG1	20:H:206:ASP:OD1	2.29	0.50
21:I:213:ILE:O	21:I:228:LEU:HG	2.11	0.50
31:s:153:VAL:HG13	31:s:166:LEU:HD11	1.93	0.50
1:U:576:PRO:HA	1:U:579:ARG:HE	1.77	0.50
2:V:33:GLN:HG3	2:V:89:LYS:HE3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:467:TYR:OH	6:Z:255:ASP:OD1	2.30	0.50
3:W:34:LEU:HB2	3:W:40:LEU:HD12	1.92	0.50
3:W:401:THR:HG23	3:W:402:ILE:HD12	1.92	0.50
9:c:197:ASN:CA	9:c:200:TYR:O	2.56	0.50
12:f:764:LEU:HD11	12:f:774:GLY:C	2.36	0.50
13:A:222:LYS:NZ	13:A:321:THR:O	2.42	0.50
13:A:310:ASP:N	13:A:311:PRO:HD3	2.26	0.50
19:G:123:GLN:O	19:G:127:GLN:HB2	2.10	0.50
21:i:40:ASN:ND2	21:i:182:GLY:O	2.43	0.50
28:P:2:SER:OG	28:P:3:ILE:N	2.44	0.50
9:c:160:PHE:HA	9:c:201:TYR:O	2.11	0.50
23:K:146:VAL:HG11	23:K:222:PRO:HA	1.94	0.50
31:s:57:PHE:HD2	31:s:60:ASP:H	1.59	0.50
1:U:644:TYR:CD2	15:C:60:ARG:NH2	2.61	0.50
2:V:496:PHE:CE1	15:C:40:GLN:CD	2.78	0.50
3:W:449:GLU:HG2	6:Z:219:LYS:HE3	1.92	0.50
4:X:252:LYS:HA	4:X:287:LEU:HD11	1.94	0.50
7:a:321:LYS:O	7:a:334:THR:OG1	2.30	0.50
12:f:119:LYS:HA	12:f:122:ALA:HB3	1.93	0.50
15:C:147:THR:HG22	15:C:150:MET:HE3	1.93	0.50
16:D:103:VAL:HG11	16:D:139:LEU:HD21	1.94	0.50
19:G:133:PRO:HD2	25:M:14:PHE:HE2	1.76	0.50
21:I:197:LEU:O	21:I:201:MET:CB	2.59	0.50
23:K:141:LEU:HB2	23:K:156:MET:HG2	1.94	0.50
32:T:1:THR:N	32:T:105:PRO:O	2.45	0.50
25:m:40:ARG:HA	25:m:45:VAL:HA	1.94	0.50
27:o:46:ALA:HB3	27:o:97:ALA:HB3	1.94	0.50
32:t:136:SER:HB2	32:t:150:LEU:HD13	1.94	0.50
1:U:133:ILE:HA	1:U:136:LYS:HB3	1.93	0.50
1:U:410:VAL:HG23	1:U:448:LEU:HD13	1.92	0.50
1:U:415:HIS:CD2	1:U:418:GLU:H	2.29	0.50
1:U:584:TYR:OH	1:U:768:GLN:NE2	2.44	0.50
12:f:369:ARG:NH2	12:f:791:VAL:O	2.41	0.50
28:P:177:ARG:NH2	31:s:150:ASP:OD2	2.41	0.50
25:m:170:GLN:HA	25:m:173:LYS:HG2	1.92	0.50
27:o:214:GLU:HA	28:p:198:ARG:HG2	1.93	0.50
31:s:125:ASP:OD1	31:s:129:SER:N	2.43	0.50
1:U:222:PHE:HE1	1:U:754:HIS:HB2	1.77	0.50
3:W:328:LEU:HB3	3:W:337:ALA:HB1	1.94	0.50
12:f:739:ALA:HB1	12:f:743:ALA:HB2	1.92	0.50
20:H:14:SER:HG	20:H:18:LYS:H	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:h:185:GLU:HA	20:h:188:ILE:HD12	1.93	0.50
31:s:198:VAL:HG22	31:s:203:ILE:HG12	1.94	0.50
32:t:1:THR:N	32:t:105:PRO:O	2.45	0.50
32:t:86:ARG:NH1	32:t:133:GLU:OE2	2.44	0.50
1:U:325:MET:O	1:U:329:LEU:HB2	2.12	0.50
2:V:211:TYR:O	2:V:215:ALA:HB2	2.12	0.50
6:Z:224:HIS:ND1	6:Z:224:HIS:N	2.60	0.50
12:f:206:ASP:OD2	12:f:245:ASN:ND2	2.45	0.50
12:f:482:ILE:HD11	12:f:517:VAL:HG23	1.94	0.50
12:f:642:ALA:N	12:f:643:PRO:CD	2.75	0.50
34:D:501:ATP:O3G	17:E:294:ARG:NH1	2.39	0.50
25:M:40:ARG:HA	25:M:45:VAL:HA	1.94	0.50
31:S:198:VAL:HG22	31:S:203:ILE:HG12	1.94	0.50
32:T:136:SER:HB2	32:T:150:LEU:HD13	1.94	0.50
31:s:35:ILE:HB	32:t:151:ARG:HH12	1.76	0.50
1:U:341:PHE:HZ	1:U:883:ARG:HB3	1.77	0.50
5:Y:262:SER:OG	5:Y:267:ARG:O	2.29	0.50
7:a:100:THR:HA	7:a:103:LYS:HG2	1.93	0.50
15:C:301:LEU:HD13	15:C:305:LEU:HD23	1.93	0.50
18:F:421:MET:HA	18:F:424:ILE:HD12	1.94	0.50
31:S:108:ASN:HB2	31:S:124:PHE:HB2	1.94	0.50
28:p:26:ARG:HH21	28:p:38:ASP:HA	1.76	0.50
1:U:456:ASP:O	1:U:460:TYR:CB	2.60	0.49
1:U:900:TYR:HB3	1:U:914:LEU:HG	1.93	0.49
2:V:358:MET:O	2:V:362:LEU:CB	2.60	0.49
3:W:49:SER:H	3:W:94:ARG:CD	2.24	0.49
7:a:292:THR:HG23	7:a:295:GLU:H	1.77	0.49
8:b:20:ASP:OD2	8:b:25:ARG:NH2	2.45	0.49
9:c:130:GLN:HE22	9:c:162:LEU:HD22	1.77	0.49
9:c:197:ASN:N	9:c:197:ASN:ND2	2.60	0.49
12:f:220:ASP:HA	12:f:223:GLU:OE1	2.11	0.49
17:E:172:LEU:HD22	17:E:301:ILE:HD11	1.93	0.49
19:G:60:LEU:O	25:M:161:TRP:N	2.41	0.49
21:I:119:GLN:HG3	22:J:78:ALA:HB1	1.93	0.49
24:L:20:HIS:HA	24:L:23:GLU:HB2	1.93	0.49
27:O:46:ALA:HB3	27:O:97:ALA:HB3	1.94	0.49
31:S:187:VAL:HG21	27:o:24:MET:HE3	1.94	0.49
24:l:117:GLN:O	24:l:120:THR:OG1	2.29	0.49
1:U:252:LEU:O	1:U:256:ALA:HB3	2.12	0.49
1:U:590:TYR:HD1	1:U:595:ASN:HD22	1.60	0.49
2:V:201:ARG:HH21	2:V:242:HIS:HB3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:335:LEU:HD21	4:X:365:LEU:HD21	1.93	0.49
9:c:33:ILE:HG23	9:c:69:VAL:HG13	1.93	0.49
12:f:649:HIS:C	12:f:651:GLY:H	2.19	0.49
12:f:759:LEU:CG	12:f:806:VAL:HG12	2.42	0.49
25:M:170:GLN:HA	25:M:173:LYS:HG2	1.92	0.49
32:T:45:VAL:HB	32:T:49:THR:HG23	1.94	0.49
21:i:15:GLU:OE2	21:i:17:ARG:NE	2.45	0.49
22:j:11:SER:OG	22:j:15:HIS:N	2.43	0.49
29:q:38:MET:HE1	29:q:44:LEU:HB2	1.94	0.49
32:t:45:VAL:HB	32:t:49:THR:HG23	1.94	0.49
1:U:337:LEU:HD21	1:U:789:ILE:HG21	1.94	0.49
3:W:200:ILE:HD12	3:W:203:GLN:HE21	1.77	0.49
7:a:159:SER:OG	7:a:175:ASP:OD2	2.26	0.49
10:d:36:LEU:HD23	10:d:38:THR:H	1.78	0.49
12:f:41:LYS:HG2	12:f:45:LEU:HD13	1.93	0.49
12:f:471:LEU:HD22	12:f:477:MET:HG3	1.93	0.49
15:C:24:TYR:HD2	16:D:40:LEU:CD2	2.24	0.49
29:Q:38:MET:HE1	29:Q:44:LEU:HB2	1.94	0.49
31:S:125:ASP:OD1	31:S:129:SER:N	2.43	0.49
32:T:15:LYS:HG2	32:T:20:VAL:HG22	1.93	0.49
32:T:86:ARG:NH1	32:T:133:GLU:OE2	2.44	0.49
24:l:20:HIS:HA	24:l:23:GLU:HB2	1.93	0.49
30:r:38:ASN:HD22	30:r:41:LEU:HD12	1.77	0.49
31:s:16:ALA:HB2	31:s:121:VAL:HG23	1.93	0.49
2:V:242:HIS:ND1	15:C:29:GLU:OE1	2.45	0.49
2:V:495:ARG:CB	15:C:44:ARG:CZ	2.85	0.49
9:c:191:ALA:HB1	9:c:196:LEU:CD1	2.41	0.49
12:f:223:GLU:OE2	14:B:59:ARG:HB2	2.12	0.49
12:f:673:ARG:NE	12:f:712:LYS:HG3	2.24	0.49
19:G:127:GLN:NE2	20:H:82:ASP:OD1	2.42	0.49
25:M:66:LEU:HD21	25:M:214:SER:HB2	1.94	0.49
29:Q:170:ARG:NH2	30:r:125:THR:OG1	2.45	0.49
30:R:1:THR:N	30:R:169:TYR:O	2.46	0.49
30:r:41:LEU:HD23	30:r:103:GLY:HA3	1.95	0.49
1:U:499:THR:O	1:U:503:GLN:NE2	2.38	0.49
4:X:177:TYR:O	4:X:182:ASN:N	2.44	0.49
12:f:673:ARG:HH22	12:f:709:THR:HA	1.77	0.49
21:I:41:ASP:OD1	21:I:41:ASP:N	2.46	0.49
25:M:37:ILE:HD11	25:M:193:VAL:HG13	1.95	0.49
19:g:202:LEU:HB2	19:g:206:LEU:HD13	1.94	0.49
23:k:141:LEU:HB2	23:k:156:MET:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:r:1:THR:N	30:r:169:TYR:O	2.46	0.49
1:U:28:ASN:HB3	1:U:59:PHE:HZ	1.77	0.49
1:U:362:ASN:HD22	9:c:173:GLU:H	1.60	0.49
2:V:159:LEU:HG	2:V:182:LYS:HD3	1.94	0.49
2:V:404:LYS:HA	2:V:407:VAL:HG12	1.94	0.49
11:e:56:LEU:CD1	11:e:56:LEU:C	2.85	0.49
12:f:93:PRO:HB2	12:f:97:LYS:HG3	1.95	0.49
12:f:219:LYS:CE	14:B:59:ARG:HB2	2.43	0.49
12:f:827:PRO:HA	12:f:862:ILE:HG13	1.95	0.49
14:B:195:GLN:O	14:B:199:GLU:HB2	2.11	0.49
15:C:31:LEU:HD22	16:D:47:LEU:CB	2.43	0.49
24:L:226:ASP:HA	24:L:229:VAL:HB	1.95	0.49
21:i:41:ASP:OD1	21:i:41:ASP:N	2.46	0.49
25:m:37:ILE:HD11	25:m:193:VAL:HG13	1.95	0.49
1:U:163:PHE:HE2	1:U:201:LEU:HD11	1.76	0.49
1:U:801:GLN:HB3	1:U:877:LEU:HD22	1.95	0.49
1:U:804:SER:HA	1:U:892:LEU:HA	1.94	0.49
3:W:104:MET:HB3	3:W:123:ARG:HH22	1.76	0.49
4:X:172:LEU:HD12	4:X:175:LYS:HD3	1.94	0.49
4:X:297:ARG:HD2	4:X:333:GLN:HE21	1.77	0.49
7:a:269:LEU:HD12	7:a:272:ILE:HD11	1.94	0.49
8:b:180:ALA:HA	8:b:183:LEU:HD13	1.94	0.49
21:I:15:GLU:OE2	21:I:17:ARG:NE	2.45	0.49
21:I:213:ILE:O	21:I:228:LEU:HD21	2.13	0.49
21:i:38:LEU:HB3	21:i:43:VAL:HG23	1.94	0.49
32:t:15:LYS:HG2	32:t:20:VAL:HG22	1.93	0.49
1:U:219:CYS:O	1:U:223:LEU:CB	2.60	0.49
3:W:158:ASP:O	3:W:162:ALA:HB3	2.13	0.49
9:c:197:ASN:ND2	9:c:197:ASN:H	2.10	0.49
10:d:200:PHE:CD1	10:d:200:PHE:N	2.81	0.49
16:D:242:GLU:O	16:D:246:MET:HB2	2.12	0.49
26:N:178:ALA:O	26:N:184:VAL:HA	2.13	0.49
1:U:126:ILE:HG21	1:U:131:GLU:HG2	1.93	0.49
3:W:177:MET:HE1	3:W:212:LYS:HE2	1.94	0.49
8:b:16:MET:HA	8:b:25:ARG:HH11	1.78	0.49
9:c:89:PRO:O	9:c:93:ALA:CB	2.60	0.49
17:E:340:GLY:C	34:E:401:ATP:C8	2.91	0.49
23:k:84:ASP:N	23:k:84:ASP:OD1	2.44	0.49
1:U:524:LYS:HB3	1:U:556:MET:HG2	1.95	0.49
1:U:898:CYS:SG	1:U:899:ARG:N	2.85	0.49
5:Y:160:ASN:O	5:Y:164:ALA:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:116:HIS:HA	10:d:119:LEU:HD23	1.95	0.49
12:f:447:ALA:HA	12:f:450:ILE:HD12	1.95	0.49
14:B:65:LEU:HD23	14:B:68:ILE:HD12	1.93	0.49
15:C:20:LEU:HD12	15:C:21:ARG:HE	1.77	0.49
16:D:170:MET:HG2	16:D:173:GLN:HB2	1.95	0.49
30:R:125:THR:OG1	29:q:170:ARG:NH2	2.46	0.49
24:l:39:LYS:HD3	24:l:144:ILE:HG12	1.95	0.49
8:b:24:THR:HG22	8:b:26:LEU:H	1.78	0.48
14:B:297:SER:OG	15:C:268:GLU:OE2	2.30	0.48
26:N:138:TYR:O	26:N:142:THR:OG1	2.28	0.48
28:P:125:ASP:OD1	28:P:129:CYS:N	2.38	0.48
30:R:38:ASN:HD22	30:R:41:LEU:HD12	1.77	0.48
20:h:91:ARG:NH1	27:o:68:LEU:O	2.46	0.48
25:m:66:LEU:HD21	25:m:214:SER:HB2	1.94	0.48
1:U:602:LEU:CD2	1:U:602:LEU:C	2.85	0.48
2:V:212:TYR:OH	2:V:287:ARG:NH2	2.45	0.48
2:V:494:MET:H	15:C:44:ARG:NH1	1.95	0.48
3:W:165:ILE:HG23	3:W:169:LEU:HD11	1.94	0.48
3:W:274:VAL:O	3:W:283:GLN:NE2	2.46	0.48
3:W:315:MET:SD	3:W:320:LEU:HD12	2.53	0.48
5:Y:23:ARG:NH1	5:Y:52:PRO:O	2.43	0.48
7:a:115:LYS:HD3	7:a:118:ILE:HD12	1.95	0.48
10:d:234:ASP:OD1	10:d:234:ASP:N	2.45	0.48
12:f:305:LEU:HB2	12:f:317:LEU:HD22	1.95	0.48
12:f:646:MET:HG3	14:B:64:LYS:HA	1.95	0.48
12:f:651:GLY:O	12:f:655:LEU:CD1	2.56	0.48
13:A:355:PHE:O	13:A:359:ALA:HB3	2.12	0.48
20:H:139:TRP:HA	20:H:144:PRO:HA	1.95	0.48
23:K:12:VAL:HG12	23:K:23:GLN:HE22	1.79	0.48
21:i:98:LEU:O	21:i:102:GLN:HA	2.13	0.48
31:s:108:ASN:HB2	31:s:124:PHE:HB2	1.94	0.48
1:U:35:TRP:HE1	1:U:67:VAL:HA	1.78	0.48
5:Y:40:GLU:O	5:Y:44:ALA:HB2	2.14	0.48
6:Z:13:PRO:HA	6:Z:16:LEU:HB3	1.95	0.48
7:a:294:GLU:OE2	7:a:298:LYS:NZ	2.47	0.48
12:f:571:GLU:HG3	12:f:573:ILE:H	1.78	0.48
12:f:759:LEU:CG	12:f:806:VAL:CG1	2.90	0.48
19:G:46:ASP:C	19:G:222:VAL:CG2	2.85	0.48
23:K:84:ASP:OD1	23:K:84:ASP:N	2.44	0.48
31:S:57:PHE:HD2	31:S:60:ASP:H	1.59	0.48
19:g:46:ASP:C	19:g:222:VAL:HG22	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:j:211:MET:HG2	22:j:213:ARG:H	1.78	0.48
24:l:189:LYS:HZ3	24:l:193:ARG:HH12	1.60	0.48
32:t:43:MET:HE3	32:t:45:VAL:HG22	1.95	0.48
3:W:90:LEU:CD2	3:W:96:GLN:CD	2.85	0.48
3:W:349:LYS:O	3:W:353:ASP:HB2	2.12	0.48
12:f:478:ARG:HG3	12:f:514:VAL:HG11	1.96	0.48
12:f:497:VAL:HA	12:f:500:LEU:HB2	1.94	0.48
12:f:810:ILE:CD1	12:f:853:VAL:C	2.85	0.48
13:A:312:ARG:HD3	13:A:312:ARG:N	2.28	0.48
16:D:370:ILE:H	16:D:370:ILE:CD1	1.97	0.48
18:F:232:GLY:HA2	36:F:501:ADP:C5'	2.39	0.48
28:P:10:ALA:O	28:P:24:ALA:HA	2.13	0.48
29:Q:85:ARG:HG2	29:Q:122:ALA:HB1	1.94	0.48
31:S:16:ALA:HB2	31:S:121:VAL:HG23	1.93	0.48
22:j:104:VAL:HA	22:j:107:ILE:HG22	1.95	0.48
28:p:10:ALA:O	28:p:24:ALA:HA	2.14	0.48
2:V:346:LEU:HD23	2:V:357:LEU:HD22	1.95	0.48
3:W:90:LEU:HD22	3:W:96:GLN:CB	2.43	0.48
5:Y:335:SER:O	5:Y:339:ALA:HB3	2.14	0.48
7:a:252:LYS:HG2	7:a:255:TRP:HE1	1.78	0.48
8:b:151:GLU:OE1	8:b:152:LYS:NZ	2.42	0.48
9:c:161:ARG:HB3	9:c:201:TYR:CZ	2.49	0.48
16:D:89:ILE:CD1	17:E:80:VAL:HG23	2.38	0.48
22:J:88:ARG:NH1	29:Q:69:MET:O	2.46	0.48
23:K:121:LEU:HD21	24:L:126:ARG:HH12	1.77	0.48
24:L:189:LYS:HZ3	24:L:193:ARG:HH22	1.61	0.48
25:M:163:CYS:SG	25:M:164:ALA:N	2.86	0.48
29:Q:141:SER:O	29:Q:145:ARG:CB	2.61	0.48
1:U:98:GLU:CD	15:C:22:GLN:OE1	2.56	0.48
1:U:177:LEU:HD22	1:U:180:SER:HB3	1.95	0.48
1:U:619:VAL:HG11	1:U:648:VAL:HG13	1.95	0.48
5:Y:72:LYS:HG3	5:Y:73:MET:HG3	1.96	0.48
5:Y:94:ASN:HD21	15:C:167:LEU:HD21	1.79	0.48
6:Z:57:PRO:HD3	9:c:102:THR:HG23	1.94	0.48
12:f:673:ARG:HE	12:f:712:LYS:HG3	1.69	0.48
12:f:840:LEU:H	12:f:840:LEU:CD1	2.25	0.48
13:A:146:LYS:HD2	13:A:148:GLN:HG2	1.95	0.48
14:B:290:ILE:HG12	14:B:305:ILE:HG23	1.95	0.48
15:C:52:LEU:CG	16:D:68:LEU:CD1	2.87	0.48
16:D:95:ALA:HA	16:D:101:ALA:HA	1.96	0.48
18:F:210:GLU:O	18:F:214:ASN:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:J:211:MET:HG2	22:J:213:ARG:H	1.78	0.48
28:P:39:PHE:HE1	28:P:61:GLN:HE21	1.61	0.48
22:j:201:SER:HA	22:j:205:ASN:HB2	1.95	0.48
25:m:163:CYS:SG	25:m:164:ALA:N	2.86	0.48
26:n:104:ASP:N	26:n:108:GLY:O	2.47	0.48
2:V:84:LYS:HA	2:V:87:SER:HB2	1.96	0.48
2:V:345:ARG:CZ	2:V:360:TYR:HD2	2.26	0.48
2:V:396:ILE:O	10:d:141:GLN:NE2	2.47	0.48
4:X:170:GLN:NE2	4:X:192:SER:OG	2.39	0.48
5:Y:173:ASP:H	15:C:335:LYS:HA	1.78	0.48
6:Z:125:ASP:HB2	6:Z:134:PRO:HB2	1.95	0.48
8:b:93:ALA:HB1	8:b:109:ILE:HD13	1.96	0.48
12:f:625:LYS:HB2	12:f:628:ASP:HB3	1.95	0.48
12:f:652:VAL:HG21	12:f:685:THR:OG1	2.14	0.48
19:G:202:LEU:HB2	19:G:206:LEU:HD13	1.94	0.48
21:I:98:LEU:O	21:I:102:GLN:HA	2.13	0.48
24:L:39:LYS:HD3	24:L:144:ILE:HG12	1.95	0.48
23:k:12:VAL:HG12	23:k:23:GLN:HE22	1.79	0.48
28:p:39:PHE:HE1	28:p:61:GLN:HE21	1.61	0.48
29:q:85:ARG:HG2	29:q:122:ALA:HB1	1.94	0.48
4:X:161:ASP:HB2	20:H:177:ARG:HA	1.95	0.48
12:f:646:MET:HE3	14:B:64:LYS:HZ2	1.78	0.48
14:B:284:ILE:HB	14:B:329:MET:HG2	1.96	0.48
18:F:313:LEU:O	18:F:317:LEU:CB	2.61	0.48
26:N:104:ASP:N	26:N:108:GLY:O	2.47	0.48
27:O:64:GLU:O	27:O:68:LEU:CB	2.61	0.48
20:h:139:TRP:HA	20:h:144:PRO:HA	1.95	0.48
29:q:13:VAL:HG11	29:q:105:ALA:HB1	1.95	0.48
32:t:126:ASP:HB2	32:t:130:VAL:O	2.14	0.48
5:Y:235:ASP:O	5:Y:239:LYS:HB3	2.14	0.48
30:R:41:LEU:HD23	30:R:103:GLY:HA3	1.95	0.48
32:T:96:MET:HE1	32:T:106:LEU:HD12	1.95	0.48
1:U:46:GLU:HA	1:U:49:TYR:HB3	1.95	0.48
3:W:82:LEU:C	3:W:82:LEU:HD13	2.39	0.48
3:W:445:LEU:HD11	6:Z:225:GLN:HE22	1.79	0.48
5:Y:279:GLU:HB2	5:Y:296:VAL:HG21	1.95	0.48
10:d:101:LEU:HG	10:d:166:PHE:HE2	1.79	0.48
12:f:691:PRO:HA	12:f:694:LEU:HB2	1.95	0.48
14:B:232:LYS:N	34:B:501:ATP:O1A	2.46	0.48
14:B:418:ASP:O	14:B:422:SER:CB	2.61	0.48
16:D:88:VAL:HG13	16:D:134:LYS:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:342:ARG:HB3	16:D:364:VAL:HG11	1.96	0.48
16:D:391:ARG:NH2	16:D:398:ASP:OD2	2.45	0.48
27:O:106:THR:OG1	27:O:109:HIS:NE2	2.42	0.48
27:O:112:SER:HB3	27:O:125:VAL:HG11	1.96	0.48
29:Q:13:VAL:HG11	29:Q:105:ALA:HB1	1.95	0.48
30:R:141:ARG:NH2	29:q:162:LYS:O	2.41	0.48
1:U:177:LEU:HD23	1:U:177:LEU:HA	1.65	0.47
3:W:365:ILE:HG22	3:W:368:LYS:HD2	1.95	0.47
7:a:149:THR:HA	7:a:152:HIS:HB3	1.95	0.47
8:b:11:ASP:OD2	8:b:114:GLY:N	2.46	0.47
13:A:368:ILE:HG22	13:A:406:GLU:HB2	1.96	0.47
14:B:221:GLY:HA3	14:B:347:ILE:HA	1.96	0.47
16:D:376:ASN:O	16:D:380:GLN:CB	2.56	0.47
20:H:150:ASP:OD1	20:H:154:ALA:N	2.46	0.47
22:J:116:GLN:O	22:J:119:THR:OG1	2.28	0.47
25:M:66:LEU:HD13	25:M:212:GLU:HG2	1.96	0.47
30:R:153:TYR:O	30:R:157:ARG:HB2	2.14	0.47
32:T:126:ASP:HB2	32:T:130:VAL:O	2.14	0.47
21:i:99:LEU:HD13	28:p:69:PHE:HB2	1.96	0.47
26:n:178:ALA:O	26:n:184:VAL:HA	2.13	0.47
12:f:834:ASP:CG	14:B:60:LEU:HD12	2.39	0.47
18:F:153:VAL:HG22	18:F:160:ILE:HG22	1.96	0.47
21:I:38:LEU:HB3	21:I:43:VAL:HG23	1.94	0.47
24:L:183:ASN:O	24:L:187:LEU:CB	2.62	0.47
30:r:153:TYR:O	30:r:157:ARG:HB2	2.14	0.47
2:V:97:ALA:H	2:V:107:ARG:HE	1.63	0.47
3:W:237:GLU:HG2	3:W:238:GLY:H	1.78	0.47
3:W:287:VAL:O	3:W:291:SER:CB	2.62	0.47
3:W:361:HIS:HA	3:W:364:ARG:HE	1.80	0.47
9:c:51:MET:HG3	9:c:82:VAL:HA	1.96	0.47
13:A:401:ARG:HH12	13:A:408:ASP:CG	2.22	0.47
17:E:291:ARG:HG2	17:E:293:GLY:H	1.78	0.47
24:L:47:VAL:HG13	24:L:212:ILE:HG13	1.97	0.47
27:O:24:MET:HE3	31:s:187:VAL:HG21	1.96	0.47
32:T:43:MET:HE3	32:T:45:VAL:HG22	1.95	0.47
20:h:150:ASP:OD1	20:h:154:ALA:N	2.46	0.47
21:i:44:LEU:HD22	21:i:190:LEU:HD23	1.97	0.47
21:i:119:GLN:NE2	22:j:79:ASP:OD1	2.47	0.47
1:U:107:HIS:HA	1:U:110:LYS:HE3	1.96	0.47
1:U:258:GLN:O	1:U:262:SER:CB	2.62	0.47
5:Y:336:ARG:O	5:Y:340:ALA:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:170:LEU:C	10:d:170:LEU:CD2	2.85	0.47
13:A:189:GLU:O	13:A:193:THR:OG1	2.32	0.47
17:E:149:ILE:HG21	17:E:276:ILE:HD11	1.96	0.47
4:X:255:LEU:HB2	4:X:287:LEU:HD13	1.95	0.47
12:f:125:ILE:HD13	12:f:129:LEU:HB2	1.96	0.47
21:I:90:LEU:HA	21:I:93:ILE:HD12	1.96	0.47
22:J:53:LEU:HD13	22:J:54:GLN:HG3	1.97	0.47
19:g:54:LYS:NZ	19:g:215:ILE:O	2.47	0.47
20:h:100:VAL:HG13	28:p:93:ASN:HD22	1.80	0.47
29:q:141:SER:O	29:q:145:ARG:CB	2.61	0.47
32:t:96:MET:HE1	32:t:106:LEU:HD12	1.95	0.47
1:U:160:LEU:HD21	1:U:196:LYS:HB3	1.97	0.47
1:U:803:LYS:HB2	1:U:875:PHE:HA	1.96	0.47
5:Y:233:ARG:HH21	5:Y:306:GLN:HE22	1.60	0.47
6:Z:20:VAL:HG21	9:c:216:MET:HE1	1.96	0.47
7:a:161:LYS:O	7:a:165:THR:OG1	2.23	0.47
7:a:273:GLN:HB3	7:a:310:LEU:HD11	1.97	0.47
11:e:57:ARG:NH1	11:e:57:ARG:CG	2.73	0.47
12:f:654:VAL:HG22	12:f:657:ILE:O	2.14	0.47
13:A:294:GLU:OE1	13:A:297:ARG:NH1	2.48	0.47
14:B:183:THR:OG1	14:B:184:TYR:N	2.47	0.47
16:D:113:VAL:HB	16:D:138:ALA:HA	1.97	0.47
17:E:300:HIS:NE2	17:E:302:ASP:OD1	2.48	0.47
21:i:90:LEU:HA	21:i:93:ILE:HD12	1.96	0.47
25:m:41:CYS:N	25:m:44:GLY:O	2.44	0.47
27:o:64:GLU:O	27:o:68:LEU:CB	2.61	0.47
1:U:336:GLU:HA	1:U:339:LEU:HB3	1.96	0.47
1:U:644:TYR:HD2	15:C:60:ARG:HH22	0.87	0.47
1:U:645:ASN:HA	15:C:60:ARG:NH1	2.30	0.47
3:W:31:CYS:O	3:W:35:ALA:CB	2.63	0.47
3:W:48:LEU:CD2	3:W:95:SER:HB3	2.03	0.47
3:W:173:THR:HG21	3:W:208:LYS:HZ3	1.79	0.47
3:W:178:GLU:C	3:W:180:LYS:H	2.22	0.47
3:W:231:ILE:O	3:W:235:GLN:CB	2.56	0.47
5:Y:192:ARG:NH2	5:Y:290:PRO:O	2.39	0.47
7:a:8:LEU:HB2	7:a:22:TRP:CE3	2.50	0.47
7:a:14:SER:H	7:a:19:PRO:HG3	1.80	0.47
7:a:70:ARG:HH21	8:b:17:ARG:HG2	1.80	0.47
10:d:155:LYS:NZ	10:d:170:LEU:CD2	2.73	0.47
12:f:548:THR:HG21	12:f:554:TYR:HE2	1.80	0.47
14:B:342:ILE:HG22	14:B:350:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:142:LYS:NZ	16:D:297:ASP:OD1	2.42	0.47
15:C:187:LEU:HB3	15:C:314:LYS:HG2	1.95	0.47
21:I:44:LEU:HD22	21:I:190:LEU:HD23	1.97	0.47
22:J:104:VAL:HA	22:J:107:ILE:HG22	1.95	0.47
21:i:229:LYS:N	21:i:232:GLU:OE2	2.48	0.47
27:o:112:SER:HB3	27:o:125:VAL:HG11	1.96	0.47
1:U:625:ILE:HG13	1:U:626:LEU:HG	1.95	0.47
5:Y:17:LEU:HD22	5:Y:212:GLU:HB2	1.96	0.47
12:f:72:ARG:HH21	12:f:112:ASN:HB3	1.80	0.47
12:f:181:ARG:HA	12:f:184:LEU:HD13	1.97	0.47
24:l:183:ASN:O	24:l:187:LEU:CB	2.62	0.47
3:W:172:GLU:CD	3:W:172:GLU:N	2.73	0.47
12:f:372:LEU:O	12:f:375:SER:OG	2.28	0.47
16:D:285:VAL:HG11	17:E:255:ARG:HH21	1.80	0.47
17:E:55:GLN:HB2	18:F:133:PHE:HB3	1.97	0.47
18:F:235:LEU:CD2	36:F:501:ADP:N7	2.78	0.47
23:K:43:SER:HA	23:K:151:PRO:HG3	1.97	0.47
24:L:216:GLY:HA3	24:L:219:LEU:HB3	1.97	0.47
2:V:85:ALA:O	2:V:89:LYS:NZ	2.42	0.47
2:V:319:HIS:HE1	2:V:324:PHE:HE1	1.62	0.47
10:d:118:GLU:HA	10:d:121:ARG:HH11	1.80	0.47
12:f:836:GLU:HB3	12:f:837:LEU:H	1.56	0.47
13:A:80:LEU:O	13:A:85:GLN:NE2	2.48	0.47
13:A:307:ASP:OD2	13:A:333:ARG:NH2	2.48	0.47
15:C:246:ILE:HB	15:C:291:VAL:HG12	1.97	0.47
19:G:47:CYS:HB3	19:G:221:THR:HG23	1.97	0.47
19:G:54:LYS:NZ	19:G:215:ILE:O	2.47	0.47
25:M:181:MET:SD	25:M:181:MET:N	2.88	0.47
22:j:40:ILE:HA	22:j:211:MET:O	2.15	0.47
23:k:195:ILE:O	23:k:198:SER:OG	2.31	0.47
24:l:47:VAL:HG13	24:l:212:ILE:HG13	1.97	0.47
2:V:408:ARG:O	2:V:412:LEU:HB2	2.16	0.46
6:Z:244:GLU:O	6:Z:248:ALA:N	2.34	0.46
9:c:195:GLY:C	9:c:200:TYR:HE1	2.08	0.46
12:f:840:LEU:HD12	12:f:840:LEU:N	2.30	0.46
13:A:113:ILE:HD11	13:A:142:VAL:HG21	1.97	0.46
15:C:381:GLU:O	15:C:385:MET:HB2	2.14	0.46
16:D:335:LEU:CG	16:D:369:LYS:HG3	2.30	0.46
19:G:165:ALA:HB1	19:G:179:LEU:HD13	1.96	0.46
26:N:110:GLN:HG3	26:N:122:ARG:CZ	2.45	0.46
20:h:204:THR:OG1	20:h:206:ASP:OD1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:m:66:LEU:HD13	25:m:212:GLU:HG2	1.96	0.46
1:U:788:VAL:HG12	1:U:909:GLY:HA2	1.97	0.46
2:V:150:ARG:O	2:V:154:ALA:HB3	2.15	0.46
10:d:46:GLN:HA	10:d:50:LEU:HD13	1.97	0.46
12:f:618:GLU:HG2	14:B:85:MET:HG3	1.97	0.46
12:f:718:ASP:CG	12:f:760:PHE:CE2	2.93	0.46
14:B:373:THR:OG1	14:B:412:MET:O	2.30	0.46
17:E:253:ILE:HG21	18:F:308:ARG:HH21	1.80	0.46
17:E:317:ALA:HA	17:E:320:ILE:HD12	1.97	0.46
22:J:40:ILE:HA	22:J:211:MET:O	2.15	0.46
27:O:138:PHE:O	27:O:142:PHE:CB	2.62	0.46
29:Q:23:SER:HB2	29:Q:28:MET:HG2	1.97	0.46
19:g:165:ALA:HB1	19:g:179:LEU:HD13	1.96	0.46
24:l:216:GLY:HA3	24:l:219:LEU:HB3	1.97	0.46
31:s:38:ARG:HH12	32:t:151:ARG:HD3	1.80	0.46
3:W:23:THR:HA	3:W:26:GLN:HB2	1.97	0.46
5:Y:144:LEU:HB3	5:Y:160:ASN:HD22	1.80	0.46
10:d:44:THR:O	10:d:47:GLN:NE2	2.48	0.46
10:d:176:ASP:HA	10:d:179:ALA:HB3	1.97	0.46
10:d:194:ALA:HB3	10:d:222:TYR:HE2	1.81	0.46
11:e:56:LEU:C	11:e:56:LEU:HD12	2.40	0.46
12:f:668:ALA:O	12:f:705:ASN:ND2	2.49	0.46
12:f:718:ASP:HB2	12:f:760:PHE:CE2	2.50	0.46
16:D:411:GLU:HG2	16:D:413:GLU:H	1.80	0.46
26:N:138:TYR:O	26:N:142:THR:CB	2.64	0.46
30:R:55:TRP:NE1	31:S:97:TYR:OH	2.49	0.46
23:k:171:GLY:H	23:k:174:SER:HB2	1.81	0.46
26:n:138:TYR:O	26:n:142:THR:OG1	2.28	0.46
29:q:38:MET:HB3	29:q:64:VAL:HG11	1.97	0.46
2:V:145:LEU:HA	2:V:151:THR:HG21	1.97	0.46
3:W:79:GLU:HA	3:W:83:LEU:HD13	1.98	0.46
3:W:178:GLU:OE2	3:W:181:GLU:CB	2.59	0.46
3:W:187:LEU:HA	3:W:190:MET:HE3	1.97	0.46
5:Y:95:LEU:HD11	5:Y:98:SER:HA	1.97	0.46
15:C:24:TYR:OH	16:D:41:TYR:HA	2.14	0.46
15:C:28:ILE:CD1	16:D:43:ARG:HB3	2.45	0.46
17:E:382:SER:HB3	18:F:340:PRO:HG3	1.98	0.46
29:Q:38:MET:HB3	29:Q:64:VAL:HG11	1.97	0.46
21:i:90:LEU:HD13	21:i:114:LEU:HD22	1.96	0.46
1:U:59:PHE:HA	1:U:62:LEU:HD13	1.98	0.46
3:W:49:SER:O	3:W:53:GLN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:233:ARG:HH12	5:Y:264:TYR:C	2.16	0.46
9:c:31:VAL:HG23	9:c:203:ILE:HG21	1.98	0.46
9:c:124:GLY:O	9:c:128:ASN:ND2	2.48	0.46
9:c:191:ALA:C	9:c:196:LEU:HD11	2.41	0.46
12:f:594:LEU:O	12:f:635:LYS:NZ	2.46	0.46
12:f:807:ARG:HE	12:f:807:ARG:HB2	1.63	0.46
13:A:97:ARG:HE	14:B:131:HIS:CD2	2.34	0.46
13:A:368:ILE:HD13	13:A:409:PHE:HE2	1.81	0.46
14:B:165:ASP:C	14:B:167:THR:H	2.23	0.46
14:B:183:THR:HG23	14:B:185:ALA:H	1.80	0.46
18:F:235:LEU:HD22	36:F:501:ADP:C8	2.50	0.46
18:F:312:GLU:O	18:F:316:GLN:CB	2.62	0.46
19:G:38:THR:HA	19:G:168:ALA:O	2.15	0.46
21:I:90:LEU:HD13	21:I:114:LEU:HD22	1.96	0.46
23:K:183:GLU:HG3	23:K:184:VAL:HG13	1.98	0.46
26:n:6:VAL:HG22	26:n:125:PHE:HB2	1.97	0.46
32:t:92:LEU:HD23	32:t:125:VAL:HG21	1.97	0.46
1:U:112:CYS:HA	1:U:115:ASN:HB2	1.98	0.46
3:W:51:GLU:N	3:W:51:GLU:CD	2.73	0.46
5:Y:60:SER:OG	5:Y:61:LEU:N	2.49	0.46
7:a:221:VAL:HG23	7:a:222:LEU:HG	1.96	0.46
12:f:654:VAL:O	12:f:657:ILE:N	2.48	0.46
12:f:801:VAL:HB	12:f:804:LEU:HD11	1.97	0.46
14:B:201:VAL:HG21	14:B:328:ILE:HD11	1.97	0.46
14:B:232:LYS:HB2	34:B:501:ATP:O1B	2.16	0.46
18:F:295:ARG:HG2	18:F:307:GLN:HG2	1.98	0.46
19:g:38:THR:HA	19:g:168:ALA:O	2.15	0.46
21:i:218:ARG:NH2	21:i:220:ASN:O	2.49	0.46
23:k:43:SER:HA	23:k:151:PRO:HG3	1.97	0.46
26:n:110:GLN:HG3	26:n:122:ARG:CZ	2.45	0.46
1:U:376:MET:HB3	1:U:735:GLY:HA2	1.98	0.46
2:V:203:LEU:O	2:V:207:ALA:CB	2.63	0.46
4:X:90:ARG:HH21	4:X:125:LEU:HA	1.81	0.46
6:Z:273:HIS:CE1	6:Z:277:ASN:HD21	2.34	0.46
12:f:673:ARG:CZ	12:f:712:LYS:HB3	2.38	0.46
12:f:681:TYR:HB3	12:f:858:LYS:HE3	1.96	0.46
17:E:168:LYS:N	17:E:296:ASP:OD2	2.43	0.46
21:I:218:ARG:NH2	21:I:220:ASN:O	2.49	0.46
12:f:209:MET:HG3	12:f:211:ILE:H	1.80	0.46
12:f:223:GLU:OE2	14:B:59:ARG:CG	2.64	0.46
16:D:352:MET:HE1	16:D:379:CYS:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:I:106:PRO:HD2	21:I:109:GLN:HE21	1.81	0.46
22:J:121:SER:OG	22:J:122:ASN:N	2.48	0.46
26:N:32:ASP:O	26:N:45:ARG:NH1	2.47	0.46
26:N:38:HIS:HB3	26:N:41:ILE:HB	1.97	0.46
29:Q:25:ILE:HG13	29:Q:26:VAL:HG13	1.98	0.46
32:T:92:LEU:HD23	32:T:125:VAL:HG21	1.97	0.46
24:l:157:ARG:HD2	24:l:176:MET:HE3	1.98	0.46
2:V:495:ARG:N	15:C:44:ARG:NH2	2.64	0.46
3:W:173:THR:HG21	3:W:208:LYS:NZ	2.30	0.46
5:Y:186:LEU:HA	5:Y:189:VAL:HG12	1.96	0.46
8:b:124:LEU:O	8:b:128:ALA:CB	2.64	0.46
9:c:89:PRO:O	9:c:93:ALA:HB2	2.16	0.46
12:f:417:ILE:HG22	12:f:418:LEU:HD12	1.97	0.46
12:f:679:LEU:HD11	12:f:686:LEU:CD1	2.46	0.46
12:f:759:LEU:HD12	12:f:808:ASN:CA	2.39	0.46
15:C:152:GLY:N	36:C:501:ADP:N1	2.64	0.46
17:E:101:ASP:OD2	17:E:104:THR:N	2.45	0.46
18:F:212:PHE:HD1	18:F:217:ILE:HD11	1.81	0.46
21:i:153:SER:OG	21:i:155:ASN:OD1	2.34	0.46
1:U:135:ASN:HA	1:U:138:PHE:HB3	1.98	0.46
1:U:367:THR:HA	1:U:370:VAL:HG22	1.98	0.46
3:W:50:LEU:HD12	3:W:50:LEU:N	2.30	0.46
5:Y:347:ILE:HG13	5:Y:354:VAL:HG22	1.98	0.46
11:e:57:ARG:NH1	11:e:58:ALA:HB2	2.31	0.46
12:f:568:GLY:H	12:f:599:ALA:HA	1.81	0.46
12:f:657:ILE:HG23	14:B:82:GLN:NE2	2.31	0.46
13:A:200:ARG:HB3	18:F:408:LEU:HD11	1.98	0.46
16:D:115:ILE:HD13	16:D:121:ARG:HH22	1.81	0.46
18:F:313:LEU:O	18:F:317:LEU:HB2	2.15	0.46
23:K:72:ALA:O	23:K:226:PHE:N	2.42	0.46
25:M:75:MET:HA	25:M:136:MET:O	2.16	0.46
27:O:120:ASP:OD1	27:O:120:ASP:N	2.49	0.46
21:i:194:ILE:O	21:i:198:ASN:HB2	2.16	0.46
23:k:183:GLU:HG3	23:k:184:VAL:HG13	1.98	0.46
29:q:23:SER:HB2	29:q:28:MET:HG2	1.97	0.46
3:W:78:LYS:CB	3:W:82:LEU:HD12	2.45	0.45
11:e:56:LEU:HD12	11:e:59:GLU:N	2.30	0.45
12:f:524:MET:HA	12:f:776:LEU:HD23	1.99	0.45
22:j:121:SER:OG	22:j:122:ASN:N	2.49	0.45
3:W:260:SER:HA	3:W:263:TRP:HB3	1.97	0.45
3:W:315:MET:SD	3:W:315:MET:C	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:135:ILE:HA	14:B:159:VAL:HB	1.98	0.45
16:D:370:ILE:HB	16:D:371:SER:H	1.52	0.45
26:N:6:VAL:HG22	26:N:125:PHE:HB2	1.97	0.45
25:m:15:SER:OG	25:m:19:ARG:N	2.45	0.45
2:V:371:ASN:OD1	2:V:427:GLN:NE2	2.49	0.45
9:c:244:VAL:HB	9:c:291:LEU:HD21	1.98	0.45
12:f:171:GLN:HE21	12:f:179:VAL:HG13	1.80	0.45
12:f:344:VAL:HG11	12:f:391:LEU:HG	1.99	0.45
12:f:650:GLN:HE22	13:A:56:LEU:HA	1.81	0.45
15:C:127:LEU:HA	15:C:128:PRO:HD2	1.75	0.45
16:D:125:LYS:C	16:D:125:LYS:CD	2.88	0.45
16:D:336:PRO:HB3	16:D:340:GLN:HB2	1.97	0.45
23:K:171:GLY:H	23:K:174:SER:HB2	1.81	0.45
23:k:60:GLU:OE1	23:k:63:SER:N	2.49	0.45
24:l:199:LEU:HD13	24:l:204:ASP:HA	1.99	0.45
1:U:247:GLN:HG3	1:U:904:LYS:HD2	1.98	0.45
1:U:469:SER:OG	1:U:470:ASN:N	2.50	0.45
3:W:312:MET:HG3	3:W:313:GLU:H	1.81	0.45
6:Z:15:VAL:HG11	6:Z:50:VAL:HG12	1.98	0.45
7:a:239:ALA:HA	7:a:242:SER:HB3	1.99	0.45
12:f:773:LYS:HB3	12:f:774:GLY:H	1.49	0.45
19:g:46:ASP:C	19:g:222:VAL:CG2	2.89	0.45
21:i:106:PRO:HD2	21:i:109:GLN:HE21	1.81	0.45
22:j:115:LYS:HG3	22:j:127:PHE:HD2	1.81	0.45
22:j:116:GLN:O	22:j:119:THR:OG1	2.28	0.45
26:n:138:TYR:O	26:n:142:THR:CB	2.64	0.45
29:q:25:ILE:HG13	29:q:26:VAL:HG13	1.98	0.45
1:U:177:LEU:HA	1:U:180:SER:HB3	1.99	0.45
3:W:85:GLU:H	3:W:85:GLU:HG3	1.50	0.45
3:W:150:ALA:HA	3:W:153:LYS:HB2	1.99	0.45
12:f:442:SER:O	12:f:446:LEU:HB2	2.16	0.45
13:A:59:ILE:HG12	14:B:72:LEU:HD11	1.99	0.45
13:A:113:ILE:HG22	13:A:121:PHE:H	1.81	0.45
16:D:85:ILE:N	16:D:86:PRO:HD2	2.30	0.45
3:W:13:ILE:HA	3:W:16:MET:HG2	1.98	0.45
3:W:198:ASP:O	3:W:202:THR:OG1	2.31	0.45
7:a:9:GLN:HE22	7:a:23:HIS:CE1	2.34	0.45
12:f:814:SER:HA	12:f:882:LEU:HD12	1.98	0.45
12:f:827:PRO:HD3	12:f:850:VAL:HG22	1.98	0.45
13:A:252:GLU:OE2	13:A:255:ARG:NH1	2.50	0.45
17:E:217:GLU:HA	17:E:220:ASN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:229:VAL:O	1:U:233:LEU:CB	2.64	0.45
1:U:401:LYS:HB3	1:U:438:GLN:HB2	1.99	0.45
1:U:645:ASN:HA	15:C:60:ARG:HH12	1.81	0.45
4:X:173:GLU:HA	4:X:176:THR:HG22	1.99	0.45
6:Z:35:VAL:HB	6:Z:97:THR:HB	1.97	0.45
6:Z:190:ARG:HH22	9:c:297:VAL:HA	1.79	0.45
10:d:191:PHE:N	10:d:220:ASN:OD1	2.37	0.45
12:f:585:GLU:HG3	12:f:588:ARG:HE	1.81	0.45
20:H:46:LEU:O	20:H:210:VAL:HA	2.17	0.45
23:K:195:ILE:O	23:K:198:SER:OG	2.31	0.45
23:K:199:LEU:HD11	23:K:217:LEU:HD11	1.99	0.45
24:l:65:HIS:O	24:l:89:ARG:NH2	2.39	0.45
31:s:140:SER:OG	31:s:186:ASP:OD2	2.33	0.45
2:V:252:ASN:ND2	2:V:284:GLU:OE2	2.50	0.45
3:W:172:GLU:N	3:W:172:GLU:OE1	2.37	0.45
4:X:357:SER:OG	4:X:358:LYS:N	2.49	0.45
5:Y:176:ARG:HD3	15:C:334:ARG:HD2	1.99	0.45
7:a:194:GLN:HB3	7:a:225:LEU:HG	1.99	0.45
7:a:279:GLU:O	7:a:283:THR:OG1	2.28	0.45
12:f:78:LEU:HA	12:f:82:ILE:HD11	1.99	0.45
13:A:221:GLY:O	13:A:225:CYS:CB	2.65	0.45
13:A:312:ARG:N	13:A:312:ARG:CD	2.79	0.45
13:A:346:PRO:HB2	13:A:351:ARG:HG3	1.99	0.45
13:A:400:ARG:HD3	13:A:400:ARG:HA	1.31	0.45
14:B:264:PRO:HG3	14:B:308:THR:HA	1.97	0.45
15:C:152:GLY:HA3	36:C:501:ADP:N6	2.29	0.45
16:D:87:LEU:HD23	16:D:131:ALA:HB2	1.89	0.45
16:D:369:LYS:N	16:D:369:LYS:CE	2.76	0.45
18:F:65:GLU:O	18:F:69:MET:CB	2.65	0.45
22:J:96:LEU:O	30:R:81:LYS:NZ	2.37	0.45
26:N:20:THR:HB	26:N:28:ASN:HB3	1.97	0.45
28:p:58:THR:O	29:q:85:ARG:NH2	2.49	0.45
1:U:576:PRO:HB2	1:U:611:ASN:HD22	1.82	0.45
3:W:6:SER:O	3:W:10:ASP:HB2	2.17	0.45
3:W:166:LEU:HA	3:W:169:LEU:HD12	1.98	0.45
4:X:53:LEU:HD23	4:X:56:LEU:HD12	1.98	0.45
5:Y:50:MET:HE2	5:Y:74:LYS:HB3	1.99	0.45
12:f:662:MET:HA	14:B:86:LYS:HE2	1.98	0.45
12:f:764:LEU:HD21	12:f:774:GLY:C	2.40	0.45
12:f:773:LYS:HD3	12:f:773:LYS:HA	1.44	0.45
16:D:50:GLU:O	16:D:54:LEU:CB	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:12:THR:HB	21:I:20:GLN:HE22	1.82	0.45
21:I:153:SER:OG	21:I:155:ASN:OD1	2.34	0.45
21:i:197:LEU:HA	21:i:200:THR:HG22	1.99	0.45
22:j:94:HIS:O	22:j:97:THR:C	2.60	0.45
25:m:75:MET:HA	25:m:136:MET:O	2.16	0.45
26:n:20:THR:HB	26:n:28:ASN:HB3	1.97	0.45
26:n:38:HIS:HB3	26:n:41:ILE:HB	1.97	0.45
28:p:125:ASP:OD1	28:p:129:CYS:N	2.38	0.45
1:U:913:ILE:H	1:U:913:ILE:HG13	1.63	0.45
2:V:373:ALA:H	2:V:427:GLN:HE21	1.65	0.45
8:b:62:THR:HG22	8:b:70:ARG:HG2	1.99	0.45
11:e:57:ARG:CZ	11:e:58:ALA:HB2	2.46	0.45
14:B:54:PRO:CB	14:B:61:LYS:CD	2.93	0.45
15:C:213:ARG:HA	15:C:247:PHE:O	2.17	0.45
15:C:235:PHE:HA	15:C:238:ALA:HB3	1.98	0.45
19:G:86:ASP:OD1	25:M:120:HIS:NE2	2.46	0.45
22:J:115:LYS:HG3	22:J:127:PHE:HD2	1.81	0.45
24:L:199:LEU:HD13	24:L:204:ASP:HA	1.98	0.45
1:U:107:HIS:HA	1:U:110:LYS:HG2	1.99	0.44
3:W:28:LEU:O	3:W:32:ALA:CB	2.65	0.44
3:W:152:ILE:HD11	3:W:165:ILE:HB	1.99	0.44
4:X:143:TYR:HD1	4:X:180:LEU:HD13	1.81	0.44
10:d:212:LYS:HD2	10:d:213:ARG:HG2	1.99	0.44
12:f:300:ARG:HE	12:f:493:ASN:HB2	1.82	0.44
12:f:760:PHE:CE1	12:f:809:ILE:HG13	2.52	0.44
15:C:196:LYS:HB2	36:C:501:ADP:O3B	2.16	0.44
21:I:194:ILE:O	21:I:198:ASN:HB2	2.16	0.44
22:j:73:PHE:HA	22:j:131:ALA:HA	1.99	0.44
1:U:261:LEU:HA	1:U:264:VAL:HG12	2.00	0.44
1:U:623:GLY:O	1:U:627:PHE:HB3	2.17	0.44
1:U:725:MET:HE3	1:U:725:MET:HB2	1.83	0.44
1:U:886:PRO:HA	1:U:889:LEU:HG	2.00	0.44
2:V:203:LEU:O	2:V:207:ALA:HB2	2.17	0.44
3:W:137:TYR:O	3:W:137:TYR:CG	2.70	0.44
5:Y:153:ASP:HB3	5:Y:156:LEU:HB2	1.99	0.44
7:a:132:LYS:O	7:a:136:GLU:CB	2.65	0.44
9:c:189:ILE:HD12	9:c:192:LEU:HD23	2.00	0.44
12:f:39:LYS:HD3	12:f:85:SER:HA	1.98	0.44
12:f:202:HIS:ND1	12:f:242:GLU:OE2	2.44	0.44
12:f:575:ALA:O	12:f:579:ALA:CB	2.64	0.44
12:f:780:PRO:O	12:f:784:ASP:CB	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:392:ALA:HA	13:A:395:PHE:HD2	1.81	0.44
13:A:413:VAL:O	13:A:417:ILE:HB	2.17	0.44
15:C:303:SER:HA	15:C:306:LEU:HB2	1.99	0.44
18:F:247:THR:HG21	18:F:278:LYS:HG3	1.99	0.44
21:I:229:LYS:N	21:I:232:GLU:OE2	2.48	0.44
23:K:60:GLU:OE1	23:K:63:SER:N	2.49	0.44
28:P:149:MET:HE3	31:s:147:PRO:HB2	2.00	0.44
19:g:17:SER:OG	19:g:21:ARG:N	2.50	0.44
30:r:26:ILE:HG21	30:r:29:GLN:HE21	1.82	0.44
1:U:567:ILE:CG2	1:U:601:ARG:CZ	2.92	0.44
6:Z:73:ASP:OD1	6:Z:77:ASN:ND2	2.51	0.44
7:a:308:GLU:HA	7:a:311:VAL:HG22	2.00	0.44
9:c:303:MET:HE2	10:d:239:SER:HA	2.00	0.44
10:d:155:LYS:CE	10:d:171:LEU:CD2	2.95	0.44
10:d:189:ILE:HG23	10:d:193:GLU:HB3	2.00	0.44
11:e:56:LEU:HG	11:e:59:GLU:HG2	1.99	0.44
13:A:333:ARG:HE	13:A:336:ARG:HH22	1.64	0.44
15:C:83:LYS:HD2	15:C:105:ILE:HD11	1.99	0.44
16:D:80:LYS:O	16:D:83:GLN:HG3	2.17	0.44
16:D:401:LYS:HA	16:D:404:LYS:HE2	1.98	0.44
17:E:33:LEU:O	17:E:37:THR:CB	2.65	0.44
22:J:94:HIS:O	22:J:97:THR:C	2.60	0.44
24:L:109:VAL:HG21	24:L:145:PHE:HD2	1.82	0.44
24:L:157:ARG:HD2	24:L:176:MET:HE3	1.98	0.44
23:k:76:CYS:SG	23:k:77:ALA:N	2.91	0.44
26:n:32:ASP:O	26:n:45:ARG:NH1	2.47	0.44
27:o:63:LEU:HD11	27:o:79:ALA:HB2	1.99	0.44
27:o:106:THR:OG1	27:o:109:HIS:NE2	2.42	0.44
27:o:120:ASP:OD1	27:o:120:ASP:N	2.49	0.44
30:r:77:ALA:O	30:r:81:LYS:HB2	2.18	0.44
2:V:318:GLN:HA	2:V:318:GLN:HE21	1.80	0.44
5:Y:215:ASP:O	5:Y:218:THR:OG1	2.36	0.44
12:f:291:GLN:HE21	12:f:879:ARG:NH2	2.15	0.44
12:f:340:MET:HE2	12:f:342:PRO:HD3	1.98	0.44
12:f:669:GLU:HA	12:f:705:ASN:HB2	1.99	0.44
12:f:676:GLY:HA3	12:f:712:LYS:HD2	1.99	0.44
12:f:760:PHE:O	12:f:760:PHE:CG	2.70	0.44
13:A:276:GLU:HB3	14:B:310:LEU:HD12	1.98	0.44
16:D:309:MET:HE1	16:D:327:LEU:HD21	1.99	0.44
18:F:189:GLY:HA3	18:F:364:ARG:HG2	2.00	0.44
22:J:91:CYS:HB2	22:J:102:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:K:17:PRO:HA	24:L:24:TYR:CZ	2.52	0.44
28:P:107:PRO:HG2	28:P:124:LEU:HB2	1.99	0.44
30:R:26:ILE:HG21	30:R:29:GLN:HE21	1.82	0.44
19:g:112:ASP:HB3	19:g:152:TYR:CZ	2.53	0.44
28:p:107:PRO:HG2	28:p:124:LEU:HB2	1.99	0.44
30:r:196:HIS:O	30:r:200:SER:OG	2.35	0.44
1:U:96:TYR:O	1:U:99:THR:OG1	2.32	0.44
2:V:417:ILE:HD13	5:Y:349:LYS:HG3	1.99	0.44
3:W:245:LYS:O	3:W:249:ALA:HB2	2.17	0.44
3:W:395:ASN:HA	3:W:398:VAL:HG22	1.98	0.44
5:Y:160:ASN:HA	5:Y:163:LYS:HB2	1.99	0.44
7:a:77:VAL:HG21	7:a:113:LEU:HD13	1.99	0.44
8:b:62:THR:HG21	8:b:71:ILE:HA	1.99	0.44
12:f:67:ASP:O	12:f:71:TYR:CB	2.66	0.44
12:f:223:GLU:OE2	14:B:59:ARG:CB	2.65	0.44
12:f:825:MET:HE3	12:f:850:VAL:HG23	2.00	0.44
17:E:251:ARG:HB3	17:E:255:ARG:HH12	1.83	0.44
18:F:180:ARG:NH1	18:F:241:ALA:O	2.50	0.44
18:F:282:ILE:HG22	18:F:327:LYS:HB2	1.98	0.44
21:I:47:ALA:O	21:I:212:GLU:N	2.43	0.44
22:J:31:THR:OG1	22:J:163:ARG:O	2.36	0.44
30:R:77:ALA:O	30:R:81:LYS:HB2	2.18	0.44
20:h:46:LEU:O	20:h:210:VAL:HA	2.17	0.44
1:U:496:LEU:HA	1:U:499:THR:HG22	1.99	0.44
4:X:73:VAL:O	4:X:77:LEU:N	2.51	0.44
8:b:58:CYS:HB3	8:b:92:VAL:HG21	2.00	0.44
12:f:460:ASP:N	12:f:460:ASP:OD1	2.49	0.44
13:A:115:VAL:HG21	13:A:118:PHE:HB2	1.99	0.44
14:B:120:HIS:HA	14:B:134:SER:HA	1.99	0.44
25:M:41:CYS:N	25:M:44:GLY:O	2.44	0.44
27:O:63:LEU:HD11	27:O:79:ALA:HB2	1.99	0.44
27:O:166:ASP:HB3	27:O:169:SER:HB2	2.00	0.44
20:h:210:VAL:HB	20:h:221:LEU:HD12	1.99	0.44
23:k:236:GLU:O	23:k:240:ASP:HB2	2.18	0.44
24:l:109:VAL:HG21	24:l:145:PHE:HD2	1.82	0.44
25:m:241:GLU:O	25:m:244:LYS:NZ	2.37	0.44
26:n:167:ASP:HB3	26:n:170:SER:HB2	2.00	0.44
28:p:36:THR:OG1	28:p:38:ASP:OD1	2.32	0.44
1:U:202:VAL:HB	1:U:216:VAL:HG23	2.00	0.44
3:W:137:TYR:CD1	3:W:137:TYR:O	2.71	0.44
3:W:178:GLU:CD	3:W:181:GLU:CA	2.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:61:GLU:HG3	7:a:79:ILE:HD13	1.99	0.44
8:b:142:ASN:HD22	8:b:172:THR:HA	1.82	0.44
12:f:371:ASN:HA	12:f:374:SER:HB2	2.00	0.44
14:B:133:VAL:HG11	14:B:157:HIS:HB2	1.99	0.44
15:C:150:MET:HA	15:C:331:ILE:HG21	1.99	0.44
15:C:337:ASN:ND2	15:C:376:VAL:O	2.50	0.44
16:D:363:TYR:CE2	16:D:399:PHE:HB3	2.51	0.44
16:D:407:ILE:HG13	16:D:408:LYS:H	1.83	0.44
17:E:244:SER:HB2	18:F:300:LYS:HG3	2.00	0.44
19:G:112:ASP:HB3	19:G:152:TYR:CZ	2.53	0.44
21:I:47:ALA:HB3	21:I:212:GLU:HB2	1.98	0.44
21:i:47:ALA:HB3	21:i:212:GLU:HB2	1.98	0.44
2:V:317:PRO:CD	11:e:4:LYS:HG3	2.48	0.44
3:W:36:LYS:HD2	3:W:84:ASN:ND2	2.32	0.44
7:a:33:LEU:HD13	7:a:36:GLN:HB2	2.00	0.44
10:d:104:LEU:HD12	10:d:107:LEU:HD13	2.00	0.44
12:f:759:LEU:H	12:f:809:ILE:HG21	1.82	0.44
14:B:252:GLY:N	14:B:285:ASP:O	2.37	0.44
16:D:107:THR:HG22	17:E:77:PRO:HG3	2.00	0.44
20:H:210:VAL:HB	20:H:221:LEU:HD12	1.99	0.44
19:g:142:GLY:O	19:g:149:PRO:HA	2.18	0.44
22:j:31:THR:OG1	22:j:163:ARG:O	2.36	0.44
23:k:72:ALA:O	23:k:226:PHE:N	2.41	0.44
27:o:138:PHE:O	27:o:142:PHE:CB	2.62	0.44
1:U:444:TYR:OH	1:U:774:PRO:O	2.33	0.44
1:U:496:LEU:O	1:U:500:ASN:HB2	2.17	0.44
3:W:17:GLU:HG3	3:W:62:SER:HB2	2.00	0.44
3:W:51:GLU:O	3:W:54:THR:N	2.51	0.44
4:X:310:ARG:HG2	4:X:314:ARG:HB3	2.00	0.44
7:a:100:THR:HG22	7:a:103:LYS:HE2	2.00	0.44
7:a:116:THR:O	7:a:120:ALA:HB2	2.18	0.44
9:c:300:LEU:HB2	10:d:246:VAL:HG11	2.00	0.44
10:d:206:MET:O	10:d:210:ALA:CB	2.66	0.44
12:f:232:TYR:HE2	12:f:263:PRO:HG2	1.83	0.44
12:f:411:ALA:HB1	12:f:444:ALA:HB2	2.00	0.44
12:f:708:ASP:HB3	12:f:787:LEU:HD22	1.80	0.44
13:A:74:PRO:HG2	13:A:77:LEU:HB2	2.00	0.44
13:A:140:VAL:HG12	13:A:152:PRO:HA	2.00	0.44
13:A:287:ASP:N	13:A:287:ASP:OD1	2.49	0.44
16:D:85:ILE:HD11	17:E:82:GLY:N	2.29	0.44
17:E:198:VAL:HG12	17:E:200:SER:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:K:196:LYS:HG3	23:K:241:ILE:HD12	1.99	0.44
26:N:167:ASP:HB3	26:N:170:SER:HB2	2.00	0.44
32:T:8:GLY:N	32:T:55:GLY:O	2.51	0.44
23:k:196:LYS:HG3	23:k:241:ILE:HD12	1.99	0.44
27:o:166:ASP:HB3	27:o:169:SER:HB2	2.00	0.44
32:t:147:GLN:HA	32:t:150:LEU:HD12	2.00	0.44
1:U:601:ARG:HA	1:U:604:HIS:HB3	1.99	0.43
3:W:117:ASP:HA	3:W:120:ILE:HG22	1.99	0.43
3:W:268:LYS:HD3	3:W:333:LEU:HB2	1.99	0.43
3:W:423:ASN:HA	3:W:426:ASN:HB3	2.00	0.43
7:a:346:ILE:O	7:a:350:LYS:HB2	2.18	0.43
8:b:138:VAL:H	8:b:160:LEU:HD21	1.82	0.43
12:f:759:LEU:N	12:f:809:ILE:HB	2.33	0.43
13:A:258:ARG:HH22	18:F:255:GLN:HA	1.82	0.43
14:B:119:ASN:HA	14:B:141:LYS:HZ1	1.82	0.43
15:C:373:GLU:HG3	15:C:375:ARG:HG3	1.99	0.43
16:D:88:VAL:O	16:D:131:ALA:CA	2.65	0.43
23:K:236:GLU:O	23:K:240:ASP:HB2	2.18	0.43
29:q:19:ARG:HB3	29:q:31:ASP:HA	2.00	0.43
1:U:474:ARG:O	1:U:478:SER:OG	2.32	0.43
1:U:688:LEU:HB3	1:U:713:TYR:HE1	1.82	0.43
1:U:789:ILE:N	1:U:910:GLY:O	2.51	0.43
5:Y:297:ARG:HD3	11:e:48:VAL:HG22	2.00	0.43
6:Z:39:LEU:H	6:Z:94:TRP:HA	1.82	0.43
9:c:192:LEU:N	9:c:196:LEU:HD21	2.30	0.43
10:d:38:THR:HG21	10:d:47:GLN:HE21	1.83	0.43
12:f:785:ARG:C	12:f:787:LEU:N	2.70	0.43
13:A:274:PHE:HB2	13:A:319:MET:HA	1.99	0.43
14:B:133:VAL:HB	14:B:158:ALA:HA	1.99	0.43
14:B:193:GLN:HG3	14:B:353:PHE:HE1	1.83	0.43
15:C:329:LEU:O	15:C:333:SER:HB3	2.17	0.43
19:G:180:GLU:HA	19:G:183:VAL:HG12	2.00	0.43
22:J:200:GLN:C	22:J:200:GLN:NE2	2.73	0.43
19:g:27:TYR:HA	19:g:30:LYS:HE2	2.00	0.43
23:k:199:LEU:HD11	23:k:217:LEU:HD11	1.99	0.43
31:s:63:THR:HG23	32:t:94:ARG:HH12	1.83	0.43
32:t:8:GLY:N	32:t:55:GLY:O	2.51	0.43
32:t:60:PHE:O	32:t:64:LYS:HB2	2.18	0.43
1:U:68:PHE:HB3	1:U:73:ALA:HB3	1.99	0.43
1:U:542:GLU:OE1	1:U:546:ARG:NH1	2.52	0.43
2:V:345:ARG:CZ	2:V:357:LEU:HA	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:454:GLU:N	10:d:187:GLU:OE2	2.39	0.43
5:Y:366:TYR:O	5:Y:369:THR:OG1	2.26	0.43
7:a:247:ARG:O	7:a:250:THR:OG1	2.32	0.43
12:f:265:ALA:HB3	12:f:268:LEU:HB2	2.01	0.43
13:A:81:ALA:HA	13:A:85:GLN:HB2	2.00	0.43
14:B:343:ARG:HE	14:B:346:ARG:NH1	2.16	0.43
14:B:423:LYS:O	14:B:427:LEU:HB2	2.19	0.43
17:E:210:GLU:OE1	17:E:213:ARG:NE	2.37	0.43
18:F:305:GLU:OE1	18:F:308:ARG:NH1	2.52	0.43
23:K:76:CYS:SG	23:K:77:ALA:N	2.91	0.43
26:N:135:ILE:HD13	26:N:163:ALA:HB2	2.01	0.43
30:R:15:ALA:HA	30:R:175:ASN:O	2.18	0.43
22:j:81:ARG:HA	22:j:84:ILE:HD12	1.99	0.43
22:j:91:CYS:HB2	22:j:102:VAL:HG21	1.99	0.43
1:U:642:GLU:C	15:C:57:ARG:NH1	2.76	0.43
2:V:363:LEU:HA	2:V:378:VAL:HG11	1.99	0.43
5:Y:348:ASP:HB2	5:Y:353:ILE:O	2.18	0.43
6:Z:209:ARG:HD2	6:Z:212:LEU:HD22	2.00	0.43
12:f:872:VAL:HG21	12:f:882:LEU:H	1.83	0.43
14:B:278:ALA:HB1	14:B:279:PRO:HD2	1.78	0.43
14:B:309:MET:O	14:B:313:LEU:HB2	2.19	0.43
15:C:155:ASP:HA	15:C:158:ILE:HD12	2.00	0.43
16:D:89:ILE:O	16:D:106:THR:HG23	2.18	0.43
16:D:208:PRO:HD3	16:D:312:ASN:HD21	1.83	0.43
21:I:197:LEU:HA	21:I:200:THR:HG22	1.99	0.43
22:J:73:PHE:HA	22:J:131:ALA:HA	2.00	0.43
24:L:196:ARG:NH2	24:L:237:GLU:O	2.44	0.43
25:M:96:SER:O	25:M:100:SER:HB3	2.18	0.43
28:P:36:THR:OG1	28:P:38:ASP:OD1	2.32	0.43
31:S:1:ARG:HH21	32:T:2:GLN:HE22	1.65	0.43
32:T:147:GLN:HA	32:T:150:LEU:HD12	2.00	0.43
26:n:135:ILE:HD13	26:n:163:ALA:HB2	2.01	0.43
27:o:1:THR:O	27:o:129:SER:N	2.51	0.43
2:V:252:ASN:HD22	2:V:284:GLU:HG2	1.82	0.43
2:V:362:LEU:HD13	2:V:378:VAL:HG22	2.01	0.43
2:V:418:SER:HB2	5:Y:350:VAL:HG11	2.00	0.43
3:W:80:TRP:CB	3:W:130:MET:HE2	2.48	0.43
5:Y:197:ALA:HB3	5:Y:226:VAL:HG21	1.99	0.43
12:f:223:GLU:HG3	14:B:59:ARG:HB3	1.69	0.43
12:f:806:VAL:C	12:f:808:ASN:H	2.26	0.43
16:D:380:GLN:HE22	17:E:167:PRO:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:322:LYS:HD3	17:E:326:ILE:HG13	2.00	0.43
18:F:81:LYS:HG2	18:F:84:LYS:HE2	2.01	0.43
22:J:81:ARG:HA	22:J:84:ILE:HD12	1.99	0.43
22:J:82:ILE:HA	22:J:85:ASN:HD22	1.84	0.43
25:M:34:SER:HA	25:M:167:LYS:HE3	2.00	0.43
19:g:53:GLN:HA	19:g:215:ILE:HA	2.01	0.43
21:i:79:ILE:HG22	21:i:82:ASP:H	1.83	0.43
25:m:34:SER:HA	25:m:167:LYS:HE3	2.00	0.43
1:U:493:VAL:O	1:U:497:LEU:HB2	2.18	0.43
1:U:571:CYS:HA	1:U:579:ARG:HG2	2.01	0.43
1:U:729:GLY:O	1:U:733:ALA:CB	2.66	0.43
3:W:253:THR:HA	3:W:254:PRO:HD3	1.88	0.43
3:W:317:TRP:CD1	3:W:358:VAL:HG21	2.53	0.43
12:f:24:THR:HG23	12:f:31:LYS:HG3	2.00	0.43
12:f:57:GLU:HG2	12:f:93:PRO:HB3	2.00	0.43
12:f:650:GLN:HA	12:f:653:ALA:H	1.83	0.43
12:f:652:VAL:CG2	12:f:685:THR:HB	2.43	0.43
15:C:69:GLN:H	15:C:69:GLN:CD	2.27	0.43
18:F:407:ALA:O	18:F:412:ALA:N	2.51	0.43
19:G:53:GLN:HA	19:G:215:ILE:HA	2.01	0.43
22:J:5:ARG:O	22:J:123:GLY:N	2.45	0.43
28:P:88:MET:HG3	28:P:124:LEU:HD11	2.00	0.43
32:T:60:PHE:O	32:T:64:LYS:HB2	2.18	0.43
19:g:103:TYR:HB2	26:n:61:TYR:CD1	2.53	0.43
3:W:46:THR:HA	3:W:50:LEU:HD13	2.00	0.43
3:W:128:LEU:HD22	3:W:147:LYS:HZ3	1.84	0.43
3:W:188:GLU:O	3:W:191:ARG:HG2	2.19	0.43
5:Y:233:ARG:HH21	5:Y:306:GLN:NE2	2.14	0.43
7:a:172:TYR:O	7:a:176:ALA:CB	2.66	0.43
12:f:291:GLN:HE21	12:f:879:ARG:HH21	1.65	0.43
12:f:808:ASN:OD1	12:f:808:ASN:N	2.52	0.43
15:C:168:PRO:HG3	15:C:175:PHE:CE2	2.54	0.43
15:C:381:GLU:HA	15:C:384:GLU:HG2	2.01	0.43
17:E:199:VAL:HG23	17:E:201:SER:H	1.83	0.43
27:O:215:LYS:O	28:P:196:THR:HA	2.19	0.43
29:Q:19:ARG:HB3	29:Q:31:ASP:HA	1.99	0.43
25:m:96:SER:O	25:m:100:SER:HB3	2.18	0.43
27:o:160:ALA:HA	27:o:163:ILE:HD12	2.00	0.43
28:p:88:MET:HG3	28:p:124:LEU:HD11	2.00	0.43
1:U:424:ALA:HA	1:U:427:LEU:HD13	2.01	0.43
1:U:791:LEU:O	1:U:914:LEU:N	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:17:GLU:HG2	3:W:63:THR:HG23	2.00	0.43
3:W:137:TYR:CE2	16:D:392:TYR:HE1	2.34	0.43
5:Y:335:SER:O	5:Y:339:ALA:CB	2.66	0.43
6:Z:238:PRO:HG2	9:c:309:PHE:HB3	2.00	0.43
9:c:113:HIS:HE1	9:c:115:HIS:CD2	2.37	0.43
9:c:192:LEU:HA	9:c:196:LEU:HD23	2.01	0.43
12:f:106:LEU:HB2	12:f:141:LYS:HD2	1.99	0.43
12:f:651:GLY:C	12:f:655:LEU:HD12	2.44	0.43
12:f:788:MET:C	12:f:790:GLN:H	2.26	0.43
13:A:312:ARG:HB2	13:A:315:ILE:HD12	2.01	0.43
16:D:125:LYS:HD2	16:D:125:LYS:HA	1.64	0.43
19:G:142:GLY:O	19:G:149:PRO:HA	2.18	0.43
25:M:39:ILE:HD11	25:M:189:ILE:HG23	2.01	0.43
27:o:44:CYS:HB2	27:o:99:VAL:HB	2.01	0.43
1:U:151:ILE:CD1	1:U:177:LEU:HG	2.49	0.43
1:U:695:MET:HE3	1:U:695:MET:HB2	1.83	0.43
2:V:81:GLN:HG3	2:V:86:VAL:HB	2.01	0.43
2:V:247:GLN:NE2	2:V:276:PHE:O	2.52	0.43
2:V:317:PRO:CG	11:e:4:LYS:CD	2.97	0.43
3:W:46:THR:CG2	3:W:50:LEU:CD1	2.81	0.43
3:W:48:LEU:HG	3:W:52:LYS:HG3	2.00	0.43
3:W:76:GLU:HA	3:W:79:GLU:CD	2.44	0.43
12:f:288:VAL:HA	12:f:291:GLN:HG2	2.01	0.43
12:f:531:ASN:HD22	12:f:534:VAL:HB	1.84	0.43
12:f:657:ILE:O	12:f:657:ILE:HG22	2.18	0.43
25:M:49:VAL:O	25:M:212:GLU:HB3	2.19	0.43
25:m:39:ILE:HD11	25:m:189:ILE:HG23	2.01	0.43
25:m:49:VAL:O	25:m:212:GLU:HB3	2.19	0.43
30:r:15:ALA:HA	30:r:175:ASN:O	2.18	0.43
1:U:500:ASN:OD1	1:U:508:THR:OG1	2.37	0.43
1:U:605:VAL:HG22	1:U:609:ASP:HB2	2.00	0.43
1:U:642:GLU:CA	15:C:57:ARG:NH1	2.81	0.43
1:U:762:GLY:O	1:U:766:PHE:HB2	2.19	0.43
2:V:317:PRO:HG3	11:e:4:LYS:HD3	2.01	0.43
2:V:495:ARG:C	15:C:44:ARG:NH2	2.77	0.43
3:W:48:LEU:HG	3:W:52:LYS:CG	2.49	0.43
3:W:94:ARG:HG3	3:W:98:LYS:HD2	2.00	0.43
3:W:312:MET:HE3	3:W:365:ILE:HD12	2.00	0.43
4:X:213:GLN:HA	4:X:216:ILE:HB	2.01	0.43
4:X:400:ALA:O	4:X:403:THR:OG1	2.35	0.43
13:A:139:ARG:HH22	14:B:122:ILE:HG21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:396:ALA:CB	13:A:401:ARG:HG2	2.48	0.43
17:E:43:SER:OG	18:F:75:GLU:OE1	2.27	0.43
17:E:253:ILE:HG13	18:F:308:ARG:HH22	1.84	0.43
18:F:376:SER:OG	18:F:415:LEU:O	2.33	0.43
21:I:187:LYS:HA	21:I:190:LEU:HD12	2.01	0.43
22:J:220:LEU:HD13	22:J:224:GLU:HB2	2.00	0.43
24:L:204:ASP:OD1	24:L:204:ASP:N	2.51	0.43
30:R:83:LEU:HD23	30:R:114:VAL:HG21	2.01	0.43
25:m:34:SER:HA	25:m:167:LYS:HG3	2.00	0.43
1:U:503:GLN:HB2	1:U:508:THR:HG21	2.01	0.42
1:U:645:ASN:CA	15:C:60:ARG:HH12	2.32	0.42
2:V:311:ASN:HA	2:V:314:ARG:HG2	2.01	0.42
2:V:346:LEU:HD12	11:e:46:ASP:CG	2.39	0.42
3:W:361:HIS:HA	3:W:364:ARG:HH11	1.83	0.42
9:c:291:LEU:O	9:c:295:ASN:ND2	2.52	0.42
10:d:125:LYS:HB3	10:d:130:ASN:HD22	1.83	0.42
10:d:155:LYS:CE	10:d:171:LEU:HG	2.40	0.42
12:f:23:GLY:HA2	12:f:27:LYS:HD3	2.01	0.42
16:D:244:PRO:HB3	16:D:291:GLU:HG3	2.00	0.42
19:G:27:TYR:HA	19:G:30:LYS:HE2	2.00	0.42
24:l:204:ASP:OD1	24:l:204:ASP:N	2.51	0.42
29:q:13:VAL:HB	29:q:183:ILE:HB	2.01	0.42
1:U:218:GLN:HG3	1:U:752:THR:HB	2.01	0.42
1:U:399:TRP:CD1	9:c:178:THR:HG21	2.54	0.42
1:U:477:GLY:O	1:U:481:LEU:HB2	2.19	0.42
2:V:150:ARG:O	2:V:154:ALA:CB	2.67	0.42
4:X:401:LEU:HD12	5:Y:369:THR:HG22	2.00	0.42
12:f:183:PRO:O	12:f:187:LEU:HB2	2.19	0.42
12:f:475:ASN:O	12:f:477:MET:N	2.52	0.42
12:f:712:LYS:CD	12:f:715:HIS:HB2	2.33	0.42
12:f:814:SER:OG	12:f:822:VAL:O	2.36	0.42
14:B:197:ILE:HG13	14:B:235:LEU:HD21	2.01	0.42
14:B:265:LYS:HA	14:B:268:ARG:HE	1.83	0.42
16:D:94:GLU:HG2	16:D:102:ILE:HD13	2.01	0.42
19:G:17:SER:OG	19:G:21:ARG:N	2.50	0.42
23:K:51:GLU:HA	23:K:215:ILE:HG22	2.02	0.42
27:O:44:CYS:HB2	27:O:99:VAL:HB	2.01	0.42
30:R:97:MET:O	30:R:116:SER:N	2.52	0.42
30:R:196:HIS:O	30:R:200:SER:OG	2.35	0.42
19:g:47:CYS:HA	19:g:221:THR:HA	2.00	0.42
22:j:68:ASN:HA	22:j:211:MET:HE1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:t:89:HIS:CE1	32:t:131:ALA:HB1	2.54	0.42
1:U:80:TYR:O	1:U:84:ALA:HB2	2.19	0.42
2:V:201:ARG:HE	2:V:242:HIS:HB3	1.83	0.42
8:b:89:GLY:HA2	8:b:92:VAL:HG12	2.01	0.42
9:c:254:ASN:HB3	9:c:280:PRO:HB3	2.01	0.42
12:f:257:ARG:HG2	12:f:272:LEU:HD13	2.01	0.42
13:A:99:THR:HG22	13:A:115:VAL:HG12	2.00	0.42
14:B:212:GLU:OE1	14:B:212:GLU:N	2.52	0.42
16:D:127:ASN:O	16:D:252:ARG:NH1	2.44	0.42
17:E:322:LYS:NZ	17:E:328:TYR:OH	2.51	0.42
21:i:15:GLU:HG3	21:i:17:ARG:HG2	2.02	0.42
24:l:148:CYS:SG	24:l:150:SER:OG	2.69	0.42
3:W:64:SER:HA	3:W:67:LEU:HB3	2.01	0.42
7:a:153:SER:O	7:a:157:ASP:HB2	2.20	0.42
12:f:171:GLN:HG3	12:f:179:VAL:HG22	2.01	0.42
16:D:254:ALA:HB2	16:D:262:ILE:HD11	2.01	0.42
17:E:88:ASP:HB3	17:E:91:LYS:HZ2	1.84	0.42
17:E:265:ASP:OD2	17:E:291:ARG:NH1	2.53	0.42
19:G:127:GLN:HA	20:H:128:ARG:NH2	2.34	0.42
21:I:79:ILE:HG22	21:I:82:ASP:H	1.83	0.42
24:L:172:LEU:O	24:L:176:MET:HB3	2.19	0.42
25:M:174:THR:O	25:M:178:LYS:NZ	2.47	0.42
31:S:93:SER:OG	31:S:128:GLY:O	2.30	0.42
24:l:172:LEU:O	24:l:176:MET:HB3	2.19	0.42
26:n:103:TRP:HA	26:n:109:GLY:HA2	2.01	0.42
32:t:177:TYR:CZ	32:t:185:ASN:HB2	2.54	0.42
1:U:94:SER:OG	1:U:95:GLU:N	2.53	0.42
3:W:96:GLN:HE21	3:W:135:LYS:N	2.17	0.42
5:Y:155:ASP:O	5:Y:158:THR:OG1	2.35	0.42
7:a:53:GLY:O	7:a:57:ILE:N	2.41	0.42
8:b:109:ILE:HB	8:b:138:VAL:HG22	2.01	0.42
9:c:238:CYS:HA	9:c:241:ASN:HD22	1.85	0.42
12:f:180:GLN:O	12:f:219:LYS:NZ	2.53	0.42
12:f:250:ARG:CZ	12:f:281:ILE:HD11	2.35	0.42
14:B:53:THR:CB	14:B:54:PRO:CD	2.90	0.42
14:B:419:PHE:HA	14:B:422:SER:HB3	2.01	0.42
15:C:59:LEU:CD1	16:D:75:ALA:CB	2.95	0.42
22:J:68:ASN:HA	22:J:211:MET:HE1	2.00	0.42
23:K:77:ALA:O	23:K:141:LEU:HA	2.20	0.42
31:S:53:GLY:O	31:S:108:ASN:HA	2.20	0.42
32:T:190:ALA:HA	32:T:198:GLU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:k:74:ILE:HA	23:k:144:GLY:O	2.20	0.42
30:r:97:MET:O	30:r:116:SER:N	2.52	0.42
1:U:680:VAL:HB	1:U:683:VAL:HG12	2.00	0.42
2:V:212:TYR:HA	2:V:215:ALA:HB3	2.02	0.42
3:W:47:LEU:HB3	3:W:94:ARG:CZ	2.49	0.42
4:X:96:PHE:HE2	4:X:106:GLU:HA	1.85	0.42
6:Z:60:GLU:HA	8:b:95:LEU:HD21	2.02	0.42
6:Z:243:GLN:C	6:Z:245:PHE:H	2.26	0.42
10:d:27:LYS:HA	10:d:30:LEU:HD12	2.02	0.42
12:f:556:ARG:NH1	12:f:786:GLN:HB2	2.35	0.42
14:B:195:GLN:O	14:B:199:GLU:CB	2.68	0.42
17:E:45:ASN:O	17:E:49:ALA:CB	2.67	0.42
18:F:164:LEU:HA	18:F:165:PRO:HD3	1.88	0.42
18:F:184:GLN:HE22	18:F:186:SER:HB3	1.83	0.42
19:G:212:PRO:HB3	19:G:235:ILE:HG22	2.01	0.42
21:I:15:GLU:HG3	21:I:17:ARG:HG2	2.02	0.42
26:N:28:ASN:HD21	27:O:122:LEU:HD21	1.85	0.42
27:O:203:ARG:HH12	28:P:158:MET:HE3	1.84	0.42
32:T:89:HIS:CE1	32:T:131:ALA:HB1	2.54	0.42
27:o:40:ASN:O	27:o:102:GLY:HA2	2.19	0.42
30:r:83:LEU:HD23	30:r:114:VAL:HG21	2.01	0.42
31:s:36:HIS:HB3	32:t:132:TYR:CZ	2.55	0.42
1:U:326:ILE:O	1:U:330:SER:OG	2.32	0.42
3:W:47:LEU:HB3	3:W:94:ARG:NH2	2.34	0.42
3:W:260:SER:O	3:W:264:GLN:N	2.53	0.42
16:D:245:ARG:HA	16:D:248:ARG:HG2	2.01	0.42
18:F:410:ARG:NH2	18:F:419:ASP:OD2	2.53	0.42
25:M:34:SER:HA	25:M:167:LYS:HG3	2.00	0.42
25:M:42:LYS:HD2	25:M:183:GLU:HA	2.02	0.42
27:O:67:SER:HB3	27:O:74:PRO:HG3	2.02	0.42
23:k:15:PHE:HE2	24:l:127:PRO:HD2	1.85	0.42
23:k:51:GLU:HA	23:k:215:ILE:HG22	2.01	0.42
28:p:159:ASP:N	28:p:159:ASP:OD1	2.52	0.42
31:s:1:ARG:HH21	32:t:2:GLN:HE22	1.68	0.42
1:U:24:LEU:HB2	1:U:59:PHE:HD2	1.84	0.42
2:V:50:GLU:HA	2:V:54:LYS:HB2	2.01	0.42
3:W:436:MET:HA	3:W:439:VAL:HG22	2.01	0.42
6:Z:237:LEU:HA	6:Z:238:PRO:HD3	1.85	0.42
13:A:425:ALA:HA	14:B:339:PRO:HB2	2.01	0.42
15:C:67:GLN:NE2	15:C:67:GLN:HA	2.32	0.42
15:C:279:GLN:HG3	15:C:284:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:115:ILE:H	16:D:115:ILE:HG13	1.68	0.42
16:D:115:ILE:HG22	16:D:139:LEU:HD12	2.02	0.42
23:K:177:ALA:O	23:K:181:LEU:HB2	2.20	0.42
24:L:189:LYS:HG3	24:L:193:ARG:HH12	1.85	0.42
26:N:7:GLN:HB3	26:N:111:VAL:HG23	2.02	0.42
26:N:103:TRP:HA	26:N:109:GLY:HA2	2.01	0.42
29:Q:172:ILE:O	29:q:174:ASN:N	2.53	0.42
27:o:14:LEU:O	27:o:175:LEU:HA	2.20	0.42
27:o:67:SER:HB3	27:o:74:PRO:HG3	2.02	0.42
1:U:443:LEU:HA	1:U:446:LEU:HB2	2.02	0.42
2:V:87:SER:HB3	2:V:126:ALA:H	1.84	0.42
2:V:262:SER:HB3	10:d:120:GLU:HB3	2.01	0.42
3:W:148:THR:O	3:W:151:THR:OG1	2.35	0.42
4:X:215:GLY:O	4:X:219:ALA:CB	2.68	0.42
4:X:400:ALA:HB1	6:Z:262:LEU:HD22	2.01	0.42
5:Y:36:ALA:O	5:Y:40:GLU:CB	2.67	0.42
7:a:77:VAL:HA	7:a:80:ILE:HG22	2.02	0.42
10:d:131:VAL:HG23	10:d:134:LYS:HE2	2.02	0.42
10:d:256:ILE:HG12	16:D:65:GLN:HG2	2.02	0.42
15:C:152:GLY:HA3	15:C:328:ILE:HG12	2.00	0.42
16:D:173:GLN:NE2	16:D:332:GLU:O	2.53	0.42
26:N:96:ALA:HB1	26:N:98:ILE:HG12	2.02	0.42
27:O:40:ASN:O	27:O:102:GLY:HA2	2.19	0.42
19:g:144:ASP:O	19:g:148:GLY:N	2.51	0.42
26:n:96:ALA:HB1	26:n:98:ILE:HG12	2.02	0.42
2:V:204:ASP:O	2:V:208:ALA:HB2	2.20	0.42
4:X:414:LEU:O	4:X:418:ALA:HB3	2.20	0.42
5:Y:88:LEU:HA	5:Y:100:ILE:HG12	2.01	0.42
12:f:733:GLY:O	12:f:746:ARG:NH1	2.45	0.42
12:f:755:ASP:OD1	12:f:755:ASP:N	2.51	0.42
15:C:45:LEU:HG	16:D:61:ILE:HG21	2.02	0.42
15:C:325:ARG:HD3	15:C:353:GLY:HA2	2.02	0.42
16:D:384:MET:HG2	17:E:159:PHE:HE1	1.85	0.42
20:H:34:PRO:HA	20:H:164:GLY:HA3	2.01	0.42
27:O:160:ALA:HA	27:O:163:ILE:HD12	2.00	0.42
29:Q:13:VAL:HB	29:Q:183:ILE:HB	2.01	0.42
21:i:187:LYS:HA	21:i:190:LEU:HD12	2.01	0.42
24:l:158:ALA:HB1	24:l:172:LEU:HD13	2.02	0.42
25:m:36:ALA:HB3	25:m:165:ILE:HG13	2.01	0.42
1:U:258:GLN:O	1:U:262:SER:HB3	2.20	0.41
3:W:78:LYS:HB3	3:W:78:LYS:HE2	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:292:GLN:NE2	4:X:296:ASN:OD1	2.44	0.41
4:X:415:TYR:HE1	5:Y:383:LEU:HD13	1.85	0.41
7:a:21:VAL:O	7:a:25:LEU:HB2	2.20	0.41
12:f:296:PHE:HA	12:f:807:ARG:CD	2.50	0.41
12:f:669:GLU:O	12:f:787:LEU:HD11	2.20	0.41
15:C:355:SER:OG	15:C:358:GLU:OE1	2.30	0.41
17:E:200:SER:HB2	17:E:232:MET:HE3	2.01	0.41
23:K:74:ILE:HA	23:K:144:GLY:O	2.20	0.41
24:L:65:HIS:NE2	24:L:220:GLU:OE2	2.53	0.41
27:O:1:THR:O	27:O:129:SER:N	2.51	0.41
32:T:141:TYR:HA	32:T:144:TYR:HD2	1.85	0.41
31:s:53:GLY:O	31:s:108:ASN:HA	2.20	0.41
32:t:190:ALA:HA	32:t:198:GLU:O	2.20	0.41
1:U:695:MET:HE1	1:U:709:PHE:HD2	1.85	0.41
2:V:172:VAL:O	2:V:176:MET:HB2	2.19	0.41
12:f:83:ARG:O	12:f:87:THR:OG1	2.33	0.41
12:f:651:GLY:O	12:f:655:LEU:CG	2.68	0.41
17:E:64:LEU:HB2	17:E:68:LYS:O	2.20	0.41
17:E:287:PRO:HA	17:E:290:LEU:HB2	2.02	0.41
22:J:104:VAL:HG13	22:J:145:TYR:HE2	1.85	0.41
25:M:36:ALA:HB3	25:M:165:ILE:HG13	2.02	0.41
26:N:5:ALA:HA	26:N:13:VAL:O	2.20	0.41
27:O:164:PHE:HE1	31:s:212:LYS:HG3	1.84	0.41
19:g:46:ASP:O	19:g:222:VAL:N	2.50	0.41
19:g:180:GLU:HA	19:g:183:VAL:HG12	2.00	0.41
24:l:228:ASP:OD1	24:l:228:ASP:N	2.53	0.41
25:m:134:SER:HB2	25:m:153:PRO:HD3	2.01	0.41
3:W:273:TYR:HE2	3:W:286:LEU:HD21	1.84	0.41
3:W:315:MET:SD	3:W:315:MET:N	2.93	0.41
4:X:212:MET:HE3	4:X:239:TYR:HE2	1.85	0.41
6:Z:138:TYR:HB3	6:Z:155:PHE:HB3	2.02	0.41
7:a:57:ILE:HD12	7:a:57:ILE:HA	1.96	0.41
12:f:811:LEU:HD21	12:f:862:ILE:HD13	2.03	0.41
14:B:252:GLY:HA2	14:B:255:LEU:HD23	2.03	0.41
15:C:136:SER:HA	15:C:139:MET:HE2	2.02	0.41
17:E:260:LEU:HG	17:E:264:MET:HE3	2.00	0.41
25:M:134:SER:HB2	25:M:153:PRO:HD3	2.01	0.41
22:j:82:ILE:HA	22:j:85:ASN:HD22	1.84	0.41
22:j:220:LEU:HD13	22:j:224:GLU:HB2	2.01	0.41
23:k:77:ALA:O	23:k:141:LEU:HA	2.20	0.41
26:n:40:ARG:NH2	26:n:181:GLU:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:r:153:TYR:HB3	30:r:157:ARG:HH22	1.85	0.41
32:t:141:TYR:HA	32:t:144:TYR:HD2	1.85	0.41
3:W:282:GLU:O	3:W:286:LEU:CB	2.59	0.41
3:W:315:MET:O	3:W:315:MET:SD	2.78	0.41
5:Y:79:ASP:HA	5:Y:82:LYS:HE2	2.02	0.41
9:c:265:MET:HE3	9:c:266:THR:HG22	2.01	0.41
12:f:75:LEU:HD13	12:f:77:GLU:HG3	2.02	0.41
14:B:407:LEU:HD23	14:B:407:LEU:HA	1.87	0.41
15:C:160:GLU:O	15:C:313:ARG:NH2	2.53	0.41
16:D:189:GLU:HA	16:D:192:LYS:HB3	2.03	0.41
16:D:353:ASN:HD22	16:D:393:ILE:HA	1.86	0.41
17:E:313:LEU:O	17:E:317:ALA:CB	2.68	0.41
20:H:74:LEU:HD21	20:H:134:LEU:HD22	2.03	0.41
28:P:159:ASP:OD1	28:P:159:ASP:N	2.52	0.41
30:R:153:TYR:HB3	30:R:157:ARG:HH22	1.85	0.41
30:R:167:ASP:HB3	30:R:170:SER:HB2	2.02	0.41
32:T:9:THR:H	32:T:41:ARG:NH2	2.19	0.41
26:n:14:LEU:HD11	26:n:101:ALA:HB3	2.03	0.41
1:U:748:LEU:HD23	1:U:760:VAL:HG22	2.02	0.41
3:W:72:LYS:O	3:W:75:TYR:N	2.53	0.41
3:W:265:GLN:OE1	3:W:335:SER:OG	2.35	0.41
3:W:355:LYS:HA	3:W:358:VAL:HG22	2.01	0.41
10:d:102:ASN:O	10:d:106:LEU:HB2	2.20	0.41
12:f:608:LYS:HA	12:f:611:GLN:HG2	2.02	0.41
14:B:54:PRO:HB2	14:B:61:LYS:HD2	1.98	0.41
15:C:90:HIS:CB	15:C:91:PRO:CD	2.61	0.41
16:D:368:ASP:OD1	16:D:368:ASP:N	2.51	0.41
23:K:48:LEU:HD21	23:K:77:ALA:HB2	2.02	0.41
24:L:158:ALA:HB1	24:L:172:LEU:HD13	2.02	0.41
27:O:164:PHE:O	31:s:38:ARG:NH2	2.54	0.41
22:j:104:VAL:HG13	22:j:145:TYR:HE2	1.85	0.41
32:t:187:PHE:O	32:t:203:LEU:N	2.52	0.41
1:U:241:ASN:HB3	1:U:244:MET:HG2	2.03	0.41
2:V:89:LYS:HD2	2:V:93:PHE:HE2	1.85	0.41
2:V:228:ARG:HA	2:V:228:ARG:HD3	1.84	0.41
4:X:397:TYR:OH	6:Z:255:ASP:OD1	2.31	0.41
5:Y:232:GLU:HG2	5:Y:233:ARG:H	1.85	0.41
5:Y:387:ILE:HD13	6:Z:275:LEU:HD12	2.02	0.41
6:Z:69:PHE:HB2	8:b:99:HIS:CE1	2.56	0.41
6:Z:116:CYS:O	6:Z:119:SER:OG	2.30	0.41
12:f:250:ARG:NH1	12:f:281:ILE:CD1	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:429:ILE:HG23	12:f:444:ALA:HB1	2.02	0.41
12:f:676:GLY:O	12:f:782:HIS:NE2	2.54	0.41
15:C:31:LEU:HD11	16:D:47:LEU:C	2.45	0.41
15:C:69:GLN:HG3	15:C:118:ASN:HD21	1.86	0.41
16:D:172:ILE:O	16:D:176:GLU:HB2	2.20	0.41
18:F:97:LEU:HB2	18:F:121:CYS:HB2	2.02	0.41
27:O:161:ALA:O	27:O:165:ASN:HB2	2.20	0.41
25:m:42:LYS:HD2	25:m:183:GLU:HA	2.02	0.41
26:n:5:ALA:HA	26:n:13:VAL:O	2.20	0.41
2:V:30:PRO:O	2:V:34:ASP:N	2.53	0.41
2:V:224:LEU:HD22	2:V:227:VAL:HB	2.02	0.41
2:V:346:LEU:CD1	11:e:46:ASP:CG	2.92	0.41
5:Y:99:GLU:HA	5:Y:102:ASP:HB3	2.02	0.41
7:a:81:LEU:HA	7:a:84:VAL:HG12	2.02	0.41
11:e:53:SER:OG	11:e:54:ASN:N	2.54	0.41
12:f:325:GLN:HE21	12:f:420:TRP:HE3	1.68	0.41
12:f:562:LEU:HA	12:f:562:LEU:HD23	1.82	0.41
12:f:637:LYS:HG2	12:f:674:THR:HA	2.02	0.41
13:A:178:GLY:HA3	13:A:353:HIS:CE1	2.56	0.41
14:B:380:LEU:HD23	14:B:383:LEU:HD12	2.03	0.41
15:C:73:VAL:CG2	15:C:127:LEU:HD13	2.49	0.41
15:C:73:VAL:HG11	16:D:110:ASN:HB2	2.02	0.41
18:F:305:GLU:HA	18:F:308:ARG:HH11	1.85	0.41
20:h:74:LEU:HD21	20:h:134:LEU:HD22	2.03	0.41
21:i:170:ALA:O	21:i:173:SER:OG	2.39	0.41
29:q:101:ASN:OD1	29:q:120:TYR:N	2.54	0.41
3:W:78:LYS:O	3:W:78:LYS:HG3	2.19	0.41
3:W:97:LEU:CD1	3:W:138:VAL:CG2	2.99	0.41
6:Z:205:LEU:HD11	7:a:357:CYS:HA	2.03	0.41
9:c:191:ALA:CA	9:c:196:LEU:HD11	2.51	0.41
12:f:759:LEU:CA	12:f:808:ASN:O	2.64	0.41
12:f:788:MET:O	12:f:790:GLN:N	2.53	0.41
13:A:84:LYS:O	13:A:88:GLN:CB	2.69	0.41
18:F:266:LYS:HA	18:F:269:ARG:HG2	2.01	0.41
20:H:69:THR:HG22	20:H:72:ILE:HB	2.03	0.41
21:I:147:LEU:HD12	21:I:159:TRP:HB2	2.02	0.41
25:M:43:ASP:N	25:M:43:ASP:OD1	2.54	0.41
29:Q:12:TYR:HA	29:Q:183:ILE:O	2.20	0.41
32:T:177:TYR:CZ	32:T:185:ASN:HB2	2.55	0.41
32:T:187:PHE:O	32:T:203:LEU:N	2.52	0.41
19:g:132:ARG:NE	25:m:123:THR:O	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:h:69:THR:HG22	20:h:72:ILE:HB	2.03	0.41
21:i:115:CYS:O	21:i:119:GLN:HB2	2.21	0.41
22:j:5:ARG:O	22:j:123:GLY:N	2.45	0.41
22:j:185:ASP:HA	22:j:188:ILE:HD12	2.03	0.41
23:k:48:LEU:HD21	23:k:77:ALA:HB2	2.02	0.41
24:l:36:VAL:HG22	24:l:160:SER:HB2	2.02	0.41
29:q:12:TYR:HA	29:q:183:ILE:O	2.20	0.41
31:s:35:ILE:O	32:t:151:ARG:NH2	2.36	0.41
1:U:188:MET:HG2	1:U:194:ARG:HD3	2.03	0.41
1:U:188:MET:HE3	1:U:194:ARG:HG3	2.03	0.41
1:U:611:ASN:HB3	1:U:614:VAL:HG12	2.03	0.41
2:V:228:ARG:NH1	2:V:254:LEU:O	2.53	0.41
3:W:408:ARG:O	4:X:346:GLN:NE2	2.45	0.41
5:Y:41:LEU:HA	5:Y:44:ALA:HB3	2.03	0.41
5:Y:225:TYR:HA	5:Y:228:MET:HE3	2.03	0.41
6:Z:43:TRP:HB3	6:Z:48:LEU:HD22	2.03	0.41
6:Z:98:GLY:HA3	6:Z:123:ILE:HG23	2.01	0.41
6:Z:121:LEU:HD11	6:Z:138:TYR:HD2	1.84	0.41
6:Z:143:GLU:HB2	6:Z:145:HIS:ND1	2.36	0.41
9:c:32:TYR:HB3	9:c:208:ARG:HD2	2.02	0.41
10:d:27:LYS:HD3	10:d:30:LEU:HD12	2.03	0.41
10:d:49:ILE:HG23	10:d:50:LEU:HD12	2.03	0.41
12:f:183:PRO:O	12:f:187:LEU:CB	2.69	0.41
12:f:221:ILE:HD12	12:f:221:ILE:HA	1.94	0.41
12:f:327:ASN:HD22	12:f:330:PHE:HB3	1.86	0.41
12:f:657:ILE:CG2	14:B:82:GLN:NE2	2.84	0.41
12:f:674:THR:O	12:f:678:LEU:CB	2.69	0.41
15:C:62:GLU:O	15:C:66:LEU:HD23	2.21	0.41
15:C:326:LEU:HD22	15:C:345:ARG:HE	1.85	0.41
17:E:45:ASN:O	17:E:49:ALA:HB2	2.20	0.41
17:E:55:GLN:HB3	17:E:99:ALA:HB1	2.03	0.41
21:I:133:SER:OG	21:I:150:SER:O	2.37	0.41
29:Q:101:ASN:OD1	29:Q:120:TYR:N	2.54	0.41
30:R:45:MET:HG3	30:R:52:CYS:HB2	2.03	0.41
19:g:97:GLU:HA	19:g:100:ASN:HD22	1.86	0.41
19:g:212:PRO:HB3	19:g:235:ILE:HG22	2.02	0.41
21:i:33:THR:HB	21:i:48:GLU:HB3	2.03	0.41
21:i:47:ALA:O	21:i:212:GLU:N	2.43	0.41
21:i:136:TYR:HB2	21:i:148:TYR:HB2	2.02	0.41
21:i:147:LEU:HD12	21:i:159:TRP:HB2	2.02	0.41
23:k:49:ALA:HB2	23:k:217:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:l:186:GLU:HA	24:l:189:LYS:HG2	2.02	0.41
26:n:7:GLN:HB3	26:n:111:VAL:HG23	2.02	0.41
27:o:19:ARG:NH1	27:o:167:LEU:O	2.54	0.41
1:U:567:ILE:CG2	1:U:601:ARG:NH1	2.84	0.41
2:V:195:ILE:HD12	15:C:25:LEU:HG	2.03	0.41
2:V:345:ARG:CZ	2:V:357:LEU:CA	2.99	0.41
2:V:407:VAL:O	2:V:411:SER:OG	2.32	0.41
3:W:61:VAL:HG12	3:W:62:SER:H	1.86	0.41
6:Z:34:ARG:HE	6:Z:102:HIS:CD2	2.39	0.41
6:Z:240:VAL:HG12	9:c:310:LYS:HG2	2.03	0.41
12:f:658:ALA:CB	14:B:78:PHE:CZ	2.88	0.41
13:A:347:ASP:OD1	13:A:347:ASP:N	2.53	0.41
14:B:381:ASP:HA	14:B:384:ILE:HD12	2.03	0.41
27:O:14:LEU:O	27:O:175:LEU:HA	2.20	0.41
30:R:5:ALA:HA	30:R:13:ILE:O	2.21	0.41
19:g:56:VAL:HG13	19:g:61:LEU:HD22	2.02	0.41
21:i:93:ILE:HA	21:i:96:ARG:HG2	2.02	0.41
24:l:189:LYS:HG3	24:l:193:ARG:HH12	1.85	0.41
30:r:167:ASP:HB3	30:r:170:SER:HB2	2.02	0.41
32:t:9:THR:H	32:t:41:ARG:NH2	2.19	0.41
3:W:101:VAL:HA	3:W:104:MET:HB2	2.02	0.40
3:W:227:TYR:O	3:W:246:HIS:NE2	2.37	0.40
4:X:221:GLU:O	4:X:223:LYS:NZ	2.46	0.40
5:Y:82:LYS:HA	5:Y:85:ASP:HB2	2.03	0.40
6:Z:243:GLN:C	6:Z:245:PHE:N	2.77	0.40
7:a:48:PRO:HB2	7:a:51:ALA:HA	2.03	0.40
7:a:156:TYR:HB3	7:a:179:PHE:HB2	2.02	0.40
8:b:125:VAL:HA	8:b:128:ALA:HB3	2.02	0.40
12:f:830:LEU:N	12:f:859:PRO:O	2.54	0.40
13:A:95:VAL:HG23	14:B:133:VAL:HG12	2.03	0.40
15:C:24:TYR:CE2	16:D:40:LEU:CD1	3.00	0.40
19:G:56:VAL:HG13	19:G:61:LEU:HD22	2.02	0.40
21:I:93:ILE:HA	21:I:96:ARG:HG2	2.01	0.40
21:I:243:GLU:O	21:I:247:ALA:CB	2.69	0.40
25:M:228:PRO:HD2	25:M:231:ILE:HD12	2.03	0.40
27:O:54:MET:HG3	28:P:96:TYR:CG	2.56	0.40
30:R:37:ILE:HG23	30:R:60:ALA:HB2	2.03	0.40
25:m:90:ILE:H	25:m:90:ILE:HG13	1.76	0.40
25:m:112:ALA:O	25:m:116:ALA:CB	2.69	0.40
27:o:63:LEU:O	27:o:67:SER:OG	2.33	0.40
30:r:182:ASP:OD1	30:r:182:ASP:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:27:LEU:HB3	1:U:63:VAL:HG11	2.03	0.40
5:Y:80:GLU:HA	5:Y:83:ARG:HG2	2.02	0.40
5:Y:215:ASP:HB3	5:Y:218:THR:HG23	2.02	0.40
6:Z:142:GLU:HB3	6:Z:153:LYS:HE2	2.03	0.40
10:d:155:LYS:CE	10:d:170:LEU:HD22	2.50	0.40
13:A:74:PRO:HA	13:A:75:PRO:HD3	1.84	0.40
14:B:52:VAL:O	14:B:52:VAL:HG22	2.20	0.40
19:G:97:GLU:HA	19:G:100:ASN:HD22	1.86	0.40
24:L:36:VAL:HG22	24:L:160:SER:HB2	2.02	0.40
27:O:19:ARG:NH1	27:O:167:LEU:O	2.54	0.40
20:h:34:PRO:HA	20:h:164:GLY:HA3	2.02	0.40
23:k:235:GLU:HA	23:k:238:ILE:HD12	2.02	0.40
1:U:458:ILE:O	1:U:462:LEU:HB2	2.20	0.40
1:U:701:ILE:HG21	1:U:810:THR:HA	2.02	0.40
6:Z:235:ASN:OD1	7:a:289:ARG:NH2	2.54	0.40
9:c:92:GLN:O	9:c:96:LEU:CB	2.65	0.40
9:c:216:MET:HE3	9:c:216:MET:HB2	1.80	0.40
12:f:408:LEU:HD21	12:f:797:LEU:HD13	2.04	0.40
12:f:760:PHE:CD2	12:f:760:PHE:O	2.75	0.40
12:f:826:GLN:HA	12:f:849:ALA:HA	2.02	0.40
13:A:143:ASP:N	13:A:143:ASP:OD1	2.53	0.40
17:E:313:LEU:O	17:E:317:ALA:HB2	2.22	0.40
24:L:94:ASP:OD1	24:L:95:SER:N	2.54	0.40
24:L:228:ASP:N	24:L:228:ASP:OD1	2.53	0.40
26:N:14:LEU:HD11	26:N:101:ALA:HB3	2.03	0.40
19:g:103:TYR:O	27:o:85:GLN:NE2	2.55	0.40
19:g:194:THR:O	19:g:198:ALA:HB2	2.22	0.40
21:i:109:GLN:OE1	29:q:71:ASN:ND2	2.52	0.40
22:j:146:GLN:HG2	22:j:154:HIS:HB3	2.03	0.40
22:j:200:GLN:HB3	22:j:201:SER:H	1.67	0.40
23:k:177:ALA:O	23:k:181:LEU:HB2	2.20	0.40
24:l:205:LEU:HB3	24:l:233:LEU:HD11	2.03	0.40
25:m:217:GLY:N	25:m:220:THR:OG1	2.54	0.40
1:U:32:ASN:HB3	2:V:232:HIS:HB2	2.04	0.40
1:U:44:LYS:HD3	1:U:47:VAL:HG21	2.02	0.40
1:U:220:LEU:HA	1:U:223:LEU:HB3	2.03	0.40
2:V:166:TYR:OH	2:V:216:ARG:HD2	2.21	0.40
6:Z:34:ARG:HH11	6:Z:58:PHE:HE2	1.68	0.40
10:d:167:ILE:O	10:d:171:LEU:HG	2.22	0.40
12:f:637:LYS:HE3	12:f:674:THR:N	2.36	0.40
18:F:305:GLU:HA	18:F:308:ARG:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:14:THR:OG1	19:G:128:ASN:O	2.39	0.40
19:G:49:VAL:HG22	19:G:219:VAL:HG23	2.02	0.40
22:J:109:ARG:O	22:J:113:SER:OG	2.38	0.40
22:J:185:ASP:HA	22:J:188:ILE:HD12	2.03	0.40
23:K:49:ALA:HB2	23:K:217:LEU:HG	2.03	0.40
25:M:112:ALA:O	25:M:116:ALA:CB	2.69	0.40
31:S:92:LEU:HA	31:S:95:ILE:HD12	2.04	0.40
30:r:45:MET:HG3	30:r:52:CYS:HB2	2.04	0.40
2:V:255:LEU:HD22	2:V:291:TYR:HB3	2.02	0.40
3:W:228:ASN:HA	3:W:231:ILE:HG23	2.04	0.40
6:Z:82:PHE:HA	6:Z:85:VAL:HG12	2.03	0.40
6:Z:83:LYS:HD2	6:Z:87:ALA:HA	2.03	0.40
7:a:212:ASN:HD21	7:a:215:GLU:HB3	1.87	0.40
16:D:161:ASP:HA	16:D:221:HIS:CD2	2.57	0.40
19:G:144:ASP:O	19:G:148:GLY:N	2.51	0.40
21:I:34:CYS:O	21:I:163:CYS:HA	2.22	0.40
30:R:97:MET:HB3	30:R:116:SER:HB3	2.03	0.40
31:S:20:PHE:HA	31:S:198:VAL:O	2.22	0.40
25:m:43:ASP:N	25:m:43:ASP:OD1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	806/953 (85%)	732 (91%)	73 (9%)	1 (0%)	48	83
2	V	506/533 (95%)	434 (86%)	67 (13%)	5 (1%)	12	47
3	W	454/456 (100%)	389 (86%)	61 (13%)	4 (1%)	14	49
4	X	378/422 (90%)	360 (95%)	18 (5%)	0	100	100
5	Y	376/389 (97%)	346 (92%)	30 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Z	284/324 (88%)	252 (89%)	30 (11%)	2 (1%)	18	55
7	a	371/376 (99%)	331 (89%)	39 (10%)	1 (0%)	36	71
8	b	189/377 (50%)	171 (90%)	18 (10%)	0	100	100
9	c	285/309 (92%)	243 (85%)	40 (14%)	2 (1%)	18	55
10	d	255/349 (73%)	213 (84%)	41 (16%)	1 (0%)	30	66
11	e	36/70 (51%)	25 (69%)	10 (28%)	1 (3%)	4	24
12	f	887/908 (98%)	705 (80%)	170 (19%)	12 (1%)	9	39
13	A	392/433 (90%)	339 (86%)	50 (13%)	3 (1%)	16	52
14	B	382/429 (89%)	339 (89%)	35 (9%)	8 (2%)	5	30
15	C	359/389 (92%)	330 (92%)	27 (8%)	2 (1%)	21	58
16	D	378/418 (90%)	331 (88%)	38 (10%)	9 (2%)	4	27
17	E	373/403 (93%)	337 (90%)	36 (10%)	0	100	100
18	F	372/439 (85%)	339 (91%)	33 (9%)	0	100	100
19	G	238/245 (97%)	229 (96%)	9 (4%)	0	100	100
19	g	238/245 (97%)	229 (96%)	9 (4%)	0	100	100
20	H	230/233 (99%)	221 (96%)	9 (4%)	0	100	100
20	h	230/233 (99%)	221 (96%)	9 (4%)	0	100	100
21	I	248/260 (95%)	223 (90%)	25 (10%)	0	100	100
21	i	248/260 (95%)	226 (91%)	22 (9%)	0	100	100
22	J	237/247 (96%)	214 (90%)	19 (8%)	4 (2%)	7	35
22	j	237/247 (96%)	219 (92%)	16 (7%)	2 (1%)	16	52
23	K	224/240 (93%)	215 (96%)	9 (4%)	0	100	100
23	k	224/240 (93%)	215 (96%)	9 (4%)	0	100	100
24	L	236/268 (88%)	219 (93%)	16 (7%)	1 (0%)	30	66
24	l	236/268 (88%)	219 (93%)	16 (7%)	1 (0%)	30	66
25	M	238/254 (94%)	223 (94%)	15 (6%)	0	100	100
25	m	238/254 (94%)	223 (94%)	15 (6%)	0	100	100
26	N	189/238 (79%)	183 (97%)	6 (3%)	0	100	100
26	n	189/238 (79%)	183 (97%)	6 (3%)	0	100	100
27	O	218/276 (79%)	210 (96%)	8 (4%)	0	100	100
27	o	218/276 (79%)	210 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	P	202/204 (99%)	189 (94%)	13 (6%)	0	100	100
28	p	202/204 (99%)	190 (94%)	12 (6%)	0	100	100
29	Q	197/201 (98%)	187 (95%)	10 (5%)	0	100	100
29	q	197/201 (98%)	187 (95%)	10 (5%)	0	100	100
30	R	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
30	r	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
31	S	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
31	s	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
32	T	213/263 (81%)	203 (95%)	10 (5%)	0	100	100
32	t	213/263 (81%)	203 (95%)	10 (5%)	0	100	100
All	All	13243/14839 (89%)	12049 (91%)	1135 (9%)	59 (0%)	31	66

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	168	GLN
2	V	349	ARG
2	V	446	VAL
3	W	83	LEU
12	f	756	PRO
12	f	838	ARG
14	B	54	PRO
14	B	141	LYS
14	B	143	LEU
14	B	278	ALA
15	C	128	PRO
16	D	126	PRO
16	D	149	SER
24	L	226	ASP
2	V	317	PRO
12	f	281	ILE
12	f	476	THR
12	f	789	SER
13	A	312	ARG
15	C	91	PRO
16	D	125	LYS
16	D	370	ILE
22	J	202	GLY

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Mol	Chain	Res	Type
22	J	203	GLY
3	W	179	LYS
6	Z	224	HIS
11	e	56	LEU
12	f	118	ASN
12	f	773	LYS
12	f	809	ILE
14	B	87	PRO
16	D	127	ASN
16	D	154	LEU
22	J	200	GLN
3	W	138	VAL
10	d	199	PHE
12	f	282	PHE
14	B	53	THR
22	j	200	GLN
2	V	351	PRO
3	W	45	GLU
7	a	149	THR
12	f	649	HIS
12	f	839	PRO
13	A	109	PRO
13	A	400	ARG
14	B	88	LEU
16	D	367	PRO
22	j	198	VAL
24	l	226	ASP
6	Z	99	PRO
9	c	116	PRO
14	B	142	ASP
1	U	174	PRO
22	J	198	VAL
12	f	642	ALA
16	D	151	ILE
9	c	156	VAL
16	D	85	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	692/816 (85%)	683 (99%)	9 (1%)	61	72
2	V	415/459 (90%)	404 (97%)	11 (3%)	39	60
3	W	416/416 (100%)	402 (97%)	14 (3%)	32	54
4	X	327/362 (90%)	326 (100%)	1 (0%)	86	84
5	Y	334/344 (97%)	332 (99%)	2 (1%)	78	80
6	Z	257/295 (87%)	251 (98%)	6 (2%)	44	64
7	a	333/336 (99%)	333 (100%)	0	100	100
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	252/267 (94%)	246 (98%)	6 (2%)	43	63
10	d	231/293 (79%)	228 (99%)	3 (1%)	61	72
11	e	38/63 (60%)	35 (92%)	3 (8%)	11	32
12	f	744/763 (98%)	721 (97%)	23 (3%)	35	56
13	A	337/372 (91%)	333 (99%)	4 (1%)	63	73
14	B	338/376 (90%)	330 (98%)	8 (2%)	43	63
15	C	314/337 (93%)	311 (99%)	3 (1%)	68	76
16	D	333/366 (91%)	319 (96%)	14 (4%)	26	48
17	E	298/353 (84%)	297 (100%)	1 (0%)	86	84
18	F	296/379 (78%)	295 (100%)	1 (0%)	86	84
19	G	193/209 (92%)	192 (100%)	1 (0%)	81	81
19	g	193/209 (92%)	191 (99%)	2 (1%)	68	76
20	H	164/190 (86%)	164 (100%)	0	100	100
20	h	164/190 (86%)	164 (100%)	0	100	100
21	I	193/220 (88%)	192 (100%)	1 (0%)	81	81
21	i	193/220 (88%)	193 (100%)	0	100	100
22	J	154/210 (73%)	151 (98%)	3 (2%)	50	66
22	j	152/210 (72%)	151 (99%)	1 (1%)	76	79
23	K	186/202 (92%)	186 (100%)	0	100	100
23	k	186/202 (92%)	186 (100%)	0	100	100
24	L	198/229 (86%)	197 (100%)	1 (0%)	81	81
24	l	198/229 (86%)	197 (100%)	1 (0%)	81	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	M	192/211 (91%)	192 (100%)	0	100	100
25	m	192/211 (91%)	192 (100%)	0	100	100
26	N	148/180 (82%)	148 (100%)	0	100	100
26	n	148/180 (82%)	148 (100%)	0	100	100
27	O	177/227 (78%)	177 (100%)	0	100	100
27	o	177/227 (78%)	177 (100%)	0	100	100
28	P	173/173 (100%)	173 (100%)	0	100	100
28	p	173/173 (100%)	173 (100%)	0	100	100
29	Q	164/171 (96%)	164 (100%)	0	100	100
29	q	164/171 (96%)	164 (100%)	0	100	100
30	R	153/201 (76%)	153 (100%)	0	100	100
30	r	153/201 (76%)	153 (100%)	0	100	100
31	S	174/198 (88%)	174 (100%)	0	100	100
31	s	175/198 (88%)	175 (100%)	0	100	100
32	T	175/214 (82%)	175 (100%)	0	100	100
32	t	175/214 (82%)	175 (100%)	0	100	100
All	All	11009/12579 (88%)	10890 (99%)	119 (1%)	63	74

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	11	LEU
1	U	177	LEU
1	U	529	ILE
1	U	602	LEU
1	U	603	LEU
1	U	629	THR
1	U	689	ILE
1	U	775	LEU
1	U	913	ILE
2	V	163	VAL
2	V	167	LEU
2	V	308	THR
2	V	318	GLN
2	V	319	HIS
2	V	333	ILE

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Mol	Chain	Res	Type
2	V	345	ARG
2	V	346	LEU
2	V	348	PHE
2	V	437	ILE
2	V	442	ILE
3	W	49	SER
3	W	78	LYS
3	W	79	GLU
3	W	82	LEU
3	W	83	LEU
3	W	85	GLU
3	W	86	ASN
3	W	90	LEU
3	W	137	TYR
3	W	138	VAL
3	W	176	SER
3	W	177	MET
3	W	179	LYS
3	W	315	MET
4	X	80	ILE
5	Y	235	ASP
5	Y	287	LEU
6	Z	91	ILE
6	Z	146	ASP
6	Z	147	ASP
6	Z	191	ILE
6	Z	224	HIS
6	Z	227	ILE
9	c	69	VAL
9	c	148	ILE
9	c	151	VAL
9	c	196	LEU
9	c	197	ASN
9	c	251	LEU
10	d	122	LEU
10	d	178	ILE
10	d	200	PHE
11	e	55	GLN
11	e	56	LEU
11	e	57	ARG
12	f	344	VAL
12	f	573	ILE

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Mol	Chain	Res	Type
12	f	615	ILE
12	f	646	MET
12	f	649	HIS
12	f	652	VAL
12	f	672	LEU
12	f	679	LEU
12	f	712	LYS
12	f	755	ASP
12	f	759	LEU
12	f	773	LYS
12	f	786	GLN
12	f	788	MET
12	f	807	ARG
12	f	808	ASN
12	f	809	ILE
12	f	822	VAL
12	f	836	GLU
12	f	837	LEU
12	f	838	ARG
12	f	840	LEU
12	f	842	VAL
13	A	312	ARG
13	A	400	ARG
13	A	401	ARG
13	A	403	ILE
14	B	53	THR
14	B	59	ARG
14	B	125	THR
14	B	139	VAL
14	B	143	LEU
14	B	166	ASP
14	B	170	LEU
14	B	277	HIS
15	C	89	VAL
15	C	90	HIS
15	C	109	THR
16	D	85	ILE
16	D	88	VAL
16	D	89	ILE
16	D	125	LYS
16	D	129	SER
16	D	149	SER

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Mol	Chain	Res	Type
16	D	150	SER
16	D	151	ILE
16	D	231	VAL
16	D	354	LEU
16	D	356	GLU
16	D	368	ASP
16	D	369	LYS
16	D	370	ILE
17	E	138	LEU
18	F	217	ILE
19	G	222	VAL
21	I	228	LEU
22	J	53	LEU
22	J	159	ASN
22	J	200	GLN
24	L	161	ILE
19	g	221	THR
19	g	222	VAL
22	j	159	ASN
24	l	161	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (208) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	111	GLN
1	U	241	ASN
1	U	345	ASN
1	U	355	ASN
1	U	362	ASN
1	U	377	HIS
1	U	415	HIS
1	U	595	ASN
1	U	647	HIS
1	U	685	GLN
1	U	721	HIS
1	U	768	GLN
2	V	78	HIS
2	V	242	HIS
2	V	247	GLN
2	V	427	GLN
2	V	459	GLN
2	V	487	HIS

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Mol	Chain	Res	Type
3	W	106	GLN
3	W	203	GLN
3	W	235	GLN
3	W	236	HIS
3	W	283	GLN
3	W	399	ASN
3	W	430	GLN
4	X	213	GLN
4	X	333	GLN
5	Y	306	GLN
5	Y	367	GLN
6	Z	104	ASN
6	Z	109	ASN
6	Z	202	ASN
6	Z	225	GLN
6	Z	243	GLN
6	Z	277	ASN
6	Z	278	ASN
7	a	9	GLN
7	a	18	GLN
7	a	35	HIS
7	a	40	GLN
7	a	164	GLN
7	a	193	GLN
7	a	212	ASN
7	a	231	GLN
7	a	249	GLN
7	a	258	GLN
7	a	267	GLN
7	a	288	HIS
7	a	290	GLN
7	a	332	HIS
7	a	337	GLN
7	a	345	GLN
7	a	370	GLN
8	b	105	HIS
8	b	142	ASN
9	c	30	GLN
9	c	44	HIS
9	c	113	HIS
9	c	130	GLN
9	c	164	ASN

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Mol	Chain	Res	Type
9	c	166	ASN
9	c	180	ASN
9	c	197	ASN
9	c	232	GLN
9	c	241	ASN
9	c	254	ASN
9	c	274	ASN
9	c	278	GLN
9	c	298	GLN
10	d	141	GLN
10	d	229	GLN
11	e	6	GLN
12	f	12	GLN
12	f	14	GLN
12	f	43	GLN
12	f	112	ASN
12	f	273	ASN
12	f	291	GLN
12	f	378	ASN
12	f	382	ASN
12	f	396	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	715	HIS
12	f	737	ASN
12	f	747	GLN
12	f	752	HIS
12	f	786	GLN
12	f	826	GLN
12	f	848	GLN
13	A	44	GLN
13	A	54	GLN
13	A	60	ASN
13	A	85	GLN
13	A	293	ASN
13	A	304	ASN
13	A	353	HIS
14	B	81	ASN
14	B	154	HIS
14	B	241	ASN
14	B	277	HIS

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Mol	Chain	Res	Type
14	B	314	ASN
15	C	36	ASN
15	C	53	ASN
15	C	64	GLN
15	C	67	GLN
15	C	90	HIS
15	C	221	GLN
16	D	67	ASN
16	D	98	GLN
16	D	133	HIS
16	D	173	GLN
16	D	221	HIS
16	D	222	HIS
16	D	237	GLN
16	D	257	ASN
16	D	312	ASN
16	D	340	GLN
16	D	353	ASN
16	D	380	GLN
17	E	75	ASN
17	E	280	ASN
18	F	83	ASN
18	F	184	GLN
18	F	208	HIS
18	F	316	GLN
18	F	380	ASN
18	F	417	HIS
19	G	12	HIS
19	G	33	ASN
19	G	68	HIS
19	G	128	ASN
20	H	63	HIS
20	H	88	HIS
20	H	102	GLN
21	I	53	HIS
21	I	220	ASN
22	J	85	ASN
22	J	92	GLN
22	J	116	GLN
22	J	120	GLN
22	J	154	HIS
22	J	159	ASN

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Mol	Chain	Res	Type
22	J	200	GLN
22	J	205	ASN
23	K	23	GLN
23	K	224	GLN
24	L	90	GLN
24	L	146	GLN
25	M	221	ASN
26	N	28	ASN
26	N	110	GLN
26	N	154	GLN
26	N	158	ASN
27	O	62	ASN
27	O	91	GLN
27	O	165	ASN
28	P	61	GLN
29	Q	8	GLN
29	Q	82	ASN
29	Q	99	HIS
29	Q	132	HIS
30	R	38	ASN
32	T	2	GLN
32	T	61	GLN
32	T	65	GLN
32	T	69	GLN
19	g	33	ASN
19	g	68	HIS
19	g	92	GLN
19	g	128	ASN
20	h	63	HIS
20	h	88	HIS
20	h	95	GLN
20	h	102	GLN
20	h	109	GLN
21	i	30	HIS
21	i	53	HIS
21	i	220	ASN
22	j	85	ASN
22	j	122	ASN
22	j	205	ASN
23	k	23	GLN
23	k	224	GLN
24	l	90	GLN

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Mol	Chain	Res	Type
24	l	146	GLN
24	l	166	GLN
25	m	180	GLN
25	m	221	ASN
26	n	7	GLN
26	n	28	ASN
26	n	110	GLN
26	n	154	GLN
26	n	158	ASN
27	o	62	ASN
27	o	66	HIS
27	o	91	GLN
28	p	93	ASN
29	q	8	GLN
29	q	82	ASN
29	q	99	HIS
29	q	132	HIS
30	r	38	ASN
30	r	70	ASN
32	t	65	GLN
32	t	69	GLN
32	t	81	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	ATP	A	501	35	32,33,33	1.37	5 (15%)	48,52,52	1.86	9 (18%)
36	ADP	F	501	35	28,29,29	1.41	4 (14%)	43,45,45	1.85	9 (20%)
36	ADP	C	501	-	28,29,29	1.42	4 (14%)	43,45,45	1.85	9 (20%)
34	ATP	B	501	35	32,33,33	1.41	4 (12%)	48,52,52	1.77	9 (18%)
34	ATP	D	501	35	32,33,33	1.32	4 (12%)	48,52,52	1.85	8 (16%)
34	ATP	E	401	35	32,33,33	1.42	4 (12%)	48,52,52	1.77	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	ATP	A	501	35	-	6/22/38/38	0/3/3/3
36	ADP	F	501	35	-	11/16/32/32	0/3/3/3
36	ADP	C	501	-	-	4/16/32/32	0/3/3/3
34	ATP	B	501	35	-	3/22/38/38	0/3/3/3
34	ATP	D	501	35	-	4/22/38/38	0/3/3/3
34	ATP	E	401	35	-	5/22/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	E	401	ATP	C5-C4	4.76	1.47	1.39
36	C	501	ADP	C5-C4	4.75	1.47	1.39
34	B	501	ATP	C5-C4	4.73	1.47	1.39
36	F	501	ADP	C5-C4	4.71	1.47	1.39
34	D	501	ATP	C5-C4	4.57	1.47	1.39
34	A	501	ATP	C5-C4	4.47	1.47	1.39
36	C	501	ADP	C5-C6	2.76	1.48	1.41
34	E	401	ATP	C5-C6	2.76	1.48	1.41
34	B	501	ATP	C5-C6	2.76	1.48	1.41
36	F	501	ADP	C5-C6	2.74	1.48	1.41
34	A	501	ATP	C5-N7	-2.73	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	D	501	ATP	C5-C6	2.64	1.48	1.41
34	A	501	ATP	C5-C6	2.61	1.48	1.41
34	D	501	ATP	C5-N7	-2.41	1.34	1.39
36	C	501	ADP	C8-N7	2.40	1.36	1.31
34	E	401	ATP	C8-N7	2.40	1.36	1.31
34	B	501	ATP	C8-N7	2.38	1.36	1.31
36	F	501	ADP	C8-N7	2.33	1.36	1.31
34	E	401	ATP	C5-N7	-2.28	1.34	1.39
34	D	501	ATP	C8-N7	2.24	1.36	1.31
36	C	501	ADP	C5-N7	-2.24	1.35	1.39
34	B	501	ATP	C5-N7	-2.20	1.35	1.39
36	F	501	ADP	C5-N7	-2.18	1.35	1.39
34	A	501	ATP	C8-N9	-2.02	1.34	1.37
34	A	501	ATP	C8-N7	2.01	1.35	1.31

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	A	501	ATP	C5-C4-N3	-6.35	117.98	126.72
34	D	501	ATP	C5-C4-N3	-6.24	118.12	126.72
36	F	501	ADP	C5-C4-N3	-5.84	118.67	126.72
36	C	501	ADP	C5-C4-N3	-5.84	118.68	126.72
34	B	501	ATP	C5-C4-N3	-5.84	118.68	126.72
34	E	401	ATP	C5-C4-N3	-5.81	118.71	126.72
34	A	501	ATP	N3-C4-N9	5.25	136.10	127.17
34	D	501	ATP	N3-C4-N9	5.09	135.82	127.17
36	F	501	ADP	N3-C4-N9	4.61	135.02	127.17
36	C	501	ADP	N3-C4-N9	4.61	135.01	127.17
34	E	401	ATP	N3-C4-N9	4.59	134.98	127.17
34	B	501	ATP	N3-C4-N9	4.58	134.96	127.17
34	D	501	ATP	C2-N3-C4	3.92	121.41	111.83
34	A	501	ATP	C2-N3-C4	3.78	121.07	111.83
36	F	501	ADP	C2-N3-C4	3.71	120.89	111.83
34	B	501	ATP	C2-N3-C4	3.70	120.88	111.83
36	C	501	ADP	C2-N3-C4	3.69	120.83	111.83
34	E	401	ATP	C2-N3-C4	3.68	120.83	111.83
34	A	501	ATP	C4-C5-N7	-3.58	106.49	110.58
34	B	501	ATP	C4-C5-N7	-3.54	106.54	110.58
36	C	501	ADP	C4-C5-N7	-3.48	106.60	110.58
34	E	401	ATP	C4-C5-N7	-3.48	106.61	110.58
36	F	501	ADP	C4-C5-N7	-3.47	106.61	110.58
34	D	501	ATP	C4-C5-N7	-3.34	106.76	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	501	ATP	N3-C2-N1	-3.34	123.52	128.58
34	B	501	ATP	N3-C2-N1	-3.22	123.71	128.58
36	F	501	ADP	N3-C2-N1	-3.20	123.73	128.58
34	E	401	ATP	N3-C2-N1	-3.18	123.76	128.58
36	C	501	ADP	N3-C2-N1	-3.17	123.78	128.58
34	A	501	ATP	N3-C2-N1	-3.09	123.90	128.58
34	A	501	ATP	C4-N9-C8	3.00	108.89	105.74
34	A	501	ATP	C5-N7-C8	2.87	107.97	103.45
34	D	501	ATP	C4-N9-C8	2.72	108.60	105.74
36	C	501	ADP	C4-N9-C8	2.64	108.51	105.74
34	E	401	ATP	C4-N9-C8	2.60	108.47	105.74
34	B	501	ATP	C4-N9-C8	2.60	108.47	105.74
36	F	501	ADP	C4-N9-C8	2.58	108.45	105.74
34	D	501	ATP	C5-N7-C8	2.55	107.46	103.45
34	E	401	ATP	C5-N7-C8	2.55	107.46	103.45
34	B	501	ATP	C5-N7-C8	2.55	107.46	103.45
36	C	501	ADP	C5-N7-C8	2.55	107.45	103.45
36	F	501	ADP	C5-N7-C8	2.53	107.43	103.45
36	F	501	ADP	C3'-C2'-C1'	2.48	106.15	101.46
36	C	501	ADP	C3'-C2'-C1'	2.48	106.15	101.46
34	E	401	ATP	C3'-C2'-C1'	2.47	106.14	101.46
34	B	501	ATP	C3'-C2'-C1'	2.46	106.11	101.46
34	A	501	ATP	C3'-C2'-C1'	2.28	105.78	101.46
34	A	501	ATP	N9-C8-N7	-2.25	110.74	113.94
34	D	501	ATP	C3'-C2'-C1'	2.24	105.70	101.46
34	B	501	ATP	C6-C5-N7	2.12	136.17	132.09
34	E	401	ATP	C6-C5-N7	2.09	136.12	132.09
36	C	501	ADP	C6-C5-N7	2.08	136.09	132.09
36	F	501	ADP	C6-C5-N7	2.07	136.08	132.09

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	501	ATP	C5'-O5'-PA-O2A
34	B	501	ATP	PB-O3B-PG-O3G
34	E	401	ATP	PB-O3B-PG-O2G
36	C	501	ADP	C5'-O5'-PA-O2A
36	C	501	ADP	C5'-O5'-PA-O3A
36	F	501	ADP	C5'-O5'-PA-O3A
36	F	501	ADP	O4'-C4'-C5'-O5'
36	F	501	ADP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
34	A	501	ATP	O4'-C4'-C5'-O5'
34	E	401	ATP	O4'-C4'-C5'-O5'
34	D	501	ATP	O4'-C1'-N9-C4
36	F	501	ADP	PA-O3A-PB-O1B
34	D	501	ATP	O4'-C1'-N9-C8
34	E	401	ATP	C3'-C4'-C5'-O5'
36	F	501	ADP	C2'-C1'-N9-C8
34	A	501	ATP	C5'-O5'-PA-O1A
34	A	501	ATP	C5'-O5'-PA-O3A
36	C	501	ADP	C5'-O5'-PA-O1A
36	F	501	ADP	C5'-O5'-PA-O1A
34	E	401	ATP	C4'-C5'-O5'-PA
36	F	501	ADP	C2'-C1'-N9-C4
34	A	501	ATP	C3'-C4'-C5'-O5'
34	E	401	ATP	PB-O3B-PG-O1G
36	F	501	ADP	O4'-C1'-N9-C4
34	B	501	ATP	PA-O3A-PB-O1B
36	F	501	ADP	O4'-C1'-N9-C8
34	D	501	ATP	C2'-C1'-N9-C8
36	F	501	ADP	PA-O3A-PB-O2B
36	F	501	ADP	PA-O3A-PB-O3B
34	A	501	ATP	PA-O3A-PB-O1B
34	B	501	ATP	PA-O3A-PB-O2B
34	D	501	ATP	PA-O3A-PB-O2B
36	C	501	ADP	PB-O3A-PA-O2A

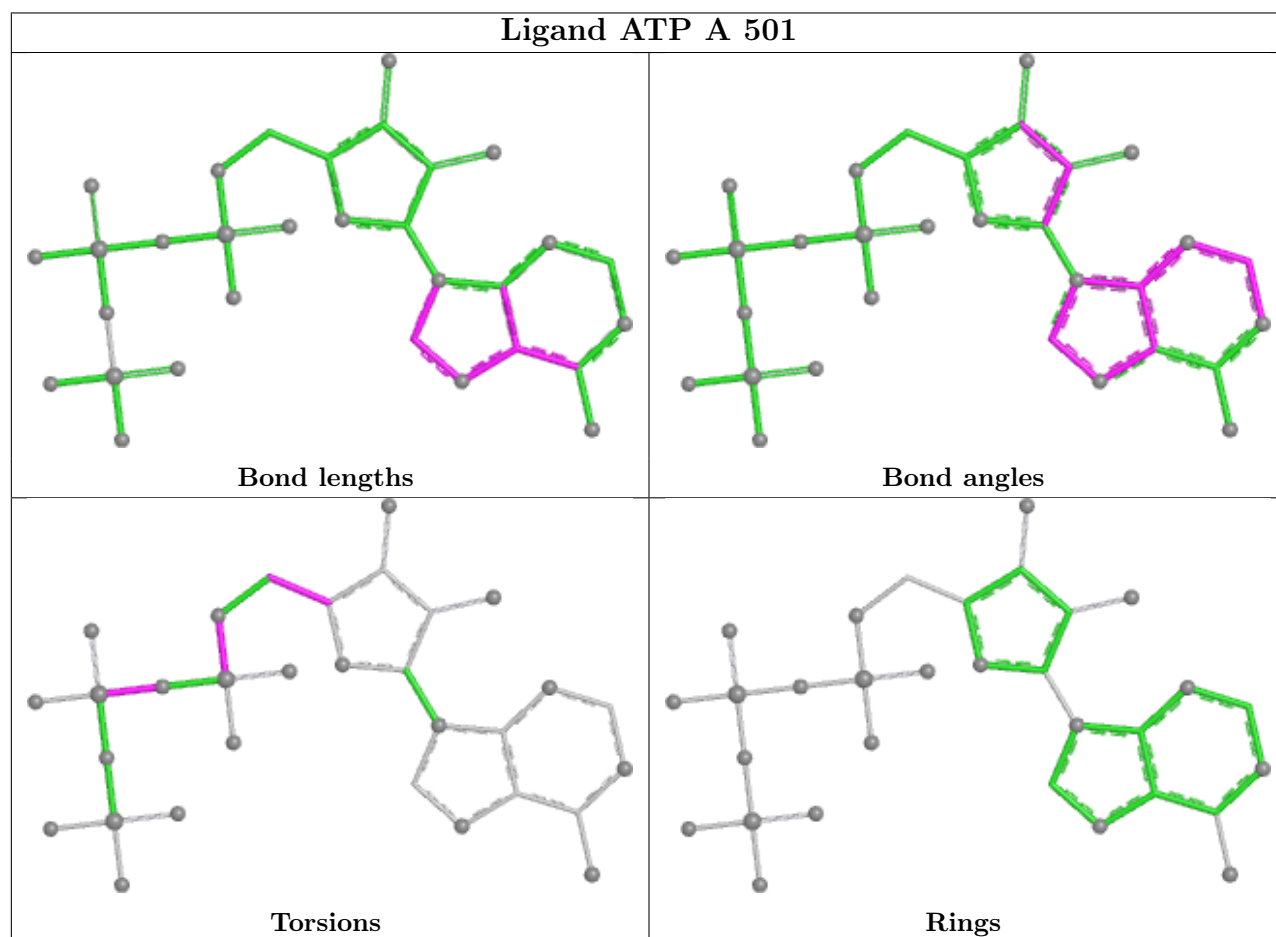
There are no ring outliers.

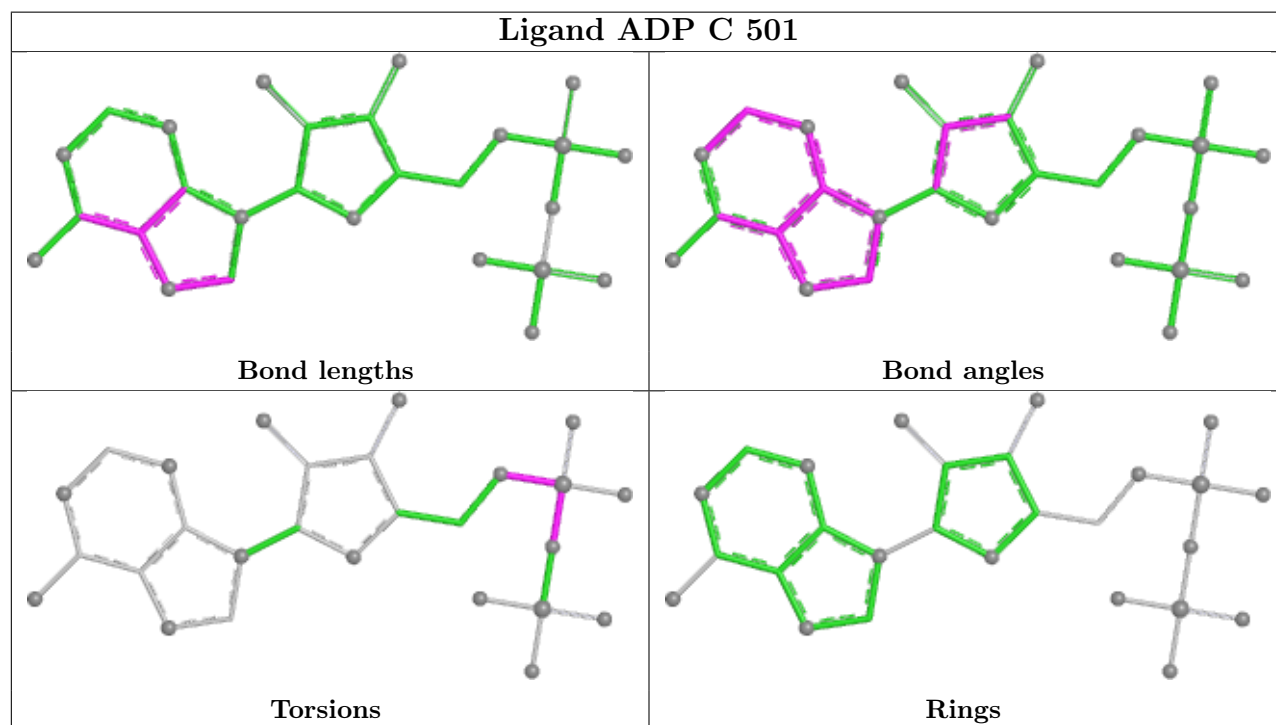
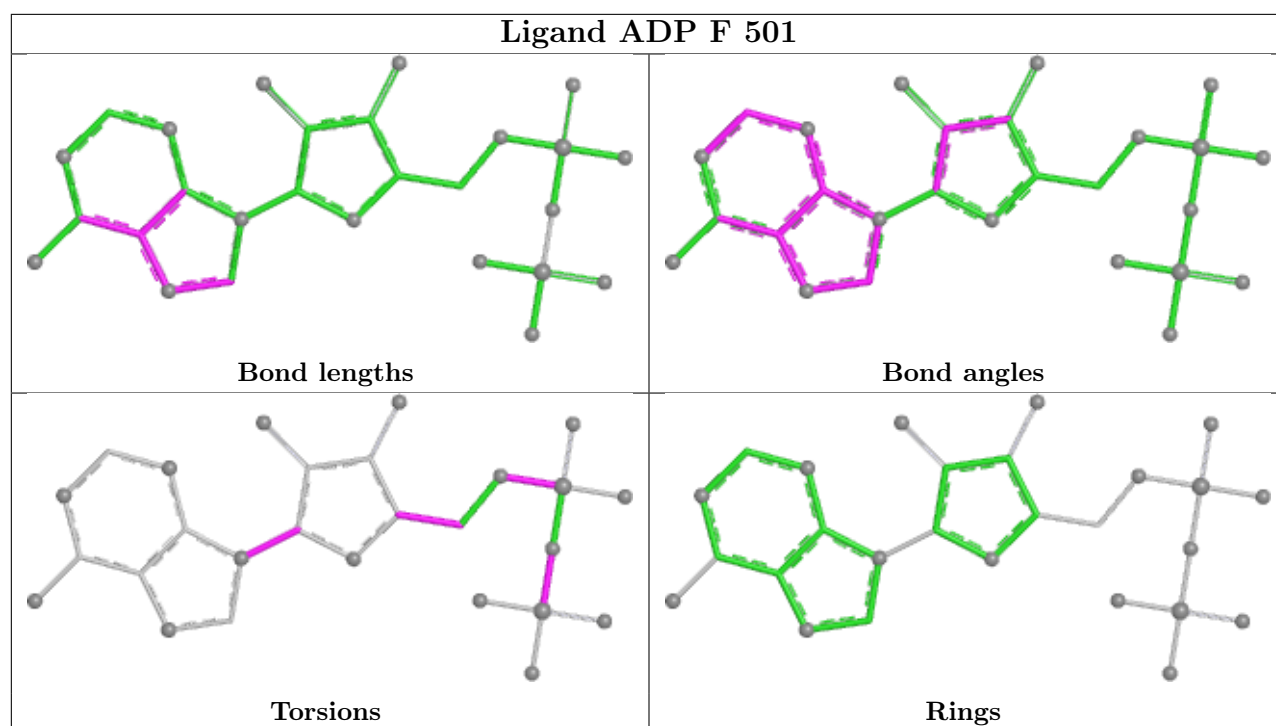
5 monomers are involved in 66 short contacts:

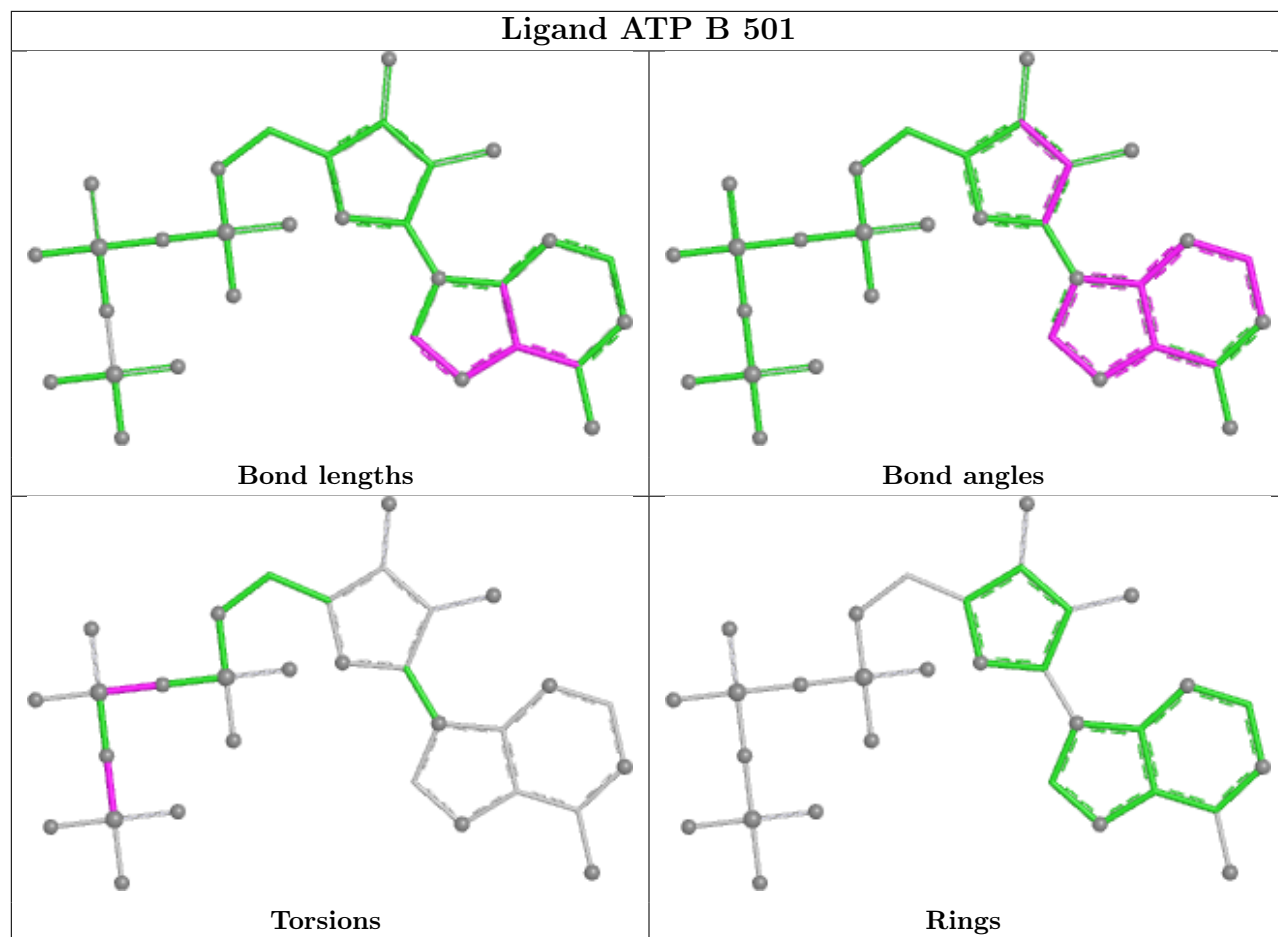
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	F	501	ADP	8	0
36	C	501	ADP	13	0
34	B	501	ATP	8	0
34	D	501	ATP	2	0
34	E	401	ATP	35	0

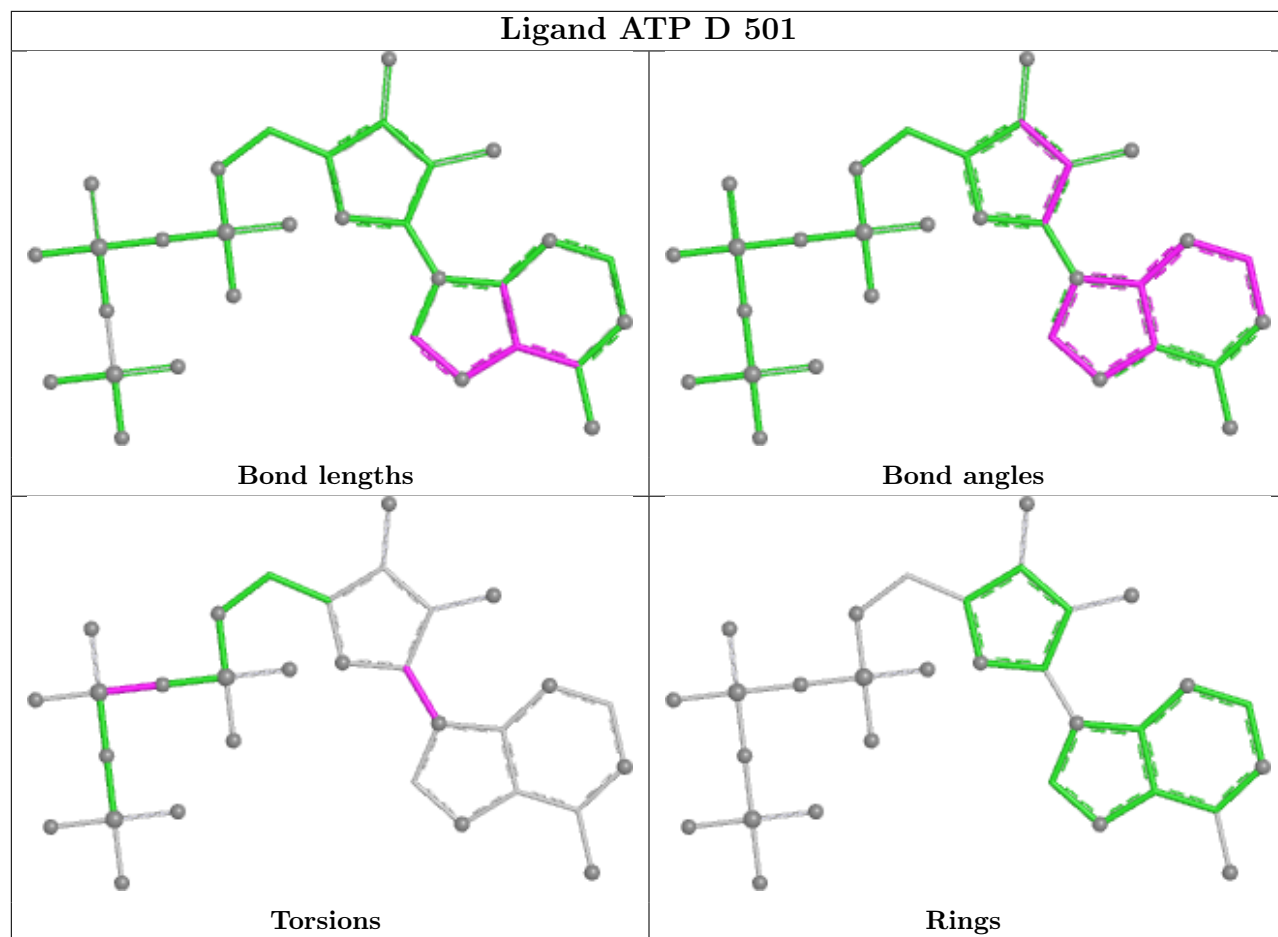
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

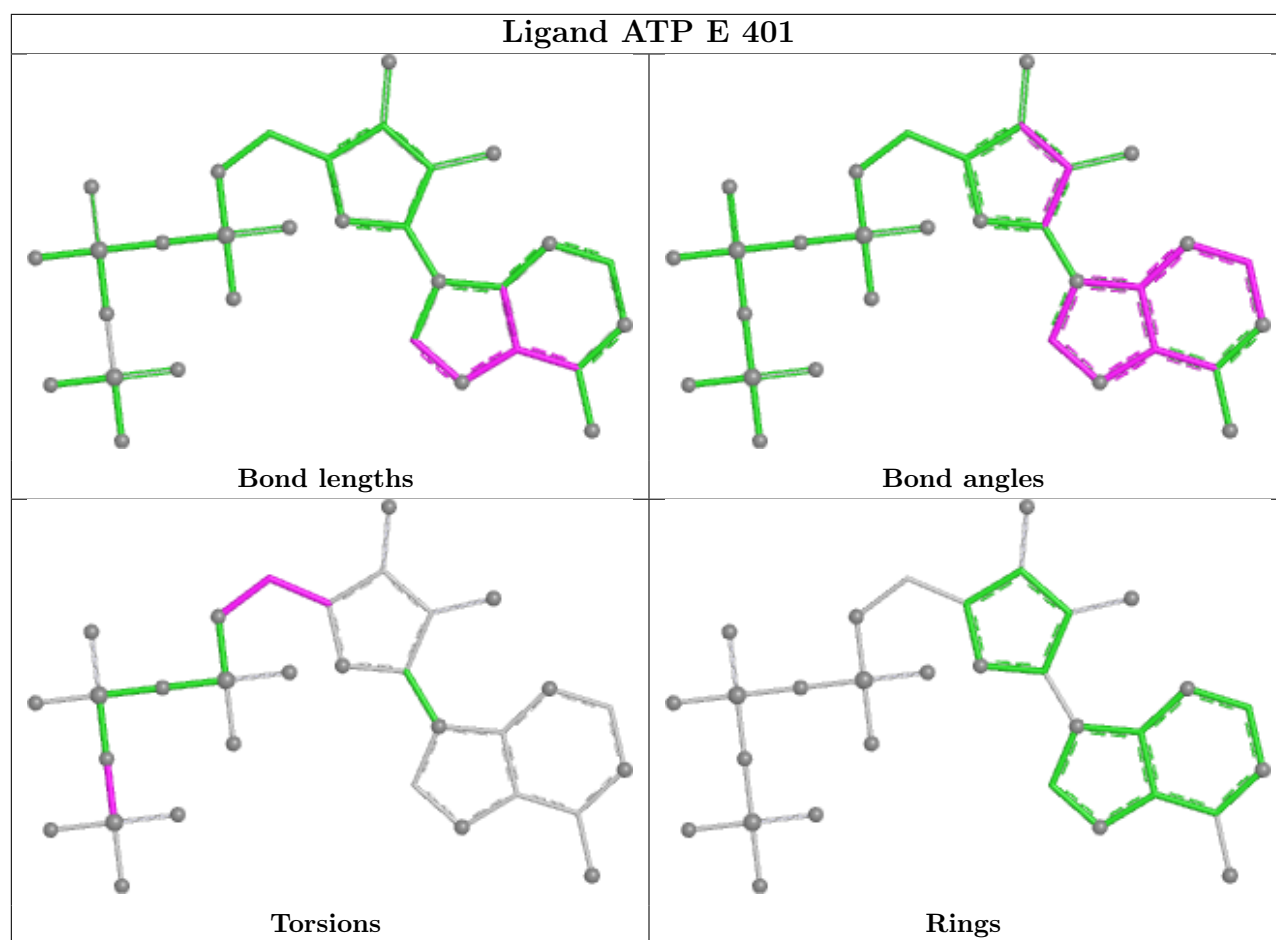
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

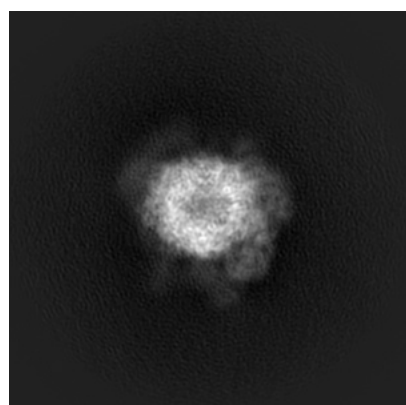
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14203. These allow visual inspection of the internal detail of the map and identification of artifacts.

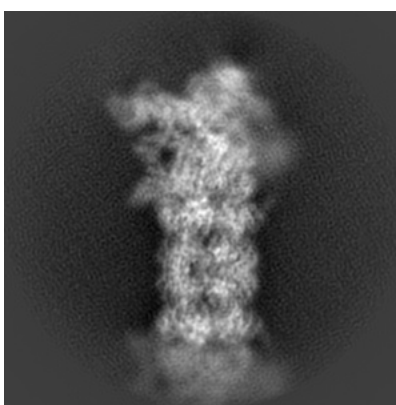
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

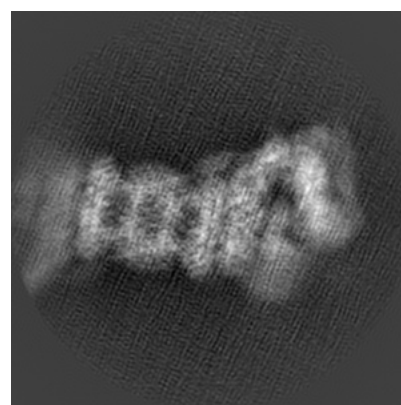
6.1.1 Primary map



X



Y

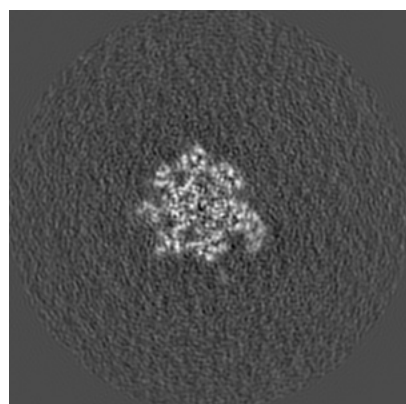


Z

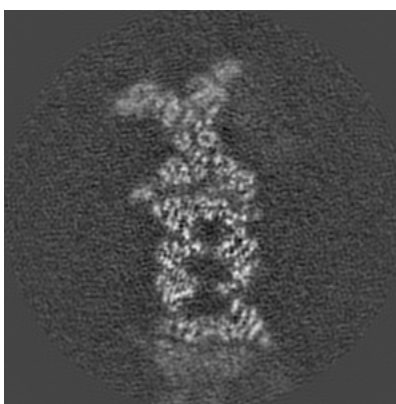
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

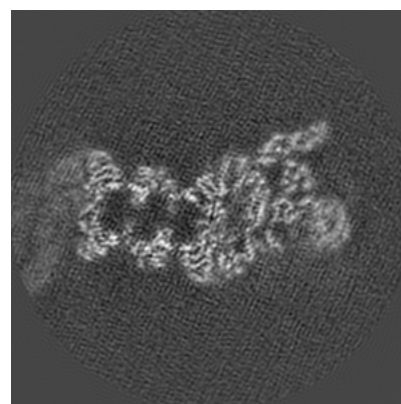
6.2.1 Primary map



X Index: 160



Y Index: 160

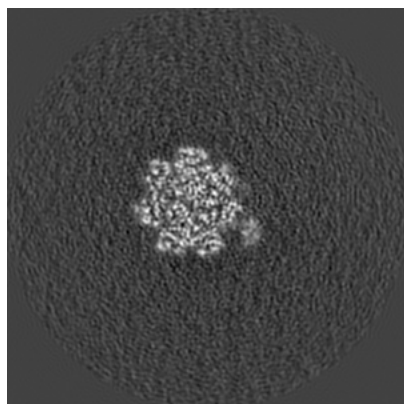


Z Index: 160

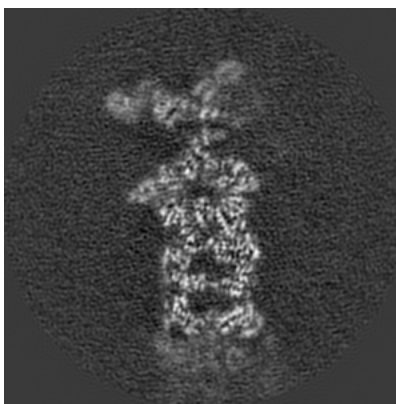
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

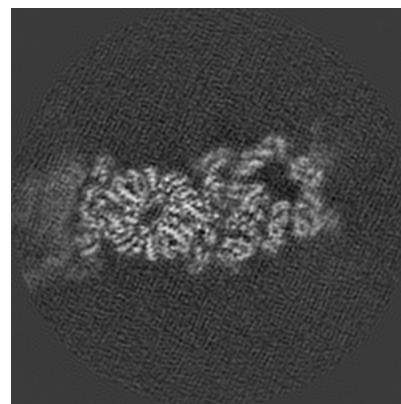
6.3.1 Primary map



X Index: 154



Y Index: 166

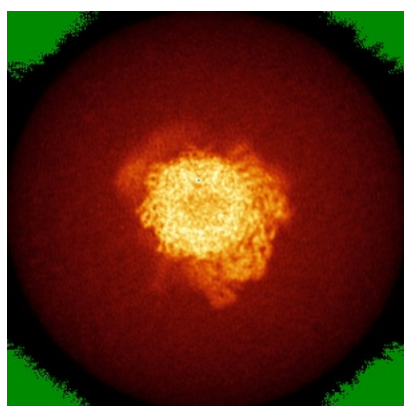


Z Index: 145

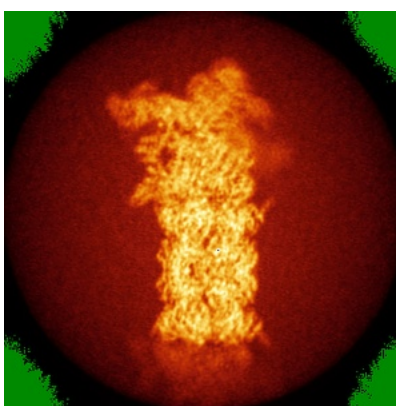
The images above show the largest variance slices of the map in three orthogonal directions.

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

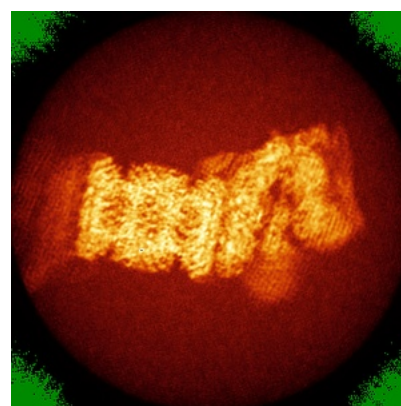
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

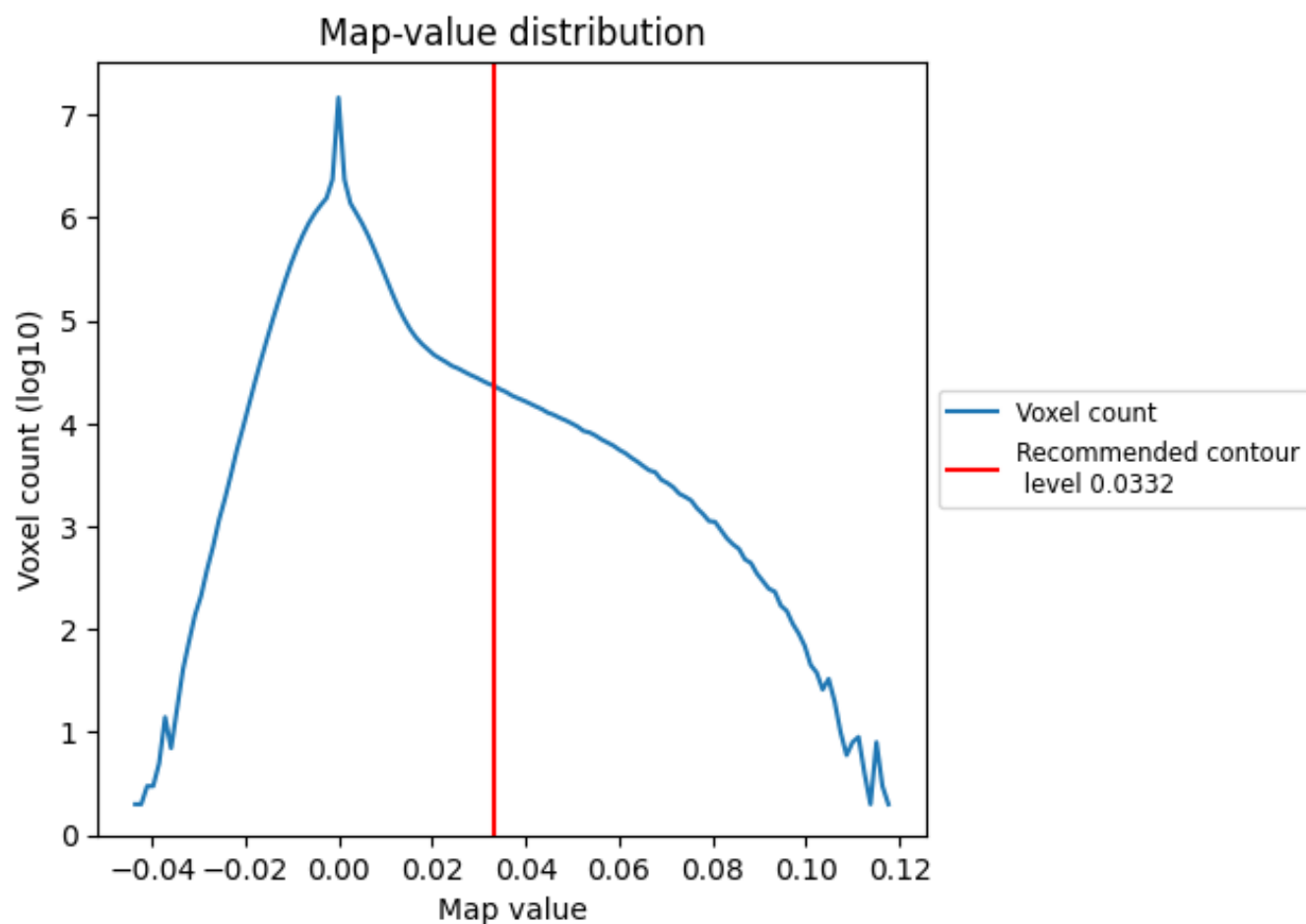
6.6 Mask visualisation

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

7 Map analysis [i](#)

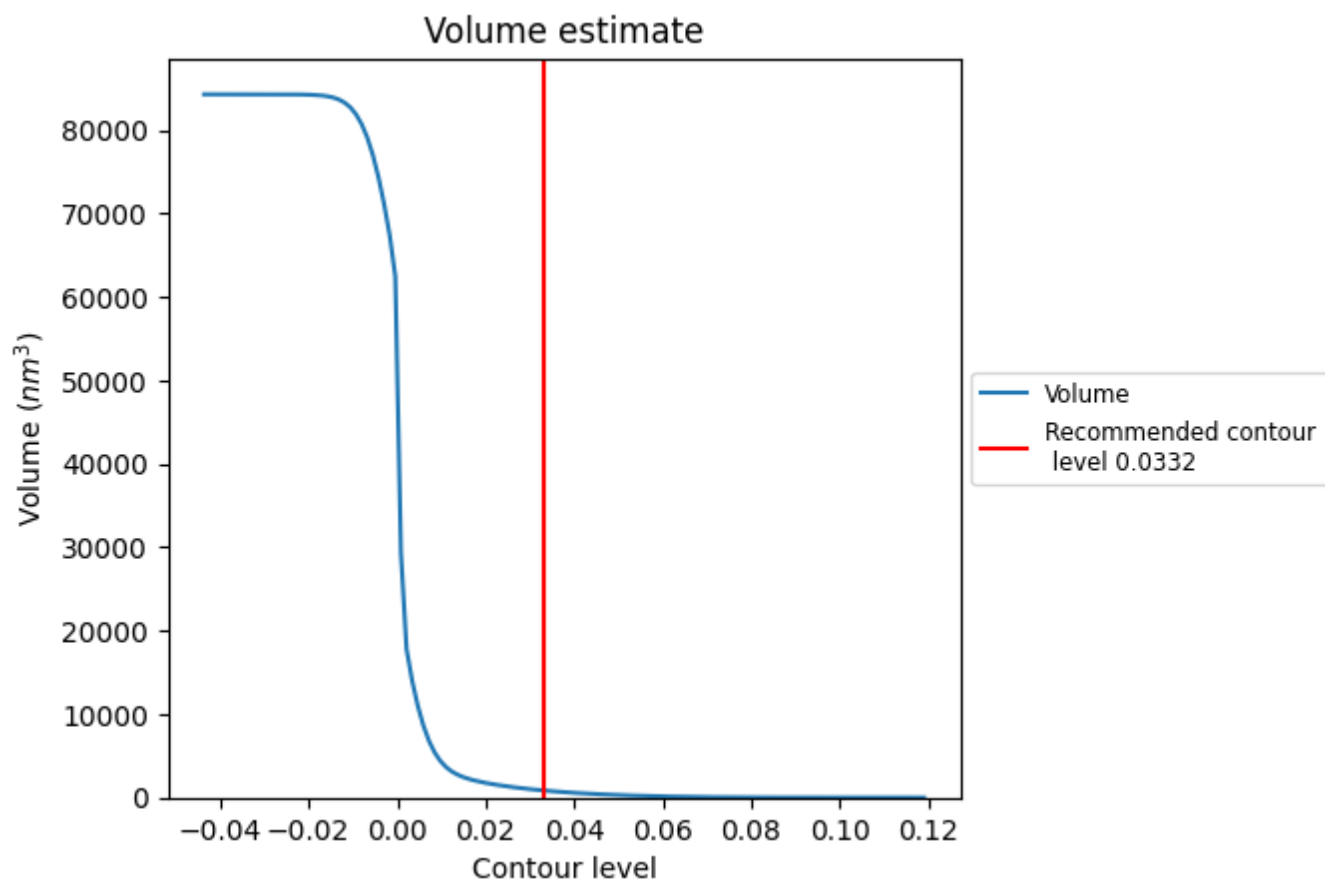
This section contains the results of statistical analysis of the map.

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.

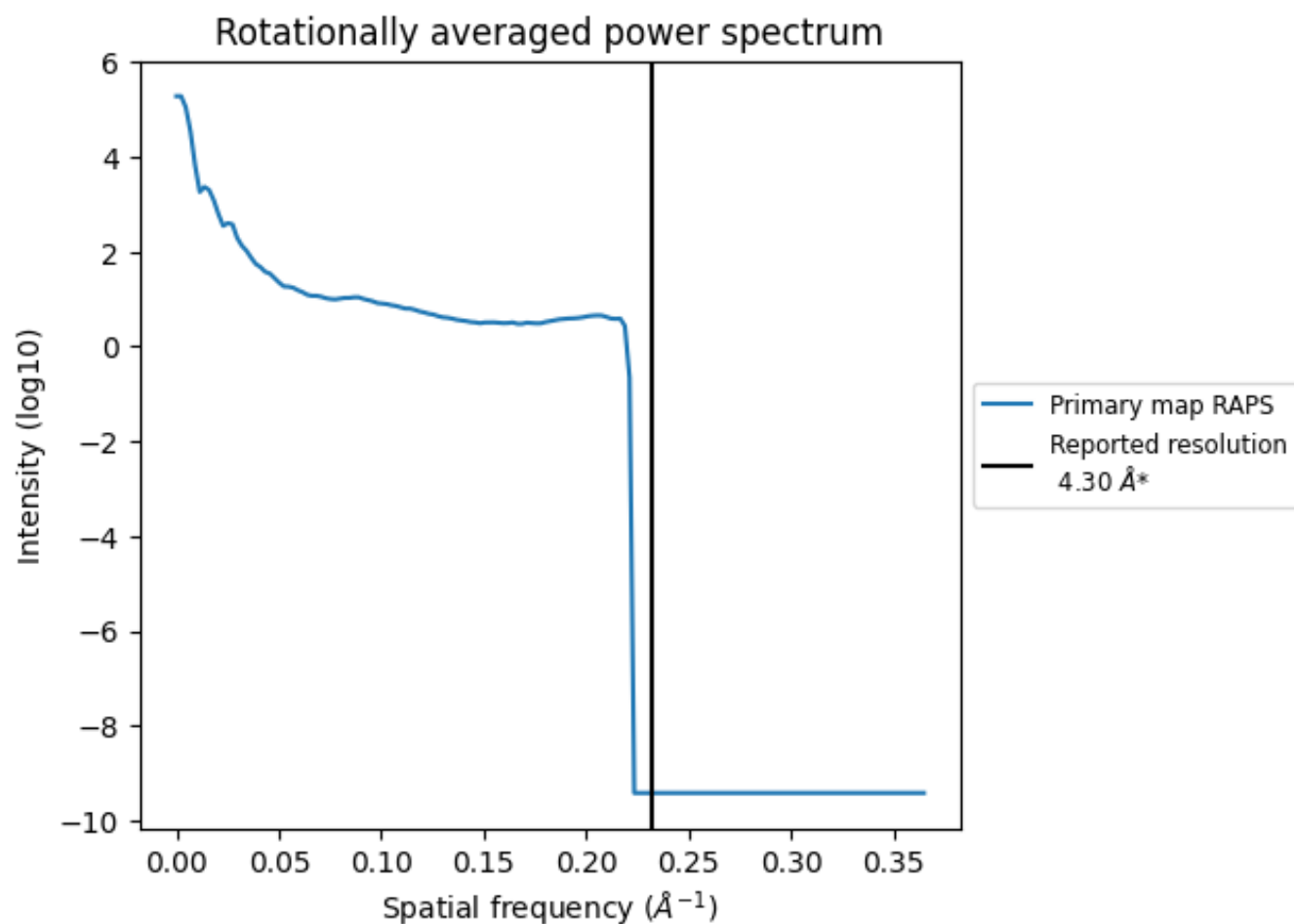
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 842 nm³; this corresponds to an approximate mass of 760 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 0.233 Å⁻¹

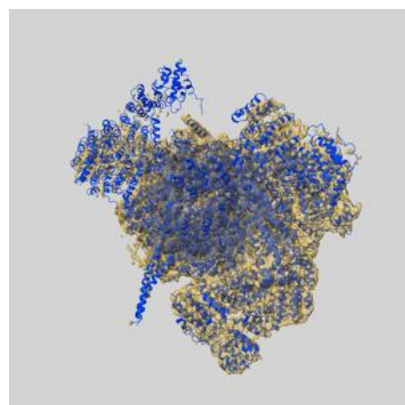
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

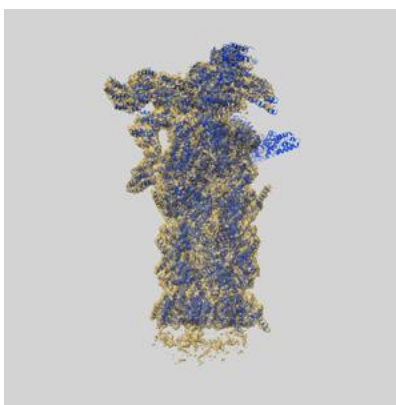
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14203 and PDB model 7QXU. Per-residue inclusion information can be found in section [3](#) on page [13](#).

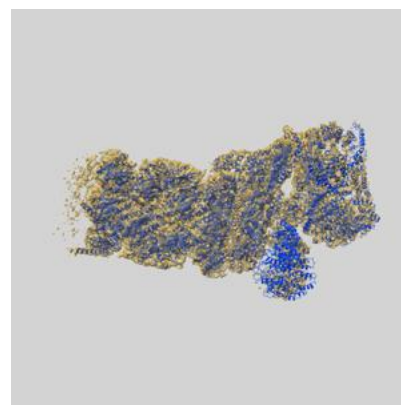
9.1 Map-model overlay [i](#)



X



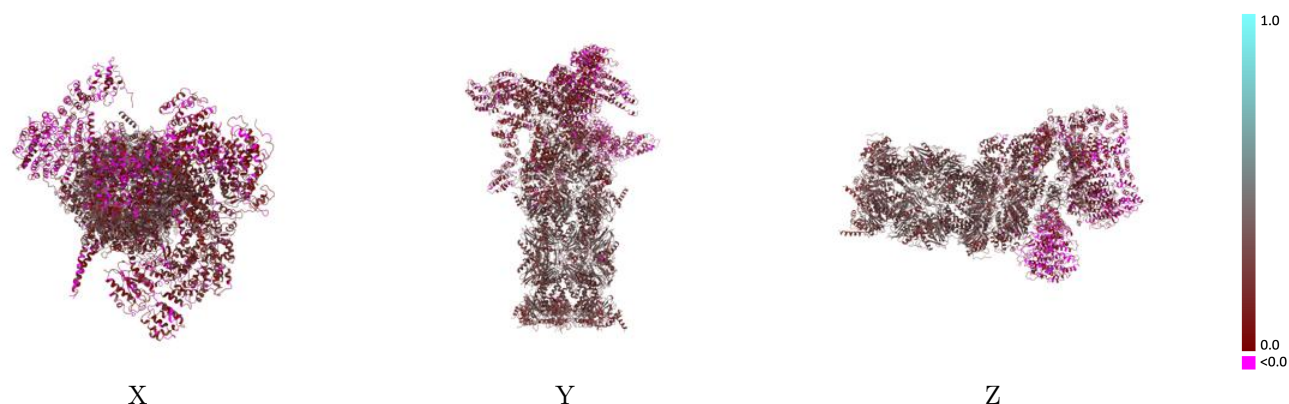
Y



Z

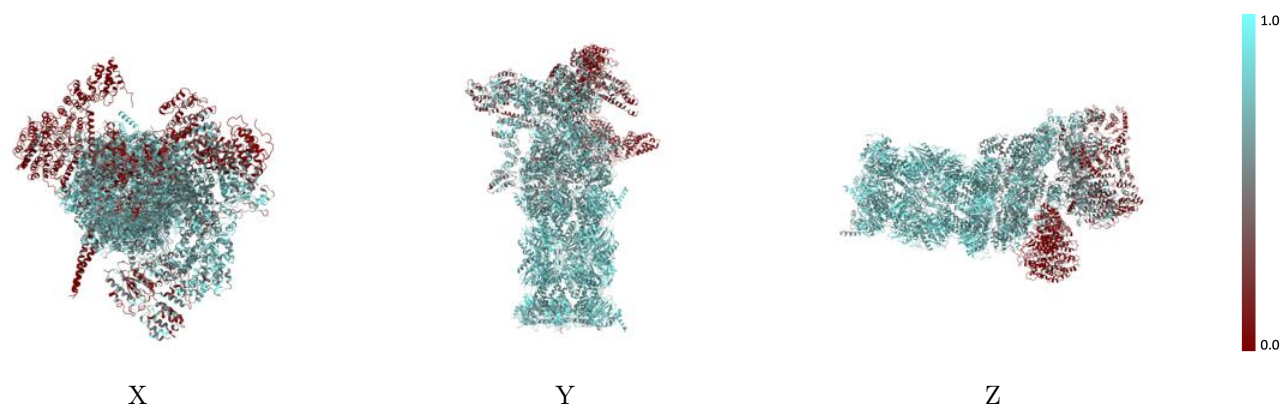
The images above show the 3D surface view of the map at the recommended contour level 0.0332 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



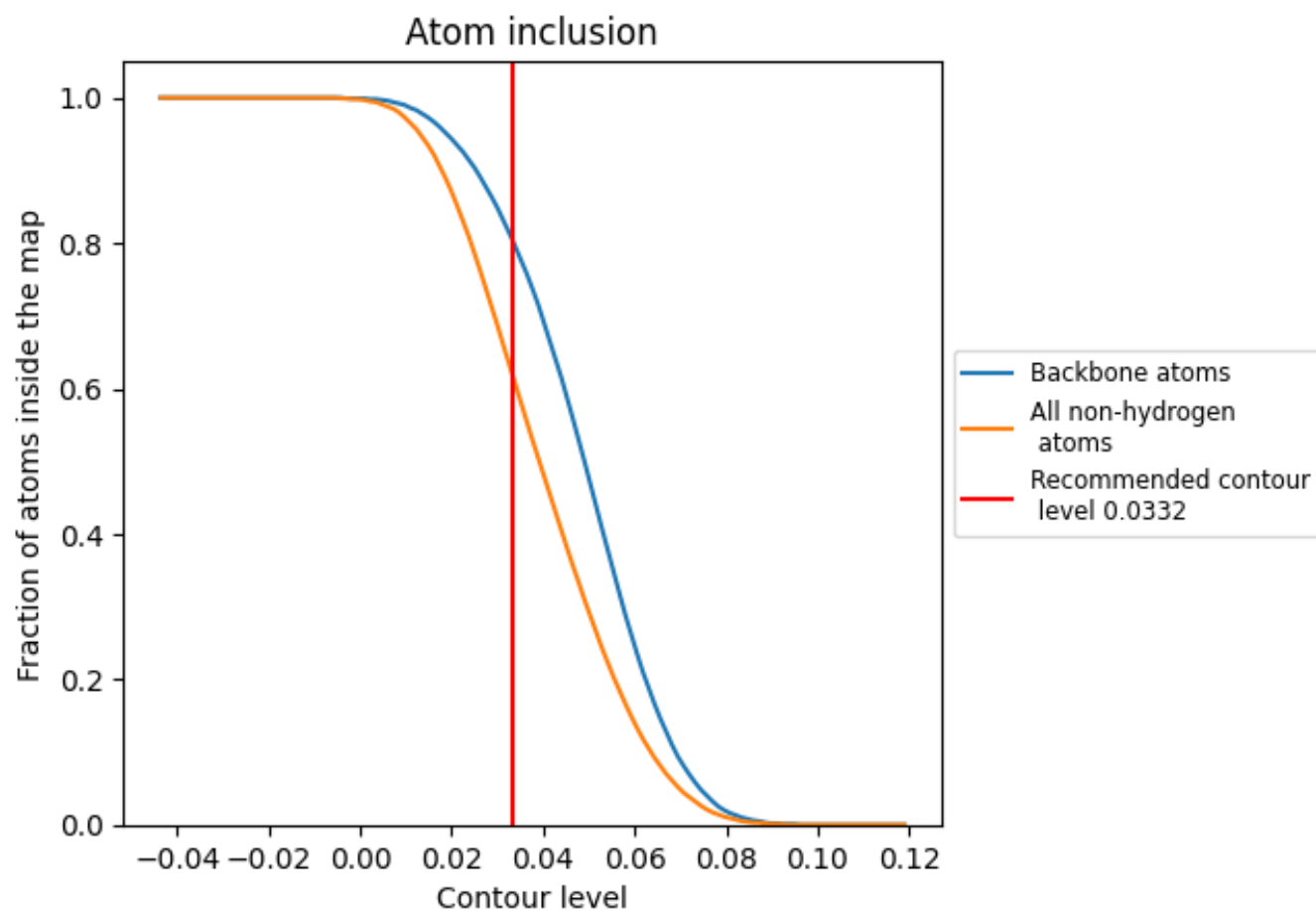
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0332).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 62% 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 (0.0332) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6210	 0.2330
A	 0.6320	 0.2630
B	 0.6190	 0.2390
C	 0.6810	 0.2610
D	 0.6450	 0.2480
E	 0.6690	 0.2490
F	 0.6630	 0.2680
G	 0.7730	 0.3080
H	 0.7870	 0.3120
I	 0.7810	 0.2920
J	 0.7960	 0.3020
K	 0.7800	 0.3080
L	 0.7890	 0.3080
M	 0.7630	 0.2980
N	 0.8200	 0.3230
O	 0.8000	 0.3180
P	 0.7850	 0.3160
Q	 0.7860	 0.3160
R	 0.8260	 0.3150
S	 0.7940	 0.3240
T	 0.8190	 0.3160
U	 0.3590	 0.0960
V	 0.3570	 0.1260
W	 0.6170	 0.1690
X	 0.5990	 0.2000
Y	 0.6810	 0.1890
Z	 0.5870	 0.1780
a	 0.5480	 0.1560
b	 0.3500	 0.1190
c	 0.6020	 0.2000
d	 0.2660	 0.1130
e	 0.3910	 0.0830
f	 0.0550	 0.0500
g	 0.7310	 0.2930
h	 0.7490	 0.2960



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Chain	Atom inclusion	Q-score
i	 0.7180	 0.2790
j	 0.7560	 0.2870
k	 0.7370	 0.2920
l	 0.7620	 0.2830
m	 0.7410	 0.3000
n	 0.7950	 0.3110
o	 0.8170	 0.3300
p	 0.7900	 0.3260
q	 0.7990	 0.3210
r	 0.8230	 0.3220
s	 0.7980	 0.3160
t	 0.8070	 0.3200