



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:27 AM UTC

PDB ID : 7QO3 / pdb_00007qo3
EMDB ID : EMD-14082
Title : Structure of the 26S proteasome-Ubp6 complex in the si state (Core Particle and Lid)
Authors : Hung, K.Y.S.; Klumpe, S.; Eisele, M.R.; Elsassner, S.; Geng, T.T.; Cheng, T.C.; Joshi, T.; Rudack, T.; Sakata, E.; Finley, D.
Deposited on : 2021-12-23
Resolution : 6.10 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:

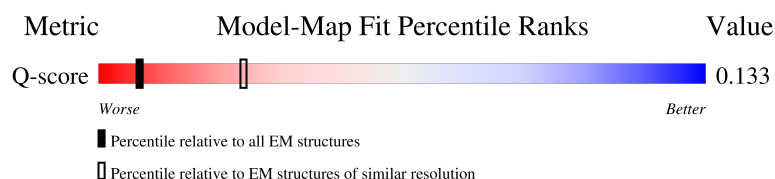
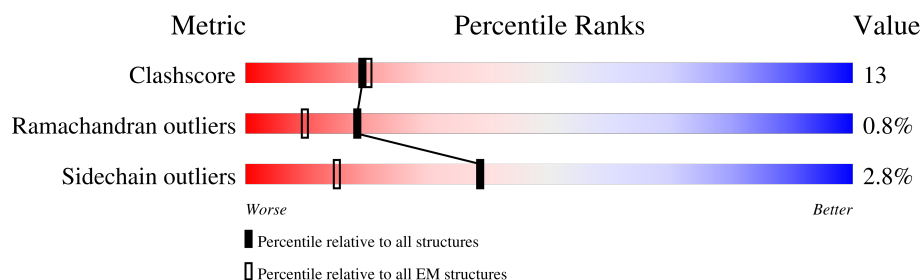
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 6.10 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	531 (5.60 - 6.60)

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

Mol	Chain	Length	Quality of chain
1	A	252	
1	a	252	
2	B	250	
2	b	250	

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Mol	Chain	Length	Quality of chain
3	C	258	
3	c	258	
4	D	254	
4	d	254	
5	E	260	
5	e	260	
6	F	234	
6	f	234	
7	G	288	
7	g	288	
8	l	215	
8	h	215	
9	2	261	
9	i	261	
10	3	205	
10	j	205	
11	4	198	
11	k	198	
12	5	287	
12	l	287	
13	6	241	
13	m	241	
14	7	266	
14	n	266	
15	W	268	

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Mol	Chain	Length	Quality of chain
16	V	306	
17	T	274	
18	X	156	
19	Y	89	
20	Z	993	
21	N	945	
22	S	523	
23	P	445	
24	Q	434	
25	R	429	
26	U	338	
27	O	393	

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 90281 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 Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		
1	A	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	249	Total	C	N	O	S	0	0
			1907	1214	314	376	3		
2	B	249	Total	C	N	O	S	0	0
			1907	1214	314	376	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		
3	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	236	Total	C	N	O	S	0	0
			1850	1158	323	365	4		
4	D	236	Total	C	N	O	S	0	0
			1850	1158	323	365	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	244	Total	C	N	O	S	0	0
			1882	1176	316	383	7		
5	E	244	Total	C	N	O	S	0	0
			1882	1176	316	383	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		
6	F	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		

- Molecule 7 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		
7	G	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		

- Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		
8	1	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		
9	2	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		
11	4	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
12	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
13	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		
14	7	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		

- Molecule 15 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	197	Total	C	N	O	S	0	0
			1534	962	269	300	3		

- Molecule 16 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	289	Total	C	N	O	S	0	0
			2274	1425	389	446	14		

- Molecule 17 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	266	Total	C	N	O	S	0	0
			2192	1405	349	432	6		

- Molecule 18 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	127	Total	C	N	O	S	0	0
			1032	664	169	195	4		

- Molecule 19 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y	89	Total	C	N	O	S	0	0
			731	447	119	164	1		

- Molecule 20 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	906	Total	C	N	O	S	0	0
			7005	4416	1150	1409	30		

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	832	Total	C	N	O	S	0	0
			6418	4078	1077	1238	25		

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	475	Total	C	N	O	S	0	0
			3894	2488	653	738	15		

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	440	Total	C	N	O	S	0	0
			3608	2297	604	697	10		

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	434	Total	C	N	O	S	0	0
			3499	2225	577	681	16		

- Molecule 25 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	405	Total	C	N	O	S	0	0
			3258	2077	535	636	10		

- Molecule 26 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	290	Total	C	N	O	S	0	0
			2306	1454	392	453	7		

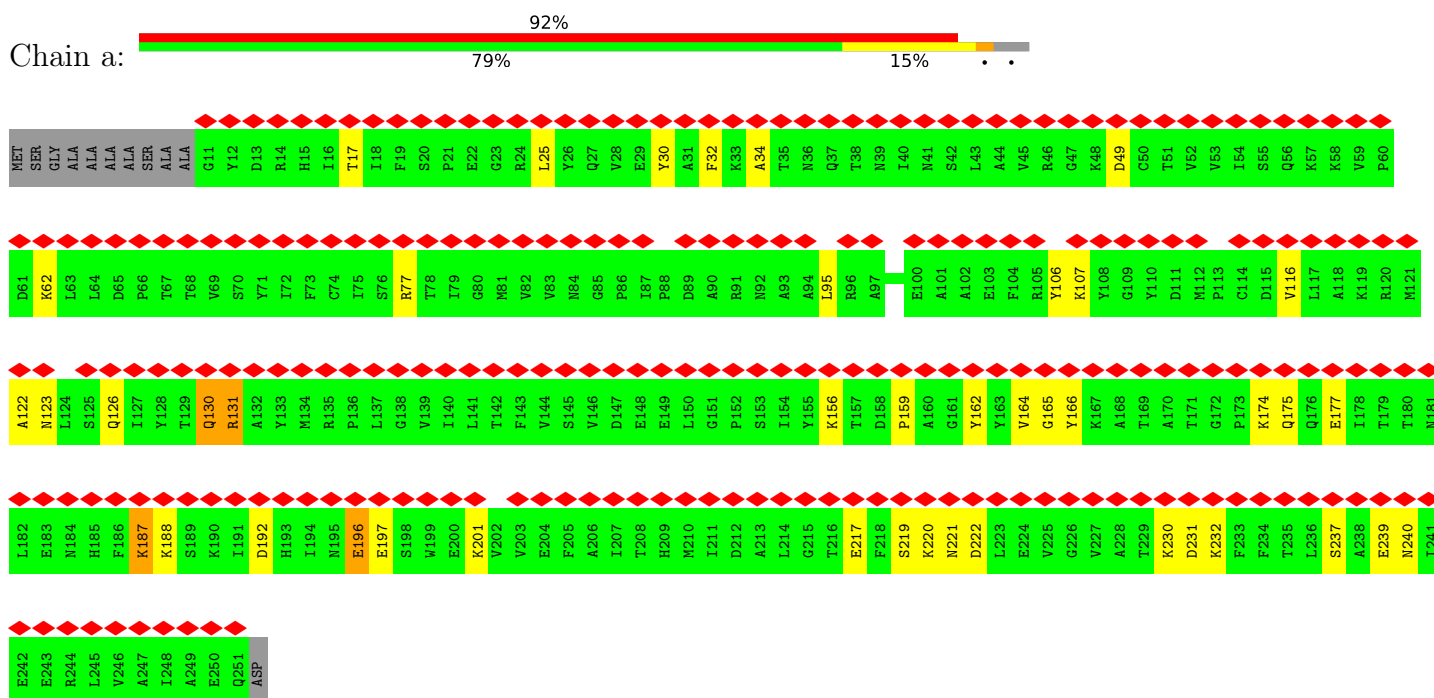
- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	O	388	Total	C	N	O	S	0	0
			3186	2051	519	608	8		

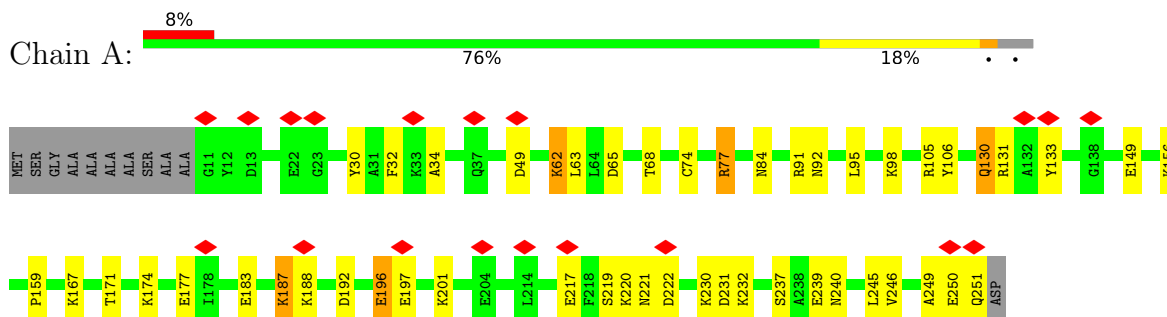
3 Residue-property plots

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

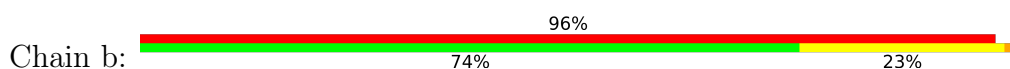
• Molecule 1: Proteasome subunit alpha type-1

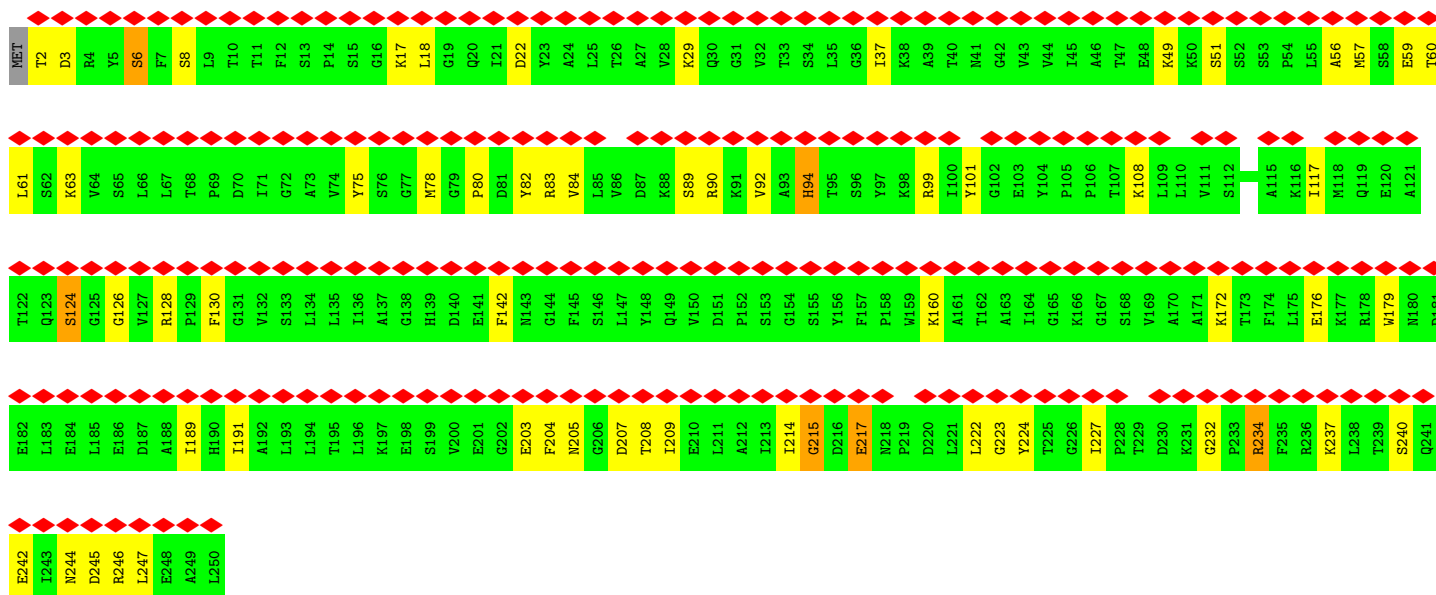


• Molecule 1: Proteasome subunit alpha type-1

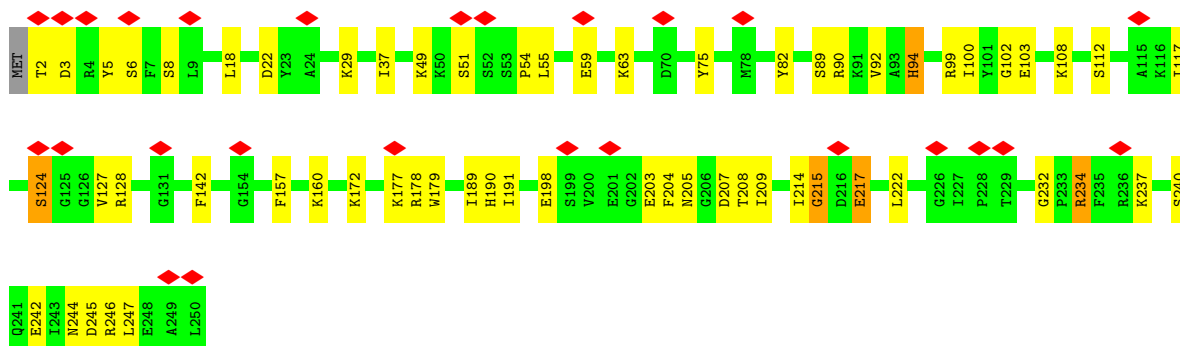
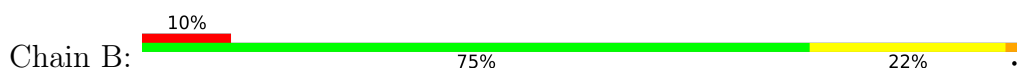


• Molecule 2: Proteasome subunit alpha type-2

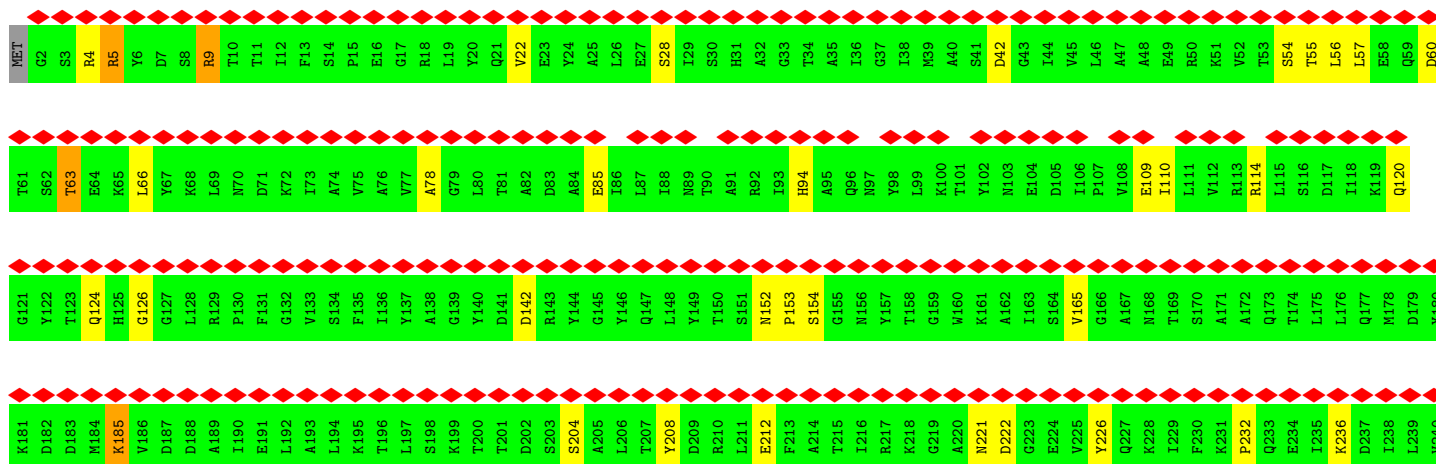
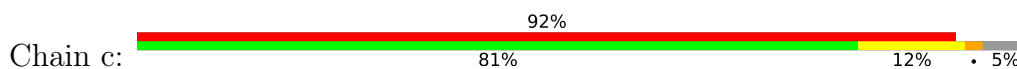


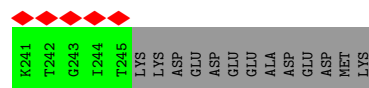


• Molecule 2: Proteasome subunit alpha type-2

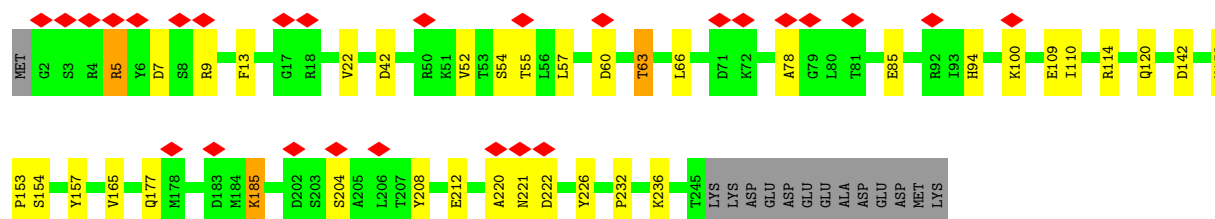
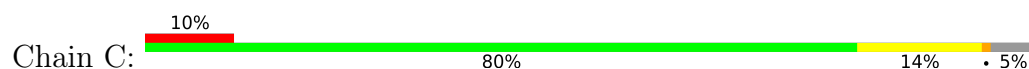


• Molecule 3: Proteasome subunit alpha type-3

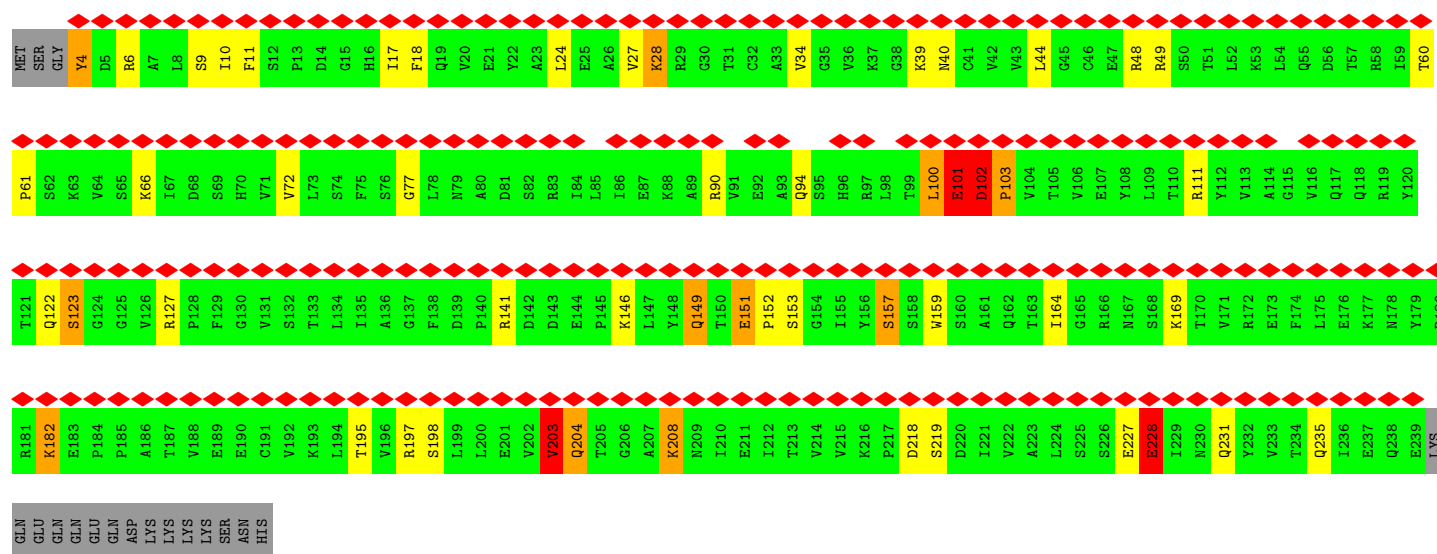
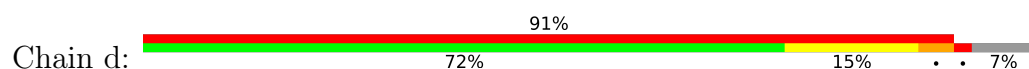




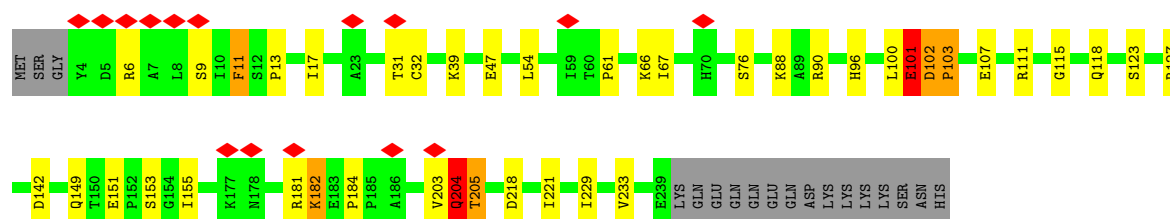
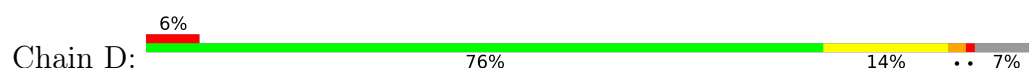
• Molecule 3: Proteasome subunit alpha type-3



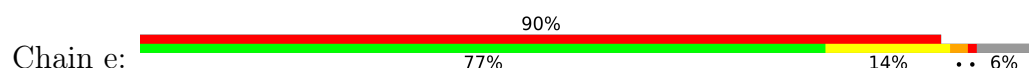
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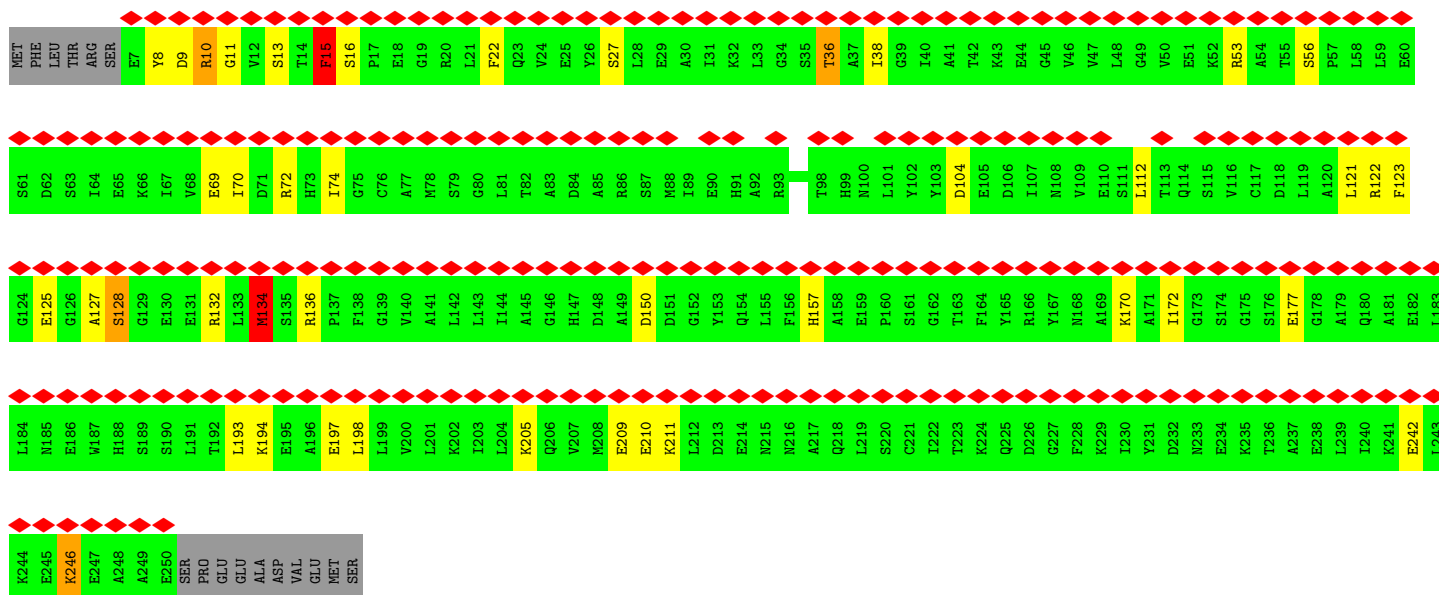


• Molecule 4: Proteasome subunit alpha type-4

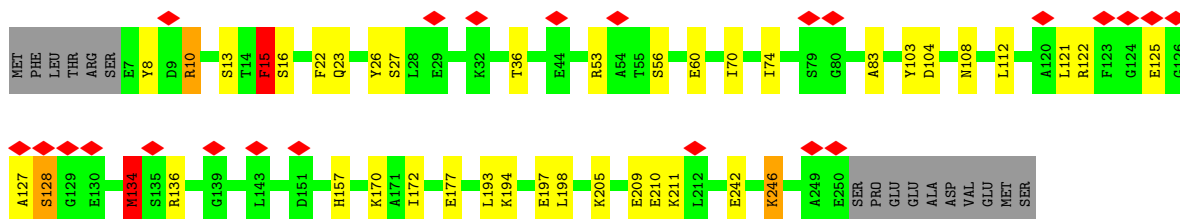
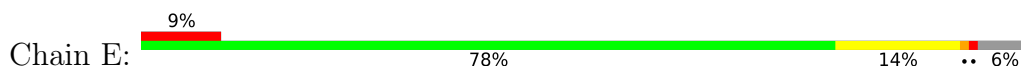


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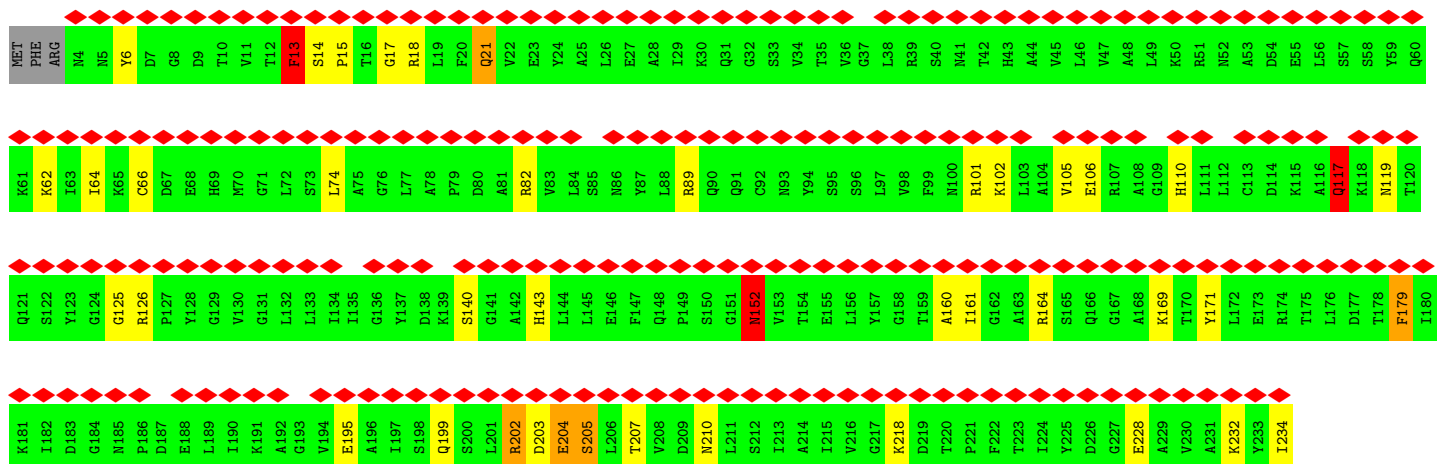
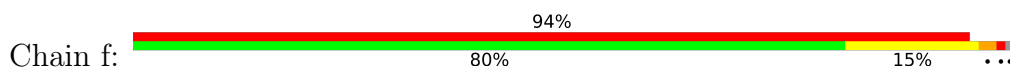




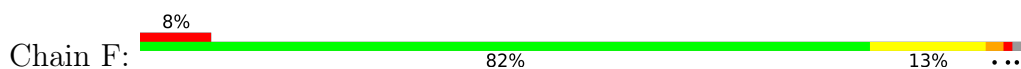
• Molecule 5: Proteasome subunit alpha type-5

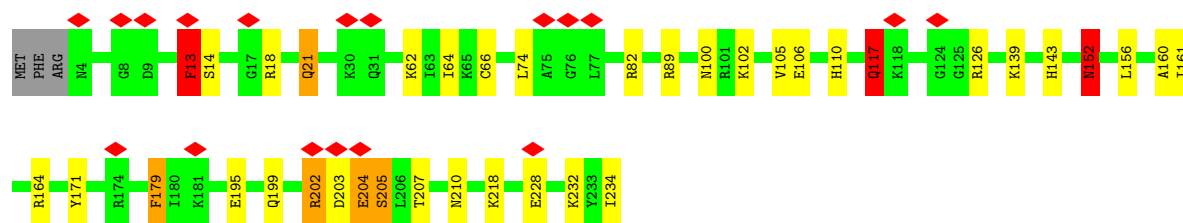


• Molecule 6: Proteasome subunit alpha type-6

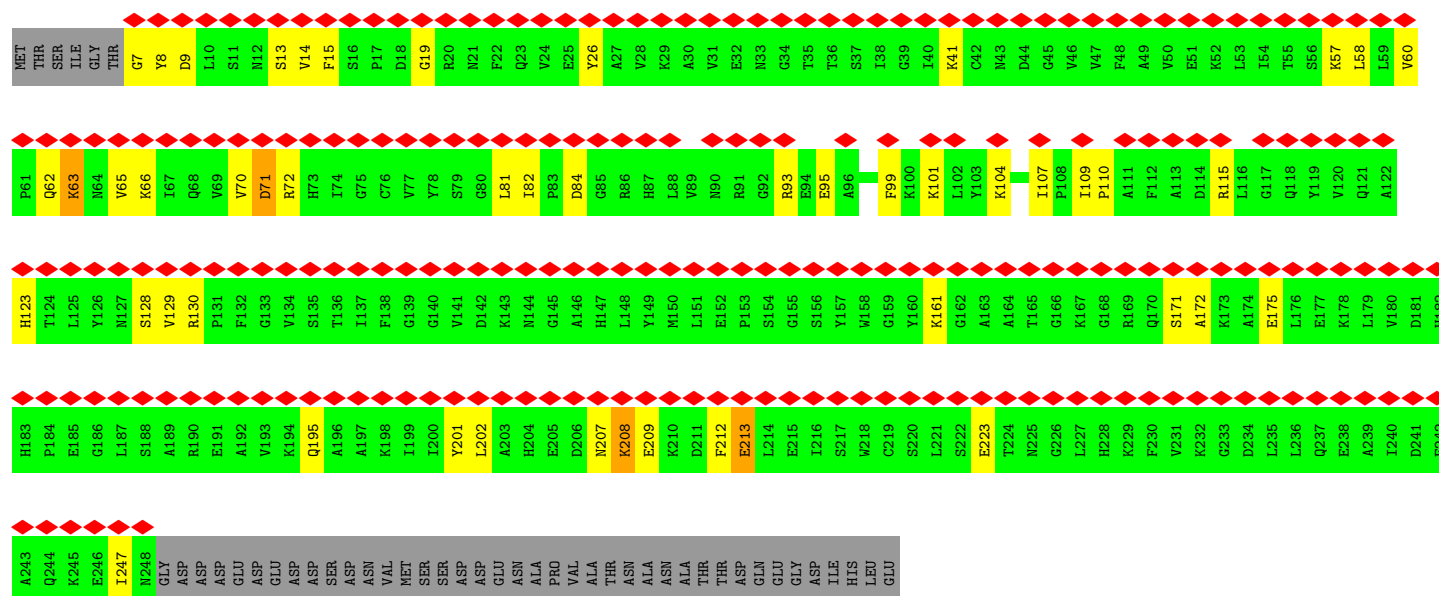
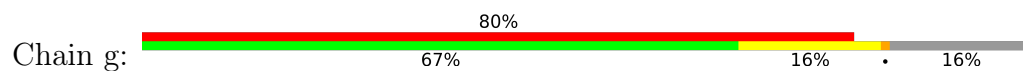


• Molecule 6: Proteasome subunit alpha type-6

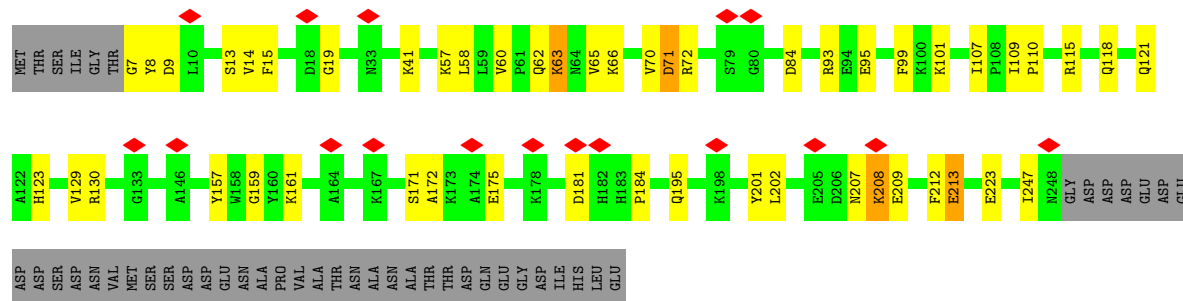




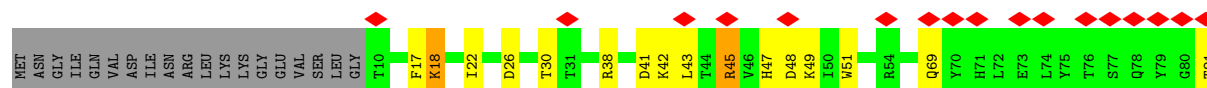
• Molecule 7: Probable proteasome subunit alpha type-7

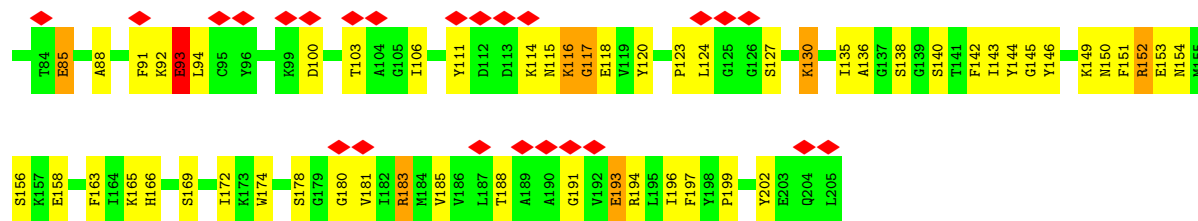


• Molecule 7: Probable proteasome subunit alpha type-7

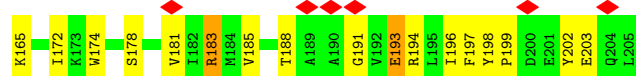


• Molecule 8: Proteasome subunit beta type-1

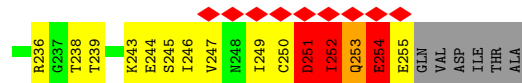
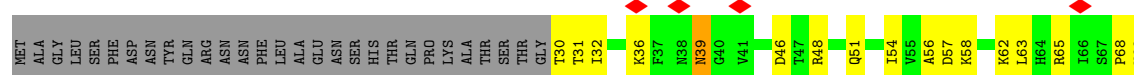




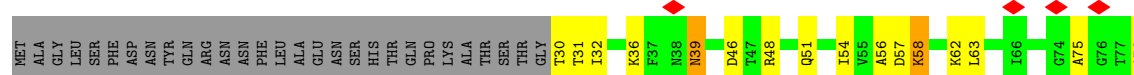
• Molecule 8: Proteasome subunit beta type-1

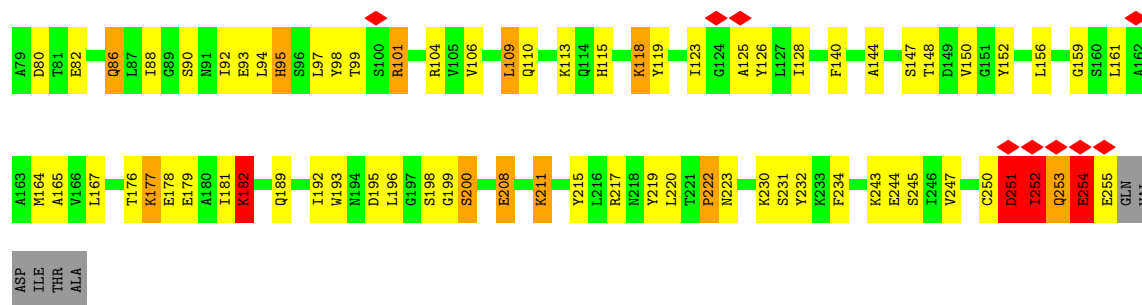


• Molecule 9: Proteasome subunit beta type-2

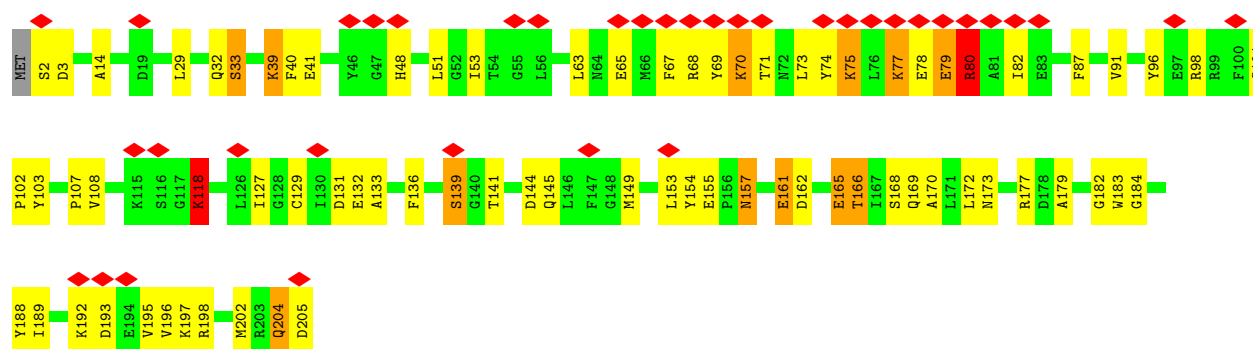


• Molecule 9: Proteasome subunit beta type-2

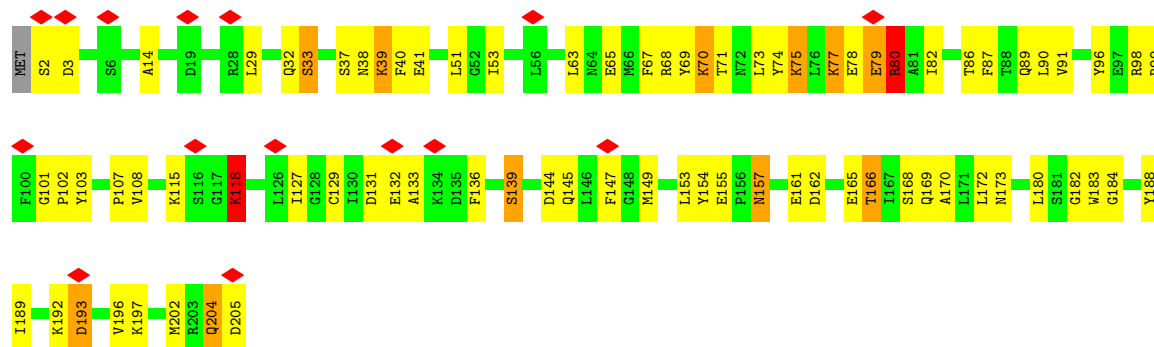




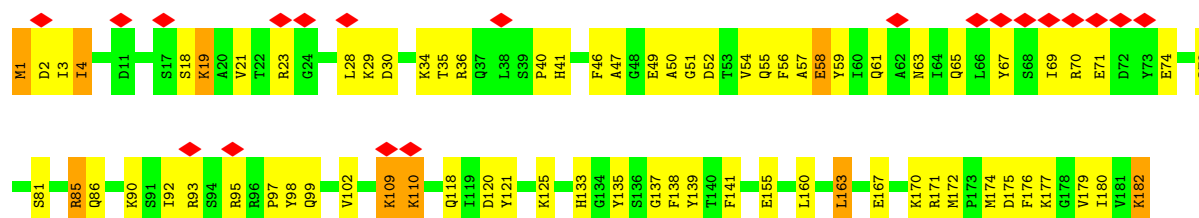
• Molecule 10: Proteasome subunit beta type-3



• Molecule 10: Proteasome subunit beta type-3

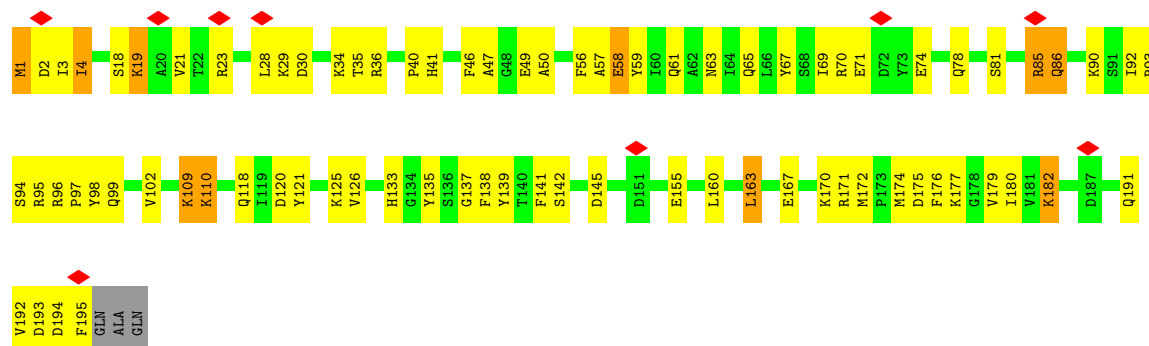


• Molecule 11: Proteasome subunit beta type-4

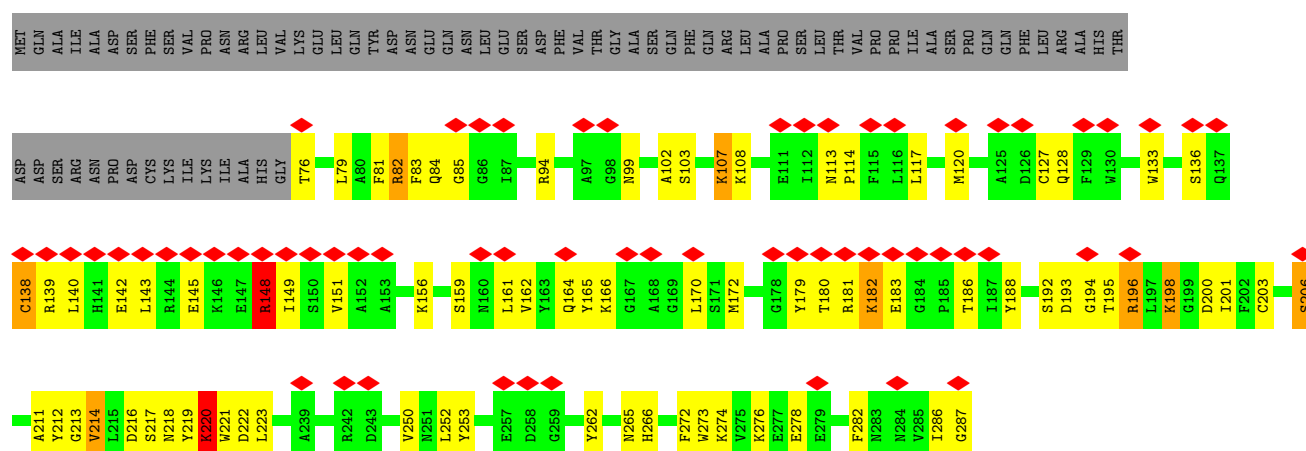
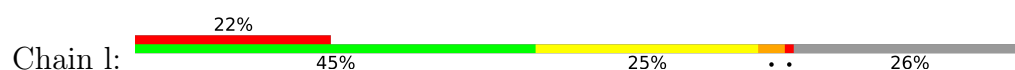




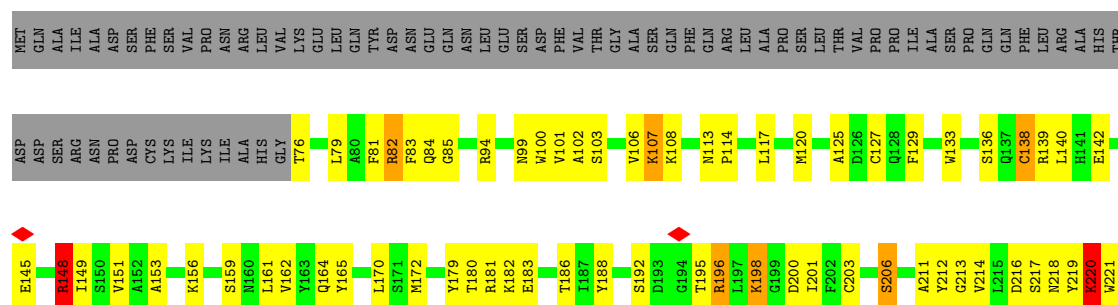
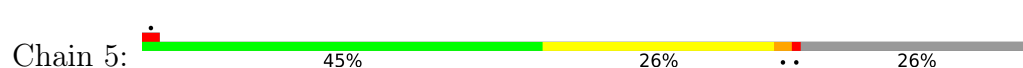
• Molecule 11: Proteasome subunit beta type-4

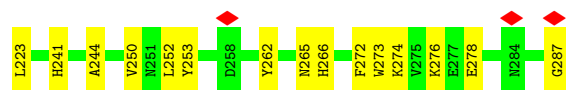


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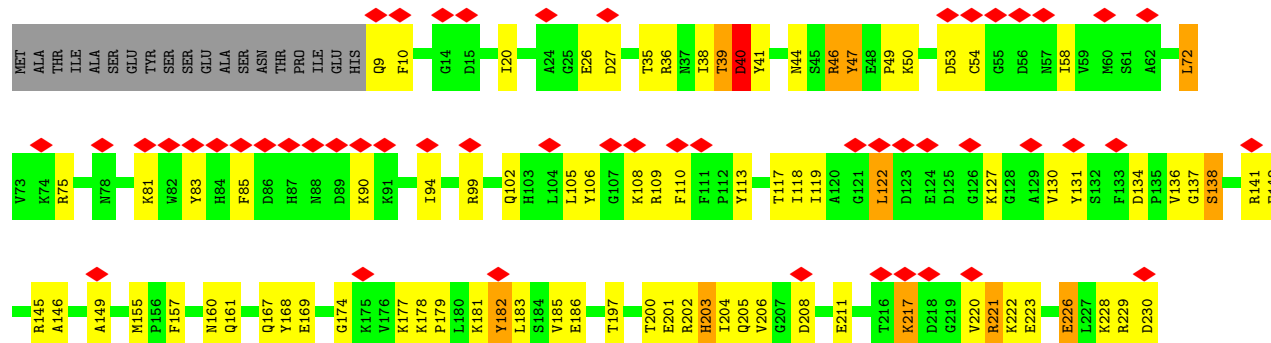


• Molecule 12: Proteasome subunit beta type-5

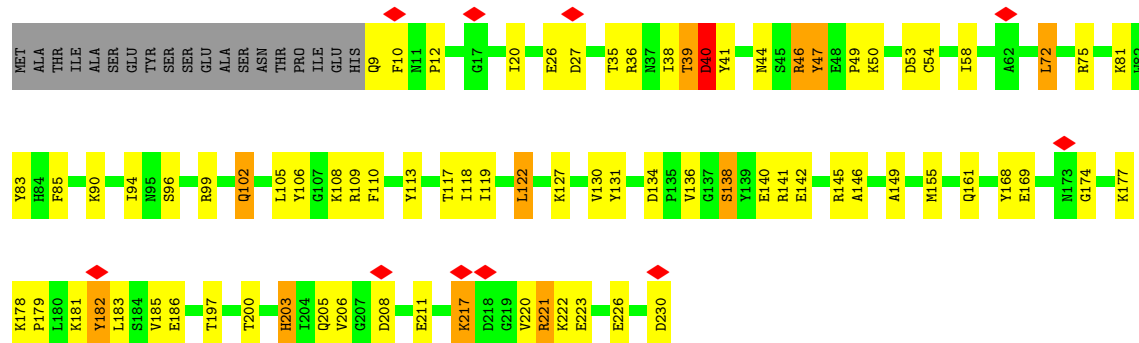




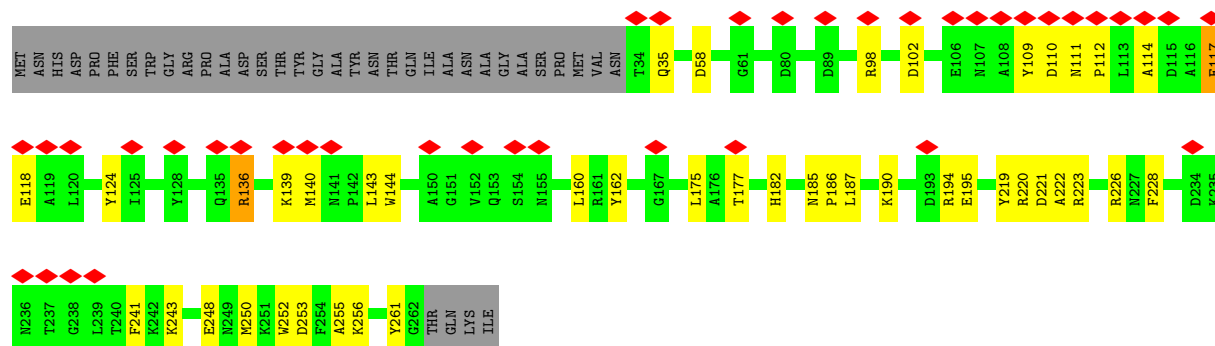
• Molecule 13: Proteasome subunit beta type-6



• Molecule 13: Proteasome subunit beta type-6



• Molecule 14: Proteasome subunit beta type-7



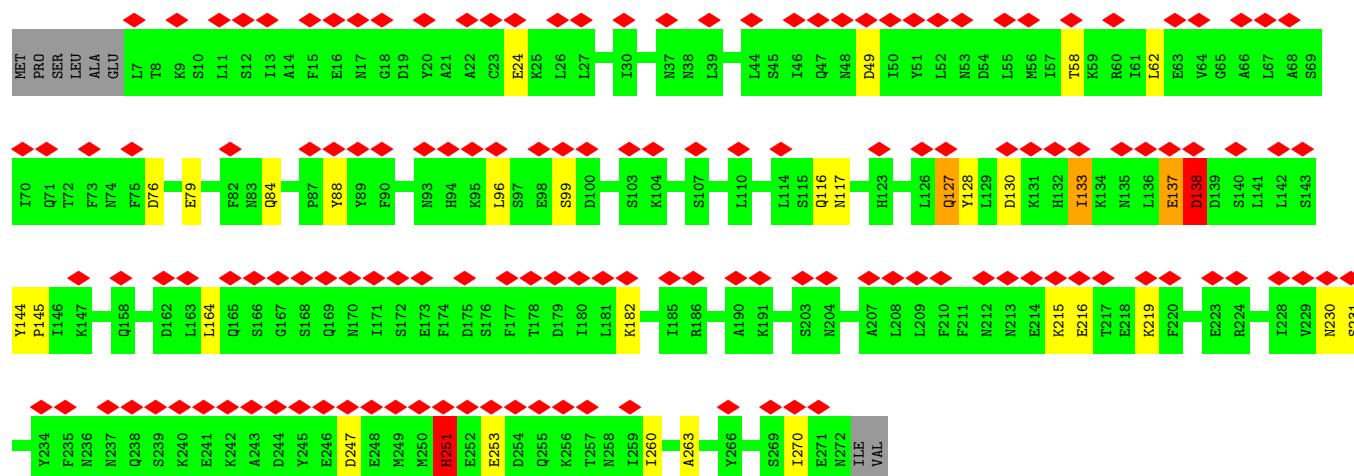
• Molecule 14: Proteasome subunit beta type-7

Chain 7:

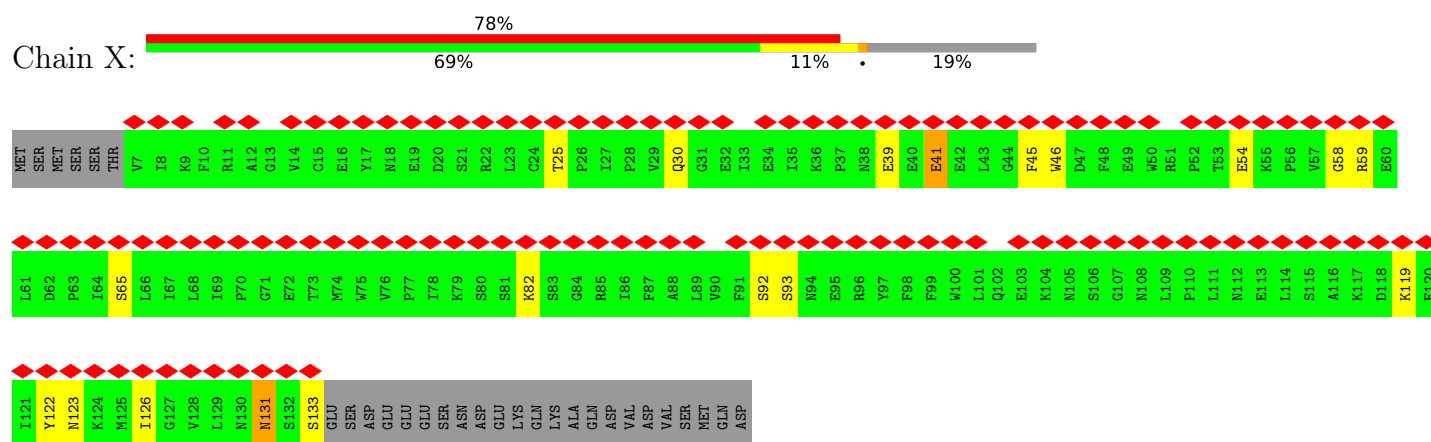
Chain W:

Chain V:

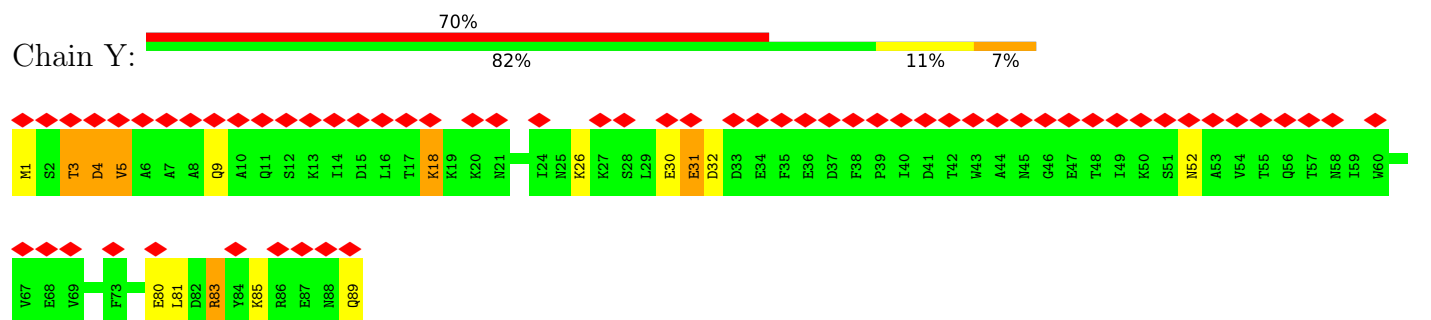
Chain T:



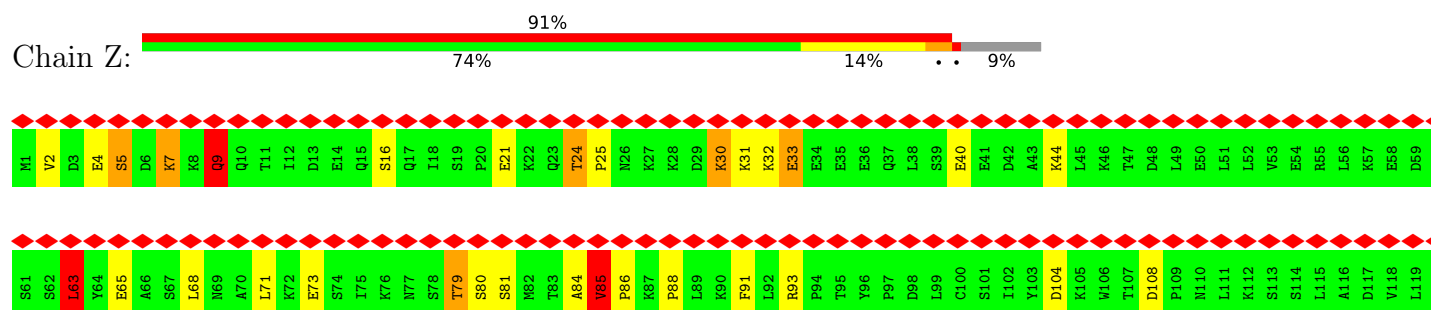
• Molecule 18: 26S proteasome regulatory subunit RPN13



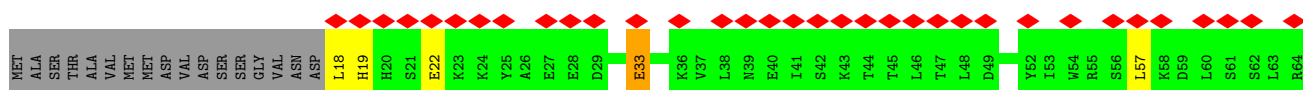
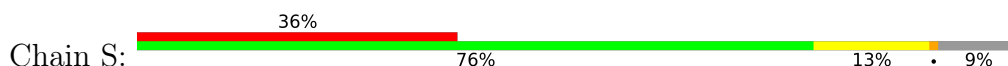
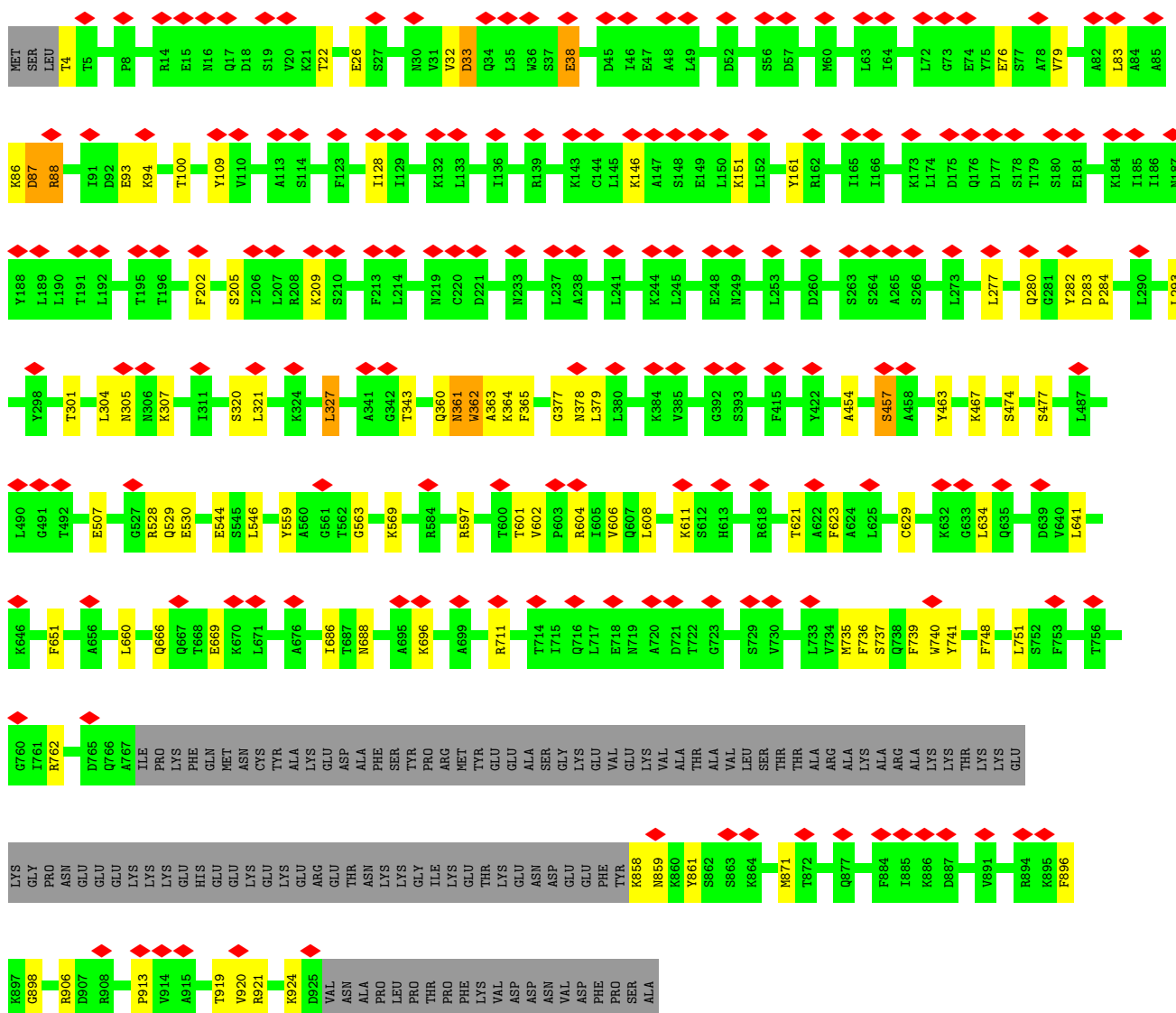
• Molecule 19: 26S proteasome complex subunit SEM1

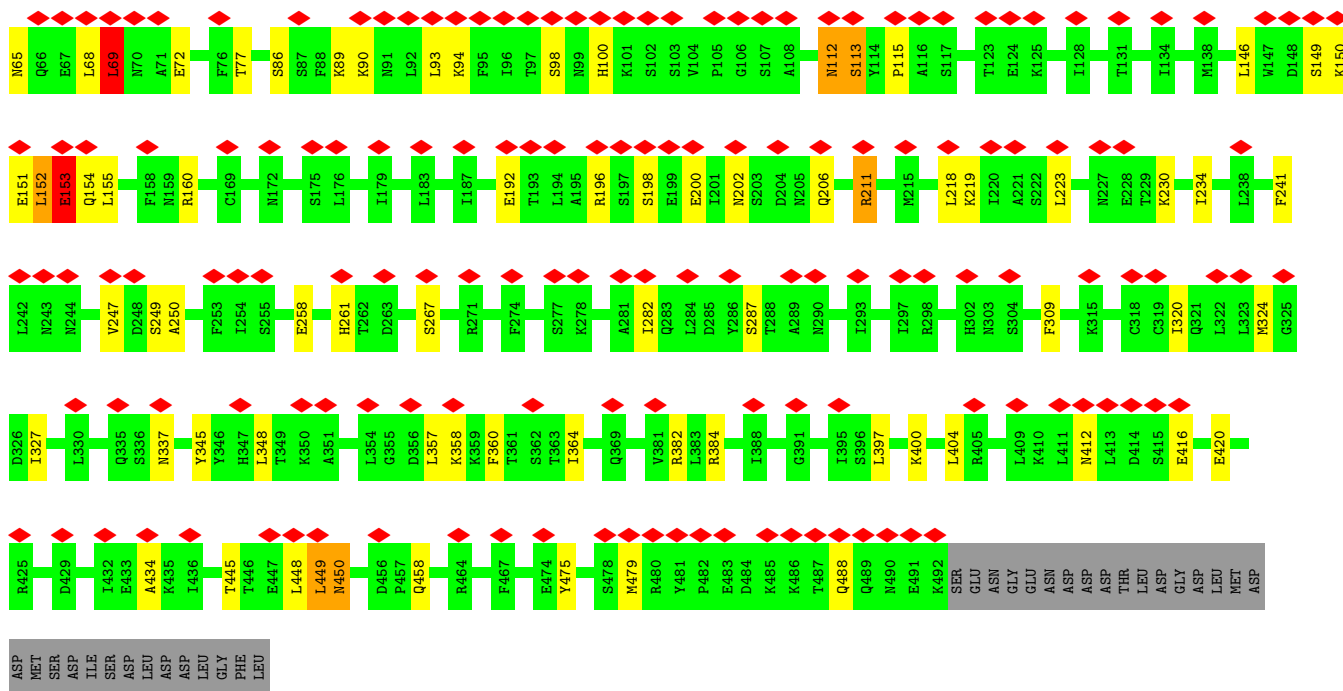


• Molecule 20: 26S proteasome regulatory subunit RPN1

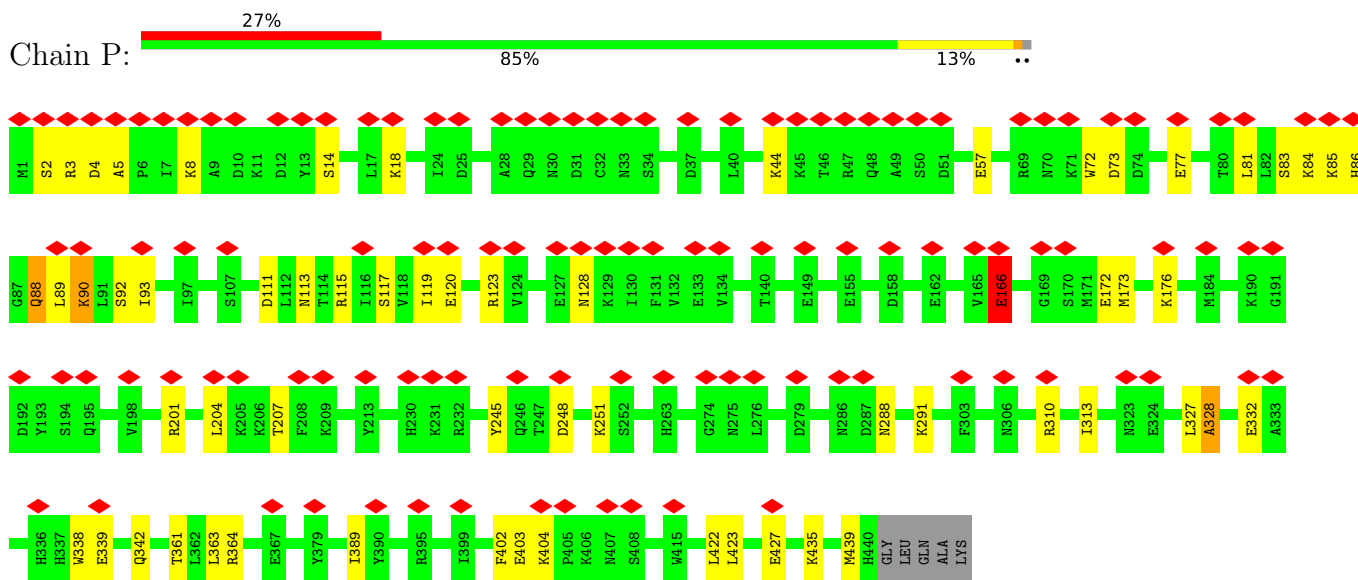


F901	E841	G781	M721	LYS	V601	D541	P481	S421	H561	T301	T241	G181	I121
Y902	Q842	I782	D722	ASN	L602	I542	D482	I422	L362	S302	F242	S182	L122
M903	D843	G783	D723	GLU	V603	T543	T483	G423	D363	D303	Q243	K183	A123
L904	A844	S784	E724	ALA	G604	T544	K484	S424	N364	P304	R244	S184	M124
N905	L845	T785	E725	TLE	S605	S545	I485	I425	S365	Y305	T245	D185	T125
A906	F846	G786	E726	GLU	C606	I546	S486	Y426	K366	M306	C246	G186	Y126
G907	I847	D787	E727	VAL	A607	M547	S487	Q427	S367	H307	Q247	S187	S127
I908	T848	F788	K728	ASP	Y608	D548	A488	W428	V368	K308	Y248	A188	E128
R909	R849	Q789	E729	GLU	T609	I549	A489	W429	F369	Q309	M249	A189	N129
P910	L850	G790	E730	MET	G610	F549	A489	I429	S370	L310	Q250	T190	G130
K911	A851	VAL	G731	VAL	T611	L551	L491	D431	S371	A311	M251	S191	K131
F912	Q852	ASP	I732	ALA	G612	E552	G492	G432	A372	Y312	C252	G192	H132
I913	G853	GLU	D733	GLU	D613	R553	L493	L433	G373	I313	V253	F193	D133
L914	L854	GLY	D734	GLY	V614	T554	G494	Q434	L374	L314	P254	E194	S134
A915	L855	GLU	E735	GLU	L615	A555	I495	Q435	D375	A315	L255	F195	L135
L916	H856	VAL	L736	VAL	L616	I556	A496	I436	S376	A316	L256	S196	R136
N917	L857	GLU	A737	GLU	I617	E557	F497	D437	A377	Q317	P257	K197	Y137
D918	C858	VAL	Y738	VAL	Q618	L558	A498	K438	Q378	K318	P258	E198	R138
E919	R859	LYS	A739	LYS	D619	K559	G499	Y439	Q379	T319	P259	D199	L139
G920	C860	ALA	V740	ALA	L620	T560	S500	I440	N380	S320	E260	T200	L140
E921	T861	GLU	L741	GLU	L621	D561	K501	Y441	L381	F321	D261	L201	S141
P922	H862	THR	G742	THR	H622	V562	N502	V442	A382	E322	V262	R202	D142
I923	T863	GLU	I743	LYS	R623	V563	D503	D443	S383	Y323	A263	L203	V143
K924	D864	LYS	A744	LYS	L624	R564	E504	E444	S384	E324	F264	C204	S144
H925	D865	ASN	L745	ASN	T625	F565	V505	P445	F385	G325	L265	L205	D145
N926	V866	GLY	E746	GLY	P626	L566	L506	E446	V386	V326	K266	D206	F146
V927	F867	SER	A747	SER	K627	A567	G507	V447	N387	Q327	T267	I207	E147
R928	N868	LEU	L748	LEU	N628	L568	L508	K448	G388	D328	A268	V208	G148
V929	D869	GLU	G749	GLU	V629	A569	L509	A449	F389	I329	Y269	P209	W149
Q930	A870	GLY	E750	GLY	K630	L570	L510	G450	L390	I330	S270	Y210	G150
Q931	H871	GLU	D751	GLU	G631	G571	P511	A451	N391	G331	I271	F211	H151
A932	L872	THR	I752	THR	E632	I572	I512	L452	L392	N332	Y272	L212	E152
V933	T873	F813	G753	THR	E633	L573	A513	L453	G393	G333	L273	K213	Y153
E934	A874	G784	K754	ASN	D634	Y574	A514	G454	Y394	K334	S274	H214	I154
T935	K875	H815	E755	ILE	A635	M575	S515	I455	C395	L335	Q275	N215	R155
V936	V876	G816	M756	ASP	ASP	G576	T516	G456	N396	S336	N276	G216	H156
G937	T877	GLU	S757	THR	GLU	Q577	D517	I457	D397	E337	E277	E217	L157
Q938	L878	C818	L758	THR	THR	G578	L518	S458	K398	H338	L278	E218	A158
A939	R879	G819	K759	ALA	THR	E579	P519	A459	L399	F339	T279	E219	L159
Q940	S880	A820	H760	GLY	ALA	Q580	I520	S460	I400	L340	D280	D219	E160
R941	I881	G821	F761	GLY	GLY	V581	E521	G461	V401	Y341	A281	V221	I161
P942	L882	T822	G762	GLN	D634	D582	T522	V462	D402	L342	I282	D222	G162
K943	T883	R823	H763	THR	A635	D583	A523	H463	M403	A343	A283	L223	E163
Q944	T884	N824	L764	ASN	ASP	V584	A524	D464	D404	K344	L284	L224	Y164
I945	A885	A825	H765	SER	GLU	L585	M525	G465	M405	E345	A285	L225	Y165
T946	V886	R826	G766	ILE	SER	E586	A526	G466	M406	L346	N286	E226	N166
G947	G887	L827	V767	ASP	ASP	T587	S527	V467	V407	N347	R287	I227	D167
W948	L888	A828	G768	PHE	PHE	I588	L528	E468	Y408	L348	L288	E228	Q168
I949	V889	Q829	H769	LEU	LEU	S589	A529	F469	K409	T349	G289	S229	V169
T950	S890	G830	E770	GLY	GLY	A590	L530	A470	T410	G350	E290	I230	G170
Q951	P891	L831	H771	GLN	VAL	I591	A531	L471	K411	P351	E291	D231	K171
S952	R892	R832	I772	ASN	ASN	E592	H532	L472	G412	K352	D292	K232	D172
T953	F893	Q833	R773	GLU	GLU	H593	V533	L473	D413	V353	M293	L233	A173
K954	T894	L834	R774	PRO	THR	P594	F534	L474	G414	P234	I294	P234	E174
L955	A895	A835	H775	THR	THR	M595	V535	Q475	M415	E355	R295	Q235	D175
V956	V896	T596	V776	THR	THR	T596	G536	D476	T416	D356	S296	F236	E176
L957	H897	G837	F777	THR	THR	S597	T537	Y477	S417	I357	V297	V237	T177
N958	R898	Y838	P778	THR	THR	A598	C538	V478	A418	Y358	F298	D238	S178
H959	Q899	S839	A779	THR	THR	I599	N539	T479	V419	K359	D299	E239	S179
Q960	L900	R840	M780	THR	THR	E600	G540	N480	A420	S360	A300	N240	D180

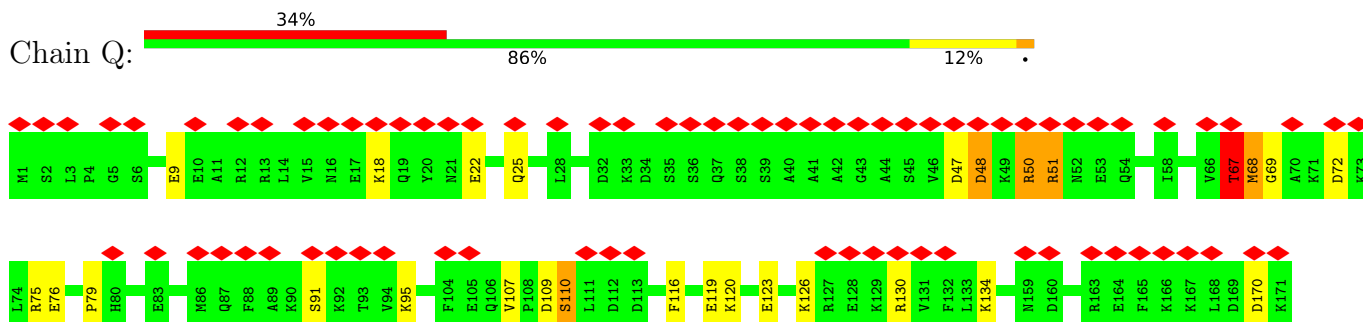


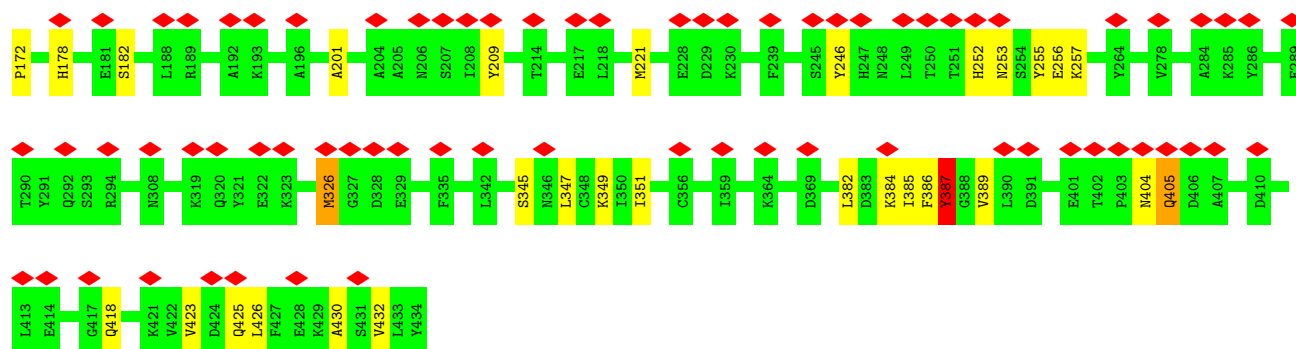


• Molecule 23: 26S proteasome regulatory subunit RPN5

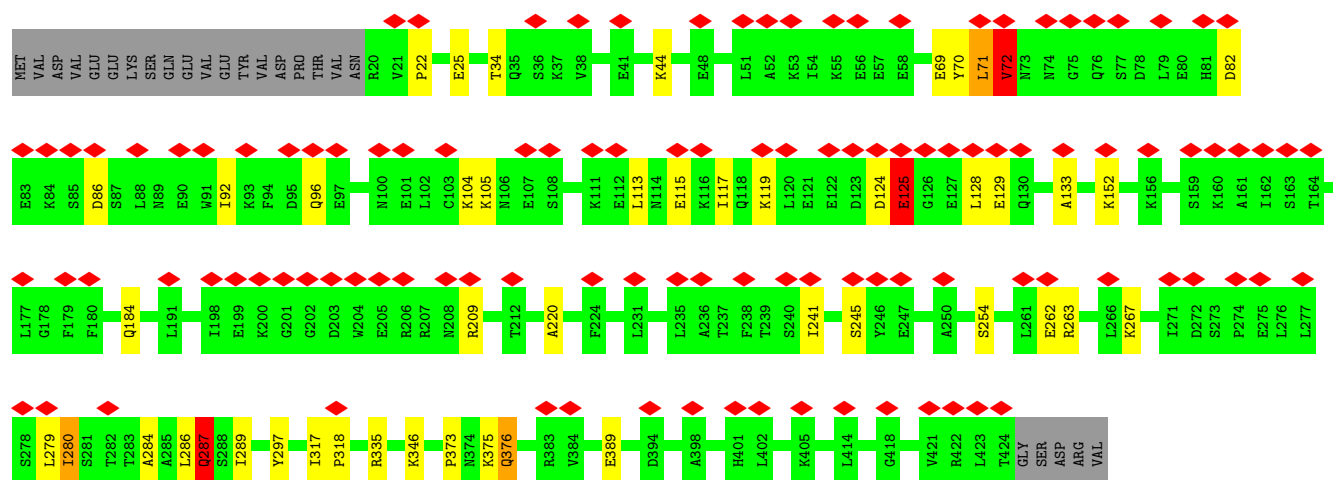
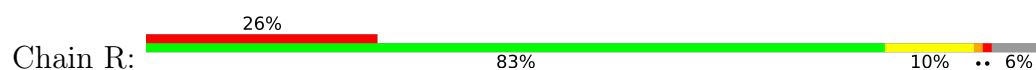


• Molecule 24: 26S proteasome regulatory subunit RPN6

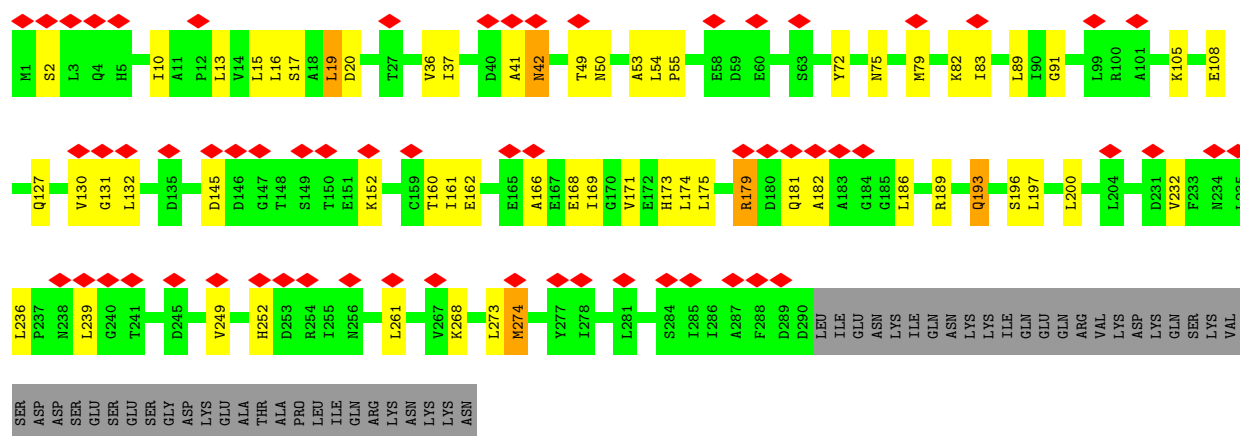




• Molecule 25: 26S proteasome regulatory subunit RPN7

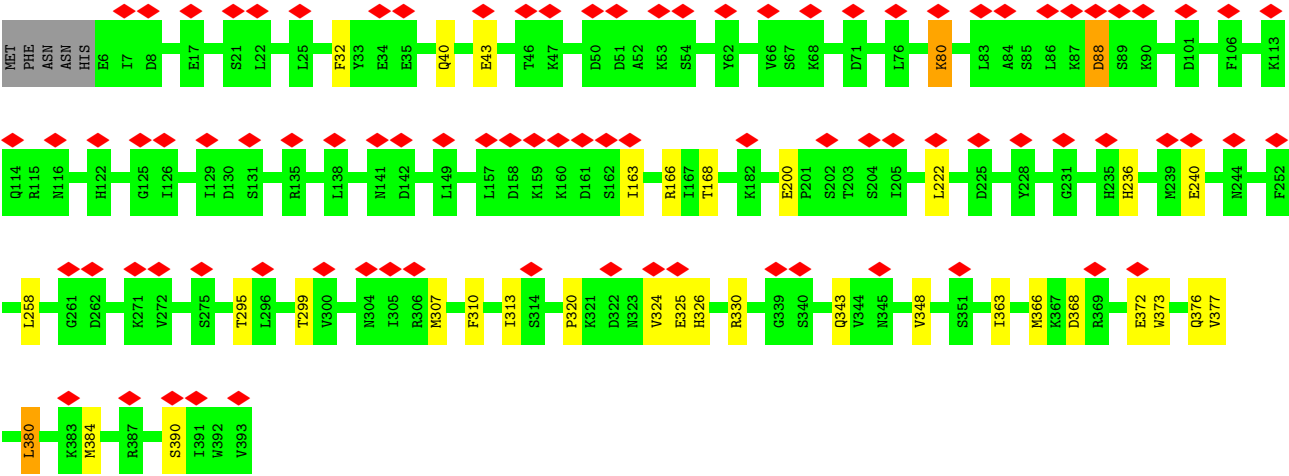


• Molecule 26: 26S proteasome regulatory subunit RPN8



• Molecule 27: 26S proteasome regulatory subunit RPN9





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88243	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	25.065	Depositor
Minimum map value	-11.917	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.815	Depositor
Recommended contour level	5.4	Depositor
Map size ($\text{\AA}$)	588.0, 588.0, 588.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.1, 2.1, 2.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.61	2/1945 (0.1%)	1.00	8/2634 (0.3%)
1	a	0.61	2/1945 (0.1%)	1.00	9/2634 (0.3%)
2	B	0.57	2/1944 (0.1%)	0.95	3/2632 (0.1%)
2	b	0.57	2/1944 (0.1%)	0.95	3/2632 (0.1%)
3	C	0.52	0/1934	0.93	3/2618 (0.1%)
3	c	0.52	0/1934	0.93	3/2618 (0.1%)
4	D	0.54	2/1879 (0.1%)	0.93	6/2546 (0.2%)
4	d	0.53	0/1879	1.21	13/2546 (0.5%)
5	E	0.65	2/1908 (0.1%)	1.04	10/2571 (0.4%)
5	e	0.65	2/1908 (0.1%)	1.04	10/2571 (0.4%)
6	F	0.72	4/1800 (0.2%)	0.98	7/2433 (0.3%)
6	f	0.72	4/1800 (0.2%)	0.98	7/2433 (0.3%)
7	G	0.57	0/1925	1.01	10/2599 (0.4%)
7	g	0.57	0/1925	1.01	10/2599 (0.4%)
8	1	0.80	2/1541 (0.1%)	1.10	12/2087 (0.6%)
8	h	0.80	2/1541 (0.1%)	1.10	12/2087 (0.6%)
9	2	0.94	5/1750 (0.3%)	1.20	15/2373 (0.6%)
9	i	0.94	5/1750 (0.3%)	1.20	16/2373 (0.7%)
10	3	0.87	4/1611 (0.2%)	1.08	9/2174 (0.4%)
10	j	0.87	4/1611 (0.2%)	1.08	9/2174 (0.4%)
11	4	0.93	7/1589 (0.4%)	1.18	14/2142 (0.7%)
11	k	0.93	7/1589 (0.4%)	1.18	14/2142 (0.7%)
12	5	0.70	0/1681	1.09	12/2274 (0.5%)
12	l	0.70	0/1681	1.09	12/2274 (0.5%)
13	6	0.87	5/1795 (0.3%)	1.11	10/2420 (0.4%)
13	m	0.87	5/1795 (0.3%)	1.11	10/2420 (0.4%)
14	7	0.45	0/1821	0.92	4/2470 (0.2%)
14	n	0.45	0/1821	0.99	9/2470 (0.4%)
15	W	0.42	0/1557	0.84	1/2111 (0.0%)
16	V	0.70	2/2309 (0.1%)	1.40	21/3115 (0.7%)
17	T	0.40	0/2235	0.92	3/3017 (0.1%)
18	X	0.45	0/1058	1.00	1/1432 (0.1%)
19	Y	0.39	0/741	1.08	3/1000 (0.3%)
20	Z	0.66	0/7122	1.44	64/9645 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
21	N	0.41	0/6521	0.84	9/8824 (0.1%)
22	S	0.41	0/3966	0.90	5/5355 (0.1%)
23	P	0.42	0/3663	0.89	8/4940 (0.2%)
24	Q	0.37	0/3556	0.92	13/4787 (0.3%)
25	R	0.40	0/3313	0.91	11/4469 (0.2%)
26	U	0.56	2/2340 (0.1%)	0.85	2/3168 (0.1%)
27	O	0.46	3/3247 (0.1%)	0.85	6/4380 (0.1%)
All	All	0.62	75/91874 (0.1%)	1.04	407/124189 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	d	0	8
5	E	0	1
5	e	0	1
6	F	0	3
6	f	0	3
7	G	0	2
7	g	0	2
8	l	0	1
8	h	0	1
9	2	0	3
9	i	0	3
12	5	0	1
12	l	0	1
15	W	0	2
16	V	0	4
17	T	0	6
18	X	0	3
19	Y	0	3
20	Z	0	41
21	N	0	2
22	S	0	2
23	P	0	3
24	Q	0	4
25	R	0	1
All	All	0	101

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	252	ILE	CG1-CD1	-12.82	1.01	1.51
9	2	252	ILE	CG1-CD1	-12.82	1.01	1.51
8	1	69	GLN	CD-NE2	-12.40	1.07	1.33
8	h	69	GLN	CD-NE2	-12.40	1.07	1.33
11	k	86	GLN	CD-NE2	-12.01	1.08	1.33
11	4	86	GLN	CD-NE2	-12.01	1.08	1.33
5	e	211	LYS	CB-CG	-11.55	1.17	1.52
5	E	211	LYS	CB-CG	-11.55	1.17	1.52
6	F	152	ASN	CG-ND2	-11.37	1.09	1.33
6	f	152	ASN	CG-ND2	-11.36	1.09	1.33
10	j	173	ASN	CG-ND2	-11.20	1.09	1.33
10	3	173	ASN	CG-ND2	-11.19	1.09	1.33
13	6	102	GLN	CD-NE2	-10.71	1.10	1.33
13	m	102	GLN	CD-NE2	-10.70	1.10	1.33
10	j	204	GLN	CD-NE2	-10.29	1.11	1.33
10	3	204	GLN	CD-NE2	-10.27	1.11	1.33
1	a	130	GLN	CD-NE2	-9.90	1.12	1.33
1	A	130	GLN	CD-NE2	-9.87	1.12	1.33
8	h	69	GLN	CD-OE1	-9.24	1.05	1.23
8	1	69	GLN	CD-OE1	-9.23	1.06	1.23
9	2	86	GLN	CD-NE2	-9.06	1.14	1.33
9	i	86	GLN	CD-NE2	-9.00	1.14	1.33
6	f	21	GLN	CD-NE2	-8.88	1.14	1.33
6	F	21	GLN	CD-NE2	-8.85	1.14	1.33
11	k	86	GLN	CD-OE1	-8.84	1.06	1.23
11	4	86	GLN	CD-OE1	-8.81	1.06	1.23
27	O	88	ASP	CG-OD1	-8.57	1.09	1.25
2	b	94	HIS	CE1-NE2	-8.54	1.24	1.32
6	f	152	ASN	CG-OD1	-8.49	1.07	1.23
6	F	152	ASN	CG-OD1	-8.48	1.07	1.23
2	B	94	HIS	CE1-NE2	-8.46	1.24	1.32
27	O	88	ASP	CG-OD2	-8.44	1.09	1.25
10	j	173	ASN	CG-OD1	-8.06	1.08	1.23
10	3	173	ASN	CG-OD1	-8.05	1.08	1.23
26	U	19	LEU	CG-CD2	-8.04	1.26	1.52
11	4	110	LYS	CG-CD	-8.04	1.28	1.52
11	k	110	LYS	CG-CD	-8.04	1.28	1.52
9	i	86	GLN	CD-OE1	-7.74	1.08	1.23
9	2	86	GLN	CD-OE1	-7.74	1.08	1.23
13	6	203	HIS	CE1-NE2	-7.68	1.24	1.32
9	i	95	HIS	CE1-NE2	-7.68	1.24	1.32
13	m	203	HIS	CE1-NE2	-7.65	1.25	1.32
9	2	95	HIS	CE1-NE2	-7.63	1.25	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	21	GLN	CD-OE1	-7.61	1.09	1.23
13	6	102	GLN	CD-OE1	-7.59	1.09	1.23
13	6	46	ARG	CZ-NH2	-7.58	1.23	1.33
6	f	21	GLN	CD-OE1	-7.58	1.09	1.23
13	m	46	ARG	CZ-NH2	-7.56	1.23	1.33
13	m	102	GLN	CD-OE1	-7.55	1.09	1.23
1	a	130	GLN	CD-OE1	-7.32	1.09	1.23
1	A	130	GLN	CD-OE1	-7.31	1.09	1.23
4	D	11	PHE	CD2-CE2	-7.06	1.17	1.38
10	j	204	GLN	CD-OE1	-6.85	1.10	1.23
10	3	204	GLN	CD-OE1	-6.83	1.10	1.23
5	E	211	LYS	CG-CD	-6.76	1.32	1.52
5	e	211	LYS	CG-CD	-6.73	1.32	1.52
4	D	11	PHE	CB-CG	-6.67	1.35	1.50
11	k	182	LYS	CE-NZ	-6.33	1.30	1.49
11	4	182	LYS	CE-NZ	-6.32	1.30	1.49
11	k	109	LYS	CG-CD	-6.28	1.33	1.52
11	4	109	LYS	CG-CD	-6.26	1.33	1.52
27	O	380	LEU	CA-CB	-6.21	1.43	1.53
16	V	205	LYS	CD-CE	-6.11	1.34	1.52
16	V	280	LEU	CG-CD2	-6.10	1.32	1.52
11	4	110	LYS	CB-CG	-6.00	1.34	1.52
11	k	110	LYS	CB-CG	-5.97	1.34	1.52
9	i	109	LEU	CG-CD1	-5.73	1.33	1.52
9	2	109	LEU	CG-CD1	-5.73	1.33	1.52
11	k	110	LYS	CE-NZ	-5.69	1.32	1.49
11	4	110	LYS	CE-NZ	-5.67	1.32	1.49
26	U	193	GLN	CA-CB	-5.62	1.44	1.53
13	6	46	ARG	CD-NE	-5.55	1.38	1.46
2	B	94	HIS	CG-CD2	-5.53	1.29	1.35
2	b	94	HIS	CG-CD2	-5.52	1.29	1.35
13	m	46	ARG	CD-NE	-5.50	1.38	1.46

All (407) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	259	LYS	CG-CD-CE	28.48	176.79	111.30
20	Z	366	LYS	CG-CD-CE	22.40	162.82	111.30
20	Z	366	LYS	CB-CG-CD	17.14	150.73	111.30
24	Q	326	MET	CB-CG-SD	14.42	155.95	112.70
4	d	208	LYS	CB-CG-CD	12.60	140.28	111.30
11	4	1	MET	CA-CB-CG	-12.12	89.85	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	1	MET	CA-CB-CG	-12.12	89.86	114.10
4	d	208	LYS	CG-CD-CE	11.82	138.48	111.30
27	O	88	ASP	OD1-CG-OD2	-11.60	95.06	122.90
1	a	201	LYS	CD-CE-NZ	-11.45	75.25	111.90
1	A	201	LYS	CD-CE-NZ	-11.44	75.28	111.90
8	1	183	ARG	CG-CD-NE	10.91	136.00	112.00
8	1	18	LYS	CD-CE-NZ	-10.89	77.06	111.90
8	h	18	LYS	CD-CE-NZ	-10.89	77.06	111.90
8	h	183	ARG	CG-CD-NE	10.88	135.94	112.00
9	i	252	ILE	CA-CB-CG1	-10.59	92.39	110.40
9	2	252	ILE	CA-CB-CG1	-10.58	92.41	110.40
20	Z	33	GLU	CG-CD-OE1	9.99	141.38	118.40
19	Y	18	LYS	CB-CG-CD	9.62	133.42	111.30
7	g	71	ASP	N-CA-C	-9.48	90.62	110.80
5	E	10	ARG	CB-CG-CD	9.46	133.07	111.30
7	G	71	ASP	N-CA-C	-9.46	90.64	110.80
5	e	10	ARG	CB-CG-CD	9.46	133.06	111.30
16	V	88	GLN	CB-CG-CD	9.27	128.35	112.60
21	N	146	LYS	CG-CD-CE	9.25	132.58	111.30
11	k	109	LYS	CG-CD-CE	9.20	132.45	111.30
11	4	109	LYS	CG-CD-CE	9.18	132.41	111.30
13	m	127	LYS	CD-CE-NZ	8.98	140.65	111.90
13	6	127	LYS	CD-CE-NZ	8.97	140.62	111.90
20	Z	33	GLU	CG-CD-OE2	-8.77	98.24	118.40
20	Z	33	GLU	OE1-CD-OE2	-8.70	102.02	122.90
20	Z	170	GLU	CB-CG-CD	8.68	127.35	112.60
11	k	1	MET	CG-SD-CE	-8.63	81.92	100.90
11	4	1	MET	CG-SD-CE	-8.62	81.93	100.90
1	A	187	LYS	CB-CG-CD	8.62	131.12	111.30
9	2	109	LEU	CB-CG-CD2	8.61	136.52	110.70
1	a	187	LYS	CB-CG-CD	8.61	131.10	111.30
9	i	109	LEU	CB-CG-CD2	8.60	136.49	110.70
25	R	287	GLN	CB-CA-C	-8.46	97.47	110.92
4	D	88	LYS	CB-CG-CD	8.44	130.70	111.30
4	D	182	LYS	CB-CG-CD	8.34	130.47	111.30
13	6	40	ASP	N-CA-C	-8.32	93.07	110.80
16	V	88	GLN	CA-CB-CG	8.32	130.75	114.10
13	m	40	ASP	N-CA-C	-8.31	93.10	110.80
24	Q	405	GLN	N-CA-C	-8.30	93.12	110.80
11	k	109	LYS	CA-CB-CG	-8.24	97.61	114.10
11	4	109	LYS	CA-CB-CG	-8.24	97.62	114.10
3	C	5	ARG	CG-CD-NE	8.20	130.04	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	48	ASP	CB-CA-C	-8.19	94.11	110.42
3	c	5	ARG	CG-CD-NE	8.19	130.02	112.00
20	Z	376	SER	N-CA-C	8.16	128.19	110.80
20	Z	33	GLU	CB-CG-CD	8.12	126.41	112.60
25	R	287	GLN	CA-CB-CG	8.11	130.31	114.10
20	Z	84	ALA	CA-C-N	8.10	137.12	122.13
20	Z	84	ALA	C-N-CA	8.10	137.12	122.13
7	g	66	LYS	CB-CG-CD	-8.10	92.68	111.30
7	G	66	LYS	CB-CG-CD	-8.09	92.70	111.30
11	4	19	LYS	CD-CE-NZ	8.07	137.72	111.90
11	k	19	LYS	CD-CE-NZ	8.07	137.71	111.90
6	f	228	GLU	CA-CB-CG	-7.99	98.12	114.10
6	F	228	GLU	CA-CB-CG	-7.98	98.14	114.10
23	P	166	GLU	CG-CD-OE2	-7.95	100.12	118.40
8	h	183	ARG	CB-CG-CD	7.92	129.53	111.30
8	l	183	ARG	CB-CG-CD	7.89	129.44	111.30
23	P	88	GLN	CA-C-N	7.72	136.29	121.54
23	P	88	GLN	C-N-CA	7.72	136.29	121.54
13	m	127	LYS	CG-CD-CE	-7.72	93.54	111.30
13	6	127	LYS	CG-CD-CE	-7.72	93.54	111.30
23	P	166	GLU	CB-CG-CD	7.71	125.70	112.60
20	Z	30	LYS	CA-CB-CG	7.64	129.39	114.10
25	R	376	GLN	N-CA-CB	-7.63	99.97	110.95
8	l	183	ARG	CA-CB-CG	-7.61	98.88	114.10
19	Y	18	LYS	CG-CD-CE	7.60	128.78	111.30
20	Z	9	GLN	CB-CG-CD	7.60	125.52	112.60
8	h	183	ARG	CA-CB-CG	-7.58	98.95	114.10
11	4	109	LYS	CB-CG-CD	7.55	128.67	111.30
11	k	109	LYS	CB-CG-CD	7.54	128.65	111.30
14	n	109	TYR	CA-C-N	7.54	135.94	121.54
14	n	109	TYR	C-N-CA	7.54	135.94	121.54
1	A	196	GLU	N-CA-C	-7.50	97.68	107.73
20	Z	366	LYS	CD-CE-NZ	-7.49	87.92	111.90
25	R	376	GLN	CA-CB-CG	7.49	129.09	114.10
1	a	196	GLU	N-CA-C	-7.48	97.70	107.73
20	Z	131	LYS	CB-CG-CD	7.44	128.42	111.30
12	l	196	ARG	NE-CZ-NH2	-7.42	112.52	119.20
20	Z	728	LYS	N-CA-C	-7.38	95.07	110.80
1	A	77	ARG	CB-CG-CD	7.38	128.26	111.30
12	5	196	ARG	NE-CZ-NH2	-7.37	112.57	119.20
19	Y	83	ARG	CG-CD-NE	7.37	128.21	112.00
1	a	77	ARG	CB-CG-CD	7.36	128.23	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	118	LYS	CA-CB-CG	7.36	128.81	114.10
20	Z	498	ALA	N-CA-CB	-7.35	98.07	110.49
5	E	211	LYS	CA-CB-CG	-7.35	99.40	114.10
10	3	118	LYS	CA-CB-CG	7.35	128.80	114.10
20	Z	802	ASP	N-CA-CB	-7.33	98.11	110.49
5	e	211	LYS	CA-CB-CG	-7.32	99.47	114.10
16	V	306	LYS	N-CA-C	-7.31	90.54	111.00
20	Z	557	GLU	N-CA-C	-7.24	101.75	113.19
9	2	182	LYS	CB-CG-CD	7.11	127.64	111.30
12	5	181	ARG	NE-CZ-NH2	7.08	125.57	119.20
9	i	182	LYS	CB-CG-CD	7.07	127.56	111.30
20	Z	9	GLN	CA-CB-CG	7.07	128.24	114.10
4	d	182	LYS	CB-CG-CD	7.07	127.56	111.30
7	g	57	LYS	CD-CE-NZ	7.04	134.42	111.90
12	l	181	ARG	NE-CZ-NH2	7.03	125.53	119.20
7	G	57	LYS	CD-CE-NZ	7.01	134.33	111.90
24	Q	48	ASP	N-CA-C	7.00	125.70	110.80
4	d	182	LYS	CG-CD-CE	-7.00	95.21	111.30
8	l	194	ARG	CG-CD-NE	6.98	127.35	112.00
8	h	194	ARG	CG-CD-NE	6.97	127.33	112.00
24	Q	387	TYR	N-CA-C	-6.96	95.97	110.80
20	Z	557	GLU	CA-CB-CG	6.93	127.97	114.10
23	P	166	GLU	CG-CD-OE1	6.93	134.33	118.40
14	7	110	ASP	N-CA-C	-6.90	96.09	110.80
23	P	338	TRP	CA-CB-CG	6.90	126.71	113.60
4	D	182	LYS	CA-CB-CG	6.88	127.86	114.10
20	Z	820	ALA	CA-C-N	6.87	127.57	119.94
20	Z	820	ALA	C-N-CA	6.87	127.57	119.94
6	f	13	PHE	CA-C-N	6.81	133.97	121.70
6	f	13	PHE	C-N-CA	6.81	133.97	121.70
20	Z	30	LYS	CB-CG-CD	6.81	126.97	111.30
6	F	13	PHE	CA-C-N	6.81	133.95	121.70
6	F	13	PHE	C-N-CA	6.81	133.95	121.70
4	d	149	GLN	CA-CB-CG	-6.79	100.52	114.10
6	F	218	LYS	CD-CE-NZ	-6.77	90.24	111.90
10	3	77	LYS	CD-CE-NZ	-6.76	90.25	111.90
10	j	77	LYS	CD-CE-NZ	-6.76	90.26	111.90
6	f	218	LYS	CD-CE-NZ	-6.76	90.28	111.90
25	R	287	GLN	N-CA-CB	6.72	120.03	109.82
16	V	259	LYS	CB-CG-CD	-6.71	95.86	111.30
12	l	196	ARG	NE-CZ-NH1	6.70	128.20	121.50
4	d	39	LYS	CD-CE-NZ	6.70	133.33	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	152	ARG	CA-CB-CG	-6.67	100.75	114.10
8	l	152	ARG	CA-CB-CG	-6.67	100.76	114.10
12	5	196	ARG	NE-CZ-NH1	6.67	128.17	121.50
6	F	228	GLU	CB-CG-CD	6.67	123.93	112.60
16	V	205	LYS	CD-CE-NZ	-6.66	90.58	111.90
5	e	10	ARG	CG-CD-NE	6.66	126.65	112.00
5	E	10	ARG	CG-CD-NE	6.66	126.65	112.00
27	O	80	LYS	CA-CB-CG	-6.65	100.80	114.10
6	f	228	GLU	CB-CG-CD	6.63	123.87	112.60
8	h	85	GLU	CA-CB-CG	6.63	127.36	114.10
8	l	85	GLU	CA-CB-CG	6.62	127.33	114.10
20	Z	85	VAL	N-CA-C	6.61	123.15	108.88
16	V	303	VAL	CA-CB-CG2	6.59	121.61	110.40
16	V	58	VAL	CA-C-N	6.59	134.13	121.54
16	V	58	VAL	C-N-CA	6.59	134.13	121.54
9	2	109	LEU	CD1-CG-CD2	-6.58	96.32	110.80
20	Z	7	LYS	CB-CG-CD	6.58	126.43	111.30
9	i	109	LEU	CD1-CG-CD2	-6.57	96.34	110.80
13	m	46	ARG	NE-CZ-NH2	-6.55	113.30	119.20
8	h	153	GLU	CB-CG-CD	6.54	123.72	112.60
27	O	80	LYS	CG-CD-CE	6.54	126.34	111.30
8	l	153	GLU	CB-CG-CD	6.54	123.71	112.60
16	V	286	GLU	CA-CB-CG	6.53	127.16	114.10
21	N	146	LYS	CD-CE-NZ	-6.53	91.00	111.90
27	O	80	LYS	CB-CG-CD	6.53	126.31	111.30
20	Z	557	GLU	CB-CG-CD	6.52	123.69	112.60
13	6	46	ARG	NE-CZ-NH2	-6.51	113.34	119.20
5	e	170	LYS	CD-CE-NZ	6.48	132.64	111.90
5	E	170	LYS	CD-CE-NZ	6.47	132.60	111.90
10	3	32	GLN	N-CA-C	6.47	124.58	110.80
20	Z	504	GLU	CA-CB-CG	6.46	127.03	114.10
10	j	32	GLN	N-CA-C	6.46	124.56	110.80
16	V	259	LYS	CD-CE-NZ	-6.46	91.23	111.90
5	e	205	LYS	CD-CE-NZ	-6.45	91.28	111.90
5	E	205	LYS	CD-CE-NZ	-6.44	91.31	111.90
22	S	152	LEU	N-CA-C	-6.41	97.14	110.80
1	A	232	LYS	CD-CE-NZ	-6.39	91.45	111.90
1	a	232	LYS	CD-CE-NZ	-6.39	91.46	111.90
14	n	110	ASP	N-CA-C	6.36	124.35	110.80
4	d	39	LYS	CG-CD-CE	6.31	125.82	111.30
16	V	306	LYS	N-CA-CB	6.29	121.19	110.50
14	n	139	LYS	CB-CG-CD	6.28	125.75	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	149	GLN	CB-CG-CD	6.28	123.28	112.60
6	f	232	LYS	CD-CE-NZ	6.28	131.99	111.90
11	4	90	LYS	CG-CD-CE	6.27	125.71	111.30
6	F	232	LYS	CD-CE-NZ	6.26	131.94	111.90
11	k	90	LYS	CG-CD-CE	6.25	125.67	111.30
3	C	9	ARG	CB-CG-CD	-6.25	96.93	111.30
9	2	208	GLU	CA-CB-CG	-6.24	101.61	114.10
9	2	217	ARG	CG-CD-NE	-6.23	98.29	112.00
20	Z	30	LYS	CG-CD-CE	-6.23	96.96	111.30
7	G	66	LYS	CG-CD-CE	6.23	125.64	111.30
7	g	66	LYS	CG-CD-CE	6.23	125.63	111.30
9	i	208	GLU	CA-CB-CG	-6.23	101.64	114.10
9	i	217	ARG	CG-CD-NE	-6.23	98.30	112.00
3	c	9	ARG	CB-CG-CD	-6.22	96.99	111.30
12	l	220	LYS	CB-CG-CD	6.22	125.61	111.30
12	5	220	LYS	CB-CG-CD	6.21	125.59	111.30
18	X	41	GLU	CG-CD-OE1	6.19	132.64	118.40
13	m	40	ASP	N-CA-CB	6.18	120.94	110.49
17	T	127	GLN	CA-CB-CG	6.18	126.46	114.10
27	O	88	ASP	CB-CG-OD1	6.18	132.62	118.40
13	6	40	ASP	N-CA-CB	6.17	120.92	110.49
20	Z	277	GLU	CA-CB-CG	-6.17	101.76	114.10
20	Z	728	LYS	N-CA-CB	6.13	120.84	110.49
20	Z	170	GLU	CA-CB-CG	6.11	126.33	114.10
9	i	167	LEU	CB-CG-CD1	-6.09	92.42	110.70
9	2	167	LEU	CB-CG-CD1	-6.09	92.42	110.70
24	Q	68	MET	N-CA-C	-6.07	93.99	111.00
26	U	19	LEU	CB-CG-CD2	-6.07	92.49	110.70
24	Q	67	THR	CA-C-N	6.07	132.62	121.70
24	Q	67	THR	C-N-CA	6.07	132.62	121.70
21	N	38	GLU	CA-CB-CG	-6.07	101.97	114.10
9	i	118	LYS	CD-CE-NZ	6.06	131.29	111.90
9	2	118	LYS	CD-CE-NZ	6.06	131.30	111.90
14	n	110	ASP	CB-CA-C	-6.01	98.47	110.42
21	N	528	ARG	CA-C-N	6.01	133.01	121.54
21	N	528	ARG	C-N-CA	6.01	133.01	121.54
4	D	204	GLN	N-CA-C	5.97	123.52	110.80
21	N	861	TYR	N-CA-C	-5.97	98.08	110.80
4	d	101	GLU	N-CA-C	-5.96	98.10	110.80
23	P	332	GLU	CB-CG-CD	-5.94	102.50	112.60
16	V	190	HIS	CB-CG-CD2	-5.93	123.49	131.20
9	i	251	ASP	CA-CB-CG	-5.92	106.69	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	69	TYR	CA-CB-CG	5.91	124.53	113.90
7	g	63	LYS	CD-CE-NZ	5.90	130.79	111.90
25	R	125	GLU	N-CA-C	5.90	123.37	110.80
14	7	136	ARG	CG-CD-NE	-5.90	99.02	112.00
10	j	69	TYR	CA-CB-CG	5.90	124.51	113.90
7	G	63	LYS	CD-CE-NZ	5.89	130.76	111.90
9	2	251	ASP	CA-CB-CG	-5.89	106.71	112.60
23	P	166	GLU	OE1-CD-OE2	-5.88	108.78	122.90
11	4	110	LYS	CA-CB-CG	-5.88	102.34	114.10
11	k	1	MET	N-CA-C	-5.88	94.54	111.00
11	4	1	MET	N-CA-C	-5.88	94.55	111.00
21	N	327	LEU	CB-CA-C	-5.87	101.05	110.79
11	k	110	LYS	CA-CB-CG	-5.87	102.36	114.10
11	4	110	LYS	CD-CE-NZ	-5.87	93.12	111.90
11	k	110	LYS	CD-CE-NZ	-5.86	93.14	111.90
20	Z	759	ARG	CB-CG-CD	5.86	124.77	111.30
13	m	177	LYS	CD-CE-NZ	-5.83	93.25	111.90
13	6	177	LYS	CD-CE-NZ	-5.83	93.25	111.90
16	V	190	HIS	N-CA-CB	5.82	118.78	110.16
14	n	117	GLU	CB-CA-C	5.82	119.33	110.37
9	2	252	ILE	CA-CB-CG2	5.80	120.35	110.50
5	e	210	GLU	N-CA-C	-5.79	98.46	110.80
13	m	46	ARG	NE-CZ-NH1	5.79	127.29	121.50
5	E	210	GLU	N-CA-C	-5.79	98.47	110.80
9	i	252	ILE	CA-CB-CG2	5.79	120.34	110.50
20	Z	5	SER	N-CA-C	-5.79	98.48	110.80
14	7	140	MET	CB-CG-SD	5.77	130.00	112.70
12	5	82	ARG	CG-CD-NE	5.76	124.68	112.00
12	l	82	ARG	CG-CD-NE	5.76	124.67	112.00
20	Z	366	LYS	N-CA-C	-5.75	98.55	110.80
20	Z	9	GLN	CG-CD-NE2	-5.74	107.79	116.40
8	h	130	LYS	CD-CE-NZ	5.73	130.25	111.90
14	n	136	ARG	CG-CD-NE	-5.73	99.40	112.00
13	6	46	ARG	NE-CZ-NH1	5.72	127.22	121.50
8	1	130	LYS	CD-CE-NZ	5.72	130.21	111.90
20	Z	918	ASP	CA-C-N	5.71	130.40	120.68
20	Z	918	ASP	C-N-CA	5.71	130.40	120.68
20	Z	512	ILE	CA-CB-CG2	-5.71	100.79	110.50
4	d	4	TYR	N-CA-C	-5.71	95.02	111.00
4	D	182	LYS	N-CA-CB	-5.71	101.69	110.20
12	5	156	LYS	CD-CE-NZ	5.70	130.15	111.90
12	l	156	LYS	CD-CE-NZ	5.69	130.12	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	161	ILE	N-CA-CB	-5.67	103.92	110.55
16	V	286	GLU	CB-CG-CD	5.65	122.21	112.60
1	A	77	ARG	CG-CD-NE	5.64	124.42	112.00
24	Q	107	VAL	N-CA-C	5.63	114.47	108.95
12	5	181	ARG	NE-CZ-NH1	-5.63	115.87	121.50
1	a	77	ARG	CG-CD-NE	5.63	124.38	112.00
26	U	179	ARG	N-CA-C	5.63	122.79	110.80
20	Z	63	LEU	CB-CA-C	-5.63	101.66	110.94
20	Z	824	ASN	CB-CA-C	5.63	118.86	109.80
11	k	4	ILE	CG1-CB-CG2	-5.62	93.83	110.70
14	7	136	ARG	CB-CG-CD	5.62	124.23	111.30
20	Z	759	ARG	NE-CZ-NH2	5.62	124.26	119.20
11	4	4	ILE	CG1-CB-CG2	-5.62	93.84	110.70
3	c	9	ARG	CG-CD-NE	5.61	124.35	112.00
3	C	9	ARG	CG-CD-NE	5.61	124.34	112.00
4	d	228	GLU	CA-CB-CG	-5.61	102.89	114.10
5	E	134	MET	CB-CG-SD	5.60	129.51	112.70
5	e	134	MET	CB-CG-SD	5.60	129.50	112.70
10	j	80	ARG	CG-CD-NE	-5.60	99.68	112.00
10	3	80	ARG	CG-CD-NE	-5.60	99.68	112.00
13	6	226	GLU	CA-CB-CG	-5.60	102.91	114.10
13	m	226	GLU	CA-CB-CG	-5.59	102.91	114.10
12	l	181	ARG	NE-CZ-NH1	-5.58	115.92	121.50
24	Q	47	ASP	CA-C-N	5.58	132.19	121.54
24	Q	47	ASP	C-N-CA	5.58	132.19	121.54
22	S	211	ARG	N-CA-CB	-5.57	101.93	110.12
9	i	58	LYS	CD-CE-NZ	-5.56	94.10	111.90
9	2	58	LYS	CD-CE-NZ	-5.55	94.12	111.90
14	n	118	GLU	N-CA-C	-5.54	105.83	112.59
12	5	182	LYS	CD-CE-NZ	5.54	129.62	111.90
22	S	261	HIS	CB-CG-CD2	-5.53	124.01	131.20
12	l	182	LYS	CD-CE-NZ	5.53	129.60	111.90
12	5	107	LYS	CD-CE-NZ	5.52	129.56	111.90
5	E	211	LYS	N-CA-CB	-5.51	102.03	110.85
12	l	107	LYS	CD-CE-NZ	5.51	129.52	111.90
7	G	208	LYS	N-CA-CB	-5.50	102.03	110.44
5	e	211	LYS	N-CA-CB	-5.49	102.07	110.85
20	Z	21	GLU	CA-CB-CG	-5.48	103.13	114.10
7	g	208	LYS	N-CA-CB	-5.48	102.05	110.44
4	d	102	ASP	CB-CA-C	-5.48	99.38	110.17
20	Z	258	PRO	N-CA-C	5.42	117.31	110.70
13	m	182	TYR	CA-CB-CG	-5.41	104.16	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	59	ASP	N-CA-C	5.41	122.32	110.80
2	b	234	ARG	CB-CG-CD	5.40	123.72	111.30
2	B	215	GLY	N-CA-C	-5.39	102.19	110.77
5	e	15	PHE	CA-C-N	5.39	131.39	121.70
5	e	15	PHE	C-N-CA	5.39	131.39	121.70
14	n	117	GLU	N-CA-CB	-5.39	100.75	110.88
2	B	234	ARG	CB-CG-CD	5.38	123.69	111.30
13	6	182	TYR	CA-CB-CG	-5.38	104.21	113.90
5	E	15	PHE	CA-C-N	5.37	131.37	121.70
5	E	15	PHE	C-N-CA	5.37	131.37	121.70
20	Z	145	ASP	CA-CB-CG	5.37	117.97	112.60
8	1	153	GLU	CA-CB-CG	5.37	124.84	114.10
8	h	153	GLU	CA-CB-CG	5.37	124.83	114.10
20	Z	759	ARG	CD-NE-CZ	-5.36	116.90	124.40
25	R	96	GLN	CA-CB-CG	-5.35	103.39	114.10
2	b	215	GLY	N-CA-C	-5.34	102.28	110.77
7	g	71	ASP	N-CA-CB	5.32	119.48	110.49
16	V	164	LEU	CA-C-N	5.31	127.74	120.46
16	V	164	LEU	C-N-CA	5.31	127.74	120.46
27	O	88	ASP	CB-CG-OD2	5.31	130.61	118.40
9	2	200	SER	N-CA-C	5.31	122.10	110.80
9	i	200	SER	N-CA-C	5.30	122.10	110.80
10	3	193	ASP	CB-CA-C	-5.30	100.12	109.02
7	G	71	ASP	N-CA-CB	5.30	119.44	110.49
10	3	204	GLN	OE1-CD-NE2	-5.30	117.30	122.60
10	j	193	ASP	CB-CA-C	-5.29	100.13	109.02
9	2	109	LEU	CB-CG-CD1	-5.29	94.82	110.70
9	i	109	LEU	CB-CG-CD1	-5.29	94.83	110.70
4	D	101	GLU	N-CA-C	-5.29	99.53	110.80
4	d	146	LYS	CA-CB-CG	-5.29	103.52	114.10
13	m	122	LEU	CD1-CG-CD2	-5.28	99.19	110.80
20	Z	309	GLN	N-CA-C	5.27	122.03	110.80
12	l	206	SER	CA-CB-OG	5.27	121.64	111.10
20	Z	728	LYS	CA-CB-CG	5.27	124.63	114.10
10	j	161	GLU	CA-CB-CG	-5.26	103.58	114.10
12	5	206	SER	CA-CB-OG	5.25	121.61	111.10
9	i	86	GLN	OE1-CD-NE2	-5.25	117.35	122.60
13	6	122	LEU	CD1-CG-CD2	-5.25	99.25	110.80
8	h	93	GLU	CA-CB-CG	5.25	124.59	114.10
20	Z	366	LYS	N-CA-CB	5.25	119.36	110.49
10	3	161	GLU	CA-CB-CG	-5.25	103.61	114.10
1	A	188	LYS	CD-CE-NZ	-5.24	95.12	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	4	19	LYS	CG-CD-CE	5.23	123.34	111.30
1	a	188	LYS	CD-CE-NZ	-5.23	95.17	111.90
8	1	93	GLU	CA-CB-CG	5.23	124.55	114.10
20	Z	738	TYR	CA-CB-CG	5.23	123.31	113.90
22	S	211	ARG	NE-CZ-NH1	-5.23	116.27	121.50
10	j	204	GLN	OE1-CD-NE2	-5.22	117.38	122.60
11	k	19	LYS	CG-CD-CE	5.22	123.31	111.30
20	Z	738	TYR	CB-CA-C	-5.22	102.13	110.79
9	2	254	GLU	CA-CB-CG	5.21	124.52	114.10
1	a	131	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	A	131	ARG	NE-CZ-NH2	5.20	123.88	119.20
2	b	234	ARG	CG-CD-NE	-5.20	100.56	112.00
2	B	234	ARG	CG-CD-NE	-5.20	100.57	112.00
9	2	86	GLN	OE1-CD-NE2	-5.19	117.41	122.60
24	Q	51	ARG	N-CA-C	5.19	121.85	110.80
9	i	254	GLU	CA-CB-CG	5.19	124.47	114.10
21	N	913	PRO	CA-C-N	5.19	130.63	122.33
21	N	913	PRO	C-N-CA	5.19	130.63	122.33
12	5	196	ARG	CD-NE-CZ	5.16	131.63	124.40
20	Z	942	PRO	CA-C-N	5.16	130.26	122.99
20	Z	942	PRO	C-N-CA	5.16	130.26	122.99
8	h	149	LYS	CD-CE-NZ	5.15	128.38	111.90
8	1	149	LYS	CD-CE-NZ	5.14	128.35	111.90
20	Z	170	GLU	CG-CD-OE1	5.14	130.22	118.40
20	Z	617	ILE	CA-C-N	5.13	127.16	120.28
20	Z	617	ILE	C-N-CA	5.13	127.16	120.28
10	3	39	LYS	CG-CD-CE	5.12	123.08	111.30
12	l	196	ARG	CD-NE-CZ	5.12	131.57	124.40
16	V	208	LYS	CD-CE-NZ	-5.12	95.51	111.90
10	j	39	LYS	CG-CD-CE	5.12	123.07	111.30
16	V	61	TYR	N-CA-C	-5.12	106.16	114.09
12	l	181	ARG	CA-CB-CG	-5.11	103.87	114.10
20	Z	79	THR	CA-C-N	5.11	131.31	121.54
20	Z	79	THR	C-N-CA	5.11	131.31	121.54
12	5	181	ARG	CA-CB-CG	-5.11	103.88	114.10
17	T	251	HIS	N-CA-C	-5.11	106.60	114.16
20	Z	376	SER	CB-CA-C	-5.10	100.27	110.42
11	4	86	GLN	OE1-CD-NE2	-5.10	117.50	122.60
25	R	375	LYS	CA-C-N	5.10	129.95	121.99
25	R	375	LYS	C-N-CA	5.10	129.95	121.99
16	V	204	HIS	CA-CB-CG	5.09	118.89	113.80
7	g	101	LYS	CA-CB-CG	-5.08	103.95	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	127	GLN	CB-CA-C	-5.07	102.70	110.81
6	f	117	GLN	N-CA-CB	-5.06	102.68	110.12
6	F	117	GLN	N-CA-CB	-5.06	102.68	110.12
11	k	86	GLN	OE1-CD-NE2	-5.05	117.55	122.60
22	S	100	HIS	N-CA-C	-5.05	108.39	114.75
25	R	376	GLN	N-CA-C	-5.05	105.91	113.89
11	k	90	LYS	CD-CE-NZ	-5.05	95.74	111.90
20	Z	557	GLU	CB-CA-C	-5.04	101.37	110.35
7	G	101	LYS	CA-CB-CG	-5.04	104.02	114.10
11	4	90	LYS	CD-CE-NZ	-5.04	95.77	111.90
7	g	207	ASN	CA-C-N	5.04	131.50	122.38
7	g	207	ASN	C-N-CA	5.04	131.50	122.38
7	G	207	ASN	CA-C-N	5.04	131.50	122.38
7	G	207	ASN	C-N-CA	5.04	131.50	122.38
25	R	72	VAL	N-CA-C	5.04	119.81	109.34
15	W	194	GLU	CA-CB-CG	5.03	124.16	114.10
20	Z	911	LYS	N-CA-CB	5.01	120.03	111.66
20	Z	33	GLU	CB-CA-C	-5.01	103.03	112.00
9	i	168	GLU	CA-CB-CG	-5.01	104.08	114.10
20	Z	432	GLY	CA-C-N	5.01	127.69	120.38
20	Z	432	GLY	C-N-CA	5.01	127.69	120.38
1	a	130	GLN	OE1-CD-NE2	-5.00	117.59	122.60
24	Q	110	SER	N-CA-C	-5.00	100.15	110.80

There are no chirality outliers.

All (101) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	30	THR	Peptide
9	2	199	GLY	Peptide
9	2	252	ILE	Peptide
9	2	253	GLN	Peptide
12	5	148	ARG	Sidechain
5	E	15	PHE	Peptide
6	F	13	PHE	Peptide
6	F	18	ARG	Peptide
6	F	204	GLU	Peptide
7	G	13	SER	Peptide
7	G	70	VAL	Mainchain
21	N	33	ASP	Sidechain
21	N	87	ASP	Mainchain
23	P	128	ASN	Sidechain

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Mol	Chain	Res	Type	Group
23	P	166	GLU	Sidechain
23	P	73	ASP	Sidechain
24	Q	109	ASP	Peptide
24	Q	404	ASN	Peptide
24	Q	50	ARG	Peptide
24	Q	67	THR	Peptide
25	R	125	GLU	Sidechain
22	S	153	GLU	Sidechain
22	S	488	GLN	Sidechain
17	T	133	ILE	Peptide
17	T	137	GLU	Peptide
17	T	138	ASP	Sidechain
17	T	247	ASP	Sidechain
17	T	251	HIS	Peptide
17	T	253	GLU	Sidechain
16	V	175	SER	Peptide
16	V	190	HIS	Sidechain
16	V	270	TYR	Peptide
16	V	59	ASP	Peptide
15	W	124	GLU	Sidechain
15	W	194	GLU	Sidechain
18	X	123	ASN	Sidechain
18	X	131	ASN	Sidechain
18	X	41	GLU	Sidechain
19	Y	3	THR	Peptide
19	Y	31	GLU	Peptide
19	Y	52	ASN	Sidechain
20	Z	104	ASP	Sidechain
20	Z	108	ASP	Sidechain
20	Z	138	ARG	Sidechain
20	Z	142	ASP	Sidechain,Mainchain
20	Z	174	GLU	Mainchain
20	Z	219	ASP	Sidechain
20	Z	222	ASP	Sidechain
20	Z	239	GLU	Sidechain
20	Z	260	GLU	Sidechain
20	Z	272	TYR	Sidechain
20	Z	321	PHE	Sidechain
20	Z	328	ASP	Sidechain
20	Z	33	GLU	Sidechain
20	Z	356	ASP	Sidechain
20	Z	363	ASP	Sidechain

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Mol	Chain	Res	Type	Group
20	Z	369	PHE	Sidechain
20	Z	394	TYR	Sidechain
20	Z	4	GLU	Peptide
20	Z	408	TYR	Sidechain
20	Z	413	ASP	Sidechain
20	Z	468	GLU	Sidechain
20	Z	503	ASP	Sidechain
20	Z	550	PHE	Sidechain
20	Z	583	ASP	Sidechain
20	Z	592	GLU	Sidechain
20	Z	633	GLU	Sidechain
20	Z	634	ASP	Sidechain
20	Z	65	GLU	Sidechain
20	Z	718	ASP	Sidechain
20	Z	727	GLU	Peptide
20	Z	73	GLU	Sidechain
20	Z	750	GLU	Sidechain
20	Z	787	ASP	Sidechain
20	Z	793	PHE	Sidechain
20	Z	799	PHE	Sidechain
20	Z	810	ASN	Sidechain
20	Z	852	GLN	Sidechain
20	Z	9	GLN	Sidechain
20	Z	91	PHE	Sidechain
20	Z	921	GLU	Sidechain
4	d	100	LEU	Peptide
4	d	151	GLU	Sidechain
4	d	18	PHE	Sidechain
4	d	203	VAL	Peptide
4	d	218	ASP	Sidechain
4	d	228	GLU	Sidechain
4	d	231	GLN	Sidechain
4	d	235	GLN	Sidechain
5	e	15	PHE	Peptide
6	f	13	PHE	Peptide
6	f	18	ARG	Peptide
6	f	204	GLU	Peptide
7	g	13	SER	Peptide
7	g	70	VAL	Mainchain
8	h	30	THR	Peptide
9	i	199	GLY	Peptide
9	i	252	ILE	Peptide

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Mol	Chain	Res	Type	Group
9	i	253	GLN	Peptide
12	l	148	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1907	0	1901	64	0
1	a	1907	0	1901	41	0
2	B	1907	0	1917	67	0
2	b	1907	0	1917	83	0
3	C	1904	0	1901	32	0
3	c	1904	0	1901	37	0
4	D	1850	0	1862	52	0
4	d	1850	0	1862	44	0
5	E	1882	0	1851	47	0
5	e	1882	0	1851	51	0
6	F	1773	0	1775	30	0
6	f	1773	0	1775	45	0
7	G	1885	0	1876	49	0
7	g	1885	0	1876	44	0
8	1	1512	0	1478	89	0
8	h	1512	0	1478	66	0
9	2	1719	0	1716	132	0
9	i	1719	0	1716	124	0
10	3	1581	0	1571	95	0
10	j	1581	0	1571	93	0
11	4	1561	0	1569	94	0
11	k	1561	0	1569	91	0
12	5	1644	0	1592	83	0
12	l	1644	0	1592	96	0
13	6	1757	0	1708	95	0
13	m	1757	0	1708	121	0
14	7	1790	0	1790	51	0
14	n	1790	0	1790	63	0
15	W	1534	0	1542	14	0
16	V	2274	0	2273	308	0
17	T	2192	0	2161	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	X	1032	0	1017	9	0
19	Y	731	0	675	14	0
20	Z	7005	0	6932	80	0
21	N	6418	0	6487	90	0
22	S	3894	0	3938	70	0
23	P	3608	0	3694	86	0
24	Q	3499	0	3524	49	0
25	R	3258	0	3263	34	0
26	U	2306	0	2331	231	0
27	O	3186	0	3213	64	0
All	All	90281	0	90064	2298	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 13.

All (2298) 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)
16:V:208:LYS:NZ	26:U:19:LEU:HD21	1.23	1.43
16:V:303:VAL:CG1	27:O:380:LEU:HB2	1.57	1.32
16:V:208:LYS:HZ1	26:U:19:LEU:CD2	1.44	1.29
16:V:303:VAL:CB	27:O:380:LEU:HD22	1.62	1.27
16:V:214:MET:O	26:U:179:ARG:NH1	1.70	1.25
16:V:295:VAL:HG11	17:T:263:ALA:CB	1.67	1.24
1:A:251:GLN:O	23:P:84:LYS:NZ	1.70	1.23
13:m:46:ARG:NH2	9:2:193:TRP:O	1.71	1.23
16:V:303:VAL:HG11	27:O:380:LEU:CB	1.68	1.22
3:C:142:ASP:OD1	11:4:110:LYS:NZ	1.75	1.18
16:V:296:LEU:CD1	26:U:193:GLN:HG2	1.75	1.17
16:V:300:VAL:HG21	26:U:193:GLN:NE2	1.55	1.17
16:V:218:LYS:NZ	26:U:132:LEU:H	1.42	1.15
16:V:303:VAL:HB	27:O:380:LEU:CD2	1.76	1.15
5:e:104:ASP:OD2	13:m:99:ARG:NE	1.79	1.15
16:V:208:LYS:NZ	26:U:19:LEU:CD2	2.05	1.15
16:V:214:MET:HA	26:U:179:ARG:CZ	1.78	1.14
16:V:280:LEU:CD2	26:U:268:LYS:HE2	1.78	1.13
20:Z:40:GLU:HB3	20:Z:44:LYS:HZ1	0.98	1.13
16:V:209:GLU:HG2	26:U:16:LEU:CD2	1.78	1.12
4:d:90:ARG:O	4:d:94:GLN:NE2	1.83	1.12
1:A:249:ALA:HA	23:P:84:LYS:CB	1.80	1.12
1:A:249:ALA:HB2	23:P:85:LYS:N	1.63	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:205:LYS:NZ	26:U:174:LEU:O	1.81	1.11
16:V:205:LYS:NZ	26:U:174:LEU:C	2.10	1.10
16:V:210:THR:HG23	26:U:175:LEU:HD11	1.30	1.10
16:V:214:MET:HA	26:U:179:ARG:NH2	1.67	1.10
16:V:303:VAL:HG21	27:O:380:LEU:HD13	1.26	1.09
16:V:292:ILE:HG21	26:U:186:LEU:HD11	1.17	1.09
16:V:177:THR:CG2	21:N:740:TRP:O	2.01	1.08
10:j:101:GLY:O	11:k:93:ARG:NH2	1.85	1.08
4:D:11:PHE:CE2	5:E:26:TYR:HB2	1.87	1.08
16:V:94:MET:SD	26:U:75:ASN:HB3	1.94	1.07
16:V:213:LEU:HD23	26:U:171:VAL:HG22	1.30	1.07
16:V:209:GLU:HG2	26:U:16:LEU:HD22	1.30	1.07
16:V:300:VAL:HG13	26:U:197:LEU:HD13	1.37	1.06
16:V:304:ALA:HB1	27:O:377:VAL:HG22	1.37	1.05
16:V:296:LEU:HD21	26:U:193:GLN:CB	1.86	1.05
4:d:141:ARG:HH21	12:l:182:LYS:HE2	1.21	1.04
16:V:303:VAL:HG11	27:O:380:LEU:HB2	1.06	1.04
16:V:214:MET:HG3	26:U:179:ARG:CD	1.86	1.04
16:V:213:LEU:HD22	26:U:171:VAL:HA	1.34	1.04
16:V:280:LEU:HD22	26:U:268:LYS:HE2	1.36	1.04
16:V:303:VAL:CG1	27:O:380:LEU:CB	2.31	1.03
16:V:213:LEU:CB	26:U:171:VAL:HG13	1.89	1.02
16:V:210:THR:HG23	26:U:175:LEU:CD1	1.90	1.02
16:V:296:LEU:HD21	26:U:193:GLN:HB3	1.41	1.01
16:V:296:LEU:CD2	26:U:193:GLN:HB2	1.90	1.01
16:V:32:ILE:HD11	26:U:16:LEU:HB3	1.38	1.01
16:V:205:LYS:HE2	26:U:174:LEU:HB3	1.41	1.01
1:A:249:ALA:HA	23:P:84:LYS:HB2	1.37	1.01
6:F:117:GLN:NE2	7:G:84:ASP:OD2	1.93	1.01
16:V:296:LEU:HD11	26:U:193:GLN:HG2	1.39	1.01
20:Z:30:LYS:HZ2	20:Z:44:LYS:NZ	1.56	1.01
2:B:99:ARG:HH21	9:2:90:SER:HB2	1.21	1.00
16:V:213:LEU:HB3	26:U:171:VAL:HG13	1.40	1.00
16:V:205:LYS:HZ1	26:U:174:LEU:C	1.65	1.00
16:V:303:VAL:HG11	27:O:380:LEU:CG	1.91	1.00
16:V:303:VAL:HB	27:O:380:LEU:HD22	1.02	1.00
11:4:35:THR:HG21	11:4:182:LYS:NZ	1.77	1.00
16:V:94:MET:CE	26:U:75:ASN:HB3	1.91	1.00
11:k:35:THR:HG21	11:k:182:LYS:NZ	1.77	1.00
16:V:300:VAL:HG21	26:U:193:GLN:CD	1.86	1.00
16:V:100:ARG:HE	26:U:53:ALA:HB3	1.23	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:304:ALA:HA	27:O:377:VAL:HA	1.45	0.99
3:c:142:ASP:OD1	11:k:110:LYS:NZ	1.98	0.97
16:V:225:LEU:HD13	23:P:423:LEU:CD2	1.94	0.97
20:Z:40:GLU:HB3	20:Z:44:LYS:NZ	1.80	0.96
16:V:205:LYS:NZ	26:U:175:LEU:HA	1.80	0.96
16:V:205:LYS:CE	26:U:174:LEU:O	2.15	0.95
9:i:48:ARG:NH2	13:6:230:ASP:OD2	2.00	0.94
16:V:218:LYS:HZ3	26:U:132:LEU:N	1.64	0.94
13:m:46:ARG:HH22	9:2:193:TRP:C	1.75	0.93
16:V:303:VAL:HG21	27:O:380:LEU:CD1	1.97	0.93
16:V:292:ILE:HG21	26:U:186:LEU:CD1	1.97	0.93
10:j:205:ASP:OD2	12:5:94:ARG:NH2	2.02	0.93
1:A:249:ALA:CA	23:P:84:LYS:HB2	1.98	0.93
16:V:295:VAL:HG11	17:T:263:ALA:HB2	1.51	0.93
16:V:213:LEU:CD2	26:U:171:VAL:HG22	1.98	0.92
2:b:90:ARG:O	2:b:94:HIS:HD2	1.51	0.92
16:V:177:THR:HG21	21:N:740:TRP:O	1.67	0.92
14:n:226:ARG:NH1	8:1:203:GLU:OE2	2.01	0.92
4:D:11:PHE:CZ	5:E:26:TYR:HB2	2.04	0.92
16:V:209:GLU:CG	26:U:16:LEU:HD22	1.98	0.91
2:B:90:ARG:O	2:B:94:HIS:HD2	1.51	0.91
16:V:303:VAL:CG1	27:O:380:LEU:HD22	2.01	0.90
25:R:335:ARG:CZ	25:R:376:GLN:HG2	2.01	0.90
16:V:296:LEU:CG	26:U:193:GLN:HG2	2.01	0.90
1:A:249:ALA:HB2	23:P:85:LYS:CA	2.01	0.90
16:V:32:ILE:HD11	26:U:16:LEU:CB	2.02	0.90
12:l:84:GLN:HE22	12:l:221:TRP:NE1	1.70	0.89
16:V:296:LEU:CD2	26:U:193:GLN:CB	2.46	0.89
12:5:102:ALA:O	13:6:145:ARG:NH1	2.05	0.89
9:i:254:GLU:OE1	9:i:254:GLU:N	2.06	0.89
4:D:66:LYS:CD	11:4:69:ILE:HD11	2.03	0.89
16:V:94:MET:HE1	26:U:75:ASN:HB3	1.53	0.89
9:i:244:GLU:HG3	10:j:198:ARG:HG2	1.53	0.88
16:V:293:VAL:HG21	26:U:189:ARG:CZ	2.03	0.88
12:5:84:GLN:HE22	12:5:221:TRP:NE1	1.70	0.88
13:m:228:LYS:HE3	9:2:223:ASN:HB3	1.55	0.88
16:V:304:ALA:CB	27:O:377:VAL:HG22	2.03	0.88
16:V:293:VAL:HG21	26:U:189:ARG:NH1	1.88	0.88
9:2:254:GLU:N	9:2:254:GLU:OE1	2.06	0.88
16:V:214:MET:HG3	26:U:179:ARG:HD3	1.56	0.88
16:V:296:LEU:HG	26:U:193:GLN:CG	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:145:ASP:HA	20:Z:149:TRP:HE1	1.37	0.88
12:l:102:ALA:O	13:m:145:ARG:NH1	2.06	0.87
6:F:164:ARG:NH2	6:F:204:GLU:OE2	2.07	0.87
6:f:164:ARG:NH2	6:f:204:GLU:OE2	2.07	0.87
12:l:139:ARG:NH1	12:l:142:GLU:OE2	2.08	0.87
15:W:122:ARG:HB2	15:W:153:LEU:HD22	1.57	0.87
16:V:280:LEU:CD2	26:U:268:LYS:CE	2.51	0.87
9:i:249:ILE:HD12	10:j:48:HIS:HB3	1.57	0.86
16:V:208:LYS:CE	26:U:19:LEU:HD21	2.04	0.86
16:V:208:LYS:HZ3	26:U:19:LEU:HD21	1.34	0.86
11:k:2:ASP:HB2	11:k:47:ALA:HB1	1.56	0.86
12:5:139:ARG:NH1	12:5:142:GLU:OE2	2.08	0.86
2:b:2:THR:HG22	2:b:3:ASP:H	1.40	0.86
2:B:2:THR:HG22	2:B:3:ASP:H	1.40	0.86
16:V:295:VAL:HG11	17:T:263:ALA:HB1	1.57	0.86
1:A:149:GLU:OE1	9:2:104:ARG:NH2	2.08	0.86
11:4:2:ASP:HB2	11:4:47:ALA:HB1	1.56	0.85
16:V:303:VAL:CG1	27:O:380:LEU:CG	2.54	0.85
16:V:205:LYS:HE2	26:U:174:LEU:CB	2.06	0.85
21:N:4:THR:CG2	22:S:211:ARG:HG2	2.06	0.85
1:A:30:TYR:HB3	7:G:15:PHE:CD2	2.12	0.84
16:V:214:MET:SD	26:U:179:ARG:HG2	2.17	0.84
4:D:181:ARG:NE	5:E:60:GLU:OE2	2.10	0.84
16:V:280:LEU:HD23	26:U:268:LYS:HE2	1.58	0.84
6:f:117:GLN:NE2	7:g:84:ASP:OD2	2.10	0.84
3:c:66:LEU:CD1	3:c:212:GLU:HB3	2.08	0.84
6:f:66:CYS:O	13:m:85:PHE:HE1	1.60	0.84
11:k:35:THR:HG21	11:k:182:LYS:HZ2	1.41	0.84
3:C:66:LEU:CD1	3:C:212:GLU:HB3	2.08	0.84
13:6:178:LYS:HD2	13:6:179:PRO:HD2	1.59	0.84
16:V:205:LYS:CE	26:U:174:LEU:C	2.49	0.84
14:n:255:ALA:O	8:1:183:ARG:NH2	2.10	0.84
11:4:30:ASP:HB2	11:4:177:LYS:HG3	1.60	0.84
13:m:178:LYS:HD2	13:m:179:PRO:HD2	1.59	0.84
4:d:149:GLN:HG3	4:d:149:GLN:O	1.77	0.83
16:V:280:LEU:HD22	26:U:268:LYS:CE	2.08	0.83
11:k:30:ASP:HB2	11:k:177:LYS:HG3	1.60	0.83
16:V:225:LEU:HB3	23:P:423:LEU:HD11	1.58	0.83
11:k:170:LYS:HD3	11:k:171:ARG:HH21	1.43	0.83
4:D:66:LYS:CE	11:4:69:ILE:HD11	2.09	0.83
12:l:286:ILE:HG23	10:3:38:ASN:OD1	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:230:ASP:OD1	9:2:48:ARG:NH1	2.12	0.83
13:m:142:GLU:OE2	13:m:145:ARG:NE	2.11	0.82
13:6:142:GLU:OE2	13:6:145:ARG:NE	2.11	0.82
6:f:15:PRO:HB3	7:g:26:TYR:CD1	2.14	0.82
11:4:170:LYS:HD3	11:4:171:ARG:HH21	1.43	0.82
16:V:306:LYS:OXT	27:O:376:GLN:HB3	1.78	0.82
12:5:103:SER:OG	13:6:145:ARG:NH2	2.13	0.82
16:V:225:LEU:HB3	23:P:423:LEU:CD1	2.10	0.82
20:Z:40:GLU:CB	20:Z:44:LYS:HZ1	1.87	0.82
16:V:305:ILE:C	16:V:306:LYS:OXT	2.20	0.82
16:V:225:LEU:HD13	23:P:423:LEU:HD21	1.63	0.81
1:A:30:TYR:HB3	7:G:15:PHE:HD2	1.45	0.81
1:A:237:SER:OG	1:A:240:ASN:OD1	1.99	0.81
5:E:242:GLU:O	5:E:246:LYS:NZ	2.14	0.81
14:n:160:LEU:HG	14:n:175:LEU:HD12	1.63	0.81
8:h:100:ASP:OD1	14:n:35:GLN:N	2.12	0.81
11:4:35:THR:HG21	11:4:182:LYS:HZ1	1.46	0.81
25:R:113:LEU:O	25:R:117:ILE:HD12	1.80	0.81
16:V:213:LEU:HD22	26:U:171:VAL:CA	2.11	0.81
4:d:141:ARG:NE	12:l:182:LYS:HB3	1.95	0.80
16:V:31:SER:OG	26:U:174:LEU:HD13	1.81	0.80
11:k:175:ASP:OD1	11:4:175:ASP:OD1	1.98	0.80
1:a:237:SER:OG	1:a:240:ASN:OD1	1.99	0.80
16:V:303:VAL:CG2	27:O:380:LEU:HD13	2.07	0.80
13:m:47:TYR:CE2	13:m:49:PRO:HD3	2.17	0.80
4:d:111:ARG:NH1	12:l:145:GLU:OE2	2.14	0.80
20:Z:30:LYS:NZ	20:Z:44:LYS:NZ	2.29	0.80
16:V:218:LYS:HZ3	26:U:132:LEU:H	0.80	0.80
16:V:215:ASN:OD1	26:U:181:GLN:OE1	1.99	0.80
16:V:210:THR:CG2	26:U:175:LEU:HD11	2.11	0.79
9:2:250:CYS:SG	10:3:193:ASP:O	2.39	0.79
13:6:47:TYR:CE2	13:6:49:PRO:HD3	2.17	0.79
16:V:205:LYS:NZ	26:U:175:LEU:CA	2.45	0.79
21:N:360:GLN:O	21:N:361:ASN:O	2.01	0.79
21:N:280:GLN:OE1	21:N:282:TYR:OH	2.01	0.79
9:i:238:THR:HB	10:j:165:GLU:OE1	1.83	0.79
5:e:242:GLU:O	5:e:246:LYS:NZ	2.14	0.79
20:Z:30:LYS:NZ	20:Z:44:LYS:HZ3	1.80	0.79
20:Z:146:PHE:H	20:Z:149:TRP:HE1	1.30	0.79
9:i:48:ARG:NH1	13:6:230:ASP:OD1	2.15	0.78
16:V:41:GLY:O	16:V:45:VAL:HG23	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:15:PRO:HA	7:g:26:TYR:HB3	1.63	0.78
13:6:81:LYS:O	13:6:85:PHE:HD2	1.66	0.78
16:V:148:LYS:O	26:U:169:ILE:HG21	1.83	0.78
2:B:172:LYS:HB3	3:C:55:THR:HG21	1.66	0.78
16:V:218:LYS:NZ	26:U:132:LEU:N	2.25	0.78
10:j:67:PHE:HE1	10:j:91:VAL:HG22	1.48	0.78
4:D:11:PHE:HE2	5:E:26:TYR:HB2	1.45	0.78
9:i:249:ILE:HD12	10:j:48:HIS:CB	2.13	0.78
2:b:227:ILE:CG1	9:i:215:TYR:HD2	1.96	0.78
16:V:292:ILE:CG2	26:U:186:LEU:HD11	2.07	0.77
16:V:303:VAL:HG12	27:O:380:LEU:HB2	1.64	0.77
2:B:103:GLU:OE1	10:3:86:THR:HG21	1.84	0.77
20:Z:145:ASP:CG	20:Z:149:TRP:HZ2	1.92	0.77
21:N:4:THR:HG23	22:S:211:ARG:HG2	1.66	0.77
9:i:181:ILE:CG2	9:i:219:TYR:HE2	1.97	0.77
16:V:304:ALA:O	27:O:377:VAL:HG23	1.84	0.77
22:S:475:TYR:CE1	26:U:273:LEU:HB2	2.20	0.77
13:m:81:LYS:O	13:m:85:PHE:HD2	1.66	0.77
8:h:41:ASP:HB2	8:h:183:ARG:HH11	1.50	0.77
16:V:303:VAL:CG1	27:O:380:LEU:CD2	2.62	0.77
16:V:245:VAL:HG13	24:Q:418:GLN:HG3	1.66	0.77
8:1:41:ASP:HB2	8:1:183:ARG:HH11	1.50	0.77
16:V:214:MET:HE3	26:U:181:GLN:CG	2.15	0.77
4:d:122:GLN:O	5:e:134:MET:HB3	1.85	0.77
16:V:94:MET:SD	26:U:75:ASN:CB	2.73	0.77
10:j:145:GLN:NE2	12:5:100:TRP:HB2	1.98	0.77
2:B:108:LYS:NZ	10:3:79:GLU:OE2	2.15	0.77
20:Z:145:ASP:HA	20:Z:149:TRP:NE1	2.00	0.76
14:n:182:HIS:ND1	9:2:161:LEU:HD13	1.99	0.76
9:2:181:ILE:CG2	9:2:219:TYR:HE2	1.97	0.76
10:3:67:PHE:HE1	10:3:91:VAL:HG22	1.48	0.76
13:6:221:ARG:HG2	13:6:221:ARG:HH11	1.50	0.76
16:V:100:ARG:NE	26:U:53:ALA:HB3	2.01	0.76
13:m:221:ARG:HG2	13:m:221:ARG:HH11	1.50	0.76
9:2:252:ILE:HG22	9:2:253:GLN:H	1.50	0.76
5:e:150:ASP:OD2	13:m:90:LYS:NZ	2.18	0.76
9:i:252:ILE:HG22	9:i:253:GLN:H	1.50	0.76
16:V:214:MET:CA	26:U:179:ARG:CZ	2.63	0.76
16:V:300:VAL:HG22	26:U:197:LEU:HD22	1.67	0.76
11:k:2:ASP:CB	11:k:47:ALA:HB1	2.15	0.76
16:V:213:LEU:HB3	26:U:171:VAL:CG1	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:93:ARG:HG2	20:Z:135:LEU:HD13	1.68	0.76
23:P:422:LEU:HD22	26:U:232:VAL:HG13	1.65	0.76
4:D:111:ARG:NH1	12:5:145:GLU:OE2	2.19	0.75
16:V:305:ILE:HA	27:O:373:TRP:NE1	2.01	0.75
14:n:226:ARG:NH1	8:1:203:GLU:CD	2.43	0.75
5:e:198:LEU:HD13	5:e:246:LYS:HE2	1.68	0.75
15:W:148:GLU:O	15:W:149:GLN:HB2	1.84	0.75
3:c:142:ASP:CG	11:k:110:LYS:HZ1	1.93	0.75
16:V:203:TYR:HB3	26:U:174:LEU:HD23	1.68	0.75
11:4:2:ASP:CB	11:4:47:ALA:HB1	2.15	0.75
14:n:256:LYS:HA	8:1:183:ARG:HH22	1.53	0.74
13:6:47:TYR:HE2	13:6:49:PRO:HD3	1.52	0.74
16:V:214:MET:HG3	26:U:179:ARG:NE	2.01	0.74
19:Y:3:THR:O	19:Y:4:ASP:O	2.05	0.74
9:i:211:LYS:HZ2	9:i:211:LYS:HB3	1.53	0.74
5:E:198:LEU:HD13	5:E:246:LYS:HE2	1.68	0.74
11:k:2:ASP:HB2	11:k:47:ALA:CB	2.18	0.74
1:A:95:LEU:CD1	7:G:118:GLN:HG3	2.17	0.74
10:j:141:THR:HB	12:5:99:ASN:HD21	1.51	0.74
12:l:219:TYR:O	12:l:220:LYS:HD3	1.88	0.74
12:5:219:TYR:O	12:5:220:LYS:HD3	1.88	0.74
10:j:29:LEU:HD22	10:j:40:PHE:CE2	2.23	0.74
13:m:46:ARG:HH22	9:2:193:TRP:CA	2.01	0.74
14:n:162:TYR:CE1	14:n:177:THR:HG22	2.23	0.73
2:B:94:HIS:HE1	9:2:93:GLU:HG2	1.53	0.73
13:6:75:ARG:NH2	13:6:113:TYR:OH	2.21	0.73
16:V:215:ASN:OD1	26:U:181:GLN:CD	2.30	0.73
21:N:529:GLN:O	21:N:559:TYR:CE1	2.41	0.73
8:h:45:ARG:HG3	8:h:51:TRP:CE2	2.24	0.73
10:3:29:LEU:HD22	10:3:40:PHE:CE2	2.23	0.73
11:4:2:ASP:HB2	11:4:47:ALA:CB	2.18	0.73
5:e:8:TYR:HB2	5:e:22:PHE:CD2	2.24	0.73
16:V:205:LYS:HE2	26:U:174:LEU:CA	2.17	0.73
16:V:220:GLN:OE1	26:U:181:GLN:OE1	2.05	0.73
4:d:141:ARG:HE	12:l:182:LYS:HB3	1.52	0.73
13:m:47:TYR:HE2	13:m:49:PRO:HD3	1.52	0.73
16:V:214:MET:HE3	26:U:181:GLN:HG3	1.71	0.73
2:b:101:TYR:OH	10:j:70:LYS:CE	2.37	0.73
8:1:45:ARG:HG3	8:1:51:TRP:CE2	2.24	0.73
16:V:40:HIS:NE2	26:U:83:ILE:HG23	2.04	0.73
16:V:306:LYS:OXT	27:O:376:GLN:CB	2.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:252:ILE:CG2	9:2:253:GLN:H	2.02	0.73
16:V:304:ALA:CA	27:O:377:VAL:HG22	2.19	0.73
9:i:150:VAL:HG21	14:7:258:ILE:HG23	1.70	0.72
9:i:161:LEU:HD13	14:7:182:HIS:CD2	2.24	0.72
16:V:303:VAL:HG11	27:O:380:LEU:CD1	2.18	0.72
12:l:113:ASN:HB3	12:l:114:PRO:HD2	1.71	0.72
16:V:296:LEU:HG	26:U:193:GLN:HG2	1.65	0.72
10:j:74:TYR:CE2	10:j:82:ILE:HG13	2.24	0.72
13:m:75:ARG:NH2	13:m:113:TYR:OH	2.21	0.72
8:1:115:ASN:O	8:1:116:LYS:O	2.08	0.72
21:N:736:PHE:O	21:N:739:PHE:HD1	1.71	0.72
5:E:8:TYR:HB2	5:E:22:PHE:CD2	2.24	0.72
16:V:225:LEU:CD1	23:P:423:LEU:HD22	2.19	0.72
8:h:18:LYS:HE2	8:h:154:ASN:HB3	1.70	0.72
9:i:252:ILE:CG2	9:i:253:GLN:H	2.02	0.72
8:h:146:TYR:CE1	8:h:150:ASN:ND2	2.58	0.72
7:G:60:VAL:HG12	7:G:63:LYS:HE2	1.71	0.72
8:h:115:ASN:O	8:h:116:LYS:O	2.08	0.72
11:k:40:PRO:C	11:k:41:HIS:HD1	1.98	0.72
16:V:303:VAL:HG12	27:O:380:LEU:CB	2.19	0.72
16:V:296:LEU:CG	26:U:193:GLN:CG	2.64	0.72
16:V:303:VAL:CB	27:O:380:LEU:CD2	2.47	0.72
12:5:252:LEU:O	12:5:253:TYR:HD1	1.73	0.72
16:V:306:LYS:C	27:O:376:GLN:HB3	2.15	0.72
12:l:252:LEU:O	12:l:253:TYR:HD1	1.73	0.71
1:A:249:ALA:HA	23:P:84:LYS:C	2.14	0.71
2:B:99:ARG:HH21	9:2:90:SER:CB	2.02	0.71
10:3:74:TYR:CE2	10:3:82:ILE:HG13	2.25	0.71
16:V:25:GLU:O	16:V:199:LEU:HD12	1.90	0.71
16:V:32:ILE:CD1	26:U:16:LEU:HB3	2.18	0.71
8:1:146:TYR:CE1	8:1:150:ASN:ND2	2.58	0.71
7:g:60:VAL:HG12	7:g:63:LYS:HE2	1.71	0.71
9:i:126:TYR:HE1	9:i:144:ALA:HB2	1.56	0.71
13:m:230:ASP:OD2	9:2:48:ARG:NH2	2.23	0.71
8:1:18:LYS:HE2	8:1:154:ASN:HB3	1.71	0.71
12:5:113:ASN:HB3	12:5:114:PRO:HD2	1.71	0.71
11:4:35:THR:HG21	11:4:182:LYS:HZ2	1.54	0.71
7:G:184:PRO:O	23:P:3:ARG:HD2	1.90	0.71
9:2:211:LYS:HZ2	9:2:211:LYS:HB3	1.56	0.71
13:6:46:ARG:HB3	13:6:208:ASP:OD2	1.90	0.71
13:m:46:ARG:HB3	13:m:208:ASP:OD2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:82:ARG:NH1	12:l:200:ASP:OD2	2.24	0.71
16:V:296:LEU:HG	26:U:193:GLN:OE1	1.91	0.71
11:k:19:LYS:HD3	11:k:177:LYS:O	1.91	0.71
11:4:19:LYS:HD3	11:4:177:LYS:O	1.91	0.71
11:4:40:PRO:C	11:4:41:HIS:HD1	1.98	0.71
16:V:225:LEU:HD13	23:P:423:LEU:HD22	1.72	0.70
22:S:153:GLU:O	22:S:155:LEU:N	2.23	0.70
16:V:177:THR:HG21	21:N:741:TYR:HA	1.73	0.70
22:S:448:LEU:O	22:S:449:LEU:O	2.09	0.70
9:2:126:TYR:HE1	9:2:144:ALA:HB2	1.56	0.70
12:5:82:ARG:NH1	12:5:200:ASP:OD2	2.24	0.70
16:V:216:LEU:CD1	26:U:168:GLU:OE2	2.38	0.70
16:V:214:MET:CE	26:U:181:GLN:HG2	2.22	0.70
11:k:67:TYR:HE2	11:k:71:GLU:HG3	1.57	0.70
16:V:209:GLU:OE1	26:U:16:LEU:HD13	1.91	0.70
10:3:118:LYS:HB2	10:3:118:LYS:HZ2	1.56	0.70
9:2:211:LYS:HB3	9:2:211:LYS:NZ	2.06	0.70
16:V:217:HIS:CE1	26:U:181:GLN:OE1	2.45	0.70
16:V:305:ILE:HA	27:O:373:TRP:HE1	1.53	0.70
2:b:224:TYR:CZ	9:i:65:ARG:HD2	2.27	0.69
11:k:54:VAL:HG11	12:l:196:ARG:H	1.57	0.69
10:3:67:PHE:CE1	10:3:91:VAL:HG22	2.27	0.69
11:4:67:TYR:HE2	11:4:71:GLU:HG3	1.57	0.69
16:V:300:VAL:CG1	26:U:197:LEU:HD13	2.19	0.69
11:4:137:GLY:O	11:4:141:PHE:HD1	1.75	0.69
13:6:75:ARG:HH22	13:6:108:LYS:HE3	1.57	0.69
11:k:137:GLY:O	11:k:141:PHE:HD1	1.75	0.69
12:l:216:ASP:OD2	11:4:167:GLU:OE2	2.09	0.69
16:V:94:MET:HE1	26:U:75:ASN:CB	2.22	0.69
8:h:165:LYS:HD2	8:h:197:PHE:CD1	2.27	0.69
13:m:75:ARG:HH22	13:m:108:LYS:HE3	1.57	0.69
8:1:165:LYS:HD2	8:1:197:PHE:CD1	2.27	0.69
3:c:66:LEU:HD11	3:c:212:GLU:HB3	1.74	0.69
2:B:189:ILE:HD13	2:B:246:ARG:NH1	2.07	0.69
13:6:208:ASP:OD2	14:7:194:ARG:CZ	2.40	0.69
16:V:32:ILE:CD1	26:U:16:LEU:CB	2.70	0.69
7:g:8:TYR:HA	7:g:14:VAL:HG21	1.75	0.69
2:B:142:PHE:HB3	10:3:80:ARG:NH2	2.08	0.69
7:G:8:TYR:HA	7:G:14:VAL:HG21	1.75	0.69
16:V:292:ILE:HD13	26:U:186:LEU:HD21	1.74	0.69
16:V:306:LYS:C	27:O:376:GLN:CD	2.61	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:306:LYS:HA	27:O:376:GLN:HE22	1.58	0.69
2:b:227:ILE:HG12	9:i:215:TYR:HD2	1.55	0.69
9:i:211:LYS:HB3	9:i:211:LYS:NZ	2.07	0.69
14:n:220:ARG:HD2	8:1:35:ILE:O	1.93	0.69
16:V:209:GLU:CD	26:U:16:LEU:HD22	2.18	0.69
2:b:6:SER:OG	4:d:4:TYR:HB2	1.92	0.69
2:b:189:ILE:HD13	2:b:246:ARG:NH1	2.07	0.69
10:j:67:PHE:CE1	10:j:91:VAL:HG22	2.27	0.69
2:b:101:TYR:OH	10:j:70:LYS:HE3	1.91	0.68
12:l:94:ARG:NH2	10:3:205:ASP:OD2	2.26	0.68
22:S:475:TYR:CE1	26:U:273:LEU:HD13	2.28	0.68
21:N:4:THR:HG22	22:S:211:ARG:HG2	1.72	0.68
5:e:8:TYR:HB2	5:e:22:PHE:CE2	2.28	0.68
16:V:306:LYS:HA	27:O:376:GLN:NE2	2.08	0.68
4:D:66:LYS:HD3	11:4:69:ILE:HD11	1.74	0.68
5:E:8:TYR:HB2	5:E:22:PHE:CE2	2.28	0.68
20:Z:382:ALA:O	20:Z:386:VAL:HG23	1.94	0.68
1:A:249:ALA:CB	23:P:85:LYS:N	2.49	0.68
24:Q:423:VAL:HA	24:Q:426:LEU:HD12	1.76	0.68
9:i:251:ASP:N	9:i:251:ASP:OD1	2.24	0.68
13:m:230:ASP:OXT	9:2:48:ARG:NH1	2.27	0.68
3:C:66:LEU:HD11	3:C:212:GLU:HB3	1.74	0.68
16:V:304:ALA:HB2	26:U:197:LEU:CD1	2.23	0.68
5:e:15:PHE:HA	5:e:16:SER:HB3	1.76	0.68
2:B:100:ILE:O	10:3:90:LEU:HA	1.93	0.68
3:C:142:ASP:CG	11:4:110:LYS:NZ	2.51	0.68
20:Z:146:PHE:H	20:Z:149:TRP:NE1	1.91	0.68
12:l:165:TYR:HB3	12:l:170:LEU:HD21	1.76	0.68
9:i:251:ASP:OD2	9:i:253:GLN:NE2	2.27	0.68
12:l:272:PHE:CE1	10:3:204:GLN:HG2	2.29	0.68
5:E:15:PHE:HA	5:E:16:SER:HB3	1.76	0.68
23:P:44:LYS:HD2	23:P:85:LYS:HE3	1.76	0.68
14:n:35:GLN:O	14:n:144:TRP:CZ3	2.48	0.67
16:V:213:LEU:O	26:U:171:VAL:HG11	1.94	0.67
3:c:9:ARG:NH2	4:d:10:ILE:HD12	2.08	0.67
8:1:114:LYS:C	8:1:115:ASN:OD1	2.37	0.67
16:V:216:LEU:HD13	26:U:168:GLU:CD	2.19	0.67
12:5:165:TYR:HB3	12:5:170:LEU:HD21	1.76	0.67
13:6:81:LYS:O	13:6:85:PHE:CD2	2.48	0.67
16:V:203:TYR:HB3	26:U:174:LEU:CD2	2.24	0.67
20:Z:30:LYS:HZ2	20:Z:44:LYS:CE	2.06	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:150:VAL:HG21	14:7:258:ILE:CG2	2.24	0.67
12:5:183:GLU:HG2	12:5:186:THR:HG21	1.76	0.67
1:a:164:VAL:HG22	2:b:57:MET:O	1.94	0.67
9:i:243:LYS:HE2	12:5:287:GLY:HA2	1.75	0.67
9:i:244:GLU:CG	10:j:198:ARG:HG2	2.23	0.67
13:m:46:ARG:HH21	9:2:193:TRP:HB3	1.60	0.67
9:2:251:ASP:OD2	9:2:253:GLN:NE2	2.27	0.67
15:W:122:ARG:HE	15:W:153:LEU:CD2	2.06	0.67
5:e:150:ASP:CG	13:m:90:LYS:NZ	2.53	0.67
5:e:150:ASP:OD1	13:m:90:LYS:NZ	2.28	0.67
8:h:145:GLY:HA2	8:1:174:TRP:HE1	1.60	0.67
16:V:245:VAL:HG13	24:Q:418:GLN:CG	2.24	0.67
9:i:193:TRP:N	9:i:193:TRP:CD1	2.58	0.67
12:l:214:VAL:HG12	11:4:142:SER:HB2	1.76	0.67
1:A:34:ALA:HB2	7:G:15:PHE:HZ	1.58	0.67
21:N:26:GLU:OE2	21:N:26:GLU:N	2.27	0.67
12:l:148:ARG:HH22	12:l:180:THR:HA	1.58	0.67
10:3:118:LYS:HB2	10:3:118:LYS:NZ	2.10	0.67
13:m:47:TYR:CD1	14:n:195:GLU:OE2	2.48	0.67
1:A:249:ALA:HA	23:P:84:LYS:CA	2.25	0.67
8:h:114:LYS:C	8:h:115:ASN:OD1	2.37	0.67
1:A:246:VAL:HA	23:P:85:LYS:HG3	1.76	0.67
16:V:177:THR:HG22	21:N:740:TRP:O	1.91	0.67
20:Z:562:TRP:O	20:Z:566:LEU:HD23	1.95	0.67
2:b:172:LYS:HB3	3:c:55:THR:HG21	1.77	0.66
12:5:148:ARG:HH22	12:5:180:THR:HA	1.58	0.66
20:Z:30:LYS:HZ2	20:Z:44:LYS:HZ2	1.39	0.66
2:b:224:TYR:CE2	9:i:65:ARG:HD2	2.30	0.66
8:h:199:PRO:HA	8:h:202:TYR:CE1	2.30	0.66
16:V:98:THR:HG23	26:U:72:TYR:CZ	2.31	0.66
25:R:279:LEU:O	25:R:280:ILE:O	2.12	0.66
1:a:164:VAL:HG23	2:b:61:LEU:HB2	1.76	0.66
3:c:4:ARG:HH12	5:e:11:GLY:HA2	1.60	0.66
8:h:85:GLU:HA	8:h:120:TYR:HE2	1.61	0.66
13:m:81:LYS:O	13:m:85:PHE:CD2	2.48	0.66
10:3:149:MET:HG2	10:3:170:ALA:HA	1.77	0.66
13:6:75:ARG:HH22	13:6:108:LYS:CE	2.08	0.66
16:V:296:LEU:HG	26:U:193:GLN:CD	2.20	0.66
12:l:183:GLU:HG2	12:l:186:THR:HG21	1.76	0.66
16:V:216:LEU:HD13	26:U:168:GLU:OE2	1.96	0.66
8:1:199:PRO:HA	8:1:202:TYR:CE1	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:150:ASP:OD1	13:m:90:LYS:CE	2.44	0.66
6:f:15:PRO:HB3	7:g:26:TYR:CG	2.29	0.66
13:m:75:ARG:HH22	13:m:108:LYS:CE	2.09	0.66
11:4:23:ARG:HE	12:5:195:THR:HG21	1.60	0.66
10:j:118:LYS:HB2	10:j:118:LYS:NZ	2.10	0.66
1:A:217:GLU:OE2	23:P:89:LEU:O	2.13	0.66
7:G:172:ALA:HA	7:G:175:GLU:OE2	1.96	0.66
13:6:26:GLU:HG2	13:6:183:LEU:HB2	1.78	0.66
1:a:166:TYR:CA	2:b:57:MET:HG3	2.26	0.66
3:c:42:ASP:OD1	3:c:185:LYS:HD2	1.96	0.66
9:2:193:TRP:N	9:2:193:TRP:CD1	2.58	0.66
16:V:296:LEU:HD23	26:U:193:GLN:HB2	1.77	0.66
14:n:226:ARG:NH2	8:1:203:GLU:OE1	2.29	0.65
9:2:32:ILE:HB	9:2:128:ILE:HD12	1.76	0.65
16:V:45:VAL:HG13	16:V:46:PRO:HA	1.78	0.65
13:m:26:GLU:HG2	13:m:183:LEU:HB2	1.77	0.65
13:m:46:ARG:NH2	9:2:193:TRP:C	2.45	0.65
6:F:100:ASN:HB2	14:7:127:GLU:HG2	1.78	0.65
2:b:101:TYR:OH	10:j:70:LYS:NZ	2.28	0.65
12:5:82:ARG:HD2	12:5:200:ASP:HA	1.79	0.65
23:P:361:THR:HG22	23:P:363:LEU:H	1.60	0.65
12:l:82:ARG:HD2	12:l:200:ASP:HA	1.79	0.65
12:l:214:VAL:CG1	11:4:142:SER:HB2	2.26	0.65
16:V:72:PRO:HG3	26:U:82:LYS:NZ	2.11	0.65
16:V:225:LEU:CD1	23:P:423:LEU:CD2	2.71	0.65
7:g:172:ALA:HA	7:g:175:GLU:OE2	1.96	0.65
9:i:32:ILE:HB	9:i:128:ILE:HD12	1.76	0.65
3:C:42:ASP:OD1	3:C:185:LYS:HD2	1.96	0.65
8:1:196:ILE:O	8:1:197:PHE:HD2	1.80	0.65
23:P:89:LEU:O	23:P:90:LYS:HG2	1.96	0.65
12:l:128:GLN:OE1	13:m:138:SER:HA	1.97	0.65
16:V:40:HIS:NE2	26:U:83:ILE:CG2	2.60	0.65
23:P:339:GLU:O	23:P:342:GLN:HG2	1.96	0.65
12:l:165:TYR:HB3	12:l:170:LEU:CD2	2.27	0.65
7:G:184:PRO:HB3	23:P:4:ASP:HB2	1.79	0.65
16:V:213:LEU:CD2	26:U:171:VAL:HG13	2.27	0.65
8:h:196:ILE:O	8:h:197:PHE:HD2	1.80	0.65
13:m:39:THR:O	13:m:40:ASP:OD1	2.15	0.65
1:a:34:ALA:HB2	7:g:15:PHE:HZ	1.62	0.65
12:l:84:GLN:HE22	12:l:221:TRP:CD1	2.14	0.65
1:A:77:ARG:NH1	8:1:48:ASP:OD1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:5:84:GLN:HE22	12:5:221:TRP:CD1	2.14	0.65
12:5:165:TYR:HB3	12:5:170:LEU:CD2	2.27	0.65
16:V:296:LEU:O	26:U:193:GLN:OE1	2.14	0.65
12:l:219:TYR:C	12:l:220:LYS:HD3	2.21	0.64
12:5:219:TYR:C	12:5:220:LYS:HD3	2.21	0.64
10:j:177:ARG:HD3	12:5:101:VAL:HB	1.79	0.64
16:V:303:VAL:HG11	27:O:380:LEU:HD13	1.78	0.64
27:O:320:PRO:O	27:O:324:VAL:HG23	1.97	0.64
9:i:150:VAL:CG2	14:7:258:ILE:HG23	2.27	0.64
1:A:95:LEU:HD12	7:G:118:GLN:HG3	1.79	0.64
4:D:13:PRO:HA	5:E:26:TYR:CD2	2.33	0.64
13:6:142:GLU:CD	13:6:145:ARG:HE	2.06	0.64
16:V:98:THR:HG22	26:U:55:PRO:N	2.12	0.64
16:V:205:LYS:HZ3	26:U:175:LEU:HA	1.63	0.64
10:j:149:MET:HG2	10:j:170:ALA:HA	1.78	0.64
2:B:240:SER:O	2:B:244:ASN:ND2	2.31	0.64
9:2:251:ASP:OD1	9:2:251:ASP:N	2.24	0.64
16:V:213:LEU:HD23	26:U:171:VAL:CG2	2.17	0.64
9:i:125:ALA:C	9:i:126:TYR:HD1	2.05	0.64
11:k:35:THR:HG21	11:k:182:LYS:HZ1	1.59	0.64
3:C:177:GLN:HA	4:D:54:LEU:HD11	1.79	0.64
9:2:250:CYS:O	9:2:251:ASP:HB3	1.97	0.64
13:6:39:THR:O	13:6:40:ASP:OD1	2.15	0.64
2:b:2:THR:N	7:g:128:SER:HB3	2.13	0.64
16:V:217:HIS:HE1	26:U:181:GLN:OE1	1.79	0.64
21:N:33:ASP:OD1	22:S:219:LYS:HD3	1.98	0.64
22:S:152:LEU:O	22:S:153:GLU:O	2.15	0.64
16:V:280:LEU:CD2	26:U:268:LYS:NZ	2.60	0.64
6:f:105:VAL:HG11	6:f:143:HIS:HB2	1.80	0.64
2:B:102:GLY:HA3	10:3:89:GLN:HG3	1.79	0.64
13:m:230:ASP:OD2	9:2:48:ARG:CZ	2.46	0.64
7:G:184:PRO:HB2	23:P:5:ALA:N	2.12	0.64
8:1:85:GLU:HA	8:1:120:TYR:HE2	1.61	0.64
8:h:180:GLY:HA2	14:7:252:TRP:CH2	2.34	0.63
3:C:94:HIS:ND1	3:C:114:ARG:HG2	2.13	0.63
6:F:117:GLN:HE22	7:G:130:ARG:HH22	1.44	0.63
9:2:125:ALA:C	9:2:126:TYR:HD1	2.05	0.63
10:j:149:MET:HE3	10:j:153:LEU:HD11	1.80	0.63
9:2:82:GLU:OE1	10:3:129:CYS:HA	1.99	0.63
10:3:74:TYR:CE2	10:3:82:ILE:HA	2.34	0.63
13:6:47:TYR:HB2	14:7:194:ARG:HH21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:62:LEU:HD13	17:T:84:GLN:HB3	1.80	0.63
21:N:33:ASP:OD1	22:S:219:LYS:CD	2.46	0.63
2:b:59:GLU:OE1	2:b:59:GLU:HA	1.99	0.63
10:j:74:TYR:CE2	10:j:82:ILE:HA	2.34	0.63
1:A:133:TYR:CD1	2:B:5:TYR:CD1	2.86	0.63
10:3:74:TYR:HE2	10:3:82:ILE:HG13	1.64	0.63
20:Z:145:ASP:OD2	20:Z:149:TRP:CZ2	2.51	0.63
13:m:142:GLU:CD	13:m:145:ARG:HE	2.06	0.63
16:V:38:LEU:HB3	26:U:166:ALA:HB1	1.80	0.63
16:V:213:LEU:CA	26:U:171:VAL:HG13	2.28	0.63
16:V:295:VAL:CG1	17:T:263:ALA:CB	2.62	0.63
3:c:94:HIS:ND1	3:c:114:ARG:HG2	2.13	0.63
1:A:249:ALA:O	23:P:84:LYS:HD3	1.99	0.63
16:V:304:ALA:HA	27:O:377:VAL:CA	2.26	0.63
5:e:13:SER:OG	6:f:126:ARG:HB3	1.99	0.63
4:D:100:LEU:O	4:D:101:GLU:HB2	1.99	0.63
16:V:209:GLU:OE1	26:U:16:LEU:HD22	1.98	0.63
12:5:133:TRP:O	12:5:136:SER:OG	2.17	0.63
16:V:222:GLN:NE2	23:P:427:GLU:OE1	2.31	0.63
16:V:300:VAL:HG13	26:U:197:LEU:CD1	2.22	0.63
1:a:165:GLY:HA3	2:b:60:THR:OG1	1.98	0.62
2:b:49:LYS:HE3	2:b:208:THR:C	2.24	0.62
2:b:240:SER:O	2:b:244:ASN:ND2	2.31	0.62
2:B:59:GLU:OE1	2:B:59:GLU:HA	1.99	0.62
8:1:41:ASP:OD2	8:1:43:LEU:N	2.32	0.62
9:i:250:CYS:O	9:i:251:ASP:HB3	1.97	0.62
12:l:84:GLN:NE2	12:l:221:TRP:CD1	2.67	0.62
6:F:105:VAL:HG11	6:F:143:HIS:HB2	1.80	0.62
11:k:175:ASP:OD2	11:4:172:MET:O	2.17	0.62
1:A:249:ALA:HA	23:P:84:LYS:HB3	1.77	0.62
12:5:84:GLN:NE2	12:5:221:TRP:CD1	2.67	0.62
16:V:224:GLY:HA3	26:U:196:SER:HB2	1.81	0.62
9:2:119:TYR:CD1	9:2:123:ILE:CD1	2.83	0.62
10:j:101:GLY:C	11:k:93:ARG:NH2	2.57	0.62
2:B:190:HIS:ND1	24:Q:95:LYS:HE2	2.14	0.62
16:V:203:TYR:CE1	26:U:173:HIS:CD2	2.87	0.62
16:V:205:LYS:NZ	26:U:175:LEU:N	2.46	0.62
20:Z:280:ASP:O	20:Z:284:LEU:HD23	1.99	0.62
10:j:118:LYS:HB2	10:j:118:LYS:HZ2	1.64	0.62
12:l:133:TRP:O	12:l:136:SER:OG	2.17	0.62
9:2:109:LEU:CD2	9:2:148:THR:HG21	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:124:GLN:OE1	4:d:127:ARG:NH1	2.32	0.62
4:d:141:ARG:HH21	12:l:182:LYS:CE	2.06	0.62
10:j:74:TYR:HE2	10:j:82:ILE:HG13	1.64	0.62
12:l:216:ASP:OD1	11:4:167:GLU:OE1	2.17	0.62
2:B:128:ARG:HD3	2:B:128:ARG:H	1.64	0.62
9:i:119:TYR:CD1	9:i:123:ILE:CD1	2.83	0.62
2:B:49:LYS:HE3	2:B:208:THR:C	2.24	0.62
4:D:11:PHE:CZ	5:E:26:TYR:CB	2.80	0.62
9:2:63:LEU:HD13	9:2:215:TYR:HE1	1.64	0.62
10:3:149:MET:HE3	10:3:153:LEU:HD11	1.80	0.62
16:V:208:LYS:HZ1	26:U:19:LEU:HD21	0.76	0.62
2:b:227:ILE:CG1	9:i:215:TYR:CD2	2.83	0.62
16:V:225:LEU:HD11	26:U:200:LEU:HB2	1.79	0.62
20:Z:40:GLU:O	20:Z:44:LYS:HD2	2.00	0.62
5:e:150:ASP:CG	13:m:90:LYS:HZ3	2.08	0.62
9:i:109:LEU:CD2	9:i:148:THR:HG21	2.30	0.62
9:i:110:GLN:OE1	9:i:110:GLN:HA	2.00	0.62
20:Z:894:MET:O	20:Z:900:LEU:HB3	2.00	0.62
12:l:188:TYR:HE2	12:l:196:ARG:NH1	1.97	0.61
16:V:177:THR:CB	21:N:740:TRP:O	2.48	0.61
16:V:216:LEU:HD13	26:U:168:GLU:OE1	1.99	0.61
10:j:77:LYS:O	10:j:79:GLU:OE1	2.18	0.61
16:V:203:TYR:CE1	26:U:173:HIS:NE2	2.67	0.61
20:Z:146:PHE:N	20:Z:149:TRP:HE1	1.96	0.61
3:c:4:ARG:NH1	5:e:11:GLY:HA2	2.15	0.61
6:f:106:GLU:O	6:f:110:HIS:ND1	2.33	0.61
9:i:239:THR:HG21	10:j:168:SER:HB2	1.82	0.61
12:5:188:TYR:HE2	12:5:196:ARG:NH1	1.97	0.61
2:b:217:GLU:OE1	2:b:217:GLU:C	2.44	0.61
6:F:106:GLU:O	6:F:110:HIS:ND1	2.33	0.61
16:V:220:GLN:HB3	26:U:181:GLN:O	1.99	0.61
5:e:15:PHE:HA	5:e:16:SER:CB	2.30	0.61
2:B:177:LYS:CE	24:Q:170:ASP:HB3	2.30	0.61
11:4:92:ILE:HG13	11:4:93:ARG:HD2	1.83	0.61
13:6:46:ARG:O	14:7:194:ARG:NH2	2.33	0.61
16:V:40:HIS:CD2	26:U:83:ILE:HG23	2.35	0.61
16:V:304:ALA:O	27:O:377:VAL:CG2	2.48	0.61
27:O:325:GLU:OE2	27:O:343:GLN:NE2	2.33	0.61
11:k:28:LEU:HD22	12:l:212:TYR:OH	2.01	0.61
8:1:43:LEU:HD13	8:1:185:VAL:HG23	1.83	0.61
22:S:458:GLN:HG3	26:U:252:HIS:ND1	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:119:TYR:CE1	9:i:123:ILE:HD11	2.36	0.61
22:S:68:LEU:O	22:S:69:LEU:O	2.18	0.61
24:Q:430:ALA:HB2	26:U:274:MET:SD	2.41	0.61
12:l:252:LEU:C	12:l:253:TYR:HD1	2.09	0.61
13:m:157:PHE:CZ	9:2:232:TYR:HE2	2.18	0.61
5:E:15:PHE:HA	5:E:16:SER:CB	2.30	0.61
10:3:65:GLU:HG2	10:3:68:ARG:NH2	2.15	0.61
16:V:304:ALA:HB2	26:U:197:LEU:HD11	1.83	0.61
20:Z:898:HIS:O	20:Z:899:GLN:HB2	2.01	0.61
21:N:277:LEU:HD22	21:N:282:TYR:CZ	2.36	0.61
23:P:117:SER:O	23:P:120:GLU:HG3	2.00	0.61
2:b:128:ARG:HD3	2:b:128:ARG:H	1.64	0.61
8:h:43:LEU:HD13	8:h:185:VAL:HG23	1.83	0.61
13:m:226:GLU:OE2	14:n:194:ARG:NH2	2.34	0.61
16:V:214:MET:HE3	26:U:181:GLN:HG2	1.82	0.61
10:j:29:LEU:HD22	10:j:40:PHE:CD2	2.36	0.61
1:A:246:VAL:HG22	23:P:85:LYS:HE2	1.83	0.61
2:B:103:GLU:OE1	10:3:86:THR:CG2	2.49	0.61
8:1:85:GLU:HA	8:1:120:TYR:CE2	2.36	0.61
9:2:110:GLN:HA	9:2:110:GLN:OE1	2.00	0.61
23:P:83:SER:HA	23:P:93:ILE:HD13	1.83	0.61
9:i:63:LEU:HD13	9:i:215:TYR:HE1	1.64	0.60
2:B:217:GLU:C	2:B:217:GLU:OE1	2.44	0.60
4:D:66:LYS:HE2	11:4:69:ILE:HD11	1.80	0.60
14:7:228:PHE:CE2	14:7:245:LEU:HD22	2.36	0.60
16:V:212:MET:SD	26:U:15:LEU:HB3	2.41	0.60
16:V:214:MET:HG3	26:U:179:ARG:CG	2.31	0.60
16:V:306:LYS:CA	27:O:376:GLN:NE2	2.63	0.60
7:g:95:GLU:OE1	7:g:115:ARG:HB3	2.01	0.60
11:k:92:ILE:HG13	11:k:93:ARG:HD2	1.83	0.60
7:G:95:GLU:OE1	7:G:115:ARG:HB3	2.01	0.60
9:2:181:ILE:HG21	9:2:219:TYR:HE2	1.66	0.60
9:2:251:ASP:C	9:2:252:ILE:HG13	2.18	0.60
12:5:252:LEU:C	12:5:253:TYR:HD1	2.09	0.60
16:V:205:LYS:HZ3	26:U:174:LEU:C	2.07	0.60
16:V:296:LEU:CG	26:U:193:GLN:CB	2.79	0.60
3:C:66:LEU:HD12	3:C:212:GLU:OE2	2.01	0.60
16:V:209:GLU:CG	26:U:16:LEU:CD2	2.64	0.60
21:N:280:GLN:OE1	21:N:282:TYR:CZ	2.54	0.60
10:j:65:GLU:HG2	10:j:68:ARG:NH2	2.15	0.60
14:n:255:ALA:HB2	8:1:39:VAL:HG12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:4:41:HIS:HD2	11:4:109:LYS:HD3	1.66	0.60
8:h:85:GLU:HA	8:h:120:TYR:CE2	2.36	0.60
9:i:231:SER:C	9:i:232:TYR:HD1	2.09	0.60
8:1:150:ASN:O	8:1:152:ARG:NH2	2.34	0.60
9:2:119:TYR:CE1	9:2:123:ILE:HD11	2.36	0.60
10:3:77:LYS:O	10:3:79:GLU:OE1	2.18	0.60
16:V:220:GLN:OE1	26:U:181:GLN:HB2	2.01	0.60
8:h:41:ASP:OD2	8:h:43:LEU:N	2.32	0.60
12:l:133:TRP:CZ3	12:l:161:LEU:HD22	2.36	0.60
1:A:183:GLU:OE1	2:B:54:PRO:HB2	2.01	0.60
16:V:292:ILE:CG2	26:U:186:LEU:CD1	2.75	0.60
11:k:59:TYR:O	11:k:63:ASN:OD1	2.20	0.60
13:m:230:ASP:CG	9:2:48:ARG:CZ	2.75	0.60
16:V:205:LYS:HZ3	26:U:175:LEU:CA	2.13	0.60
16:V:214:MET:HG2	26:U:181:GLN:NE2	2.17	0.60
24:Q:252:HIS:ND1	24:Q:253:ASN:HB2	2.16	0.60
13:m:47:TYR:CD1	14:n:195:GLU:CD	2.80	0.60
12:5:133:TRP:CZ3	12:5:161:LEU:HD22	2.36	0.60
11:k:41:HIS:HD2	11:k:109:LYS:HD3	1.66	0.60
7:G:223:GLU:HA	7:G:223:GLU:OE2	2.02	0.60
10:3:29:LEU:HD22	10:3:40:PHE:CD2	2.36	0.60
11:k:55:GLN:HG2	12:l:194:GLY:O	2.02	0.59
14:n:220:ARG:HG2	8:1:34:TYR:HE1	1.66	0.59
7:G:171:SER:O	7:G:175:GLU:OE2	2.20	0.59
16:V:205:LYS:HE2	26:U:174:LEU:C	2.27	0.59
16:V:205:LYS:HZ1	26:U:175:LEU:CA	2.13	0.59
13:m:58:ILE:HD11	13:m:119:ILE:HD12	1.83	0.59
1:A:230:LYS:O	1:A:231:ASP:HB2	2.02	0.59
12:5:113:ASN:HB3	12:5:114:PRO:CD	2.31	0.59
13:6:58:ILE:HD11	13:6:119:ILE:HD12	1.83	0.59
15:W:122:ARG:HE	15:W:153:LEU:HD22	1.67	0.59
21:N:601:THR:HG22	21:N:604:ARG:HH21	1.67	0.59
2:b:227:ILE:HD11	9:i:215:TYR:CD2	2.37	0.59
8:h:150:ASN:O	8:h:152:ARG:NH2	2.34	0.59
9:i:193:TRP:N	9:i:193:TRP:HD1	1.98	0.59
2:B:198:GLU:OE2	24:Q:209:TYR:HB2	2.02	0.59
19:Y:26:LYS:O	19:Y:30:GLU:OE1	2.21	0.59
3:c:63:THR:HG22	3:c:63:THR:O	2.02	0.59
3:c:66:LEU:HD12	3:c:212:GLU:OE2	2.01	0.59
4:D:13:PRO:HA	5:E:26:TYR:CE2	2.37	0.59
21:N:463:TYR:CZ	21:N:467:LYS:HD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:736:PHE:O	21:N:739:PHE:CD1	2.55	0.59
1:a:165:GLY:C	2:b:57:MET:HB2	2.28	0.59
9:2:231:SER:C	9:2:232:TYR:HD1	2.10	0.59
21:N:602:VAL:O	21:N:606:VAL:HG22	2.01	0.59
7:g:223:GLU:OE2	7:g:223:GLU:HA	2.02	0.59
9:i:177:LYS:O	9:i:181:ILE:HG13	2.02	0.59
13:m:130:VAL:C	13:m:131:TYR:HD2	2.11	0.59
1:A:249:ALA:CA	23:P:84:LYS:C	2.75	0.59
8:1:93:GLU:CD	8:1:93:GLU:C	2.70	0.59
9:2:195:ASP:OD1	9:2:196:LEU:N	2.36	0.59
16:V:72:PRO:HG3	26:U:82:LYS:HZ2	1.67	0.59
20:Z:30:LYS:HZ2	20:Z:44:LYS:CD	2.15	0.59
9:i:181:ILE:HG21	9:i:219:TYR:HE2	1.66	0.59
10:j:74:TYR:HD2	10:j:82:ILE:HB	1.68	0.59
13:m:46:ARG:NH2	9:2:193:TRP:CA	2.65	0.59
13:m:46:ARG:NH2	9:2:193:TRP:HB3	2.16	0.59
3:C:63:THR:HG22	3:C:63:THR:O	2.02	0.59
6:F:139:LYS:NZ	14:7:124:TYR:OH	2.25	0.59
11:4:59:TYR:O	11:4:63:ASN:OD1	2.20	0.59
13:6:130:VAL:C	13:6:131:TYR:HD2	2.11	0.59
16:V:208:LYS:HZ3	26:U:19:LEU:CD2	1.98	0.59
16:V:209:GLU:HG2	26:U:16:LEU:HD21	1.80	0.59
20:Z:40:GLU:CB	20:Z:44:LYS:NZ	2.55	0.59
20:Z:308:LYS:O	20:Z:309:GLN:O	2.19	0.59
20:Z:763:HIS:CE1	20:Z:795:THR:HG22	2.38	0.59
8:h:93:GLU:C	8:h:93:GLU:CD	2.70	0.59
9:i:195:ASP:OD1	9:i:196:LEU:N	2.36	0.59
10:j:172:LEU:HA	10:j:202:MET:CE	2.33	0.59
16:V:225:LEU:CB	23:P:423:LEU:CD1	2.79	0.59
2:b:207:ASP:OD1	2:b:240:SER:OG	2.21	0.58
9:i:251:ASP:C	9:i:252:ILE:HG13	2.18	0.58
2:B:207:ASP:OD1	2:B:240:SER:OG	2.21	0.58
16:V:214:MET:C	26:U:179:ARG:NH1	2.55	0.58
20:Z:395:CYS:SG	20:Z:842:GLN:NE2	2.70	0.58
20:Z:842:GLN:NE2	20:Z:845:LEU:HD22	2.18	0.58
3:C:100:LYS:HG3	10:3:65:GLU:HB3	1.85	0.58
16:V:225:LEU:O	23:P:423:LEU:CD1	2.51	0.58
22:S:211:ARG:NH1	22:S:241:PHE:CD1	2.71	0.58
1:a:230:LYS:O	1:a:231:ASP:HB2	2.02	0.58
3:c:152:ASN:HB2	3:c:153:PRO:HD2	1.86	0.58
7:g:171:SER:O	7:g:175:GLU:OE2	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:3:ILE:HD12	11:k:176:PHE:CD1	2.38	0.58
4:D:123:SER:HA	5:E:134:MET:HA	1.85	0.58
18:X:92:SER:O	18:X:93:SER:HB2	2.02	0.58
14:n:187:LEU:O	14:n:190:LYS:HB3	2.03	0.58
9:2:177:LYS:O	9:2:181:ILE:HG13	2.02	0.58
12:5:253:TYR:CE1	12:5:262:TYR:CD1	2.92	0.58
16:V:302:SER:O	16:V:306:LYS:HB2	2.03	0.58
5:e:53:ARG:HH12	5:e:209:GLU:HG3	1.68	0.58
12:l:113:ASN:HB3	12:l:114:PRO:CD	2.31	0.58
9:2:193:TRP:N	9:2:193:TRP:HD1	1.99	0.58
23:P:77:GLU:O	23:P:81:LEU:HD23	2.03	0.58
12:l:253:TYR:CE1	12:l:262:TYR:CD1	2.92	0.58
1:A:105:ARG:HG2	8:1:73:GLU:OE1	2.04	0.58
21:N:361:ASN:O	21:N:363:ALA:N	2.36	0.58
10:j:204:GLN:OE1	10:j:204:GLN:HA	2.03	0.58
10:3:74:TYR:HD2	10:3:82:ILE:HB	1.68	0.58
10:3:172:LEU:HA	10:3:202:MET:CE	2.33	0.58
11:4:3:ILE:HD12	11:4:176:PHE:CD1	2.38	0.58
22:S:475:TYR:CD1	26:U:273:LEU:HD13	2.38	0.58
16:V:221:TRP:HH2	23:P:427:GLU:HG3	1.68	0.58
20:Z:85:VAL:O	20:Z:85:VAL:CG1	2.51	0.58
5:E:53:ARG:HH12	5:E:209:GLU:HG3	1.68	0.58
10:3:63:LEU:O	10:3:67:PHE:HD2	1.87	0.58
17:T:127:GLN:HG3	22:S:247:VAL:HG21	1.86	0.58
22:S:475:TYR:CE1	26:U:273:LEU:CB	2.87	0.58
3:c:9:ARG:NH2	4:d:10:ILE:CD1	2.67	0.57
19:Y:4:ASP:O	19:Y:5:VAL:C	2.46	0.57
11:k:85:ARG:HG3	11:k:125:LYS:HB2	1.86	0.57
12:l:138:CYS:SG	12:l:149:ILE:HG21	2.44	0.57
2:B:142:PHE:CE1	10:3:115:LYS:HE2	2.39	0.57
2:B:178:ARG:HH12	24:Q:130:ARG:HD3	1.69	0.57
10:3:204:GLN:HA	10:3:204:GLN:OE1	2.03	0.57
11:4:85:ARG:HG3	11:4:125:LYS:HB2	1.87	0.57
16:V:296:LEU:C	26:U:193:GLN:OE1	2.47	0.57
21:N:93:GLU:O	21:N:94:LYS:HD2	2.04	0.57
22:S:77:THR:CG2	22:S:86:SER:HA	2.34	0.57
2:b:142:PHE:HB3	10:j:80:ARG:HH22	1.68	0.57
9:i:57:ASP:OD2	10:j:132:GLU:O	2.22	0.57
9:i:243:LYS:O	9:i:244:GLU:OE2	2.22	0.57
11:k:2:ASP:HA	11:k:47:ALA:HB1	1.87	0.57
3:C:152:ASN:HB2	3:C:153:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:5:129:PHE:HD1	13:6:102:GLN:OE1	1.86	0.57
12:5:138:CYS:SG	12:5:149:ILE:HG21	2.44	0.57
13:6:168:TYR:CD2	13:6:174:GLY:HA2	2.39	0.57
4:d:90:ARG:C	4:d:94:GLN:NE2	2.61	0.57
10:j:63:LEU:O	10:j:67:PHE:HD2	1.87	0.57
11:k:30:ASP:CB	11:k:177:LYS:HG3	2.34	0.57
20:Z:145:ASP:CA	20:Z:149:TRP:HE1	2.13	0.57
2:b:90:ARG:O	2:b:94:HIS:CD2	2.44	0.57
9:i:211:LYS:HZ2	9:i:211:LYS:CB	2.16	0.57
9:i:211:LYS:NZ	9:i:211:LYS:CB	2.67	0.57
14:n:140:MET:HA	14:n:140:MET:HE3	1.86	0.57
6:F:62:LYS:O	6:F:74:LEU:HD23	2.05	0.57
21:N:277:LEU:HB3	21:N:282:TYR:CE2	2.39	0.57
25:R:113:LEU:O	25:R:117:ILE:CD1	2.52	0.57
9:i:119:TYR:HD1	9:i:123:ILE:CD1	2.18	0.57
11:k:36:ARG:NE	11:k:58:GLU:OE1	2.38	0.57
12:l:286:ILE:HG21	10:3:39:LYS:HB2	1.87	0.57
10:3:169:GLN:HA	10:3:172:LEU:HD12	1.87	0.57
11:4:36:ARG:NE	11:4:58:GLU:OE1	2.38	0.57
20:Z:30:LYS:HZ2	20:Z:44:LYS:HD3	1.67	0.57
26:U:37:ILE:HG22	26:U:91:GLY:C	2.30	0.57
9:i:94:LEU:HB3	9:i:98:TYR:HE2	1.70	0.57
16:V:296:LEU:CG	26:U:193:GLN:HB2	2.35	0.57
2:b:75:TYR:CD1	2:b:82:TYR:CD2	2.92	0.57
5:e:104:ASP:OD2	13:m:99:ARG:CD	2.52	0.57
9:i:244:GLU:HG3	10:j:198:ARG:CG	2.31	0.57
2:B:75:TYR:CD1	2:B:82:TYR:CD2	2.93	0.57
5:E:10:ARG:O	5:E:10:ARG:HG3	2.04	0.57
13:6:142:GLU:OE2	13:6:145:ARG:HB2	2.04	0.57
4:d:48:ARG:HE	4:d:60:THR:CG2	2.18	0.56
6:f:171:TYR:OH	6:f:195:GLU:OE1	2.23	0.56
9:i:208:GLU:HB2	9:i:211:LYS:HD2	1.87	0.56
10:j:71:THR:O	10:j:75:LYS:HG3	2.05	0.56
20:Z:145:ASP:CG	20:Z:149:TRP:CZ2	2.79	0.56
6:f:62:LYS:O	6:f:74:LEU:HD23	2.05	0.56
13:m:168:TYR:CD2	13:m:174:GLY:HA2	2.39	0.56
21:N:293:LEU:HD22	21:N:379:LEU:HD13	1.86	0.56
24:Q:252:HIS:CE1	24:Q:253:ASN:HB2	2.40	0.56
1:a:106:TYR:CZ	9:i:114:GLN:NE2	2.74	0.56
8:h:17:PHE:CE1	8:h:22:ILE:HG13	2.40	0.56
8:h:193:GLU:HA	8:h:193:GLU:OE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:88:ILE:O	9:i:92:ILE:HG12	2.06	0.56
10:j:118:LYS:NZ	10:j:118:LYS:CB	2.68	0.56
14:n:220:ARG:HG2	8:1:34:TYR:CE1	2.39	0.56
9:2:88:ILE:O	9:2:92:ILE:HG12	2.06	0.56
9:2:94:LEU:HB3	9:2:98:TYR:HE2	1.70	0.56
11:4:2:ASP:HA	11:4:47:ALA:HB1	1.87	0.56
16:V:205:LYS:CE	26:U:174:LEU:HB3	2.24	0.56
24:Q:123:GLU:OE1	24:Q:126:LYS:NZ	2.28	0.56
11:k:1:MET:C	11:k:1:MET:HE2	2.31	0.56
1:A:149:GLU:CD	9:2:104:ARG:HH21	2.12	0.56
2:B:203:GLU:OE1	2:B:204:PHE:N	2.39	0.56
9:2:243:LYS:O	9:2:244:GLU:OE2	2.22	0.56
23:P:173:MET:HE2	23:P:173:MET:N	2.21	0.56
9:i:220:LEU:HG	9:i:222:PRO:HD3	1.87	0.56
10:j:169:GLN:HA	10:j:172:LEU:HD12	1.87	0.56
6:F:74:LEU:HD23	6:F:74:LEU:H	1.69	0.56
10:3:71:THR:O	10:3:75:LYS:HG3	2.05	0.56
11:4:30:ASP:CB	11:4:177:LYS:HG3	2.35	0.56
21:N:205:SER:O	21:N:209:LYS:HG2	2.05	0.56
6:f:74:LEU:HD23	6:f:74:LEU:H	1.69	0.56
11:k:55:GLN:OE1	12:l:159:SER:OG	2.22	0.56
5:E:127:ALA:O	5:E:128:SER:O	2.24	0.56
8:1:17:PHE:CE1	8:1:22:ILE:HG13	2.40	0.56
9:2:208:GLU:HB2	9:2:211:LYS:HD2	1.87	0.56
14:7:215:ARG:HD3	14:7:248:GLU:O	2.06	0.56
20:Z:442:VAL:O	20:Z:443:ASP:O	2.24	0.56
1:a:126:GLN:HG3	2:b:80:PRO:O	2.05	0.56
2:b:203:GLU:OE1	2:b:204:PHE:N	2.39	0.56
5:e:127:ALA:O	5:e:128:SER:O	2.24	0.56
12:l:183:GLU:CG	12:l:186:THR:HG21	2.36	0.56
13:m:142:GLU:OE2	13:m:145:ARG:HB2	2.04	0.56
14:7:215:ARG:HD2	14:7:249:ASN:O	2.04	0.56
21:N:277:LEU:HD22	21:N:282:TYR:CE2	2.41	0.56
22:S:65:ASN:ND2	22:S:72:GLU:OE2	2.32	0.56
9:i:46:ASP:OD2	9:i:198:SER:HA	2.06	0.56
13:m:20:ILE:HD12	13:m:118:ILE:HG13	1.88	0.56
13:m:39:THR:OG1	13:m:44:ASN:ND2	2.38	0.56
5:E:134:MET:HB2	5:E:136:ARG:H	1.70	0.56
10:3:118:LYS:NZ	10:3:118:LYS:CB	2.68	0.56
25:R:335:ARG:NH2	25:R:376:GLN:HG2	2.20	0.56
12:l:203:CYS:SG	12:l:211:ALA:HB3	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:194:LYS:HD2	5:E:197:GLU:OE1	2.06	0.56
13:6:20:ILE:HD12	13:6:118:ILE:HG13	1.88	0.56
13:6:149:ALA:HB1	13:6:205:GLN:OE1	2.06	0.56
23:P:361:THR:HB	23:P:364:ARG:HG2	1.87	0.56
5:e:134:MET:HB2	5:e:136:ARG:H	1.70	0.56
8:h:100:ASP:OD1	14:n:35:GLN:HA	2.06	0.56
8:h:120:TYR:HE1	8:h:130:LYS:HG3	1.71	0.56
14:n:222:ALA:HB2	8:1:30:THR:HG21	1.88	0.56
13:6:49:PRO:O	13:6:50:LYS:HD3	2.06	0.56
14:7:228:PHE:HE2	14:7:245:LEU:HD22	1.70	0.56
20:Z:842:GLN:HG2	20:Z:842:GLN:O	2.05	0.56
9:i:48:ARG:CZ	13:6:230:ASP:OD2	2.54	0.55
14:n:220:ARG:CG	8:1:34:TYR:CE1	2.89	0.55
14:n:256:LYS:HE3	8:1:198:TYR:OH	2.05	0.55
23:P:339:GLU:OE2	23:P:342:GLN:NE2	2.39	0.55
8:h:150:ASN:O	8:h:152:ARG:NH1	2.40	0.55
11:k:2:ASP:CA	11:k:47:ALA:HB1	2.36	0.55
13:m:41:TYR:CD2	13:m:41:TYR:N	2.72	0.55
13:m:161:GLN:HE22	9:2:234:PHE:HZ	1.53	0.55
21:N:32:VAL:HG13	21:N:33:ASP:OD2	2.06	0.55
21:N:94:LYS:HA	21:N:94:LYS:HE3	1.89	0.55
11:k:167:GLU:OE1	12:5:213:GLY:HA2	2.06	0.55
13:m:49:PRO:O	13:m:50:LYS:HD3	2.06	0.55
8:1:150:ASN:O	8:1:152:ARG:NH1	2.40	0.55
12:5:83:PHE:HD2	12:5:84:GLN:N	2.05	0.55
15:W:87:MET:SD	15:W:125:LEU:HD13	2.45	0.55
16:V:304:ALA:C	27:O:377:VAL:HG22	2.32	0.55
26:U:36:VAL:HG21	26:U:89:LEU:CD1	2.35	0.55
10:j:192:LYS:HD2	10:j:192:LYS:C	2.32	0.55
6:F:171:TYR:OH	6:F:195:GLU:OE1	2.23	0.55
8:1:120:TYR:HE1	8:1:130:LYS:HG3	1.72	0.55
9:2:220:LEU:HG	9:2:222:PRO:HD3	1.87	0.55
10:3:205:ASP:OD1	10:3:205:ASP:OXT	2.24	0.55
12:5:76:THR:HG23	12:5:108:LYS:HE2	1.88	0.55
12:5:183:GLU:CG	12:5:186:THR:HG21	2.36	0.55
12:5:203:CYS:SG	12:5:211:ALA:HB3	2.46	0.55
19:Y:80:GLU:HA	19:Y:83:ARG:HD3	1.88	0.55
20:Z:727:GLU:O	20:Z:728:LYS:CG	2.55	0.55
5:e:10:ARG:O	5:e:10:ARG:HG3	2.04	0.55
5:e:194:LYS:HD2	5:e:197:GLU:OE1	2.06	0.55
7:g:104:LYS:NZ	14:n:98:ARG:NH1	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:205:ASP:OXT	10:j:205:ASP:OD1	2.24	0.55
9:2:119:TYR:HD1	9:2:123:ILE:CD1	2.18	0.55
11:4:1:MET:C	11:4:1:MET:HE2	2.31	0.55
5:e:70:ILE:HG21	5:e:112:LEU:HD21	1.88	0.55
13:m:149:ALA:HB1	13:m:205:GLN:OE1	2.06	0.55
8:1:193:GLU:HA	8:1:193:GLU:OE2	2.05	0.55
13:6:41:TYR:N	13:6:41:TYR:CD2	2.72	0.55
16:V:217:HIS:CE1	26:U:181:GLN:CD	2.85	0.55
25:R:184:GLN:NE2	25:R:220:ALA:HB1	2.22	0.55
13:m:142:GLU:CD	13:m:145:ARG:HH21	2.15	0.55
8:1:47:HIS:ND1	8:1:48:ASP:N	2.55	0.55
10:3:96:TYR:HD1	10:3:127:ILE:CG2	2.20	0.55
15:W:194:GLU:CD	15:W:195:GLY:N	2.65	0.55
10:j:96:TYR:HD1	10:j:127:ILE:CG2	2.20	0.55
2:B:90:ARG:O	2:B:94:HIS:CD2	2.44	0.55
5:E:108:ASN:OD1	13:6:90:LYS:HE2	2.07	0.55
9:2:46:ASP:OD2	9:2:198:SER:HA	2.06	0.55
12:5:188:TYR:CZ	12:5:198:LYS:HD3	2.41	0.55
16:V:225:LEU:CB	23:P:423:LEU:HD13	2.37	0.55
16:V:288:LEU:HD21	17:T:270:ILE:HD11	1.88	0.55
12:l:83:PHE:HD2	12:l:84:GLN:N	2.05	0.55
5:E:70:ILE:HG21	5:E:112:LEU:HD21	1.88	0.55
9:2:252:ILE:HG22	9:2:253:GLN:N	2.21	0.55
13:6:142:GLU:CD	13:6:145:ARG:HH21	2.15	0.55
10:j:70:LYS:HD2	10:j:73:LEU:HD12	1.89	0.55
16:V:148:LYS:O	26:U:169:ILE:CG2	2.54	0.55
16:V:305:ILE:HA	27:O:373:TRP:CD1	2.42	0.55
19:Y:31:GLU:HG3	19:Y:31:GLU:O	2.06	0.55
9:i:252:ILE:HG22	9:i:253:GLN:N	2.21	0.54
22:S:475:TYR:OH	22:S:479:MET:SD	2.60	0.54
4:d:203:VAL:O	4:d:204:GLN:HB2	2.07	0.54
5:e:128:SER:N	6:f:119:ASN:OD1	2.39	0.54
10:j:74:TYR:CD2	10:j:82:ILE:HB	2.42	0.54
11:4:2:ASP:CA	11:4:47:ALA:HB1	2.36	0.54
11:4:95:ARG:O	11:4:97:PRO:HD3	2.07	0.54
20:Z:269:TYR:CE2	20:Z:293:MET:HG3	2.42	0.54
23:P:435:LYS:O	23:P:439:MET:HG2	2.07	0.54
13:m:105:LEU:HB3	13:m:136:VAL:O	2.08	0.54
12:5:216:ASP:OD1	12:5:217:SER:N	2.40	0.54
21:N:920:VAL:O	21:N:924:LYS:HG2	2.08	0.54
22:S:230:LYS:O	22:S:234:ILE:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:125:GLU:HB3	25:R:129:GLU:OE2	2.06	0.54
6:f:13:PHE:HE1	7:g:130:ARG:HG2	1.72	0.54
8:h:47:HIS:ND1	8:h:48:ASP:N	2.55	0.54
15:W:128:LEU:O	15:W:131:THR:OG1	2.23	0.54
11:k:95:ARG:O	11:k:97:PRO:HD3	2.07	0.54
10:3:78:GLU:OE2	10:3:80:ARG:NH1	2.41	0.54
2:b:215:GLY:O	2:b:234:ARG:HG2	2.08	0.54
3:c:142:ASP:CG	11:k:110:LYS:NZ	2.60	0.54
12:l:188:TYR:CZ	12:l:198:LYS:HD3	2.42	0.54
10:3:192:LYS:HD2	10:3:192:LYS:C	2.32	0.54
14:7:136:ARG:HD2	14:7:141:ASN:O	2.08	0.54
15:W:194:GLU:CD	15:W:195:GLY:H	2.16	0.54
10:j:102:PRO:CB	10:j:127:ILE:HD11	2.38	0.54
12:l:76:THR:HG23	12:l:108:LYS:HE2	1.88	0.54
12:l:216:ASP:OD1	12:l:217:SER:N	2.41	0.54
14:n:220:ARG:CD	8:1:35:ILE:O	2.55	0.54
10:3:70:LYS:HD2	10:3:73:LEU:HD12	1.90	0.54
10:3:74:TYR:CD2	10:3:82:ILE:HB	2.42	0.54
11:4:135:TYR:HB2	11:4:138:PHE:CD2	2.43	0.54
13:6:105:LEU:HB3	13:6:136:VAL:O	2.07	0.54
16:V:213:LEU:CA	26:U:171:VAL:CG1	2.86	0.54
17:T:144:TYR:HB3	17:T:145:PRO:CD	2.38	0.54
11:k:49:GLU:HG2	11:k:99:GLN:OE1	2.08	0.54
11:k:135:TYR:HB2	11:k:138:PHE:CD2	2.43	0.54
9:2:232:TYR:HD2	10:3:153:LEU:HD23	1.72	0.54
16:V:300:VAL:CG2	26:U:193:GLN:CD	2.73	0.54
10:j:2:SER:OG	10:j:3:ASP:N	2.40	0.54
9:2:78:ALA:HB1	10:3:129:CYS:SG	2.47	0.54
13:6:39:THR:OG1	13:6:44:ASN:ND2	2.38	0.54
16:V:40:HIS:CD2	26:U:83:ILE:CG2	2.91	0.54
19:Y:30:GLU:OE2	22:S:309:PHE:HD1	1.91	0.54
14:n:219:TYR:O	8:1:35:ILE:HD12	2.08	0.54
16:V:210:THR:HG23	26:U:175:LEU:HD12	1.86	0.54
1:a:164:VAL:CG2	2:b:57:MET:O	2.56	0.53
16:V:91:MET:HA	26:U:79:MET:HE2	1.89	0.53
16:V:303:VAL:HG12	27:O:380:LEU:HD22	1.88	0.53
17:T:219:LYS:HD3	17:T:219:LYS:N	2.23	0.53
25:R:113:LEU:HG	25:R:117:ILE:HD11	1.90	0.53
3:c:4:ARG:HH12	5:e:11:GLY:CA	2.20	0.53
9:i:119:TYR:HD1	9:i:123:ILE:HG13	1.73	0.53
9:i:161:LEU:HB3	14:7:182:HIS:HD2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:52:ASP:OD1	12:l:166:LYS:NZ	2.41	0.53
1:A:249:ALA:HB2	23:P:85:LYS:CB	2.38	0.53
2:B:160:LYS:HD3	2:B:179:TRP:CZ2	2.43	0.53
12:5:159:SER:O	12:5:162:VAL:HG12	2.09	0.53
13:6:47:TYR:CB	14:7:194:ARG:HH21	2.21	0.53
16:V:25:GLU:H	16:V:199:LEU:CD1	2.22	0.53
16:V:213:LEU:CD2	26:U:171:VAL:CG2	2.81	0.53
27:O:368:ASP:O	27:O:372:GLU:OE2	2.26	0.53
10:j:78:GLU:OE2	10:j:80:ARG:NH1	2.41	0.53
2:B:94:HIS:CE1	9:2:93:GLU:HG2	2.38	0.53
9:2:119:TYR:HD1	9:2:123:ILE:HG13	1.74	0.53
16:V:292:ILE:HD13	26:U:186:LEU:CD2	2.36	0.53
16:V:306:LYS:NZ	26:U:239:LEU:HG	2.24	0.53
22:S:458:GLN:HG3	26:U:252:HIS:CE1	2.43	0.53
3:c:9:ARG:CZ	4:d:10:ILE:HD12	2.38	0.53
7:g:175:GLU:OE1	7:g:202:LEU:HB2	2.09	0.53
11:k:21:VAL:HG12	11:k:29:LYS:O	2.09	0.53
12:l:159:SER:O	12:l:162:VAL:HG12	2.09	0.53
13:m:131:TYR:CE2	13:m:141:ARG:HD2	2.44	0.53
4:D:11:PHE:CE2	5:E:23:GLN:O	2.62	0.53
8:1:103:THR:OG1	8:1:124:LEU:HD22	2.09	0.53
8:1:181:VAL:HG23	8:1:183:ARG:HD3	1.90	0.53
9:2:211:LYS:NZ	9:2:211:LYS:CB	2.66	0.53
21:N:569:LYS:HD3	21:N:569:LYS:C	2.33	0.53
4:d:27:VAL:HA	4:d:77:GLY:HA2	1.91	0.53
13:m:47:TYR:CD2	13:m:49:PRO:HD3	2.44	0.53
10:3:51:LEU:HD21	10:3:53:ILE:HD11	1.91	0.53
13:6:178:LYS:HD2	13:6:179:PRO:CD	2.36	0.53
3:c:4:ARG:HG2	4:d:6:ARG:HG3	1.89	0.53
14:n:252:TRP:CH2	8:1:38:ARG:HD2	2.44	0.53
10:3:102:PRO:CB	10:3:127:ILE:HD11	2.38	0.53
13:6:131:TYR:CE2	13:6:141:ARG:HD2	2.43	0.53
16:V:296:LEU:HD12	27:O:384:MET:HE1	1.91	0.53
20:Z:85:VAL:O	20:Z:85:VAL:HG12	2.08	0.53
7:G:175:GLU:OE1	7:G:202:LEU:HB2	2.09	0.53
9:2:178:GLU:HA	9:2:181:ILE:HD12	1.90	0.53
25:R:117:ILE:HG23	25:R:133:ALA:HB1	1.89	0.53
9:i:192:ILE:C	9:i:193:TRP:HD1	2.17	0.53
16:V:288:LEU:HD21	17:T:270:ILE:CD1	2.39	0.53
17:T:260:ILE:HD12	17:T:260:ILE:H	1.74	0.53
24:Q:68:MET:HG2	24:Q:69:GLY:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:209:ARG:HD2	25:R:241:ILE:HD11	1.91	0.53
2:b:160:LYS:HD3	2:b:179:TRP:CZ2	2.43	0.53
9:i:109:LEU:HD12	9:i:140:PHE:CD2	2.44	0.53
12:l:148:ARG:NH2	12:l:179:TYR:O	2.42	0.53
2:B:215:GLY:O	2:B:234:ARG:HG2	2.08	0.53
16:V:39:LYS:HE3	26:U:49:THR:HG22	1.89	0.53
20:Z:352:LYS:HG2	20:Z:462:VAL:HG23	1.91	0.53
4:d:102:ASP:O	4:d:103:PRO:C	2.51	0.53
9:2:109:LEU:HD12	9:2:140:PHE:CD2	2.44	0.53
9:2:211:LYS:HZ2	9:2:211:LYS:CB	2.20	0.53
16:V:32:ILE:CD1	26:U:16:LEU:HB2	2.38	0.53
21:N:293:LEU:CD2	21:N:379:LEU:HD13	2.38	0.53
21:N:529:GLN:O	21:N:559:TYR:CZ	2.62	0.53
23:P:8:LYS:N	23:P:8:LYS:HD2	2.24	0.53
23:P:402:PHE:O	23:P:403:GLU:HB3	2.09	0.53
4:d:11:PHE:CE1	5:e:136:ARG:HB2	2.45	0.52
13:m:229:ARG:HD3	9:2:193:TRP:CG	2.43	0.52
18:X:58:GLY:O	18:X:59:ARG:HB3	2.09	0.52
20:Z:93:ARG:HG3	20:Z:135:LEU:HD22	1.90	0.52
6:f:202:ARG:O	6:f:203:ASP:HB2	2.10	0.52
8:h:181:VAL:HG23	8:h:183:ARG:HD3	1.90	0.52
6:F:199:GLN:OE1	6:F:199:GLN:HA	2.09	0.52
11:4:21:VAL:HG12	11:4:29:LYS:O	2.09	0.52
12:5:148:ARG:NH2	12:5:179:TYR:O	2.42	0.52
16:V:98:THR:HG23	26:U:72:TYR:CE1	2.44	0.52
16:V:214:MET:HE2	26:U:181:GLN:HG2	1.90	0.52
21:N:38:GLU:OE1	22:S:249:SER:HB3	2.08	0.52
3:c:60:ASP:O	3:c:232:PRO:HG3	2.09	0.52
5:e:128:SER:HA	6:f:119:ASN:OD1	2.08	0.52
10:j:51:LEU:HD21	10:j:53:ILE:HD11	1.91	0.52
10:j:145:GLN:HE21	12:5:100:TRP:HB2	1.75	0.52
1:A:62:LYS:HA	23:P:2:SER:HA	1.91	0.52
7:G:109:ILE:HB	7:G:110:PRO:HD3	1.92	0.52
10:3:2:SER:OG	10:3:3:ASP:N	2.40	0.52
20:Z:63:LEU:HD23	20:Z:63:LEU:H	1.73	0.52
20:Z:352:LYS:CG	20:Z:462:VAL:HG23	2.40	0.52
25:R:286:LEU:O	25:R:287:GLN:C	2.50	0.52
2:b:17:LYS:H	3:c:28:SER:HB3	1.74	0.52
13:6:208:ASP:OD2	14:7:194:ARG:NH1	2.42	0.52
22:S:77:THR:HG22	22:S:86:SER:HA	1.92	0.52
1:A:62:LYS:HB3	23:P:2:SER:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:HA	7:G:161:LYS:HB2	1.92	0.52
2:B:99:ARG:HA	9:2:86:GLN:OE1	2.08	0.52
7:G:181:ASP:HA	23:P:4:ASP:OD1	2.08	0.52
10:3:40:PHE:CE1	10:3:41:GLU:O	2.63	0.52
25:R:152:LYS:HA	25:R:152:LYS:HE3	1.91	0.52
7:g:62:GLN:O	7:g:63:LYS:HD3	2.10	0.52
8:h:103:THR:OG1	8:h:124:LEU:HD22	2.09	0.52
10:j:40:PHE:CE1	10:j:41:GLU:O	2.63	0.52
4:D:181:ARG:CZ	5:E:60:GLU:OE2	2.57	0.52
5:E:13:SER:OG	6:F:126:ARG:HB3	2.09	0.52
20:Z:305:VAL:HG12	20:Z:307:HIS:H	1.74	0.52
1:a:107:LYS:O	9:i:111:MET:HG3	2.10	0.52
4:d:90:ARG:C	4:d:94:GLN:HE22	2.17	0.52
1:A:32:PHE:CE1	1:A:159:PRO:HD2	2.45	0.52
1:A:65:ASP:HB2	7:G:161:LYS:HD2	1.91	0.52
7:G:62:GLN:O	7:G:63:LYS:HD3	2.10	0.52
11:4:49:GLU:HG2	11:4:99:GLN:OE1	2.08	0.52
11:4:192:VAL:HG22	11:4:194:ASP:H	1.74	0.52
16:V:208:LYS:HZ2	16:V:208:LYS:HB2	1.74	0.52
8:h:47:HIS:HE2	8:h:81:THR:HG22	1.73	0.52
12:l:286:ILE:CG2	10:3:38:ASN:OD1	2.53	0.52
13:6:47:TYR:CD2	13:6:49:PRO:HD3	2.44	0.52
16:V:296:LEU:HD11	26:U:193:GLN:CG	2.25	0.52
24:Q:349:LYS:N	24:Q:349:LYS:HD3	2.25	0.52
27:O:295:THR:O	27:O:299:THR:HG23	2.10	0.52
6:f:199:GLN:OE1	6:f:199:GLN:HA	2.09	0.52
8:h:41:ASP:HB2	8:h:183:ARG:NH1	2.24	0.52
9:i:125:ALA:O	9:i:126:TYR:HD1	1.93	0.52
9:i:178:GLU:HA	9:i:181:ILE:HD12	1.90	0.52
10:j:145:GLN:HE22	12:5:100:TRP:HB2	1.73	0.52
11:k:192:VAL:HG22	11:k:194:ASP:H	1.74	0.52
14:n:223:ARG:HH11	14:n:223:ARG:HG3	1.75	0.52
16:V:221:TRP:CH2	23:P:427:GLU:OE1	2.63	0.52
18:X:25:THR:HG22	18:X:82:LYS:HZ3	1.75	0.52
22:S:475:TYR:HE1	26:U:273:LEU:HD13	1.71	0.52
25:R:92:ILE:HG23	25:R:92:ILE:O	2.10	0.52
9:i:252:ILE:CG2	9:i:253:GLN:N	2.72	0.52
13:m:35:THR:HG22	13:m:49:PRO:HA	1.93	0.52
3:C:13:PHE:CE2	4:D:127:ARG:HD2	2.44	0.52
8:1:47:HIS:HE2	8:1:81:THR:HG22	1.73	0.52
8:1:49:LYS:CE	8:1:111:TYR:HD2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:6:35:THR:HG22	13:6:211:GLU:OE1	2.10	0.52
17:T:127:GLN:O	17:T:130:ASP:HB2	2.10	0.52
22:S:475:TYR:CD1	26:U:273:LEU:HD22	2.44	0.52
3:C:60:ASP:O	3:C:232:PRO:HG3	2.09	0.51
8:1:99:LYS:HZ1	14:7:136:ARG:NH2	2.07	0.51
16:V:213:LEU:CD2	26:U:171:VAL:HA	2.24	0.51
16:V:296:LEU:HG	26:U:193:GLN:CB	2.39	0.51
23:P:364:ARG:HG2	23:P:364:ARG:HH11	1.76	0.51
7:g:109:ILE:HB	7:g:110:PRO:HD3	1.92	0.51
16:V:221:TRP:HH2	23:P:427:GLU:CG	2.23	0.51
21:N:669:GLU:OE2	21:N:669:GLU:N	2.43	0.51
9:i:189:GLN:OE1	9:i:193:TRP:NE1	2.44	0.51
9:i:222:PRO:O	9:i:223:ASN:CG	2.53	0.51
10:j:78:GLU:O	10:j:79:GLU:HB2	2.10	0.51
13:6:47:TYR:CA	14:7:194:ARG:HH21	2.22	0.51
15:W:64:THR:HG22	15:W:65:PHE:N	2.25	0.51
16:V:304:ALA:HB1	26:U:200:LEU:HD23	1.92	0.51
21:N:623:PHE:HZ	21:N:739:PHE:HE1	1.59	0.51
8:h:180:GLY:HA2	14:7:252:TRP:CZ3	2.45	0.51
1:A:91:ARG:HH12	7:G:157:TYR:H	1.59	0.51
6:F:202:ARG:O	6:F:203:ASP:HB2	2.09	0.51
9:2:222:PRO:O	9:2:223:ASN:CG	2.53	0.51
13:6:35:THR:HG22	13:6:49:PRO:HA	1.92	0.51
21:N:606:VAL:HB	21:N:621:THR:HG23	1.93	0.51
3:C:226:TYR:CE2	9:2:254:GLU:OE1	2.63	0.51
9:2:250:CYS:SG	10:3:193:ASP:C	2.93	0.51
1:a:130:GLN:NE2	2:b:130:PHE:HZ	2.09	0.51
13:m:230:ASP:OD1	9:2:48:ARG:CZ	2.58	0.51
14:n:255:ALA:HA	8:1:39:VAL:HB	1.93	0.51
1:A:92:ASN:HB2	7:G:121:GLN:HG2	1.92	0.51
10:3:78:GLU:O	10:3:79:GLU:HB2	2.10	0.51
17:T:127:GLN:HG3	22:S:247:VAL:CG2	2.41	0.51
10:j:102:PRO:HB2	10:j:127:ILE:HD11	1.92	0.51
13:m:167:GLN:OE1	10:3:169:GLN:NE2	2.40	0.51
19:Y:89:GLN:HG2	19:Y:89:GLN:OXT	2.10	0.51
23:P:44:LYS:HD2	23:P:85:LYS:CE	2.39	0.51
1:a:32:PHE:CE1	1:a:159:PRO:HD2	2.45	0.51
7:g:213:GLU:OE1	7:g:213:GLU:HA	2.11	0.51
9:2:189:GLN:OE1	9:2:193:TRP:NE1	2.44	0.51
10:3:102:PRO:HB2	10:3:127:ILE:HD11	1.92	0.51
16:V:212:MET:SD	26:U:15:LEU:CB	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:188:TYR:CE2	12:l:196:ARG:NH1	2.79	0.51
13:m:35:THR:HG22	13:m:211:GLU:OE1	2.10	0.51
2:B:198:GLU:OE2	24:Q:209:TYR:CG	2.64	0.51
8:1:140:SER:HA	8:1:143:ILE:HG12	1.93	0.51
9:2:192:ILE:C	9:2:193:TRP:HD1	2.17	0.51
13:6:20:ILE:HD12	13:6:118:ILE:CG1	2.41	0.51
16:V:205:LYS:HZ3	26:U:175:LEU:N	2.07	0.51
20:Z:145:ASP:CB	20:Z:149:TRP:HZ2	2.23	0.51
20:Z:171:LYS:H	20:Z:171:LYS:HD3	1.75	0.51
2:b:189:ILE:HD13	2:b:246:ARG:HH12	1.76	0.51
8:h:49:LYS:CE	8:h:111:TYR:HD2	2.23	0.51
9:i:228:LYS:HZ1	10:j:155:GLU:HG3	1.76	0.51
1:A:249:ALA:C	23:P:84:LYS:HB2	2.36	0.51
14:7:228:PHE:CE2	14:7:245:LEU:HB2	2.46	0.51
22:S:449:LEU:O	22:S:450:ASN:CB	2.59	0.51
1:a:25:LEU:HD12	2:b:78:MET:HE1	1.92	0.50
13:6:46:ARG:O	13:6:208:ASP:OD2	2.30	0.50
14:7:65:SER:HA	14:7:223:ARG:HH22	1.76	0.50
14:7:109:TYR:O	14:7:110:ASP:HB2	2.10	0.50
22:S:360:PHE:CE2	22:S:384:ARG:HD3	2.46	0.50
10:j:168:SER:O	10:j:172:LEU:HD12	2.11	0.50
2:b:2:THR:CG2	2:b:3:ASP:H	2.16	0.50
5:e:74:ILE:HG21	5:e:112:LEU:CD2	2.41	0.50
9:i:236:ARG:HE	10:j:161:GLU:HB3	1.76	0.50
10:j:149:MET:CG	10:j:170:ALA:HA	2.40	0.50
13:m:109:ARG:HH11	13:m:109:ARG:HG3	1.77	0.50
7:G:15:PHE:CE2	7:G:19:GLY:HA2	2.47	0.50
7:G:213:GLU:OE1	7:G:213:GLU:HA	2.11	0.50
12:5:183:GLU:CD	12:5:186:THR:HG21	2.37	0.50
26:U:108:GLU:CD	26:U:152:LYS:HZ3	2.18	0.50
1:a:30:TYR:HB3	7:g:15:PHE:CD2	2.46	0.50
4:d:90:ARG:NH1	11:k:70:ARG:HG3	2.26	0.50
9:i:46:ASP:O	9:i:62:LYS:HG3	2.12	0.50
13:m:20:ILE:HD12	13:m:118:ILE:CG1	2.41	0.50
14:n:226:ARG:CZ	8:1:203:GLU:CD	2.84	0.50
2:B:99:ARG:NH2	9:2:90:SER:HB2	2.06	0.50
9:2:125:ALA:O	9:2:126:TYR:HD1	1.93	0.50
24:Q:75:ARG:O	24:Q:79:PRO:HD2	2.11	0.50
6:f:13:PHE:CE1	7:g:130:ARG:HG2	2.46	0.50
8:h:116:LYS:O	8:h:117:GLY:C	2.55	0.50
8:h:140:SER:HA	8:h:143:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:1:MET:N	11:k:3:ILE:HG13	2.26	0.50
12:l:183:GLU:CD	12:l:186:THR:HG21	2.37	0.50
12:l:287:GLY:HA2	9:2:243:LYS:HE2	1.94	0.50
13:m:157:PHE:CE1	9:2:232:TYR:HE2	2.29	0.50
5:E:125:GLU:OE2	5:E:134:MET:O	2.30	0.50
10:3:154:TYR:CE1	10:3:155:GLU:O	2.65	0.50
13:6:203:HIS:HE1	13:6:205:GLN:OE1	1.95	0.50
16:V:94:MET:SD	26:U:75:ASN:C	2.94	0.50
12:l:282:PHE:CE1	11:4:145:ASP:OD1	2.65	0.50
13:m:46:ARG:O	13:m:208:ASP:OD2	2.30	0.50
3:C:110:ILE:HD11	11:4:71:GLU:OE1	2.12	0.50
3:C:208:TYR:CD2	3:C:236:LYS:HE2	2.47	0.50
5:E:74:ILE:HG21	5:E:112:LEU:CD2	2.41	0.50
16:V:25:GLU:C	16:V:199:LEU:HD12	2.37	0.50
22:S:155:LEU:HD12	22:S:155:LEU:H	1.77	0.50
5:e:8:TYR:CD1	5:e:22:PHE:HE2	2.30	0.50
9:i:150:VAL:CG2	14:7:258:ILE:CG2	2.89	0.50
10:j:108:VAL:CG2	10:j:139:SER:OG	2.60	0.50
10:j:154:TYR:CE1	10:j:155:GLU:O	2.65	0.50
12:l:273:TRP:HE3	12:l:276:LYS:HE2	1.75	0.50
13:m:203:HIS:HE1	13:m:205:GLN:OE1	1.95	0.50
14:n:111:ASN:HB2	14:n:114:ALA:HB2	1.94	0.50
2:B:189:ILE:HD13	2:B:246:ARG:HH12	1.76	0.50
9:2:119:TYR:HE1	9:2:123:ILE:HD11	1.77	0.50
10:3:149:MET:CG	10:3:170:ALA:HA	2.40	0.50
13:6:109:ARG:HG3	13:6:109:ARG:HH11	1.77	0.50
14:7:193:ASP:C	14:7:194:ARG:HG3	2.37	0.50
1:a:220:LYS:HG3	1:a:221:ASN:OD1	2.12	0.50
3:c:4:ARG:HG2	4:d:6:ARG:CG	2.41	0.50
7:g:15:PHE:CE2	7:g:19:GLY:HA2	2.47	0.50
1:A:105:ARG:HG2	8:1:73:GLU:CD	2.36	0.50
4:D:115:GLY:O	4:D:118:GLN:HG3	2.12	0.50
5:E:8:TYR:CD1	5:E:22:PHE:HE2	2.30	0.50
7:G:201:TYR:HD2	7:G:247:ILE:HD13	1.76	0.50
12:5:273:TRP:HE3	12:5:276:LYS:HE2	1.75	0.50
14:7:126:PHE:HZ	14:7:169:THR:OG1	1.95	0.50
3:c:208:TYR:CD2	3:c:236:LYS:HE2	2.47	0.50
7:g:201:TYR:HD2	7:g:247:ILE:HD13	1.76	0.50
9:i:51:GLN:NE2	9:i:54:ILE:HB	2.27	0.50
10:3:168:SER:O	10:3:172:LEU:HD12	2.11	0.50
11:4:1:MET:N	11:4:3:ILE:HG13	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:327:LEU:O	23:P:328:ALA:HB3	2.12	0.50
26:U:193:GLN:NE2	26:U:193:GLN:O	2.43	0.50
4:d:44:LEU:HD12	4:d:72:VAL:HG23	1.94	0.49
14:n:253:ASP:HA	8:1:198:TYR:OH	2.12	0.49
9:2:51:GLN:NE2	9:2:54:ILE:HB	2.27	0.49
20:Z:30:LYS:NZ	20:Z:44:LYS:HD3	2.27	0.49
24:Q:389:VAL:HG23	25:R:346:LYS:HD2	1.94	0.49
10:j:162:ASP:O	10:j:166:THR:OG1	2.30	0.49
14:n:221:ASP:HA	8:1:33:ALA:O	2.12	0.49
1:A:167:LYS:HG3	2:B:55:LEU:O	2.12	0.49
10:3:162:ASP:O	10:3:166:THR:OG1	2.30	0.49
16:V:306:LYS:O	27:O:376:GLN:HB3	2.12	0.49
19:Y:3:THR:C	19:Y:4:ASP:O	2.55	0.49
21:N:544:GLU:OE1	21:N:546:LEU:HD23	2.12	0.49
5:e:157:HIS:NE2	5:e:172:ILE:HG21	2.27	0.49
9:i:159:GLY:CA	9:i:195:ASP:OD2	2.60	0.49
9:i:228:LYS:NZ	10:j:155:GLU:HG3	2.26	0.49
14:n:162:TYR:CE1	14:n:177:THR:CG2	2.93	0.49
14:n:182:HIS:HD1	9:2:161:LEU:HD13	1.76	0.49
14:n:220:ARG:HG3	8:1:34:TYR:CD1	2.47	0.49
1:A:220:LYS:HG3	1:A:221:ASN:OD1	2.12	0.49
9:2:46:ASP:O	9:2:62:LYS:HG3	2.12	0.49
10:3:108:VAL:CG2	10:3:139:SER:OG	2.60	0.49
11:4:40:PRO:HD2	11:4:74:GLU:OE2	2.13	0.49
24:Q:25:GLN:H	24:Q:25:GLN:CD	2.20	0.49
7:g:104:LYS:HZ2	14:n:98:ARG:NH1	2.10	0.49
1:A:251:GLN:C	23:P:84:LYS:HZ1	1.98	0.49
16:V:59:ASP:C	16:V:59:ASP:OD2	2.55	0.49
16:V:205:LYS:HZ1	26:U:175:LEU:HA	1.69	0.49
16:V:306:LYS:CA	27:O:376:GLN:CD	2.86	0.49
17:T:137:GLU:O	17:T:138:ASP:O	2.29	0.49
22:S:434:ALA:HA	22:S:445:THR:HA	1.95	0.49
26:U:72:TYR:O	26:U:75:ASN:HB2	2.11	0.49
2:b:172:LYS:HB3	3:c:55:THR:CG2	2.42	0.49
8:1:41:ASP:HB2	8:1:183:ARG:NH1	2.24	0.49
2:b:108:LYS:NZ	10:j:79:GLU:OE2	2.41	0.49
11:k:160:LEU:O	11:k:163:LEU:HB2	2.13	0.49
3:C:157:TYR:CE1	4:D:61:PRO:HD3	2.48	0.49
4:D:39:LYS:HZ3	4:D:184:PRO:HD2	1.78	0.49
6:F:156:LEU:HD23	7:G:58:LEU:HB2	1.95	0.49
13:6:181:LYS:HG3	13:6:182:TYR:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:X:25:THR:HG22	18:X:82:LYS:NZ	2.27	0.49
21:N:301:THR:O	21:N:305:ASN:OD1	2.30	0.49
21:N:688:ASN:O	21:N:696:LYS:HD3	2.12	0.49
5:e:122:ARG:HB3	5:e:134:MET:HE3	1.95	0.49
5:e:125:GLU:OE2	5:e:134:MET:O	2.30	0.49
10:j:101:GLY:C	11:k:93:ARG:HH21	2.13	0.49
13:m:181:LYS:HG3	13:m:182:TYR:N	2.26	0.49
16:V:214:MET:CE	26:U:181:GLN:CG	2.84	0.49
7:G:60:VAL:CG1	7:G:63:LYS:HE2	2.41	0.49
8:1:116:LYS:O	8:1:117:GLY:C	2.55	0.49
11:4:160:LEU:O	11:4:163:LEU:HB2	2.13	0.49
16:V:98:THR:HG22	26:U:55:PRO:CD	2.43	0.49
21:N:762:ARG:HD3	21:N:762:ARG:N	2.28	0.49
22:S:211:ARG:NH1	22:S:241:PHE:CE1	2.81	0.49
3:c:221:ASN:O	3:c:222:ASP:HB2	2.12	0.49
9:i:246:ILE:HD12	10:j:195:VAL:O	2.12	0.49
7:G:7:GLY:O	7:G:9:ASP:OD1	2.31	0.49
9:2:159:GLY:CA	9:2:195:ASP:OD2	2.60	0.49
16:V:295:VAL:HG11	17:T:263:ALA:HB3	1.81	0.49
22:S:112:ASN:O	22:S:113:SER:C	2.55	0.49
23:P:111:ASP:O	23:P:115:ARG:HG3	2.13	0.49
1:a:166:TYR:HA	2:b:57:MET:HG3	1.95	0.49
7:g:123:HIS:HA	7:g:129:VAL:CG2	2.43	0.49
9:i:177:LYS:HD3	9:i:208:GLU:OE1	2.13	0.49
5:E:157:HIS:NE2	5:E:172:ILE:HG21	2.27	0.49
6:F:117:GLN:HE22	7:G:130:ARG:NH2	2.10	0.49
12:5:250:VAL:HG12	12:5:266:HIS:O	2.13	0.49
20:Z:314:LEU:HD12	20:Z:956:LEU:HD21	1.95	0.49
21:N:463:TYR:OH	21:N:467:LYS:HD2	2.13	0.49
11:k:58:GLU:HA	11:k:58:GLU:OE2	2.13	0.48
11:k:58:GLU:OE2	11:k:61:GLN:OE1	2.31	0.48
12:l:81:PHE:HB3	12:l:201:ILE:HG22	1.94	0.48
4:D:102:ASP:O	4:D:103:PRO:C	2.55	0.48
12:5:81:PHE:HB3	12:5:201:ILE:HG22	1.94	0.48
12:5:188:TYR:CE2	12:5:196:ARG:NH1	2.79	0.48
16:V:213:LEU:CG	26:U:171:VAL:HG13	2.41	0.48
21:N:22:THR:O	21:N:26:GLU:OE2	2.31	0.48
23:P:120:GLU:HB3	23:P:123:ARG:NH2	2.27	0.48
25:R:335:ARG:NH1	25:R:376:GLN:HG2	2.26	0.48
12:l:250:VAL:HG12	12:l:266:HIS:O	2.13	0.48
13:m:202:ARG:HD2	10:3:147:PHE:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:17:ILE:HD11	5:E:136:ARG:CZ	2.43	0.48
7:G:8:TYR:HD1	7:G:14:VAL:HB	1.78	0.48
3:C:221:ASN:O	3:C:222:ASP:HB2	2.12	0.48
7:G:123:HIS:HA	7:G:129:VAL:CG2	2.43	0.48
13:6:94:ILE:HG12	13:6:122:LEU:O	2.14	0.48
16:V:293:VAL:HG11	26:U:189:ARG:HH11	1.77	0.48
1:a:17:THR:O	2:b:128:ARG:NE	2.42	0.48
3:c:226:TYR:CE2	9:i:254:GLU:OE1	2.66	0.48
4:d:149:GLN:HG2	4:d:159:TRP:CD1	2.49	0.48
5:e:194:LYS:CD	5:e:197:GLU:OE1	2.61	0.48
7:g:60:VAL:CG1	7:g:63:LYS:HE2	2.41	0.48
9:i:39:ASN:N	9:i:39:ASN:OD1	2.45	0.48
11:k:49:GLU:HG2	11:k:99:GLN:HB3	1.96	0.48
12:l:253:TYR:HE1	12:l:262:TYR:CE1	2.32	0.48
13:m:197:THR:O	13:m:200:THR:OG1	2.31	0.48
9:2:39:ASN:OD1	9:2:39:ASN:N	2.45	0.48
9:2:80:ASP:OD2	10:3:99:ARG:NH1	2.47	0.48
10:3:74:TYR:CD2	10:3:82:ILE:CG1	2.96	0.48
11:4:118:GLN:HG3	11:4:133:HIS:CE1	2.49	0.48
16:V:303:VAL:HG12	27:O:380:LEU:CD2	2.42	0.48
22:S:449:LEU:O	22:S:450:ASN:HB2	2.13	0.48
11:k:40:PRO:HD2	11:k:74:GLU:OE2	2.12	0.48
11:k:67:TYR:HE2	11:k:71:GLU:CG	2.25	0.48
13:m:160:ASN:HD22	10:3:149:MET:HE1	1.79	0.48
9:2:109:LEU:HD23	9:2:148:THR:HG21	1.95	0.48
9:2:119:TYR:CD1	9:2:123:ILE:HD11	2.49	0.48
11:4:58:GLU:OE2	11:4:61:GLN:OE1	2.31	0.48
11:4:67:TYR:HE2	11:4:71:GLU:CG	2.25	0.48
22:S:211:ARG:CZ	22:S:241:PHE:CE1	2.96	0.48
22:S:404:LEU:HB3	22:S:416:GLU:HB2	1.95	0.48
9:i:119:TYR:HE1	9:i:123:ILE:HD11	1.77	0.48
13:m:131:TYR:HE2	13:m:141:ARG:HD2	1.79	0.48
1:A:74:CYS:O	8:1:77:SER:HB2	2.13	0.48
4:D:181:ARG:NH2	5:E:60:GLU:OE2	2.47	0.48
6:F:234:ILE:HG22	6:F:234:ILE:OXT	2.13	0.48
8:1:115:ASN:C	8:1:116:LYS:O	2.56	0.48
12:5:172:MET:H	12:5:192:SER:HB3	1.79	0.48
16:V:177:THR:HB	21:N:740:TRP:O	2.13	0.48
20:Z:462:VAL:HG13	20:Z:462:VAL:O	2.13	0.48
5:e:121:LEU:C	5:e:121:LEU:CD2	2.87	0.48
12:l:103:SER:OG	13:m:145:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:272:PHE:CZ	10:3:204:GLN:HG2	2.48	0.48
5:E:209:GLU:HA	5:E:209:GLU:OE2	2.14	0.48
1:a:122:ALA:HB3	2:b:83:ARG:HD3	1.96	0.48
1:a:196:GLU:OE1	1:a:196:GLU:HA	2.13	0.48
7:g:175:GLU:OE1	7:g:202:LEU:CB	2.62	0.48
11:k:118:GLN:HG3	11:k:133:HIS:CE1	2.49	0.48
5:E:194:LYS:CD	5:E:197:GLU:OE1	2.62	0.48
7:G:175:GLU:OE1	7:G:202:LEU:CB	2.62	0.48
9:2:115:HIS:HA	9:2:118:LYS:NZ	2.29	0.48
9:2:250:CYS:C	9:2:251:ASP:OD1	2.57	0.48
11:4:41:HIS:CD2	11:4:109:LYS:HD3	2.47	0.48
13:6:46:ARG:CB	14:7:194:ARG:NE	2.77	0.48
16:V:287:THR:HB	26:U:261:LEU:CD2	2.44	0.48
1:a:196:GLU:O	1:a:197:GLU:HG3	2.14	0.48
4:d:123:SER:HA	5:e:134:MET:HA	1.96	0.48
9:i:255:GLU:CD	9:i:255:GLU:H	2.22	0.48
4:D:39:LYS:CE	4:D:184:PRO:HD2	2.44	0.48
4:D:229:ILE:O	4:D:233:VAL:HG23	2.13	0.48
13:6:131:TYR:HE2	13:6:141:ARG:HD2	1.79	0.48
24:Q:347:LEU:O	24:Q:351:ILE:HG12	2.14	0.48
7:g:7:GLY:O	7:g:9:ASP:OD1	2.31	0.48
10:j:74:TYR:CD2	10:j:82:ILE:CG1	2.96	0.48
2:B:142:PHE:CD1	10:3:115:LYS:NZ	2.80	0.48
8:1:150:ASN:O	8:1:152:ARG:CZ	2.62	0.48
12:5:253:TYR:HE1	12:5:262:TYR:CE1	2.32	0.48
13:6:161:GLN:OE1	13:6:161:GLN:HA	2.14	0.48
7:g:8:TYR:HD1	7:g:14:VAL:HB	1.78	0.47
9:i:250:CYS:O	9:i:251:ASP:CB	2.61	0.47
11:k:4:ILE:HD13	11:k:4:ILE:HG21	1.70	0.47
13:m:41:TYR:N	13:m:41:TYR:HD2	2.12	0.47
9:2:250:CYS:O	9:2:251:ASP:CB	2.60	0.47
9:2:254:GLU:H	9:2:254:GLU:CD	2.09	0.47
16:V:35:LEU:HB2	26:U:13:LEU:HD13	1.95	0.47
16:V:203:TYR:CZ	26:U:173:HIS:CD2	3.02	0.47
17:T:58:THR:HG21	17:T:88:TYR:OH	2.13	0.47
25:R:317:ILE:HB	25:R:318:PRO:HD3	1.96	0.47
4:d:40:ASN:OD1	4:d:40:ASN:O	2.32	0.47
11:k:41:HIS:HD2	11:k:109:LYS:CD	2.26	0.47
12:l:83:PHE:HD2	12:l:85:GLY:H	1.60	0.47
5:E:122:ARG:HB3	5:E:134:MET:HE3	1.95	0.47
9:2:109:LEU:HD21	9:2:148:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:3:132:GLU:OE1	10:3:133:ALA:N	2.47	0.47
11:4:28:LEU:HD22	12:5:212:TYR:OH	2.14	0.47
11:4:41:HIS:HD2	11:4:109:LYS:CD	2.26	0.47
11:4:49:GLU:HG2	11:4:99:GLN:HB3	1.95	0.47
13:6:47:TYR:HE2	13:6:49:PRO:CD	2.24	0.47
14:7:193:ASP:O	14:7:194:ARG:HG3	2.13	0.47
21:N:100:THR:HG22	22:S:223:LEU:HD22	1.96	0.47
22:S:357:LEU:HD11	22:S:384:ARG:NE	2.29	0.47
24:Q:72:ASP:O	24:Q:76:GLU:HG3	2.14	0.47
7:g:104:LYS:HZ2	14:n:98:ARG:HH11	1.61	0.47
8:h:115:ASN:C	8:h:116:LYS:O	2.56	0.47
8:h:150:ASN:O	8:h:152:ARG:CZ	2.62	0.47
12:l:172:MET:H	12:l:192:SER:HB3	1.79	0.47
13:m:47:TYR:HD1	14:n:195:GLU:CD	2.22	0.47
2:B:222:LEU:HD13	2:B:232:GLY:HA2	1.96	0.47
10:3:39:LYS:HG2	10:3:39:LYS:O	2.14	0.47
11:4:56:PHE:HD1	11:4:98:TYR:HE2	1.62	0.47
11:4:58:GLU:OE2	11:4:58:GLU:HA	2.13	0.47
11:4:92:ILE:HG13	11:4:93:ARG:N	2.28	0.47
12:5:203:CYS:HB3	12:5:212:TYR:CE1	2.49	0.47
16:V:36:LYS:NZ	26:U:50:ASN:OD1	2.47	0.47
20:Z:24:THR:HB	20:Z:25:PRO:CD	2.44	0.47
26:U:105:LYS:HA	26:U:108:GLU:HG2	1.96	0.47
26:U:160:THR:O	26:U:161:ILE:HD13	2.15	0.47
1:a:126:GLN:OE1	2:b:84:VAL:HG21	2.13	0.47
2:b:222:LEU:HD13	2:b:232:GLY:HA2	1.96	0.47
9:i:115:HIS:HA	9:i:118:LYS:NZ	2.29	0.47
9:i:119:TYR:CD1	9:i:123:ILE:HD11	2.49	0.47
13:m:94:ILE:HG12	13:m:122:LEU:O	2.14	0.47
1:A:30:TYR:O	7:G:15:PHE:CE2	2.67	0.47
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.13	0.47
6:F:179:PHE:CD1	6:F:179:PHE:C	2.92	0.47
21:N:919:THR:HG22	21:N:921:ARG:H	1.79	0.47
4:d:24:LEU:O	4:d:28:LYS:HG3	2.14	0.47
5:e:72:ARG:HB2	12:l:139:ARG:NH2	2.29	0.47
5:e:193:LEU:O	5:e:197:GLU:HG3	2.14	0.47
6:f:234:ILE:HG22	6:f:234:ILE:OXT	2.13	0.47
7:g:7:GLY:C	7:g:9:ASP:OD1	2.58	0.47
9:i:119:TYR:CE1	9:i:123:ILE:CD1	2.97	0.47
9:i:250:CYS:C	9:i:251:ASP:OD1	2.57	0.47
10:j:154:TYR:CD1	10:j:155:GLU:N	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:41:HIS:CD2	11:k:109:LYS:HD3	2.47	0.47
11:k:51:GLY:HA3	12:l:193:ASP:HB2	1.97	0.47
12:l:83:PHE:CD2	12:l:84:GLN:N	2.83	0.47
13:m:230:ASP:OXT	13:m:230:ASP:CG	2.57	0.47
1:A:133:TYR:CD1	2:B:5:TYR:CE1	3.02	0.47
1:A:196:GLU:O	1:A:197:GLU:HG3	2.14	0.47
6:F:179:PHE:C	6:F:179:PHE:HD1	2.23	0.47
9:2:177:LYS:HD3	9:2:208:GLU:OE1	2.13	0.47
9:2:255:GLU:H	9:2:255:GLU:CD	2.22	0.47
13:6:197:THR:O	13:6:200:THR:OG1	2.31	0.47
16:V:293:VAL:HG11	26:U:189:ARG:NH1	2.30	0.47
21:N:277:LEU:HB3	21:N:282:TYR:CD2	2.49	0.47
22:S:149:SER:C	22:S:150:LYS:HG2	2.39	0.47
25:R:113:LEU:HG	25:R:117:ILE:CD1	2.44	0.47
1:a:123:ASN:OD1	2:b:83:ARG:HG2	2.13	0.47
6:f:13:PHE:HA	6:f:14:SER:CB	2.45	0.47
9:i:109:LEU:HD21	9:i:148:THR:HG21	1.96	0.47
10:j:132:GLU:OE1	10:j:133:ALA:N	2.47	0.47
14:n:182:HIS:CE1	9:2:161:LEU:HD13	2.49	0.47
2:B:37:ILE:HD11	2:B:191:ILE:HG22	1.97	0.47
2:B:203:GLU:OE1	2:B:204:PHE:C	2.58	0.47
5:E:121:LEU:CD2	5:E:121:LEU:C	2.87	0.47
11:4:61:GLN:O	11:4:65:GLN:HG3	2.15	0.47
13:6:41:TYR:N	13:6:41:TYR:HD2	2.12	0.47
14:7:153:GLN:HB2	14:7:157:ASP:OD2	2.15	0.47
16:V:214:MET:HG3	26:U:179:ARG:HG2	1.97	0.47
24:Q:182:SER:HB3	24:Q:221:MET:HE2	1.96	0.47
24:Q:345:SER:O	24:Q:349:LYS:HG2	2.14	0.47
1:a:116:VAL:HG21	9:i:99:THR:HG22	1.97	0.47
1:a:219:SER:H	1:a:222:ASP:HB2	1.80	0.47
2:b:203:GLU:CD	2:b:204:PHE:H	2.23	0.47
2:b:227:ILE:HD11	9:i:215:TYR:CE2	2.49	0.47
4:d:66:LYS:HE2	11:k:69:ILE:HD11	1.95	0.47
5:e:209:GLU:HA	5:e:209:GLU:OE2	2.14	0.47
6:f:66:CYS:O	13:m:85:PHE:CE1	2.52	0.47
6:f:179:PHE:CD1	6:f:179:PHE:C	2.92	0.47
6:f:207:THR:OG1	6:f:210:ASN:CG	2.58	0.47
9:i:193:TRP:O	13:6:46:ARG:NH2	2.47	0.47
10:j:29:LEU:HD22	10:j:40:PHE:HE2	1.76	0.47
11:k:92:ILE:HG13	11:k:93:ARG:N	2.29	0.47
14:n:221:ASP:OD1	8:1:33:ALA:HB1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:193:LEU:O	5:E:197:GLU:HG3	2.14	0.47
10:3:74:TYR:CD2	10:3:82:ILE:CB	2.98	0.47
10:3:101:GLY:O	11:4:93:ARG:NH2	2.48	0.47
10:3:188:TYR:CZ	10:3:197:LYS:HD2	2.49	0.47
11:4:46:PHE:CE2	11:4:57:ALA:CB	2.97	0.47
14:7:39:VAL:HG23	14:7:90:ILE:H	1.77	0.47
16:V:214:MET:CG	26:U:179:ARG:HG2	2.45	0.47
21:N:277:LEU:HD22	21:N:282:TYR:OH	2.14	0.47
24:Q:246:TYR:CZ	24:Q:257:LYS:HG2	2.48	0.47
26:U:10:ILE:O	26:U:161:ILE:HG23	2.15	0.47
27:O:363:ILE:O	27:O:366:MET:HG3	2.14	0.47
4:d:90:ARG:CZ	11:k:70:ARG:HA	2.45	0.47
4:d:149:GLN:HE21	4:d:157:SER:HB2	1.80	0.47
10:j:188:TYR:CZ	10:j:197:LYS:HD2	2.49	0.47
11:k:1:MET:HE2	11:k:1:MET:O	2.15	0.47
11:k:23:ARG:HE	12:l:195:THR:HG21	1.80	0.47
11:k:61:GLN:O	11:k:65:GLN:HG3	2.15	0.47
4:D:100:LEU:HD22	12:5:153:ALA:HB1	1.95	0.47
6:F:13:PHE:HA	6:F:14:SER:CB	2.45	0.47
7:G:7:GLY:C	7:G:9:ASP:OD1	2.58	0.47
14:7:136:ARG:CG	14:7:143:LEU:HG	2.45	0.47
16:V:177:THR:CG2	21:N:741:TYR:HA	2.41	0.47
20:Z:439:TYR:HA	20:Z:442:VAL:HG22	1.97	0.47
27:O:166:ARG:HG2	27:O:200:GLU:OE1	2.15	0.47
27:O:236:HIS:N	27:O:240:GLU:OE2	2.47	0.47
2:b:37:ILE:HD11	2:b:191:ILE:HG22	1.97	0.47
2:b:203:GLU:OE1	2:b:204:PHE:C	2.58	0.47
4:d:60:THR:OG1	4:d:61:PRO:HD2	2.15	0.47
6:f:179:PHE:C	6:f:179:PHE:HD1	2.23	0.47
7:g:104:LYS:NZ	14:n:98:ARG:HH11	2.12	0.47
13:m:36:ARG:NH1	13:m:206:VAL:O	2.48	0.47
1:A:133:TYR:CE1	2:B:5:TYR:CD1	3.03	0.47
2:B:203:GLU:CD	2:B:204:PHE:H	2.23	0.47
4:D:155:ILE:HG13	5:E:83:ALA:HB2	1.95	0.47
12:5:83:PHE:CD2	12:5:84:GLN:N	2.83	0.47
22:S:218:LEU:HD11	22:S:258:GLU:OE2	2.14	0.47
6:f:101:ARG:HG3	14:n:124:TYR:CZ	2.50	0.47
8:h:100:ASP:OD1	14:n:35:GLN:CA	2.62	0.47
10:j:204:GLN:HG2	12:5:241:HIS:ND1	2.30	0.47
12:l:203:CYS:HB3	12:l:212:TYR:CE1	2.49	0.47
12:l:203:CYS:HB3	12:l:212:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:151:GLU:HG3	4:D:153:SER:H	1.80	0.47
6:F:207:THR:OG1	6:F:210:ASN:CG	2.58	0.47
6:F:207:THR:H	6:F:210:ASN:HB2	1.80	0.47
9:2:119:TYR:CE1	9:2:123:ILE:CD1	2.97	0.47
16:V:72:PRO:HD3	26:U:82:LYS:HD3	1.96	0.47
16:V:151:VAL:HB	26:U:173:HIS:CD2	2.49	0.47
20:Z:149:TRP:HA	20:Z:152:GLU:HB3	1.96	0.47
20:Z:700:GLU:OE1	20:Z:700:GLU:N	2.48	0.47
24:Q:18:LYS:HG2	24:Q:22:GLU:OE2	2.15	0.47
1:a:166:TYR:CD1	2:b:56:ALA:HA	2.49	0.46
7:g:65:VAL:HG11	14:n:112:PRO:CD	2.45	0.46
9:i:109:LEU:HD23	9:i:148:THR:HG21	1.95	0.46
10:j:14:ALA:O	10:j:136:PHE:HB2	2.16	0.46
1:A:219:SER:H	1:A:222:ASP:HB2	1.80	0.46
5:E:103:TYR:O	13:6:96:SER:HA	2.15	0.46
12:5:203:CYS:HB3	12:5:212:TYR:CZ	2.50	0.46
14:7:136:ARG:HG2	14:7:143:LEU:HG	1.97	0.46
16:V:280:LEU:HD21	26:U:268:LYS:NZ	2.29	0.46
20:Z:30:LYS:HZ3	20:Z:44:LYS:HZ3	1.56	0.46
20:Z:788:PRO:O	20:Z:789:GLN:HB2	2.15	0.46
27:O:222:LEU:HD23	27:O:258:LEU:HD11	1.97	0.46
27:O:313:ILE:CG2	27:O:324:VAL:HG13	2.45	0.46
1:a:166:TYR:N	2:b:57:MET:HG3	2.31	0.46
1:A:249:ALA:O	23:P:84:LYS:HB2	2.16	0.46
2:B:198:GLU:OE2	24:Q:209:TYR:CB	2.63	0.46
4:D:17:ILE:HD11	5:E:136:ARG:NE	2.30	0.46
4:D:149:GLN:HE22	4:D:151:GLU:HB3	1.81	0.46
7:G:184:PRO:HB2	23:P:5:ALA:H	1.80	0.46
8:1:114:LYS:HB2	8:1:115:ASN:OD1	2.15	0.46
13:6:47:TYR:CD2	13:6:47:TYR:C	2.93	0.46
21:N:623:PHE:HZ	21:N:739:PHE:CE1	2.33	0.46
3:c:66:LEU:CD1	3:c:212:GLU:CB	2.90	0.46
4:d:10:ILE:CG2	5:e:9:ASP:O	2.64	0.46
11:k:56:PHE:HD1	11:k:98:TYR:HE2	1.62	0.46
11:k:67:TYR:O	11:k:67:TYR:HD2	1.99	0.46
12:l:83:PHE:CE2	12:l:85:GLY:N	2.83	0.46
13:m:35:THR:CG2	13:m:211:GLU:OE1	2.63	0.46
13:m:46:ARG:NH2	9:2:193:TRP:CB	2.78	0.46
13:m:185:VAL:HG12	13:m:186:GLU:OE1	2.15	0.46
2:B:204:PHE:CE2	2:B:247:LEU:HD22	2.50	0.46
12:5:79:LEU:C	12:5:79:LEU:HD12	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:6:35:THR:CG2	13:6:211:GLU:OE1	2.63	0.46
16:V:31:SER:O	16:V:35:LEU:HD12	2.16	0.46
25:R:184:GLN:NE2	25:R:220:ALA:CB	2.78	0.46
2:b:204:PHE:CE2	2:b:247:LEU:HD22	2.50	0.46
8:h:93:GLU:OE1	8:h:94:LEU:HG	2.15	0.46
9:i:189:GLN:HE22	9:i:222:PRO:HG3	1.80	0.46
10:j:39:LYS:O	10:j:39:LYS:HG2	2.14	0.46
10:j:74:TYR:CD2	10:j:82:ILE:CB	2.98	0.46
11:k:46:PHE:CE2	11:k:57:ALA:CB	2.97	0.46
4:D:39:LYS:NZ	4:D:184:PRO:HD2	2.30	0.46
13:6:46:ARG:HB3	14:7:194:ARG:NE	2.30	0.46
13:6:185:VAL:HG12	13:6:186:GLU:OE1	2.15	0.46
13:6:230:ASP:CG	13:6:230:ASP:OXT	2.57	0.46
14:7:35:GLN:HG2	14:7:144:TRP:HB2	1.97	0.46
16:V:203:TYR:CB	26:U:174:LEU:HD23	2.41	0.46
27:O:40:GLN:NE2	27:O:43:GLU:HB2	2.31	0.46
27:O:310:PHE:HE1	27:O:343:GLN:OE1	1.98	0.46
4:d:228:GLU:H	4:d:228:GLU:HG2	1.52	0.46
8:h:114:LYS:HB2	8:h:115:ASN:OD1	2.15	0.46
12:l:117:LEU:HD11	12:l:253:TYR:HD2	1.81	0.46
13:m:228:LYS:HE3	9:2:223:ASN:CB	2.38	0.46
14:n:256:LYS:HB3	8:1:196:ILE:HD12	1.97	0.46
8:1:183:ARG:HH21	8:1:183:ARG:HD2	1.52	0.46
15:W:122:ARG:CB	15:W:153:LEU:HD22	2.36	0.46
25:R:115:GLU:OE2	25:R:119:LYS:HE2	2.14	0.46
4:d:151:GLU:HB2	4:d:152:PRO:HD2	1.96	0.46
10:j:74:TYR:HD2	10:j:82:ILE:CB	2.29	0.46
10:j:87:PHE:O	10:j:91:VAL:HG23	2.16	0.46
13:m:47:TYR:CD2	13:m:47:TYR:C	2.93	0.46
13:m:161:GLN:OE1	13:m:161:GLN:HA	2.14	0.46
8:1:93:GLU:OE1	8:1:94:LEU:HG	2.15	0.46
12:5:83:PHE:CE2	12:5:85:GLY:N	2.83	0.46
12:5:165:TYR:CB	12:5:170:LEU:HD21	2.44	0.46
13:6:36:ARG:NH1	13:6:206:VAL:O	2.48	0.46
14:7:148:ILE:HG23	14:7:175:LEU:HD23	1.97	0.46
16:V:296:LEU:HG	26:U:193:GLN:HB2	1.97	0.46
18:X:122:TYR:O	18:X:126:ILE:HG13	2.15	0.46
2:b:92:VAL:HG21	2:b:117:ILE:HD11	1.97	0.46
8:h:188:THR:OG1	8:h:191:GLY:O	2.33	0.46
12:l:79:LEU:C	12:l:79:LEU:HD12	2.40	0.46
12:l:151:VAL:HG21	12:l:186:THR:OG1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:178:LYS:HD2	13:m:179:PRO:CD	2.36	0.46
12:5:117:LEU:HD11	12:5:253:TYR:HD2	1.81	0.46
13:6:83:TYR:HE2	13:6:90:LYS:HG2	1.81	0.46
5:e:132:ARG:HH22	6:f:126:ARG:HH12	1.64	0.46
5:e:150:ASP:OD1	13:m:90:LYS:CD	2.64	0.46
10:3:74:TYR:HD2	10:3:82:ILE:CB	2.29	0.46
10:3:87:PHE:O	10:3:91:VAL:HG23	2.16	0.46
19:Y:1:MET:HG2	22:S:337:ASN:HB2	1.96	0.46
20:Z:386:VAL:HG13	20:Z:837:TYR:CD2	2.51	0.46
23:P:119:ILE:O	23:P:123:ARG:HG3	2.16	0.46
24:Q:25:GLN:CD	24:Q:25:GLN:N	2.73	0.46
25:R:279:LEU:O	25:R:279:LEU:HG	2.15	0.46
1:a:95:LEU:HD23	1:a:95:LEU:C	2.41	0.46
1:a:162:TYR:HA	2:b:83:ARG:NH1	2.31	0.46
9:i:31:THR:OG1	9:i:159:GLY:HA3	2.16	0.46
11:k:51:GLY:HA3	12:l:193:ASP:CB	2.45	0.46
13:m:46:ARG:HH22	9:2:193:TRP:HA	1.77	0.46
14:n:241:PHE:HE1	14:n:243:LYS:HZ3	1.63	0.46
2:B:203:GLU:OE1	2:B:204:PHE:O	2.34	0.46
3:C:109:GLU:OE1	3:C:110:ILE:HD13	2.16	0.46
10:3:154:TYR:CD1	10:3:155:GLU:N	2.83	0.46
11:4:1:MET:HE2	11:4:1:MET:O	2.15	0.46
15:W:188:SER:OG	15:W:189:PRO:HD2	2.15	0.46
16:V:94:MET:O	26:U:72:TYR:CE1	2.68	0.46
21:N:641:LEU:HD13	21:N:660:LEU:HG	1.98	0.46
22:S:345:TYR:HA	22:S:348:LEU:HD12	1.98	0.46
27:O:32:PHE:CZ	27:O:40:GLN:HG3	2.51	0.46
4:d:100:LEU:C	4:d:101:GLU:HG2	2.41	0.46
11:k:36:ARG:CZ	11:k:58:GLU:OE1	2.64	0.46
3:C:66:LEU:CD1	3:C:212:GLU:CB	2.90	0.46
11:4:193:ASP:OD2	11:4:193:ASP:N	2.49	0.46
22:S:400:LYS:CD	25:R:389:GLU:OE2	2.64	0.46
25:R:22:PRO:HA	25:R:25:GLU:CD	2.41	0.46
2:b:223:GLY:HA2	9:i:69:LYS:NZ	2.30	0.45
3:c:109:GLU:OE1	3:c:110:ILE:HD13	2.16	0.45
6:f:64:ILE:HG21	6:f:89:ARG:HH21	1.81	0.45
1:A:95:LEU:HD23	1:A:95:LEU:C	2.41	0.45
9:2:189:GLN:HE22	9:2:222:PRO:HG3	1.80	0.45
13:6:134:ASP:C	13:6:134:ASP:OD1	2.58	0.45
14:7:110:ASP:O	14:7:111:ASN:C	2.59	0.45
20:Z:727:GLU:O	20:Z:728:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:37:ILE:CD1	2:b:191:ILE:HG22	2.46	0.45
10:j:98:ARG:HH21	10:j:103:TYR:HA	1.81	0.45
13:m:169:GLU:OE1	13:m:179:PRO:CD	2.64	0.45
4:D:11:PHE:HZ	5:E:26:TYR:C	2.24	0.45
10:3:14:ALA:O	10:3:136:PHE:HB2	2.16	0.45
11:4:67:TYR:CE2	11:4:71:GLU:HG3	2.45	0.45
16:V:225:LEU:HB2	23:P:423:LEU:HD13	1.97	0.45
20:Z:601:VAL:HG23	20:Z:622:HIS:CE1	2.51	0.45
21:N:277:LEU:O	21:N:282:TYR:HD2	1.99	0.45
25:R:128:LEU:HB2	25:R:129:GLU:OE2	2.16	0.45
26:U:17:SER:O	26:U:20:ASP:OD2	2.33	0.45
2:b:203:GLU:OE1	2:b:204:PHE:O	2.34	0.45
8:h:142:PHE:CE1	14:7:66:LEU:HD13	2.52	0.45
9:i:181:ILE:HG21	9:i:219:TYR:CE2	2.49	0.45
10:j:157:ASN:N	10:j:157:ASN:OD1	2.49	0.45
3:C:66:LEU:HD11	3:C:212:GLU:CB	2.45	0.45
7:G:99:PHE:CD2	7:G:107:ILE:HA	2.52	0.45
9:2:31:THR:OG1	9:2:159:GLY:HA3	2.16	0.45
14:7:39:VAL:O	14:7:89:ASP:HA	2.16	0.45
16:V:188:LEU:HD23	16:V:188:LEU:C	2.40	0.45
16:V:217:HIS:NE2	26:U:181:GLN:NE2	2.64	0.45
16:V:217:HIS:NE2	26:U:182:ALA:HB2	2.30	0.45
20:Z:386:VAL:CG1	20:Z:837:TYR:CD2	3.00	0.45
22:S:364:ILE:HD11	22:S:384:ARG:NH1	2.31	0.45
24:Q:252:HIS:CG	24:Q:253:ASN:N	2.84	0.45
25:R:267:LYS:HB2	25:R:297:TYR:CD2	2.51	0.45
10:j:74:TYR:CD2	10:j:82:ILE:HG13	2.52	0.45
12:l:165:TYR:CB	12:l:170:LEU:HD21	2.44	0.45
4:D:90:ARG:NH1	11:4:69:ILE:HG23	2.30	0.45
11:4:67:TYR:HD2	11:4:67:TYR:O	1.99	0.45
16:V:214:MET:CG	26:U:179:ARG:HD3	2.39	0.45
24:Q:119:GLU:HG3	24:Q:120:LYS:N	2.31	0.45
8:h:136:ALA:C	8:h:140:SER:HG	2.24	0.45
13:m:46:ARG:CZ	9:2:193:TRP:O	2.52	0.45
13:m:222:LYS:C	13:m:223:GLU:HG3	2.41	0.45
14:n:255:ALA:HB2	8:1:39:VAL:CG1	2.46	0.45
4:D:203:VAL:O	4:D:204:GLN:O	2.35	0.45
9:2:179:GLU:HA	9:2:182:LYS:HD3	1.99	0.45
11:4:69:ILE:HG23	11:4:70:ARG:N	2.31	0.45
22:S:416:GLU:O	22:S:420:GLU:HG3	2.17	0.45
24:Q:126:LYS:HA	24:Q:134:LYS:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:237:SER:OG	1:a:239:GLU:OE1	2.34	0.45
11:k:69:ILE:HG23	11:k:70:ARG:N	2.31	0.45
12:l:148:ARG:NH2	12:l:180:THR:HA	2.30	0.45
8:1:91:PHE:CD2	8:1:106:ILE:HD13	2.52	0.45
8:1:123:PRO:HD2	8:1:127:SER:O	2.16	0.45
11:4:36:ARG:CZ	11:4:58:GLU:OE1	2.64	0.45
13:6:230:ASP:OD1	13:6:230:ASP:OXT	2.34	0.45
16:V:72:PRO:CG	26:U:82:LYS:NZ	2.79	0.45
16:V:98:THR:HG22	26:U:54:LEU:C	2.42	0.45
16:V:208:LYS:NZ	16:V:208:LYS:HB2	2.32	0.45
16:V:215:ASN:OD1	26:U:181:GLN:NE2	2.49	0.45
25:R:104:LYS:HD3	25:R:105:LYS:N	2.31	0.45
26:U:249:VAL:HA	26:U:252:HIS:CD2	2.52	0.45
7:g:99:PHE:CD2	7:g:107:ILE:HA	2.52	0.45
13:m:230:ASP:OD1	13:m:230:ASP:OXT	2.35	0.45
2:B:37:ILE:CD1	2:B:191:ILE:HG22	2.46	0.45
4:D:31:THR:O	4:D:76:SER:HB3	2.17	0.45
4:D:39:LYS:HE2	4:D:184:PRO:HD2	1.99	0.45
4:D:101:GLU:O	4:D:102:ASP:O	2.34	0.45
6:F:64:ILE:HG21	6:F:89:ARG:HH21	1.81	0.45
10:3:98:ARG:HH21	10:3:103:TYR:HA	1.81	0.45
20:Z:759:ARG:HH11	20:Z:759:ARG:HD3	1.46	0.45
25:R:44:LYS:HD3	25:R:44:LYS:C	2.41	0.45
6:f:207:THR:H	6:f:210:ASN:HB2	1.80	0.45
8:h:123:PRO:HD2	8:h:127:SER:O	2.16	0.45
14:n:136:ARG:HD3	14:n:143:LEU:HD11	1.98	0.45
14:n:250:MET:SD	14:n:250:MET:N	2.88	0.45
1:A:237:SER:OG	1:A:239:GLU:OE1	2.34	0.45
2:B:92:VAL:HG21	2:B:117:ILE:HD11	1.97	0.45
5:E:8:TYR:HB2	5:E:22:PHE:HD2	1.80	0.45
9:2:93:GLU:O	9:2:97:LEU:CD1	2.65	0.45
12:5:151:VAL:HG21	12:5:186:THR:OG1	2.16	0.45
16:V:221:TRP:CD1	26:U:130:VAL:O	2.70	0.45
21:N:304:LEU:HA	21:N:307:LYS:HE3	1.98	0.45
24:Q:255:TYR:CD2	24:Q:256:GLU:N	2.85	0.45
11:k:3:ILE:CD1	11:k:176:PHE:CD1	3.00	0.45
13:m:201:GLU:OE1	9:2:58:LYS:HD2	2.17	0.45
2:B:18:LEU:O	2:B:22:ASP:OD1	2.35	0.45
4:D:107:GLU:HG2	4:D:111:ARG:HH11	1.82	0.45
8:1:115:ASN:HB3	8:1:118:GLU:OE2	2.17	0.45
16:V:208:LYS:HZ1	26:U:19:LEU:HD23	1.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:31:GLU:HA	19:Y:31:GLU:OE2	2.17	0.45
7:g:41:LYS:HB3	7:g:161:LYS:O	2.16	0.45
9:i:109:LEU:HD21	9:i:148:THR:CG2	2.47	0.45
11:k:67:TYR:CE2	11:k:71:GLU:HG3	2.45	0.45
14:n:58:ASP:HA	14:n:228:PHE:HA	1.99	0.45
14:n:250:MET:HG2	14:n:252:TRP:HD1	1.82	0.45
10:3:70:LYS:HD2	10:3:70:LYS:HA	1.76	0.45
10:3:74:TYR:CD2	10:3:82:ILE:HG13	2.52	0.45
13:6:94:ILE:CG1	13:6:122:LEU:O	2.65	0.45
13:6:169:GLU:OE1	13:6:179:PRO:CD	2.64	0.45
14:7:136:ARG:CD	14:7:141:ASN:O	2.65	0.45
16:V:213:LEU:HD22	26:U:171:VAL:CB	2.46	0.45
17:T:215:LYS:HG3	17:T:216:GLU:N	2.32	0.45
20:Z:81:SER:HA	20:Z:88:PRO:HB2	1.99	0.45
20:Z:879:ALA:O	20:Z:883:THR:HG23	2.16	0.45
21:N:161:TYR:HA	21:N:202:PHE:CE1	2.52	0.45
5:e:69:GLU:OE1	12:l:143:LEU:HD23	2.18	0.44
8:h:49:LYS:HE3	8:h:111:TYR:HB3	1.99	0.44
9:i:179:GLU:HA	9:i:182:LYS:HD3	1.99	0.44
11:k:34:LYS:HA	11:k:46:PHE:CE1	2.52	0.44
11:k:46:PHE:CD2	11:k:57:ALA:HB2	2.52	0.44
13:m:134:ASP:C	13:m:134:ASP:OD1	2.58	0.44
14:n:248:GLU:HA	14:n:250:MET:CE	2.48	0.44
7:G:41:LYS:HB3	7:G:161:LYS:O	2.16	0.44
9:2:181:ILE:HG21	9:2:219:TYR:CE2	2.49	0.44
12:5:83:PHE:CD2	12:5:85:GLY:N	2.81	0.44
13:6:12:PRO:HB2	14:7:137:ARG:HH21	1.81	0.44
16:V:217:HIS:CE1	26:U:181:GLN:O	2.70	0.44
18:X:45:PHE:HA	18:X:133:SER:O	2.17	0.44
1:a:126:GLN:HB3	2:b:84:VAL:HG11	1.99	0.44
4:d:149:GLN:NE2	4:d:159:TRP:HE1	2.15	0.44
8:h:115:ASN:HB3	8:h:118:GLU:OE2	2.17	0.44
9:i:48:ARG:NH2	13:6:230:ASP:CG	2.71	0.44
11:k:78:GLN:O	11:k:125:LYS:NZ	2.50	0.44
12:l:99:ASN:OD1	10:3:180:LEU:CD1	2.65	0.44
13:m:83:TYR:HE2	13:m:90:LYS:HG2	1.81	0.44
8:1:150:ASN:C	8:1:152:ARG:HH12	2.24	0.44
11:4:56:PHE:HD1	11:4:98:TYR:CE2	2.35	0.44
13:6:222:LYS:C	13:6:223:GLU:HG3	2.41	0.44
16:V:153:ILE:O	16:V:153:ILE:HG23	2.18	0.44
8:h:91:PHE:CD2	8:h:106:ILE:HD13	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:119:TYR:HD1	9:i:123:ILE:CG1	2.31	0.44
10:j:51:LEU:HD11	10:j:107:PRO:HB3	1.99	0.44
13:m:230:ASP:CG	9:2:48:ARG:NH2	2.75	0.44
1:A:106:TYR:HB2	8:1:70:TYR:HB2	1.98	0.44
5:E:177:GLU:H	5:E:177:GLU:CD	2.25	0.44
11:4:46:PHE:CD2	11:4:57:ALA:HB2	2.52	0.44
20:Z:80:SER:O	20:Z:81:SER:HB2	2.17	0.44
22:S:320:ILE:O	22:S:324:MET:HG3	2.17	0.44
8:h:174:TRP:HE1	8:1:145:GLY:HA2	1.81	0.44
10:j:182:GLY:O	10:j:184:GLY:N	2.51	0.44
11:k:56:PHE:HD1	11:k:98:TYR:CE2	2.35	0.44
11:k:167:GLU:OE2	12:5:216:ASP:OD2	2.36	0.44
14:n:185:ASN:N	14:n:186:PRO:CD	2.80	0.44
5:E:104:ASP:OD2	13:6:99:ARG:NE	2.40	0.44
14:7:193:ASP:O	14:7:194:ARG:CG	2.65	0.44
16:V:45:VAL:CG1	16:V:46:PRO:HA	2.44	0.44
21:N:629:CYS:SG	21:N:634:LEU:HD12	2.58	0.44
6:f:62:LYS:HA	6:f:74:LEU:HD21	1.98	0.44
13:m:27:ASP:O	13:m:122:LEU:HD21	2.17	0.44
13:m:94:ILE:CG1	13:m:122:LEU:O	2.65	0.44
14:n:250:MET:HG2	14:n:252:TRP:CD1	2.52	0.44
2:B:214:ILE:HD12	2:B:214:ILE:N	2.33	0.44
8:1:188:THR:OG1	8:1:191:GLY:O	2.33	0.44
21:N:277:LEU:O	21:N:282:TYR:CD2	2.71	0.44
2:b:18:LEU:O	2:b:22:ASP:OD1	2.35	0.44
2:b:227:ILE:CD1	9:i:215:TYR:CD2	3.01	0.44
10:j:204:GLN:CG	12:5:241:HIS:ND1	2.81	0.44
11:k:172:MET:HG2	11:k:174:MET:H	1.83	0.44
11:k:193:ASP:OD2	11:k:193:ASP:N	2.49	0.44
14:n:248:GLU:HA	14:n:250:MET:HE1	1.99	0.44
6:F:89:ARG:HD3	13:6:85:PHE:CD1	2.53	0.44
10:3:182:GLY:O	10:3:184:GLY:N	2.51	0.44
11:4:36:ARG:HD2	11:4:58:GLU:OE2	2.18	0.44
15:W:64:THR:CG2	15:W:65:PHE:N	2.80	0.44
20:Z:135:LEU:CD1	20:Z:138:ARG:HH21	2.30	0.44
21:N:858:LYS:NZ	21:N:859:ASN:H	2.15	0.44
24:Q:389:VAL:HB	25:R:346:LYS:HB3	1.98	0.44
11:k:36:ARG:HD2	11:k:58:GLU:OE2	2.18	0.44
1:A:130:GLN:OE1	2:B:127:VAL:HG12	2.17	0.44
6:F:66:CYS:O	13:6:85:PHE:HE1	2.01	0.44
8:1:49:LYS:HE3	8:1:111:TYR:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:109:LEU:HD21	9:2:148:THR:CG2	2.47	0.44
9:2:176:THR:HG22	9:2:178:GLU:H	1.82	0.44
11:4:180:ILE:HD11	11:4:191:GLN:OE1	2.17	0.44
13:6:130:VAL:O	13:6:131:TYR:HD2	2.01	0.44
16:V:91:MET:SD	26:U:79:MET:HE3	2.57	0.44
16:V:221:TRP:CH2	23:P:427:GLU:HG3	2.51	0.44
16:V:304:ALA:C	27:O:377:VAL:CG2	2.90	0.44
22:S:19:HIS:O	22:S:22:GLU:HG2	2.18	0.44
2:b:99:ARG:NH2	9:i:91:ASN:OD1	2.51	0.44
5:e:177:GLU:H	5:e:177:GLU:CD	2.24	0.44
9:i:93:GLU:O	9:i:97:LEU:CD1	2.65	0.44
2:B:157:PHE:CE1	3:C:52:VAL:HG21	2.53	0.44
3:C:7:ASP:HB3	4:D:6:ARG:HH21	1.83	0.44
10:3:51:LEU:HD11	10:3:107:PRO:HB3	2.00	0.44
10:3:157:ASN:N	10:3:157:ASN:OD1	2.49	0.44
22:S:198:SER:O	22:S:200:GLU:OE1	2.36	0.44
3:c:94:HIS:HD1	3:c:114:ARG:HG2	1.82	0.44
6:f:152:ASN:OD1	6:f:152:ASN:C	2.61	0.44
6:f:152:ASN:HD22	7:g:82:ILE:HG21	1.82	0.44
11:k:180:ILE:HD11	11:k:191:GLN:OE1	2.17	0.44
3:C:94:HIS:HD1	3:C:114:ARG:HG2	1.82	0.44
4:D:96:HIS:CE1	4:D:102:ASP:O	2.71	0.44
10:3:29:LEU:HD22	10:3:40:PHE:HE2	1.76	0.44
11:4:3:ILE:CD1	11:4:176:PHE:CD1	3.00	0.44
16:V:98:THR:HG22	26:U:55:PRO:HD3	2.00	0.44
22:S:152:LEU:O	22:S:153:GLU:C	2.61	0.44
24:Q:382:LEU:C	24:Q:384:LYS:HD2	2.42	0.44
1:a:30:TYR:HB3	7:g:15:PHE:HD2	1.83	0.43
8:h:150:ASN:C	8:h:152:ARG:HH12	2.25	0.43
12:l:218:ASN:O	12:l:220:LYS:NZ	2.51	0.43
1:A:98:LYS:HD3	8:1:78:GLN:HG2	2.00	0.43
4:D:66:LYS:CG	11:4:69:ILE:HD11	2.48	0.43
6:F:62:LYS:HA	6:F:74:LEU:HD21	1.99	0.43
9:2:119:TYR:CD2	9:2:119:TYR:N	2.85	0.43
11:4:78:GLN:O	11:4:125:LYS:NZ	2.50	0.43
11:4:179:VAL:O	11:4:195:PHE:CD1	2.71	0.43
21:N:623:PHE:CZ	21:N:739:PHE:HE1	2.36	0.43
25:R:34:THR:HG21	25:R:69:GLU:OE1	2.18	0.43
11:k:35:THR:CG2	11:k:182:LYS:NZ	2.66	0.43
13:m:47:TYR:HE2	13:m:49:PRO:CD	2.24	0.43
8:1:152:ARG:NH1	8:1:152:ARG:HG3	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:126:TYR:N	9:2:126:TYR:CD1	2.85	0.43
9:2:128:ILE:HD11	9:2:156:LEU:N	2.33	0.43
10:3:189:ILE:HB	10:3:196:VAL:HG12	2.00	0.43
13:6:27:ASP:O	13:6:122:LEU:HD21	2.17	0.43
16:V:98:THR:CG2	26:U:55:PRO:HD3	2.48	0.43
16:V:214:MET:HG2	26:U:181:GLN:HE21	1.80	0.43
16:V:280:LEU:HD23	26:U:268:LYS:CE	2.31	0.43
21:N:86:LYS:O	21:N:87:ASP:HB2	2.19	0.43
22:S:400:LYS:HD3	25:R:389:GLU:OE2	2.17	0.43
24:Q:345:SER:O	24:Q:349:LYS:HE2	2.17	0.43
4:d:34:VAL:HG23	4:d:195:THR:HG23	2.00	0.43
10:j:189:ILE:HB	10:j:196:VAL:HG12	2.00	0.43
3:C:22:VAL:HG11	3:C:154:SER:HB2	2.00	0.43
4:D:13:PRO:HA	5:E:26:TYR:CG	2.54	0.43
14:7:109:TYR:O	14:7:110:ASP:CB	2.65	0.43
18:X:30:GLN:H	18:X:54:GLU:HB3	1.82	0.43
21:N:361:ASN:O	21:N:362:TRP:C	2.59	0.43
21:N:608:LEU:O	21:N:611:LYS:HB3	2.18	0.43
24:Q:252:HIS:CE1	24:Q:253:ASN:CB	3.01	0.43
1:a:174:LYS:O	1:a:177:GLU:OE2	2.36	0.43
3:c:22:VAL:HG11	3:c:154:SER:HB2	2.00	0.43
8:h:172:ILE:HA	8:h:178:SER:OG	2.19	0.43
11:k:69:ILE:CG2	11:k:70:ARG:N	2.82	0.43
13:m:122:LEU:HD13	13:m:217:LYS:HG2	2.00	0.43
1:A:174:LYS:O	1:A:177:GLU:OE2	2.36	0.43
4:D:11:PHE:CE2	5:E:23:GLN:HA	2.54	0.43
4:D:11:PHE:CD2	5:E:23:GLN:HA	2.53	0.43
7:G:99:PHE:CE2	7:G:107:ILE:HA	2.54	0.43
11:4:35:THR:CG2	11:4:182:LYS:NZ	2.66	0.43
13:6:122:LEU:HD13	13:6:217:LYS:HG2	2.00	0.43
15:W:188:SER:OG	15:W:189:PRO:CD	2.66	0.43
16:V:208:LYS:HA	26:U:127:GLN:NE2	2.34	0.43
19:Y:3:THR:O	19:Y:4:ASP:C	2.60	0.43
20:Z:24:THR:HB	20:Z:25:PRO:HD3	1.99	0.43
20:Z:829:GLN:O	20:Z:833:GLN:HG3	2.17	0.43
22:S:192:GLU:O	22:S:196:ARG:HG2	2.18	0.43
9:i:128:ILE:HD11	9:i:156:LEU:N	2.33	0.43
12:l:216:ASP:OD2	11:4:167:GLU:CD	2.61	0.43
14:n:223:ARG:HG3	14:n:223:ARG:NH1	2.33	0.43
1:A:62:LYS:O	7:G:161:LYS:HG3	2.17	0.43
11:4:40:PRO:O	11:4:41:HIS:ND1	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:4:172:MET:HG2	11:4:174:MET:H	1.83	0.43
13:6:105:LEU:HD23	13:6:113:TYR:HD2	1.84	0.43
20:Z:591:ILE:H	20:Z:591:ILE:HD12	1.83	0.43
21:N:87:ASP:O	21:N:88:ARG:CB	2.66	0.43
21:N:735:MET:HG3	21:N:748:PHE:CD2	2.53	0.43
23:P:86:HIS:HB3	23:P:88:GLN:H	1.83	0.43
1:a:166:TYR:C	2:b:57:MET:HG3	2.44	0.43
2:b:222:LEU:O	9:i:68:PRO:CB	2.67	0.43
3:c:66:LEU:HD11	3:c:212:GLU:CB	2.45	0.43
8:h:152:ARG:NH1	8:h:152:ARG:HG3	2.33	0.43
9:i:93:GLU:O	9:i:97:LEU:HD12	2.19	0.43
9:i:126:TYR:N	9:i:126:TYR:CD1	2.85	0.43
10:j:129:CYS:O	10:j:131:ASP:OD2	2.36	0.43
11:k:40:PRO:O	11:k:41:HIS:ND1	2.44	0.43
13:m:130:VAL:O	13:m:131:TYR:HD2	2.01	0.43
9:2:56:ALA:C	9:2:57:ASP:OD1	2.61	0.43
17:T:133:ILE:O	17:T:133:ILE:HG13	2.18	0.43
21:N:377:GLY:O	21:N:378:ASN:HB2	2.18	0.43
21:N:454:ALA:C	21:N:457:SER:HG	2.26	0.43
21:N:474:SER:OG	21:N:477:SER:HB2	2.17	0.43
2:b:75:TYR:CE1	2:b:82:TYR:CD2	3.06	0.43
11:k:179:VAL:O	11:k:195:PHE:CD1	2.71	0.43
12:l:213:GLY:HA2	11:4:167:GLU:OE1	2.19	0.43
1:A:30:TYR:CB	7:G:15:PHE:CD2	2.94	0.43
4:D:66:LYS:O	4:D:90:ARG:CZ	2.66	0.43
7:G:184:PRO:CB	23:P:4:ASP:H	2.32	0.43
9:2:30:THR:OG1	9:2:75:ALA:HB2	2.19	0.43
9:2:93:GLU:O	9:2:97:LEU:HD12	2.18	0.43
10:3:51:LEU:CD2	10:3:53:ILE:HD11	2.48	0.43
12:5:84:GLN:NE2	12:5:221:TRP:NE1	2.51	0.43
12:5:252:LEU:C	12:5:253:TYR:CD1	2.93	0.43
13:6:26:GLU:OE2	13:6:183:LEU:HD12	2.19	0.43
14:7:136:ARG:NE	14:7:141:ASN:O	2.51	0.43
22:S:241:PHE:CD2	22:S:250:ALA:HB2	2.53	0.43
24:Q:67:THR:N	24:Q:68:MET:HB2	2.33	0.43
24:Q:116:PHE:HA	24:Q:119:GLU:HG2	2.00	0.43
2:b:101:TYR:CZ	10:j:70:LYS:HE3	2.54	0.43
3:c:185:LYS:HD3	3:c:185:LYS:HA	1.74	0.43
8:h:88:ALA:CB	8:h:120:TYR:HD2	2.31	0.43
9:i:196:LEU:HD12	13:6:41:TYR:HA	2.01	0.43
12:l:128:GLN:HE21	13:m:99:ARG:HH12	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:TYR:CE1	2:B:82:TYR:CD2	3.06	0.43
2:B:190:HIS:ND1	24:Q:95:LYS:CE	2.81	0.43
10:3:144:ASP:OD1	10:3:145:GLN:N	2.51	0.43
16:V:288:LEU:CD2	17:T:270:ILE:HD13	2.49	0.43
16:V:305:ILE:O	27:O:376:GLN:NE2	2.52	0.43
21:N:4:THR:HG23	22:S:211:ARG:CG	2.43	0.43
22:S:18:LEU:HD23	22:S:18:LEU:HA	1.91	0.43
22:S:149:SER:O	22:S:150:LYS:CB	2.67	0.43
22:S:160:ARG:HH12	22:S:206:GLN:HB3	1.83	0.43
23:P:364:ARG:HG2	23:P:364:ARG:NH1	2.34	0.43
24:Q:178:HIS:HB3	24:Q:201:ALA:HB2	2.01	0.43
24:Q:385:ILE:O	24:Q:385:ILE:HG13	2.19	0.43
8:h:151:PHE:O	8:h:152:ARG:HG3	2.19	0.43
9:i:30:THR:OG1	9:i:75:ALA:HB2	2.19	0.43
9:i:56:ALA:C	9:i:57:ASP:OD1	2.61	0.43
11:4:34:LYS:HA	11:4:46:PHE:CE1	2.52	0.43
11:4:46:PHE:HB3	11:4:102:VAL:HG12	2.01	0.43
20:Z:560:THR:O	20:Z:563:VAL:HG22	2.19	0.43
21:N:666:GLN:HA	21:N:711:ARG:HH21	1.83	0.43
22:S:89:LYS:HZ1	22:S:93:LEU:HD21	1.83	0.43
23:P:88:GLN:HB2	23:P:92:SER:HB2	2.00	0.43
23:P:173:MET:SD	23:P:176:LYS:NZ	2.85	0.43
26:U:41:ALA:O	26:U:42:ASN:HB2	2.19	0.43
3:C:220:ALA:HB2	9:2:253:GLN:O	2.18	0.43
4:D:32:CYS:H	4:D:47:GLU:HB3	1.84	0.43
9:2:99:THR:O	9:2:101:ARG:HG3	2.19	0.43
9:2:189:GLN:NE2	9:2:222:PRO:HG3	2.33	0.43
10:3:129:CYS:O	10:3:131:ASP:OD2	2.36	0.43
20:Z:386:VAL:HG13	20:Z:837:TYR:CG	2.54	0.43
27:O:326:HIS:HB3	27:O:330:ARG:NH1	2.34	0.43
7:g:175:GLU:OE1	7:g:202:LEU:HD13	2.19	0.42
8:h:115:ASN:O	8:h:116:LYS:C	2.62	0.42
13:m:169:GLU:OE1	13:m:179:PRO:HD2	2.19	0.42
14:n:261:TYR:O	9:2:150:VAL:HG13	2.18	0.42
2:B:177:LYS:HE3	24:Q:170:ASP:HB3	2.00	0.42
3:C:54:SER:HB3	3:C:57:LEU:HB2	2.00	0.42
12:5:120:MET:HA	12:5:127:CYS:SG	2.59	0.42
12:5:203:CYS:CB	12:5:212:TYR:CE1	3.02	0.42
16:V:213:LEU:HD22	26:U:171:VAL:HG13	2.00	0.42
21:N:686:ILE:HA	21:N:696:LYS:HG2	2.01	0.42
21:N:896:PHE:CE2	21:N:898:GLY:HA2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:89:LYS:NZ	22:S:93:LEU:HD21	2.34	0.42
22:S:94:LYS:HA	22:S:98:SER:HA	1.99	0.42
4:d:90:ARG:HH11	11:k:70:ARG:HG3	1.84	0.42
6:f:106:GLU:O	6:f:110:HIS:CE1	2.73	0.42
10:j:144:ASP:OD1	10:j:145:GLN:N	2.51	0.42
8:l:88:ALA:CB	8:l:120:TYR:HD2	2.31	0.42
9:2:219:TYR:CD1	9:2:219:TYR:O	2.72	0.42
16:V:178:GLY:O	21:N:651:PHE:CZ	2.72	0.42
20:Z:149:TRP:CD2	20:Z:149:TRP:C	2.97	0.42
22:S:358:LYS:HE2	22:S:412:ASN:OD1	2.19	0.42
23:P:86:HIS:CB	23:P:88:GLN:H	2.33	0.42
23:P:288:ASN:O	23:P:291:LYS:HG2	2.19	0.42
2:b:214:ILE:N	2:b:214:ILE:HD12	2.33	0.42
2:b:215:GLY:O	2:b:234:ARG:CG	2.67	0.42
3:c:152:ASN:HB2	3:c:153:PRO:CD	2.49	0.42
6:f:17:GLY:O	7:g:81:LEU:HD21	2.18	0.42
6:f:117:GLN:C	6:f:117:GLN:OE1	2.62	0.42
9:i:176:THR:HG22	9:i:178:GLU:H	1.82	0.42
9:i:189:GLN:NE2	9:i:222:PRO:HG3	2.33	0.42
10:j:51:LEU:CD2	10:j:53:ILE:HD11	2.48	0.42
10:j:204:GLN:OE1	10:j:204:GLN:CA	2.60	0.42
12:l:120:MET:HA	12:l:127:CYS:SG	2.59	0.42
7:G:161:LYS:HB3	7:G:161:LYS:HZ3	1.84	0.42
13:6:47:TYR:C	13:6:47:TYR:HD2	2.26	0.42
17:T:230:ASN:O	17:T:231:SER:HB2	2.18	0.42
20:Z:31:LYS:HE3	20:Z:79:THR:HA	2.02	0.42
2:b:2:THR:HG22	2:b:3:ASP:N	2.21	0.42
7:g:65:VAL:HG11	14:n:112:PRO:HD2	2.00	0.42
8:h:26:ASP:O	8:h:42:LYS:HD2	2.20	0.42
12:l:252:LEU:C	12:l:253:TYR:CD1	2.93	0.42
13:m:26:GLU:OE2	13:m:183:LEU:HD12	2.19	0.42
6:F:117:GLN:OE1	6:F:117:GLN:C	2.62	0.42
6:F:152:ASN:OD1	6:F:152:ASN:C	2.61	0.42
13:6:53:ASP:OD1	13:6:220:VAL:HG21	2.20	0.42
13:6:169:GLU:OE1	13:6:179:PRO:HD2	2.19	0.42
24:Q:386:PHE:CZ	24:Q:387:TYR:O	2.73	0.42
1:a:122:ALA:CB	2:b:83:ARG:HD3	2.49	0.42
3:c:54:SER:HB3	3:c:57:LEU:HB2	2.00	0.42
6:f:105:VAL:HG11	6:f:143:HIS:CB	2.49	0.42
7:g:99:PHE:CE2	7:g:107:ILE:HA	2.54	0.42
11:k:177:LYS:HE3	11:4:170:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:165:TYR:CB	12:l:170:LEU:CD2	2.97	0.42
1:A:68:THR:HB	7:G:159:GLY:HA3	2.01	0.42
1:A:249:ALA:HB2	23:P:85:LYS:H	1.70	0.42
7:G:175:GLU:OE1	7:G:202:LEU:HD13	2.19	0.42
8:1:26:ASP:O	8:1:42:LYS:HD2	2.20	0.42
9:2:94:LEU:HA	9:2:94:LEU:HD23	1.83	0.42
10:3:37:SER:HB3	11:4:126:VAL:HG11	2.02	0.42
10:3:80:ARG:HE	10:3:80:ARG:HB2	1.46	0.42
20:Z:68:LEU:HA	20:Z:71:LEU:HD12	2.00	0.42
21:N:544:GLU:HG3	21:N:546:LEU:N	2.34	0.42
10:j:204:GLN:HG2	12:5:272:PHE:CE1	2.54	0.42
12:l:83:PHE:CD2	12:l:83:PHE:C	2.98	0.42
13:m:47:TYR:C	13:m:47:TYR:HD2	2.26	0.42
13:m:160:ASN:ND2	10:3:149:MET:HE1	2.35	0.42
2:B:215:GLY:O	2:B:234:ARG:CG	2.67	0.42
3:C:78:ALA:CB	3:C:165:VAL:HG23	2.50	0.42
4:D:67:ILE:HD13	4:D:90:ARG:HD3	2.00	0.42
11:4:4:ILE:HD13	11:4:4:ILE:HG21	1.70	0.42
13:6:9:GLN:NE2	13:6:10:PHE:O	2.53	0.42
16:V:252:SER:HB2	24:Q:425:GLN:OE1	2.19	0.42
16:V:306:LYS:HZ2	26:U:239:LEU:HG	1.84	0.42
17:T:76:ASP:O	17:T:79:GLU:HG3	2.19	0.42
23:P:172:GLU:C	23:P:173:MET:HE2	2.45	0.42
1:a:122:ALA:HB1	2:b:83:ARG:HD2	2.01	0.42
1:a:130:GLN:NE2	2:b:130:PHE:CZ	2.87	0.42
4:d:141:ARG:NH1	4:d:141:ARG:HG3	2.35	0.42
8:h:183:ARG:HH21	8:h:183:ARG:HD2	1.52	0.42
9:i:99:THR:O	9:i:101:ARG:HG3	2.19	0.42
9:i:219:TYR:O	9:i:219:TYR:CD1	2.72	0.42
12:l:83:PHE:CD2	12:l:85:GLY:N	2.81	0.42
12:l:214:VAL:HG12	11:4:142:SER:CB	2.46	0.42
1:A:245:LEU:O	23:P:85:LYS:O	2.37	0.42
2:B:8:SER:HA	2:B:124:SER:O	2.20	0.42
3:C:152:ASN:HB2	3:C:153:PRO:CD	2.49	0.42
4:D:66:LYS:HE3	4:D:221:ILE:HD12	2.02	0.42
8:1:151:PHE:O	8:1:152:ARG:HG3	2.19	0.42
14:7:246:GLN:HB2	14:7:248:GLU:OE2	2.20	0.42
16:V:41:GLY:O	16:V:45:VAL:CG2	2.60	0.42
16:V:135:ARG:HA	16:V:135:ARG:CZ	2.49	0.42
21:N:277:LEU:CD2	21:N:282:TYR:CE2	3.02	0.42
22:S:33:GLU:HG3	22:S:57:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:72:VAL:HG22	25:R:72:VAL:O	2.19	0.42
25:R:254:SER:OG	25:R:289:ILE:HG13	2.19	0.42
2:b:8:SER:HA	2:b:124:SER:O	2.20	0.42
2:b:49:LYS:HE3	2:b:208:THR:O	2.20	0.42
8:h:38:ARG:NH2	9:i:168:GLU:OE2	2.50	0.42
6:F:106:GLU:O	6:F:110:HIS:CE1	2.73	0.42
6:F:160:ALA:O	6:F:161:ILE:HG23	2.20	0.42
8:1:49:LYS:HA	8:1:49:LYS:HD2	1.85	0.42
8:1:172:ILE:HA	8:1:178:SER:OG	2.19	0.42
12:5:165:TYR:CB	12:5:170:LEU:CD2	2.97	0.42
16:V:218:LYS:CD	26:U:131:GLY:HA3	2.50	0.42
23:P:18:LYS:HE2	23:P:57:GLU:HG3	2.02	0.42
1:a:49:ASP:OD1	1:a:49:ASP:N	2.53	0.42
2:b:176:GLU:HA	3:c:56:LEU:HD11	2.02	0.42
5:e:8:TYR:HB2	5:e:22:PHE:HD2	1.80	0.42
5:e:127:ALA:HB2	6:f:125:GLY:HA2	2.01	0.42
11:k:23:ARG:CZ	11:k:50:ALA:HB1	2.50	0.42
11:k:46:PHE:HB3	11:k:102:VAL:HG12	2.01	0.42
11:k:139:TYR:CE1	11:k:171:ARG:HB3	2.55	0.42
12:l:203:CYS:CB	12:l:212:TYR:CE1	3.02	0.42
13:m:53:ASP:OD1	13:m:220:VAL:HG21	2.20	0.42
2:B:49:LYS:HE3	2:B:208:THR:O	2.20	0.42
6:F:204:GLU:O	6:F:205:SER:O	2.37	0.42
9:2:119:TYR:HD1	9:2:123:ILE:CG1	2.31	0.42
11:4:69:ILE:CG2	11:4:70:ARG:N	2.82	0.42
13:6:54:CYS:HB2	13:6:58:ILE:HG23	2.01	0.42
14:7:47:MET:SD	14:7:210:ILE:HD11	2.60	0.42
20:Z:546:ILE:HG22	20:Z:574:TYR:OH	2.20	0.42
21:N:79:VAL:O	21:N:83:LEU:HD13	2.20	0.42
23:P:120:GLU:HA	23:P:123:ARG:NE	2.34	0.42
24:Q:126:LYS:HB3	24:Q:134:LYS:HD2	2.02	0.42
26:U:15:LEU:H	26:U:15:LEU:HD12	1.84	0.42
8:h:152:ARG:HG3	8:h:152:ARG:HH11	1.85	0.42
13:m:109:ARG:NH1	13:m:110:PHE:CE1	2.88	0.42
13:m:146:ALA:HB3	13:m:155:MET:HG2	2.02	0.42
14:n:255:ALA:CB	8:1:39:VAL:HG12	2.48	0.42
1:A:95:LEU:HD12	7:G:118:GLN:CG	2.47	0.42
4:D:205:THR:O	4:D:205:THR:HG22	2.19	0.42
8:1:18:LYS:HD3	8:1:18:LYS:HA	1.85	0.42
8:1:152:ARG:HG3	8:1:152:ARG:HH11	1.85	0.42
9:2:119:TYR:CD1	9:2:123:ILE:HD12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:3:74:TYR:HE2	10:3:82:ILE:HA	1.83	0.42
13:6:109:ARG:NH1	13:6:110:PHE:CE1	2.88	0.42
16:V:304:ALA:HB1	27:O:377:VAL:CG2	2.28	0.42
19:Y:26:LYS:HD2	22:S:309:PHE:CD2	2.55	0.42
20:Z:443:ASP:O	20:Z:444:GLU:O	2.38	0.42
22:S:90:LYS:O	22:S:94:LYS:HG2	2.20	0.42
22:S:146:LEU:CD1	22:S:151:GLU:HG2	2.50	0.42
2:b:222:LEU:O	9:i:68:PRO:HB2	2.20	0.41
5:e:15:PHE:CA	5:e:16:SER:HB3	2.49	0.41
8:h:166:HIS:O	8:h:169:SER:OG	2.35	0.41
10:3:98:ARG:NH2	10:3:103:TYR:HA	2.35	0.41
11:4:139:TYR:CE1	11:4:171:ARG:HB3	2.55	0.41
12:5:83:PHE:HD2	12:5:85:GLY:H	1.60	0.41
12:5:106:VAL:HA	13:6:140:GLU:OE2	2.19	0.41
21:N:906:ARG:HA	21:N:906:ARG:NE	2.34	0.41
24:Q:126:LYS:CA	24:Q:134:LYS:HD2	2.50	0.41
2:b:223:GLY:HA2	9:i:69:LYS:HZ3	1.85	0.41
5:e:123:PHE:HE2	6:f:126:ARG:HD3	1.84	0.41
6:f:6:TYR:HE1	7:g:9:ASP:O	2.03	0.41
7:g:175:GLU:OE1	7:g:202:LEU:CD1	2.68	0.41
13:m:105:LEU:HD23	13:m:113:TYR:HD2	1.84	0.41
13:m:204:ILE:HB	9:2:196:LEU:HB3	2.02	0.41
2:B:100:ILE:HG22	10:3:90:LEU:HD13	2.02	0.41
2:B:242:GLU:O	2:B:245:ASP:HB2	2.20	0.41
3:C:185:LYS:HD3	3:C:185:LYS:HA	1.74	0.41
10:3:74:TYR:HD2	10:3:82:ILE:CG1	2.33	0.41
10:3:204:GLN:OE1	10:3:204:GLN:CA	2.60	0.41
12:5:198:LYS:HA	12:5:198:LYS:HD2	1.84	0.41
13:6:146:ALA:HB3	13:6:155:MET:HG2	2.02	0.41
21:N:76:GLU:OE1	21:N:76:GLU:N	2.53	0.41
21:N:739:PHE:CD2	21:N:739:PHE:C	2.98	0.41
6:f:204:GLU:O	6:f:205:SER:O	2.37	0.41
13:m:9:GLN:NE2	13:m:10:PHE:O	2.53	0.41
13:m:54:CYS:HB2	13:m:58:ILE:HG23	2.01	0.41
8:1:196:ILE:C	8:1:197:PHE:CD2	2.99	0.41
11:4:23:ARG:CZ	11:4:50:ALA:HB1	2.50	0.41
11:4:120:ASP:CG	11:4:121:TYR:N	2.78	0.41
12:5:218:ASN:O	12:5:220:LYS:NZ	2.51	0.41
16:V:217:HIS:HE1	26:U:181:GLN:CD	2.24	0.41
20:Z:314:LEU:CD1	20:Z:956:LEU:HD21	2.50	0.41
21:N:361:ASN:C	21:N:363:ALA:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:284:ALA:HA	25:R:287:GLN:HE21	1.85	0.41
26:U:197:LEU:HD21	27:O:380:LEU:CD2	2.49	0.41
27:O:163:ILE:HD12	27:O:168:THR:HG21	2.02	0.41
3:c:78:ALA:CB	3:c:165:VAL:HG23	2.50	0.41
8:h:49:LYS:HE2	8:h:111:TYR:HD2	1.84	0.41
9:i:36:LYS:HB3	9:i:152:TYR:HA	2.01	0.41
12:l:99:ASN:OD1	10:3:180:LEU:HD11	2.21	0.41
7:G:175:GLU:OE1	7:G:202:LEU:CD1	2.68	0.41
21:N:307:LYS:HE2	21:N:343:THR:HG21	2.01	0.41
23:P:117:SER:C	23:P:120:GLU:HG3	2.45	0.41
23:P:245:TYR:CE2	23:P:251:LYS:NZ	2.88	0.41
24:Q:126:LYS:HB3	24:Q:134:LYS:CE	2.50	0.41
1:a:175:GLN:OE1	1:a:175:GLN:N	2.50	0.41
10:j:70:LYS:HD2	10:j:70:LYS:HA	1.76	0.41
12:l:220:LYS:HG2	12:l:223:LEU:HD13	2.03	0.41
5:E:121:LEU:C	5:E:121:LEU:HD23	2.46	0.41
12:5:83:PHE:CD2	12:5:83:PHE:C	2.98	0.41
12:5:148:ARG:NH2	12:5:180:THR:HA	2.30	0.41
12:5:165:TYR:O	12:5:170:LEU:HD23	2.20	0.41
16:V:39:LYS:HE3	26:U:49:THR:CG2	2.49	0.41
16:V:178:GLY:HA3	21:N:651:PHE:HE2	1.85	0.41
20:Z:495:ILE:HD13	20:Z:884:THR:HG21	2.03	0.41
22:S:200:GLU:N	22:S:200:GLU:OE2	2.53	0.41
22:S:282:ILE:HA	22:S:382:ARG:HH12	1.86	0.41
6:f:169:LYS:HB3	7:g:58:LEU:CD1	2.51	0.41
9:i:119:TYR:N	9:i:119:TYR:CD2	2.85	0.41
1:A:49:ASP:OD1	1:A:49:ASP:N	2.53	0.41
4:D:11:PHE:HZ	5:E:26:TYR:CB	2.33	0.41
8:1:156:SER:HB3	8:1:158:GLU:OE1	2.21	0.41
9:2:232:TYR:N	9:2:232:TYR:CD1	2.88	0.41
12:5:84:GLN:NE2	12:5:221:TRP:CE2	2.89	0.41
13:6:47:TYR:HB2	14:7:194:ARG:NH2	2.34	0.41
16:V:245:VAL:HG22	24:Q:418:GLN:HG3	2.03	0.41
20:Z:287:ARG:HB2	20:Z:855:LEU:HD11	2.03	0.41
21:N:87:ASP:C	21:N:88:ARG:HG3	2.45	0.41
21:N:563:GLY:H	21:N:597:ARG:HE	1.67	0.41
23:P:204:LEU:HB2	23:P:207:THR:HG23	2.02	0.41
27:O:307:MET:HA	27:O:348:VAL:O	2.20	0.41
27:O:326:HIS:HB3	27:O:330:ARG:CZ	2.51	0.41
6:f:13:PHE:HA	6:f:14:SER:HB3	2.03	0.41
6:f:140:SER:OG	14:n:117:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:98:ARG:NH2	10:j:103:TYR:HA	2.35	0.41
11:k:1:MET:H2	11:k:3:ILE:HG13	1.86	0.41
11:k:120:ASP:CG	11:k:121:TYR:N	2.78	0.41
13:m:38:ILE:HD11	13:m:205:GLN:HG2	2.03	0.41
13:m:178:LYS:HD3	13:m:178:LYS:HA	1.74	0.41
2:B:2:THR:CG2	2:B:3:ASP:H	2.16	0.41
9:2:113:LYS:HD2	9:2:148:THR:HG23	2.03	0.41
11:4:86:GLN:OE1	11:4:86:GLN:HA	2.21	0.41
12:5:139:ARG:HA	12:5:139:ARG:HD3	1.92	0.41
17:T:96:LEU:O	17:T:96:LEU:HG	2.19	0.41
18:X:119:LYS:HZ2	18:X:122:TYR:HD2	1.67	0.41
19:Y:81:LEU:HG	19:Y:85:LYS:NZ	2.35	0.41
23:P:120:GLU:HA	23:P:123:ARG:CZ	2.51	0.41
24:Q:172:PRO:HB2	24:Q:209:TYR:CE1	2.56	0.41
10:j:145:GLN:HE21	12:5:100:TRP:CB	2.33	0.41
12:l:265:ASN:OD1	12:l:265:ASN:C	2.64	0.41
2:B:59:GLU:OE1	2:B:59:GLU:CA	2.68	0.41
2:B:178:ARG:NH1	24:Q:130:ARG:HH11	2.19	0.41
9:2:32:ILE:CB	9:2:128:ILE:HD12	2.48	0.41
9:2:36:LYS:HB3	9:2:152:TYR:HA	2.01	0.41
9:2:95:HIS:HA	9:2:98:TYR:HD2	1.86	0.41
10:3:127:ILE:O	10:3:127:ILE:HG22	2.21	0.41
13:6:12:PRO:HB2	14:7:137:ARG:HE	1.86	0.41
20:Z:123:ALA:HB1	20:Z:132:HIS:CE1	2.56	0.41
23:P:422:LEU:CD1	26:U:236:LEU:HD12	2.51	0.41
26:U:161:ILE:HG22	26:U:162:GLU:N	2.36	0.41
2:b:205:ASN:O	2:b:209:ILE:HG12	2.21	0.41
2:b:242:GLU:O	2:b:245:ASP:HB2	2.21	0.41
4:d:66:LYS:HG3	11:k:69:ILE:HD11	2.02	0.41
5:e:132:ARG:NH2	6:f:126:ARG:HH12	2.19	0.41
8:h:18:LYS:HA	8:h:18:LYS:HD3	1.85	0.41
8:h:165:LYS:HD2	8:h:197:PHE:CE1	2.55	0.41
8:h:196:ILE:C	8:h:197:PHE:CD2	2.99	0.41
9:i:95:HIS:HA	9:i:98:TYR:HD2	1.86	0.41
11:k:81:SER:C	11:k:125:LYS:HD2	2.46	0.41
14:n:102:ASP:OD2	14:n:102:ASP:C	2.64	0.41
9:2:253:GLN:C	9:2:254:GLU:O	2.63	0.41
12:5:125:ALA:HA	13:6:138:SER:H	1.86	0.41
12:5:220:LYS:HG2	12:5:223:LEU:HD13	2.03	0.41
15:W:122:ARG:HB2	15:W:153:LEU:CD2	2.40	0.41
16:V:22:ASP:HB3	16:V:157:ARG:HH22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:98:THR:CG2	26:U:72:TYR:CZ	3.03	0.41
16:V:178:GLY:HA3	21:N:651:PHE:CE2	2.56	0.41
17:T:127:GLN:CG	22:S:247:VAL:HG21	2.49	0.41
18:X:46:TRP:HZ2	18:X:131:ASN:HD22	1.68	0.41
20:Z:165:TYR:HA	20:Z:168:GLN:HE21	1.86	0.41
21:N:87:ASP:O	21:N:88:ARG:HB2	2.21	0.41
21:N:530:GLU:OE1	21:N:530:GLU:N	2.54	0.41
21:N:751:LEU:N	21:N:751:LEU:HD12	2.36	0.41
22:S:211:ARG:NH2	22:S:241:PHE:CE1	2.89	0.41
23:P:327:LEU:O	23:P:328:ALA:CB	2.68	0.41
25:R:70:TYR:HB2	25:R:71:LEU:H	1.67	0.41
5:e:150:ASP:OD1	13:m:90:LYS:HE2	2.19	0.41
10:j:74:TYR:HD2	10:j:82:ILE:CG1	2.33	0.41
13:m:106:TYR:O	13:m:109:ARG:HG2	2.21	0.41
1:A:84:ASN:HB2	1:A:171:THR:HG21	2.03	0.41
1:A:250:GLU:OE2	23:P:81:LEU:CD1	2.69	0.41
7:G:65:VAL:HG11	14:7:112:PRO:HD3	2.02	0.41
8:1:120:TYR:CE1	8:1:130:LYS:HG3	2.54	0.41
9:2:219:TYR:CD1	9:2:219:TYR:C	2.98	0.41
11:4:1:MET:H2	11:4:3:ILE:HG13	1.85	0.41
16:V:60:ASP:O	16:V:60:ASP:CG	2.64	0.41
21:N:283:ASP:CG	21:N:284:PRO:HD2	2.46	0.41
21:N:305:ASN:OD1	21:N:871:MET:HE1	2.21	0.41
22:S:475:TYR:CZ	22:S:479:MET:SD	3.13	0.41
26:U:197:LEU:HD21	27:O:380:LEU:HD23	2.02	0.41
4:d:34:VAL:HG23	4:d:195:THR:CG2	2.50	0.40
9:i:113:LYS:HD2	9:i:148:THR:HG23	2.03	0.40
10:j:118:LYS:CB	10:j:118:LYS:HZ3	2.34	0.40
10:j:179:ALA:O	12:5:244:ALA:HB1	2.21	0.40
13:m:49:PRO:C	13:m:50:LYS:HD3	2.46	0.40
2:B:112:SER:CB	10:3:77:LYS:HE3	2.51	0.40
12:5:265:ASN:OD1	12:5:265:ASN:C	2.64	0.40
13:6:106:TYR:O	13:6:109:ARG:HG2	2.21	0.40
23:P:310:ARG:H	23:P:313:ILE:HD12	1.86	0.40
2:b:63:LYS:HE2	2:b:75:TYR:OH	2.21	0.40
4:d:141:ARG:HE	12:l:182:LYS:CB	2.26	0.40
5:e:121:LEU:C	5:e:121:LEU:HD23	2.46	0.40
6:f:160:ALA:O	6:f:161:ILE:HG23	2.20	0.40
8:h:135:ILE:HD11	8:h:144:TYR:CD2	2.56	0.40
8:h:174:TRP:CZ3	8:1:144:TYR:CZ	3.09	0.40
12:l:84:GLN:NE2	12:l:221:TRP:CE2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:72:LEU:CD2	13:m:117:THR:OG1	2.69	0.40
14:n:187:LEU:HB2	9:2:165:ALA:HB1	2.03	0.40
8:1:49:LYS:HE2	8:1:111:TYR:HD2	1.85	0.40
8:1:150:ASN:O	8:1:163:PHE:HE2	2.04	0.40
11:4:94:SER:C	11:4:96:ARG:H	2.29	0.40
13:6:72:LEU:CD2	13:6:117:THR:OG1	2.69	0.40
16:V:32:ILE:HD11	26:U:16:LEU:C	2.46	0.40
16:V:225:LEU:HD12	23:P:423:LEU:HD22	2.00	0.40
17:T:24:GLU:OE1	17:T:24:GLU:HA	2.22	0.40
20:Z:842:GLN:HE22	20:Z:845:LEU:HD22	1.84	0.40
21:N:360:GLN:O	21:N:364:LYS:HB3	2.20	0.40
23:P:72:TRP:CE2	23:P:113:ASN:OD1	2.75	0.40
24:Q:386:PHE:O	24:Q:387:TYR:CD1	2.74	0.40
24:Q:432:VAL:O	24:Q:432:VAL:HG12	2.20	0.40
1:a:131:ARG:HA	2:b:126:GLY:O	2.20	0.40
2:b:6:SER:O	3:c:126:GLY:O	2.39	0.40
4:d:227:GLU:OE2	4:d:227:GLU:N	2.51	0.40
8:h:26:ASP:OD1	8:h:42:LYS:HE2	2.22	0.40
8:h:150:ASN:O	8:h:163:PHE:HE2	2.04	0.40
9:i:119:TYR:CD1	9:i:123:ILE:HD12	2.54	0.40
9:i:126:TYR:HD1	9:i:126:TYR:N	2.19	0.40
9:i:253:GLN:C	9:i:254:GLU:O	2.63	0.40
12:l:165:TYR:HB3	12:l:170:LEU:HD23	2.00	0.40
13:m:146:ALA:CB	13:m:155:MET:HG2	2.51	0.40
2:B:63:LYS:HE2	2:B:75:TYR:OH	2.21	0.40
2:B:205:ASN:O	2:B:209:ILE:HG12	2.21	0.40
3:C:110:ILE:HD11	11:4:71:GLU:CD	2.46	0.40
4:D:66:LYS:HD3	11:4:69:ILE:CD1	2.47	0.40
8:1:49:LYS:HG3	8:1:111:TYR:O	2.22	0.40
8:1:62:GLN:HB3	9:2:113:LYS:NZ	2.37	0.40
13:6:146:ALA:CB	13:6:155:MET:HG2	2.51	0.40
14:7:198:ILE:HB	14:7:199:PRO:HD3	2.04	0.40
20:Z:249:MET:HB3	20:Z:265:LEU:HD21	2.03	0.40
22:S:397:LEU:HD13	25:R:373:PRO:HA	2.03	0.40
5:e:36:THR:CG2	5:e:38:ILE:HG13	2.51	0.40
8:h:174:TRP:CZ3	8:1:144:TYR:OH	2.74	0.40
9:i:232:TYR:N	9:i:232:TYR:CD1	2.88	0.40
11:k:3:ILE:HD12	11:k:176:PHE:CG	2.56	0.40
8:1:135:ILE:HD11	8:1:144:TYR:CD2	2.56	0.40
10:3:74:TYR:CE2	10:3:82:ILE:CG1	3.02	0.40
11:4:81:SER:C	11:4:125:LYS:HD2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:6:38:ILE:HD11	13:6:205:GLN:HG2	2.03	0.40
16:V:72:PRO:HG3	26:U:82:LYS:CD	2.51	0.40
16:V:303:VAL:CG1	27:O:380:LEU:HD13	2.47	0.40
17:T:164:LEU:HD13	17:T:182:LYS:HG3	2.03	0.40
17:T:251:HIS:ND1	17:T:251:HIS:O	2.55	0.40
20:Z:309:GLN:C	20:Z:311:ALA:N	2.79	0.40
23:P:86:HIS:HB3	23:P:88:GLN:N	2.36	0.40
6:f:15:PRO:HB3	7:g:26:TYR:CE1	2.55	0.40
8:h:156:SER:HB3	8:h:158:GLU:OE1	2.21	0.40
9:i:162:ALA:HA	14:7:186:PRO:HG2	2.03	0.40
12:l:83:PHE:HE2	12:l:85:GLY:HA3	1.86	0.40
12:l:128:GLN:OE1	13:m:138:SER:CA	2.68	0.40
13:m:134:ASP:OD1	13:m:137:GLY:O	2.40	0.40
13:m:157:PHE:HZ	9:2:232:TYR:HE2	1.63	0.40
9:2:115:HIS:HA	9:2:118:LYS:HZ2	1.86	0.40
17:T:116:GLN:O	17:T:117:ASN:HB2	2.21	0.40
17:T:127:GLN:O	17:T:128:TYR:C	2.64	0.40
19:Y:81:LEU:O	19:Y:85:LYS:HG3	2.21	0.40
21:N:320:SER:HB2	21:N:321:LEU:HD12	2.03	0.40
23:P:4:ASP:O	23:P:8:LYS:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/252 (95%)	228 (95%)	11 (5%)	0	100	100
1	a	239/252 (95%)	228 (95%)	11 (5%)	0	100	100
2	B	247/250 (99%)	237 (96%)	9 (4%)	1 (0%)	30	67
2	b	247/250 (99%)	237 (96%)	9 (4%)	1 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	242/258 (94%)	229 (95%)	13 (5%)	0	100	100
3	c	242/258 (94%)	229 (95%)	13 (5%)	0	100	100
4	D	234/254 (92%)	218 (93%)	11 (5%)	5 (2%)	5	29
4	d	234/254 (92%)	215 (92%)	14 (6%)	5 (2%)	5	29
5	E	242/260 (93%)	228 (94%)	13 (5%)	1 (0%)	30	67
5	e	242/260 (93%)	228 (94%)	13 (5%)	1 (0%)	30	67
6	F	229/234 (98%)	219 (96%)	9 (4%)	1 (0%)	30	67
6	f	229/234 (98%)	219 (96%)	9 (4%)	1 (0%)	30	67
7	G	240/288 (83%)	234 (98%)	5 (2%)	1 (0%)	30	67
7	g	240/288 (83%)	234 (98%)	5 (2%)	1 (0%)	30	67
8	1	194/215 (90%)	182 (94%)	10 (5%)	2 (1%)	12	48
8	h	194/215 (90%)	182 (94%)	10 (5%)	2 (1%)	12	48
9	2	224/261 (86%)	209 (93%)	11 (5%)	4 (2%)	6	34
9	i	224/261 (86%)	209 (93%)	11 (5%)	4 (2%)	6	34
10	3	202/205 (98%)	186 (92%)	14 (7%)	2 (1%)	12	48
10	j	202/205 (98%)	186 (92%)	14 (7%)	2 (1%)	12	48
11	4	193/198 (98%)	182 (94%)	11 (6%)	0	100	100
11	k	193/198 (98%)	182 (94%)	11 (6%)	0	100	100
12	5	210/287 (73%)	201 (96%)	8 (4%)	1 (0%)	24	63
12	l	210/287 (73%)	201 (96%)	8 (4%)	1 (0%)	24	63
13	6	220/241 (91%)	207 (94%)	11 (5%)	2 (1%)	14	50
13	m	220/241 (91%)	207 (94%)	11 (5%)	2 (1%)	14	50
14	7	227/266 (85%)	199 (88%)	27 (12%)	1 (0%)	30	67
14	n	227/266 (85%)	211 (93%)	16 (7%)	0	100	100
15	W	195/268 (73%)	181 (93%)	13 (7%)	1 (0%)	24	63
16	V	287/306 (94%)	258 (90%)	26 (9%)	3 (1%)	12	48
17	T	264/274 (96%)	240 (91%)	23 (9%)	1 (0%)	30	67
18	X	125/156 (80%)	112 (90%)	12 (10%)	1 (1%)	16	54
19	Y	87/89 (98%)	76 (87%)	8 (9%)	3 (3%)	3	21
20	Z	902/993 (91%)	817 (91%)	70 (8%)	15 (2%)	7	36
21	N	828/945 (88%)	789 (95%)	36 (4%)	3 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	S	473/523 (90%)	438 (93%)	26 (6%)	9 (2%)	6	32
23	P	438/445 (98%)	417 (95%)	19 (4%)	2 (0%)	24	63
24	Q	432/434 (100%)	400 (93%)	26 (6%)	6 (1%)	9	40
25	R	403/429 (94%)	383 (95%)	17 (4%)	3 (1%)	18	56
26	U	288/338 (85%)	274 (95%)	13 (4%)	1 (0%)	36	72
27	O	386/393 (98%)	376 (97%)	10 (3%)	0	100	100
All	All	11394/12531 (91%)	10688 (94%)	617 (5%)	89 (1%)	18	54

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	124	SER
4	d	101	GLU
4	d	204	GLN
5	e	128	SER
6	f	205	SER
7	g	71	ASP
8	h	116	LYS
9	i	251	ASP
9	i	254	GLU
10	j	183	TRP
13	m	40	ASP
2	B	124	SER
4	D	101	GLU
4	D	204	GLN
5	E	128	SER
6	F	205	SER
7	G	71	ASP
8	1	116	LYS
9	2	251	ASP
9	2	254	GLU
10	3	183	TRP
13	6	40	ASP
14	7	110	ASP
16	V	60	ASP
16	V	271	VAL
17	T	138	ASP
19	Y	4	ASP
20	Z	5	SER
20	Z	85	VAL

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Mol	Chain	Res	Type
20	Z	142	ASP
20	Z	173	ALA
20	Z	174	GLU
20	Z	309	GLN
20	Z	366	LYS
20	Z	377	ALA
20	Z	443	ASP
20	Z	444	GLU
20	Z	498	ALA
20	Z	728	LYS
20	Z	802	ASP
20	Z	926	ASN
21	N	88	ARG
21	N	361	ASN
22	S	69	LEU
22	S	153	GLU
22	S	154	GLN
22	S	449	LEU
24	Q	110	SER
24	Q	387	TYR
24	Q	405	GLN
25	R	71	LEU
25	R	72	VAL
25	R	280	ILE
4	d	203	VAL
15	W	149	GLN
19	Y	32	ASP
21	N	362	TRP
22	S	113	SER
22	S	450	ASN
24	Q	48	ASP
24	Q	51	ARG
10	j	33	SER
13	m	138	SER
10	3	33	SER
13	6	138	SER
18	X	39	GLU
23	P	328	ALA
9	i	200	SER
4	D	102	ASP
4	D	103	PRO
9	2	200	SER

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Mol	Chain	Res	Type
16	V	84	ASP
23	P	90	LYS
4	d	103	PRO
12	l	278	GLU
4	D	205	THR
12	5	278	GLU
19	Y	5	VAL
22	S	112	ASN
24	Q	50	ARG
4	d	102	ASP
8	h	117	GLY
9	i	222	PRO
8	1	117	GLY
9	2	222	PRO
20	Z	24	THR
26	U	42	ASN
22	S	327	ILE
22	S	115	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/210 (98%)	202 (98%)	4 (2%)	50	67
1	a	206/210 (98%)	201 (98%)	5 (2%)	43	63
2	B	208/209 (100%)	202 (97%)	6 (3%)	37	58
2	b	208/209 (100%)	202 (97%)	6 (3%)	37	58
3	C	203/216 (94%)	197 (97%)	6 (3%)	36	57
3	c	203/216 (94%)	197 (97%)	6 (3%)	36	57
4	D	209/226 (92%)	205 (98%)	4 (2%)	50	67
4	d	209/226 (92%)	195 (93%)	14 (7%)	15	36
5	E	200/215 (93%)	195 (98%)	5 (2%)	42	62
5	e	200/215 (93%)	195 (98%)	5 (2%)	42	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	190/193 (98%)	183 (96%)	7 (4%)	30	51
6	f	190/193 (98%)	183 (96%)	7 (4%)	30	51
7	G	200/239 (84%)	193 (96%)	7 (4%)	32	53
7	g	200/239 (84%)	193 (96%)	7 (4%)	32	53
8	1	162/178 (91%)	157 (97%)	5 (3%)	35	56
8	h	162/178 (91%)	157 (97%)	5 (3%)	35	56
9	2	185/214 (86%)	173 (94%)	12 (6%)	15	37
9	i	185/214 (86%)	173 (94%)	12 (6%)	15	37
10	3	172/173 (99%)	162 (94%)	10 (6%)	18	40
10	j	172/173 (99%)	162 (94%)	10 (6%)	18	40
11	4	173/175 (99%)	168 (97%)	5 (3%)	37	58
11	k	173/175 (99%)	168 (97%)	5 (3%)	37	58
12	5	169/235 (72%)	158 (94%)	11 (6%)	15	37
12	l	169/235 (72%)	158 (94%)	11 (6%)	15	37
13	6	185/201 (92%)	179 (97%)	6 (3%)	34	56
13	m	185/201 (92%)	179 (97%)	6 (3%)	34	56
14	7	195/224 (87%)	194 (100%)	1 (0%)	81	83
14	n	195/224 (87%)	195 (100%)	0	100	100
15	W	171/230 (74%)	167 (98%)	4 (2%)	44	64
16	V	253/268 (94%)	248 (98%)	5 (2%)	48	66
17	T	249/256 (97%)	247 (99%)	2 (1%)	73	80
18	X	116/144 (81%)	115 (99%)	1 (1%)	70	79
19	Y	81/81 (100%)	79 (98%)	2 (2%)	42	62
20	Z	773/850 (91%)	734 (95%)	39 (5%)	22	43
21	N	698/797 (88%)	690 (99%)	8 (1%)	65	76
22	S	447/489 (91%)	442 (99%)	5 (1%)	65	76
23	P	412/415 (99%)	406 (98%)	6 (2%)	57	72
24	Q	391/391 (100%)	388 (99%)	3 (1%)	73	80
25	R	356/379 (94%)	349 (98%)	7 (2%)	48	66
26	U	263/308 (85%)	260 (99%)	3 (1%)	65	76
27	O	363/368 (99%)	360 (99%)	3 (1%)	73	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9887/10792 (92%)	9611 (97%)	276 (3%)	38 59

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	62	LYS
1	a	156	LYS
1	a	187	LYS
1	a	192	ASP
1	a	217	GLU
2	b	6	SER
2	b	29	LYS
2	b	51	SER
2	b	89	SER
2	b	217	GLU
2	b	237	LYS
3	c	5	ARG
3	c	63	THR
3	c	85	GLU
3	c	120	GLN
3	c	185	LYS
3	c	204	SER
4	d	9	SER
4	d	17	ILE
4	d	28	LYS
4	d	49	ARG
4	d	123	SER
4	d	153	SER
4	d	157	SER
4	d	164	ILE
4	d	169	LYS
4	d	182	LYS
4	d	197	ARG
4	d	198	SER
4	d	208	LYS
4	d	219	SER
5	e	27	SER
5	e	36	THR
5	e	56	SER
5	e	134	MET
5	e	246	LYS
6	f	21	GLN

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Mol	Chain	Res	Type
6	f	82	ARG
6	f	102	LYS
6	f	117	GLN
6	f	152	ASN
6	f	179	PHE
6	f	202	ARG
7	g	72	ARG
7	g	93	ARG
7	g	195	GLN
7	g	208	LYS
7	g	209	GLU
7	g	212	PHE
7	g	213	GLU
8	h	45	ARG
8	h	92	LYS
8	h	93	GLU
8	h	138	SER
8	h	193	GLU
9	i	39	ASN
9	i	101	ARG
9	i	106	VAL
9	i	147	SER
9	i	164	MET
9	i	177	LYS
9	i	182	LYS
9	i	211	LYS
9	i	230	LYS
9	i	245	SER
9	i	247	VAL
9	i	254	GLU
10	j	33	SER
10	j	70	LYS
10	j	75	LYS
10	j	79	GLU
10	j	80	ARG
10	j	118	LYS
10	j	139	SER
10	j	157	ASN
10	j	165	GLU
10	j	166	THR
11	k	18	SER
11	k	58	GLU

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Mol	Chain	Res	Type
11	k	85	ARG
11	k	155	GLU
11	k	163	LEU
12	l	107	LYS
12	l	138	CYS
12	l	140	LEU
12	l	148	ARG
12	l	164	GLN
12	l	198	LYS
12	l	206	SER
12	l	214	VAL
12	l	220	LYS
12	l	222	ASP
12	l	274	LYS
13	m	39	THR
13	m	40	ASP
13	m	47	TYR
13	m	72	LEU
13	m	217	LYS
13	m	221	ARG
1	A	62	LYS
1	A	156	LYS
1	A	187	LYS
1	A	192	ASP
2	B	6	SER
2	B	29	LYS
2	B	51	SER
2	B	89	SER
2	B	217	GLU
2	B	237	LYS
3	C	5	ARG
3	C	63	THR
3	C	85	GLU
3	C	120	GLN
3	C	185	LYS
3	C	204	SER
4	D	9	SER
4	D	142	ASP
4	D	182	LYS
4	D	218	ASP
5	E	27	SER
5	E	36	THR

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Mol	Chain	Res	Type
5	E	56	SER
5	E	134	MET
5	E	246	LYS
6	F	21	GLN
6	F	82	ARG
6	F	102	LYS
6	F	117	GLN
6	F	152	ASN
6	F	179	PHE
6	F	202	ARG
7	G	72	ARG
7	G	93	ARG
7	G	195	GLN
7	G	208	LYS
7	G	209	GLU
7	G	212	PHE
7	G	213	GLU
8	1	45	ARG
8	1	92	LYS
8	1	93	GLU
8	1	138	SER
8	1	193	GLU
9	2	39	ASN
9	2	101	ARG
9	2	106	VAL
9	2	147	SER
9	2	164	MET
9	2	177	LYS
9	2	182	LYS
9	2	211	LYS
9	2	230	LYS
9	2	245	SER
9	2	247	VAL
9	2	254	GLU
10	3	33	SER
10	3	70	LYS
10	3	75	LYS
10	3	79	GLU
10	3	80	ARG
10	3	118	LYS
10	3	139	SER
10	3	157	ASN

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Mol	Chain	Res	Type
10	3	165	GLU
10	3	166	THR
11	4	18	SER
11	4	58	GLU
11	4	85	ARG
11	4	155	GLU
11	4	163	LEU
12	5	107	LYS
12	5	138	CYS
12	5	140	LEU
12	5	148	ARG
12	5	164	GLN
12	5	198	LYS
12	5	206	SER
12	5	214	VAL
12	5	220	LYS
12	5	222	ASP
12	5	274	LYS
13	6	39	THR
13	6	40	ASP
13	6	47	TYR
13	6	72	LEU
13	6	217	LYS
13	6	221	ARG
14	7	127	GLU
15	W	99	LYS
15	W	119	SER
15	W	120	ASP
15	W	121	SER
16	V	88	GLN
16	V	110	SER
16	V	175	SER
16	V	259	LYS
16	V	286	GLU
17	T	49	ASP
17	T	99	SER
18	X	65	SER
19	Y	9	GLN
19	Y	18	LYS
20	Z	2	VAL
20	Z	7	LYS
20	Z	9	GLN

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Mol	Chain	Res	Type
20	Z	16	SER
20	Z	32	LYS
20	Z	63	LEU
20	Z	86	PRO
20	Z	131	LYS
20	Z	164	VAL
20	Z	170	GLU
20	Z	171	LYS
20	Z	179	SER
20	Z	239	GLU
20	Z	267	THR
20	Z	290	GLU
20	Z	366	LYS
20	Z	376	SER
20	Z	387	ASN
20	Z	434	GLN
20	Z	471	LEU
20	Z	479	THR
20	Z	504	GLU
20	Z	512	ILE
20	Z	557	GLU
20	Z	561	ASP
20	Z	583	ASP
20	Z	589	SER
20	Z	627	LYS
20	Z	738	TYR
20	Z	751	ASP
20	Z	759	ARG
20	Z	811	SER
20	Z	817	LEU
20	Z	822	THR
20	Z	840	ARG
20	Z	848	THR
20	Z	880	SER
20	Z	899	GLN
20	Z	916	LEU
21	N	109	TYR
21	N	128	ILE
21	N	151	LYS
21	N	327	LEU
21	N	365	PHE
21	N	457	SER

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Mol	Chain	Res	Type
21	N	507	GLU
21	N	737	SER
22	S	33	GLU
22	S	69	LEU
22	S	202	ASN
22	S	267	SER
22	S	287	SER
23	P	14	SER
23	P	166	GLU
23	P	201	ARG
23	P	248	ASP
23	P	389	ILE
23	P	404	LYS
24	Q	9	GLU
24	Q	91	SER
24	Q	326	MET
25	R	82	ASP
25	R	86	ASP
25	R	124	ASP
25	R	245	SER
25	R	262	GLU
25	R	263	ARG
25	R	287	GLN
26	U	2	SER
26	U	145	ASP
26	U	274	MET
27	O	80	LYS
27	O	88	ASP
27	O	390	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (159) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	56	GLN
1	a	130	GLN
1	a	181	ASN
1	a	209	HIS
2	b	20	GLN
2	b	94	HIS
2	b	139	HIS
3	c	21	GLN
3	c	103	ASN

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Mol	Chain	Res	Type
3	c	173	GLN
3	c	227	GLN
4	d	94	GLN
4	d	96	HIS
4	d	204	GLN
5	e	23	GLN
5	e	99	HIS
5	e	147	HIS
5	e	218	GLN
6	f	5	ASN
6	f	43	HIS
7	g	23	GLN
7	g	87	HIS
7	g	127	ASN
7	g	195	GLN
8	h	71	HIS
8	h	98	ASN
8	h	154	ASN
9	i	86	GLN
9	i	114	GLN
9	i	145	HIS
9	i	201	ASN
9	i	248	ASN
11	k	65	GLN
12	l	84	GLN
12	l	283	ASN
13	m	44	ASN
13	m	84	HIS
13	m	87	HIS
13	m	102	GLN
14	n	36	GLN
14	n	155	ASN
14	n	236	ASN
14	n	246	GLN
1	A	56	GLN
1	A	181	ASN
1	A	209	HIS
2	B	94	HIS
2	B	139	HIS
3	C	31	HIS
3	C	89	ASN
3	C	120	GLN

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Mol	Chain	Res	Type
3	C	227	GLN
4	D	96	HIS
4	D	149	GLN
4	D	178	ASN
5	E	99	HIS
5	E	147	HIS
6	F	43	HIS
7	G	195	GLN
8	1	98	ASN
8	1	154	ASN
9	2	114	GLN
9	2	143	HIS
9	2	145	HIS
9	2	201	ASN
9	2	248	ASN
10	3	72	ASN
11	4	65	GLN
12	5	84	GLN
12	5	283	ASN
13	6	84	HIS
13	6	87	HIS
14	7	35	GLN
14	7	70	ASN
14	7	141	ASN
14	7	246	GLN
15	W	29	GLN
15	W	102	GLN
15	W	103	ASN
15	W	162	ASN
15	W	163	ASN
16	V	73	GLN
16	V	97	GLN
16	V	176	ASN
16	V	217	HIS
17	T	37	ASN
17	T	118	ASN
17	T	192	ASN
18	X	131	ASN
20	Z	23	GLN
20	Z	37	GLN
20	Z	151	HIS
20	Z	168	GLN

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Mol	Chain	Res	Type
20	Z	243	GLN
20	Z	276	ASN
20	Z	391	ASN
20	Z	593	HIS
20	Z	622	HIS
20	Z	763	HIS
20	Z	766	HIS
20	Z	823	ASN
20	Z	829	GLN
20	Z	833	GLN
20	Z	868	ASN
20	Z	874	ASN
20	Z	951	GLN
21	N	30	ASN
21	N	116	GLN
21	N	199	ASN
21	N	219	ASN
21	N	226	ASN
21	N	306	ASN
21	N	329	HIS
21	N	336	ASN
21	N	346	ASN
21	N	580	ASN
21	N	679	ASN
21	N	703	GLN
21	N	738	GLN
22	S	20	HIS
22	S	66	GLN
22	S	205	ASN
22	S	207	ASN
22	S	225	HIS
22	S	244	ASN
22	S	335	GLN
22	S	339	GLN
22	S	417	GLN
23	P	128	ASN
23	P	164	GLN
23	P	315	GLN
23	P	337	HIS
23	P	348	HIS
24	Q	114	GLN
24	Q	135	HIS

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Mol	Chain	Res	Type
24	Q	145	HIS
24	Q	159	ASN
24	Q	206	ASN
24	Q	334	HIS
24	Q	392	GLN
24	Q	404	ASN
24	Q	420	ASN
25	R	114	ASN
25	R	184	GLN
25	R	208	ASN
25	R	287	GLN
25	R	374	ASN
26	U	5	HIS
26	U	107	ASN
26	U	142	GLN
26	U	156	HIS
26	U	181	GLN
26	U	216	ASN
26	U	252	HIS
26	U	262	GLN
27	O	40	GLN
27	O	318	HIS
27	O	376	GLN
27	O	389	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

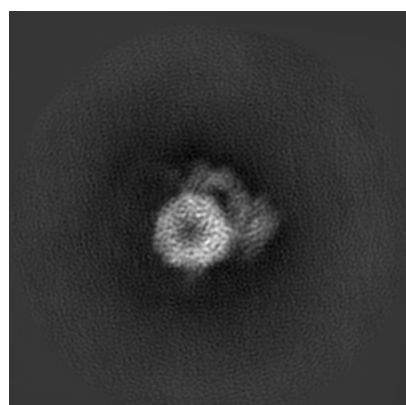
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14082. These allow visual inspection of the internal detail of the map and identification of artifacts.

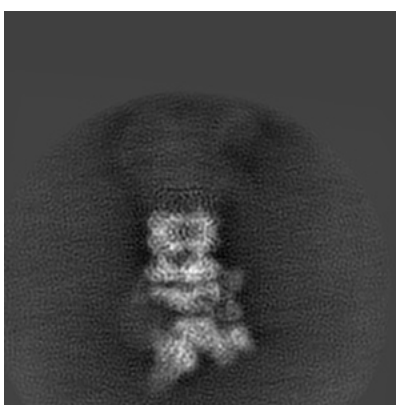
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

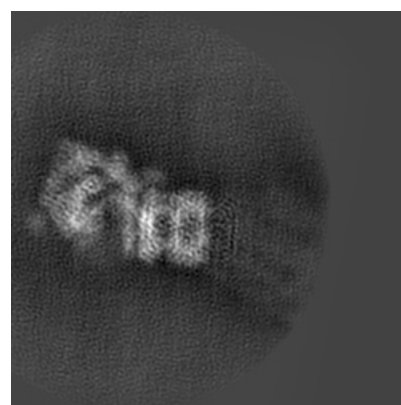
6.1.1 Primary map



X



Y

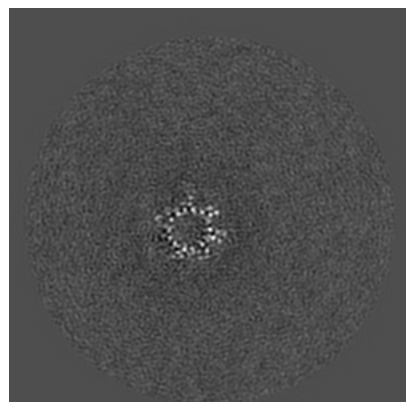


Z

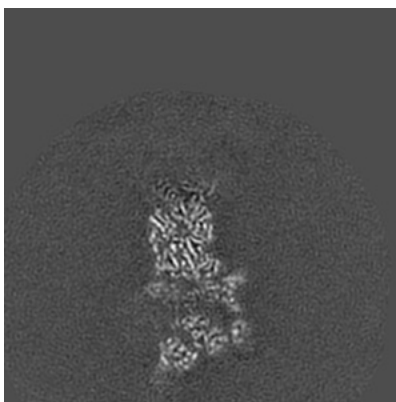
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

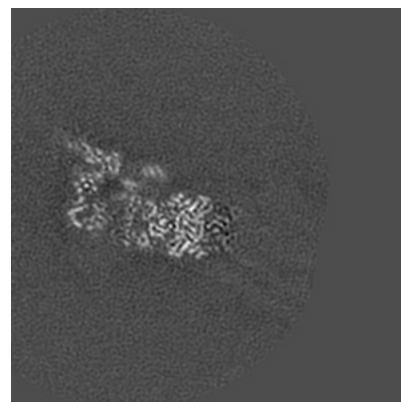
6.2.1 Primary map



X Index: 140



Y Index: 140

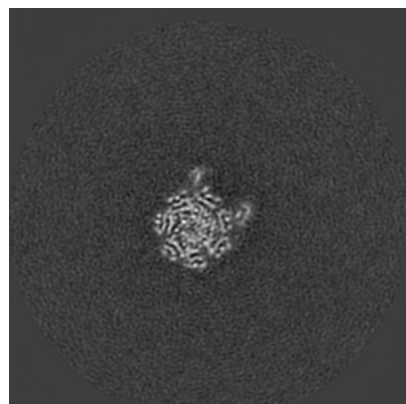


Z Index: 140

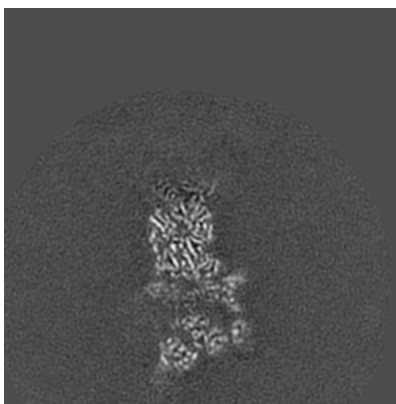
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

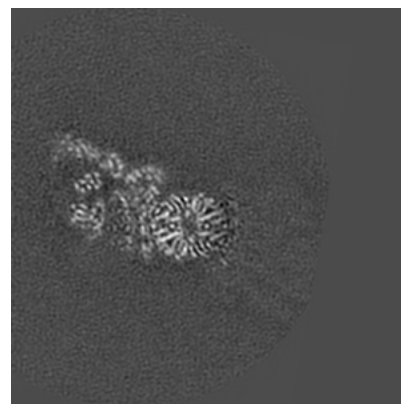
6.3.1 Primary map



X Index: 97



Y Index: 140

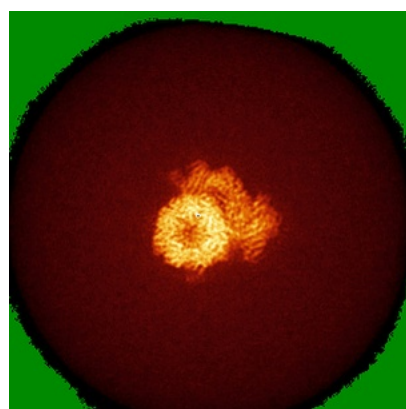


Z Index: 136

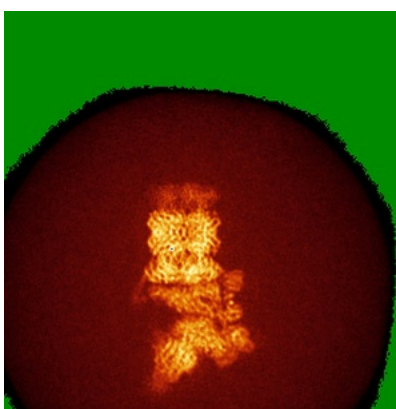
The images above show the largest variance slices of the map in three orthogonal directions.

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

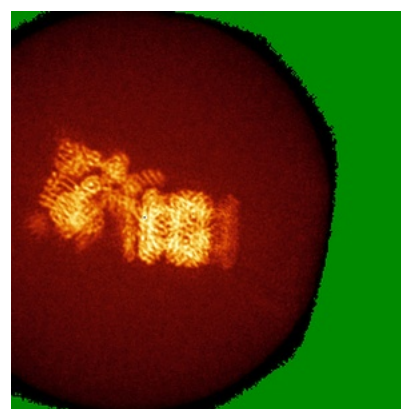
6.4.1 Primary map



X



Y

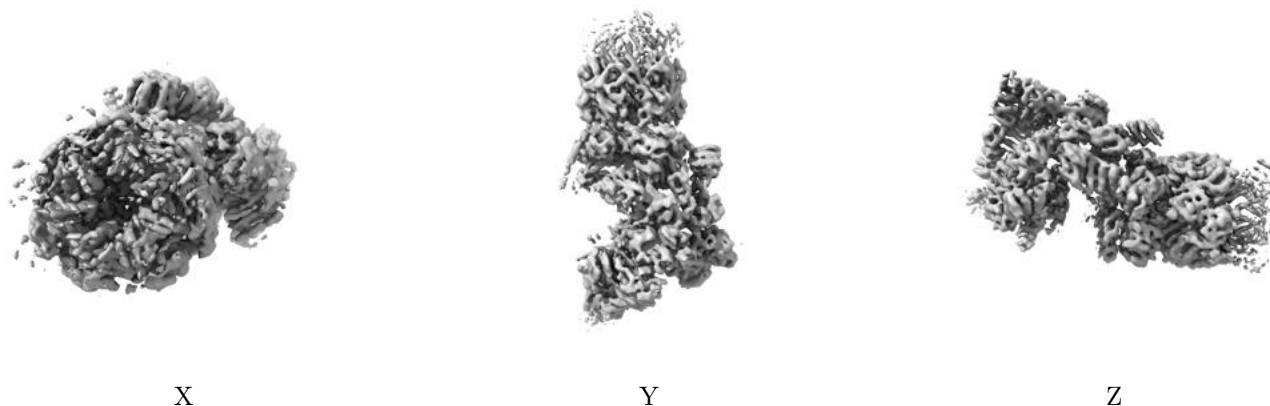


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

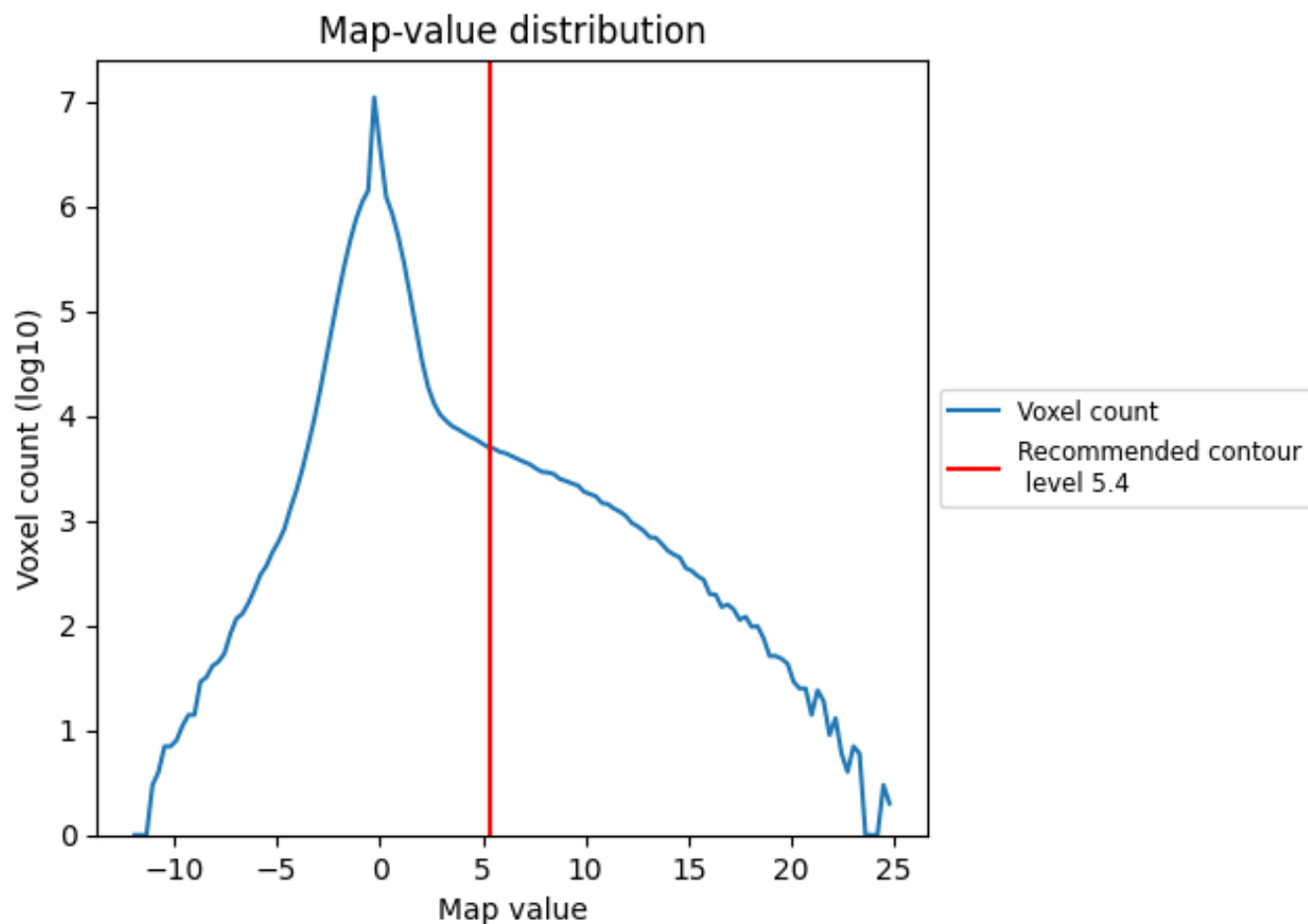
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

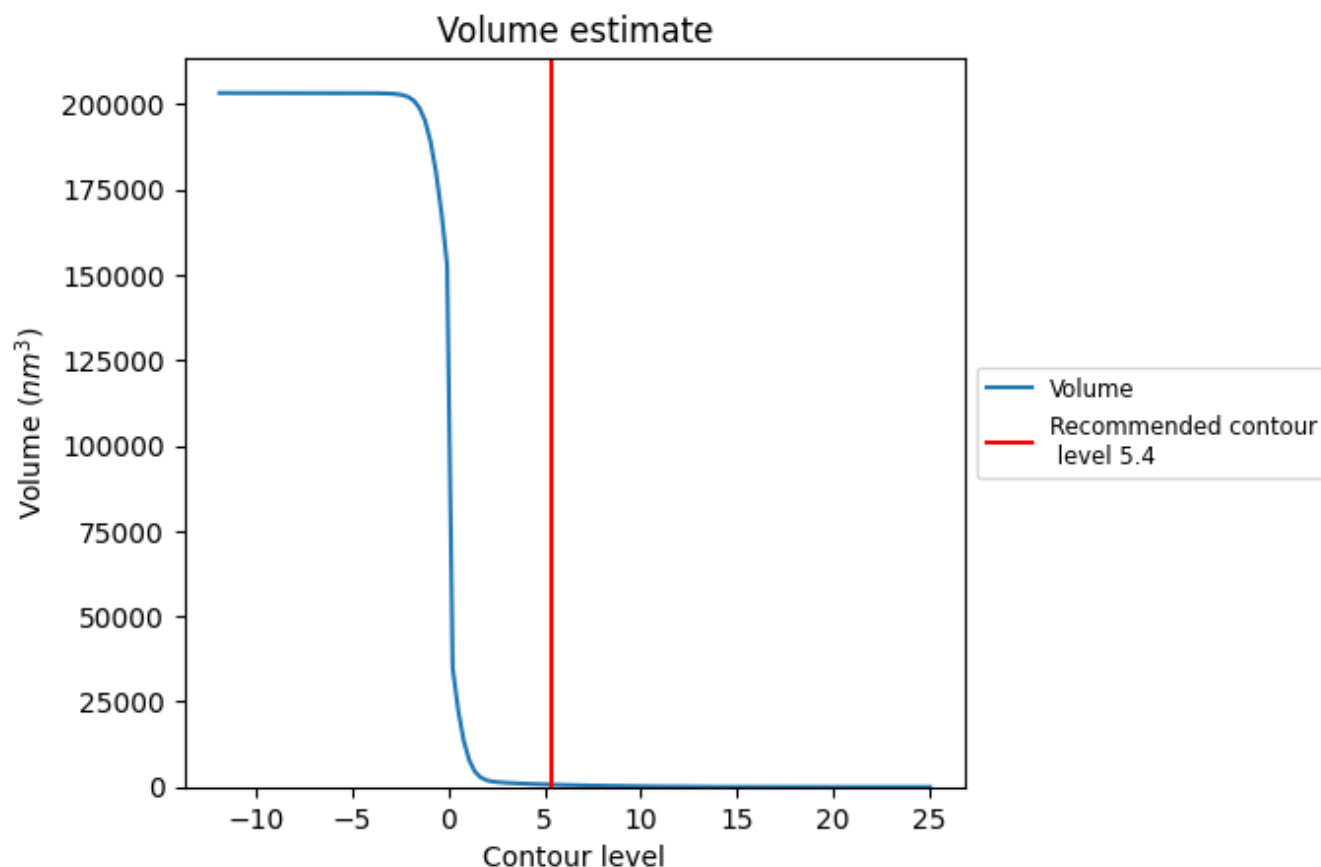
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

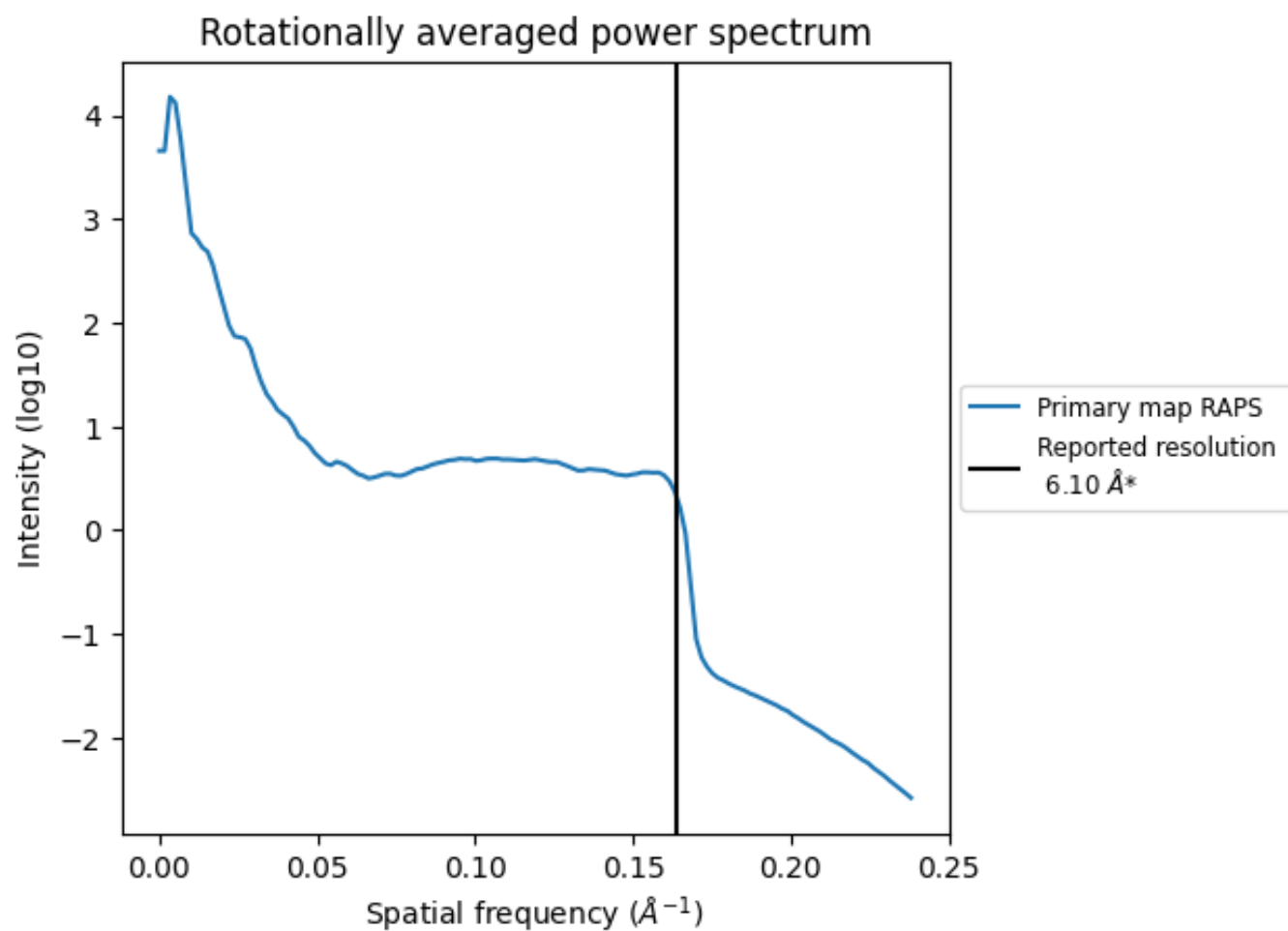
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 678 nm^3 ; this corresponds to an approximate mass of 613 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 0.164 Å⁻¹

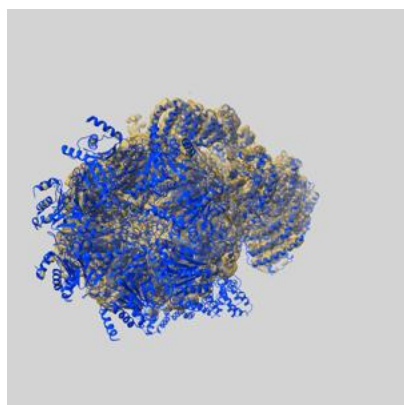
8 Fourier-Shell correlation

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

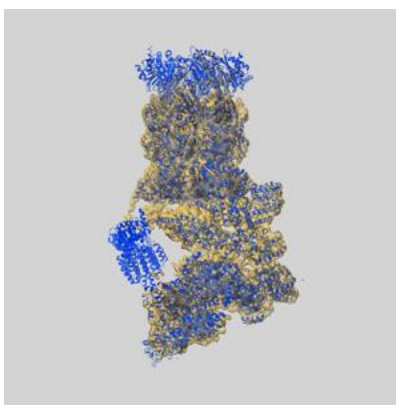
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14082 and PDB model 7QO3. Per-residue inclusion information can be found in section 3 on page 10.

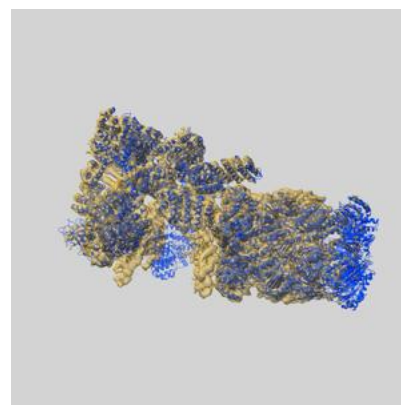
9.1 Map-model overlay [i](#)



X



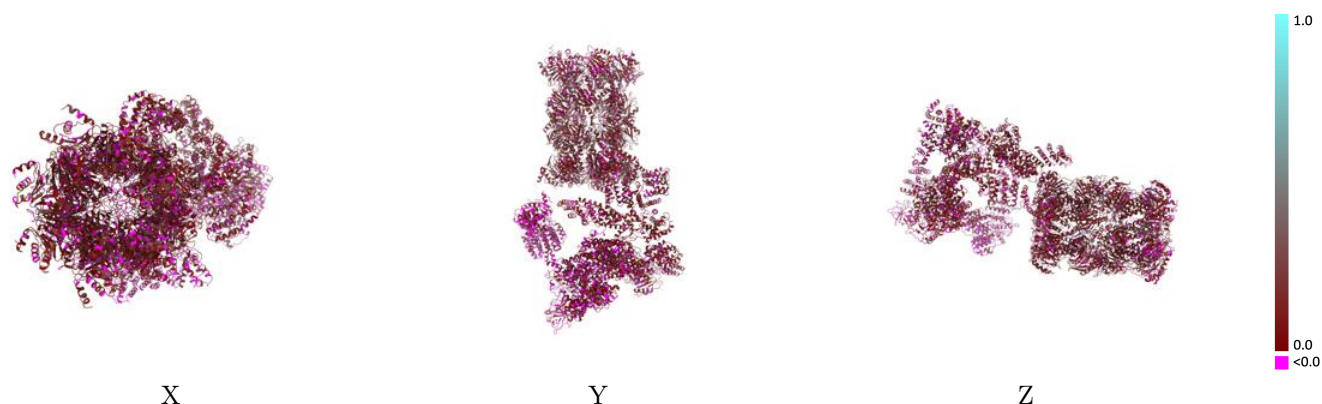
Y



Z

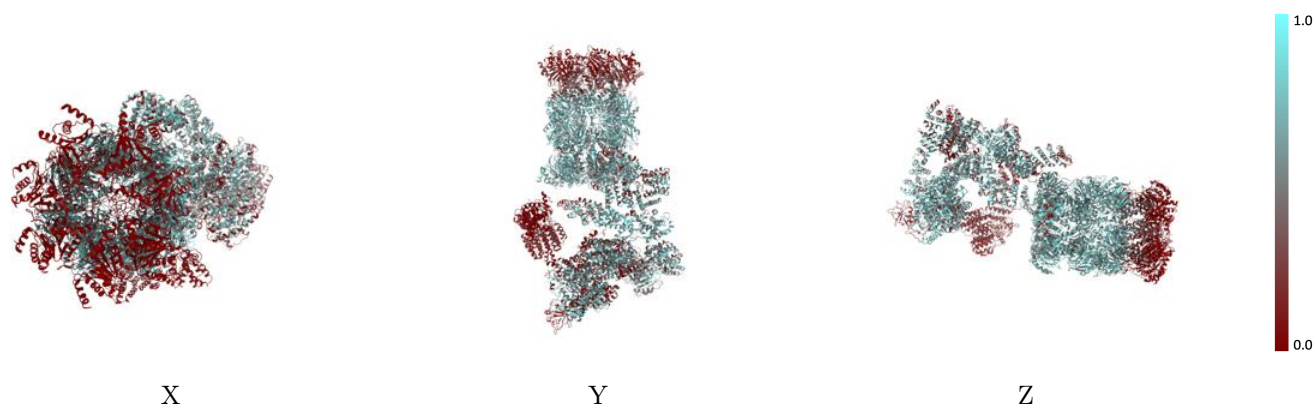
The images above show the 3D surface view of the map at the recommended contour level 5.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



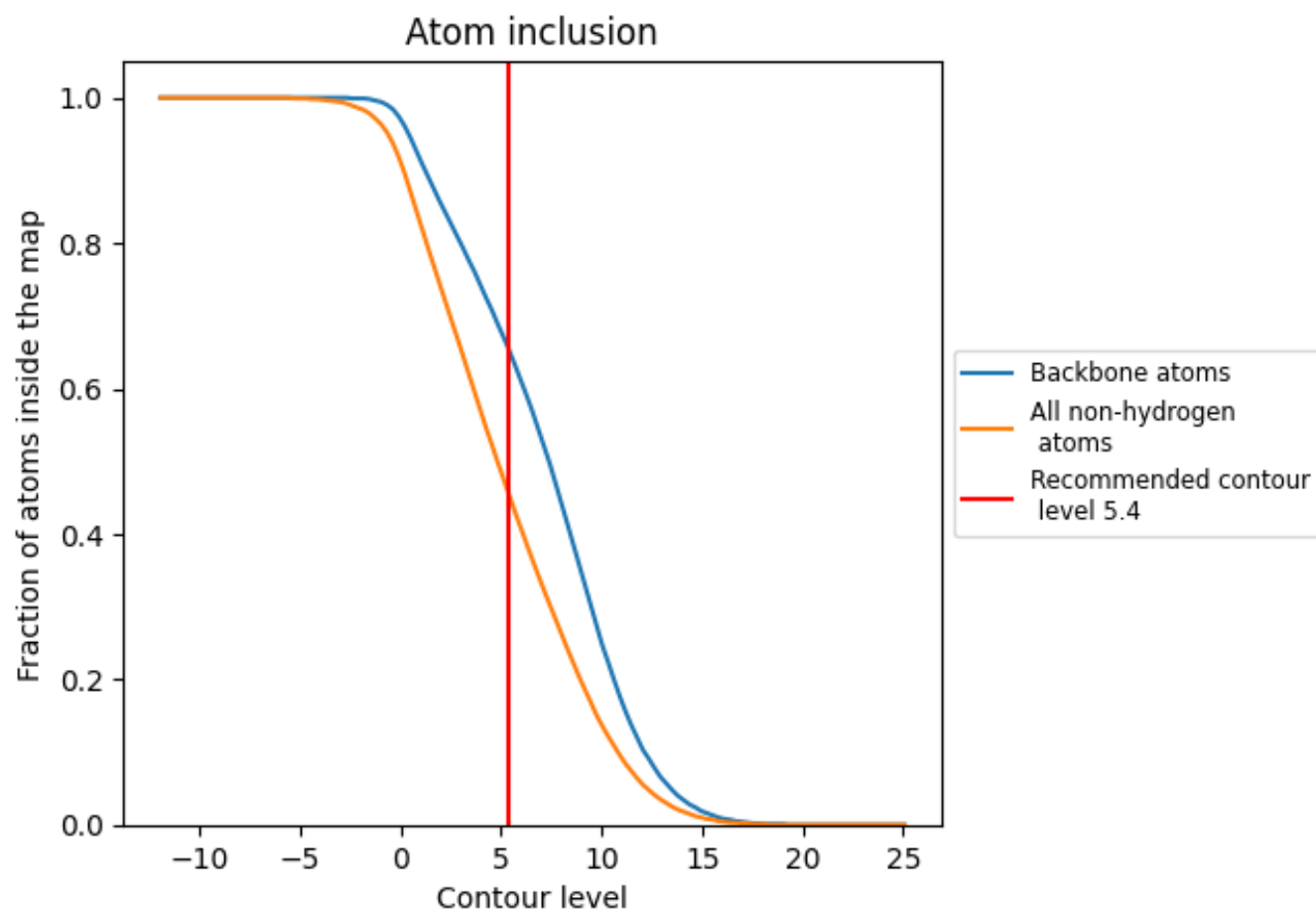
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 45% 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 (5.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4540	 0.1330
1	 0.6980	 0.1590
2	 0.6650	 0.1830
3	 0.6500	 0.1630
4	 0.6870	 0.1730
5	 0.7310	 0.1720
6	 0.6970	 0.1740
7	 0.6820	 0.1550
A	 0.6370	 0.1620
B	 0.6190	 0.1560
C	 0.6180	 0.1640
D	 0.6450	 0.1610
E	 0.6400	 0.1460
F	 0.6790	 0.1660
G	 0.6720	 0.1690
N	 0.5790	 0.1210
O	 0.5680	 0.1320
P	 0.5480	 0.1290
Q	 0.4930	 0.1280
R	 0.5400	 0.1200
S	 0.4710	 0.1080
T	 0.3670	 0.1020
U	 0.5670	 0.1400
V	 0.5230	 0.1270
W	 0.5320	 0.1110
X	 0.0590	 0.0300
Y	 0.2610	 0.0620
Z	 0.0030	 0.0320
a	 0.0620	 0.1440
b	 0.0650	 0.1320
c	 0.0480	 0.1300
d	 0.0390	 0.1350
e	 0.0410	 0.1310
f	 0.0750	 0.1300
g	 0.0720	 0.1490



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Chain	Atom inclusion	Q-score
h	 0.5900	 0.1610
i	 0.5710	 0.1740
j	 0.5690	 0.1690
k	 0.6310	 0.1700
l	 0.5340	 0.1540
m	 0.5590	 0.1650
n	 0.5960	 0.1610