



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:33 AM UTC

PDB ID : 6B43 / pdb_00006b43
EMDB ID : EMD-7047
Title : CryoEM structure and atomic model of the Kaposi's sarcoma-associated herpesvirus capsid
Authors : Dai, X.H.; Gong, D.Y.; Sun, R.; Zhou, Z.H.
Deposited on : 2017-09-25
Resolution : 4.20 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:

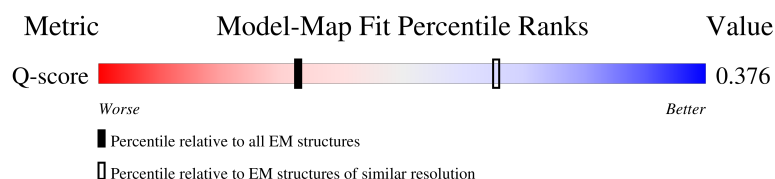
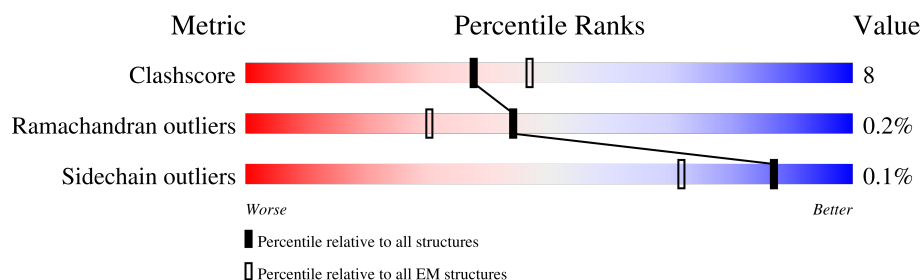
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.20 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	5410 (3.70 - 4.70)

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	4	1376	58% 69% 19% 12%
1	A	1376	9% 80% 19% .
1	B	1376	10% 79% 19% .
1	C	1376	11% 76% 22% ..

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Mol	Chain	Length	Quality of chain
1	D	1376	
1	E	1376	
1	F	1376	
1	M	1376	
1	N	1376	
1	O	1376	
1	S	1376	
1	T	1376	
1	U	1376	
1	V	1376	
1	W	1376	
1	X	1376	
2	0	170	
2	1	170	
2	2	170	
2	3	170	
2	G	170	
2	H	170	
2	I	170	
2	J	170	
2	K	170	
2	L	170	
2	P	170	
2	Q	170	
2	R	170	

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Mol	Chain	Length	Quality of chain
2	Y	170	
2	Z	170	
3	5	331	
3	8	331	
3	b	331	
3	e	331	
3	h	331	
4	6	305	
4	7	305	
4	9	305	
4	a	305	
4	c	305	
4	d	305	
4	f	305	
4	g	305	
4	i	305	
4	j	305	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 214334 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1363	Total	C	N	O	S	0	0
			10682	6786	1854	1969	73		
1	B	1355	Total	C	N	O	S	0	0
			10627	6751	1843	1960	73		
1	C	1354	Total	C	N	O	S	0	0
			10621	6748	1842	1959	72		
1	D	1355	Total	C	N	O	S	0	0
			10627	6751	1843	1960	73		
1	E	1363	Total	C	N	O	S	0	0
			10682	6786	1854	1969	73		
1	F	1356	Total	C	N	O	S	0	0
			10638	6757	1847	1961	73		
1	M	1355	Total	C	N	O	S	0	0
			10627	6751	1843	1960	73		
1	N	1363	Total	C	N	O	S	0	0
			10682	6786	1854	1969	73		
1	O	1355	Total	C	N	O	S	0	0
			10627	6751	1843	1960	73		
1	S	1281	Total	C	N	O	S	0	0
			10060	6397	1737	1855	71		
1	T	1360	Total	C	N	O	S	0	0
			10666	6776	1851	1966	73		
1	U	1355	Total	C	N	O	S	0	0
			10627	6751	1843	1960	73		
1	V	1352	Total	C	N	O	S	0	0
			10604	6739	1839	1954	72		
1	W	1354	Total	C	N	O	S	0	0
			10621	6748	1842	1959	72		
1	X	1345	Total	C	N	O	S	0	0
			10548	6701	1829	1946	72		
1	4	1216	Total	C	N	O	S	0	0
			9586	6102	1665	1748	71		

- Molecule 2 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	H	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	I	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	J	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	K	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	L	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	P	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	Q	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	R	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	Y	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	Z	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	0	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	1	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	2	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
2	3	78	Total	C	N	O	S	0	0
			666	418	130	115	3		

- Molecule 3 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	319	Total	C	N	O	S	0	0
			2463	1578	421	449	15		
3	8	321	Total	C	N	O	S	0	0
			2477	1586	424	452	15		
3	b	321	Total	C	N	O	S	0	0
			2477	1586	424	452	15		
3	e	319	Total	C	N	O	S	0	0
			2460	1575	422	448	15		
3	h	321	Total	C	N	O	S	0	0
			2477	1586	424	452	15		

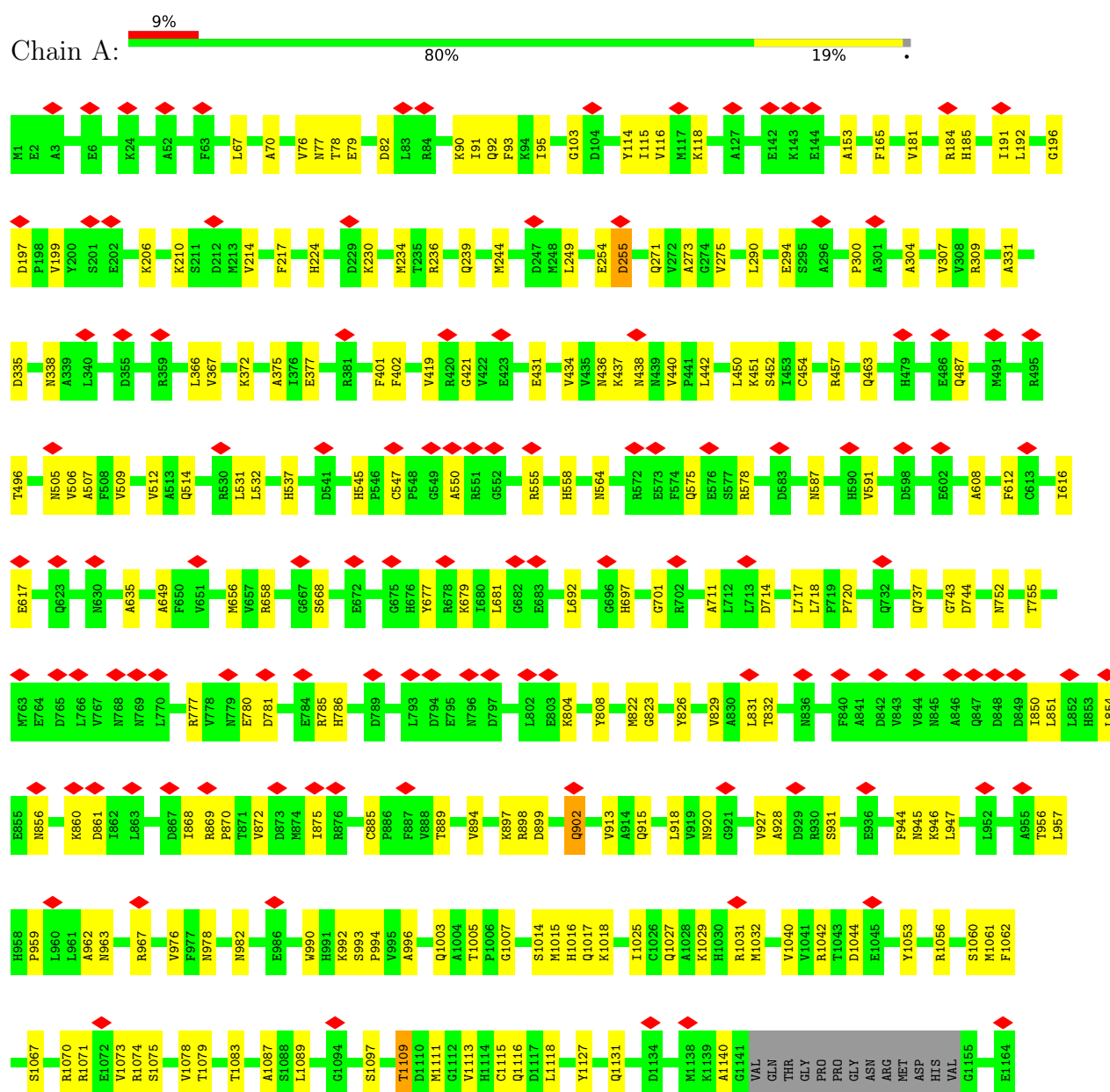
- Molecule 4 is a protein called Triplex capsid protein 2.

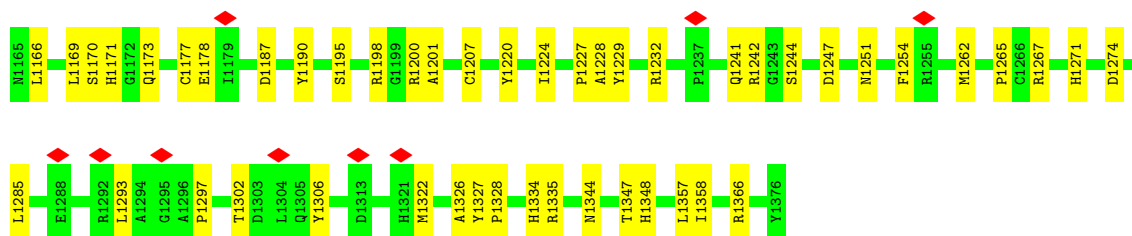
Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	7	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		
4	9	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	a	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		
4	c	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	d	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		
4	f	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	g	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		
4	i	294	Total	C	N	O	S	0	0
			2329	1485	397	433	14		
4	j	300	Total	C	N	O	S	0	0
			2364	1505	401	443	15		

3 Residue-property plots

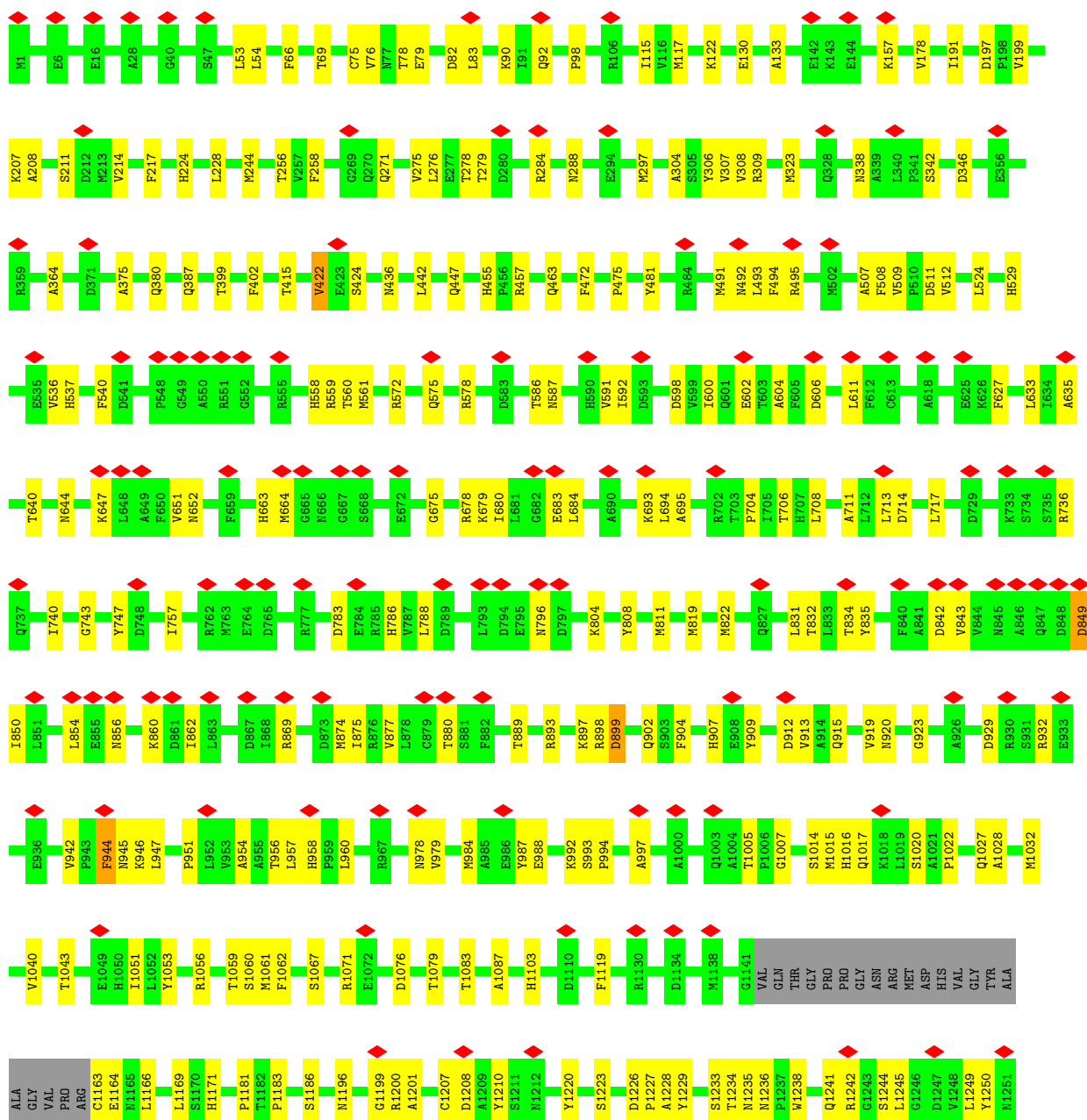
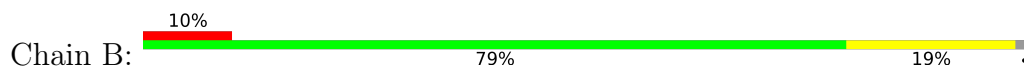
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

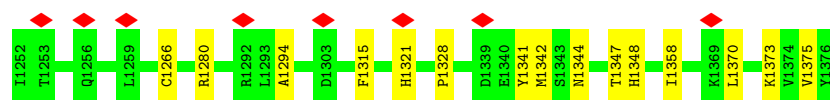
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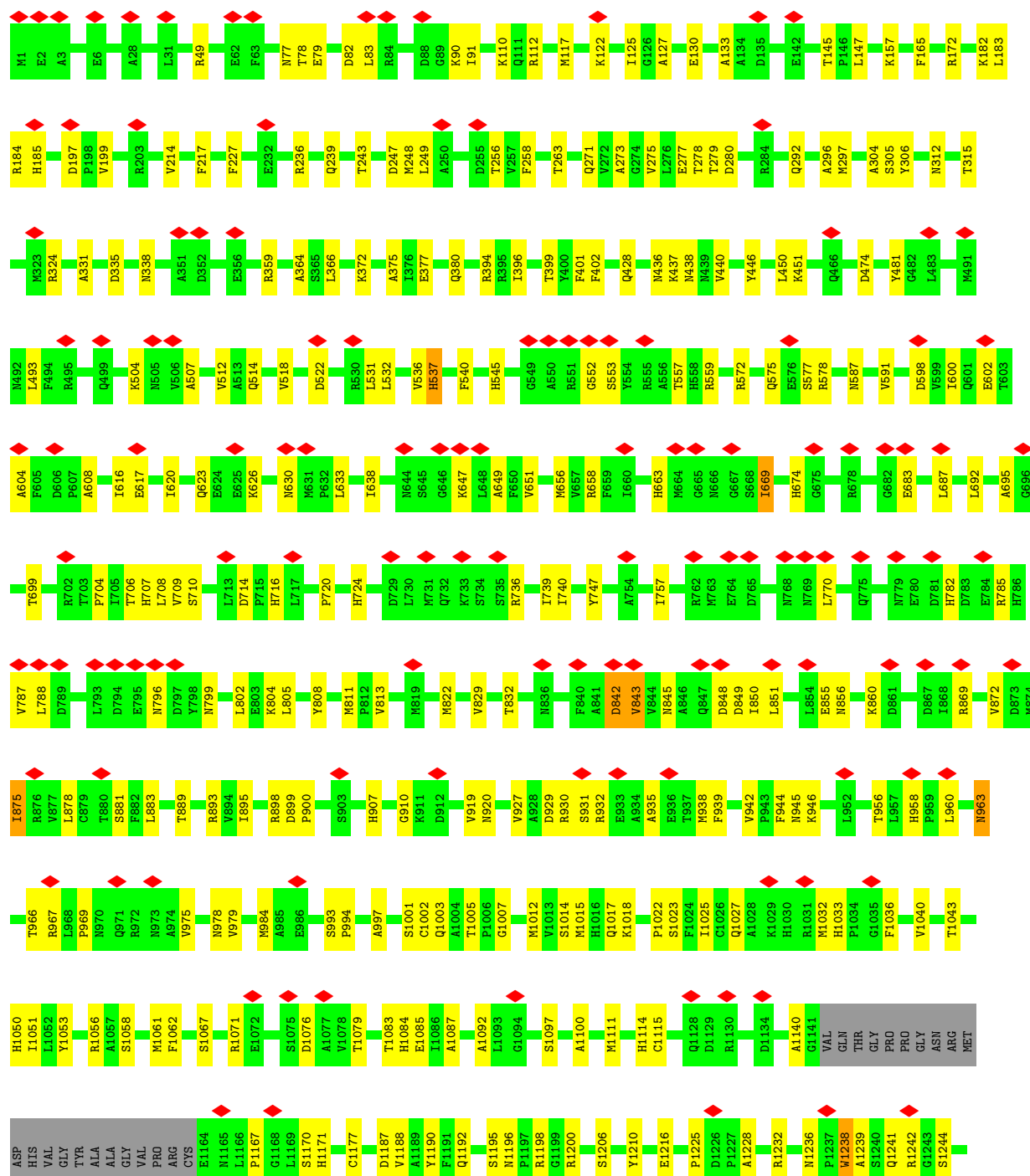
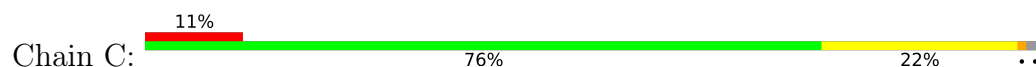


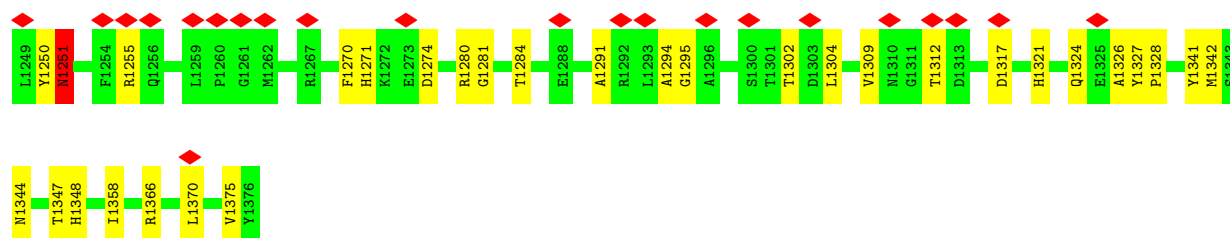
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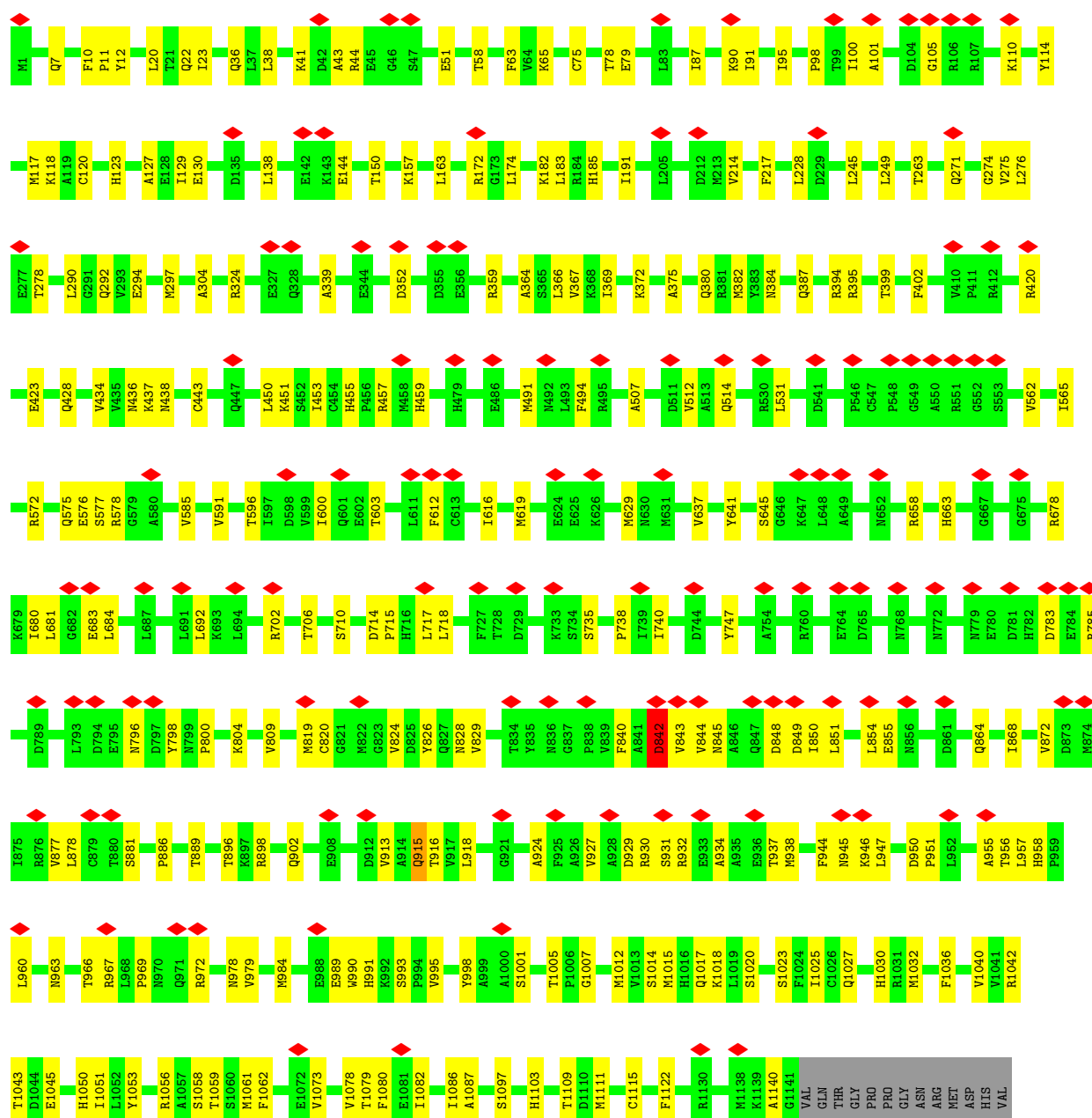
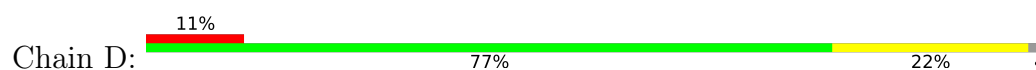


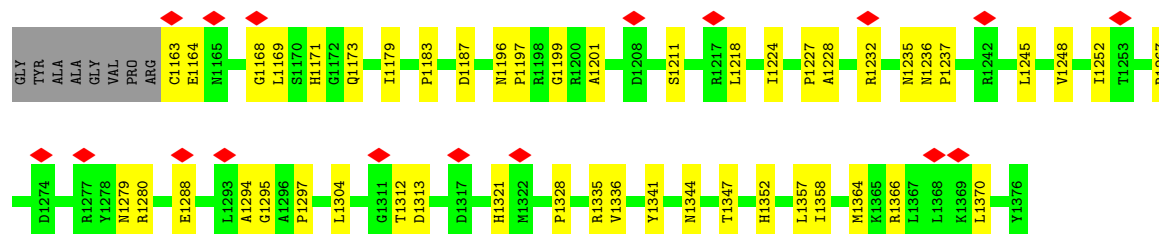
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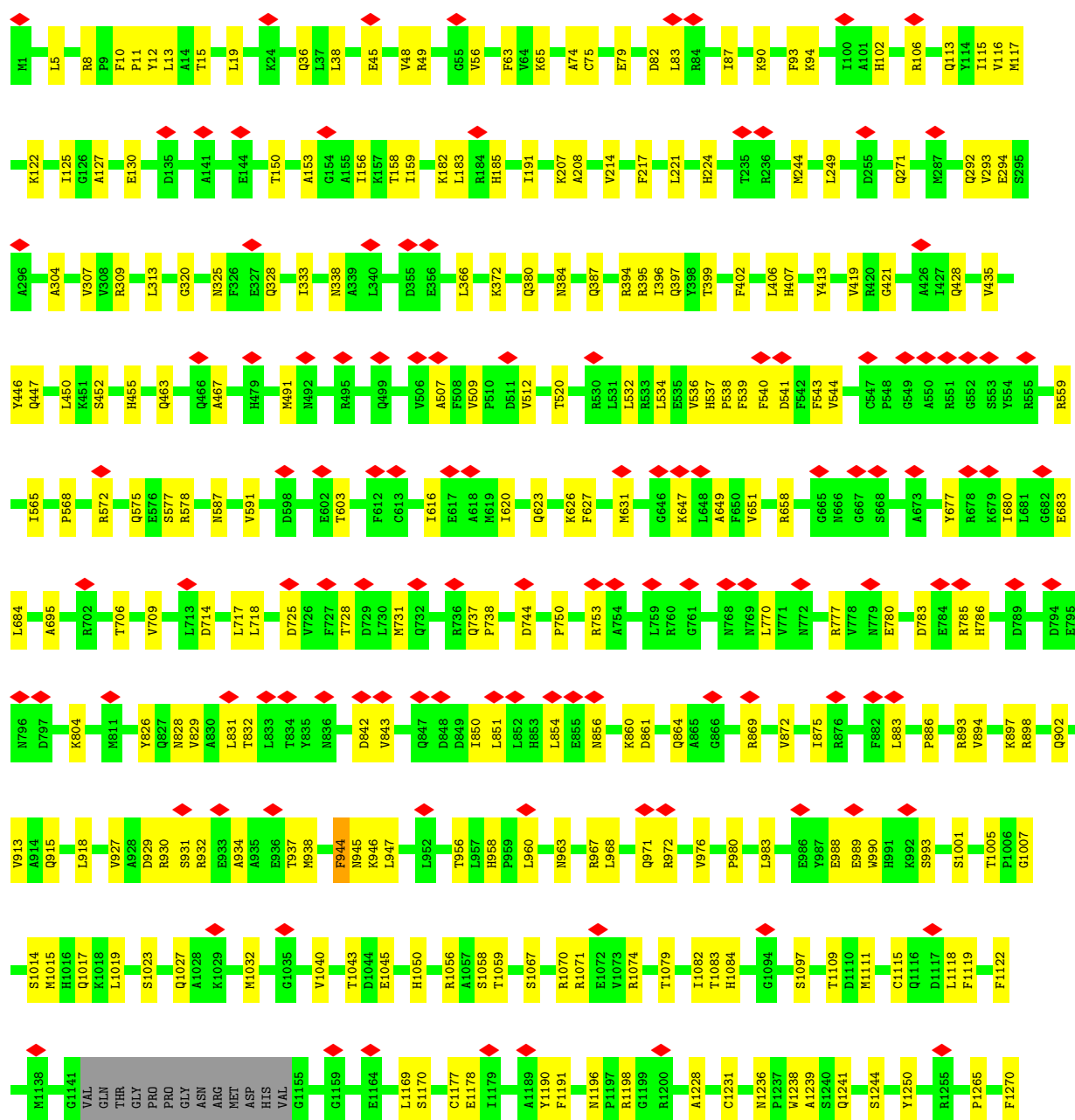
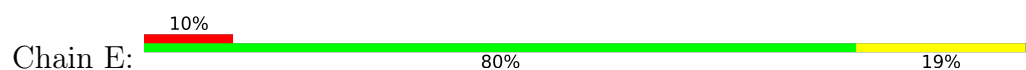


• Molecule 1: Major capsid protein



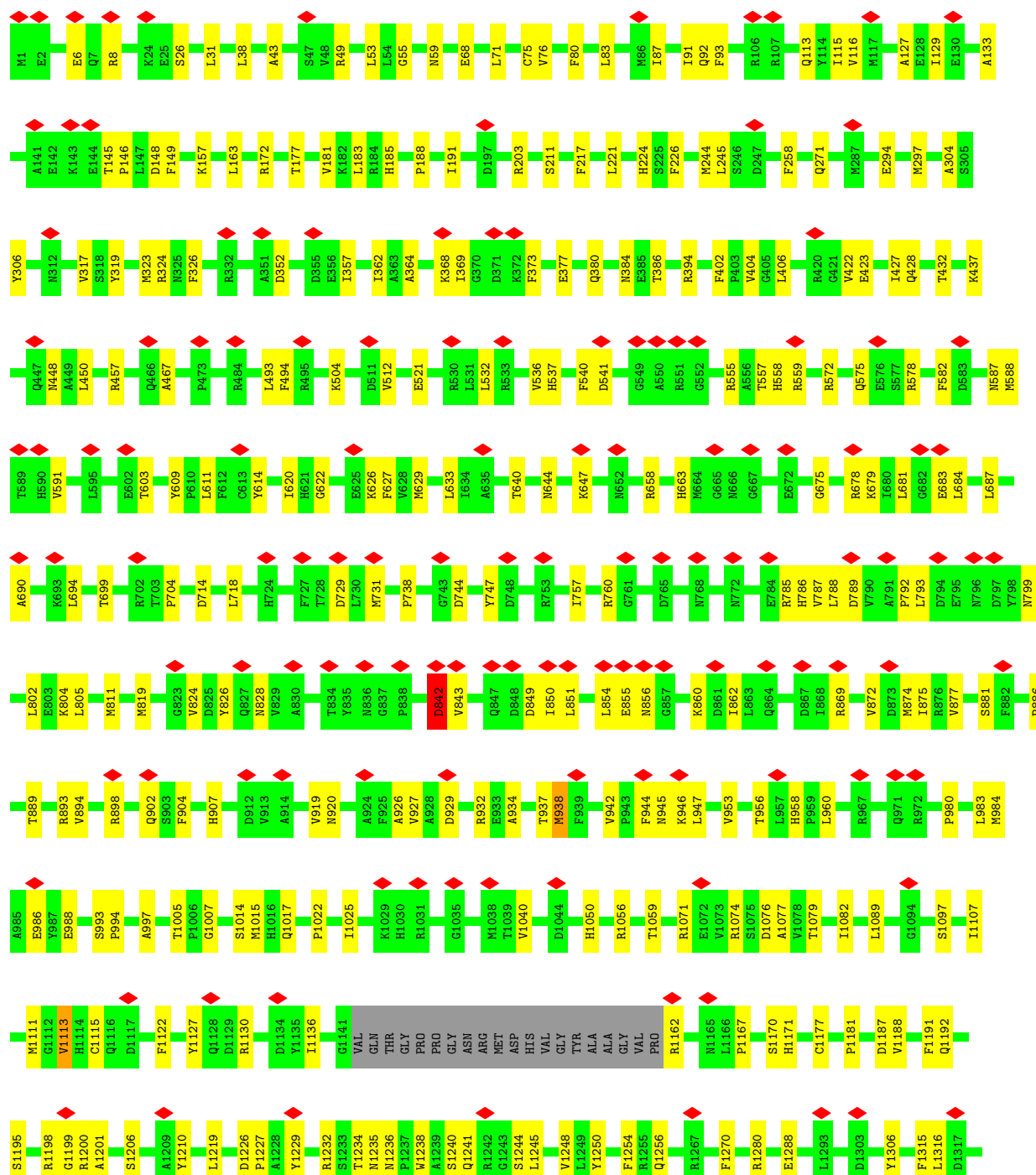
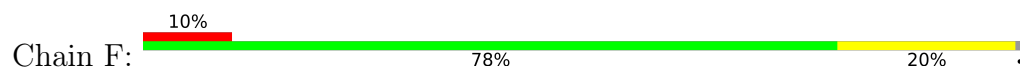


• Molecule 1: Major capsid protein



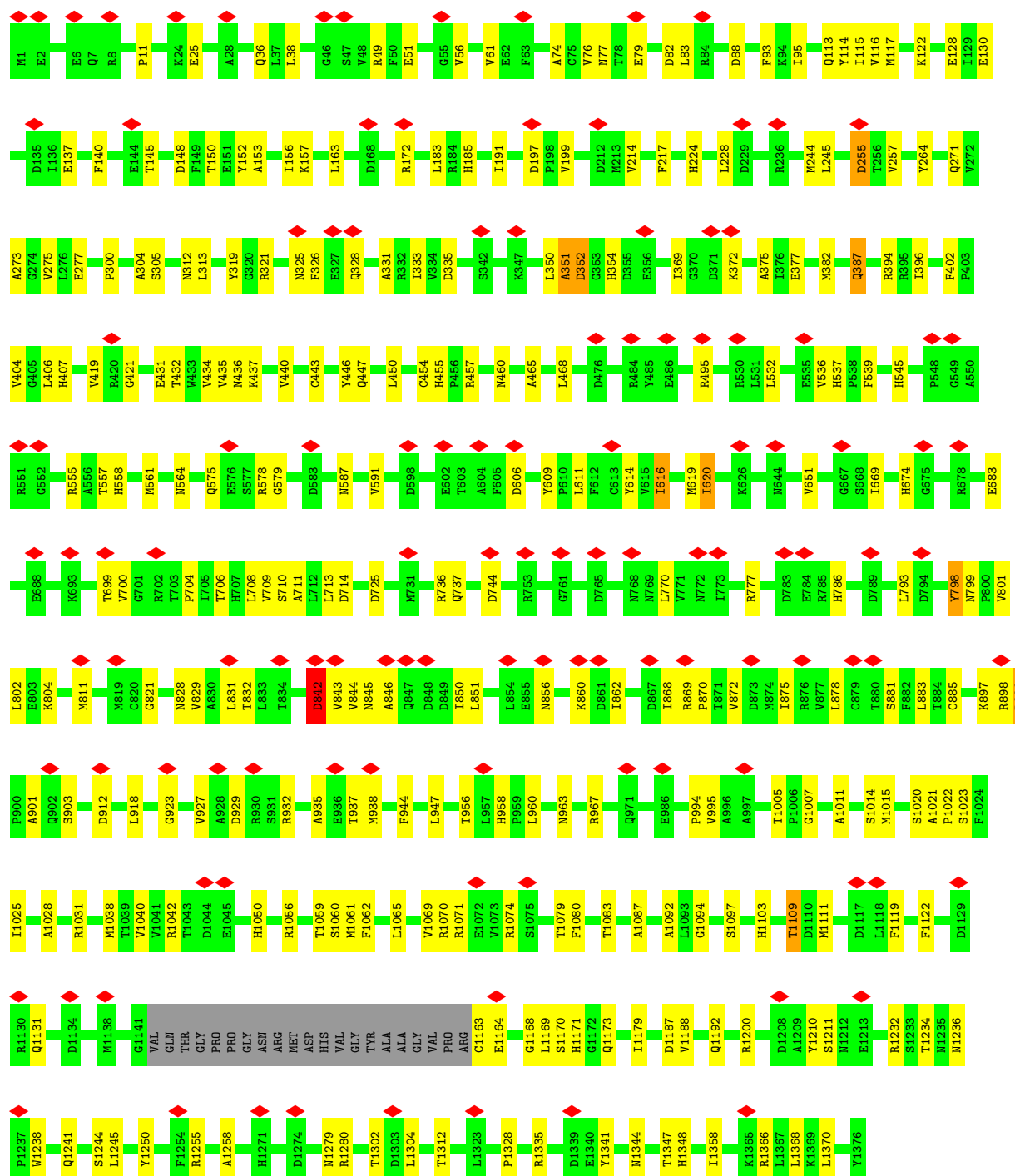
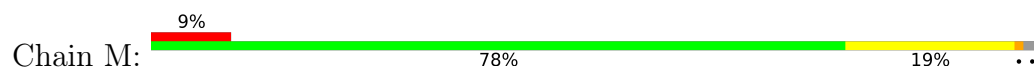


• Molecule 1: Major capsid protein

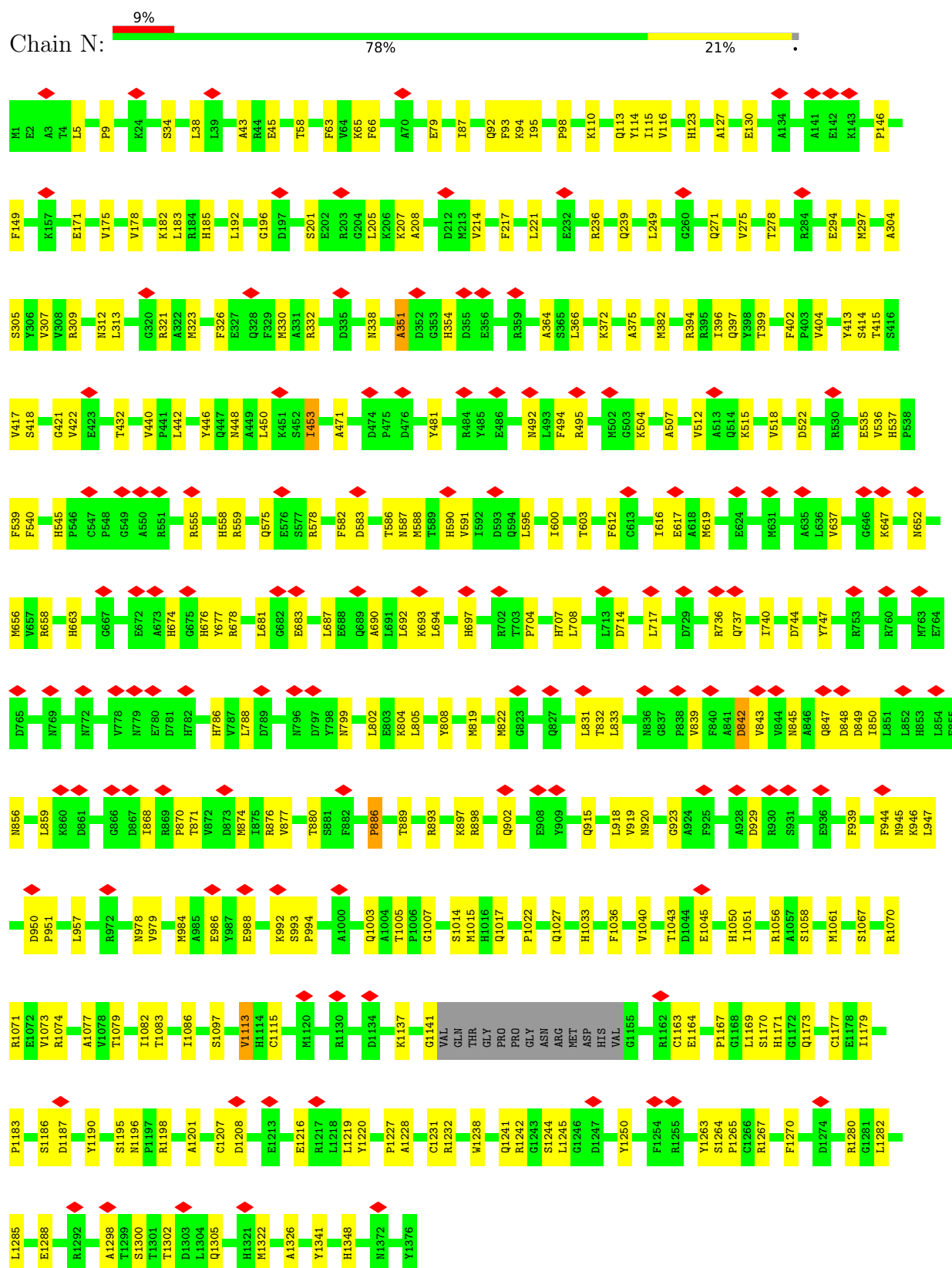




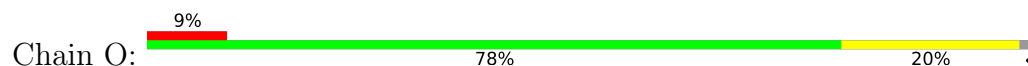
• Molecule 1: Major capsid protein



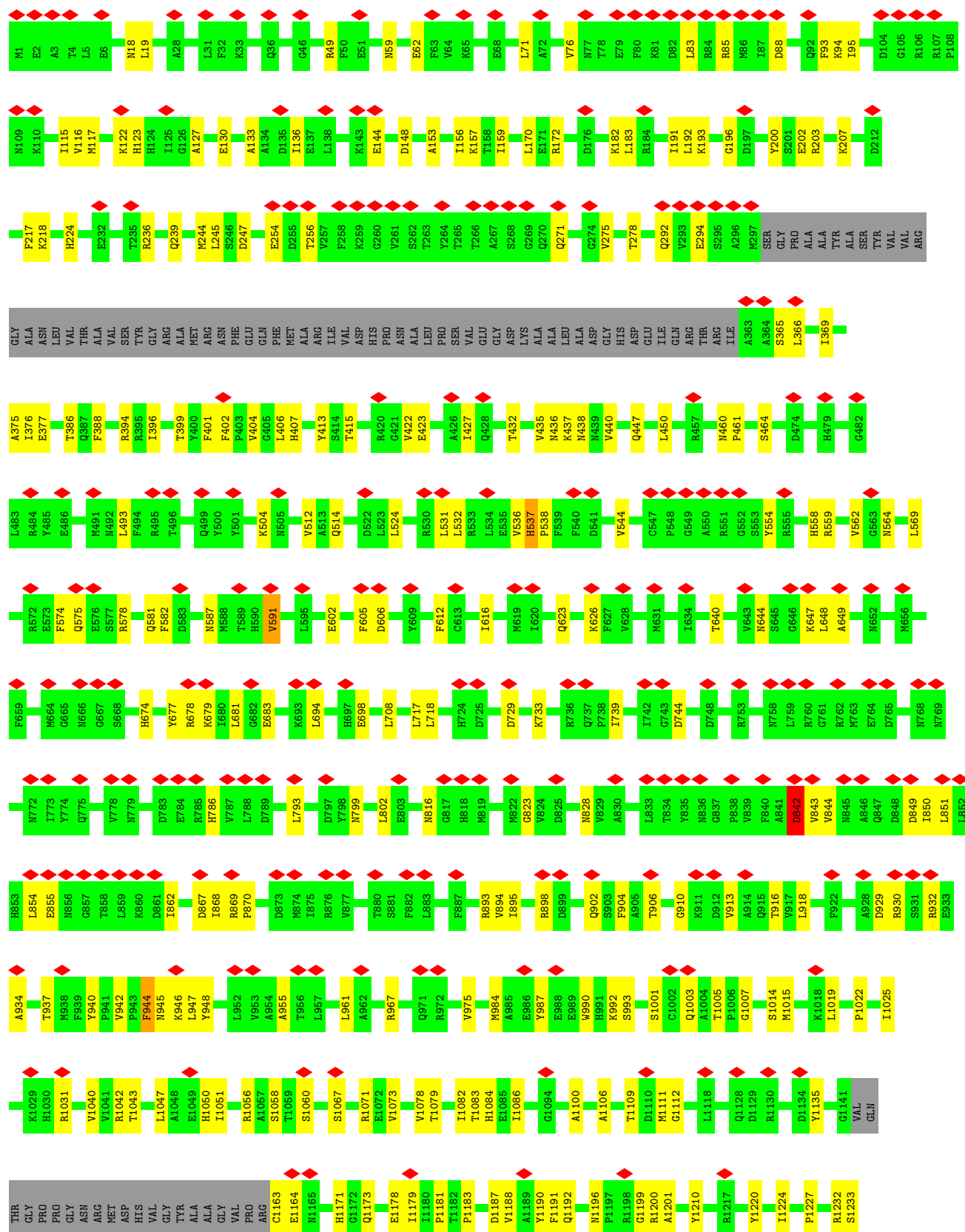
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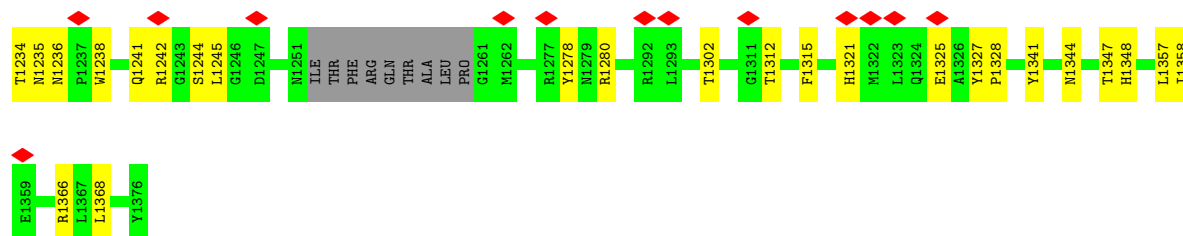


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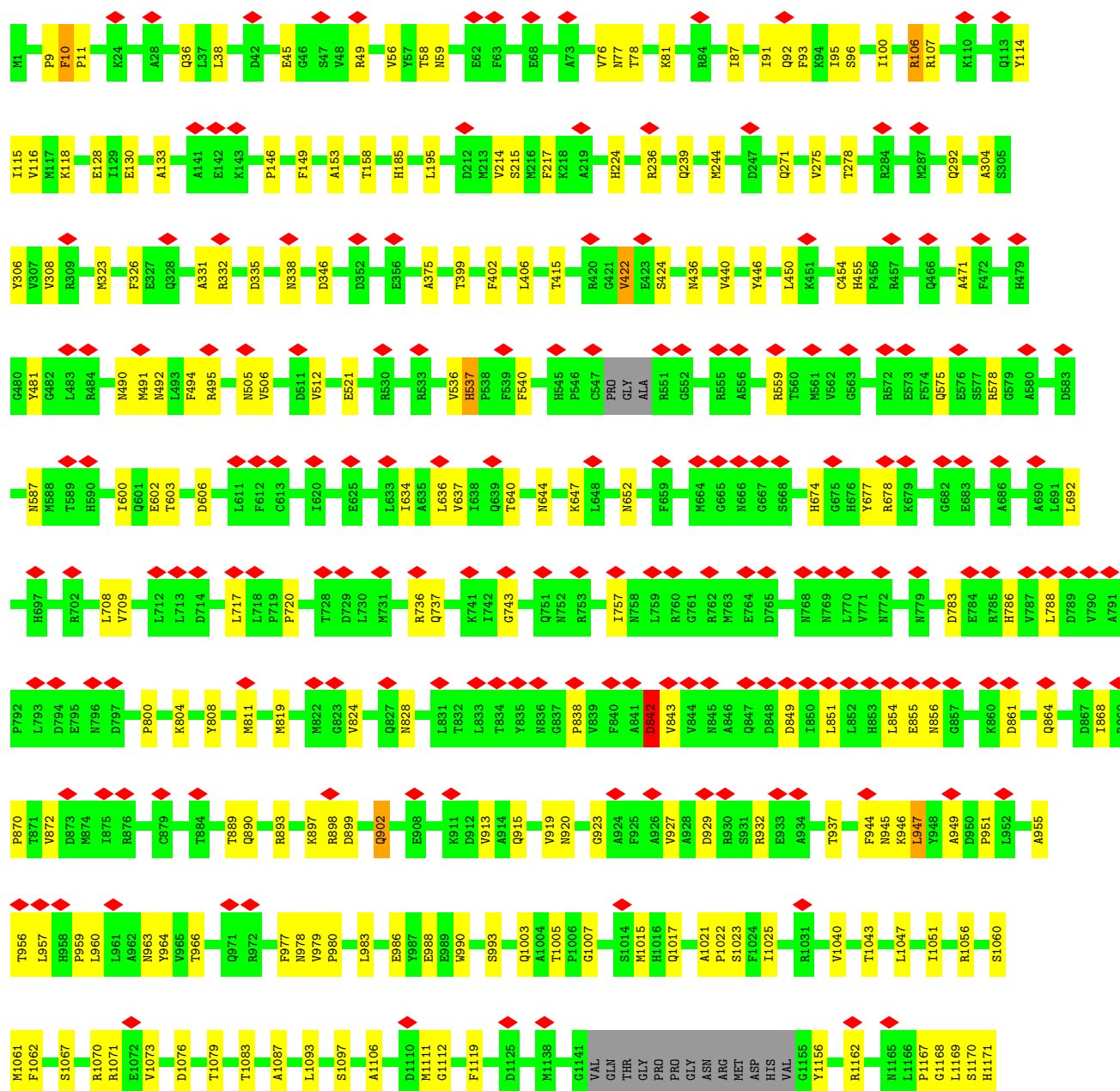
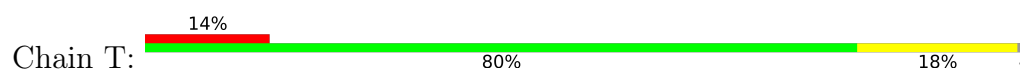


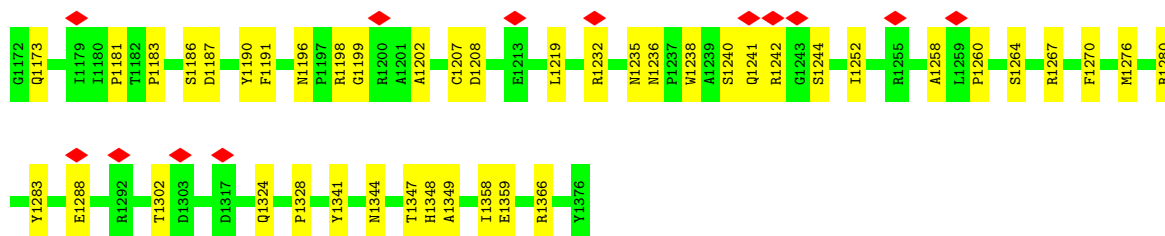




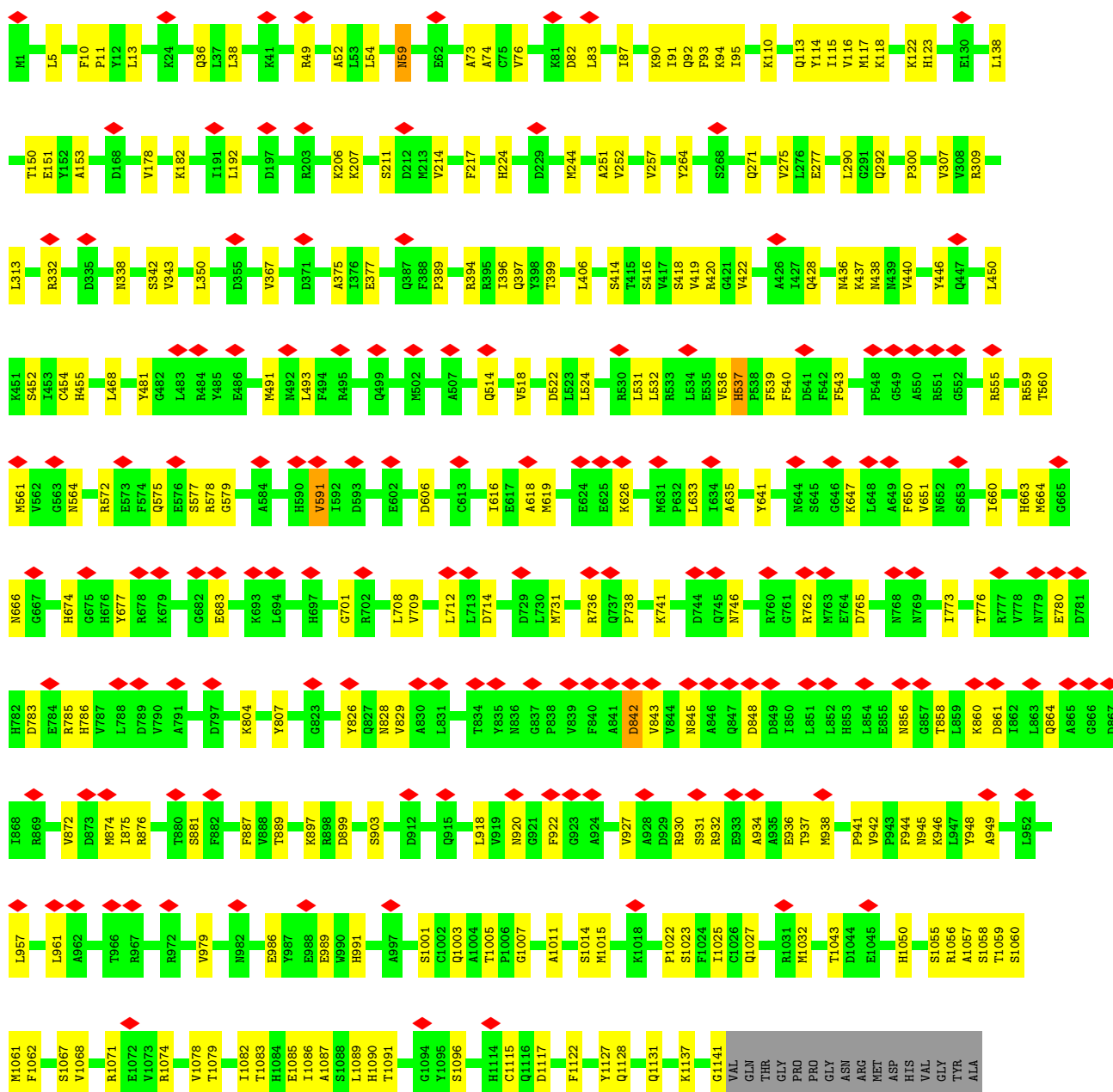
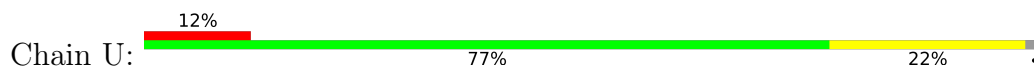


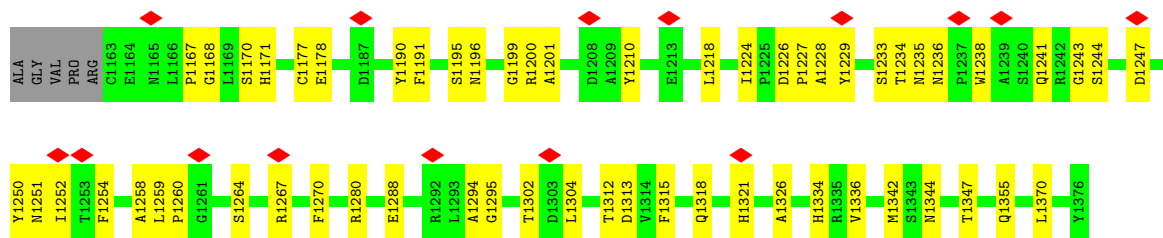
• Molecule 1: Major capsid protein



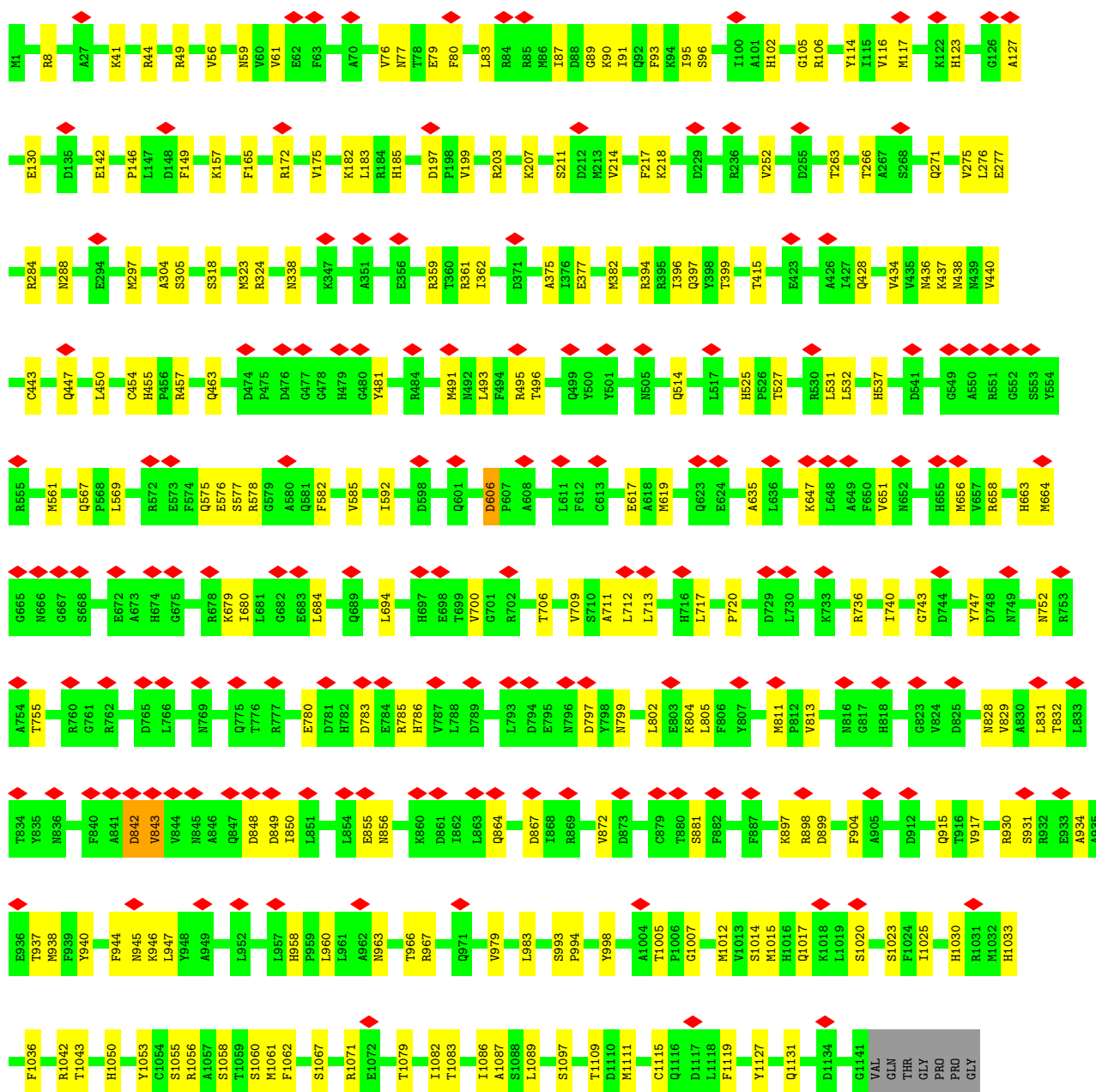
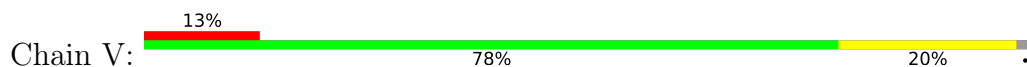


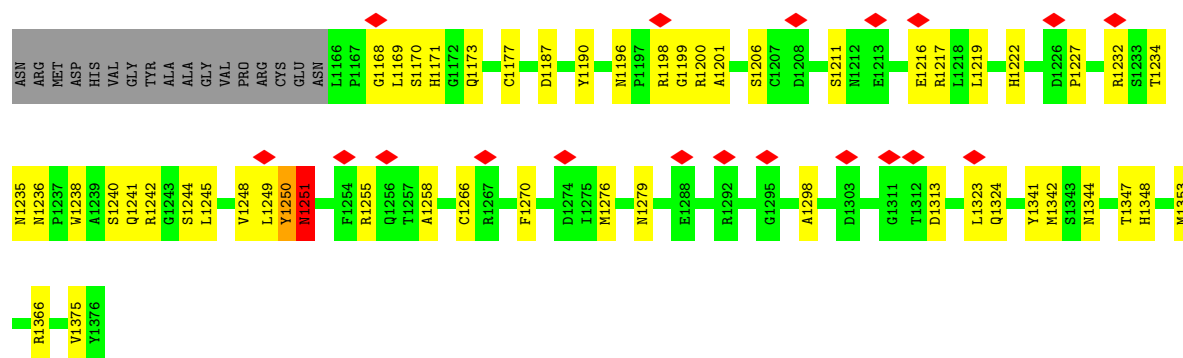
• Molecule 1: Major capsid protein



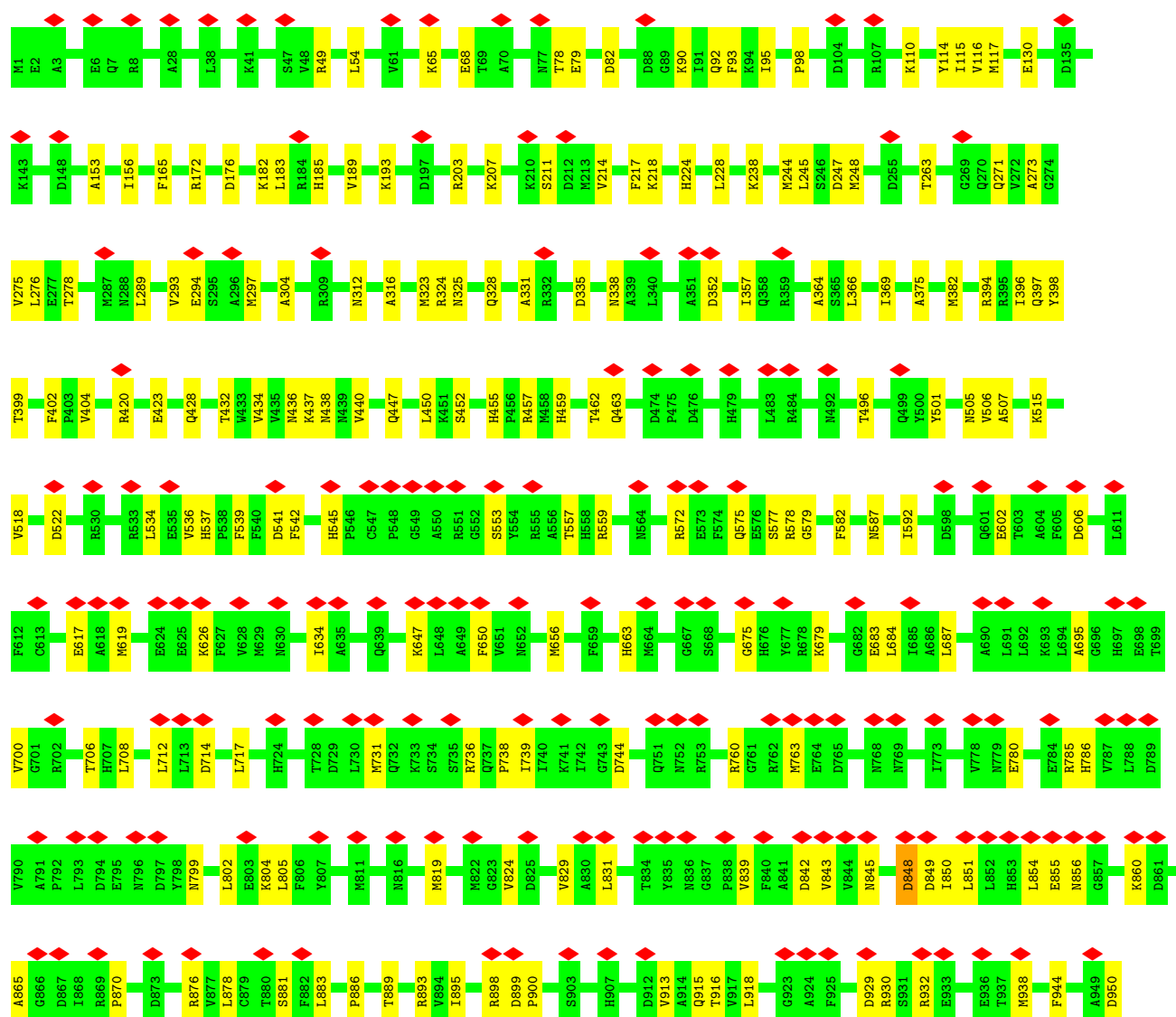
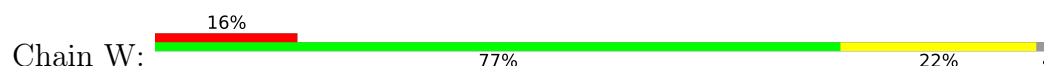


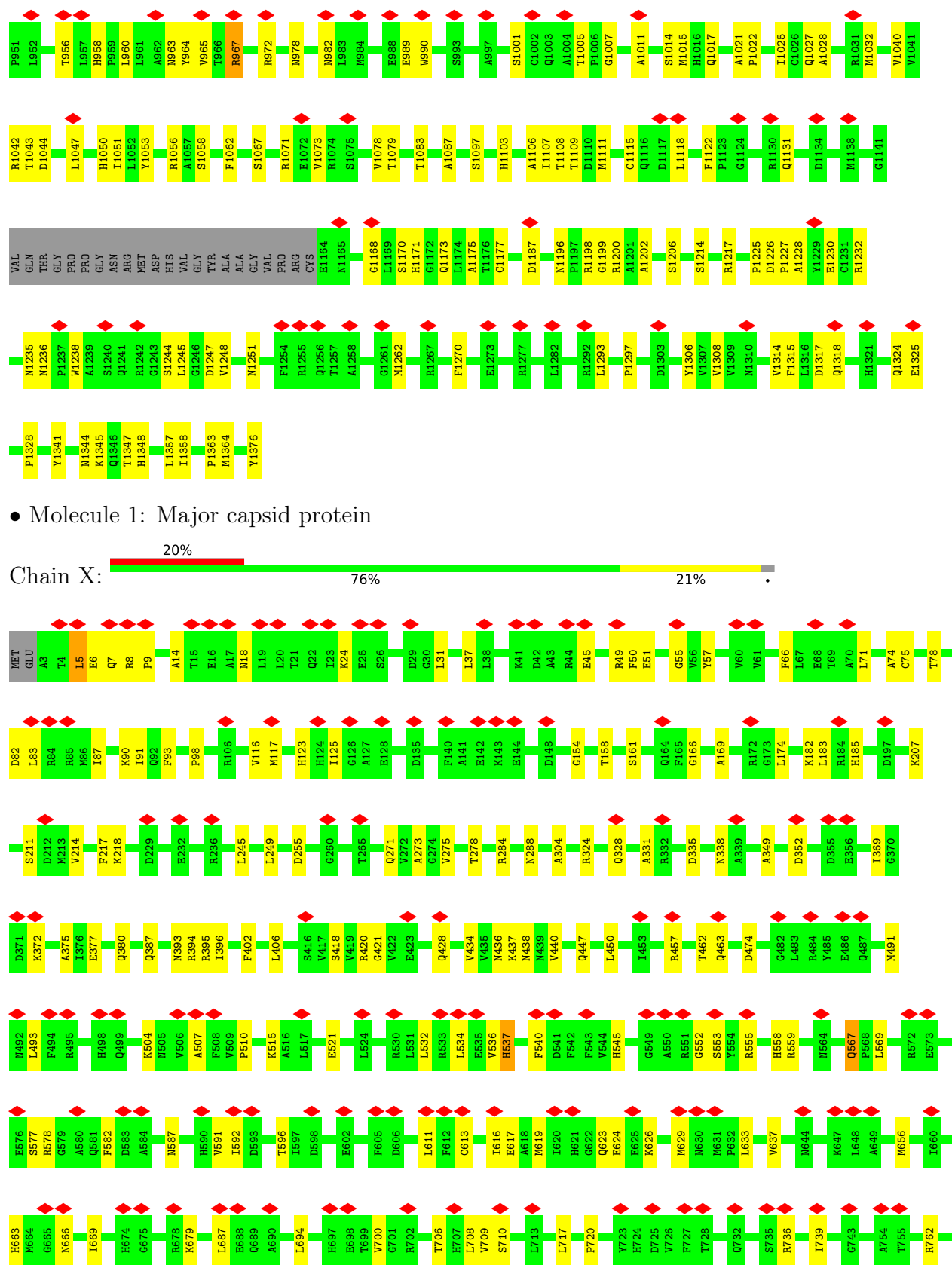
• Molecule 1: Major capsid protein

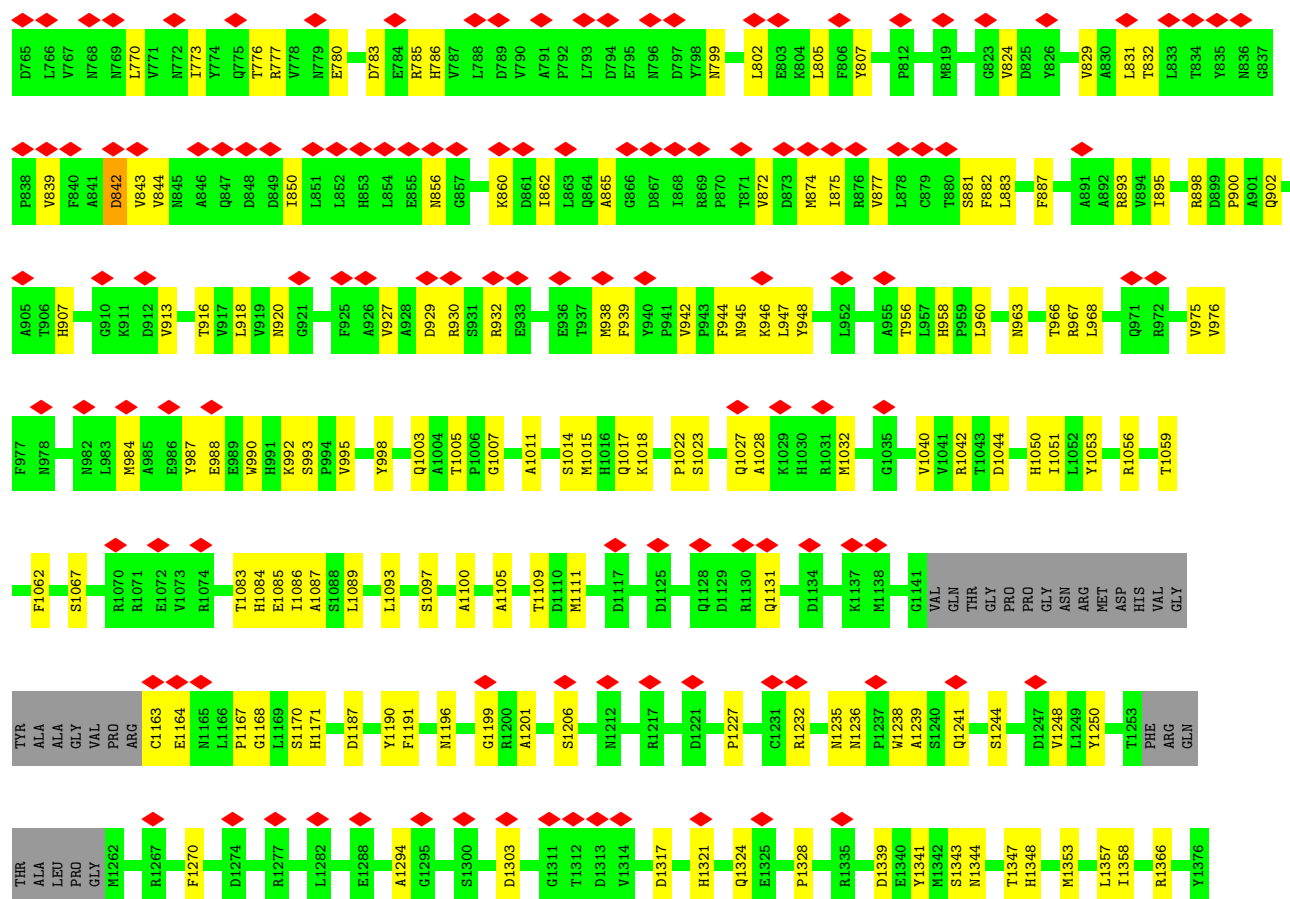




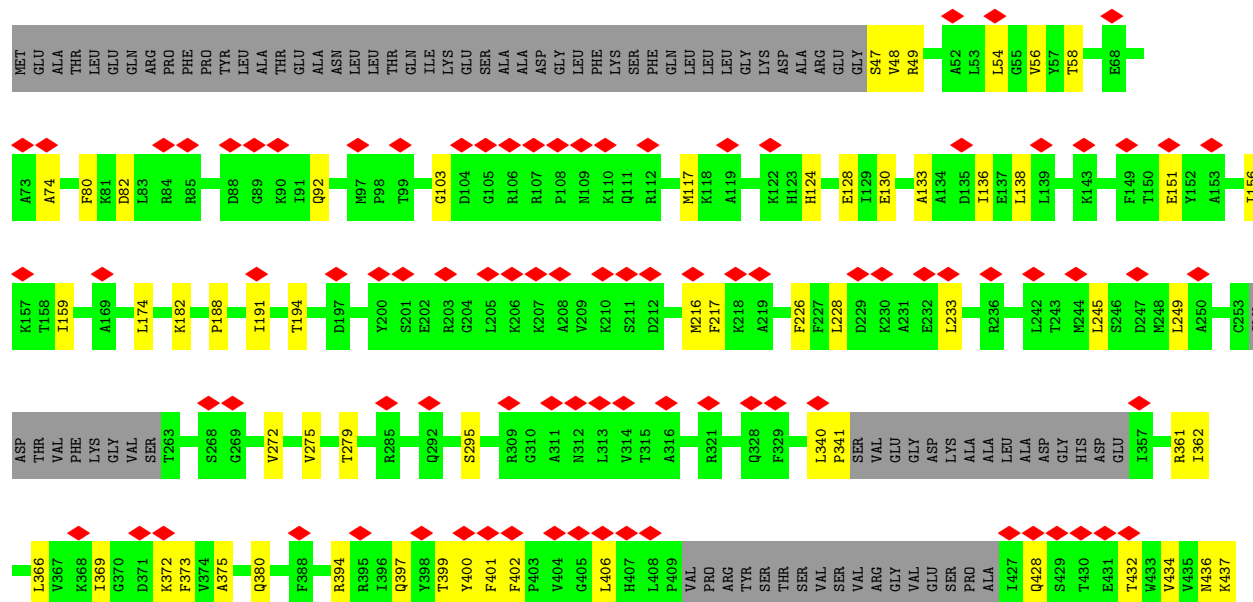
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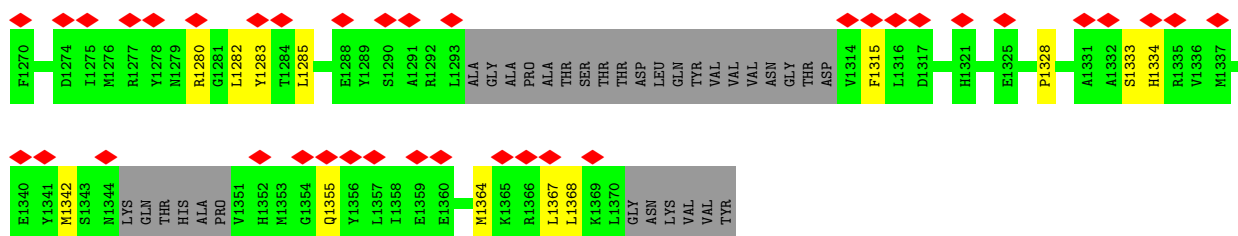




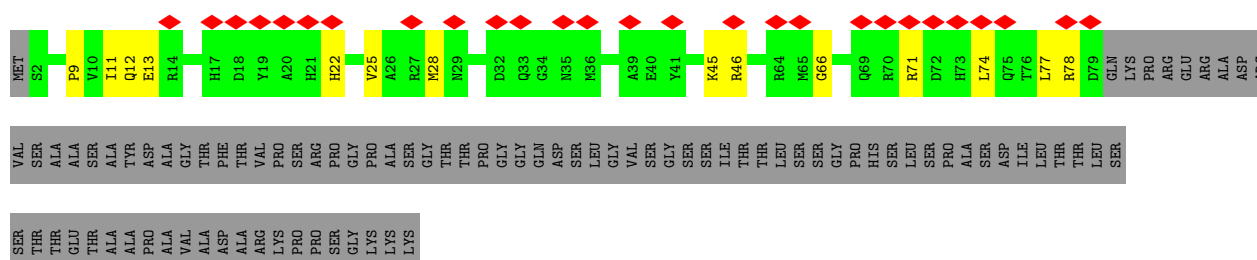
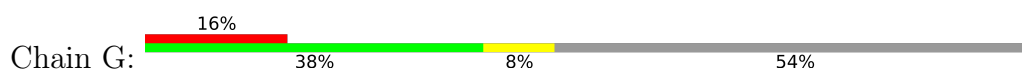
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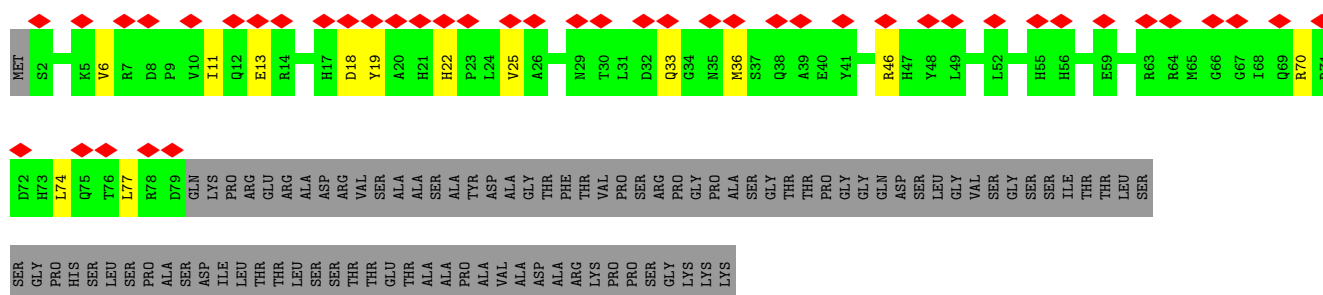
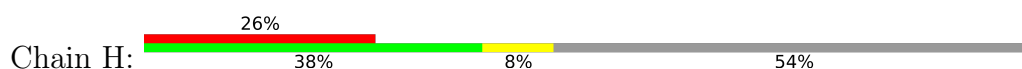
GLY	GLY	T1043	L983	G923	L863	E803	G743	E683	Q623	G563	G503	M438
PRO	PRO	D1044	M884	A924	Q864	K804	D744	L884	E624	N564	K504	M439
GLY	GLY	E1045	A885	F925	A865	L805	Q745	I885	E625	I565	N505	L442
ASN	ASN	Y1210	E986	A926	Q866	F806	N746	A886	K526	P566	V506	
ARG	ARG	S1058	E987	Y927	Q867	Y807	Y747	D867	F627	Q567	A507	
ASP	ASP	V1063	E988	A928	I868	Y808	D748	E888	V628	P568	F508	Y446
HIS	HIS	G1064	E989	D929	I869	Y809	N749	Q889	M629	L569	V509	Q447
VAL	VAL	L1065	W990	R930	P870	L810	P750	A690	N630	A570	P510	M448
GLY	GLY	H991	H991	R931	T871	M811	Q751	L691	M631	P571	D511	A449
ALA	ALA	R1071	K992	S932	V872	P812	Q752	L692	P632	P572	V512	L450
ALA	ALA	V1072	S993	E933	D873	V813	R753	K693	L633	E573	A513	K451
GLY	GLY	R1073	P994	A934	M874	C814	R754	L694	I634	F574	Q514	S452
VAL	VAL	S1074	V995	A935	I875	S815	T755	A695	A635	Q575	I453	I453
ARG	ARG	D1076	A996	E936	R876	N816	F756	G696	L636	E576	K515	C454
CYS	CYS	A1077	A997	T937	V877	G817	I757	H697	V637	S577	L517	H455
GLU	GLU	V1078	Y998	N938	L878	H818	N758	E698	I638	R578	V518	P456
ASN	ASN	T1079	A999	F939	C879	M819	L759	T699	Q639	G579	T519	R457
LEU	LEU	H1084	A1000	Y940	T880	C820	R760	V700	T640	A580	T520	M458
PRO	PRO	E1085	S1001	P941	S881	G821	G761	G701	Y641	E521	E521	H459
GLY	GLY	I1086	C1002	V942	F882	M822	R762	R702	W642	D522	D522	M460
LEU	LEU	A1087	L883	P943	T884	V824	M763	I703	N643	L523	L523	P461
GLN	GLN	H1103	T884	F944	T884	V824	E764	P704	N644	A584	L524	T462
LEU	LEU	M1111	C885	N945	C885	D825	D765	I705	S645	V585	H525	Q463
A1175	A1175	P1006	P886	K946	P886	Y826	L766	T706	G646	T586	P526	Q466
T1176	T1176	G1007	F887	L947	F887	Q827	V767	H707	K647	N587	T527	A467
C1177	C1177	A1008	V888	Y948	V888	N828	M768	L708	L648	M588	S528	L468
E1178	E1178	I1009	T889	Y949	T889	V829	M769	V709	A649	T589	H529	M469
I1180	I1180	S1010	Q890	D950	Q890	A830	L770	S710	F650	H590	B530	Q470
P1183	P1183	A1011	A891	P951	A891	L831	V771	A711	N651	V591	L531	
V1184	V1184	M1012	A892	L952	A892	T832	I772	L712	N652	I592	L532	P473
T1185	T1185	V1013	R893	V953	R893	L833	I773	L713	S653	D593	R533	D474
S1186	S1186	S1014	V894	A954	V894	T834	V774	D714	Y654	Q594	L534	P475
D1187	D1187	M1015	I895	A955	I895	Y835	Q775	P715	H655	L595	E535	D476
V1188	V1188	H1016	T896	T956	T896	N836	I776	H716	M656	T596	V536	C477
A1189	A1189	Q1017	R897	L957	R897	G837	R777	L717	V657	I597	H537	G478
Y1190	Y1190	K1018	R898	H958	R898	P838	V778	L718	R658	D598	P538	H479
F1191	F1191	L1019	D899	P959	D899	V839	N779	P719	F659	V599	F539	G480
Q1192	Q1192	S1020	P900	L960	P900	F840	E780	F720	I660	I600	F540	Y481
S1195	S1195	A1021	A901	L961	A901	A841	D781	F721	C661	Q601	D541	G482
N1196	N1196	P1022	Q902	A962	Q902	D842	A722	A722	T662	E602	F542	L483
P1197	P1197	S1023	S903	N963	S903	V843	D783	H724	H663	T603	F543	R484
R1198	R1198	F1024	F904	Y964	F904	V844	E784	D725	M664	A604	V544	Y485
G1199	G1199	I1025	A905	V965	A905	N845	R785	D726	G665	F605	H545	E486
A1200	A1200	C1026	T906	T966	T906	A846	H786	V726	N666	D606	P546	Q487
R1200	R1200	Q1027	H907	R967	H907	Q847	V787	F727	G667	P607	C547	T488
G1201	G1201	A1028	E908	L968	E908	D848	L788	T728	S668	A608	P548	P489
A1202	A1202	K1029	Y909	P969	Y909	D849	D789	D729	I669	Y609	G549	M490
I1203	I1203	H1030	Q910	N970	Q910	L850	V790	L730	P670	P610	A550	M491
V1204	V1204	R1031	X911	Q971	X911	L851	A791	Q732	K671	L611	R551	M492
V1205	V1205	M1032	D912	R972	L852	L852	P792	K733	E672	F612	G552	L493
S1206	S1206	H1033	V913	N973	H853	H853	L793	S734	A673	C613	S553	F494
VAL	VAL	P1034	A914	A974	L854	L854	D794	S735	H674	Y614	Y554	R495
GLN	GLN	F1036	Q915	V976	E955	E955	E795	R736	G675	V615	R555	T496
THR	THR	A1037	T916	V976	N856	N856	N796	Q737	H676	I616	A556	F497
ALA	ALA	M1038	V917	F977	G857	G857	D797	P738	V677	T557	H558	H498
LEU	LEU	T1039	L918	N978	T858	T858	Y798	R678	K679	A618	R559	Q499
PRO	PRO	V1040	V919	V979	L859	L859	N799	K679	I680	M619	T560	Y501
G1261	G1261	V1041	N920	P980	K860	K860	P900	I740	L681	I620	M561	M502
Y1263	Y1263	R1042	G921	S981	G921	D861	V801	I742	G822	G622	V562	
S1264	S1264		F922	N982	F922	L862	L302					
R1267	R1267											
Q1268	Q1268											
F1269	F1269											



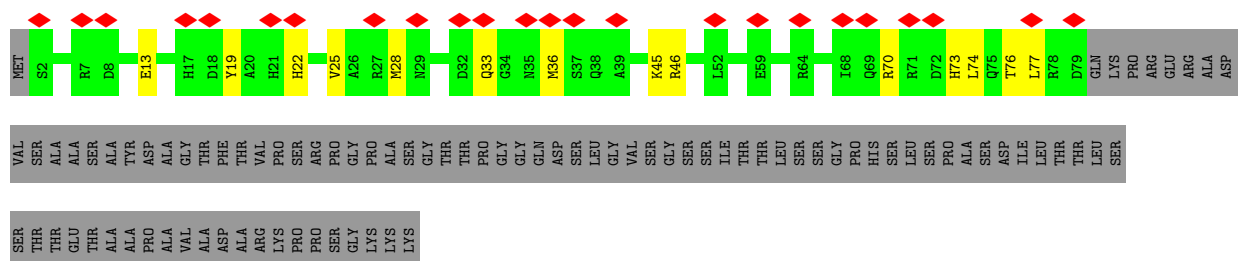
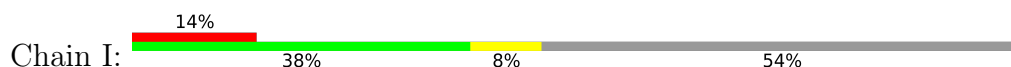
• Molecule 2: Small capsomere-interacting protein



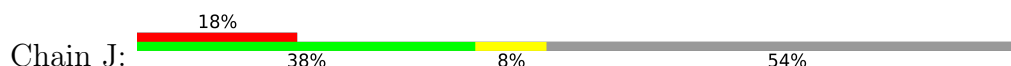
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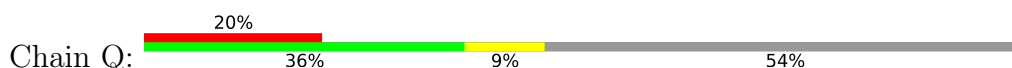


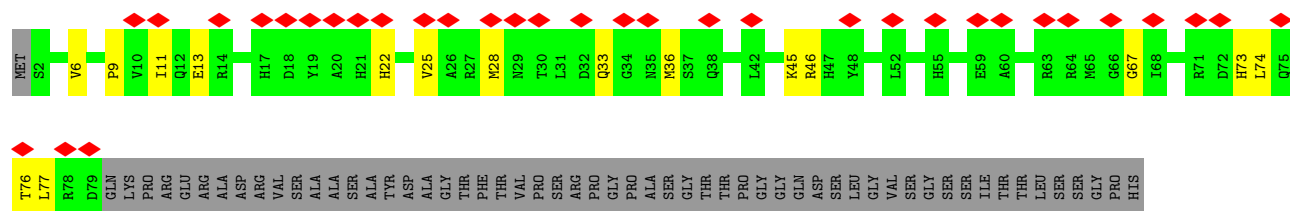
• Molecule 2: Small capsomere-interacting protein



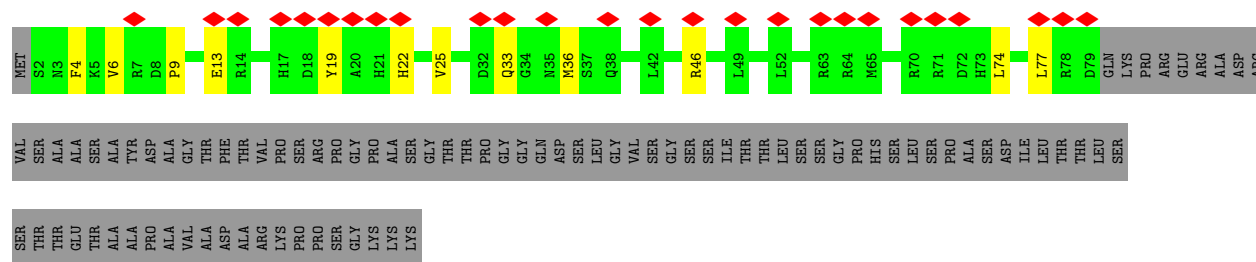
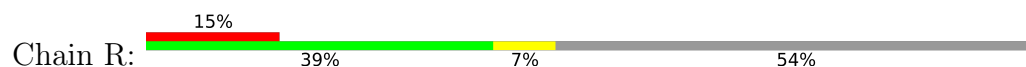
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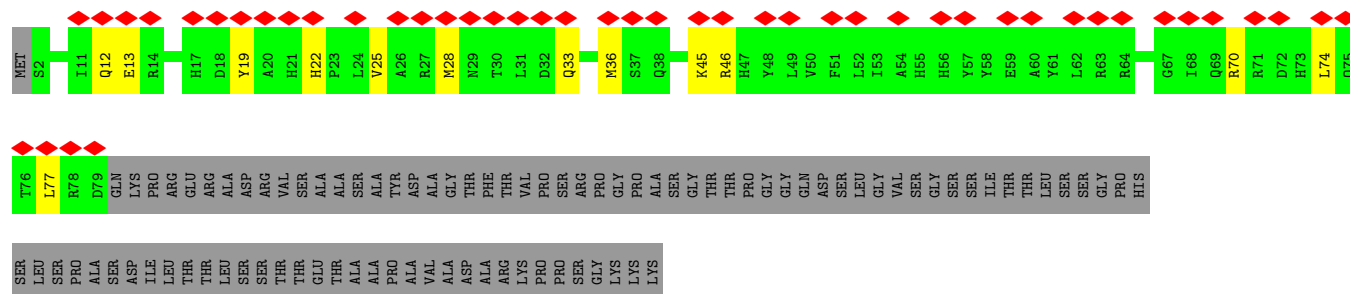
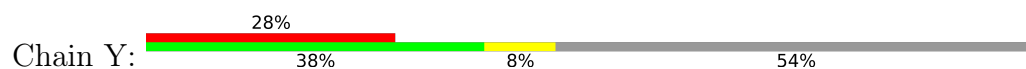




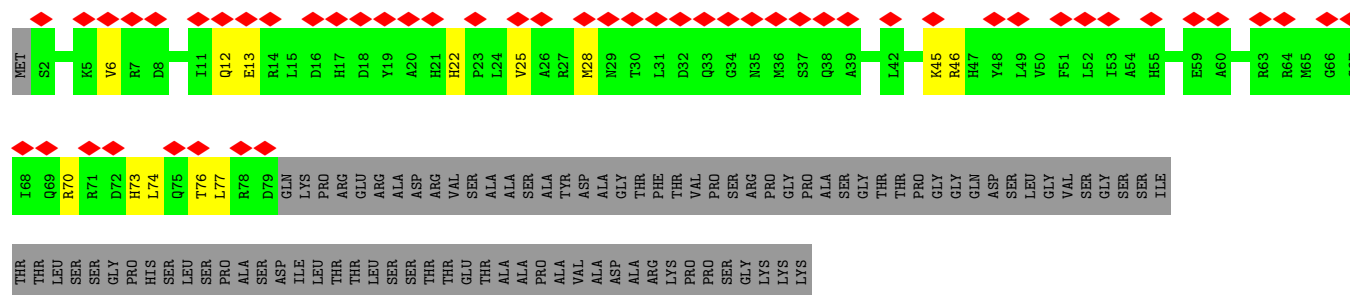
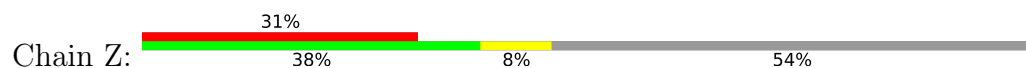
- Molecule 2: Small capsomere-interacting protein



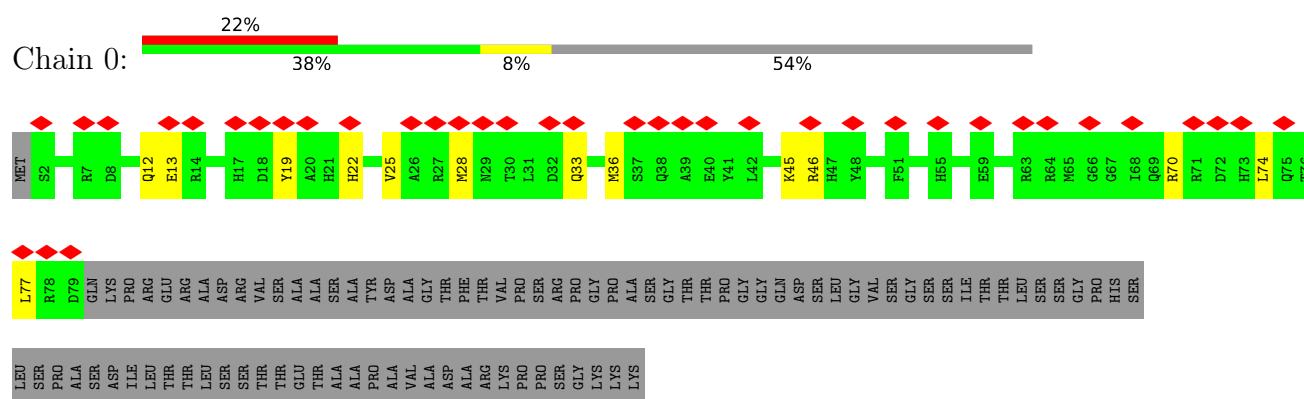
- Molecule 2: Small capsomere-interacting protein



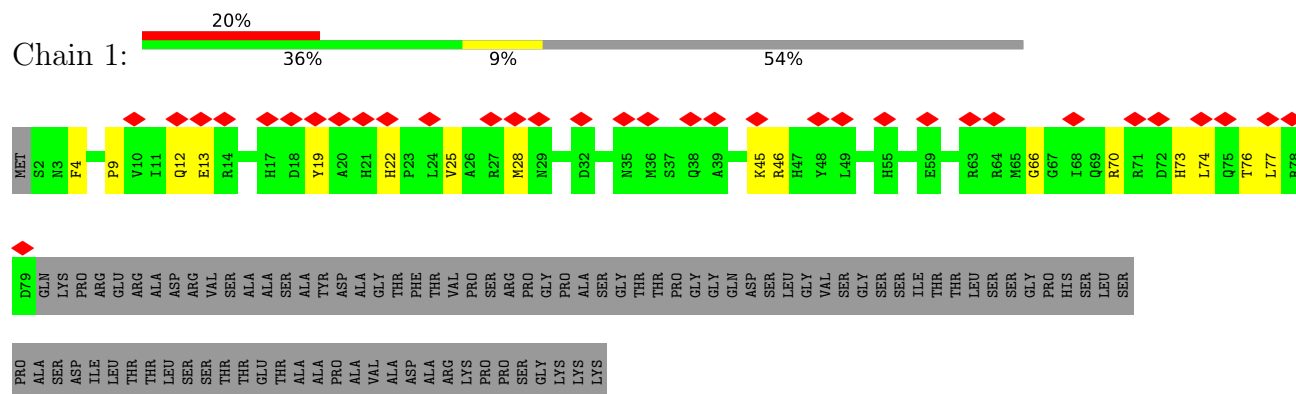
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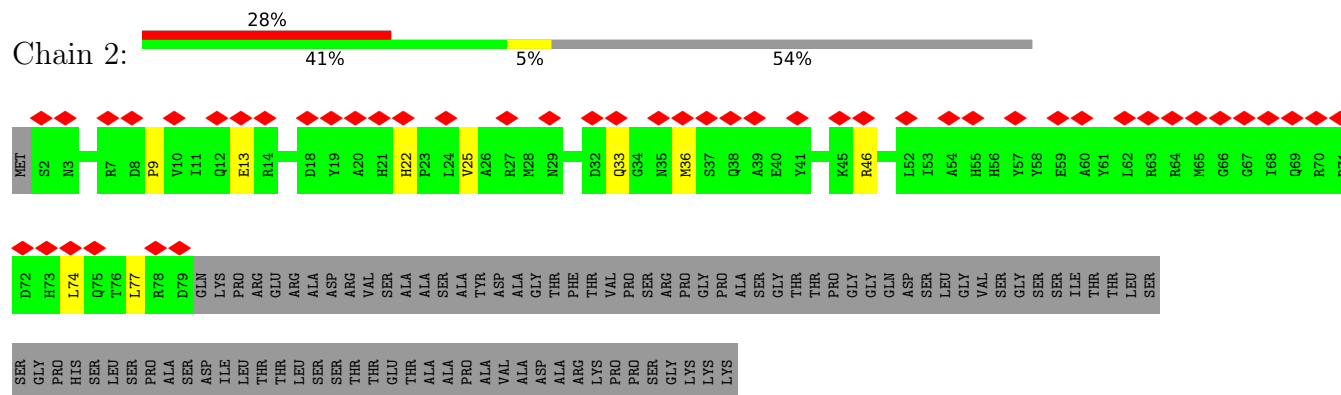
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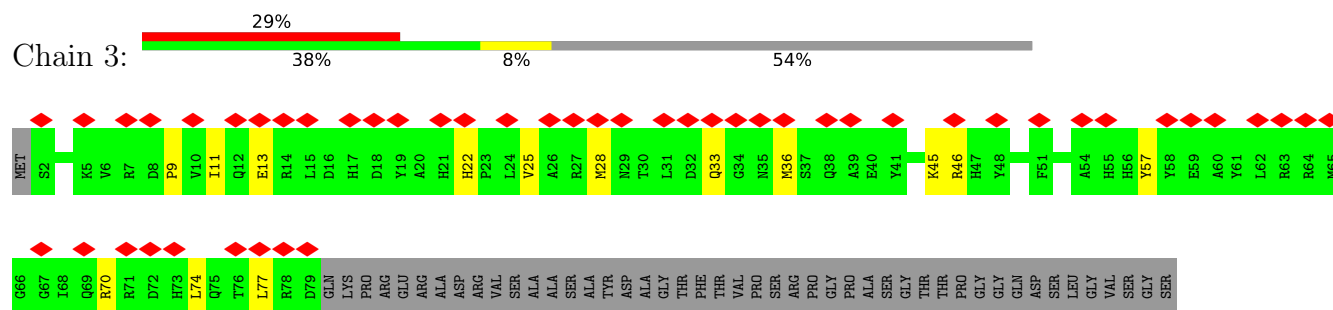
- Molecule 2: Small capsomere-interacting protein



- Molecule 2: Small capsomere-interacting protein



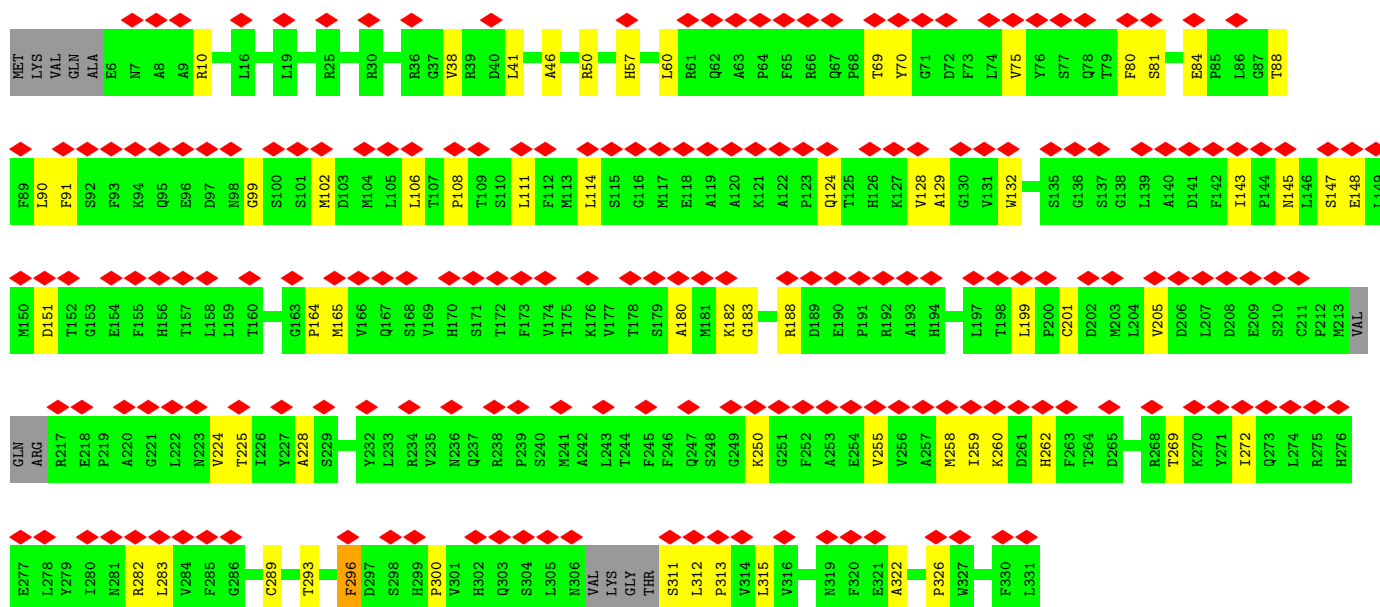
- Molecule 2: Small capsomere-interacting protein



SER ILE THR THR LEU SER SER GLY HIS SER LEU SER PRO ALA ALA SER ASP SER LEU THR THR SER SER THR THR THR GLU THR ALA ALA ALA PRO ALA VAL ASP ALA ARG LYS PRO PRO SER GLY LYS LYS

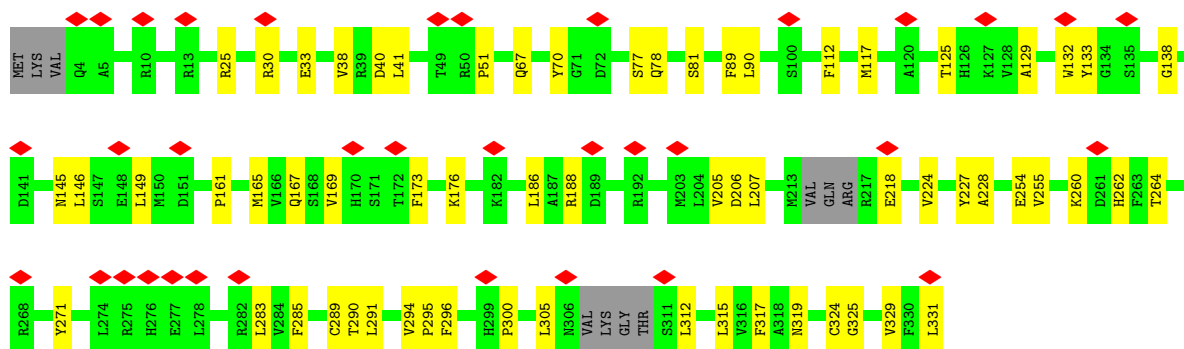
• Molecule 3: Triplex capsid protein 1

Chain 5: 



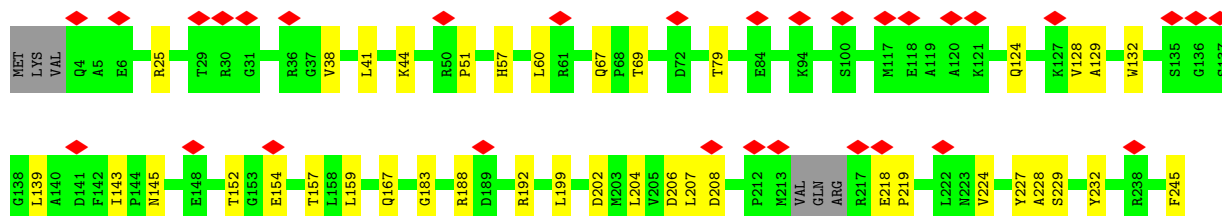
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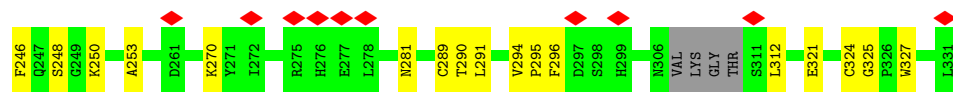
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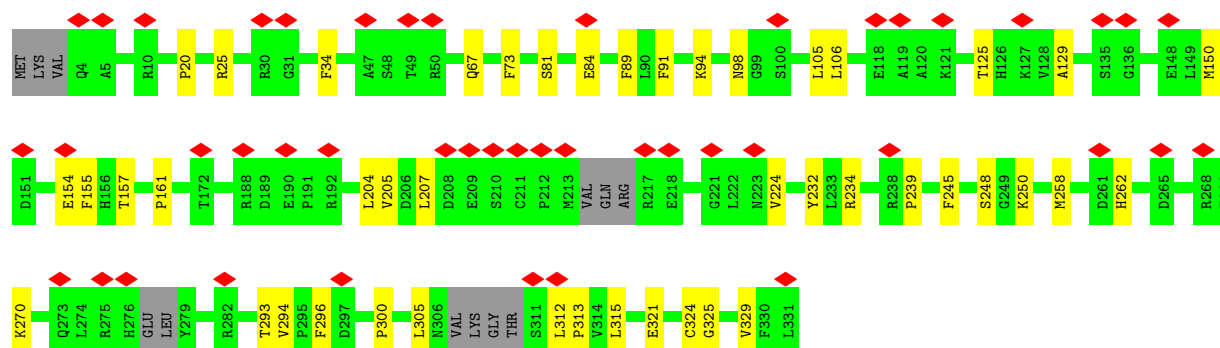
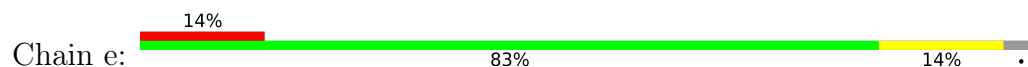
• Molecule 3: Triplex capsid protein 1

Chain b: 

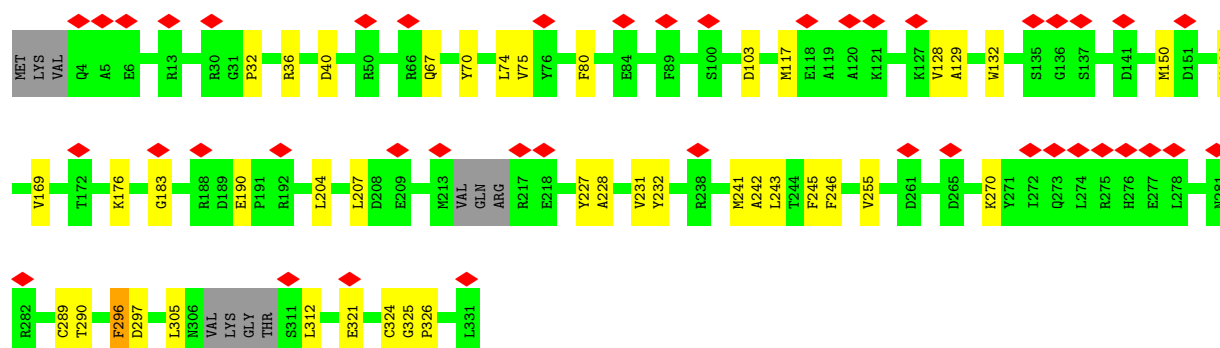
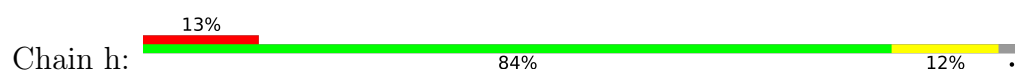




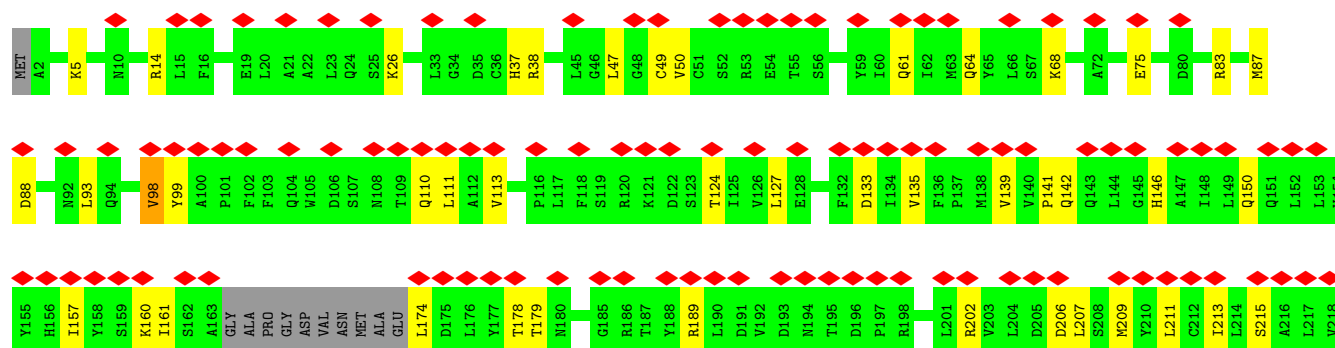
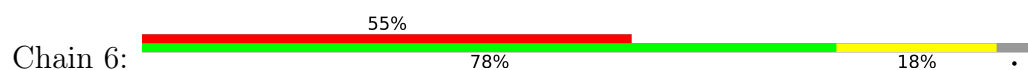
• Molecule 3: Triplex capsid protein 1



• Molecule 3: Triplex capsid protein 1

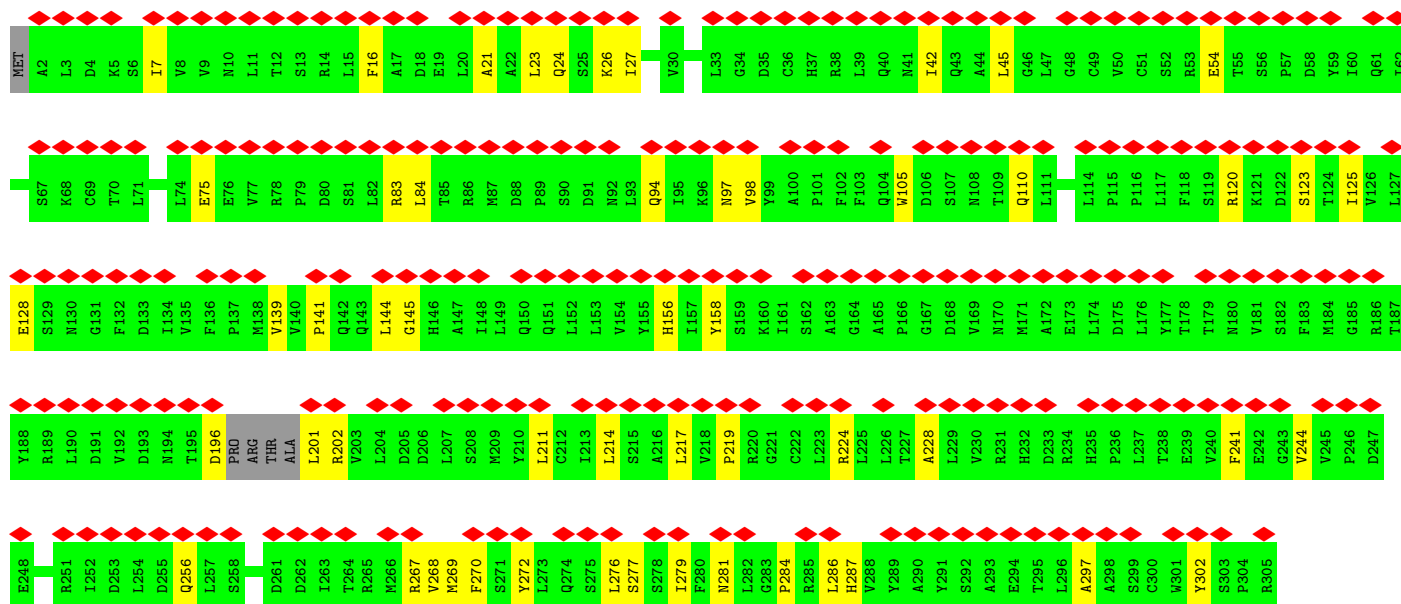
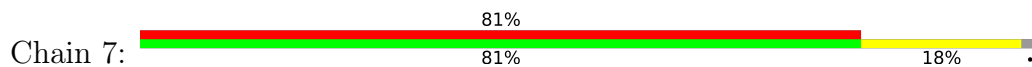


• Molecule 4: Triplex capsid protein 2

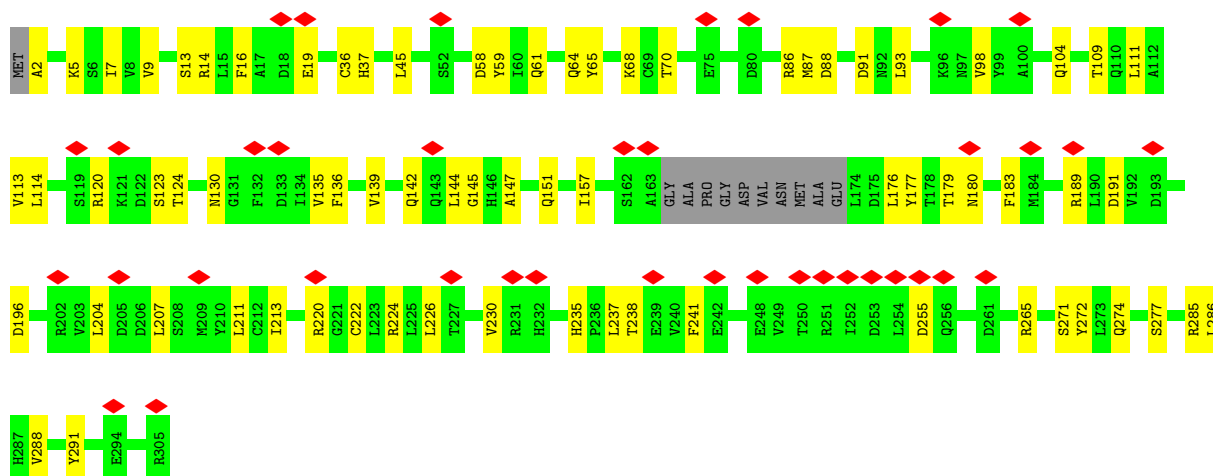




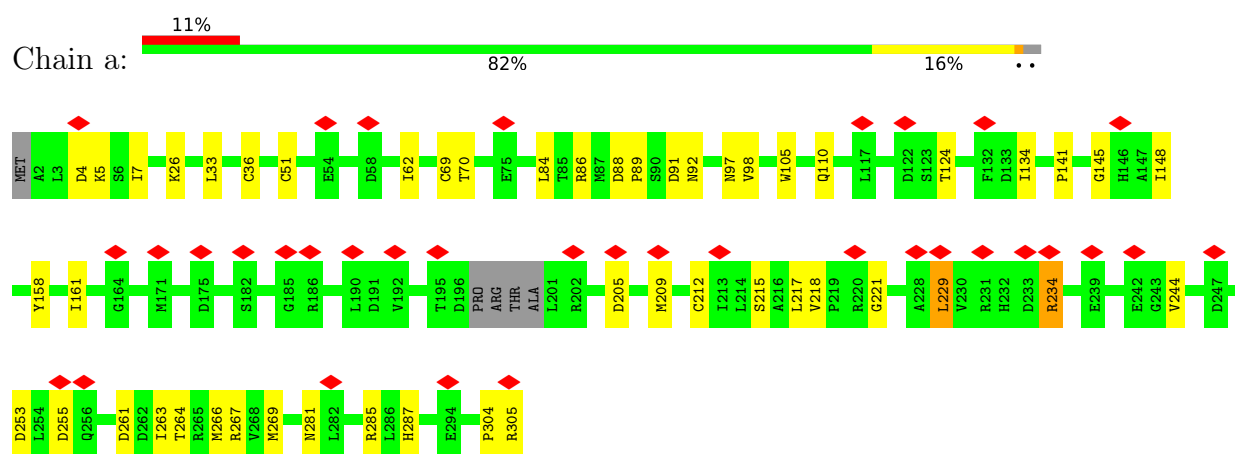
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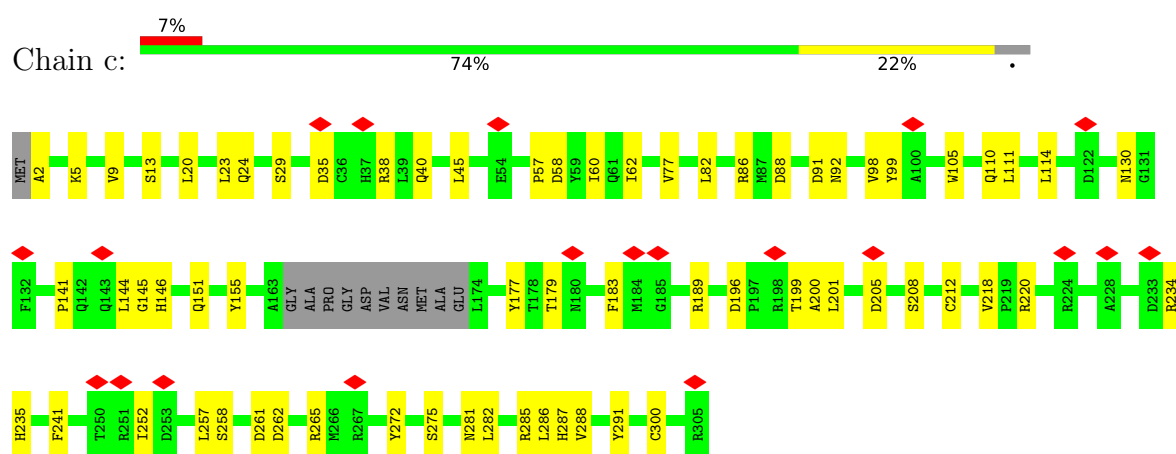
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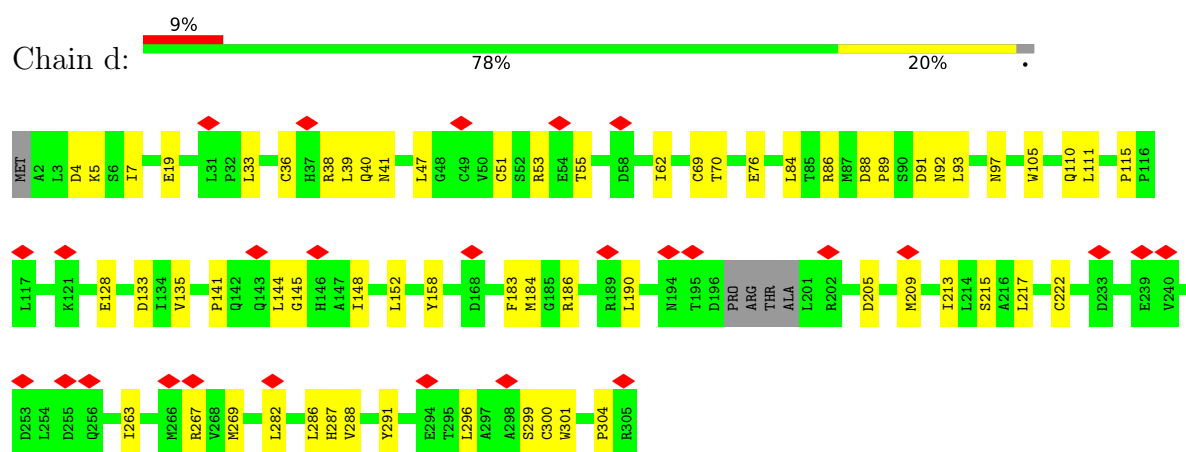
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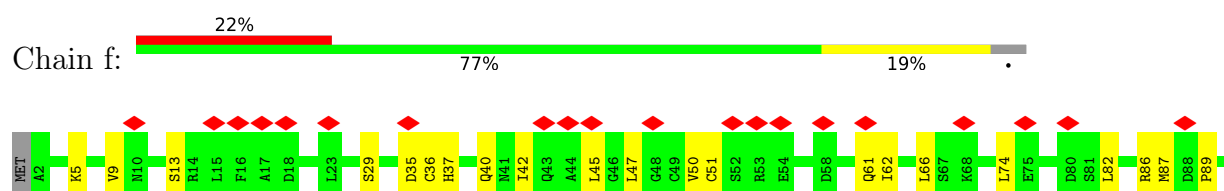
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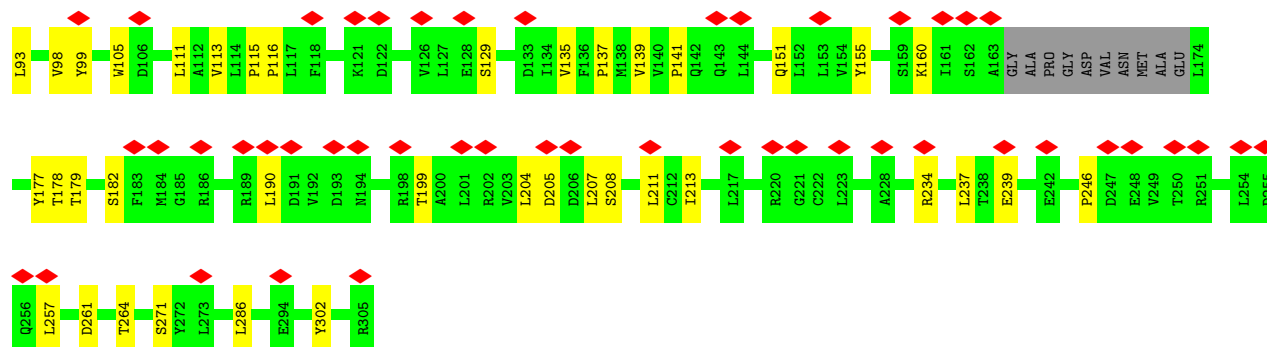


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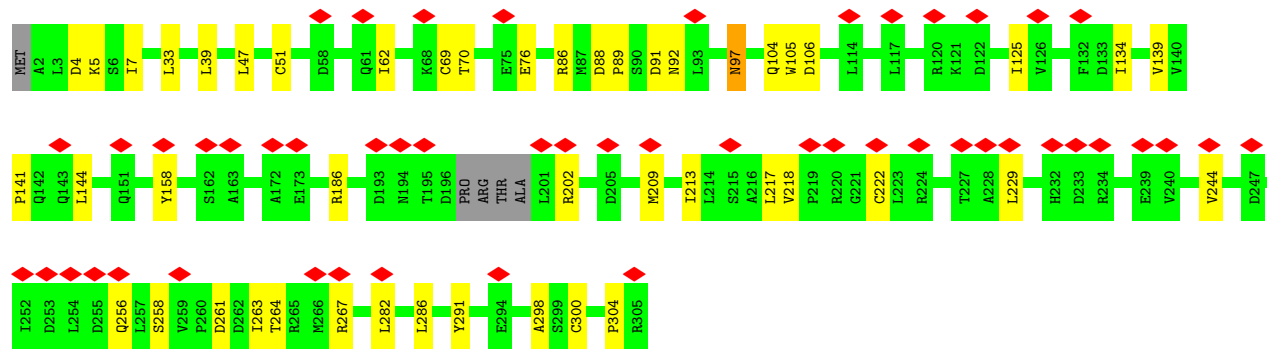
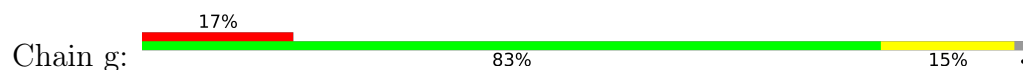


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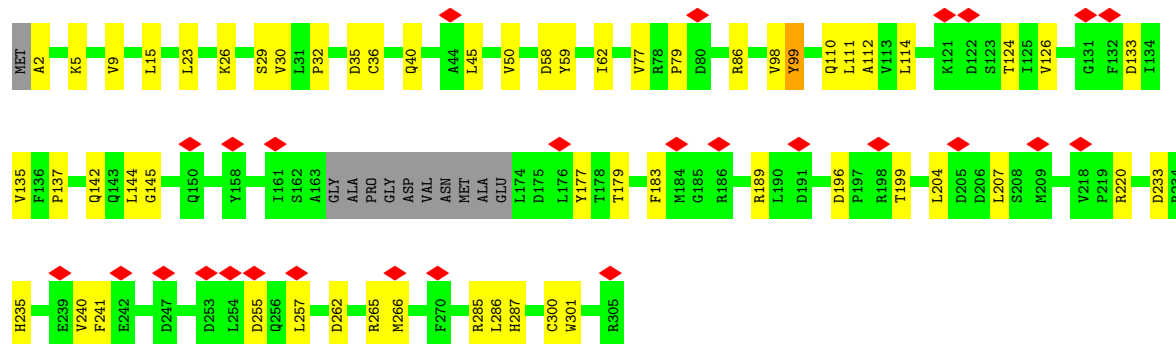
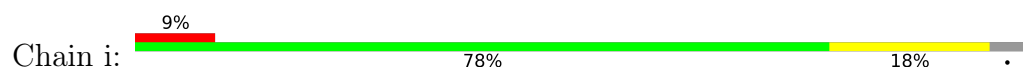




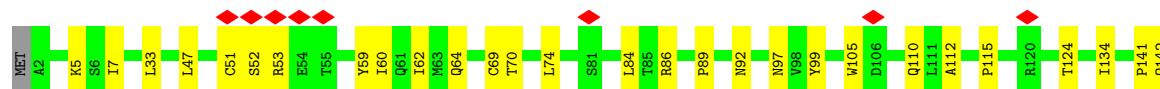
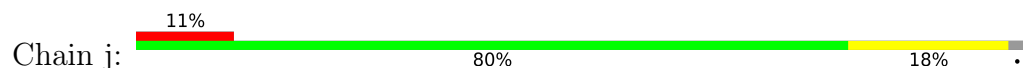
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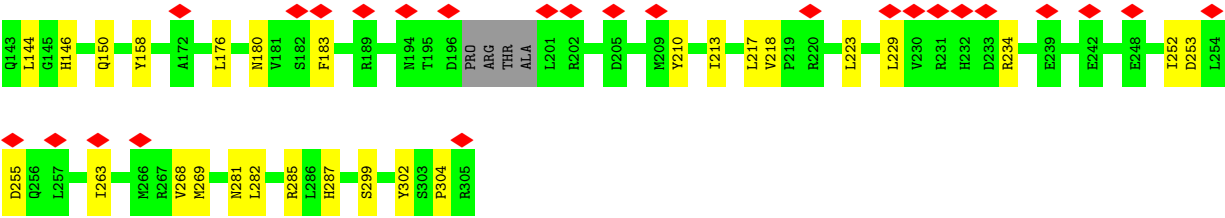


• Molecule 4: Triplex capsid protein 2



• Molecule 4: Triplex capsid protein 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	25315	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 ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	24271	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	15.720	Depositor
Minimum map value	-11.596	Depositor
Average map value	0.008	Depositor
Map value standard deviation	1.070	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	1318.3999, 1318.3999, 1318.3999	wwPDB
Map dimensions	1280, 1280, 1280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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	4	0.26	0/9812	0.61	4/13326 (0.0%)
1	A	0.36	0/10936	0.63	1/14866 (0.0%)
1	B	0.37	0/10879	0.67	10/14788 (0.1%)
1	C	0.35	0/10873	0.63	6/14780 (0.0%)
1	D	0.36	0/10879	0.66	2/14788 (0.0%)
1	E	0.37	0/10936	0.64	2/14866 (0.0%)
1	F	0.37	0/10890	0.65	7/14802 (0.0%)
1	M	0.38	0/10879	0.66	6/14788 (0.0%)
1	N	0.37	0/10936	0.66	10/14866 (0.1%)
1	O	0.37	0/10879	0.65	2/14788 (0.0%)
1	S	0.33	0/10298	0.64	3/13995 (0.0%)
1	T	0.35	0/10918	0.65	4/14839 (0.0%)
1	U	0.36	0/10879	0.65	4/14788 (0.0%)
1	V	0.36	0/10856	0.65	3/14757 (0.0%)
1	W	0.37	1/10873 (0.0%)	0.63	0/14780
1	X	0.33	0/10797	0.62	4/14676 (0.0%)
2	0	0.38	0/682	0.47	0/919
2	1	0.38	0/682	0.47	0/919
2	2	0.37	0/682	0.47	0/919
2	3	0.38	0/682	0.48	0/919
2	G	0.38	0/682	0.47	0/919
2	H	0.38	0/682	0.48	0/919
2	I	0.37	0/682	0.47	0/919
2	J	0.37	0/682	0.47	0/919
2	K	0.38	0/682	0.47	0/919
2	L	0.37	0/682	0.47	0/919
2	P	0.37	0/682	0.47	0/919
2	Q	0.37	0/682	0.47	0/919
2	R	0.37	0/682	0.47	0/919
2	Y	0.38	0/682	0.48	0/919
2	Z	0.37	0/682	0.48	0/919
3	5	0.26	0/2525	0.58	2/3433 (0.1%)
3	8	0.35	0/2539	0.58	2/3452 (0.1%)
3	b	0.35	0/2539	0.58	2/3452 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	e	0.33	0/2521	0.56	2/3426 (0.1%)
3	h	0.34	0/2539	0.57	2/3452 (0.1%)
4	6	0.28	0/2375	0.60	0/3234
4	7	0.26	0/2410	0.58	1/3281 (0.0%)
4	9	0.36	0/2375	0.63	0/3234
4	a	0.41	2/2410 (0.1%)	0.61	0/3281
4	c	0.38	0/2375	0.62	0/3234
4	d	0.38	0/2410	0.62	0/3281
4	f	0.32	0/2375	0.59	0/3234
4	g	0.36	0/2410	0.60	0/3281
4	i	0.37	0/2375	0.60	0/3234
4	j	0.38	0/2410	0.63	0/3281
All	All	0.36	3/219338 (0.0%)	0.63	79/298068 (0.0%)

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
1	4	0	9
1	A	0	4
1	B	0	7
1	C	0	8
1	D	0	10
1	E	0	5
1	F	0	4
1	M	0	6
1	N	0	7
1	O	0	6
1	S	0	6
1	T	0	11
1	U	0	4
1	V	0	6
1	W	0	2
1	X	0	1
3	h	0	1
4	6	0	1
4	7	0	1
4	9	0	2
4	a	0	1
4	c	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
4	d	0	1
4	f	0	2
4	g	0	2
4	i	0	1
4	j	0	2
All	All	0	111

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	a	234	ARG	CZ-NH2	-6.90	1.24	1.33
1	W	967	ARG	CD-NE	-6.15	1.37	1.46
4	a	234	ARG	CD-NE	5.45	1.53	1.46

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1181	PRO	CA-C-N	9.55	148.86	120.69
1	B	1181	PRO	C-N-CA	9.55	148.86	120.69
1	F	1113	VAL	N-CA-C	-8.53	105.01	113.20
1	T	308	VAL	N-CA-C	-7.42	105.31	111.91
1	N	417	VAL	N-CA-C	-7.03	105.20	113.42
1	C	1309	VAL	N-CA-C	-6.83	107.22	113.71
3	5	296	PHE	CA-C-N	6.67	134.29	121.54
3	5	296	PHE	C-N-CA	6.67	134.29	121.54
1	B	308	VAL	N-CA-C	-6.67	105.97	111.91
1	F	1113	VAL	CB-CA-C	6.58	117.22	110.70
1	V	842	ASP	CA-C-N	6.43	133.54	121.97
1	V	842	ASP	C-N-CA	6.43	133.54	121.97
1	U	591	VAL	N-CA-C	-6.19	106.77	112.96
1	C	842	ASP	CA-C-N	6.06	132.87	121.97
1	C	842	ASP	C-N-CA	6.06	132.87	121.97
1	S	591	VAL	N-CA-C	-6.03	106.36	113.42
1	E	842	ASP	CA-C-N	5.85	132.50	121.97
1	E	842	ASP	C-N-CA	5.85	132.50	121.97
1	X	842	ASP	CA-C-N	5.84	132.49	121.97
1	X	842	ASP	C-N-CA	5.84	132.49	121.97
1	F	842	ASP	CA-C-N	5.82	132.44	121.97
1	F	842	ASP	C-N-CA	5.82	132.44	121.97
3	h	296	PHE	CA-C-N	5.80	132.62	121.54
3	h	296	PHE	C-N-CA	5.80	132.62	121.54
1	S	842	ASP	CA-C-N	5.79	132.39	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	842	ASP	C-N-CA	5.79	132.39	121.97
1	T	902	GLN	CA-CB-CG	5.79	125.67	114.10
1	U	842	ASP	CA-C-N	5.76	132.33	121.97
1	U	842	ASP	C-N-CA	5.76	132.33	121.97
1	B	842	ASP	CA-C-N	5.75	132.32	121.97
1	B	842	ASP	C-N-CA	5.75	132.32	121.97
1	B	944	PHE	CA-C-N	5.61	132.26	121.54
1	B	944	PHE	C-N-CA	5.61	132.26	121.54
1	C	1251	ASN	N-CA-C	5.56	122.64	110.80
1	D	842	ASP	CA-C-N	5.54	131.94	121.97
1	D	842	ASP	C-N-CA	5.54	131.94	121.97
1	M	842	ASP	CA-C-N	5.50	131.87	121.97
1	M	842	ASP	C-N-CA	5.50	131.87	121.97
1	4	848	ASP	CA-C-N	5.48	132.00	121.54
1	4	848	ASP	C-N-CA	5.48	132.00	121.54
1	C	875	ILE	N-CA-C	-5.47	107.49	112.96
1	U	875	ILE	N-CA-C	-5.47	108.17	113.53
1	T	842	ASP	CA-C-N	5.44	131.77	121.97
1	T	842	ASP	C-N-CA	5.44	131.77	121.97
3	8	296	PHE	CA-C-N	5.43	131.91	121.54
3	8	296	PHE	C-N-CA	5.43	131.91	121.54
3	b	296	PHE	CA-C-N	5.38	130.05	122.46
3	b	296	PHE	C-N-CA	5.38	130.05	122.46
1	N	504	LYS	CA-C-N	5.34	135.56	123.16
1	N	504	LYS	C-N-CA	5.34	135.56	123.16
1	N	453	ILE	N-CA-C	-5.34	105.54	113.39
1	4	103	GLY	CA-C-N	5.33	131.72	121.54
1	4	103	GLY	C-N-CA	5.33	131.72	121.54
3	e	296	PHE	CA-C-N	5.30	131.67	121.54
3	e	296	PHE	C-N-CA	5.30	131.67	121.54
1	O	842	ASP	CA-C-N	5.26	131.44	121.97
1	O	842	ASP	C-N-CA	5.26	131.44	121.97
1	V	1251	ASN	N-CA-C	5.23	121.95	110.80
1	X	5	LEU	CA-CB-CG	5.22	134.58	116.30
1	A	902	GLN	CA-CB-CG	5.21	124.53	114.10
1	B	415	THR	N-CA-C	-5.21	107.95	114.56
1	N	421	GLY	CA-C-N	5.18	131.29	121.97
1	N	421	GLY	C-N-CA	5.18	131.29	121.97
1	N	351	ALA	CA-C-N	5.17	131.41	121.54
1	N	351	ALA	C-N-CA	5.17	131.41	121.54
1	N	842	ASP	CA-C-N	5.17	131.27	121.97
1	N	842	ASP	C-N-CA	5.17	131.27	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	55	GLY	N-CA-C	5.15	121.89	110.66
1	B	835	TYR	CA-C-N	5.15	128.98	121.31
1	B	835	TYR	C-N-CA	5.15	128.98	121.31
1	M	351	ALA	CA-C-N	5.12	131.32	121.54
1	M	351	ALA	C-N-CA	5.12	131.32	121.54
1	M	1109	THR	CA-C-N	5.12	131.31	121.54
1	M	1109	THR	C-N-CA	5.12	131.31	121.54
1	X	567	GLN	N-CA-C	5.11	121.11	109.81
1	C	1238	TRP	CA-CB-CG	-5.08	103.95	113.60
4	7	27	ILE	N-CA-C	-5.06	108.91	113.71
1	F	504	LYS	CA-C-N	5.04	129.68	122.23
1	F	504	LYS	C-N-CA	5.04	129.68	122.23

There are no chirality outliers.

All (111) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	4	1016	HIS	Peptide
1	4	1084	HIS	Peptide
1	4	1334	HIS	Peptide
1	4	735	SER	Peptide
1	4	842	ASP	Peptide
1	4	844	VAL	Peptide
1	4	848	ASP	Peptide
1	4	850	ILE	Peptide
1	4	899	ASP	Peptide
4	6	98	VAL	Peptide
4	7	284	PRO	Peptide
4	9	37	HIS	Peptide
4	9	98	VAL	Peptide
1	A	1109	THR	Peptide
1	A	255	ASP	Peptide
1	A	537	HIS	Peptide
1	A	899	ASP	Peptide
1	B	1315	PHE	Peptide
1	B	422	VAL	Peptide
1	B	651	VAL	Peptide
1	B	849	ASP	Peptide
1	B	899	ASP	Peptide
1	B	913	VAL	Peptide
1	B	946	LYS	Peptide
1	C	1017	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	C	1250	TYR	Peptide
1	C	1255	ARG	Peptide
1	C	292	GLN	Peptide
1	C	537	HIS	Peptide
1	C	900	PRO	Peptide
1	C	944	PHE	Peptide
1	C	963	ASN	Peptide
1	D	138	LEU	Peptide
1	D	144	GLU	Peptide
1	D	292	GLN	Peptide
1	D	457	ARG	Peptide
1	D	459	HIS	Peptide
1	D	596	THR	Peptide
1	D	798	TYR	Peptide
1	D	842	ASP	Peptide
1	D	849	ASP	Peptide
1	D	915	GLN	Peptide
1	E	1017	GLN	Peptide
1	E	292	GLN	Peptide
1	E	320	GLY	Peptide
1	E	651	VAL	Peptide
1	E	944	PHE	Peptide
1	F	1017	GLN	Peptide
1	F	1316	LEU	Peptide
1	F	938	MET	Peptide
1	F	944	PHE	Peptide
1	M	1312	THR	Peptide
1	M	255	ASP	Peptide
1	M	351	ALA	Peptide
1	M	387	GLN	Peptide
1	M	798	TYR	Peptide
1	M	899	ASP	Peptide
1	N	1113	VAL	Peptide
1	N	842	ASP	Peptide
1	N	849	ASP	Peptide
1	N	886	PRO	Peptide
1	N	918	LEU	Peptide
1	N	929	ASP	Peptide
1	N	944	PHE	Peptide
1	O	1042	ARG	Peptide
1	O	1252	ILE	Peptide
1	O	293	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	O	536	VAL	Peptide
1	O	537	HIS	Peptide
1	O	842	ASP	Peptide
1	S	292	GLN	Peptide
1	S	537	HIS	Peptide
1	S	606	ASP	Peptide
1	S	844	VAL	Peptide
1	S	850	ILE	Peptide
1	S	944	PHE	Peptide
1	T	10	PHE	Peptide
1	T	106	ARG	Peptide
1	T	1112	GLY	Peptide
1	T	1181	PRO	Peptide
1	T	292	GLN	Peptide
1	T	422	VAL	Peptide
1	T	537	HIS	Peptide
1	T	842	ASP	Peptide
1	T	849	ASP	Peptide
1	T	899	ASP	Peptide
1	T	944	PHE	Peptide
1	U	292	GLN	Peptide
1	U	537	HIS	Peptide
1	U	59	ASN	Peptide
1	U	651	VAL	Peptide
1	V	1250	TYR	Peptide
1	V	142	GLU	Peptide
1	V	606	ASP	Peptide
1	V	797	ASP	Peptide
1	V	849	ASP	Peptide
1	V	899	ASP	Peptide
1	W	848	ASP	Peptide
1	W	849	ASP	Peptide
1	X	537	HIS	Peptide
4	a	229	LEU	Peptide
4	c	98	VAL	Peptide
4	d	300	CYS	Peptide
4	f	182	SER	Peptide
4	f	98	VAL	Peptide
4	g	282	LEU	Peptide
4	g	97	ASN	Peptide
3	h	296	PHE	Peptide
4	i	99	TYR	Peptide

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Mol	Chain	Res	Type	Group
4	j	281	ASN	Peptide
4	j	59	TYR	Peptide

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	4	9586	0	9478	160	0
1	A	10682	0	10559	167	0
1	B	10627	0	10504	164	0
1	C	10621	0	10498	195	0
1	D	10627	0	10503	194	0
1	E	10682	0	10558	187	0
1	F	10638	0	10517	180	0
1	M	10627	0	10503	185	0
1	N	10682	0	10558	182	0
1	O	10627	0	10505	178	0
1	S	10060	0	9942	176	0
1	T	10666	0	10542	159	0
1	U	10627	0	10504	211	0
1	V	10604	0	10486	177	0
1	W	10621	0	10499	198	0
1	X	10548	0	10422	186	0
2	0	666	0	647	9	0
2	1	666	0	647	11	0
2	2	666	0	647	5	0
2	3	666	0	647	10	0
2	G	666	0	647	10	0
2	H	666	0	647	9	0
2	I	666	0	647	8	0
2	J	666	0	647	8	0
2	K	666	0	647	8	0
2	L	666	0	647	8	0
2	P	666	0	647	8	0
2	Q	666	0	647	11	0
2	R	666	0	647	8	0
2	Y	666	0	647	8	0
2	Z	666	0	647	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	5	2463	0	2453	38	0
3	8	2477	0	2466	39	0
3	b	2477	0	2465	35	0
3	e	2460	0	2448	29	0
3	h	2477	0	2466	26	0
4	6	2329	0	2354	42	0
4	7	2364	0	2379	36	0
4	9	2329	0	2354	46	0
4	a	2364	0	2379	36	0
4	c	2329	0	2354	47	0
4	d	2364	0	2379	50	0
4	f	2329	0	2354	42	0
4	g	2364	0	2379	34	0
4	i	2329	0	2354	35	0
4	j	2364	0	2379	40	0
All	All	214334	0	212246	3214	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (3214) 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)
1:C:736:ARG:HH22	1:C:899:ASP:HA	1.49	0.77
1:F:172:ARG:HH12	1:F:386:THR:HG21	1.49	0.77
1:X:558:HIS:HB3	1:X:898:ARG:HH12	1.50	0.76
1:4:457:ARG:HH12	1:4:463:GLN:HB3	1.50	0.75
1:W:865:ALA:HA	1:W:930:ARG:HH12	1.51	0.75
4:f:177:TYR:HB3	4:g:263:ILE:HG21	1.70	0.74
4:j:62:ILE:HG21	4:j:115:PRO:HB3	1.69	0.74
1:T:855:GLU:HG2	2:Y:70:ARG:HE	1.52	0.73
1:D:387:GLN:HE22	1:M:25:GLU:H	1.35	0.73
1:T:536:VAL:HG13	1:T:1244:SER:HA	1.70	0.73
1:V:1241:GLN:HB3	1:V:1244:SER:HB3	1.71	0.73
1:S:1241:GLN:HB3	1:S:1244:SER:HB3	1.73	0.71
1:E:115:ILE:HB	1:M:36:GLN:HB3	1.73	0.70
1:M:113:GLN:HB3	1:U:38:LEU:HB2	1.72	0.70
1:U:1241:GLN:HB3	1:U:1244:SER:HB3	1.72	0.70
1:C:799:ASN:HD21	1:C:802:LEU:HG	1.55	0.70
1:M:575:GLN:NE2	1:M:1015:MET:SD	2.61	0.70
1:U:389:PRO:HB3	1:V:203:ARG:HH12	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:443:CYS:SG	1:V:447:GLN:NE2	2.65	0.70
1:D:1199:GLY:HA3	1:D:1235:ASN:H	1.56	0.70
1:M:1241:GLN:HB3	1:M:1244:SER:HB3	1.73	0.69
1:C:1241:GLN:HB3	1:C:1244:SER:HB3	1.74	0.69
1:M:736:ARG:HH12	1:M:899:ASP:HA	1.57	0.69
1:D:829:VAL:HA	1:D:938:MET:HE1	1.74	0.69
1:T:1183:PRO:HG2	1:T:1186:SER:HB3	1.74	0.69
1:S:575:GLN:NE2	1:S:1015:MET:SD	2.60	0.69
1:B:602:GLU:HB3	1:B:647:LYS:HE2	1.75	0.69
1:N:591:VAL:HB	1:N:683:GLU:HB2	1.75	0.68
1:S:203:ARG:HH21	1:X:395:ARG:HH22	1.41	0.68
4:9:36:CYS:SG	4:9:86:ARG:NH2	2.67	0.68
4:9:111:LEU:HB2	4:9:286:LEU:HB2	1.75	0.68
1:N:575:GLN:NE2	1:N:1015:MET:SD	2.67	0.68
1:V:91:ILE:HD12	1:V:1089:LEU:HD22	1.74	0.68
3:5:90:LEU:HD11	3:5:165:MET:HG3	1.76	0.68
4:7:286:LEU:HB3	4:7:302:TYR:HD1	1.59	0.68
1:O:963:ASN:O	1:O:967:ARG:N	2.27	0.68
1:D:120:CYS:O	4:9:14:ARG:NH2	2.27	0.68
1:T:575:GLN:NE2	1:T:1015:MET:SD	2.68	0.67
3:h:232:TYR:O	3:h:270:LYS:NZ	2.28	0.67
1:U:514:GLN:HG3	1:U:531:LEU:HD21	1.76	0.67
1:B:157:LYS:HD2	1:C:338:ASN:HA	1.76	0.67
1:C:736:ARG:NH2	1:C:899:ASP:OD1	2.27	0.67
1:D:663:HIS:HA	1:E:930:ARG:HD2	1.77	0.67
1:U:1127:TYR:O	4:c:234:ARG:NH2	2.27	0.67
1:U:736:ARG:HD2	1:U:897:LYS:H	1.59	0.67
1:U:450:LEU:HD21	1:U:1025:ILE:HG13	1.76	0.67
4:c:35:ASP:HB2	4:c:40:GLN:HE22	1.60	0.67
1:A:617:GLU:HG3	1:A:656:MET:HG3	1.76	0.67
1:B:663:HIS:HA	1:C:930:ARG:HD2	1.76	0.67
1:T:1111:MET:SD	1:T:1366:ARG:NH2	2.68	0.67
1:N:886:PRO:O	1:N:920:ASN:ND2	2.27	0.67
1:U:1295:GLY:H	1:U:1321:HIS:HE1	1.42	0.67
3:h:289:CYS:SG	3:h:290:THR:N	2.67	0.66
1:E:850:ILE:HD12	1:E:875:ILE:HD12	1.78	0.66
1:F:828:ASN:ND2	1:F:937:THR:O	2.28	0.66
1:C:591:VAL:HB	1:C:683:GLU:HB2	1.77	0.66
1:E:399:THR:HG22	1:E:1043:THR:HG22	1.76	0.66
1:V:95:ILE:HB	1:V:114:TYR:HB2	1.76	0.66
1:N:736:ARG:HG3	1:N:737:GLN:HG2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:927:VAL:H	1:M:956:THR:HG21	1.61	0.66
1:W:399:THR:HG22	1:W:1043:THR:HG22	1.78	0.66
1:E:709:VAL:HG22	1:E:1023:SER:HA	1.78	0.66
1:M:1169:LEU:HD11	1:N:208:ALA:HA	1.78	0.66
1:4:1211:SER:HB2	1:4:1214:SER:HB3	1.78	0.66
1:M:777:ARG:NH2	1:M:885:CYS:O	2.28	0.66
1:U:275:VAL:HG22	1:U:375:ALA:HB3	1.77	0.65
1:U:290:LEU:HB3	1:U:367:VAL:HG21	1.79	0.65
1:X:1111:MET:SD	1:X:1366:ARG:NH2	2.67	0.65
4:9:142:GLN:HE22	4:9:285:ARG:HG2	1.61	0.65
1:E:532:LEU:O	1:E:1241:GLN:NE2	2.30	0.65
1:E:856:ASN:HA	1:E:860:LYS:HE3	1.78	0.65
1:E:1170:SER:HA	1:F:211:SER:HB3	1.77	0.65
1:N:1285:LEU:HB3	1:N:1322:MET:HE1	1.76	0.65
1:W:1236:ASN:HB2	1:W:1238:TRP:HE3	1.60	0.65
1:A:290:LEU:HB3	1:A:367:VAL:HG21	1.77	0.65
4:d:89:PRO:HB3	4:d:304:PRO:HG3	1.78	0.65
1:A:558:HIS:HD2	1:A:902:GLN:HE22	1.45	0.65
1:B:1062:PHE:HB2	1:B:1087:ALA:HB3	1.77	0.65
1:C:575:GLN:NE2	1:C:1015:MET:SD	2.70	0.65
1:W:963:ASN:O	1:W:967:ARG:N	2.30	0.65
1:W:965:VAL:O	1:W:972:ARG:NH1	2.29	0.65
1:M:850:ILE:HD12	1:M:875:ILE:HD12	1.78	0.65
1:S:399:THR:HG22	1:S:1043:THR:HG22	1.76	0.65
1:S:828:ASN:ND2	1:S:937:THR:O	2.29	0.65
4:6:220:ARG:HG2	4:6:265:ARG:HH12	1.62	0.65
3:h:204:LEU:HA	3:h:245:PHE:HB2	1.77	0.65
1:V:606:ASP:OD1	1:V:647:LYS:NZ	2.30	0.65
1:4:757:ILE:HG12	1:4:788:LEU:HD22	1.78	0.65
1:B:575:GLN:NE2	1:B:1015:MET:SD	2.70	0.65
1:O:450:LEU:HD21	1:O:1025:ILE:HG13	1.77	0.65
1:U:829:VAL:HA	1:U:938:MET:HE1	1.77	0.65
1:X:1027:GLN:HB3	1:X:1032:MET:HB2	1.78	0.65
1:N:492:ASN:HD22	1:N:495:ARG:HE	1.45	0.65
1:4:275:VAL:HG22	1:4:375:ALA:HB3	1.77	0.65
1:F:575:GLN:NE2	1:F:1015:MET:SD	2.70	0.64
1:E:93:PHE:HB2	1:E:116:VAL:HB	1.78	0.64
1:D:172:ARG:NH1	1:D:382:MET:O	2.30	0.64
1:F:1162:ARG:N	1:F:1306:TYR:HH	1.95	0.64
1:M:93:PHE:HB2	1:M:116:VAL:HB	1.78	0.64
1:4:943:PRO:HB3	1:4:977:PHE:HE2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:855:GLU:HG2	2:3:70:ARG:HE	1.63	0.64
1:A:718:LEU:O	1:A:915:GLN:NE2	2.31	0.64
1:O:93:PHE:HB2	1:O:116:VAL:HB	1.77	0.64
1:X:434:VAL:HG11	1:X:1042:ARG:HH22	1.61	0.64
1:N:1074:ARG:HD2	1:N:1077:ALA:HB3	1.79	0.64
1:N:832:THR:HG22	2:Q:11:ILE:HD11	1.80	0.64
1:U:54:LEU:HB2	1:V:91:ILE:HG12	1.79	0.64
1:A:701:GLY:HA3	1:A:1131:GLN:HE21	1.62	0.64
1:C:893:ARG:NH1	1:C:984:MET:SD	2.71	0.64
1:S:930:ARG:HD2	1:X:663:HIS:HA	1.80	0.64
1:4:182:LYS:NZ	1:4:1058:SER:OG	2.30	0.64
1:4:477:GLY:HA2	1:4:546:PRO:HG3	1.80	0.64
4:a:69:CYS:SG	4:a:70:THR:N	2.71	0.64
1:W:193:LYS:NZ	1:W:247:ASP:OD2	2.30	0.64
1:F:760:ARG:HH22	1:F:886:PRO:HA	1.60	0.64
1:A:777:ARG:NH2	1:A:885:CYS:O	2.31	0.63
1:O:1196:ASN:HD21	1:O:1324:GLN:HG3	1.63	0.63
1:U:701:GLY:HA3	1:U:1131:GLN:HE21	1.63	0.63
1:U:736:ARG:NH2	1:U:899:ASP:OD1	2.30	0.63
1:V:1111:MET:SD	1:V:1366:ARG:NH2	2.70	0.63
4:9:5:LYS:HB3	4:9:86:ARG:HB3	1.81	0.63
1:4:828:ASN:ND2	1:4:938:MET:SD	2.71	0.63
4:c:177:TYR:HB3	4:d:263:ILE:HG21	1.80	0.63
1:A:153:ALA:HB1	1:B:338:ASN:HB3	1.79	0.63
1:V:271:GLN:OE1	1:V:1056:ARG:NH1	2.31	0.63
1:A:514:GLN:HG3	1:A:531:LEU:HD21	1.80	0.63
1:W:92:GLN:HE22	1:W:115:ILE:HG23	1.63	0.63
1:4:743:GLY:HA3	1:4:786:HIS:HE1	1.63	0.63
1:A:1111:MET:SD	1:A:1366:ARG:NH2	2.68	0.63
1:B:1342:MET:HE1	1:B:1370:LEU:H	1.64	0.63
1:C:1312:THR:HG21	1:D:105:GLY:H	1.64	0.63
1:F:394:ARG:HD3	1:F:1315:PHE:HB3	1.79	0.63
4:7:26:LYS:HE2	4:7:98:VAL:HB	1.81	0.63
1:A:575:GLN:NE2	1:A:1015:MET:SD	2.71	0.63
1:C:855:GLU:HG2	2:H:70:ARG:HE	1.63	0.63
1:F:898:ARG:HD3	1:F:902:GLN:HG3	1.81	0.63
1:M:115:ILE:HB	1:U:36:GLN:HB3	1.81	0.63
4:i:111:LEU:HB2	4:i:286:LEU:HB2	1.79	0.63
1:D:157:LYS:HD2	1:E:338:ASN:HA	1.81	0.63
1:A:1241:GLN:HB3	1:A:1244:SER:HB3	1.81	0.63
1:C:813:VAL:HG21	1:C:1012:MET:HG3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1167:PRO:HD3	1:D:1224:ILE:HD13	1.80	0.63
1:N:93:PHE:HB2	1:N:116:VAL:HB	1.80	0.63
1:T:153:ALA:HB1	1:U:338:ASN:HB3	1.80	0.63
1:W:1293:LEU:HD21	1:W:1297:PRO:HG3	1.81	0.63
1:X:37:LEU:HB2	1:X:50:PHE:HB2	1.81	0.63
3:5:91:PHE:HB2	3:5:106:LEU:HB2	1.79	0.63
1:B:256:THR:HG22	1:B:258:PHE:H	1.64	0.63
1:E:540:PHE:O	1:E:559:ARG:NH1	2.32	0.63
1:A:1070:ARG:NH1	3:h:67:GLN:OE1	2.32	0.62
1:A:1228:ALA:HA	1:F:1171:HIS:HE1	1.65	0.62
1:E:915:GLN:HG2	1:E:989:GLU:HG3	1.79	0.62
1:X:611:LEU:HD22	1:X:862:ILE:HG12	1.81	0.62
4:c:111:LEU:HB2	4:c:286:LEU:HB2	1.81	0.62
1:M:856:ASN:HA	1:M:860:LYS:HE3	1.80	0.62
1:S:514:GLN:HG3	1:S:531:LEU:HD21	1.80	0.62
1:W:714:ASP:O	1:W:804:LYS:NZ	2.31	0.62
1:W:1005:THR:HG22	1:W:1007:GLY:H	1.64	0.62
1:X:537:HIS:HA	1:X:1238:TRP:HD1	1.63	0.62
1:W:447:GLN:NE2	1:X:521:GLU:OE1	2.32	0.62
1:B:214:VAL:HA	1:B:217:PHE:HD2	1.65	0.62
1:B:893:ARG:NH2	1:B:988:GLU:OE1	2.31	0.62
1:D:1111:MET:SD	1:D:1366:ARG:NH2	2.69	0.62
1:S:415:THR:HG23	1:X:418:SER:HB3	1.81	0.62
4:9:58:ASP:HB3	4:9:196:ASP:HB3	1.81	0.62
1:E:1005:THR:HG22	1:E:1007:GLY:H	1.64	0.62
1:F:799:ASN:HD21	1:F:802:LEU:HG	1.65	0.62
1:M:1069:VAL:HG22	3:b:44:LYS:HG2	1.82	0.62
1:W:325:ASN:ND2	1:W:352:ASP:OD2	2.32	0.62
2:2:13:GLU:OE1	2:2:46:ARG:NH2	2.31	0.62
1:4:935:ALA:HA	1:4:938:MET:HB2	1.81	0.62
2:G:71:ARG:HD2	2:H:18:ASP:HA	1.81	0.62
1:O:829:VAL:HA	1:O:938:MET:HE1	1.81	0.62
1:U:828:ASN:ND2	1:U:937:THR:O	2.33	0.62
1:V:157:LYS:HD2	1:W:338:ASN:HA	1.80	0.62
1:W:663:HIS:HA	1:X:930:ARG:HD2	1.79	0.62
1:X:1005:THR:HG22	1:X:1007:GLY:H	1.64	0.62
1:E:828:ASN:ND2	1:E:937:THR:O	2.30	0.62
1:F:714:ASP:O	1:F:804:LYS:NZ	2.32	0.62
1:4:1267:ARG:NH2	4:7:54:GLU:OE1	2.33	0.62
1:C:709:VAL:HG22	1:C:1023:SER:HA	1.82	0.62
1:N:708:LEU:HD21	1:N:1022:PRO:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:428:GLN:NE2	1:U:577:SER:OG	2.32	0.62
1:V:399:THR:HG22	1:V:1043:THR:HG22	1.81	0.62
3:b:129:ALA:HA	3:b:132:TRP:HD1	1.63	0.62
1:E:19:LEU:HB2	1:T:59:ASN:HD21	1.65	0.62
2:G:13:GLU:OE1	2:G:46:ARG:NH2	2.30	0.62
2:J:13:GLU:OE1	2:J:46:ARG:NH2	2.31	0.62
1:N:442:LEU:HD13	1:N:1113:VAL:HG23	1.82	0.62
1:T:58:THR:HG22	1:U:94:LYS:HB3	1.82	0.62
1:T:946:LYS:NZ	1:T:986:GLU:OE1	2.33	0.62
2:1:13:GLU:OE1	2:1:46:ARG:NH2	2.30	0.62
1:B:275:VAL:HG22	1:B:375:ALA:HB3	1.82	0.62
1:F:760:ARG:HH21	1:F:789:ASP:HB3	1.64	0.62
1:M:275:VAL:HG22	1:M:375:ALA:HB3	1.82	0.62
1:N:399:THR:HG22	1:N:1043:THR:HG22	1.80	0.62
1:O:1295:GLY:H	1:O:1321:HIS:HE1	1.46	0.62
1:V:428:GLN:NE2	1:V:577:SER:OG	2.33	0.62
1:A:271:GLN:OE1	1:A:1056:ARG:NH1	2.33	0.61
1:B:811:MET:HB3	1:B:819:MET:HE1	1.82	0.61
1:S:1163:CYS:SG	1:S:1164:GLU:N	2.72	0.61
1:C:946:LYS:HE2	1:C:993:SER:HA	1.82	0.61
1:N:471:ALA:HA	1:N:1242:ARG:HH12	1.65	0.61
1:B:808:TYR:HB3	1:B:1016:HIS:HE1	1.66	0.61
1:T:275:VAL:HG22	1:T:375:ALA:HB3	1.82	0.61
1:X:271:GLN:OE1	1:X:1056:ARG:NH1	2.33	0.61
1:X:709:VAL:HG22	1:X:1023:SER:HA	1.82	0.61
1:S:144:GLU:OE2	3:5:10:ARG:NH2	2.34	0.61
1:V:1344:ASN:ND2	1:V:1347:THR:OG1	2.28	0.61
1:W:214:VAL:HA	1:W:217:PHE:HD2	1.65	0.61
1:B:1294:ALA:HB1	1:B:1321:HIS:HE1	1.64	0.61
1:N:704:PRO:HG2	1:O:969:PRO:HD2	1.83	0.61
1:U:1236:ASN:HB2	1:U:1238:TRP:HE3	1.65	0.61
1:W:572:ARG:NH2	1:W:1001:SER:O	2.33	0.61
1:B:507:ALA:HB1	1:B:978:ASN:HD22	1.66	0.61
1:B:856:ASN:ND2	2:G:66:GLY:O	2.33	0.61
1:U:95:ILE:HB	1:U:114:TYR:HB2	1.82	0.61
1:U:1005:THR:HG22	1:U:1007:GLY:H	1.65	0.61
1:X:617:GLU:HG3	1:X:656:MET:HG3	1.82	0.61
3:8:329:VAL:HG21	4:9:271:SER:HB2	1.82	0.61
4:f:5:LYS:HB2	4:f:86:ARG:HB3	1.82	0.61
1:D:1005:THR:HG22	1:D:1007:GLY:H	1.65	0.61
1:N:687:LEU:HB3	1:N:805:LEU:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:111:LEU:HA	3:5:114:LEU:HD13	1.82	0.61
3:b:152:THR:HA	3:b:281:ASN:HB3	1.81	0.61
1:N:58:THR:HG22	1:O:94:LYS:HB3	1.83	0.61
1:T:107:ARG:HG3	4:6:37:HIS:HE1	1.66	0.61
1:B:90:LYS:HE2	1:B:117:MET:HE1	1.82	0.61
1:E:1027:GLN:HB3	1:E:1032:MET:HB2	1.83	0.61
1:M:313:LEU:HD21	1:U:150:THR:HG21	1.83	0.61
1:V:813:VAL:HG21	1:V:1012:MET:HG3	1.83	0.61
1:W:850:ILE:HD12	1:W:870:PRO:HG2	1.82	0.61
2:Z:13:GLU:OE1	2:Z:46:ARG:NH2	2.30	0.61
4:i:300:CYS:SG	4:i:301:TRP:N	2.73	0.61
1:B:919:VAL:HG12	1:B:920:ASN:HB2	1.82	0.61
1:C:829:VAL:HA	1:C:938:MET:HE1	1.82	0.61
4:j:218:VAL:HA	4:j:269:MET:HE1	1.81	0.61
1:B:54:LEU:HB2	1:C:91:ILE:HG12	1.81	0.60
1:B:1027:GLN:HB3	1:B:1032:MET:HB2	1.83	0.60
1:S:898:ARG:HD3	1:S:902:GLN:HG3	1.83	0.60
1:T:709:VAL:HG22	1:T:1023:SER:HA	1.82	0.60
1:X:83:LEU:HD22	1:X:1085:GLU:HB3	1.83	0.60
1:F:540:PHE:O	1:F:559:ARG:NH1	2.33	0.60
1:M:1211:SER:O	1:M:1279:ASN:ND2	2.35	0.60
1:N:1005:THR:HG22	1:N:1007:GLY:H	1.66	0.60
1:V:1236:ASN:HB2	1:V:1238:TRP:HE3	1.65	0.60
1:X:1067:SER:HG	1:X:1083:THR:HG1	1.50	0.60
1:M:799:ASN:HD21	1:M:802:LEU:HG	1.66	0.60
1:N:537:HIS:HA	1:N:1238:TRP:CD1	2.36	0.60
1:O:828:ASN:ND2	1:O:937:THR:O	2.31	0.60
1:T:1171:HIS:HE1	1:U:1228:ALA:HA	1.66	0.60
1:W:447:GLN:HB3	1:W:1028:ALA:HB1	1.84	0.60
1:X:394:ARG:NH1	1:X:1317:ASP:OD2	2.34	0.60
3:8:289:CYS:SG	3:8:290:THR:N	2.74	0.60
4:g:47:LEU:HD23	4:g:62:ILE:HD12	1.82	0.60
1:C:90:LYS:HE2	1:C:117:MET:HE1	1.81	0.60
1:D:36:GLN:HB3	1:N:115:ILE:HB	1.82	0.60
1:O:1005:THR:HG22	1:O:1007:GLY:H	1.66	0.60
1:X:82:ASP:OD1	1:X:82:ASP:N	2.34	0.60
4:c:58:ASP:HB3	4:c:196:ASP:H	1.66	0.60
1:S:207:LYS:HD3	1:X:1168:GLY:HA2	1.83	0.60
1:W:1027:GLN:HB3	1:W:1032:MET:HB2	1.83	0.60
1:X:578:ARG:NH1	1:X:1014:SER:OG	2.34	0.60
3:5:228:ALA:HB3	3:5:289:CYS:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:211:LEU:HA	4:7:214:LEU:HB2	1.83	0.60
1:B:536:VAL:HG13	1:B:1244:SER:HA	1.84	0.60
1:C:1027:GLN:HB3	1:C:1032:MET:HB2	1.83	0.60
1:D:855:GLU:HG2	2:I:70:ARG:HE	1.67	0.60
1:O:578:ARG:NH1	1:O:1014:SER:O	2.35	0.60
1:S:157:LYS:HD2	1:T:338:ASN:HA	1.83	0.60
1:S:182:LYS:NZ	1:S:1058:SER:OG	2.35	0.60
1:V:93:PHE:HB2	1:V:116:VAL:HB	1.82	0.60
1:W:626:LYS:NZ	1:W:881:SER:O	2.35	0.60
1:W:799:ASN:HD21	1:W:802:LEU:HG	1.65	0.60
3:b:324:CYS:SG	3:b:325:GLY:N	2.75	0.60
1:E:271:GLN:OE1	1:E:1056:ARG:NH1	2.35	0.60
1:M:587:ASN:OD1	1:N:1003:GLN:NE2	2.35	0.60
1:N:850:ILE:HD12	1:N:870:PRO:HG2	1.84	0.60
1:O:575:GLN:NE2	1:O:1015:MET:SD	2.74	0.60
1:O:799:ASN:HD21	1:O:802:LEU:HG	1.65	0.60
1:T:49:ARG:HD3	1:U:87:ILE:HD11	1.84	0.60
1:T:1162:ARG:HH22	1:U:206:LYS:HB3	1.66	0.60
1:U:575:GLN:NE2	1:U:1015:MET:SD	2.74	0.60
1:V:829:VAL:HA	1:V:938:MET:HE1	1.84	0.60
1:4:74:ALA:HB1	1:4:182:LYS:HE3	1.82	0.60
1:4:611:LEU:HB3	1:4:862:ILE:HG21	1.84	0.60
3:8:324:CYS:SG	3:8:325:GLY:N	2.75	0.60
1:A:1201:ALA:HB3	1:A:1227:PRO:HG2	1.84	0.60
1:D:578:ARG:NH1	1:D:1014:SER:O	2.34	0.60
1:F:93:PHE:HB2	1:F:116:VAL:HB	1.84	0.60
1:M:537:HIS:HA	1:M:1238:TRP:HD1	1.67	0.60
1:W:964:TYR:HA	1:W:967:ARG:HB2	1.83	0.60
1:X:491:MET:HB2	1:X:783:ASP:HA	1.84	0.60
4:6:245:VAL:O	4:7:256:GLN:NE2	2.35	0.60
1:A:512:VAL:HG12	1:A:993:SER:HB3	1.82	0.60
1:E:249:LEU:HD21	1:E:372:LYS:HB2	1.82	0.60
1:O:1241:GLN:HB3	1:O:1244:SER:HB3	1.84	0.60
1:U:271:GLN:OE1	1:U:1056:ARG:NH1	2.31	0.60
1:C:77:ASN:HA	1:C:1061:MET:HB2	1.83	0.60
1:E:572:ARG:NH2	1:E:1001:SER:O	2.35	0.60
1:U:264:TYR:HE1	1:U:300:PRO:HD2	1.67	0.60
4:a:285:ARG:HE	4:a:305:ARG:HD3	1.67	0.60
1:A:711:ALA:HB3	1:A:1016:HIS:HB3	1.84	0.59
1:C:197:ASP:HB3	1:C:199:VAL:HG12	1.84	0.59
1:M:1168:GLY:HA2	1:N:207:LYS:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:93:PHE:HB2	1:W:116:VAL:HB	1.83	0.59
1:W:325:ASN:HB3	1:W:328:GLN:HB3	1.84	0.59
1:X:438:ASN:HD22	1:X:1171:HIS:HD2	1.49	0.59
1:4:394:ARG:NH1	1:4:1315:PHE:O	2.34	0.59
1:C:399:THR:HG22	1:C:1043:THR:HG22	1.84	0.59
1:F:683:GLU:O	1:F:687:LEU:N	2.32	0.59
1:F:1280:ARG:NH2	1:F:1288:GLU:OE1	2.35	0.59
2:K:13:GLU:OE1	2:K:46:ARG:NH2	2.31	0.59
2:H:13:GLU:OE1	2:H:46:ARG:NH2	2.30	0.59
1:O:450:LEU:HD11	1:O:1025:ILE:HA	1.82	0.59
1:S:1200:ARG:NH1	1:S:1233:SER:O	2.35	0.59
1:V:450:LEU:HD11	1:V:1025:ILE:HG13	1.83	0.59
1:4:194:THR:HG21	1:4:216:MET:HB3	1.83	0.59
4:j:47:LEU:HD23	4:j:62:ILE:HD12	1.84	0.59
1:A:850:ILE:HD12	1:A:875:ILE:HD12	1.83	0.59
1:F:658:ARG:HA	1:F:681:LEU:HD11	1.83	0.59
1:M:1163:CYS:SG	1:M:1164:GLU:N	2.74	0.59
1:T:1280:ARG:NH2	1:T:1288:GLU:OE1	2.35	0.59
1:4:1115:CYS:HA	1:4:1177:CYS:H	1.67	0.59
3:5:151:ASP:O	3:5:282:ARG:NH1	2.36	0.59
1:B:537:HIS:HA	1:B:1238:TRP:CD1	2.36	0.59
1:O:572:ARG:NH2	1:O:1001:SER:O	2.35	0.59
2:P:13:GLU:OE1	2:P:46:ARG:NH2	2.30	0.59
1:X:214:VAL:HA	1:X:217:PHE:HD2	1.67	0.59
1:4:456:PRO:O	1:4:460:ASN:N	2.35	0.59
1:4:539:PHE:O	1:4:559:ARG:NH1	2.34	0.59
1:4:963:ASN:O	1:4:967:ARG:N	2.33	0.59
1:F:856:ASN:OD1	1:F:860:LYS:NZ	2.31	0.59
1:W:1187:ASP:OD2	1:W:1232:ARG:NH1	2.33	0.59
1:4:1241:GLN:HG3	1:4:1243:GLY:H	1.68	0.59
3:8:218:GLU:OE1	4:9:68:LYS:NZ	2.36	0.59
4:c:9:VAL:HG21	4:c:45:LEU:HD21	1.83	0.59
1:A:578:ARG:NH2	1:A:1017:GLN:OE1	2.36	0.59
1:A:1169:LEU:HD11	1:B:208:ALA:HA	1.85	0.59
1:C:536:VAL:HG13	1:C:1244:SER:HA	1.83	0.59
1:D:275:VAL:HG22	1:D:375:ALA:HB3	1.84	0.59
1:F:919:VAL:HG12	1:F:920:ASN:HB2	1.85	0.59
1:V:90:LYS:HE2	1:V:117:MET:HE1	1.85	0.59
1:A:91:ILE:HB	1:A:118:LYS:HB2	1.85	0.59
1:B:578:ARG:NH1	1:B:1014:SER:OG	2.36	0.59
1:B:678:ARG:HH22	1:C:608:ALA:HB3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:ARG:NH1	1:C:1317:ASP:OD2	2.35	0.59
1:E:36:GLN:HB3	1:U:115:ILE:HB	1.85	0.59
1:O:428:GLN:NE2	1:O:577:SER:OG	2.34	0.59
1:V:575:GLN:NE2	1:V:1015:MET:SD	2.76	0.59
1:4:886:PRO:HD2	1:4:920:ASN:HD22	1.67	0.59
1:4:1342:MET:HG2	1:4:1368:LEU:HB3	1.84	0.59
4:f:111:LEU:HB2	4:f:286:LEU:HB2	1.83	0.59
4:j:89:PRO:HB3	4:j:304:PRO:HG3	1.84	0.59
1:A:275:VAL:HG22	1:A:375:ALA:HB3	1.85	0.59
2:L:13:GLU:OE1	2:L:46:ARG:NH2	2.30	0.59
1:M:396:ILE:HD11	1:M:1050:HIS:HE1	1.66	0.59
1:S:537:HIS:HA	1:S:1238:TRP:HD1	1.66	0.59
1:4:946:LYS:NZ	1:4:977:PHE:O	2.35	0.59
1:C:157:LYS:NZ	1:D:339:ALA:O	2.35	0.59
1:C:704:PRO:HG2	1:D:969:PRO:HD2	1.84	0.59
1:D:575:GLN:HE21	1:D:1015:MET:HG3	1.67	0.59
1:O:536:VAL:HG22	1:O:1241:GLN:HG2	1.83	0.59
4:a:229:LEU:HB2	4:a:234:ARG:HH21	1.68	0.59
1:O:777:ARG:NH2	1:O:885:CYS:O	2.36	0.58
1:U:1027:GLN:HB3	1:U:1032:MET:HB2	1.84	0.58
1:U:1342:MET:HE1	1:U:1370:LEU:H	1.67	0.58
1:X:850:ILE:HD11	1:X:872:VAL:HA	1.85	0.58
1:E:56:VAL:HG13	1:F:92:GLN:HB3	1.85	0.58
1:E:428:GLN:NE2	1:E:577:SER:OG	2.36	0.58
1:F:893:ARG:NH2	1:F:988:GLU:OE1	2.36	0.58
1:M:714:ASP:O	1:M:804:LYS:NZ	2.35	0.58
1:U:93:PHE:HB2	1:U:116:VAL:HB	1.84	0.58
1:U:422:VAL:HG11	1:U:1355:GLN:HE22	1.68	0.58
4:6:179:THR:OG1	4:6:189:ARG:NH1	2.35	0.58
1:A:532:LEU:O	1:A:1241:GLN:NE2	2.37	0.58
1:E:384:ASN:O	1:E:387:GLN:NE2	2.36	0.58
1:E:770:LEU:HD11	1:E:883:LEU:HD13	1.85	0.58
1:F:555:ARG:HH21	1:F:907:HIS:HA	1.68	0.58
1:S:504:LYS:O	1:S:967:ARG:NH1	2.37	0.58
1:V:1196:ASN:HD21	1:V:1324:GLN:HG3	1.69	0.58
1:W:278:THR:HG22	1:W:1051:ILE:HG12	1.85	0.58
1:4:130:GLU:HG2	1:4:1079:THR:HG22	1.85	0.58
1:4:399:THR:HG22	1:4:1043:THR:HG22	1.84	0.58
1:4:652:ASN:ND2	1:4:923:GLY:O	2.33	0.58
1:C:757:ILE:HG12	1:C:788:LEU:HD22	1.84	0.58
1:M:56:VAL:HG13	1:N:92:GLN:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:611:LEU:HD11	1:M:935:ALA:HB2	1.85	0.58
1:O:555:ARG:HH21	1:O:910:GLY:HA2	1.66	0.58
1:T:77:ASN:HA	1:T:1061:MET:HB2	1.84	0.58
2:Y:13:GLU:OE1	2:Y:46:ARG:NH2	2.31	0.58
1:4:716:HIS:O	1:4:915:GLN:NE2	2.36	0.58
1:4:723:TYR:OH	1:4:921:GLY:O	2.21	0.58
3:e:324:CYS:SG	3:e:325:GLY:N	2.74	0.58
1:C:145:THR:HG22	1:C:147:LEU:H	1.68	0.58
1:E:829:VAL:HA	1:E:938:MET:HE1	1.86	0.58
1:F:1005:THR:HG22	1:F:1007:GLY:H	1.69	0.58
1:N:95:ILE:HB	1:N:114:TYR:HB2	1.85	0.58
1:N:448:ASN:ND2	1:O:1231:CYS:SG	2.76	0.58
1:S:1328:PRO:HB2	1:S:1358:ILE:HG21	1.85	0.58
1:T:1198:ARG:HB3	1:T:1270:PHE:HE1	1.66	0.58
1:X:1241:GLN:HB3	1:X:1244:SER:HB3	1.84	0.58
1:B:898:ARG:NH1	1:B:904:PHE:O	2.37	0.58
1:M:128:GLU:OE2	1:N:110:LYS:NZ	2.35	0.58
1:M:163:LEU:HD21	3:b:51:PRO:HG2	1.86	0.58
1:O:918:LEU:HB2	1:O:944:PHE:HE2	1.69	0.58
2:Q:13:GLU:OE1	2:Q:46:ARG:NH2	2.30	0.58
1:4:711:ALA:O	1:4:804:LYS:NZ	2.35	0.58
4:g:69:CYS:SG	4:g:70:THR:N	2.76	0.58
1:A:338:ASN:HA	1:F:157:LYS:HD2	1.86	0.58
1:C:263:THR:O	1:C:359:ARG:NH1	2.35	0.58
1:S:271:GLN:OE1	1:S:1056:ARG:NH1	2.36	0.58
1:T:491:MET:HB2	1:T:783:ASP:HA	1.83	0.58
1:V:457:ARG:HH22	1:V:463:GLN:HG2	1.67	0.58
1:4:799:ASN:HD21	1:4:802:LEU:HG	1.68	0.58
4:f:246:PRO:HA	4:g:256:GLN:HE22	1.68	0.58
1:C:1342:MET:HE1	1:C:1370:LEU:H	1.67	0.58
1:N:1173:GLN:NE2	1:N:1302:THR:OG1	2.36	0.58
1:S:49:ARG:HD3	1:T:87:ILE:HD11	1.86	0.58
1:U:714:ASP:O	1:U:804:LYS:NZ	2.35	0.58
1:U:1062:PHE:HB2	1:U:1087:ALA:HB3	1.85	0.58
1:A:711:ALA:HB2	1:A:1018:LYS:HD3	1.86	0.58
1:D:678:ARG:HD3	1:E:647:LYS:HZ1	1.69	0.58
1:V:275:VAL:HG22	1:V:375:ALA:HB3	1.86	0.58
1:V:1062:PHE:HB2	1:V:1087:ALA:HB3	1.86	0.58
1:4:965:VAL:HG13	1:4:972:ARG:HG2	1.84	0.58
1:D:163:LEU:HD21	3:8:51:PRO:HG2	1.85	0.58
1:D:228:LEU:HD22	1:D:1103:HIS:HD2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1027:GLN:HE22	1:D:1032:MET:HB2	1.67	0.58
1:E:850:ILE:HD11	1:E:872:VAL:HA	1.86	0.58
1:S:1067:SER:HG	1:S:1083:THR:HG1	1.49	0.58
1:4:279:THR:HB	1:4:380:GLN:HE21	1.69	0.58
4:a:89:PRO:HB3	4:a:304:PRO:HG3	1.85	0.58
1:A:963:ASN:O	1:A:967:ARG:N	2.36	0.57
1:E:958:HIS:HE1	1:E:960:LEU:HB3	1.68	0.57
1:N:5:LEU:HD23	1:N:34:SER:HB2	1.86	0.57
1:U:1178:GLU:OE2	1:U:1250:TYR:OH	2.22	0.57
1:O:192:LEU:HD22	1:O:251:ALA:HB1	1.85	0.57
1:U:903:SER:HB2	1:U:1128:GLN:HE22	1.69	0.57
1:W:293:VAL:HG13	1:W:294:GLU:HG3	1.84	0.57
1:B:757:ILE:HG12	1:B:788:LEU:HD22	1.85	0.57
1:C:1198:ARG:NH1	1:C:1200:ARG:O	2.37	0.57
1:D:38:LEU:HB2	1:N:113:GLN:HB3	1.86	0.57
1:D:123:HIS:HB2	1:D:1086:ILE:HB	1.85	0.57
1:M:1005:THR:HG22	1:M:1007:GLY:H	1.69	0.57
1:N:1201:ALA:HB3	1:N:1227:PRO:HG2	1.85	0.57
1:O:197:ASP:HB3	1:O:199:VAL:HG12	1.86	0.57
1:T:49:ARG:NH1	4:d:76:GLU:OE2	2.38	0.57
1:U:1137:LYS:O	1:U:1141:GLY:N	2.36	0.57
1:X:893:ARG:NH2	1:X:988:GLU:OE1	2.36	0.57
1:X:902:GLN:NE2	1:X:1018:LYS:O	2.37	0.57
3:e:329:VAL:HG21	4:f:271:SER:HB2	1.84	0.57
1:A:1074:ARG:NH2	4:j:299:SER:OG	2.36	0.57
1:F:729:ASP:HB2	1:F:793:LEU:HD11	1.86	0.57
1:N:271:GLN:OE1	1:N:1056:ARG:NH1	2.38	0.57
1:O:77:ASN:HA	1:O:1061:MET:HB2	1.87	0.57
1:T:898:ARG:HD3	1:T:902:GLN:HG3	1.86	0.57
1:4:581:GLN:NE2	1:4:1031:ARG:O	2.38	0.57
3:5:129:ALA:HA	3:5:132:TRP:HD1	1.69	0.57
4:j:124:THR:OG1	4:j:134:ILE:O	2.21	0.57
1:B:1226:ASP:HB2	1:B:1229:TYR:H	1.69	0.57
1:M:963:ASN:O	1:M:967:ARG:N	2.36	0.57
1:O:1071:ARG:O	1:O:1079:THR:OG1	2.21	0.57
1:T:1071:ARG:O	1:T:1079:THR:OG1	2.23	0.57
1:M:828:ASN:ND2	1:M:937:THR:O	2.31	0.57
2:R:13:GLU:OE1	2:R:46:ARG:NH2	2.30	0.57
1:4:340:LEU:HD12	1:4:341:PRO:HD2	1.87	0.57
4:d:111:LEU:HD22	4:d:286:LEU:HD11	1.87	0.57
4:f:35:ASP:HB2	4:f:40:GLN:HE22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:5:LYS:HD2	4:g:86:ARG:HB3	1.85	0.57
1:B:1163:CYS:SG	1:B:1164:GLU:N	2.77	0.57
1:F:929:ASP:OD1	1:F:932:ARG:NH2	2.38	0.57
1:S:365:SER:HB2	1:S:376:ILE:H	1.70	0.57
1:S:532:LEU:O	1:S:1241:GLN:NE2	2.37	0.57
1:V:438:ASN:HD22	1:V:1171:HIS:HD2	1.53	0.57
1:V:578:ARG:NH1	1:V:1014:SER:OG	2.37	0.57
3:8:305:LEU:HD12	3:8:312:LEU:HD23	1.85	0.57
4:i:177:TYR:HB3	4:j:263:ILE:HG21	1.86	0.57
1:C:275:VAL:HG22	1:C:375:ALA:HB3	1.87	0.57
1:T:214:VAL:HA	1:T:217:PHE:HD2	1.69	0.57
1:U:1201:ALA:HB3	1:U:1227:PRO:HG2	1.85	0.57
1:V:77:ASN:HA	1:V:1061:MET:HB2	1.87	0.57
4:6:220:ARG:NH1	4:6:252:ILE:O	2.38	0.57
4:j:69:CYS:SG	4:j:70:THR:N	2.77	0.57
1:O:1198:ARG:NH2	1:O:1219:LEU:O	2.38	0.57
1:X:275:VAL:HG22	1:X:375:ALA:HB3	1.87	0.57
4:c:29:SER:OG	4:c:99:TYR:OH	2.23	0.57
3:e:91:PHE:HB2	3:e:106:LEU:HB2	1.86	0.57
1:A:1285:LEU:HD13	1:A:1322:MET:HE1	1.87	0.57
1:E:963:ASN:O	1:E:967:ARG:N	2.32	0.57
1:M:117:MET:HB2	1:U:5:LEU:HD12	1.86	0.57
1:S:85:ARG:HH21	1:4:138:LEU:HD22	1.69	0.57
4:7:110:GLN:HG2	4:7:287:HIS:HE1	1.70	0.57
1:A:717:LEU:HB2	1:A:990:TRP:HZ3	1.70	0.56
1:E:893:ARG:NH2	1:E:988:GLU:OE1	2.37	0.56
1:E:968:LEU:HD11	1:E:971:GLN:HE21	1.69	0.56
1:V:79:GLU:HB3	1:V:305:SER:HA	1.87	0.56
1:X:946:LYS:NZ	1:X:975:VAL:O	2.36	0.56
3:h:40:ASP:O	4:i:2:ALA:N	2.38	0.56
1:E:587:ASN:HB2	1:F:572:ARG:HH22	1.69	0.56
1:S:117:MET:HE2	1:X:24:LYS:HG3	1.85	0.56
1:S:537:HIS:HA	1:S:1238:TRP:CD1	2.40	0.56
1:T:93:PHE:HB2	1:T:116:VAL:HB	1.87	0.56
1:4:839:VAL:HG11	1:4:875:ILE:HD12	1.86	0.56
4:7:217:LEU:HB2	4:7:269:MET:HG3	1.86	0.56
4:9:144:LEU:HD21	4:9:183:PHE:HB2	1.87	0.56
1:B:633:LEU:HA	1:B:874:MET:HE3	1.86	0.56
1:D:23:ILE:H	1:M:387:GLN:HE22	1.52	0.56
1:D:572:ARG:NH2	1:D:1001:SER:O	2.38	0.56
1:F:946:LYS:NZ	1:F:986:GLU:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1071:ARG:HH22	4:c:38:ARG:H	1.51	0.56
1:T:130:GLU:HG2	1:T:1079:THR:HG22	1.86	0.56
1:T:490:ASN:OD1	1:T:495:ARG:NH1	2.38	0.56
1:T:537:HIS:HA	1:T:1238:TRP:CD1	2.40	0.56
1:T:757:ILE:HG12	1:T:788:LEU:HD22	1.87	0.56
1:T:929:ASP:OD1	1:T:932:ARG:NH2	2.38	0.56
1:U:663:HIS:HA	1:V:930:ARG:HD2	1.86	0.56
1:V:828:ASN:ND2	1:V:937:THR:O	2.37	0.56
1:W:575:GLN:NE2	1:W:1015:MET:SD	2.78	0.56
1:X:428:GLN:NE2	1:X:577:SER:OG	2.35	0.56
1:X:927:VAL:HB	1:X:956:THR:HG21	1.86	0.56
1:4:901:ALA:HB3	1:4:1020:SER:HB3	1.86	0.56
4:c:88:ASP:HB2	4:c:91:ASP:HB2	1.86	0.56
1:E:435:VAL:HG11	1:E:1368:LEU:HD22	1.88	0.56
1:N:249:LEU:HD21	1:N:372:LYS:HB2	1.88	0.56
1:S:88:ASP:OD2	4:6:14:ARG:NH2	2.36	0.56
1:S:536:VAL:HG13	1:S:1244:SER:HA	1.86	0.56
1:S:581:GLN:NE2	1:S:1031:ARG:O	2.38	0.56
1:T:91:ILE:HB	1:T:118:LYS:HB2	1.87	0.56
1:U:252:VAL:HG11	1:U:1055:SER:HB3	1.88	0.56
1:U:626:LYS:NZ	1:U:881:SER:O	2.37	0.56
1:V:1201:ALA:HB3	1:V:1227:PRO:HG2	1.86	0.56
1:W:915:GLN:HG2	1:W:989:GLU:HG3	1.88	0.56
1:4:849:ASP:HB3	1:4:869:ARG:HB3	1.87	0.56
4:7:141:PRO:O	4:7:145:GLY:N	2.37	0.56
4:a:97:ASN:HD22	4:a:105:TRP:HE1	1.54	0.56
4:i:114:LEU:HD11	4:i:145:GLY:HA2	1.86	0.56
1:A:214:VAL:HA	1:A:217:PHE:HD2	1.70	0.56
1:B:1071:ARG:O	1:B:1079:THR:OG1	2.24	0.56
1:C:782:HIS:HA	1:C:785:ARG:HD2	1.87	0.56
1:D:1252:ILE:HD11	1:D:1267:ARG:HG3	1.87	0.56
1:E:75:CYS:SG	1:E:1059:THR:OG1	2.59	0.56
1:T:236:ARG:NH1	1:T:239:GLN:OE1	2.39	0.56
1:U:1251:ASN:HB3	1:U:1254:PHE:HB3	1.87	0.56
1:V:61:VAL:HG11	1:W:98:PRO:HG3	1.87	0.56
1:W:829:VAL:HA	1:W:938:MET:HE1	1.87	0.56
1:X:57:TYR:O	1:4:47:SER:N	2.38	0.56
4:7:156:HIS:NE2	4:7:201:LEU:O	2.38	0.56
1:C:739:ILE:HB	1:C:895:ILE:HB	1.87	0.56
1:N:1241:GLN:HB3	1:N:1244:SER:HB3	1.86	0.56
1:X:183:LEU:HD13	1:X:394:ARG:HH21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:177:TYR:HB3	4:a:263:ILE:HG21	1.88	0.56
1:B:832:THR:HG22	2:H:11:ILE:HD11	1.87	0.56
1:D:91:ILE:HB	1:D:118:LYS:HB2	1.87	0.56
1:O:929:ASP:OD1	1:O:932:ARG:NH2	2.38	0.56
3:8:300:PRO:HB3	3:8:317:PHE:HE1	1.70	0.56
1:A:1071:ARG:O	1:A:1079:THR:OG1	2.24	0.56
1:B:944:PHE:HA	1:B:984:MET:HE1	1.88	0.56
1:M:325:ASN:HB3	1:M:328:GLN:HB3	1.88	0.56
1:N:182:LYS:NZ	1:N:1058:SER:OG	2.37	0.56
1:V:514:GLN:HG3	1:V:531:LEU:HD21	1.87	0.56
1:V:946:LYS:HE2	1:V:993:SER:HA	1.88	0.56
1:W:396:ILE:HD11	1:W:1050:HIS:HE1	1.69	0.56
3:e:25:ARG:NH2	4:g:4:ASP:OD2	2.39	0.56
3:h:117:MET:HE1	3:h:243:LEU:H	1.70	0.56
1:B:717:LEU:HA	1:B:915:GLN:HE22	1.70	0.56
1:D:796:ASN:OD1	1:E:932:ARG:NH1	2.38	0.56
1:S:946:LYS:NZ	1:S:975:VAL:O	2.39	0.56
1:W:182:LYS:NZ	1:W:1058:SER:OG	2.39	0.56
1:4:432:THR:HG22	1:4:1333:SER:HA	1.88	0.56
1:4:1071:ARG:O	1:4:1079:THR:OG1	2.24	0.56
3:h:183:GLY:HA3	3:h:321:GLU:HA	1.87	0.56
1:B:271:GLN:OE1	1:B:1056:ARG:NH1	2.39	0.56
1:C:514:GLN:HG3	1:C:531:LEU:HD21	1.88	0.56
1:N:822:MET:HE1	1:N:957:LEU:HD13	1.88	0.56
1:X:74:ALA:HB1	1:X:182:LYS:HE3	1.88	0.56
4:c:58:ASP:OD2	4:c:199:THR:OG1	2.24	0.56
3:h:324:CYS:SG	3:h:325:GLY:N	2.76	0.56
1:D:182:LYS:NZ	1:D:1058:SER:OG	2.39	0.55
1:D:1173:GLN:NE2	1:D:1304:LEU:O	2.38	0.55
1:F:406:LEU:HD21	1:F:1191:PHE:HE2	1.72	0.55
2:I:13:GLU:OE1	2:I:46:ARG:NH2	2.31	0.55
1:S:130:GLU:HG2	1:S:1079:THR:HG22	1.87	0.55
1:V:663:HIS:HA	1:W:930:ARG:HD2	1.88	0.55
1:V:1198:ARG:NH2	1:V:1219:LEU:O	2.39	0.55
1:X:447:GLN:HA	1:X:450:LEU:HB2	1.88	0.55
1:4:1005:THR:HG22	1:4:1007:GLY:H	1.71	0.55
4:6:47:LEU:HB3	4:6:135:VAL:HB	1.88	0.55
4:9:179:THR:OG1	4:9:189:ARG:NH1	2.40	0.55
4:a:253:ASP:HB3	4:a:255:ASP:H	1.71	0.55
4:c:220:ARG:HG2	4:c:265:ARG:HH12	1.71	0.55
1:B:1207:CYS:SG	1:B:1208:ASP:N	2.79	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:889:THR:HA	1:C:920:ASN:HB3	1.87	0.55
1:F:591:VAL:HB	1:F:683:GLU:HB2	1.89	0.55
1:M:616:ILE:HG23	1:M:620:ILE:HD13	1.87	0.55
1:W:537:HIS:HA	1:W:1238:TRP:HE1	1.70	0.55
4:a:221:GLY:HA2	4:a:266:MET:HE1	1.89	0.55
1:D:947:LEU:HD21	1:D:995:VAL:HG12	1.87	0.55
1:E:182:LYS:NZ	1:E:1058:SER:OG	2.39	0.55
1:E:394:ARG:NH1	1:E:1317:ASP:OD2	2.39	0.55
1:S:460:ASN:HB3	1:S:904:PHE:HB3	1.89	0.55
1:S:1042:ARG:NH2	1:S:1112:GLY:O	2.38	0.55
1:T:492:ASN:HD22	1:T:495:ARG:HE	1.54	0.55
1:X:331:ALA:HA	1:X:335:ASP:HB2	1.87	0.55
4:6:127:LEU:HD13	4:6:133:ASP:HA	1.89	0.55
4:a:36:CYS:HA	4:a:86:ARG:HH12	1.70	0.55
1:F:1130:ARG:HH22	4:f:239:GLU:HG2	1.71	0.55
1:N:578:ARG:NH1	1:N:1014:SER:O	2.39	0.55
1:S:1173:GLN:NE2	1:S:1302:THR:O	2.39	0.55
1:T:399:THR:HG22	1:T:1043:THR:HG22	1.89	0.55
4:c:13:SER:OG	4:c:130:ASN:ND2	2.40	0.55
1:A:1187:ASP:OD2	1:A:1232:ARG:NH2	2.40	0.55
1:D:399:THR:HG22	1:D:1043:THR:HG22	1.87	0.55
1:E:512:VAL:HG12	1:E:993:SER:HB3	1.88	0.55
1:F:626:LYS:HZ1	1:F:881:SER:HA	1.71	0.55
1:M:271:GLN:OE1	1:M:1056:ARG:NH1	2.34	0.55
1:N:1264:SER:HB2	1:N:1267:ARG:HB2	1.88	0.55
1:S:591:VAL:HG12	1:S:679:LYS:HG2	1.87	0.55
1:U:1280:ARG:NH2	1:U:1288:GLU:OE1	2.39	0.55
1:V:537:HIS:HB3	1:V:1245:LEU:HB2	1.88	0.55
1:X:93:PHE:HB2	1:X:116:VAL:HB	1.88	0.55
1:4:626:LYS:O	1:4:630:ASN:ND2	2.39	0.55
1:A:1254:PHE:HD1	1:A:1267:ARG:HH12	1.55	0.55
1:C:540:PHE:O	1:C:559:ARG:NH1	2.40	0.55
1:D:428:GLN:NE2	1:D:577:SER:OG	2.39	0.55
1:D:578:ARG:NH2	1:D:1017:GLN:OE1	2.39	0.55
1:D:929:ASP:OD1	1:D:932:ARG:NH2	2.40	0.55
1:D:963:ASN:O	1:D:967:ARG:N	2.37	0.55
1:F:271:GLN:OE1	1:F:1056:ARG:NH1	2.37	0.55
1:T:471:ALA:HA	1:T:1242:ARG:HH12	1.71	0.55
1:T:736:ARG:HB3	1:T:897:LYS:HB2	1.88	0.55
1:U:606:ASP:OD2	1:U:641:TYR:OH	2.22	0.55
1:V:635:ALA:HB2	1:V:664:MET:HE1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1051:ILE:HB	1:X:1100:ALA:HB3	1.88	0.55
4:j:176:LEU:O	4:j:180:ASN:ND2	2.38	0.55
1:B:402:PHE:HD2	1:B:1040:VAL:HB	1.70	0.55
1:B:587:ASN:ND2	1:C:1001:SER:O	2.40	0.55
1:B:743:GLY:HA3	1:B:786:HIS:HE1	1.72	0.55
1:C:692:LEU:HD21	1:D:972:ARG:HE	1.70	0.55
1:C:1111:MET:SD	1:C:1366:ARG:NH2	2.77	0.55
1:O:263:THR:HA	1:O:359:ARG:HH12	1.72	0.55
1:S:144:GLU:HB2	1:S:148:ASP:HB2	1.89	0.55
2:3:13:GLU:OE1	2:3:46:ARG:NH2	2.31	0.55
1:4:434:VAL:HG11	1:4:1042:ARG:HH12	1.72	0.55
1:C:438:ASN:HD22	1:C:1171:HIS:HD2	1.54	0.55
1:D:150:THR:HG21	1:N:313:LEU:HD21	1.89	0.55
1:F:183:LEU:HD13	1:F:394:ARG:HH22	1.72	0.55
1:N:494:PHE:HZ	2:Q:6:VAL:HG22	1.71	0.55
1:N:587:ASN:HD22	1:O:572:ARG:HH12	1.54	0.55
1:O:1163:CYS:SG	1:O:1164:GLU:N	2.79	0.55
1:U:666:ASN:ND2	1:V:867:ASP:OD2	2.39	0.55
4:6:161:ILE:HG12	4:7:224:ARG:HE	1.72	0.55
3:b:208:ASP:HA	3:b:250:LYS:HZ1	1.71	0.55
1:A:1027:GLN:HB3	1:A:1032:MET:HB2	1.89	0.55
1:D:75:CYS:SG	1:D:1059:THR:OG1	2.64	0.55
1:D:420:ARG:HH11	1:E:1353:MET:HE1	1.71	0.55
1:F:1250:TYR:HB2	1:F:1270:PHE:HD2	1.70	0.55
1:X:396:ILE:HD11	1:X:1050:HIS:HE1	1.72	0.55
1:X:532:LEU:O	1:X:1241:GLN:NE2	2.40	0.55
1:F:532:LEU:O	1:F:1241:GLN:NE2	2.39	0.55
1:M:1173:GLN:NE2	1:M:1302:THR:OG1	2.40	0.55
1:N:586:THR:HA	1:N:693:LYS:HD2	1.89	0.55
1:N:946:LYS:NZ	1:N:986:GLU:OE1	2.40	0.55
1:T:92:GLN:HE22	1:T:115:ILE:HG23	1.72	0.55
1:T:271:GLN:OE1	1:T:1056:ARG:NH1	2.38	0.55
1:T:828:ASN:ND2	1:T:937:THR:O	2.40	0.55
1:T:893:ARG:NH2	1:T:988:GLU:OE1	2.40	0.55
1:V:592:ILE:HG12	1:V:679:LYS:HB3	1.89	0.55
1:W:90:LYS:HE2	1:W:117:MET:HE1	1.88	0.55
1:4:563:GLY:HA3	1:4:1015:MET:HG3	1.88	0.55
4:6:111:LEU:HB2	4:6:286:LEU:HB2	1.89	0.55
1:B:578:ARG:NH1	1:B:1014:SER:O	2.40	0.54
1:B:635:ALA:HB2	1:B:664:MET:HE1	1.89	0.54
1:C:450:LEU:HD11	1:C:1025:ILE:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1073:VAL:HG13	1:D:1078:VAL:HG22	1.89	0.54
1:D:1335:ARG:HH22	1:D:1370:LEU:HD11	1.71	0.54
1:M:842:ASP:OD2	2:P:19:TYR:OH	2.25	0.54
1:U:452:SER:HB3	1:U:1117:ASP:HA	1.89	0.54
1:X:829:VAL:HA	1:X:938:MET:HE1	1.90	0.54
1:X:1163:CYS:N	1:X:1303:ASP:OD2	2.40	0.54
1:X:1344:ASN:ND2	1:X:1347:THR:OG1	2.40	0.54
3:5:164:PRO:HG2	3:5:180:ALA:HB3	1.88	0.54
4:d:7:ILE:HB	4:d:84:LEU:HB2	1.89	0.54
3:h:128:VAL:HG21	3:h:312:LEU:HD13	1.88	0.54
1:B:492:ASN:HD22	1:B:495:ARG:HE	1.53	0.54
1:F:115:ILE:HB	1:T:36:GLN:HB3	1.90	0.54
1:S:564:ASN:ND2	1:S:990:TRP:O	2.40	0.54
1:T:964:TYR:OH	1:T:978:ASN:ND2	2.41	0.54
2:0:13:GLU:OE1	2:0:46:ARG:NH2	2.31	0.54
4:f:36:CYS:HB3	4:f:86:ARG:HH22	1.71	0.54
1:A:587:ASN:HB2	1:B:572:ARG:HH22	1.72	0.54
1:C:182:LYS:NZ	1:C:1058:SER:OG	2.40	0.54
1:C:273:ALA:O	1:C:1053:TYR:OH	2.24	0.54
1:D:1115:CYS:HB2	1:D:1179:ILE:HD11	1.88	0.54
1:F:640:THR:O	1:F:644:ASN:ND2	2.40	0.54
1:M:214:VAL:HA	1:M:217:PHE:HD2	1.71	0.54
1:O:714:ASP:O	1:O:804:LYS:NZ	2.41	0.54
1:U:591:VAL:N	1:U:683:GLU:OE1	2.40	0.54
1:A:826:TYR:OH	1:A:920:ASN:O	2.26	0.54
1:A:1220:TYR:HD2	1:A:1242:ARG:HH11	1.55	0.54
1:C:1187:ASP:OD2	1:C:1232:ARG:NH2	2.41	0.54
1:D:38:LEU:HD12	1:N:113:GLN:HG2	1.88	0.54
1:M:95:ILE:HB	1:M:114:TYR:HB2	1.89	0.54
1:O:438:ASN:HD22	1:O:1171:HIS:HD2	1.55	0.54
1:S:396:ILE:HD11	1:S:1050:HIS:HE1	1.72	0.54
1:U:536:VAL:HG13	1:U:1244:SER:HA	1.89	0.54
1:U:561:MET:H	1:U:564:ASN:HD22	1.55	0.54
1:4:1282:LEU:HD23	1:4:1285:LEU:HD12	1.88	0.54
1:A:1173:GLN:NE2	1:A:1302:THR:OG1	2.41	0.54
1:C:1196:ASN:HD21	1:C:1324:GLN:HG3	1.73	0.54
1:F:1198:ARG:NH2	1:F:1219:LEU:O	2.41	0.54
1:S:867:ASP:OD2	1:X:666:ASN:ND2	2.41	0.54
1:T:1070:ARG:HH22	3:e:20:PRO:HG3	1.72	0.54
1:U:633:LEU:HA	1:U:874:MET:HE3	1.90	0.54
1:U:1167:PRO:HG3	1:V:1217:ARG:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:8:ARG:NH2	1:W:316:ALA:O	2.40	0.54
3:5:75:VAL:HG11	3:5:80:PHE:HB2	1.89	0.54
4:9:104:GLN:NE2	4:9:291:TYR:OH	2.41	0.54
1:C:518:VAL:HG13	1:C:522:ASP:HB3	1.88	0.54
1:C:929:ASP:OD1	1:C:932:ARG:NH2	2.40	0.54
1:D:1280:ARG:NH2	1:D:1288:GLU:OE1	2.41	0.54
1:O:959:PRO:HA	1:O:962:ALA:HB3	1.89	0.54
1:S:192:LEU:O	1:S:196:GLY:N	2.38	0.54
1:S:1220:TYR:HD2	1:S:1242:ARG:HH11	1.56	0.54
1:S:1236:ASN:HB2	1:S:1238:TRP:HE3	1.72	0.54
1:T:1167:PRO:HD3	1:U:1224:ILE:HD13	1.90	0.54
1:V:8:ARG:NH1	1:V:49:ARG:O	2.39	0.54
1:V:537:HIS:HA	1:V:1238:TRP:CD1	2.42	0.54
1:V:780:GLU:OE1	1:V:785:ARG:NH1	2.32	0.54
1:4:756:PHE:O	1:4:788:LEU:N	2.41	0.54
3:b:167:GLN:HB2	3:b:188:ARG:HG3	1.90	0.54
1:C:620:ILE:HD11	1:C:630:ASN:HD22	1.72	0.54
1:D:963:ASN:HA	1:D:966:THR:HG22	1.90	0.54
1:E:333:ILE:HD11	1:M:11:PRO:HD3	1.89	0.54
1:F:1111:MET:HE1	1:F:1366:ARG:HH22	1.73	0.54
1:F:1248:VAL:HG13	1:F:1254:PHE:HD2	1.73	0.54
1:M:83:LEU:HD21	1:M:122:LYS:HD2	1.90	0.54
1:M:578:ARG:NH1	1:M:1014:SER:O	2.39	0.54
1:N:717:LEU:HD23	1:N:804:LYS:HD3	1.88	0.54
1:N:1207:CYS:SG	1:N:1208:ASP:N	2.80	0.54
1:T:1005:THR:HG22	1:T:1007:GLY:H	1.71	0.54
1:U:83:LEU:HD22	1:U:1085:GLU:HB3	1.87	0.54
1:W:331:ALA:HA	1:W:335:ASP:HB2	1.90	0.54
1:W:1071:ARG:O	1:W:1079:THR:OG1	2.25	0.54
1:X:436:ASN:HB3	1:X:440:VAL:H	1.72	0.54
1:4:934:ALA:O	1:4:938:MET:N	2.33	0.54
1:D:600:ILE:O	1:D:603:THR:OG1	2.26	0.54
1:D:706:THR:O	1:D:710:SER:OG	2.25	0.54
1:E:507:ALA:HB2	1:E:971:GLN:HE22	1.73	0.54
1:E:1342:MET:HE1	1:E:1370:LEU:H	1.73	0.54
1:M:725:ASP:HB3	1:M:793:LEU:HD22	1.88	0.54
1:O:1295:GLY:H	1:O:1321:HIS:CE1	2.26	0.54
1:V:1249:LEU:O	1:V:1255:ARG:NH2	2.40	0.54
4:d:36:CYS:HB2	4:d:86:ARG:HH22	1.73	0.54
4:d:97:ASN:HD22	4:d:105:TRP:HD1	1.56	0.54
1:C:278:THR:HG22	1:C:1051:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:709:VAL:HG22	1:M:1023:SER:HA	1.89	0.54
1:O:736:ARG:HD2	1:O:897:LYS:HB2	1.90	0.54
1:T:1241:GLN:HB3	1:T:1244:SER:HB3	1.89	0.54
1:U:491:MET:HE3	1:U:786:HIS:H	1.73	0.54
1:U:532:LEU:O	1:U:1241:GLN:NE2	2.40	0.54
1:A:450:LEU:HD11	1:A:1025:ILE:HA	1.90	0.54
1:E:491:MET:HE3	1:E:786:HIS:H	1.73	0.54
2:G:78:ARG:HH21	2:H:19:TYR:HE1	1.55	0.54
1:X:629:MET:HE3	1:X:877:VAL:HG13	1.90	0.54
1:4:226:PHE:HD2	1:4:1364:MET:HB3	1.72	0.54
1:4:777:ARG:NH2	1:4:885:CYS:O	2.38	0.54
1:4:1333:SER:HB2	1:4:1355:GLN:HB2	1.89	0.54
4:j:7:ILE:HG21	4:j:33:LEU:HD21	1.90	0.54
1:D:1245:LEU:HA	1:D:1248:VAL:HB	1.90	0.53
1:E:15:THR:HG21	1:U:257:VAL:HG13	1.89	0.53
1:F:1256:GLN:OE1	4:g:202:ARG:NH2	2.41	0.53
1:N:893:ARG:NH2	1:N:988:GLU:OE1	2.41	0.53
1:S:739:ILE:HB	1:S:895:ILE:HB	1.88	0.53
1:S:946:LYS:HE2	1:S:993:SER:HA	1.88	0.53
1:U:153:ALA:HB1	1:V:338:ASN:HB3	1.91	0.53
1:U:1260:PRO:HG3	4:d:55:THR:HG22	1.89	0.53
1:V:963:ASN:O	1:V:967:ARG:N	2.36	0.53
2:Y:12:GLN:HB2	2:3:70:ARG:CZ	2.39	0.53
1:4:133:ALA:HA	1:4:136:ILE:HD12	1.91	0.53
1:C:1344:ASN:ND2	1:C:1347:THR:OG1	2.41	0.53
1:E:929:ASP:OD1	1:E:932:ARG:NH2	2.41	0.53
1:N:448:ASN:HD21	1:N:1113:VAL:HG13	1.73	0.53
1:O:1236:ASN:HB2	1:O:1238:TRP:HE3	1.73	0.53
1:T:195:LEU:HD23	1:T:1283:TYR:HE1	1.74	0.53
1:U:1295:GLY:H	1:U:1321:HIS:CE1	2.26	0.53
1:V:799:ASN:HD21	1:V:802:LEU:HG	1.73	0.53
1:X:537:HIS:HA	1:X:1238:TRP:CD1	2.43	0.53
1:4:743:GLY:O	1:4:746:ASN:ND2	2.40	0.53
1:4:1236:ASN:HB2	1:4:1238:TRP:HE3	1.73	0.53
1:E:591:VAL:N	1:E:683:GLU:OE1	2.38	0.53
1:E:1043:THR:HG23	1:E:1265:PRO:HG3	1.91	0.53
1:M:708:LEU:HD21	1:M:1022:PRO:HG2	1.90	0.53
1:M:897:LYS:HA	1:M:912:ASP:HA	1.90	0.53
1:U:90:LYS:HE2	1:U:117:MET:HE1	1.91	0.53
1:A:547:CYS:HB2	1:A:550:ALA:HB3	1.90	0.53
1:B:1171:HIS:HE1	1:C:1228:ALA:HA	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1187:ASP:OD2	1:D:1232:ARG:NH2	2.42	0.53
1:S:893:ARG:HG3	1:S:916:THR:HG22	1.90	0.53
1:S:987:TYR:O	1:S:992:LYS:NZ	2.42	0.53
1:S:1179:ILE:HG22	1:S:1181:PRO:HD3	1.91	0.53
1:U:1071:ARG:HH22	4:d:38:ARG:H	1.56	0.53
1:W:932:ARG:HE	1:W:956:THR:HG23	1.73	0.53
1:X:1201:ALA:HB3	1:X:1227:PRO:HG2	1.91	0.53
1:A:206:LYS:HD3	1:F:1162:ARG:HH22	1.72	0.53
1:B:493:LEU:HD13	1:B:942:VAL:HG21	1.90	0.53
1:C:963:ASN:HA	1:C:966:THR:HG22	1.91	0.53
1:D:491:MET:HB2	1:D:783:ASP:HA	1.89	0.53
1:D:819:MET:N	1:D:950:ASP:OD2	2.40	0.53
1:F:826:TYR:HE2	1:F:886:PRO:HG2	1.73	0.53
1:M:606:ASP:HB3	1:M:609:TYR:HB2	1.91	0.53
1:S:640:THR:O	1:S:644:ASN:ND2	2.40	0.53
1:U:491:MET:HB2	1:U:783:ASP:HA	1.90	0.53
1:W:851:LEU:HD23	1:W:854:LEU:HD12	1.89	0.53
1:X:457:ARG:NH1	1:X:462:THR:OG1	2.34	0.53
3:5:81:SER:OG	3:5:84:GLU:OE2	2.27	0.53
3:5:260:LYS:HD3	4:6:209:MET:HE1	1.91	0.53
3:8:25:ARG:NH2	4:a:4:ASP:OD2	2.42	0.53
4:j:229:LEU:H	4:j:234:ARG:HH21	1.56	0.53
1:A:737:GLN:HG2	1:A:897:LYS:HE2	1.89	0.53
1:A:1005:THR:HG22	1:A:1007:GLY:H	1.74	0.53
1:A:1062:PHE:HB2	1:A:1087:ALA:HB3	1.89	0.53
1:C:451:LYS:HG2	1:C:1140:ALA:HB1	1.91	0.53
1:D:20:LEU:O	1:M:387:GLN:NE2	2.41	0.53
1:D:214:VAL:HA	1:D:217:PHE:HD2	1.73	0.53
1:D:715:PRO:HB3	1:D:800:PRO:HG3	1.89	0.53
1:O:214:VAL:HA	1:O:217:PHE:HD2	1.72	0.53
1:T:540:PHE:O	1:T:559:ARG:NH1	2.42	0.53
1:T:640:THR:O	1:T:644:ASN:ND2	2.38	0.53
1:W:153:ALA:HB1	1:X:338:ASN:HB3	1.91	0.53
1:X:963:ASN:O	1:X:967:ARG:N	2.42	0.53
3:e:204:LEU:HA	3:e:245:PHE:HB2	1.90	0.53
1:B:736:ARG:HD2	1:B:897:LYS:HB2	1.91	0.53
1:B:1005:THR:HG22	1:B:1007:GLY:H	1.73	0.53
1:B:1201:ALA:HB3	1:B:1227:PRO:HG2	1.90	0.53
1:D:641:TYR:O	1:D:645:SER:OG	2.26	0.53
1:E:402:PHE:HD2	1:E:1040:VAL:HB	1.73	0.53
1:E:649:ALA:O	1:E:677:TYR:OH	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:LEU:HD22	1:F:43:ALA:HA	1.91	0.53
1:F:448:ASN:ND2	1:F:1113:VAL:O	2.42	0.53
1:M:579:GLY:HA3	1:M:1011:ALA:HA	1.90	0.53
1:M:829:VAL:HA	1:M:938:MET:HE1	1.91	0.53
1:O:491:MET:HE1	1:O:742:ILE:HG22	1.90	0.53
1:O:824:VAL:H	1:O:889:THR:HG21	1.74	0.53
1:U:864:GLN:O	1:U:930:ARG:NH2	2.42	0.53
1:V:617:GLU:HG3	1:V:656:MET:HG3	1.91	0.53
1:W:965:VAL:HG13	1:W:972:ARG:HD3	1.89	0.53
1:A:578:ARG:NH1	1:A:1014:SER:O	2.42	0.53
1:D:79:GLU:N	1:D:304:ALA:O	2.42	0.53
1:E:48:VAL:HG21	1:F:317:VAL:HA	1.90	0.53
1:E:575:GLN:NE2	1:E:1015:MET:SD	2.82	0.53
1:M:255:ASP:HB2	1:M:1092:ALA:HB1	1.90	0.53
1:N:540:PHE:O	1:N:559:ARG:NH1	2.42	0.53
1:S:708:LEU:HD21	1:S:1022:PRO:HG2	1.90	0.53
1:X:324:ARG:NE	1:X:352:ASP:OD2	2.42	0.53
4:6:87:MET:HE3	4:6:93:LEU:HD21	1.90	0.53
4:7:7:ILE:N	4:7:84:LEU:O	2.38	0.53
4:d:97:ASN:HD21	4:d:296:LEU:HD22	1.74	0.53
4:i:58:ASP:OD2	4:i:199:THR:OG1	2.25	0.53
1:C:1005:THR:HG22	1:C:1007:GLY:H	1.74	0.53
1:F:406:LEU:O	1:F:428:GLN:NE2	2.42	0.53
1:M:435:VAL:HG11	1:M:1368:LEU:HD22	1.91	0.53
1:M:557:THR:HA	1:M:898:ARG:HH22	1.74	0.53
1:M:1083:THR:HG21	4:c:38:ARG:HD3	1.91	0.53
1:O:271:GLN:OE1	1:O:1056:ARG:NH1	2.41	0.53
1:T:56:VAL:HG13	1:U:92:GLN:HB3	1.91	0.53
1:U:399:THR:HG22	1:U:1043:THR:HG22	1.90	0.53
1:V:578:ARG:NH1	1:V:1014:SER:O	2.41	0.53
1:X:1187:ASP:OD2	1:X:1232:ARG:NH2	2.42	0.53
1:4:822:MET:H	1:4:944:PHE:HE2	1.56	0.53
4:a:7:ILE:HB	4:a:84:LEU:HB2	1.91	0.53
1:B:540:PHE:O	1:B:559:ARG:NH1	2.42	0.53
1:D:324:ARG:NH2	1:D:352:ASP:OD1	2.42	0.53
1:F:1241:GLN:HB3	1:F:1244:SER:HB3	1.90	0.53
1:O:1187:ASP:OD2	1:O:1232:ARG:NH2	2.42	0.53
1:W:428:GLN:NE2	1:W:577:SER:OG	2.42	0.53
1:X:8:ARG:HH22	1:X:18:ASN:HD21	1.55	0.53
1:X:706:THR:O	1:X:710:SER:OG	2.27	0.53
4:7:120:ARG:NH1	4:7:123:SER:OG	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:151:GLN:O	4:c:155:TYR:N	2.40	0.53
1:C:714:ASP:O	1:C:804:LYS:NZ	2.43	0.52
1:C:1071:ARG:O	1:C:1079:THR:OG1	2.27	0.52
1:D:828:ASN:ND2	1:D:937:THR:O	2.41	0.52
1:E:927:VAL:HB	1:E:956:THR:HG21	1.90	0.52
1:N:178:VAL:HG22	1:N:1061:MET:HE2	1.90	0.52
1:N:307:VAL:HG12	1:N:309:ARG:H	1.75	0.52
1:U:1210:TYR:HE1	1:U:1280:ARG:HG2	1.72	0.52
1:W:958:HIS:CE1	1:W:960:LEU:HB3	2.45	0.52
1:X:1341:TYR:HB2	1:X:1357:LEU:HD11	1.90	0.52
3:5:225:THR:HG22	3:5:293:THR:HG22	1.91	0.52
4:6:99:TYR:HE2	4:6:139:VAL:H	1.55	0.52
4:j:60:ILE:HG22	4:j:64:GLN:HG2	1.90	0.52
1:A:331:ALA:HA	1:A:335:ASP:HB2	1.90	0.52
1:C:256:THR:HG22	1:C:258:PHE:H	1.74	0.52
1:C:602:GLU:HB3	1:C:647:LYS:HE2	1.91	0.52
1:D:585:VAL:HG11	1:D:1030:HIS:HB3	1.91	0.52
1:D:864:GLN:O	1:D:930:ARG:NH2	2.41	0.52
1:M:744:ASP:H	1:M:786:HIS:HE1	1.56	0.52
1:O:770:LEU:HD11	1:O:883:LEU:HD13	1.91	0.52
1:S:461:PRO:HG2	1:S:906:THR:H	1.74	0.52
1:T:708:LEU:HD21	1:T:1022:PRO:HG2	1.91	0.52
1:T:898:ARG:HE	1:T:913:VAL:HG23	1.75	0.52
1:U:1068:VAL:HG22	1:U:1082:ILE:HG12	1.91	0.52
1:U:1122:PHE:HE1	1:U:1258:ALA:HB2	1.74	0.52
1:C:785:ARG:HG2	1:C:787:VAL:H	1.74	0.52
1:D:450:LEU:HD11	1:D:1025:ILE:HG13	1.90	0.52
1:M:82:ASP:N	1:M:82:ASP:OD1	2.41	0.52
1:N:1263:TYR:OH	1:N:1305:GLN:NE2	2.40	0.52
1:U:572:ARG:NH2	1:U:1001:SER:O	2.41	0.52
1:A:856:ASN:OD1	1:A:860:LYS:NZ	2.42	0.52
1:B:611:LEU:HD22	1:B:862:ILE:HG12	1.90	0.52
1:B:958:HIS:CE1	1:B:960:LEU:HB3	2.44	0.52
1:C:130:GLU:OE1	1:D:110:LYS:NZ	2.40	0.52
1:C:849:ASP:HB2	1:C:869:ARG:HH21	1.75	0.52
1:E:958:HIS:CE1	1:E:960:LEU:HB3	2.44	0.52
1:F:588:MET:HB3	1:F:690:ALA:HB2	1.92	0.52
1:N:1071:ARG:O	1:N:1079:THR:OG1	2.25	0.52
1:O:842:ASP:OD2	2:R:19:TYR:OH	2.28	0.52
1:X:799:ASN:HD21	1:X:802:LEU:HG	1.73	0.52
1:4:927:VAL:O	1:4:956:THR:OG1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LEU:HD21	1:A:372:LYS:HB2	1.91	0.52
1:E:11:PRO:HB2	1:U:332:ARG:HD2	1.92	0.52
1:E:731:MET:HE2	1:E:738:PRO:HB2	1.91	0.52
1:O:532:LEU:O	1:O:1241:GLN:NE2	2.42	0.52
1:U:537:HIS:HA	1:U:1238:TRP:HE1	1.74	0.52
1:V:1005:THR:HG22	1:V:1007:GLY:H	1.72	0.52
1:X:1199:GLY:HA2	1:X:1235:ASN:HB3	1.91	0.52
1:A:1262:MET:HA	1:A:1306:TYR:HA	1.90	0.52
1:F:849:ASP:HB2	1:F:869:ARG:HH21	1.73	0.52
1:O:742:ILE:HG12	1:O:788:LEU:HD11	1.91	0.52
1:S:95:ILE:HD12	1:S:116:VAL:HG21	1.92	0.52
1:T:1190:TYR:OH	1:T:1196:ASN:O	2.27	0.52
1:V:578:ARG:NH2	1:V:1017:GLN:OE1	2.43	0.52
1:V:1187:ASP:OD2	1:V:1232:ARG:NH2	2.42	0.52
1:W:545:HIS:N	1:W:553:SER:O	2.43	0.52
1:4:655:HIS:O	1:4:659:PHE:N	2.42	0.52
3:b:289:CYS:SG	3:b:290:THR:N	2.83	0.52
4:g:88:ASP:HB2	4:g:91:ASP:HB2	1.91	0.52
4:i:266:MET:O	4:j:150:GLN:NE2	2.42	0.52
1:D:1197:PRO:O	1:D:1236:ASN:ND2	2.42	0.52
1:E:1071:ARG:O	1:E:1079:THR:OG1	2.25	0.52
1:M:77:ASN:HA	1:M:1061:MET:HB2	1.92	0.52
1:M:172:ARG:NH1	1:M:382:MET:O	2.42	0.52
1:U:842:ASP:OD2	2:0:19:TYR:OH	2.27	0.52
1:W:420:ARG:NH1	1:X:1353:MET:SD	2.82	0.52
1:W:856:ASN:ND2	2:1:66:GLY:O	2.35	0.52
1:X:49:ARG:HB2	1:4:56:VAL:HB	1.90	0.52
1:D:878:LEU:O	1:D:881:SER:OG	2.28	0.52
1:F:394:ARG:HB3	1:F:1050:HIS:CD2	2.45	0.52
1:F:850:ILE:HD12	1:F:875:ILE:HD12	1.92	0.52
1:F:1341:TYR:HA	1:F:1348:HIS:HD2	1.74	0.52
1:N:236:ARG:NH1	1:N:239:GLN:OE1	2.43	0.52
1:N:1183:PRO:HG2	1:N:1186:SER:HB3	1.91	0.52
1:S:294:GLU:HB2	1:S:366:LEU:HD22	1.91	0.52
1:T:455:HIS:HD2	1:T:1119:PHE:HD1	1.56	0.52
1:U:858:THR:HG22	1:U:934:ALA:HB1	1.92	0.52
1:V:396:ILE:HD11	1:V:1050:HIS:HE1	1.75	0.52
1:W:185:HIS:O	1:W:1097:SER:OG	2.27	0.52
1:W:438:ASN:HD22	1:W:1171:HIS:HD2	1.56	0.52
3:5:124:GLN:NE2	3:5:311:SER:O	2.40	0.52
4:7:277:SER:O	4:7:281:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ASP:HB3	1:A:199:VAL:HG12	1.92	0.52
1:B:387:GLN:OE1	1:C:112:ARG:NH1	2.43	0.52
1:B:714:ASP:O	1:B:804:LYS:NZ	2.43	0.52
1:C:699:THR:HA	1:C:704:PRO:HA	1.91	0.52
1:F:558:HIS:CE1	1:F:902:GLN:HE22	2.27	0.52
1:N:130:GLU:HG3	1:O:110:LYS:HD2	1.91	0.52
1:O:588:MET:HE1	1:O:687:LEU:HA	1.92	0.52
1:S:193:LYS:NZ	1:S:247:ASP:OD2	2.41	0.52
1:T:402:PHE:HD2	1:T:1040:VAL:HB	1.74	0.52
3:8:254:GLU:HG2	4:9:64:GLN:HE21	1.74	0.52
4:d:5:LYS:HD2	4:d:86:ARG:HB3	1.91	0.52
3:e:207:LEU:HD11	3:e:258:MET:HB3	1.92	0.52
1:E:1196:ASN:HD21	1:E:1324:GLN:HG3	1.74	0.52
1:N:127:ALA:HB3	1:N:1082:ILE:HB	1.92	0.52
1:N:1280:ARG:NH2	1:N:1288:GLU:OE1	2.42	0.52
1:O:182:LYS:NZ	1:O:1058:SER:OG	2.42	0.52
1:O:402:PHE:HD2	1:O:1040:VAL:HB	1.74	0.52
1:W:536:VAL:HB	1:W:542:PHE:HE2	1.74	0.52
1:W:839:VAL:O	1:W:876:ARG:NH2	2.43	0.52
1:X:619:MET:SD	1:X:881:SER:OG	2.65	0.52
3:8:78:GLN:NE2	3:8:138:GLY:O	2.43	0.52
3:8:112:PHE:HA	3:8:117:MET:HE3	1.91	0.52
1:E:185:HIS:O	1:E:1097:SER:OG	2.28	0.51
1:N:536:VAL:HG13	1:N:1244:SER:HA	1.91	0.51
1:O:717:LEU:HB2	1:O:990:TRP:HZ3	1.74	0.51
1:X:578:ARG:NH1	1:X:1014:SER:O	2.43	0.51
3:8:300:PRO:HB2	3:8:315:LEU:HD22	1.92	0.51
1:C:537:HIS:HA	1:C:1238:TRP:CD1	2.45	0.51
1:C:878:LEU:O	1:C:881:SER:OG	2.28	0.51
1:N:889:THR:HA	1:N:920:ASN:HB3	1.92	0.51
1:O:79:GLU:N	1:O:304:ALA:O	2.44	0.51
1:O:467:ALA:HB2	1:O:1254:PHE:HE2	1.75	0.51
1:S:648:LEU:HD13	1:S:677:TYR:HE1	1.74	0.51
1:T:606:ASP:OD1	1:T:647:LYS:NZ	2.36	0.51
1:V:214:VAL:HA	1:V:217:PHE:HD2	1.75	0.51
1:V:585:VAL:HG11	1:V:1030:HIS:HB3	1.90	0.51
1:V:720:PRO:HA	1:V:917:VAL:HG13	1.91	0.51
1:W:275:VAL:HG22	1:W:375:ALA:HB3	1.92	0.51
1:4:578:ARG:NH1	1:4:1014:SER:O	2.43	0.51
1:4:620:ILE:HG22	1:4:622:GLY:H	1.75	0.51
4:6:215:SER:HB2	4:7:219:PRO:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:284:PRO:HA	4:6:305:ARG:HB3	1.93	0.51
1:A:191:ILE:HA	1:A:217:PHE:HE1	1.74	0.51
1:A:854:LEU:HD13	1:A:860:LYS:HG2	1.92	0.51
1:M:1062:PHE:HB2	1:M:1087:ALA:HB3	1.91	0.51
4:6:26:LYS:HA	4:6:98:VAL:HG21	1.92	0.51
1:B:704:PRO:HG2	1:C:969:PRO:HD2	1.92	0.51
1:E:82:ASP:OD1	1:E:82:ASP:N	2.42	0.51
1:M:450:LEU:HD11	1:M:1025:ILE:HG13	1.91	0.51
1:M:1170:SER:OG	1:N:1227:PRO:O	2.27	0.51
1:N:1163:CYS:SG	1:N:1164:GLU:N	2.84	0.51
1:O:1190:TYR:OH	1:O:1196:ASN:O	2.27	0.51
1:S:200:TYR:HE1	1:X:1105:ALA:HB1	1.75	0.51
1:T:1167:PRO:HG2	1:U:1218:LEU:HD23	1.91	0.51
1:U:82:ASP:N	1:U:82:ASP:OD1	2.43	0.51
1:X:898:ARG:HH21	1:X:913:VAL:HG21	1.75	0.51
3:8:224:VAL:HG13	3:8:294:VAL:HB	1.93	0.51
4:c:288:VAL:HG22	4:c:300:CYS:HB2	1.92	0.51
4:i:15:LEU:HD12	4:i:79:PRO:HA	1.92	0.51
1:A:236:ARG:HH21	1:A:239:GLN:HG3	1.76	0.51
1:A:438:ASN:HD22	1:A:1171:HIS:CD2	2.28	0.51
1:A:1003:GLN:NE2	1:F:587:ASN:OD1	2.43	0.51
1:A:1227:PRO:O	1:F:1170:SER:OG	2.28	0.51
1:C:850:ILE:HD11	1:C:872:VAL:HA	1.92	0.51
1:D:278:THR:HG22	1:D:1051:ILE:HA	1.93	0.51
1:D:395:ARG:HD3	1:D:1045:GLU:HB3	1.93	0.51
1:F:785:ARG:HG2	1:F:787:VAL:H	1.76	0.51
1:M:706:THR:O	1:M:710:SER:OG	2.28	0.51
1:S:587:ASN:OD1	1:T:1003:GLN:NE2	2.44	0.51
1:W:736:ARG:HH22	1:W:900:PRO:HD3	1.75	0.51
1:X:510:PRO:HD2	1:X:976:VAL:HG13	1.92	0.51
1:4:514:GLN:HE21	1:4:531:LEU:HD21	1.75	0.51
4:9:13:SER:OG	4:9:130:ASN:ND2	2.43	0.51
1:B:606:ASP:OD1	1:B:647:LYS:NZ	2.33	0.51
1:B:1241:GLN:HB3	1:B:1244:SER:HB3	1.92	0.51
1:D:629:MET:HE3	1:D:877:VAL:HG13	1.93	0.51
1:F:68:GLU:HA	1:F:362:ILE:HD12	1.93	0.51
1:F:127:ALA:HB3	1:F:1082:ILE:HB	1.92	0.51
1:M:561:MET:HE2	1:M:711:ALA:HB1	1.93	0.51
1:N:788:LEU:HD21	1:N:919:VAL:HG21	1.92	0.51
1:O:82:ASP:HB2	1:O:85:ARG:HB2	1.93	0.51
1:O:537:HIS:HA	1:O:1238:TRP:HE1	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:83:LEU:HD21	1:S:122:LYS:HD2	1.91	0.51
1:T:800:PRO:HB2	1:T:804:LYS:HE3	1.91	0.51
1:V:266:THR:HA	1:V:297:MET:HA	1.92	0.51
1:4:1204:VAL:O	1:4:1283:TYR:OH	2.28	0.51
4:7:16:PHE:HZ	4:7:128:GLU:HB2	1.74	0.51
1:A:90:LYS:HB3	1:F:53:LEU:HD23	1.93	0.51
1:A:635:ALA:HB1	1:A:668:SER:HB3	1.92	0.51
1:C:474:ASP:OD1	1:C:552:GLY:N	2.40	0.51
1:N:66:PHE:HD1	1:N:175:VAL:HG22	1.76	0.51
1:U:450:LEU:HD11	1:U:1025:ILE:HA	1.91	0.51
1:V:850:ILE:HD11	1:V:872:VAL:HA	1.91	0.51
1:V:1245:LEU:HA	1:V:1248:VAL:HB	1.92	0.51
1:W:450:LEU:HD11	1:W:1025:ILE:HG13	1.93	0.51
1:W:929:ASP:OD1	1:W:932:ARG:NH2	2.43	0.51
4:a:51:CYS:HB2	4:a:62:ILE:HD11	1.93	0.51
4:d:51:CYS:HB2	4:d:62:ILE:HD11	1.93	0.51
4:j:51:CYS:HB2	4:j:62:ILE:HD11	1.91	0.51
1:A:273:ALA:O	1:A:1053:TYR:OH	2.27	0.51
1:C:214:VAL:HA	1:C:217:PHE:HD2	1.76	0.51
1:C:617:GLU:HG3	1:C:656:MET:HG3	1.92	0.51
1:C:899:ASP:OD2	1:C:1018:LYS:NZ	2.32	0.51
1:E:127:ALA:HB3	1:E:1082:ILE:HB	1.91	0.51
1:N:1187:ASP:OD2	1:N:1232:ARG:NH2	2.44	0.51
1:O:130:GLU:HG2	1:O:1079:THR:HG22	1.91	0.51
1:V:197:ASP:HB3	1:V:199:VAL:HG12	1.91	0.51
1:V:436:ASN:HB3	1:V:440:VAL:H	1.75	0.51
1:X:687:LEU:HD23	1:X:805:LEU:HD22	1.93	0.51
1:A:230:LYS:HB3	1:A:234:MET:HE3	1.93	0.51
1:A:658:ARG:HA	1:A:681:LEU:HD11	1.92	0.51
1:C:125:ILE:HB	1:C:1084:HIS:HB3	1.93	0.51
1:E:737:GLN:HB3	1:E:897:LYS:H	1.74	0.51
1:N:603:THR:HG22	1:N:647:LYS:HB3	1.93	0.51
1:S:1051:ILE:O	1:S:1100:ALA:N	2.44	0.51
1:T:1196:ASN:HD22	1:T:1202:ALA:H	1.58	0.51
1:W:780:GLU:OE1	1:W:785:ARG:NH1	2.41	0.51
1:X:6:GLU:HG3	1:X:7:GLN:HG3	1.93	0.51
1:4:539:PHE:HE1	1:4:565:ILE:HD11	1.76	0.51
1:4:836:ASN:HD21	1:4:839:VAL:HB	1.75	0.51
4:d:69:CYS:SG	4:d:70:THR:N	2.83	0.51
1:A:210:LYS:NZ	1:A:1207:CYS:O	2.42	0.51
1:O:536:VAL:HB	1:O:542:PHE:HE2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1073:VAL:O	4:g:92:ASN:ND2	2.43	0.51
1:U:454:CYS:O	1:U:1127:TYR:OH	2.27	0.51
1:U:1059:THR:HG22	1:U:1090:HIS:HA	1.93	0.51
1:V:79:GLU:N	1:V:304:ALA:O	2.44	0.51
1:4:1074:ARG:HH12	4:6:83:ARG:HG3	1.75	0.51
4:d:19:GLU:OE2	4:d:128:GLU:N	2.40	0.51
1:B:932:ARG:HE	1:B:956:THR:HG23	1.77	0.50
1:F:297:MET:HE3	1:F:364:ALA:HB3	1.93	0.50
2:J:74:LEU:HD23	2:J:77:LEU:HD12	1.94	0.50
1:M:898:ARG:O	1:M:903:SER:OG	2.29	0.50
1:T:1196:ASN:HD21	1:T:1324:GLN:HG3	1.76	0.50
1:T:1258:ALA:HB1	3:e:98:ASN:HD22	1.76	0.50
1:U:1200:ARG:NH1	1:U:1233:SER:O	2.44	0.50
1:W:224:HIS:CD2	1:W:244:MET:HE1	2.45	0.50
1:W:399:THR:HA	1:W:1043:THR:HA	1.93	0.50
1:4:737:GLN:NE2	1:4:749:ASN:OD1	2.44	0.50
4:f:113:VAL:HG22	4:f:139:VAL:HG12	1.93	0.50
1:A:67:LEU:HD11	1:A:300:PRO:HG2	1.91	0.50
1:D:902:GLN:NE2	1:D:1018:LYS:O	2.43	0.50
1:D:1196:ASN:HD22	1:D:1201:ALA:HA	1.76	0.50
1:E:5:LEU:HD12	1:U:117:MET:HB2	1.92	0.50
1:N:396:ILE:HD11	1:N:1050:HIS:HE1	1.77	0.50
1:O:224:HIS:CD2	1:O:244:MET:HE1	2.46	0.50
1:O:436:ASN:HB3	1:O:440:VAL:H	1.76	0.50
1:O:537:HIS:HB3	1:O:1245:LEU:HB2	1.93	0.50
1:O:821:GLY:HA2	1:O:923:GLY:HA2	1.93	0.50
1:X:540:PHE:O	1:X:559:ARG:NH1	2.45	0.50
1:4:397:GLN:NE2	1:4:1263:TYR:OH	2.44	0.50
4:a:33:LEU:N	4:a:69:CYS:SG	2.75	0.50
4:f:151:GLN:O	4:f:155:TYR:N	2.40	0.50
1:C:83:LEU:HD13	1:C:1085:GLU:HB3	1.93	0.50
1:D:249:LEU:HD21	1:D:372:LYS:HB2	1.93	0.50
1:E:13:LEU:O	1:T:58:THR:N	2.42	0.50
1:E:380:GLN:O	1:E:384:ASN:N	2.45	0.50
1:F:113:GLN:HB3	1:T:38:LEU:HB2	1.91	0.50
1:F:855:GLU:HG2	2:K:70:ARG:HE	1.76	0.50
1:F:1210:TYR:HE1	1:F:1280:ARG:HG2	1.75	0.50
2:R:74:LEU:HD23	2:R:77:LEU:HD12	1.94	0.50
1:U:1199:GLY:HA2	1:U:1235:ASN:HB3	1.93	0.50
1:W:958:HIS:HE1	1:W:960:LEU:HB3	1.77	0.50
1:W:1199:GLY:HA2	1:W:1235:ASN:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:278:THR:HG22	1:X:1051:ILE:HA	1.93	0.50
4:9:176:LEU:O	4:9:180:ASN:ND2	2.43	0.50
1:A:564:ASN:ND2	1:A:990:TRP:O	2.45	0.50
1:D:826:TYR:HE2	1:D:886:PRO:HG2	1.75	0.50
1:E:770:LEU:HD21	1:E:883:LEU:HD22	1.92	0.50
1:S:438:ASN:HD22	1:S:1171:HIS:HD2	1.58	0.50
1:T:636:LEU:HD23	1:T:870:PRO:HA	1.93	0.50
1:U:1168:GLY:HA2	1:V:207:LYS:HD3	1.93	0.50
1:V:277:GLU:HG2	1:V:377:GLU:HB2	1.92	0.50
1:W:183:LEU:HD13	1:W:394:ARG:HH21	1.75	0.50
2:Z:74:LEU:HD23	2:Z:77:LEU:HD12	1.94	0.50
1:4:47:SER:OG	1:4:48:VAL:N	2.44	0.50
4:a:88:ASP:HB2	4:a:91:ASP:HB2	1.92	0.50
3:h:70:TYR:HE1	3:h:166:VAL:HG21	1.77	0.50
1:A:434:VAL:HG11	1:A:1042:ARG:HH22	1.77	0.50
1:B:640:THR:O	1:B:644:ASN:ND2	2.45	0.50
1:B:856:ASN:OD1	1:B:860:LYS:NZ	2.41	0.50
1:D:90:LYS:HE2	1:D:117:MET:HE1	1.93	0.50
1:E:578:ARG:NH1	1:E:1014:SER:OG	2.45	0.50
1:N:871:THR:OG1	1:N:874:MET:SD	2.68	0.50
1:S:94:LYS:HG2	1:S:115:ILE:HG12	1.93	0.50
1:S:224:HIS:HD2	1:S:244:MET:HE1	1.77	0.50
1:S:423:GLU:OE2	1:X:420:ARG:NH2	2.45	0.50
1:T:332:ARG:NH2	1:T:346:ASP:OD1	2.45	0.50
1:T:450:LEU:HD21	1:T:1025:ILE:HG13	1.92	0.50
1:U:397:GLN:HB3	1:U:1318:GLN:HB3	1.92	0.50
1:U:619:MET:SD	1:U:881:SER:OG	2.63	0.50
2:1:74:LEU:HD23	2:1:77:LEU:HD12	1.94	0.50
2:2:74:LEU:HD23	2:2:77:LEU:HD12	1.94	0.50
1:4:455:HIS:HE2	1:4:1122:PHE:HB2	1.76	0.50
4:d:53:ARG:NH2	4:d:133:ASP:OD2	2.44	0.50
1:C:481:TYR:OH	1:C:979:VAL:N	2.45	0.50
1:F:1187:ASP:OD2	1:F:1232:ARG:NH2	2.44	0.50
1:M:319:TYR:OH	1:V:323:MET:SD	2.59	0.50
1:M:609:TYR:HE2	1:M:614:TYR:HB2	1.76	0.50
1:N:683:GLU:O	1:N:687:LEU:N	2.38	0.50
1:N:714:ASP:O	1:N:804:LYS:NZ	2.45	0.50
1:S:1201:ALA:HB3	1:S:1227:PRO:HG2	1.94	0.50
1:V:56:VAL:HG22	1:W:92:GLN:HB3	1.93	0.50
1:V:855:GLU:HG2	2:0:70:ARG:HE	1.76	0.50
2:Y:74:LEU:HD23	2:Y:77:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:114:LEU:HD11	4:9:145:GLY:HA2	1.94	0.50
4:g:7:ILE:HG21	4:g:33:LEU:HD21	1.93	0.50
1:C:507:ALA:HB1	1:C:978:ASN:HD21	1.76	0.50
1:C:963:ASN:O	1:C:967:ARG:NE	2.39	0.50
1:C:1171:HIS:HE1	1:D:1228:ALA:HA	1.76	0.50
1:D:41:LYS:O	1:D:44:ARG:NH1	2.44	0.50
1:D:619:MET:SD	1:D:881:SER:OG	2.69	0.50
1:D:1062:PHE:HB2	1:D:1087:ALA:HB3	1.94	0.50
1:M:918:LEU:HB2	1:M:944:PHE:HE2	1.76	0.50
1:T:9:PRO:HG3	1:T:45:GLU:HB3	1.94	0.50
1:T:743:GLY:HA3	1:T:786:HIS:HE1	1.75	0.50
1:T:1173:GLN:NE2	1:T:1302:THR:OG1	2.44	0.50
1:U:537:HIS:HA	1:U:1238:TRP:NE1	2.27	0.50
1:V:397:GLN:HE22	1:V:1298:ALA:HB3	1.76	0.50
1:V:569:LEU:HD13	1:V:1238:TRP:HH2	1.76	0.50
1:W:394:ARG:NH1	1:W:1317:ASP:OD2	2.45	0.50
1:X:773:ILE:O	1:X:776:THR:OG1	2.29	0.50
3:8:295:PRO:HG3	3:8:319:ASN:HB2	1.94	0.50
3:b:224:VAL:HG13	3:b:294:VAL:HB	1.93	0.50
1:M:228:LEU:HD22	1:M:1103:HIS:HD2	1.77	0.50
1:O:1137:LYS:HA	1:O:1140:ALA:HB3	1.93	0.50
1:S:438:ASN:HD22	1:S:1171:HIS:CD2	2.30	0.50
1:T:600:ILE:O	1:T:603:THR:OG1	2.28	0.50
1:T:1067:SER:OG	1:T:1083:THR:OG1	2.29	0.50
1:T:1207:CYS:SG	1:T:1208:ASP:N	2.84	0.50
1:U:446:TYR:O	1:U:450:LEU:N	2.44	0.50
1:V:525:HIS:HD2	1:V:527:THR:HG22	1.77	0.50
1:V:864:GLN:O	1:V:930:ARG:NH2	2.45	0.50
2:0:74:LEU:HD23	2:0:77:LEU:HD12	1.94	0.50
1:4:699:THR:HG22	1:4:704:PRO:HG3	1.93	0.50
1:4:708:LEU:HD22	1:4:1022:PRO:HG2	1.93	0.50
4:i:5:LYS:HB2	4:i:86:ARG:HB3	1.94	0.50
1:A:823:GLY:HA2	1:A:889:THR:HG21	1.94	0.50
1:C:770:LEU:HD11	1:C:883:LEU:HD13	1.94	0.50
1:D:434:VAL:HG11	1:D:1042:ARG:HH22	1.76	0.50
1:E:718:LEU:HD12	1:E:894:VAL:HG21	1.94	0.50
1:F:163:LEU:HD12	3:e:34:PHE:HE1	1.76	0.50
1:M:699:THR:HA	1:M:704:PRO:HA	1.94	0.50
1:N:898:ARG:HB3	1:N:902:GLN:HB2	1.94	0.50
1:N:1033:HIS:NE2	1:N:1036:PHE:O	2.43	0.50
1:O:419:VAL:HG11	1:O:1352:HIS:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:842:ASP:OD2	2:Y:19:TYR:OH	2.29	0.50
1:U:406:LEU:HD21	1:U:1191:PHE:HE2	1.77	0.50
1:U:1226:ASP:HB2	1:U:1229:TYR:H	1.76	0.50
1:W:1344:ASN:ND2	1:W:1347:THR:OG1	2.44	0.50
1:X:273:ALA:O	1:X:1053:TYR:OH	2.29	0.50
1:X:708:LEU:HD21	1:X:1022:PRO:HG2	1.93	0.50
1:X:887:PHE:O	1:X:920:ASN:ND2	2.44	0.50
3:5:269:THR:HA	3:5:272:ILE:HD12	1.94	0.50
3:8:77:SER:N	3:8:173:PHE:O	2.45	0.50
4:a:158:TYR:HA	4:a:161:ILE:HD12	1.93	0.50
3:b:128:VAL:HG11	3:b:312:LEU:HD22	1.92	0.50
4:i:204:LEU:HD23	4:i:207:LEU:HD12	1.94	0.50
1:A:545:HIS:HE1	1:A:555:ARG:HD2	1.76	0.49
1:B:1067:SER:OG	1:B:1083:THR:OG1	2.29	0.49
1:C:133:ALA:HB2	1:C:1076:ASP:HA	1.94	0.49
1:C:493:LEU:HD13	1:C:942:VAL:HG21	1.93	0.49
1:C:1281:GLY:O	1:C:1284:THR:OG1	2.26	0.49
1:D:1169:LEU:HD21	1:E:208:ALA:HA	1.93	0.49
1:E:396:ILE:HD11	1:E:1050:HIS:HE1	1.75	0.49
2:G:74:LEU:HD23	2:G:77:LEU:HD12	1.94	0.49
2:K:74:LEU:HD23	2:K:77:LEU:HD12	1.94	0.49
2:L:74:LEU:HD23	2:L:77:LEU:HD12	1.93	0.49
1:N:740:ILE:HB	1:N:747:TYR:HB3	1.94	0.49
1:O:255:ASP:HB3	1:O:1093:LEU:HB3	1.92	0.49
1:T:185:HIS:O	1:T:1097:SER:OG	2.30	0.49
1:T:1047:LEU:HD12	1:T:1106:ALA:HB3	1.93	0.49
1:U:918:LEU:HB2	1:U:944:PHE:CE2	2.47	0.49
1:W:579:GLY:HA3	1:W:1011:ALA:HA	1.94	0.49
1:X:536:VAL:HG13	1:X:1244:SER:HA	1.93	0.49
1:4:174:LEU:HD11	1:4:1084:HIS:HE1	1.76	0.49
1:4:731:MET:HG2	1:4:738:PRO:HD2	1.94	0.49
4:j:5:LYS:HB2	4:j:86:ARG:HB3	1.94	0.49
1:D:714:ASP:O	1:D:804:LYS:NZ	2.44	0.49
1:D:840:PHE:HE1	2:J:49:LEU:HD11	1.76	0.49
1:D:1168:GLY:HA2	1:E:207:LYS:HD3	1.94	0.49
1:E:49:ARG:NH2	4:g:76:GLU:OE2	2.45	0.49
1:E:130:GLU:HG2	1:E:1079:THR:HG22	1.94	0.49
1:F:757:ILE:HG12	1:F:788:LEU:HD22	1.93	0.49
1:F:842:ASP:OD2	2:L:19:TYR:OH	2.27	0.49
1:F:1344:ASN:ND2	1:F:1347:THR:OG1	2.45	0.49
2:H:74:LEU:HD23	2:H:77:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:851:LEU:HD12	1:M:869:ARG:HD2	1.93	0.49
1:N:600:ILE:O	1:N:603:THR:OG1	2.26	0.49
1:T:578:ARG:NH2	1:T:1017:GLN:OE1	2.45	0.49
1:V:712:LEU:O	1:V:804:LYS:NZ	2.45	0.49
1:V:1255:ARG:HB2	1:V:1258:ALA:HB2	1.92	0.49
1:W:1062:PHE:HB2	1:W:1087:ALA:HB3	1.94	0.49
1:A:718:LEU:HD12	1:A:894:VAL:HG21	1.93	0.49
1:B:850:ILE:HD12	1:B:875:ILE:HD12	1.93	0.49
1:F:71:LEU:N	1:F:377:GLU:OE2	2.46	0.49
1:F:146:PRO:HA	1:F:149:PHE:HD2	1.77	0.49
1:M:619:MET:SD	1:M:881:SER:OG	2.67	0.49
1:N:839:VAL:HG13	1:N:876:ARG:HG2	1.93	0.49
1:N:1115:CYS:HA	1:N:1177:CYS:HB2	1.93	0.49
1:O:504:LYS:HE2	1:O:507:ALA:HB2	1.93	0.49
1:U:414:SER:OG	1:U:416:SER:OG	2.29	0.49
1:V:182:LYS:NZ	1:V:1058:SER:OG	2.46	0.49
1:V:1251:ASN:ND2	1:V:1270:PHE:O	2.36	0.49
2:3:74:LEU:HD23	2:3:77:LEU:HD12	1.94	0.49
4:6:5:LYS:HD3	4:6:88:ASP:HB2	1.93	0.49
1:B:854:LEU:HD13	1:B:860:LYS:HG2	1.93	0.49
1:C:706:THR:O	1:C:710:SER:OG	2.30	0.49
1:E:491:MET:HB2	1:E:783:ASP:HA	1.94	0.49
1:E:1115:CYS:HA	1:E:1177:CYS:HB2	1.95	0.49
1:S:582:PHE:HE1	1:S:694:LEU:HD11	1.78	0.49
1:V:592:ILE:HD11	1:V:680:ILE:HA	1.93	0.49
1:V:831:LEU:HD22	2:1:9:PRO:HG2	1.93	0.49
1:W:49:ARG:HD3	1:X:87:ILE:HD11	1.94	0.49
1:4:92:GLN:HB3	1:4:117:MET:HG2	1.93	0.49
4:6:124:THR:HG22	4:6:135:VAL:HG22	1.94	0.49
3:b:79:THR:HA	3:b:139:LEU:HD21	1.95	0.49
1:A:918:LEU:HB2	1:A:944:PHE:CE2	2.48	0.49
1:A:1293:LEU:HD21	1:A:1297:PRO:HG3	1.93	0.49
1:B:600:ILE:O	1:B:604:ALA:N	2.46	0.49
1:B:1169:LEU:O	1:C:1206:SER:OG	2.24	0.49
1:C:438:ASN:HD22	1:C:1171:HIS:CD2	2.31	0.49
1:M:183:LEU:HD13	1:M:394:ARG:HH21	1.77	0.49
1:M:1171:HIS:HE1	1:N:1228:ALA:HA	1.76	0.49
1:N:294:GLU:HB2	1:N:366:LEU:HD22	1.92	0.49
1:N:831:LEU:HD22	2:Q:9:PRO:HG2	1.94	0.49
1:O:537:HIS:HA	1:O:1238:TRP:NE1	2.27	0.49
2:Q:74:LEU:HD23	2:Q:77:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:1187:ASP:OD2	1:T:1232:ARG:NH2	2.45	0.49
1:U:1078:VAL:HG21	3:b:41:LEU:HD23	1.93	0.49
1:U:1312:THR:HG22	4:d:41:ASN:HD22	1.77	0.49
1:W:447:GLN:HA	1:W:450:LEU:HB2	1.95	0.49
1:W:760:ARG:HH12	1:W:886:PRO:HA	1.77	0.49
1:4:945:ASN:HB3	1:4:948:TYR:HD2	1.78	0.49
3:5:128:VAL:HG11	3:5:312:LEU:HD13	1.94	0.49
1:A:714:ASP:O	1:A:804:LYS:NZ	2.44	0.49
1:C:907:HIS:HB2	1:C:910:GLY:H	1.78	0.49
1:C:1210:TYR:HE1	1:C:1280:ARG:HG2	1.76	0.49
1:F:1071:ARG:O	1:F:1079:THR:OG1	2.30	0.49
1:N:38:LEU:HD11	1:N:43:ALA:HA	1.94	0.49
1:O:624:GLU:HB2	1:O:762:ARG:HH12	1.78	0.49
1:O:684:LEU:HA	1:O:687:LEU:HB2	1.94	0.49
1:U:1071:ARG:HH22	4:d:38:ARG:N	2.11	0.49
1:W:172:ARG:O	1:W:176:ASP:N	2.38	0.49
1:W:1328:PRO:HB2	1:W:1358:ILE:HG21	1.94	0.49
1:X:633:LEU:HA	1:X:874:MET:HE3	1.94	0.49
1:X:850:ILE:HD12	1:X:875:ILE:HD12	1.94	0.49
3:5:183:GLY:HA2	3:5:322:ALA:H	1.76	0.49
4:f:160:LYS:HG2	4:g:229:LEU:HA	1.95	0.49
1:A:1109:THR:O	1:A:1111:MET:N	2.46	0.49
1:B:491:MET:HB2	1:B:783:ASP:HA	1.95	0.49
1:B:537:HIS:HA	1:B:1238:TRP:HD1	1.78	0.49
1:B:877:VAL:O	1:B:880:THR:OG1	2.30	0.49
1:C:183:LEU:HD13	1:C:394:ARG:HH21	1.77	0.49
1:C:557:THR:HA	1:C:898:ARG:HH22	1.78	0.49
1:D:738:PRO:HB3	1:D:896:THR:HG22	1.94	0.49
1:D:889:THR:HB	1:D:918:LEU:HD11	1.94	0.49
1:E:183:LEU:HD13	1:E:394:ARG:HH21	1.77	0.49
1:M:257:VAL:HG12	1:M:350:LEU:HD21	1.95	0.49
1:N:481:TYR:OH	1:N:979:VAL:N	2.46	0.49
1:U:418:SER:HB3	1:V:415:THR:HG23	1.94	0.49
1:U:618:ALA:HB2	1:U:922:PHE:HE1	1.77	0.49
1:U:1195:SER:O	1:U:1326:ALA:N	2.43	0.49
1:U:1259:LEU:HD12	1:U:1260:PRO:HD2	1.94	0.49
1:W:1247:ASP:O	1:W:1251:ASN:ND2	2.46	0.49
3:5:147:SER:O	3:5:151:ASP:N	2.43	0.49
4:j:33:LEU:N	4:j:69:CYS:SG	2.86	0.49
1:B:279:THR:HB	1:B:380:GLN:HE21	1.77	0.49
1:E:452:SER:HB2	1:E:1118:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:536:VAL:HG12	1:E:537:HIS:HD2	1.78	0.49
1:M:185:HIS:O	1:M:1097:SER:OG	2.31	0.49
1:M:1236:ASN:HB2	1:M:1238:TRP:HE3	1.78	0.49
1:N:418:SER:HB3	1:O:415:THR:HG23	1.95	0.49
1:N:652:ASN:ND2	1:N:923:GLY:O	2.45	0.49
1:S:578:ARG:NH1	1:S:1014:SER:OG	2.46	0.49
1:V:717:LEU:HD12	1:V:915:GLN:HE22	1.77	0.49
1:W:541:ASP:N	1:W:557:THR:O	2.46	0.49
1:W:578:ARG:NH1	1:W:1014:SER:O	2.45	0.49
1:4:249:LEU:HD21	1:4:372:LYS:HB2	1.95	0.49
3:8:228:ALA:HB3	3:8:289:CYS:HB3	1.94	0.49
4:9:87:MET:HE3	4:9:93:LEU:HD21	1.94	0.49
4:9:213:ILE:HG12	4:a:244:VAL:HG11	1.95	0.49
4:9:277:SER:OG	4:a:281:ASN:ND2	2.45	0.49
4:c:9:VAL:HB	4:c:82:LEU:HB2	1.95	0.49
1:B:695:ALA:HB1	1:B:706:THR:HG22	1.95	0.49
1:C:79:GLU:N	1:C:304:ALA:O	2.45	0.49
1:C:172:ARG:HG3	1:D:100:ILE:HA	1.95	0.49
1:E:463:GLN:HE21	1:E:467:ALA:HB2	1.78	0.49
1:E:539:PHE:O	1:E:559:ARG:N	2.45	0.49
1:F:629:MET:HE3	1:F:877:VAL:HG13	1.95	0.49
1:M:495:ARG:NH1	2:P:3:ASN:O	2.46	0.49
1:O:279:THR:OG1	1:O:280:ASP:N	2.43	0.49
1:S:729:ASP:HB2	1:S:793:LEU:HD11	1.95	0.49
1:U:918:LEU:HB2	1:U:944:PHE:HE2	1.78	0.49
1:V:658:ARG:NH2	1:W:929:ASP:OD2	2.46	0.49
1:V:1169:LEU:O	1:W:1206:SER:OG	2.24	0.49
1:W:684:LEU:HA	1:W:687:LEU:HD13	1.94	0.49
1:W:893:ARG:HG3	1:W:916:THR:HG22	1.94	0.49
1:X:770:LEU:HD11	1:X:883:LEU:HD13	1.94	0.49
1:X:1062:PHE:HB2	1:X:1087:ALA:HB3	1.95	0.49
4:6:213:ILE:HG23	4:7:244:VAL:HG11	1.94	0.49
4:7:196:ASP:HB2	4:7:202:ARG:HH12	1.76	0.49
4:d:144:LEU:O	4:d:148:ILE:N	2.44	0.49
3:h:228:ALA:HB3	3:h:289:CYS:HB3	1.95	0.49
1:B:1341:TYR:HA	1:B:1348:HIS:HD2	1.78	0.49
1:C:249:LEU:HD21	1:C:372:LYS:HB2	1.95	0.49
1:C:277:GLU:HG2	1:C:377:GLU:HB2	1.94	0.49
1:F:80:PHE:HD2	1:F:83:LEU:HD12	1.77	0.49
1:M:79:GLU:HB3	1:M:305:SER:HA	1.94	0.49
1:N:877:VAL:O	1:N:880:THR:OG1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:606:ASP:OD1	1:O:647:LYS:NZ	2.35	0.49
1:W:1225:PRO:HB2	1:W:1230:GLU:HG3	1.94	0.49
1:X:406:LEU:HD21	1:X:1191:PHE:HE2	1.77	0.49
1:4:361:ARG:NH1	1:4:362:ILE:O	2.46	0.49
1:4:851:LEU:HD22	1:4:863:LEU:HB3	1.94	0.49
3:8:90:LEU:HD11	3:8:165:MET:HG3	1.94	0.49
3:b:25:ARG:NH2	4:d:4:ASP:OD2	2.46	0.49
1:A:889:THR:HB	1:A:918:LEU:HD11	1.95	0.48
1:A:1171:HIS:HE1	1:B:1228:ALA:HA	1.78	0.48
1:B:342:SER:O	1:B:346:ASP:N	2.45	0.48
1:C:79:GLU:HB3	1:C:305:SER:HA	1.95	0.48
1:E:307:VAL:HG12	1:E:309:ARG:H	1.78	0.48
1:E:537:HIS:CE1	1:E:539:PHE:HB2	2.48	0.48
1:E:1250:TYR:HB2	1:E:1270:PHE:HD2	1.76	0.48
1:M:331:ALA:HA	1:M:335:ASP:HB2	1.94	0.48
1:N:717:LEU:HD11	1:N:808:TYR:HE2	1.78	0.48
1:O:245:LEU:HD22	1:O:369:ILE:HG21	1.95	0.48
2:P:74:LEU:HD23	2:P:77:LEU:HD12	1.94	0.48
1:S:1224:ILE:HD13	1:X:1167:PRO:HD3	1.95	0.48
1:T:436:ASN:HD22	1:T:440:VAL:HB	1.77	0.48
1:T:824:VAL:H	1:T:889:THR:HG21	1.78	0.48
1:U:927:VAL:HG21	1:U:957:LEU:HD21	1.94	0.48
1:V:276:LEU:HB3	1:V:1053:TYR:HD1	1.78	0.48
1:V:1020:SER:N	1:V:1023:SER:OG	2.45	0.48
1:W:402:PHE:HD2	1:W:1040:VAL:HB	1.77	0.48
1:W:578:ARG:NH2	1:W:1017:GLN:OE1	2.45	0.48
1:4:676:HIS:HA	1:4:679:LYS:HB2	1.94	0.48
4:6:262:ASP:OD2	4:7:158:TYR:OH	2.30	0.48
4:a:205:ASP:O	4:a:209:MET:N	2.42	0.48
3:b:227:TYR:HB2	3:b:246:PHE:HB2	1.93	0.48
4:f:89:PRO:HA	4:f:302:TYR:HD2	1.77	0.48
4:f:151:GLN:HG2	4:f:179:THR:HA	1.95	0.48
4:i:257:LEU:HD13	4:j:158:TYR:HE1	1.78	0.48
1:A:91:ILE:HD11	1:A:1089:LEU:HD11	1.95	0.48
1:D:290:LEU:HD23	1:D:367:VAL:HG21	1.95	0.48
1:D:1163:CYS:SG	1:D:1164:GLU:N	2.85	0.48
1:E:158:THR:OG1	1:T:45:GLU:OE1	2.31	0.48
1:E:945:ASN:OD1	1:E:946:LYS:N	2.46	0.48
1:E:1070:ARG:NH1	3:b:67:GLN:OE1	2.46	0.48
1:E:1190:TYR:OH	1:E:1196:ASN:O	2.30	0.48
1:E:1301:THR:HG21	1:F:203:ARG:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:224:HIS:HD2	1:M:244:MET:HE1	1.78	0.48
1:M:421:GLY:HA3	1:N:413:TYR:HA	1.95	0.48
1:M:564:ASN:HA	1:M:994:PRO:HG2	1.95	0.48
1:M:1210:TYR:HE1	1:M:1280:ARG:HG2	1.78	0.48
1:O:740:ILE:HB	1:O:747:TYR:HB3	1.94	0.48
1:O:1134:ASP:O	1:O:1138:MET:N	2.47	0.48
1:S:945:ASN:HB3	1:S:948:TYR:H	1.77	0.48
1:T:406:LEU:HD21	1:T:1191:PHE:HE2	1.78	0.48
1:U:277:GLU:HG2	1:U:377:GLU:HB2	1.95	0.48
1:X:447:GLN:HB3	1:X:1028:ALA:HB1	1.95	0.48
1:X:555:ARG:HA	1:X:907:HIS:HE1	1.79	0.48
4:7:23:LEU:HD11	4:7:125:ILE:HG21	1.95	0.48
3:8:283:LEU:O	4:9:272:TYR:OH	2.32	0.48
4:i:35:ASP:HB2	4:i:40:GLN:HE22	1.77	0.48
1:F:75:CYS:HG	1:F:1059:THR:HG1	1.56	0.48
1:F:1130:ARG:HH11	4:f:234:ARG:HD2	1.78	0.48
2:I:74:LEU:HD23	2:I:77:LEU:HD12	1.94	0.48
1:M:878:LEU:O	1:M:881:SER:OG	2.32	0.48
1:N:582:PHE:HE1	1:N:694:LEU:HD11	1.77	0.48
1:N:663:HIS:HA	1:O:930:ARG:HD2	1.95	0.48
1:W:312:ASN:ND2	1:W:323:MET:O	2.46	0.48
1:W:394:ARG:HD3	1:W:1315:PHE:HB3	1.96	0.48
1:X:623:GLN:HB2	1:X:626:LYS:HB2	1.95	0.48
4:f:61:GLN:HB2	4:f:199:THR:HG21	1.95	0.48
4:f:205:ASP:O	4:f:208:SER:OG	2.26	0.48
4:i:36:CYS:SG	4:i:86:ARG:NH2	2.79	0.48
1:C:504:LYS:HB3	1:C:967:ARG:HH12	1.78	0.48
1:C:927:VAL:HB	1:C:956:THR:HG21	1.95	0.48
1:D:22:GLN:NE2	1:N:201:SER:OG	2.44	0.48
1:D:276:LEU:HB3	1:D:1053:TYR:HD1	1.79	0.48
1:D:423:GLU:HA	1:D:1352:HIS:HE1	1.78	0.48
1:E:217:PHE:O	1:E:221:LEU:N	2.41	0.48
1:O:745:GLN:OE1	1:O:786:HIS:ND1	2.46	0.48
1:S:406:LEU:HD21	1:S:1191:PHE:HE2	1.79	0.48
1:T:861:ASP:HA	1:T:864:GLN:HB2	1.95	0.48
1:T:1168:GLY:HA2	1:U:207:LYS:HD3	1.95	0.48
1:W:1109:THR:HG22	1:W:1175:ALA:HB2	1.95	0.48
1:W:1341:TYR:HA	1:W:1348:HIS:CD2	2.48	0.48
1:4:727:PHE:HA	1:4:730:LEU:HB3	1.95	0.48
4:j:89:PRO:HA	4:j:302:TYR:HD2	1.79	0.48
4:j:282:LEU:HD13	4:j:285:ARG:HH21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LEU:O	1:A:196:GLY:N	2.45	0.48
1:B:1196:ASN:HD22	1:B:1201:ALA:HA	1.79	0.48
1:C:402:PHE:HB3	1:C:1040:VAL:HB	1.96	0.48
1:C:796:ASN:OD1	1:D:932:ARG:NH1	2.46	0.48
1:C:1236:ASN:HB2	1:C:1238:TRP:HE3	1.78	0.48
1:E:717:LEU:HB2	1:E:990:TRP:HZ3	1.79	0.48
1:F:760:ARG:HB2	1:F:792:PRO:HD3	1.95	0.48
1:F:927:VAL:HB	1:F:956:THR:HG21	1.95	0.48
1:M:153:ALA:HA	1:M:156:ILE:HG22	1.95	0.48
1:M:1111:MET:HE1	1:M:1366:ARG:HH22	1.77	0.48
1:O:436:ASN:OD1	1:O:437:LYS:N	2.47	0.48
1:O:515:LYS:NZ	1:O:534:LEU:O	2.44	0.48
1:O:1344:ASN:ND2	1:O:1347:THR:OG1	2.47	0.48
1:S:717:LEU:HB2	1:S:990:TRP:HZ3	1.78	0.48
1:V:59:ASN:HD22	1:W:95:ILE:HA	1.76	0.48
1:V:185:HIS:O	1:V:1097:SER:OG	2.32	0.48
1:V:1071:ARG:O	1:V:1079:THR:OG1	2.31	0.48
1:W:708:LEU:HD21	1:W:1022:PRO:HG2	1.95	0.48
4:7:120:ARG:HA	4:7:123:SER:HB3	1.94	0.48
4:f:35:ASP:HB3	4:f:37:HIS:HD2	1.77	0.48
3:h:128:VAL:HG11	3:h:312:LEU:HD22	1.95	0.48
1:A:808:TYR:OH	1:A:915:GLN:NE2	2.47	0.48
1:A:1198:ARG:NH1	1:A:1200:ARG:O	2.46	0.48
1:B:1341:TYR:HA	1:B:1348:HIS:CD2	2.47	0.48
1:C:1114:HIS:O	1:C:1177:CYS:N	2.43	0.48
1:D:931:SER:HB2	1:D:934:ALA:HB3	1.95	0.48
1:E:8:ARG:NH1	1:F:319:TYR:O	2.46	0.48
1:M:1250:TYR:HA	1:M:1255:ARG:HH21	1.78	0.48
1:N:402:PHE:HD2	1:N:1040:VAL:HB	1.78	0.48
1:N:440:VAL:HG22	1:O:1193:THR:HG21	1.95	0.48
1:O:512:VAL:HG12	1:O:993:SER:HB3	1.95	0.48
1:S:275:VAL:HG22	1:S:375:ALA:HB3	1.95	0.48
1:U:83:LEU:HD21	1:U:122:LYS:HD2	1.95	0.48
1:U:419:VAL:HG23	1:U:1336:VAL:HG11	1.95	0.48
1:U:708:LEU:HD21	1:U:1022:PRO:HG2	1.94	0.48
1:V:211:SER:OG	1:V:1206:SER:OG	2.30	0.48
1:V:619:MET:SD	1:V:881:SER:OG	2.71	0.48
1:X:45:GLU:O	1:4:58:THR:OG1	2.30	0.48
1:4:272:VAL:HA	1:4:373:PHE:HB2	1.94	0.48
4:d:38:ARG:HG3	4:d:39:LEU:HG	1.94	0.48
1:B:587:ASN:OD1	1:C:1003:GLN:NE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ASP:OD1	1:C:82:ASP:N	2.43	0.48
1:C:428:GLN:NE2	1:C:577:SER:OG	2.34	0.48
1:C:720:PRO:HD3	1:C:808:TYR:CZ	2.49	0.48
1:E:714:ASP:O	1:E:804:LYS:NZ	2.46	0.48
1:F:245:LEU:HD22	1:F:369:ILE:HG21	1.95	0.48
1:O:558:HIS:CD2	1:O:902:GLN:HE22	2.31	0.48
1:O:658:ARG:HA	1:O:681:LEU:HD11	1.96	0.48
1:T:481:TYR:OH	1:T:979:VAL:N	2.45	0.48
1:U:49:ARG:HD3	1:V:87:ILE:HD11	1.95	0.48
1:U:1067:SER:HG	1:U:1083:THR:HG1	1.58	0.48
1:V:931:SER:HB2	1:V:934:ALA:HB3	1.95	0.48
1:W:587:ASN:OD1	1:X:1003:GLN:NE2	2.46	0.48
1:X:436:ASN:OD1	1:X:437:LYS:N	2.47	0.48
1:X:929:ASP:OD1	1:X:932:ARG:NH2	2.46	0.48
1:4:537:HIS:CE1	1:4:539:PHE:HB2	2.49	0.48
1:4:1188:VAL:HG12	1:4:1192:GLN:HE22	1.78	0.48
1:A:851:LEU:HD12	1:A:869:ARG:HD2	1.95	0.48
1:B:76:VAL:HB	1:B:1060:SER:HA	1.96	0.48
1:C:532:LEU:O	1:C:1241:GLN:NE2	2.46	0.48
1:C:919:VAL:HG12	1:C:920:ASN:HB2	1.95	0.48
1:C:1033:HIS:NE2	1:C:1036:PHE:O	2.45	0.48
1:D:845:ASN:N	1:D:848:ASP:OD2	2.45	0.48
1:E:831:LEU:HD22	2:K:9:PRO:HG2	1.95	0.48
1:E:1344:ASN:ND2	1:E:1347:THR:OG1	2.46	0.48
1:F:304:ALA:HB2	1:F:357:ILE:HD11	1.96	0.48
1:M:536:VAL:HG13	1:M:1244:SER:HA	1.95	0.48
1:M:850:ILE:HD11	1:M:872:VAL:HA	1.96	0.48
1:N:518:VAL:HG13	1:N:522:ASP:HB3	1.94	0.48
1:O:877:VAL:O	1:O:880:THR:OG1	2.30	0.48
1:U:123:HIS:N	1:U:1086:ILE:O	2.42	0.48
1:U:396:ILE:HD11	1:U:1050:HIS:HE1	1.77	0.48
1:U:438:ASN:HD22	1:U:1171:HIS:HD2	1.61	0.48
1:V:218:LYS:NZ	1:V:1323:LEU:O	2.47	0.48
1:V:1067:SER:OG	1:V:1083:THR:OG1	2.32	0.48
1:W:763:MET:HE3	1:W:883:LEU:HB2	1.94	0.48
1:X:1196:ASN:HD21	1:X:1324:GLN:HG3	1.78	0.48
4:c:234:ARG:H	4:c:234:ARG:HD3	1.77	0.48
4:i:144:LEU:HD21	4:i:183:PHE:HB2	1.96	0.48
1:A:402:PHE:HD2	1:A:1040:VAL:HB	1.79	0.48
1:C:185:HIS:O	1:C:1097:SER:OG	2.32	0.48
1:C:851:LEU:HD12	1:C:869:ARG:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:GLU:HB3	1:E:87:ILE:HB	1.96	0.48
1:D:512:VAL:HG12	1:D:993:SER:HB3	1.95	0.48
1:D:718:LEU:H	1:D:915:GLN:HE22	1.62	0.48
1:F:217:PHE:O	1:F:221:LEU:N	2.47	0.48
1:F:536:VAL:HG13	1:F:1244:SER:HA	1.95	0.48
1:F:578:ARG:NH1	1:F:1014:SER:O	2.44	0.48
1:M:457:ARG:HH11	1:M:460:ASN:HD21	1.61	0.48
1:N:744:ASP:H	1:N:786:HIS:HE1	1.62	0.48
1:N:1198:ARG:NH2	1:N:1219:LEU:O	2.42	0.48
1:O:191:ILE:HA	1:O:217:PHE:HE1	1.79	0.48
1:S:127:ALA:HB3	1:S:1082:ILE:HB	1.96	0.48
1:S:278:THR:HG22	1:S:1051:ILE:HA	1.96	0.48
1:T:95:ILE:HB	1:T:114:TYR:HB2	1.96	0.48
1:T:1236:ASN:HB2	1:T:1238:TRP:HE3	1.78	0.48
1:W:224:HIS:HD2	1:W:244:MET:HE1	1.78	0.48
1:W:700:VAL:O	1:W:1131:GLN:NE2	2.47	0.48
1:W:898:ARG:HE	1:W:913:VAL:HG23	1.77	0.48
1:X:91:ILE:HD11	1:X:1089:LEU:HD22	1.95	0.48
1:X:463:GLN:HB3	1:X:1248:VAL:HG13	1.95	0.48
1:4:759:LEU:HD22	1:4:792:PRO:HB3	1.95	0.48
1:4:1027:GLN:HB3	1:4:1032:MET:HB2	1.96	0.48
1:4:1073:VAL:HG13	1:4:1078:VAL:HA	1.96	0.48
4:9:226:LEU:HD11	4:a:212:CYS:HB3	1.96	0.48
4:c:110:GLN:HE22	4:c:287:HIS:CE1	2.31	0.48
3:e:293:THR:OG1	3:e:321:GLU:OE2	2.32	0.48
1:A:831:LEU:HD22	2:G:9:PRO:HG2	1.95	0.48
1:B:481:TYR:OH	1:B:979:VAL:O	2.25	0.48
1:B:1199:GLY:HA2	1:B:1235:ASN:HB3	1.94	0.48
1:C:436:ASN:OD1	1:C:437:LYS:N	2.47	0.48
1:D:1183:PRO:HG3	1:D:1237:PRO:HD2	1.96	0.48
1:E:49:ARG:HD3	1:F:87:ILE:HD11	1.95	0.48
1:F:224:HIS:HD2	1:F:244:MET:HE1	1.78	0.48
1:O:537:HIS:HA	1:O:1238:TRP:CD1	2.49	0.48
1:S:955:ALA:HA	1:S:961:LEU:HD22	1.95	0.48
1:T:811:MET:HB3	1:T:819:MET:HE1	1.96	0.48
1:U:561:MET:H	1:U:564:ASN:ND2	2.11	0.48
1:V:1168:GLY:HA2	1:W:207:LYS:HD3	1.96	0.48
1:V:1199:GLY:HA2	1:V:1235:ASN:HB3	1.96	0.48
1:X:700:VAL:O	1:X:1131:GLN:NE2	2.47	0.48
1:4:128:GLU:OE2	1:4:1071:ARG:NH2	2.47	0.48
1:4:567:GLN:HE21	1:4:998:TYR:HA	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:129:ALA:HA	3:8:132:TRP:HD1	1.79	0.48
3:8:146:LEU:HD23	3:8:149:LEU:HD12	1.95	0.48
1:B:508:PHE:O	1:B:978:ASN:ND2	2.38	0.47
1:D:1171:HIS:HE1	1:E:1228:ALA:HA	1.77	0.47
1:D:1294:ALA:HB3	1:D:1297:PRO:HD3	1.96	0.47
1:M:224:HIS:CD2	1:M:244:MET:HE1	2.49	0.47
1:O:224:HIS:HD2	1:O:244:MET:HE1	1.78	0.47
1:V:743:GLY:HA3	1:V:786:HIS:HE1	1.79	0.47
1:X:123:HIS:HB2	1:X:1086:ILE:HB	1.95	0.47
1:X:515:LYS:NZ	1:X:534:LEU:O	2.47	0.47
1:X:856:ASN:HA	1:X:860:LYS:HD2	1.95	0.47
1:4:634:ILE:HB	1:4:638:ILE:HD12	1.95	0.47
3:b:69:THR:HG21	4:d:92:ASN:HD22	1.79	0.47
3:h:326:PRO:HG2	4:j:285:ARG:HH22	1.79	0.47
1:C:127:ALA:HB2	1:D:101:ALA:HB2	1.95	0.47
1:D:717:LEU:HA	1:D:990:TRP:HZ3	1.79	0.47
1:E:15:THR:HG22	1:U:350:LEU:HD11	1.96	0.47
1:E:38:LEU:HB2	1:U:113:GLN:HB3	1.95	0.47
1:O:394:ARG:HD3	1:O:1315:PHE:HB3	1.95	0.47
1:T:868:ILE:HG22	1:T:870:PRO:HD3	1.96	0.47
4:c:220:ARG:NH1	4:c:252:ILE:O	2.47	0.47
4:c:257:LEU:HD13	4:d:158:TYR:HE1	1.79	0.47
4:c:262:ASP:OD2	4:d:158:TYR:OH	2.32	0.47
4:i:262:ASP:OD2	4:j:158:TYR:OH	2.32	0.47
1:B:78:THR:HG22	1:B:304:ALA:HB3	1.96	0.47
1:B:82:ASP:N	1:B:82:ASP:OD1	2.46	0.47
1:C:716:HIS:CE1	1:C:736:ARG:HG3	2.49	0.47
1:D:294:GLU:HB2	1:D:366:LEU:HD22	1.95	0.47
1:D:850:ILE:HD11	1:D:872:VAL:HA	1.96	0.47
1:D:1294:ALA:HB1	1:D:1321:HIS:HE1	1.80	0.47
1:F:6:GLU:OE1	1:F:8:ARG:NH1	2.47	0.47
1:T:306:TYR:OH	1:T:323:MET:O	2.31	0.47
1:T:1252:ILE:O	1:T:1267:ARG:NH2	2.45	0.47
1:V:436:ASN:OD1	1:V:437:LYS:N	2.48	0.47
1:X:380:GLN:NE2	1:X:393:ASN:HD21	2.12	0.47
3:5:199:LEU:O	3:5:315:LEU:N	2.45	0.47
4:6:111:LEU:HA	4:6:141:PRO:HA	1.96	0.47
3:b:143:ILE:HG22	3:b:145:ASN:H	1.79	0.47
4:f:5:LYS:HB2	4:f:86:ARG:HD3	1.97	0.47
3:h:32:PRO:O	3:h:36:ARG:NH1	2.47	0.47
1:A:1224:ILE:HD13	1:F:1167:PRO:HD3	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:687:LEU:HB3	1:C:805:LEU:HD13	1.95	0.47
1:D:183:LEU:HD13	1:D:394:ARG:HH21	1.80	0.47
1:D:927:VAL:HB	1:D:956:THR:HG21	1.96	0.47
1:D:1341:TYR:HB2	1:D:1357:LEU:HD11	1.95	0.47
1:E:455:HIS:HD2	1:E:1119:PHE:HD1	1.63	0.47
1:M:49:ARG:HD3	1:N:87:ILE:HD11	1.95	0.47
1:M:191:ILE:HA	1:M:217:PHE:HE1	1.79	0.47
1:M:1122:PHE:HE1	1:M:1258:ALA:HB2	1.79	0.47
1:O:312:ASN:HD21	1:O:326:PHE:HB2	1.80	0.47
1:O:406:LEU:HD21	1:O:1191:PHE:HE2	1.79	0.47
1:S:59:ASN:HD22	1:T:96:SER:H	1.62	0.47
1:S:388:PHE:HE2	1:T:100:ILE:H	1.62	0.47
1:S:913:VAL:HG11	1:S:990:TRP:CD1	2.50	0.47
1:T:1170:SER:HA	1:U:211:SER:HB3	1.96	0.47
1:U:1264:SER:HB2	1:U:1267:ARG:HG3	1.95	0.47
1:X:624:GLU:HB2	1:X:762:ARG:HH12	1.79	0.47
3:8:40:ASP:O	4:9:2:ALA:N	2.48	0.47
4:i:23:LEU:HB3	4:i:77:VAL:HG21	1.95	0.47
4:j:52:SER:OG	4:j:53:ARG:N	2.47	0.47
1:A:927:VAL:HB	1:A:956:THR:HG21	1.97	0.47
1:C:994:PRO:HA	1:C:997:ALA:HB3	1.96	0.47
1:M:770:LEU:HD11	1:M:883:LEU:HD13	1.96	0.47
1:N:275:VAL:HG22	1:N:375:ALA:HB3	1.96	0.47
1:T:947:LEU:H	1:T:947:LEU:HG	1.44	0.47
1:U:606:ASP:OD1	1:U:647:LYS:NZ	2.40	0.47
1:U:780:GLU:OE1	1:U:785:ARG:NH1	2.48	0.47
1:U:1344:ASN:ND2	1:U:1347:THR:OG1	2.47	0.47
1:V:491:MET:HE3	1:V:786:HIS:H	1.79	0.47
1:W:617:GLU:HG3	1:W:656:MET:HG3	1.96	0.47
1:X:284:ARG:O	1:X:288:ASN:ND2	2.48	0.47
1:X:493:LEU:HD13	1:X:942:VAL:HG21	1.97	0.47
1:4:245:LEU:HD22	1:4:369:ILE:HG21	1.96	0.47
1:4:1212:ASN:HA	1:4:1280:ARG:HH22	1.80	0.47
4:f:105:TRP:HE1	4:f:141:PRO:HD3	1.79	0.47
1:D:402:PHE:HD2	1:D:1040:VAL:HB	1.79	0.47
1:D:637:VAL:HG22	1:D:868:ILE:HD13	1.96	0.47
1:D:1027:GLN:NE2	1:D:1032:MET:HB2	2.29	0.47
1:M:899:ASP:O	1:M:901:ALA:N	2.47	0.47
1:S:1051:ILE:HB	1:S:1100:ALA:HB3	1.95	0.47
1:U:887:PHE:O	1:U:920:ASN:ND2	2.43	0.47
1:V:576:GLU:OE1	1:V:998:TYR:OH	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:404:VAL:HG23	1:W:432:THR:HG23	1.96	0.47
1:W:913:VAL:HG11	1:W:990:TRP:CD1	2.49	0.47
1:4:652:ASN:HA	1:4:925:PHE:HE2	1.79	0.47
3:5:46:ALA:HB1	3:5:50:ARG:HH12	1.78	0.47
4:6:113:VAL:HG22	4:6:139:VAL:HG12	1.95	0.47
3:e:155:PHE:N	3:e:232:TYR:OH	2.48	0.47
1:A:93:PHE:HB2	1:A:116:VAL:HB	1.95	0.47
1:A:831:LEU:HD23	2:G:11:ILE:HD12	1.97	0.47
1:B:306:TYR:OH	1:B:323:MET:O	2.32	0.47
1:B:889:THR:HA	1:B:920:ASN:HB3	1.97	0.47
1:B:951:PRO:HA	1:B:954:ALA:HB3	1.96	0.47
1:B:1344:ASN:ND2	1:B:1347:THR:OG1	2.48	0.47
1:C:1342:MET:HA	1:C:1375:VAL:HG21	1.96	0.47
1:D:958:HIS:CE1	1:D:960:LEU:HB3	2.50	0.47
1:E:125:ILE:HB	1:E:1084:HIS:HB3	1.97	0.47
1:F:512:VAL:HG12	1:F:993:SER:HB3	1.95	0.47
1:F:609:TYR:HE2	1:F:614:TYR:HB2	1.80	0.47
1:F:889:THR:HA	1:F:920:ASN:HB3	1.97	0.47
1:M:404:VAL:HG23	1:M:432:THR:HG23	1.97	0.47
1:M:1302:THR:OG1	1:M:1304:LEU:O	2.31	0.47
1:N:397:GLN:HE22	1:N:1298:ALA:HB3	1.80	0.47
1:N:558:HIS:CE1	1:N:902:GLN:HE22	2.33	0.47
1:N:588:MET:HB3	1:N:690:ALA:HB2	1.95	0.47
1:O:404:VAL:HG23	1:O:432:THR:HG23	1.97	0.47
1:O:455:HIS:HE2	1:O:1122:PHE:HB2	1.79	0.47
1:O:1062:PHE:HB2	1:O:1087:ALA:HB3	1.95	0.47
1:S:62:GLU:O	1:S:172:ARG:NH2	2.46	0.47
1:S:1187:ASP:OD2	1:S:1232:ARG:NH2	2.41	0.47
1:T:889:THR:HA	1:T:920:ASN:HB3	1.97	0.47
1:U:92:GLN:NE2	1:U:116:VAL:O	2.47	0.47
1:U:436:ASN:OD1	1:U:437:LYS:N	2.47	0.47
1:U:493:LEU:HD13	1:U:942:VAL:HG21	1.97	0.47
1:U:856:ASN:OD1	1:U:860:LYS:NZ	2.47	0.47
1:U:989:GLU:HG2	1:U:991:HIS:H	1.80	0.47
1:V:123:HIS:HB2	1:V:1086:ILE:HB	1.96	0.47
1:V:493:LEU:HB2	1:V:940:TYR:HE2	1.79	0.47
1:V:651:VAL:HG12	1:V:811:MET:HE1	1.96	0.47
1:V:944:PHE:HE1	1:V:983:LEU:HD22	1.80	0.47
1:V:1219:LEU:HD11	1:V:1276:MET:HE3	1.97	0.47
1:V:1342:MET:HA	1:V:1375:VAL:HG21	1.97	0.47
1:W:263:THR:OG1	1:W:1056:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:918:LEU:HD22	1:W:944:PHE:HZ	1.78	0.47
1:4:669:ILE:HD11	1:4:674:HIS:CD2	2.50	0.47
3:5:69:THR:H	3:5:182:LYS:HD2	1.80	0.47
3:8:167:GLN:HB2	3:8:188:ARG:HG3	1.96	0.47
4:9:274:GLN:O	4:a:281:ASN:ND2	2.42	0.47
3:e:234:ARG:HG2	3:e:239:PRO:HB3	1.97	0.47
4:g:213:ILE:HG23	4:g:217:LEU:HD12	1.97	0.47
4:j:142:GLN:O	4:j:146:HIS:ND1	2.36	0.47
1:A:451:LYS:HG2	1:A:1140:ALA:HB1	1.95	0.47
1:E:79:GLU:N	1:E:304:ALA:O	2.48	0.47
1:E:102:HIS:HE1	1:E:106:ARG:HD2	1.80	0.47
1:E:851:LEU:HD12	1:E:869:ARG:HD2	1.95	0.47
1:M:277:GLU:HG2	1:M:377:GLU:HB2	1.96	0.47
1:M:312:ASN:HD21	1:M:326:PHE:HB2	1.79	0.47
1:N:175:VAL:HG21	1:N:382:MET:HE1	1.96	0.47
1:O:9:PRO:HB3	1:O:45:GLU:HB3	1.97	0.47
1:O:576:GLU:OE1	1:O:998:TYR:OH	2.33	0.47
1:W:1168:GLY:HA2	1:X:207:LYS:HD3	1.97	0.47
1:X:592:ILE:HG23	1:X:596:THR:HG23	1.95	0.47
3:5:70:TYR:HE2	3:5:188:ARG:HH22	1.61	0.47
3:5:326:PRO:HA	4:7:110:GLN:HE22	1.80	0.47
4:c:20:LEU:O	4:c:24:GLN:N	2.42	0.47
4:f:257:LEU:HD13	4:g:158:TYR:HE1	1.80	0.47
1:B:399:THR:HG22	1:B:1043:THR:HG22	1.97	0.47
1:C:856:ASN:OD1	1:C:860:LYS:NZ	2.46	0.47
1:D:450:LEU:HD11	1:D:1025:ILE:HA	1.97	0.47
1:E:913:VAL:HG11	1:E:990:TRP:CD1	2.50	0.47
1:O:1122:PHE:HE1	1:O:1258:ALA:HB2	1.78	0.47
1:O:1137:LYS:O	1:O:1141:GLY:N	2.37	0.47
1:S:224:HIS:CD2	1:S:244:MET:HE1	2.50	0.47
1:T:678:ARG:HD3	1:U:647:LYS:HZ1	1.80	0.47
1:U:214:VAL:HA	1:U:217:PHE:HD2	1.80	0.47
1:W:271:GLN:OE1	1:W:1056:ARG:NH1	2.48	0.47
1:X:57:TYR:HD2	1:4:49:ARG:HD2	1.80	0.47
1:4:457:ARG:HH21	1:4:1248:VAL:HA	1.79	0.47
1:4:461:PRO:HB2	1:4:556:ALA:HB1	1.97	0.47
3:5:88:THR:HB	3:5:108:PRO:HD2	1.97	0.47
4:c:57:PRO:HB2	4:c:62:ILE:HD11	1.97	0.47
4:f:116:PRO:HD3	4:f:137:PRO:HA	1.96	0.47
1:A:850:ILE:HD11	1:A:872:VAL:HA	1.97	0.47
1:C:49:ARG:HD3	1:D:87:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:450:LEU:HD11	1:F:1025:ILE:HG13	1.97	0.47
1:M:821:GLY:HA2	1:M:923:GLY:HA2	1.97	0.47
1:N:1250:TYR:HB2	1:N:1270:PHE:HD2	1.80	0.47
1:O:918:LEU:HB2	1:O:944:PHE:CE2	2.48	0.47
1:S:461:PRO:HA	1:S:464:SER:HB3	1.97	0.47
1:S:602:GLU:HB3	1:S:647:LYS:HE3	1.97	0.47
1:T:587:ASN:HD21	1:U:1003:GLN:HE21	1.63	0.47
1:T:1156:TYR:HE1	1:T:1260:PRO:HB3	1.80	0.47
1:U:1074:ARG:HA	4:c:92:ASN:HB2	1.96	0.47
1:V:736:ARG:NH1	1:V:897:LYS:O	2.47	0.47
1:V:856:ASN:HB2	2:1:12:GLN:HE21	1.79	0.47
1:X:1294:ALA:HB3	1:X:1321:HIS:CE1	2.50	0.47
1:4:1042:ARG:NE	1:4:1177:CYS:SG	2.85	0.47
4:c:146:HIS:HD2	4:c:282:LEU:HD21	1.80	0.47
1:A:1067:SER:OG	1:A:1083:THR:OG1	2.32	0.46
1:B:512:VAL:HG11	1:B:992:LYS:HB3	1.98	0.46
1:B:1220:TYR:HB3	1:B:1242:ARG:HE	1.80	0.46
1:C:271:GLN:OE1	1:C:1056:ARG:NH1	2.48	0.46
1:E:63:PHE:HE2	1:E:65:LYS:HE2	1.79	0.46
1:E:294:GLU:HB2	1:E:366:LEU:HD22	1.97	0.46
1:E:851:LEU:HD23	1:E:854:LEU:HD21	1.96	0.46
1:F:49:ARG:NH2	3:h:190:GLU:OE2	2.48	0.46
1:F:185:HIS:O	1:F:1097:SER:OG	2.33	0.46
1:N:79:GLU:HB3	1:N:305:SER:HA	1.96	0.46
1:N:1137:LYS:O	1:N:1141:GLY:N	2.46	0.46
1:O:92:GLN:HE22	1:O:115:ILE:HG23	1.79	0.46
1:O:228:LEU:HD22	1:O:1103:HIS:HB2	1.96	0.46
1:S:1199:GLY:HA2	1:S:1235:ASN:HB3	1.95	0.46
1:T:932:ARG:HE	1:T:956:THR:HG23	1.80	0.46
1:T:1169:LEU:HD12	1:U:211:SER:HB2	1.96	0.46
1:U:1115:CYS:HA	1:U:1177:CYS:HB2	1.97	0.46
1:V:700:VAL:O	1:V:1131:GLN:NE2	2.48	0.46
1:V:706:THR:HB	1:V:713:LEU:HD13	1.96	0.46
1:W:731:MET:HG2	1:W:738:PRO:HG3	1.97	0.46
1:X:51:GLU:HB3	1:4:54:LEU:HB3	1.97	0.46
3:5:255:VAL:HA	3:5:258:MET:HB2	1.97	0.46
3:b:183:GLY:HA2	3:b:321:GLU:HB2	1.96	0.46
4:c:218:VAL:HG13	4:d:215:SER:HB2	1.97	0.46
4:g:258:SER:H	4:g:261:ASP:HB2	1.79	0.46
1:A:959:PRO:HA	1:A:962:ALA:HB3	1.96	0.46
1:B:652:ASN:ND2	1:B:923:GLY:O	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1195:SER:O	1:C:1326:ALA:N	2.45	0.46
1:D:271:GLN:OE1	1:D:1056:ARG:NH1	2.36	0.46
1:D:989:GLU:HG2	1:D:991:HIS:H	1.79	0.46
1:M:51:GLU:H	1:N:321:ARG:HA	1.80	0.46
1:M:537:HIS:HB3	1:M:1245:LEU:HB2	1.97	0.46
1:M:651:VAL:HG12	1:M:811:MET:HE1	1.97	0.46
1:S:1005:THR:HG22	1:S:1007:GLY:H	1.80	0.46
1:T:851:LEU:HD23	1:T:854:LEU:HD21	1.97	0.46
1:T:856:ASN:ND2	2:Z:12:GLN:HE21	2.13	0.46
1:T:1070:ARG:HG3	3:e:67:GLN:HE22	1.79	0.46
1:U:946:LYS:HD3	1:U:986:GLU:HG2	1.96	0.46
1:V:172:ARG:HD2	1:V:382:MET:HE1	1.97	0.46
1:V:454:CYS:O	1:V:1127:TYR:OH	2.33	0.46
1:V:481:TYR:OH	1:V:979:VAL:O	2.30	0.46
1:V:1250:TYR:CZ	1:V:1266:CYS:HB2	2.50	0.46
1:W:1170:SER:OG	1:X:1227:PRO:O	2.32	0.46
1:4:402:PHE:HB3	1:4:1040:VAL:HB	1.97	0.46
1:4:428:GLN:NE2	1:4:577:SER:OG	2.39	0.46
1:4:654:TYR:HE2	1:4:803:GLU:HG2	1.80	0.46
3:5:99:GLY:H	3:5:102:MET:HG3	1.80	0.46
3:8:30:ARG:HH11	3:8:33:GLU:HG2	1.79	0.46
3:e:300:PRO:HB2	3:e:315:LEU:HD22	1.97	0.46
3:h:231:VAL:HB	3:h:242:ALA:HB3	1.96	0.46
4:i:26:LYS:HG2	4:i:98:VAL:HG11	1.97	0.46
1:A:1344:ASN:ND2	1:A:1347:THR:OG1	2.48	0.46
1:C:638:ILE:HG12	1:C:649:ALA:HB3	1.98	0.46
1:E:980:PRO:HD2	1:E:983:LEU:HD12	1.98	0.46
1:F:1236:ASN:HB2	1:F:1238:TRP:HE3	1.80	0.46
1:M:197:ASP:HB3	1:M:199:VAL:HG12	1.96	0.46
1:N:674:HIS:CE1	1:N:678:ARG:HE	2.34	0.46
1:S:436:ASN:HB3	1:S:440:VAL:H	1.79	0.46
1:S:718:LEU:HD12	1:S:894:VAL:HG21	1.97	0.46
1:U:52:ALA:H	1:V:89:GLY:HA2	1.79	0.46
1:U:420:ARG:NH1	1:V:1353:MET:SD	2.88	0.46
1:W:1199:GLY:HA3	1:W:1236:ASN:H	1.80	0.46
1:W:1345:LYS:NZ	1:W:1376:TYR:O	2.49	0.46
1:X:717:LEU:HB2	1:X:990:TRP:HZ3	1.81	0.46
1:X:1236:ASN:HB2	1:X:1238:TRP:HE3	1.81	0.46
4:c:23:LEU:HB3	4:c:77:VAL:HG21	1.97	0.46
4:g:291:TYR:HD1	4:g:298:ALA:HB2	1.80	0.46
1:A:78:THR:HG22	1:A:304:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1247:ASP:HB3	1:A:1251:ASN:HD21	1.80	0.46
1:B:83:LEU:HD21	1:B:122:LYS:HD2	1.96	0.46
1:B:578:ARG:NH2	1:B:1017:GLN:OE1	2.47	0.46
1:C:616:ILE:HG21	1:C:633:LEU:HD22	1.95	0.46
1:C:1190:TYR:OH	1:C:1196:ASN:O	2.32	0.46
1:E:620:ILE:HG23	1:E:626:LYS:HB2	1.97	0.46
1:N:1171:HIS:HE1	1:O:1228:ALA:HA	1.79	0.46
1:S:254:GLU:O	1:S:256:THR:OG1	2.29	0.46
1:T:913:VAL:HG11	1:T:990:TRP:CD1	2.50	0.46
1:U:537:HIS:HA	1:U:1238:TRP:CD1	2.50	0.46
1:V:829:VAL:O	1:V:832:THR:OG1	2.31	0.46
1:X:567:GLN:HE22	1:X:998:TYR:N	2.13	0.46
1:X:958:HIS:CE1	1:X:960:LEU:HB3	2.50	0.46
1:4:617:GLU:OE2	1:4:723:TYR:OH	2.17	0.46
3:5:300:PRO:HB2	3:5:315:LEU:HD22	1.96	0.46
4:c:60:ILE:HG13	4:c:200:ALA:HA	1.96	0.46
3:e:224:VAL:HG13	3:e:294:VAL:HB	1.97	0.46
4:i:9:VAL:HG21	4:i:45:LEU:HD21	1.98	0.46
4:j:112:ALA:HB2	4:j:282:LEU:HD23	1.98	0.46
1:A:781:ASP:O	1:A:785:ARG:NH1	2.45	0.46
1:B:1020:SER:HB3	1:B:1022:PRO:HD2	1.98	0.46
1:E:731:MET:HB3	1:E:750:PRO:HG3	1.97	0.46
1:S:493:LEU:HD13	1:S:942:VAL:HG21	1.98	0.46
1:W:397:GLN:HB3	1:W:1318:GLN:HB3	1.97	0.46
1:X:66:PHE:HE1	1:X:174:LEU:HD13	1.81	0.46
3:8:271:TYR:HE2	3:8:331:LEU:HD11	1.79	0.46
4:c:201:LEU:O	4:c:205:ASP:N	2.49	0.46
3:e:205:VAL:HG21	3:e:262:HIS:HE1	1.80	0.46
4:f:204:LEU:HD23	4:f:207:LEU:HD12	1.97	0.46
4:i:58:ASP:HB3	4:i:196:ASP:H	1.80	0.46
1:A:419:VAL:HG22	1:A:421:GLY:H	1.80	0.46
1:B:1183:PRO:HG2	1:B:1186:SER:HB3	1.98	0.46
1:C:227:PHE:HE1	1:C:1100:ALA:HB1	1.80	0.46
1:D:1073:VAL:HG22	1:D:1078:VAL:HG13	1.98	0.46
1:E:293:VAL:HG13	1:E:294:GLU:HG3	1.96	0.46
1:M:419:VAL:HG22	1:M:421:GLY:H	1.81	0.46
1:M:1071:ARG:O	1:M:1079:THR:OG1	2.31	0.46
1:N:736:ARG:HB3	1:N:897:LYS:HD3	1.97	0.46
1:S:156:ILE:HA	1:S:159:ILE:HG22	1.96	0.46
1:S:1047:LEU:HD12	1:S:1106:ALA:HB3	1.96	0.46
1:W:537:HIS:HA	1:W:1238:TRP:NE1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:245:LEU:HD22	1:X:369:ILE:HG21	1.97	0.46
1:X:739:ILE:HB	1:X:895:ILE:HB	1.98	0.46
3:8:70:TYR:OH	3:8:186:LEU:N	2.49	0.46
4:a:261:ASP:O	4:a:264:THR:OG1	2.28	0.46
4:d:152:LEU:HD21	4:d:190:LEU:HD11	1.98	0.46
1:A:452:SER:HB3	1:A:1118:LEU:H	1.81	0.46
1:A:1328:PRO:HB2	1:A:1358:ILE:HG21	1.97	0.46
1:B:284:ARG:O	1:B:288:ASN:ND2	2.48	0.46
1:B:831:LEU:O	1:B:834:THR:OG1	2.32	0.46
1:C:78:THR:OG1	1:C:1061:MET:O	2.27	0.46
1:E:578:ARG:NH1	1:E:1014:SER:O	2.41	0.46
1:M:455:HIS:HD2	1:M:1119:PHE:HD1	1.62	0.46
1:M:1328:PRO:HB2	1:M:1358:ILE:HG21	1.98	0.46
1:N:617:GLU:HG3	1:N:656:MET:HG3	1.97	0.46
1:O:491:MET:HG3	1:O:785:ARG:H	1.81	0.46
1:T:331:ALA:HA	1:T:335:ASP:HB3	1.98	0.46
1:V:1170:SER:OG	1:W:1227:PRO:O	2.28	0.46
1:V:1222:HIS:CE1	1:V:1241:GLN:HA	2.50	0.46
1:W:276:LEU:HA	1:W:1053:TYR:HA	1.97	0.46
1:W:744:ASP:H	1:W:786:HIS:HE1	1.62	0.46
1:W:1198:ARG:HG2	1:W:1270:PHE:HE1	1.81	0.46
1:X:249:LEU:HD21	1:X:372:LYS:HB2	1.98	0.46
1:4:812:PRO:HB2	1:4:999:ALA:HB1	1.98	0.46
1:4:904:PHE:HZ	1:4:1127:TYR:HA	1.80	0.46
4:7:105:TRP:HH2	4:7:139:VAL:HG12	1.81	0.46
4:9:157:ILE:HA	4:a:229:LEU:HD21	1.98	0.46
3:h:207:LEU:HD11	3:h:246:PHE:HD1	1.81	0.46
1:A:103:GLY:HA2	4:g:39:LEU:HD13	1.98	0.46
1:A:436:ASN:HB3	1:A:440:VAL:H	1.81	0.46
1:B:1245:LEU:O	1:B:1249:LEU:N	2.48	0.46
1:C:1062:PHE:HB2	1:C:1087:ALA:HB3	1.97	0.46
1:C:1251:ASN:HD21	1:C:1270:PHE:C	2.24	0.46
1:D:692:LEU:HD21	1:E:972:ARG:HH21	1.80	0.46
1:D:958:HIS:HE1	1:D:960:LEU:HB3	1.80	0.46
1:F:76:VAL:HG21	1:F:258:PHE:HD2	1.81	0.46
1:F:394:ARG:HB3	1:F:1050:HIS:HD2	1.81	0.46
1:N:404:VAL:HG23	1:N:432:THR:HG23	1.98	0.46
1:O:326:PHE:O	1:O:330:MET:N	2.48	0.46
1:S:623:GLN:HG3	1:S:626:LYS:HD3	1.96	0.46
1:S:744:ASP:H	1:S:786:HIS:HE1	1.62	0.46
1:S:1188:VAL:HG12	1:S:1192:GLN:HE22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:903:SER:O	1:U:1128:GLN:NE2	2.49	0.46
1:V:740:ILE:HB	1:V:747:TYR:HB3	1.96	0.46
1:V:1033:HIS:NE2	1:V:1036:PHE:O	2.48	0.46
1:W:273:ALA:O	1:W:1053:TYR:OH	2.33	0.46
1:X:211:SER:OG	1:X:1206:SER:OG	2.33	0.46
1:X:504:LYS:HB2	1:X:967:ARG:HH12	1.81	0.46
1:4:898:ARG:O	1:4:903:SER:OG	2.28	0.46
4:9:70:THR:HG21	4:9:86:ARG:HH12	1.80	0.46
4:9:204:LEU:HD23	4:9:207:LEU:HD12	1.98	0.46
3:h:169:VAL:HB	3:h:176:LYS:HB3	1.98	0.46
1:A:436:ASN:OD1	1:A:437:LYS:N	2.49	0.46
1:B:75:CYS:SG	1:B:1059:THR:OG1	2.72	0.46
1:B:494:PHE:HZ	2:H:6:VAL:HG22	1.80	0.46
1:B:822:MET:HE1	1:B:957:LEU:HD11	1.98	0.46
1:C:663:HIS:HA	1:D:930:ARG:HD2	1.98	0.46
1:C:1341:TYR:HA	1:C:1348:HIS:CD2	2.51	0.46
1:D:1109:THR:O	1:D:1111:MET:N	2.49	0.46
1:E:224:HIS:CD2	1:E:244:MET:HE1	2.51	0.46
1:F:493:LEU:HD13	1:F:942:VAL:HG21	1.97	0.46
1:M:1344:ASN:ND2	1:M:1347:THR:OG1	2.49	0.46
1:N:185:HIS:O	1:N:1097:SER:OG	2.34	0.46
1:N:819:MET:N	1:N:950:ASP:OD2	2.46	0.46
1:N:1341:TYR:HA	1:N:1348:HIS:HD2	1.80	0.46
1:O:148:ASP:O	1:O:152:TYR:N	2.44	0.46
1:V:434:VAL:HG11	1:V:1042:ARG:HH12	1.81	0.46
1:4:191:ILE:HA	1:4:217:PHE:HE1	1.81	0.46
4:6:61:GLN:HA	4:6:64:GLN:HB3	1.98	0.46
4:6:174:LEU:O	4:6:178:THR:OG1	2.32	0.46
4:c:5:LYS:HZ1	4:c:91:ASP:CG	2.24	0.46
4:d:88:ASP:HB2	4:d:91:ASP:HB2	1.98	0.46
4:i:126:VAL:HG23	4:i:133:ASP:HB3	1.98	0.46
1:A:496:THR:HG21	1:A:982:ASN:HD22	1.81	0.46
1:A:507:ALA:HB1	1:A:978:ASN:HD22	1.80	0.46
1:B:178:VAL:HG22	1:B:1061:MET:HE2	1.98	0.46
1:C:401:PHE:N	1:C:1327:TYR:O	2.48	0.46
1:C:600:ILE:O	1:C:604:ALA:N	2.48	0.46
1:C:946:LYS:HZ2	1:C:975:VAL:HA	1.81	0.46
1:C:1167:PRO:HG2	1:D:1218:LEU:HD23	1.99	0.46
1:D:898:ARG:HE	1:D:913:VAL:HG23	1.80	0.46
1:S:407:HIS:CE1	1:S:574:PHE:HB2	2.51	0.46
1:S:1190:TYR:OH	1:S:1196:ASN:O	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:128:GLU:HG2	1:U:110:LYS:HG3	1.96	0.46
1:T:737:GLN:H	1:T:897:LYS:HD3	1.81	0.46
1:U:1071:ARG:HH12	4:d:38:ARG:HB3	1.81	0.46
1:W:211:SER:OG	1:W:1206:SER:OG	2.33	0.46
1:W:436:ASN:OD1	1:W:437:LYS:N	2.49	0.46
1:W:592:ILE:HG13	1:W:683:GLU:HG2	1.98	0.46
1:4:566:PRO:HB2	1:4:568:PRO:HD2	1.98	0.46
1:4:838:PRO:HA	1:4:841:ALA:HB3	1.98	0.46
3:5:148:GLU:HA	3:5:151:ASP:HB2	1.97	0.46
3:8:89:PHE:HZ	3:8:161:PRO:HB3	1.81	0.46
3:8:260:LYS:O	3:8:264:THR:OG1	2.28	0.46
4:a:145:GLY:HA2	4:a:148:ILE:HG22	1.96	0.46
4:d:105:TRP:HB2	4:d:291:TYR:CZ	2.51	0.46
4:g:47:LEU:O	4:g:51:CYS:N	2.48	0.46
1:A:82:ASP:N	1:A:82:ASP:OD1	2.47	0.45
1:A:913:VAL:HG22	1:A:990:TRP:HE1	1.81	0.45
1:D:174:LEU:HD23	1:D:1086:ILE:HD11	1.99	0.45
1:E:125:ILE:N	1:E:1084:HIS:O	2.49	0.45
1:F:537:HIS:HA	1:F:1238:TRP:CD1	2.51	0.45
1:F:611:LEU:HD22	1:F:862:ILE:HG12	1.96	0.45
1:F:854:LEU:HD13	1:F:860:LYS:HG2	1.97	0.45
1:M:352:ASP:HB2	1:M:354:HIS:CD2	2.51	0.45
1:N:453:ILE:HG12	1:N:1179:ILE:HG21	1.97	0.45
1:O:457:ARG:NH2	1:O:1254:PHE:O	2.50	0.45
1:S:436:ASN:OD1	1:S:437:LYS:N	2.50	0.45
1:S:569:LEU:HD22	1:S:1183:PRO:HB2	1.99	0.45
1:T:323:MET:HG3	1:T:326:PHE:HD1	1.81	0.45
1:T:1341:TYR:HE1	1:T:1359:GLU:HG2	1.81	0.45
1:V:41:LYS:O	1:V:44:ARG:NH1	2.49	0.45
1:V:712:LEU:HD13	1:V:805:LEU:HD21	1.98	0.45
1:W:739:ILE:HB	1:W:895:ILE:HB	1.97	0.45
1:W:845:ASN:N	1:W:848:ASP:OD2	2.49	0.45
1:X:9:PRO:HA	1:X:387:GLN:HG2	1.98	0.45
4:i:220:ARG:HG2	4:i:265:ARG:HH12	1.81	0.45
1:A:752:ASN:O	1:A:755:THR:OG1	2.33	0.45
1:B:92:GLN:HE22	1:B:115:ILE:HG23	1.81	0.45
1:C:842:ASP:OD2	2:I:19:TYR:OH	2.29	0.45
1:D:514:GLN:HG3	1:D:531:LEU:HD21	1.98	0.45
1:E:10:PHE:HB2	1:E:12:TYR:CE1	2.52	0.45
1:E:394:ARG:HD3	1:E:1315:PHE:HB3	1.99	0.45
1:F:224:HIS:CD2	1:F:244:MET:HE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:467:ALA:HB2	1:F:1254:PHE:HE2	1.81	0.45
1:F:994:PRO:HA	1:F:997:ALA:HB3	1.98	0.45
1:M:130:GLU:HB2	1:N:110:LYS:HD2	1.96	0.45
1:N:217:PHE:O	1:N:221:LEU:N	2.50	0.45
1:N:1017:GLN:HE21	1:N:1027:GLN:HE21	1.62	0.45
1:S:934:ALA:O	1:S:937:THR:OG1	2.30	0.45
1:T:602:GLU:HB3	1:T:647:LYS:HE2	1.99	0.45
1:T:652:ASN:ND2	1:T:923:GLY:O	2.39	0.45
1:T:720:PRO:HD3	1:T:808:TYR:CZ	2.50	0.45
1:U:826:TYR:OH	1:U:920:ASN:O	2.33	0.45
1:U:941:PRO:HB3	1:U:957:LEU:HD12	1.98	0.45
1:V:263:THR:HA	1:V:359:ARG:HH12	1.81	0.45
1:W:244:MET:HE2	1:W:244:MET:HB2	1.81	0.45
1:X:1190:TYR:OH	1:X:1196:ASN:O	2.30	0.45
1:4:228:LEU:HD22	1:4:1103:HIS:HB2	1.96	0.45
1:4:401:PHE:HD2	1:4:1328:PRO:HB3	1.81	0.45
4:9:235:HIS:HB2	4:9:238:THR:HG22	1.98	0.45
3:b:154:GLU:O	3:b:157:THR:OG1	2.33	0.45
4:c:179:THR:OG1	4:c:189:ARG:NH1	2.50	0.45
4:i:142:GLN:HE22	4:i:285:ARG:HG2	1.81	0.45
1:A:743:GLY:HA3	1:A:786:HIS:HE1	1.81	0.45
1:B:79:GLU:N	1:B:304:ALA:O	2.49	0.45
1:E:113:GLN:HB3	1:M:38:LEU:HB2	1.97	0.45
1:E:446:TYR:O	1:E:450:LEU:N	2.50	0.45
1:F:145:THR:HG23	1:F:148:ASP:H	1.81	0.45
1:F:850:ILE:HD11	1:F:872:VAL:HA	1.98	0.45
1:F:980:PRO:HD2	1:F:983:LEU:HD12	1.97	0.45
1:M:74:ALA:O	1:M:1059:THR:OG1	2.33	0.45
1:O:435:VAL:HG11	1:O:1368:LEU:HD22	1.98	0.45
1:O:964:TYR:HA	1:O:967:ARG:HB2	1.97	0.45
1:O:1195:SER:O	1:O:1326:ALA:N	2.49	0.45
1:S:422:VAL:HG13	1:S:427:ILE:HG21	1.97	0.45
1:S:1109:THR:HG22	1:S:1111:MET:H	1.81	0.45
1:W:218:LYS:NZ	1:W:1325:GLU:OE2	2.37	0.45
1:X:945:ASN:H	1:X:948:TYR:HB2	1.82	0.45
1:4:699:THR:HA	1:4:704:PRO:HA	1.99	0.45
3:8:169:VAL:HB	3:8:176:LYS:HB3	1.99	0.45
1:B:228:LEU:HD22	1:B:1103:HIS:HB2	1.97	0.45
1:B:958:HIS:HE1	1:B:960:LEU:HB3	1.81	0.45
1:B:994:PRO:HA	1:B:997:ALA:HB3	1.97	0.45
1:C:842:ASP:HB3	1:C:843:VAL:H	1.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:THR:OG1	1:D:1061:MET:O	2.30	0.45
1:D:129:ILE:HB	1:D:1080:PHE:HB2	1.98	0.45
1:E:918:LEU:HB2	1:E:944:PHE:CE2	2.52	0.45
1:F:582:PHE:HE1	1:F:694:LEU:HD11	1.81	0.45
2:K:22:HIS:HB3	2:K:25:VAL:HG23	1.99	0.45
1:T:634:ILE:HA	1:T:637:VAL:HB	1.99	0.45
1:T:1219:LEU:HD11	1:T:1276:MET:HE3	1.98	0.45
1:V:495:ARG:HH12	2:1:4:PHE:HB3	1.82	0.45
1:V:842:ASP:HB3	1:V:843:VAL:H	1.53	0.45
1:W:130:GLU:HG2	1:W:1079:THR:HG22	1.98	0.45
1:W:1044:ASP:HA	1:W:1109:THR:HG21	1.99	0.45
1:X:31:LEU:HD22	1:X:55:GLY:HA2	1.97	0.45
1:X:214:VAL:HG12	1:X:218:LYS:HE2	1.97	0.45
1:4:824:VAL:HG13	1:4:939:PHE:CZ	2.51	0.45
4:d:205:ASP:O	4:d:209:MET:N	2.40	0.45
4:i:29:SER:OG	4:i:30:VAL:N	2.48	0.45
1:D:578:ARG:NH1	1:D:1014:SER:OG	2.49	0.45
1:F:633:LEU:HA	1:F:874:MET:HE3	1.99	0.45
1:M:431:GLU:OE1	1:M:1031:ARG:NH1	2.48	0.45
1:S:93:PHE:HB2	1:S:116:VAL:HB	1.99	0.45
1:T:146:PRO:HA	1:T:149:PHE:HD2	1.81	0.45
1:U:54:LEU:HD23	1:V:324:ARG:HB2	1.99	0.45
1:U:709:VAL:HG22	1:U:1023:SER:HA	1.98	0.45
1:W:95:ILE:HB	1:W:114:TYR:HB2	1.97	0.45
1:W:619:MET:SD	1:W:881:SER:OG	2.65	0.45
1:W:634:ILE:HG22	1:W:650:PHE:HE2	1.80	0.45
1:X:78:THR:HA	1:X:304:ALA:HB3	1.99	0.45
2:2:22:HIS:HB3	2:2:25:VAL:HG23	1.99	0.45
4:d:145:GLY:HA2	4:d:148:ILE:HG22	1.98	0.45
4:f:42:ILE:HA	4:f:45:LEU:HD13	1.99	0.45
4:f:47:LEU:HB3	4:f:135:VAL:HB	1.98	0.45
4:f:237:LEU:HD21	4:g:209:MET:HE3	1.99	0.45
1:F:1074:ARG:HD2	1:F:1077:ALA:HB3	1.99	0.45
1:M:264:TYR:CE1	1:M:300:PRO:HD2	2.52	0.45
1:N:183:LEU:HD22	1:N:394:ARG:HH22	1.82	0.45
1:S:245:LEU:HD22	1:S:369:ILE:HG21	1.98	0.45
1:V:1341:TYR:HA	1:V:1348:HIS:CD2	2.52	0.45
1:W:1073:VAL:HG13	1:W:1078:VAL:HG22	1.98	0.45
2:Z:22:HIS:HB3	2:Z:25:VAL:HG23	1.99	0.45
2:0:22:HIS:HB3	2:0:25:VAL:HG23	1.99	0.45
2:1:22:HIS:HB3	2:1:25:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:38:VAL:HA	3:5:41:LEU:HD13	1.99	0.45
4:7:214:LEU:HD21	4:7:272:TYR:HB3	1.99	0.45
4:9:61:GLN:O	4:9:65:TYR:N	2.46	0.45
1:A:76:VAL:HB	1:A:1060:SER:HA	1.99	0.45
1:B:224:HIS:HD2	1:B:244:MET:HE1	1.81	0.45
1:B:511:ASP:H	1:B:987:TYR:HH	1.64	0.45
1:C:623:GLN:HB2	1:C:626:LYS:HB2	1.98	0.45
1:D:63:PHE:HE2	1:D:65:LYS:HE2	1.81	0.45
1:F:684:LEU:HA	1:F:687:LEU:HB2	1.99	0.45
1:M:76:VAL:HB	1:M:1060:SER:HA	1.99	0.45
1:S:558:HIS:O	1:S:902:GLN:NE2	2.30	0.45
1:S:1227:PRO:O	1:X:1170:SER:OG	2.28	0.45
1:U:579:GLY:HA3	1:U:1011:ALA:HA	1.98	0.45
1:U:1071:ARG:O	1:U:1079:THR:OG1	2.35	0.45
1:X:578:ARG:NH2	1:X:1017:GLN:OE1	2.41	0.45
1:X:1250:TYR:HB2	1:X:1270:PHE:HD2	1.82	0.45
2:3:22:HIS:HB3	2:3:25:VAL:HG23	1.99	0.45
1:4:839:VAL:HG13	1:4:872:VAL:HG13	1.99	0.45
1:A:79:GLU:N	1:A:304:ALA:O	2.50	0.45
1:A:254:GLU:HG3	1:A:255:ASP:H	1.82	0.45
1:A:307:VAL:HG12	1:A:309:ARG:H	1.82	0.45
1:B:1342:MET:HE2	1:B:1373:LYS:HG3	1.99	0.45
1:C:280:ASP:O	1:C:380:GLN:NE2	2.49	0.45
1:C:578:ARG:NH1	1:C:1014:SER:O	2.45	0.45
1:E:214:VAL:HA	1:E:217:PHE:HD2	1.82	0.45
1:F:603:THR:HG22	1:F:647:LYS:HB3	1.99	0.45
1:F:744:ASP:H	1:F:786:HIS:HE1	1.64	0.45
1:M:1038:MET:HE1	1:M:1179:ILE:HG13	1.99	0.45
1:N:946:LYS:HE2	1:N:993:SER:HA	1.99	0.45
1:N:1170:SER:OG	1:O:1227:PRO:O	2.34	0.45
1:O:826:TYR:HE2	1:O:886:PRO:HG2	1.81	0.45
2:Q:22:HIS:HB3	2:Q:25:VAL:HG23	1.99	0.45
1:S:218:LYS:NZ	1:S:1325:GLU:OE2	2.37	0.45
1:T:717:LEU:HA	1:T:915:GLN:HE22	1.82	0.45
1:U:91:ILE:HD11	1:U:1089:LEU:HD11	1.99	0.45
1:U:481:TYR:OH	1:U:979:VAL:N	2.47	0.45
1:U:1170:SER:OG	1:V:1227:PRO:O	2.27	0.45
1:V:146:PRO:HA	1:V:149:PHE:HD2	1.81	0.45
1:W:602:GLU:C	1:W:647:LYS:HZ3	2.24	0.45
2:Y:22:HIS:HB3	2:Y:25:VAL:HG23	1.99	0.45
1:4:893:ARG:HH21	1:4:914:ALA:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:204:LEU:HA	3:b:245:PHE:HB2	1.98	0.45
1:A:487:GLN:NE2	1:A:744:ASP:O	2.50	0.45
1:A:692:LEU:HD23	1:A:692:LEU:HA	1.80	0.45
1:A:1195:SER:O	1:A:1326:ALA:N	2.47	0.45
1:C:931:SER:O	1:C:935:ALA:N	2.50	0.45
1:D:58:THR:HG22	1:E:94:LYS:HB3	1.98	0.45
1:D:245:LEU:HD22	1:D:369:ILE:HG21	1.98	0.45
1:F:323:MET:HG3	1:F:326:PHE:HD1	1.81	0.45
1:F:437:LYS:HD3	1:F:1107:ILE:HB	1.99	0.45
1:F:904:PHE:HZ	1:F:1127:TYR:HA	1.82	0.45
1:M:88:ASP:HB2	1:M:321:ARG:HH22	1.82	0.45
1:M:436:ASN:OD1	1:M:437:LYS:N	2.50	0.45
1:M:465:ALA:HA	1:M:468:LEU:HB3	1.98	0.45
1:N:537:HIS:HB3	1:N:1245:LEU:HB2	1.98	0.45
1:N:1073:VAL:O	4:a:92:ASN:ND2	2.50	0.45
1:S:136:ILE:HG23	3:5:60:LEU:HD23	1.98	0.45
1:S:401:PHE:N	1:S:1327:TYR:O	2.50	0.45
1:X:945:ASN:OD1	1:X:946:LYS:N	2.49	0.45
1:4:233:LEU:HD11	1:4:1367:LEU:HD21	1.99	0.45
4:9:16:PHE:HB2	4:9:19:GLU:HG2	1.98	0.45
1:C:658:ARG:NH2	1:D:929:ASP:OD2	2.50	0.45
1:D:443:CYS:N	1:E:1231:CYS:SG	2.90	0.45
1:D:680:ILE:O	1:D:684:LEU:N	2.45	0.45
1:E:419:VAL:HG22	1:E:421:GLY:H	1.82	0.45
1:E:534:LEU:HD11	1:E:544:VAL:HG23	1.98	0.45
1:E:1109:THR:O	1:E:1111:MET:N	2.50	0.45
1:F:1348:HIS:CE1	1:F:1357:LEU:HD22	2.52	0.45
2:I:22:HIS:HB3	2:I:25:VAL:HG23	1.99	0.45
1:M:137:GLU:CD	3:b:192:ARG:HE	2.25	0.45
1:N:1195:SER:O	1:N:1326:ALA:N	2.50	0.45
1:O:700:VAL:O	1:O:1131:GLN:NE2	2.50	0.45
1:O:945:ASN:O	1:O:949:ALA:N	2.50	0.45
1:O:1341:TYR:HB2	1:O:1357:LEU:HD11	1.99	0.45
1:S:202:GLU:HA	1:X:387:GLN:HE22	1.82	0.45
1:U:635:ALA:HB2	1:U:664:MET:HE1	1.99	0.45
1:U:945:ASN:O	1:U:949:ALA:N	2.50	0.45
1:X:166:GLY:HA2	1:X:169:ALA:HB3	1.99	0.45
1:4:1241:GLN:HB3	1:4:1244:SER:HA	1.98	0.45
4:7:214:LEU:HD11	4:7:272:TYR:CG	2.52	0.45
1:A:95:ILE:HB	1:A:114:TYR:HB2	1.99	0.44
1:A:1044:ASP:HA	1:A:1109:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:LEU:HD23	1:D:367:VAL:HG11	1.99	0.44
1:E:74:ALA:HB1	1:E:182:LYS:HE3	1.98	0.44
1:E:695:ALA:HB1	1:E:706:THR:HG22	1.98	0.44
1:F:188:PRO:HD2	1:F:191:ILE:HD12	1.99	0.44
1:F:540:PHE:HA	1:F:558:HIS:HA	1.97	0.44
1:F:1115:CYS:HA	1:F:1177:CYS:HB2	1.99	0.44
1:F:1181:PRO:HG3	1:F:1245:LEU:HD22	1.98	0.44
2:G:22:HIS:HB3	2:G:25:VAL:HG23	1.99	0.44
1:M:611:LEU:HD22	1:M:862:ILE:HG12	1.99	0.44
1:O:481:TYR:OH	1:O:979:VAL:N	2.50	0.44
1:S:183:LEU:HD13	1:S:394:ARG:HH21	1.82	0.44
1:T:454:CYS:HA	1:T:1021:ALA:HB1	1.99	0.44
1:T:512:VAL:HG12	1:T:993:SER:HB3	1.99	0.44
1:W:79:GLU:N	1:W:304:ALA:O	2.48	0.44
1:W:606:ASP:OD1	1:W:647:LYS:NZ	2.35	0.44
1:X:154:GLY:O	1:X:158:THR:OG1	2.30	0.44
2:Z:70:ARG:NH2	2:O:12:GLN:HB2	2.32	0.44
2:3:33:GLN:NE2	2:3:36:MET:O	2.46	0.44
1:4:566:PRO:HD2	1:4:569:LEU:HD12	1.97	0.44
4:6:49:CYS:SG	4:6:50:VAL:N	2.90	0.44
3:h:305:LEU:HD12	3:h:312:LEU:HD23	1.98	0.44
1:C:587:ASN:HD22	1:D:572:ARG:HH12	1.65	0.44
1:C:598:ASP:O	1:C:602:GLU:N	2.42	0.44
1:C:1067:SER:OG	1:C:1083:THR:OG1	2.33	0.44
1:C:1200:ARG:NH1	1:C:1225:PRO:O	2.48	0.44
1:D:562:VAL:HG13	1:D:565:ILE:HD12	1.99	0.44
1:D:945:ASN:OD1	1:D:946:LYS:N	2.50	0.44
1:E:946:LYS:HE2	1:E:993:SER:HA	1.99	0.44
1:N:79:GLU:N	1:N:304:ALA:O	2.50	0.44
1:N:992:LYS:HB2	1:N:994:PRO:HD2	1.99	0.44
2:R:22:HIS:HB3	2:R:25:VAL:HG23	1.99	0.44
1:U:59:ASN:ND2	1:V:96:SER:O	2.50	0.44
1:V:183:LEU:HD13	1:V:394:ARG:HH21	1.81	0.44
1:V:567:GLN:NE2	1:V:994:PRO:O	2.50	0.44
1:W:324:ARG:HH22	1:W:352:ASP:HB2	1.83	0.44
1:W:1196:ASN:HD22	1:W:1202:ALA:H	1.65	0.44
1:X:947:LEU:HD21	1:X:995:VAL:HG12	1.98	0.44
1:X:1341:TYR:HA	1:X:1348:HIS:CD2	2.53	0.44
1:4:850:ILE:HD12	1:4:870:PRO:HG2	1.99	0.44
3:5:205:VAL:HG21	3:5:262:HIS:HE1	1.82	0.44
4:9:124:THR:HG22	4:9:135:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:50:VAL:HG13	4:f:62:ILE:HG12	1.98	0.44
1:A:236:ARG:HE	1:A:239:GLN:HB2	1.83	0.44
1:A:946:LYS:HE2	1:A:993:SER:HA	1.98	0.44
1:B:276:LEU:HA	1:B:1053:TYR:HA	1.99	0.44
1:D:7:GLN:HE21	1:D:36:GLN:HG2	1.82	0.44
1:F:1200:ARG:H	1:F:1240:SER:HG	1.62	0.44
1:M:264:TYR:HE1	1:M:300:PRO:HD2	1.82	0.44
1:M:455:HIS:HD2	1:M:1119:PHE:CD1	2.36	0.44
1:N:658:ARG:HA	1:N:681:LEU:HD11	1.98	0.44
1:N:1045:GLU:OE1	1:N:1300:SER:OG	2.32	0.44
1:S:236:ARG:HH21	1:S:239:GLN:HG3	1.81	0.44
1:S:1341:TYR:HA	1:S:1348:HIS:CD2	2.52	0.44
1:T:76:VAL:HB	1:T:1060:SER:HA	1.99	0.44
1:T:224:HIS:HD2	1:T:244:MET:HE1	1.82	0.44
1:U:945:ASN:OD1	1:U:946:LYS:N	2.51	0.44
1:V:842:ASP:OD2	2:1:19:TYR:OH	2.25	0.44
1:V:898:ARG:NH1	1:V:904:PHE:O	2.51	0.44
1:V:1344:ASN:HD21	1:V:1347:THR:HG1	1.62	0.44
1:X:75:CYS:SG	1:X:1059:THR:OG1	2.63	0.44
1:X:865:ALA:HA	1:X:930:ARG:HH22	1.83	0.44
4:d:287:HIS:HB2	4:d:301:TRP:NE1	2.32	0.44
1:A:76:VAL:O	1:A:1061:MET:N	2.42	0.44
1:B:447:GLN:HB2	1:B:1028:ALA:HB1	1.99	0.44
1:B:1200:ARG:HG3	1:B:1234:THR:HG23	1.98	0.44
1:C:172:ARG:HB3	1:D:100:ILE:HG23	1.98	0.44
1:D:185:HIS:O	1:D:1097:SER:OG	2.36	0.44
1:E:1074:ARG:HB3	4:d:93:LEU:HA	1.99	0.44
1:F:324:ARG:HH21	1:F:352:ASP:HB3	1.82	0.44
1:F:380:GLN:O	1:F:384:ASN:N	2.36	0.44
1:O:723:TYR:HE1	1:O:921:GLY:H	1.64	0.44
1:O:1033:HIS:NE2	1:O:1036:PHE:O	2.51	0.44
1:S:823:GLY:N	1:S:940:TYR:O	2.50	0.44
1:V:361:ARG:NH1	1:V:362:ILE:O	2.51	0.44
1:V:455:HIS:HD2	1:V:1119:PHE:HD1	1.66	0.44
1:W:675:GLY:O	1:W:679:LYS:N	2.43	0.44
1:4:989:GLU:HB3	1:4:992:LYS:HD3	1.99	0.44
3:5:283:LEU:O	4:6:272:TYR:OH	2.35	0.44
4:7:97:ASN:HD22	4:7:105:TRP:HE1	1.64	0.44
4:9:7:ILE:HD11	4:9:86:ARG:HH11	1.83	0.44
4:9:113:VAL:HG22	4:9:139:VAL:HG12	2.00	0.44
4:f:29:SER:HB3	4:f:74:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:104:GLN:HG2	4:g:186:ARG:HH12	1.83	0.44
1:C:1294:ALA:HB1	1:C:1321:HIS:CE1	2.53	0.44
1:D:191:ILE:HA	1:D:217:PHE:HE1	1.83	0.44
1:D:453:ILE:HD13	1:D:1036:PHE:HZ	1.83	0.44
1:E:603:THR:HG22	1:E:647:LYS:HB3	1.99	0.44
1:F:699:THR:HA	1:F:704:PRO:HA	1.98	0.44
1:F:1195:SER:O	1:F:1326:ALA:N	2.50	0.44
2:H:22:HIS:HB3	2:H:25:VAL:HG23	1.99	0.44
1:M:333:ILE:HD11	1:U:11:PRO:HD3	1.99	0.44
1:N:1170:SER:HA	1:O:211:SER:HB3	1.99	0.44
1:O:856:ASN:HD21	2:Q:67:GLY:HA3	1.82	0.44
1:O:1074:ARG:HG2	1:O:1076:ASP:H	1.82	0.44
1:S:435:VAL:HG11	1:S:1368:LEU:HD22	1.99	0.44
1:S:524:LEU:O	1:S:1233:SER:N	2.49	0.44
1:S:605:PHE:HZ	1:S:816:ASN:HD22	1.64	0.44
1:T:838:PRO:HB2	1:T:872:VAL:HG11	1.99	0.44
1:V:848:ASP:H	1:V:872:VAL:HG23	1.82	0.44
1:W:153:ALA:HA	1:W:156:ILE:HG22	1.99	0.44
1:4:537:HIS:HB3	1:4:1245:LEU:HD12	2.00	0.44
1:4:561:MET:H	1:4:564:ASN:HD22	1.66	0.44
1:4:627:PHE:O	1:4:631:MET:N	2.51	0.44
4:6:110:GLN:HG2	4:6:142:GLN:HE21	1.82	0.44
3:8:145:ASN:O	3:8:149:LEU:N	2.44	0.44
1:C:850:ILE:HD12	1:C:875:ILE:HD12	2.00	0.44
1:D:38:LEU:HD13	1:D:43:ALA:HA	2.00	0.44
1:E:150:THR:HG21	1:U:313:LEU:HD21	1.98	0.44
1:E:829:VAL:O	1:E:832:THR:OG1	2.32	0.44
1:F:1226:ASP:HB2	1:F:1229:TYR:H	1.82	0.44
1:N:507:ALA:HB1	1:N:978:ASN:HD21	1.82	0.44
1:O:994:PRO:HA	1:O:997:ALA:HB3	1.99	0.44
2:Q:33:GLN:NE2	2:Q:36:MET:O	2.46	0.44
1:S:674:HIS:O	1:S:678:ARG:N	2.40	0.44
1:U:1067:SER:OG	1:U:1083:THR:OG1	2.27	0.44
1:W:65:LYS:HB2	1:W:68:GLU:HB2	2.00	0.44
1:W:304:ALA:HB2	1:W:357:ILE:HD11	1.98	0.44
4:6:75:GLU:OE1	4:6:83:ARG:NE	2.50	0.44
4:9:123:SER:OG	4:9:136:PHE:O	2.34	0.44
3:b:232:TYR:O	3:b:270:LYS:NZ	2.38	0.44
3:e:234:ARG:HA	3:e:239:PRO:HA	1.99	0.44
4:i:220:ARG:NH1	4:i:255:ASP:OD2	2.51	0.44
1:A:224:HIS:CD2	1:A:244:MET:HE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:ASN:OD1	1:A:946:LYS:N	2.50	0.44
1:B:130:GLU:HG3	1:C:110:LYS:HD2	1.99	0.44
1:C:1294:ALA:HB1	1:C:1321:HIS:HE1	1.82	0.44
1:D:394:ARG:HB2	1:D:1050:HIS:NE2	2.33	0.44
1:D:576:GLU:OE1	1:D:998:TYR:OH	2.36	0.44
1:E:541:ASP:HB2	1:E:559:ARG:HG3	1.99	0.44
1:F:402:PHE:HD2	1:F:1040:VAL:HB	1.83	0.44
1:F:402:PHE:O	1:F:1040:VAL:N	2.45	0.44
1:F:541:ASP:HB2	1:F:559:ARG:HG3	2.00	0.44
1:M:454:CYS:HA	1:M:1021:ALA:HB1	1.99	0.44
1:O:518:VAL:HG13	1:O:522:ASP:HB3	2.00	0.44
1:T:78:THR:HG22	1:T:304:ALA:HB3	2.00	0.44
1:U:578:ARG:NH1	1:U:1014:SER:O	2.46	0.44
1:W:238:LYS:HG2	1:W:289:LEU:HD22	2.00	0.44
1:W:294:GLU:HB2	1:W:366:LEU:HD22	2.00	0.44
1:X:507:ALA:HB2	1:X:968:LEU:HD11	1.99	0.44
2:Z:73:HIS:O	2:Z:76:THR:OG1	2.34	0.44
3:5:57:HIS:HA	3:5:60:LEU:HD13	2.00	0.44
1:A:1166:LEU:O	1:B:207:LYS:NZ	2.48	0.44
1:B:561:MET:HE2	1:B:711:ALA:HB1	1.99	0.44
1:B:740:ILE:HB	1:B:747:TYR:HB3	1.99	0.44
1:B:1328:PRO:HB2	1:B:1358:ILE:HG21	2.00	0.44
1:C:83:LEU:HD11	1:C:122:LYS:HD2	2.00	0.44
1:D:1344:ASN:ND2	1:D:1347:THR:OG1	2.51	0.44
1:F:1201:ALA:HB3	1:F:1227:PRO:HG2	2.00	0.44
1:M:115:ILE:HG22	1:U:5:LEU:HD11	2.00	0.44
1:O:731:MET:HE2	1:O:738:PRO:HG2	2.00	0.44
2:P:22:HIS:HB3	2:P:25:VAL:HG23	1.99	0.44
1:S:386:THR:HG21	1:T:100:ILE:HG13	1.99	0.44
1:S:438:ASN:ND2	1:T:215:SER:OG	2.50	0.44
1:U:807:TYR:O	1:U:948:TYR:OH	2.31	0.44
1:W:856:ASN:OD1	1:W:860:LYS:NZ	2.36	0.44
1:W:1196:ASN:HD21	1:W:1324:GLN:HG3	1.82	0.44
1:X:185:HIS:O	1:X:1097:SER:OG	2.35	0.44
1:X:491:MET:HE3	1:X:786:HIS:H	1.83	0.44
4:6:240:VAL:HG21	4:7:268:VAL:HG21	2.00	0.44
4:9:230:VAL:HG11	4:9:241:PHE:HD2	1.82	0.44
4:j:217:LEU:HB3	4:j:269:MET:SD	2.58	0.44
1:C:958:HIS:CE1	1:C:960:LEU:HB3	2.53	0.44
1:C:1018:LYS:HB2	1:C:1023:SER:HB3	1.99	0.44
1:E:406:LEU:HD21	1:E:1191:PHE:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:ILE:HD11	1:F:1089:LEU:HD21	2.00	0.44
1:F:448:ASN:HD22	1:F:1113:VAL:HG12	1.82	0.44
1:F:851:LEU:HD12	1:F:869:ARG:HD2	1.99	0.44
1:M:669:ILE:HD13	1:M:674:HIS:HB2	2.00	0.44
1:N:312:ASN:ND2	1:N:323:MET:HB2	2.32	0.44
1:O:1198:ARG:HA	1:O:1239:ALA:HB3	2.00	0.44
1:O:1271:HIS:ND1	1:O:1274:ASP:OD2	2.51	0.44
1:T:1199:GLY:HA2	1:T:1235:ASN:HB3	1.99	0.44
1:T:1341:TYR:HA	1:T:1348:HIS:CD2	2.53	0.44
1:U:872:VAL:HG12	1:U:876:ARG:HG3	1.99	0.44
1:W:537:HIS:HB3	1:W:1245:LEU:HB2	2.00	0.44
1:X:158:THR:O	1:X:161:SER:OG	2.30	0.44
1:X:736:ARG:HH21	1:X:900:PRO:HG3	1.81	0.44
1:X:1328:PRO:HB2	1:X:1358:ILE:HG21	2.00	0.44
4:7:94:GLN:HE21	4:7:297:ALA:HB1	1.83	0.44
3:b:124:GLN:HB3	3:b:202:ASP:HB2	1.99	0.44
1:B:591:VAL:O	1:B:679:LYS:NZ	2.44	0.43
1:C:279:THR:OG1	1:C:280:ASP:N	2.50	0.43
1:D:591:VAL:HB	1:D:683:GLU:HB2	1.99	0.43
1:E:1241:GLN:HB3	1:E:1244:SER:HB3	1.98	0.43
2:L:22:HIS:HB3	2:L:25:VAL:HG23	1.99	0.43
1:M:434:VAL:HG11	1:M:1042:ARG:HH22	1.83	0.43
1:M:1187:ASP:OD2	1:M:1232:ARG:NH2	2.50	0.43
1:N:446:TYR:O	1:N:450:LEU:N	2.51	0.43
1:O:361:ARG:NH1	1:O:362:ILE:O	2.51	0.43
1:S:153:ALA:HA	1:S:156:ILE:HG22	1.99	0.43
1:S:538:PRO:O	1:S:559:ARG:NH1	2.51	0.43
1:S:868:ILE:HG22	1:S:870:PRO:HD3	1.99	0.43
1:T:116:VAL:HG11	1:T:1093:LEU:HD12	2.00	0.43
1:U:524:LEU:O	1:U:1233:SER:N	2.40	0.43
1:U:1313:ASP:OD1	1:V:106:ARG:NH1	2.51	0.43
1:X:125:ILE:HD12	1:X:1084:HIS:HB3	2.00	0.43
2:0:33:GLN:NE2	2:0:36:MET:O	2.46	0.43
1:4:80:PHE:HB3	1:4:1063:VAL:H	1.83	0.43
1:4:188:PRO:HD2	1:4:191:ILE:HD12	2.00	0.43
1:4:704:PRO:HD2	1:4:707:HIS:CE1	2.53	0.43
3:b:229:SER:HB3	3:b:246:PHE:HE2	1.82	0.43
3:e:248:SER:HB2	3:e:250:LYS:HG3	2.00	0.43
4:g:51:CYS:HB2	4:g:62:ILE:HD11	2.00	0.43
4:g:141:PRO:HG2	4:g:144:LEU:HD12	1.99	0.43
4:g:261:ASP:O	4:g:264:THR:OG1	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:LEU:HD23	1:A:996:ALA:HB2	2.00	0.43
1:B:66:PHE:O	1:B:69:THR:OG1	2.35	0.43
1:B:897:LYS:HA	1:B:912:ASP:HA	2.00	0.43
1:E:90:LYS:HE2	1:E:117:MET:HE1	2.00	0.43
1:E:931:SER:HB2	1:E:934:ALA:HB3	1.99	0.43
1:F:537:HIS:HA	1:F:1238:TRP:NE1	2.33	0.43
1:F:811:MET:HB3	1:F:819:MET:HE1	2.00	0.43
1:F:934:ALA:O	1:F:937:THR:OG1	2.30	0.43
1:O:558:HIS:HD2	1:O:560:THR:HA	1.84	0.43
1:O:1190:TYR:HD1	1:O:1229:TYR:HE2	1.66	0.43
1:S:562:VAL:HA	1:S:1019:LEU:HD11	1.98	0.43
1:T:415:THR:HB	1:T:1349:ALA:HB1	2.01	0.43
1:T:1344:ASN:ND2	1:T:1347:THR:OG1	2.52	0.43
1:U:578:ARG:NH1	1:U:1014:SER:OG	2.51	0.43
1:W:1047:LEU:HD12	1:W:1106:ALA:HB3	1.99	0.43
1:W:1262:MET:HA	1:W:1306:TYR:HA	2.00	0.43
1:X:57:TYR:CD2	1:4:49:ARG:HD2	2.53	0.43
1:4:964:TYR:OH	1:4:978:ASN:ND2	2.51	0.43
3:e:125:THR:O	3:e:129:ALA:N	2.46	0.43
4:g:105:TRP:HH2	4:g:139:VAL:HG12	1.84	0.43
3:h:150:MET:HB3	3:h:150:MET:HE3	1.77	0.43
4:i:240:VAL:HG21	4:j:268:VAL:HG11	2.00	0.43
4:j:144:LEU:HD21	4:j:183:PHE:HB3	2.00	0.43
1:A:861:ASP:O	1:A:931:SER:OG	2.35	0.43
1:C:945:ASN:OD1	1:C:946:LYS:N	2.51	0.43
1:E:1067:SER:OG	1:E:1083:THR:OG1	2.36	0.43
1:F:380:GLN:HB3	1:F:384:ASN:ND2	2.33	0.43
1:M:245:LEU:HD22	1:M:369:ILE:HG21	2.00	0.43
1:S:591:VAL:N	1:S:683:GLU:OE1	2.50	0.43
1:S:744:ASP:H	1:S:786:HIS:CE1	2.35	0.43
1:S:1312:THR:O	1:T:106:ARG:NH1	2.44	0.43
1:U:178:VAL:HG22	1:U:1061:MET:HE2	2.01	0.43
1:U:1294:ALA:HB1	1:U:1321:HIS:CE1	2.53	0.43
1:V:752:ASN:O	1:V:755:THR:OG1	2.31	0.43
1:W:245:LEU:HD22	1:W:369:ILE:HD13	1.99	0.43
1:W:1196:ASN:ND2	1:W:1202:ALA:H	2.17	0.43
1:X:591:VAL:HG12	1:X:679:LYS:HG2	1.99	0.43
1:4:454:CYS:O	1:4:1127:TYR:OH	2.24	0.43
3:8:38:VAL:HG13	3:8:41:LEU:HD13	2.01	0.43
4:a:217:LEU:O	4:a:221:GLY:N	2.51	0.43
4:c:141:PRO:O	4:c:145:GLY:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:141:PRO:HG2	4:d:144:LEU:HB2	2.00	0.43
4:f:62:ILE:HG21	4:f:115:PRO:HB3	2.00	0.43
1:A:431:GLU:OE1	1:A:1031:ARG:NH1	2.51	0.43
1:C:1302:THR:OG1	1:C:1304:LEU:O	2.33	0.43
1:F:92:GLN:HE22	1:F:115:ILE:HG23	1.82	0.43
1:F:306:TYR:OH	1:F:323:MET:O	2.32	0.43
2:I:33:GLN:NE2	2:I:36:MET:O	2.46	0.43
1:M:447:GLN:HB3	1:M:1028:ALA:HB1	2.00	0.43
1:N:123:HIS:N	1:N:1086:ILE:O	2.51	0.43
1:N:637:VAL:HG22	1:N:868:ILE:HD13	1.99	0.43
1:S:450:LEU:HD11	1:S:1025:ILE:HA	2.00	0.43
1:V:1313:ASP:OD2	1:W:203:ARG:NH2	2.40	0.43
1:W:54:LEU:HB2	1:X:91:ILE:HG13	2.00	0.43
1:W:744:ASP:H	1:W:786:HIS:CE1	2.36	0.43
1:W:855:GLU:HG2	2:1:70:ARG:HG3	2.01	0.43
1:X:5:LEU:HD22	1:X:14:ALA:HB1	2.01	0.43
1:X:893:ARG:HA	1:X:916:THR:HG22	2.00	0.43
1:4:436:ASN:OD1	1:4:437:LYS:N	2.51	0.43
1:A:442:LEU:HB2	1:A:1113:VAL:HG21	2.01	0.43
1:A:1073:VAL:HG13	1:A:1078:VAL:HG22	2.01	0.43
1:B:907:HIS:HB3	1:B:909:TYR:H	1.83	0.43
1:C:165:PHE:HE1	1:D:98:PRO:HA	1.84	0.43
1:D:491:MET:HG3	1:D:785:ARG:H	1.83	0.43
1:E:534:LEU:HD13	1:E:543:PHE:HA	2.00	0.43
1:E:627:PHE:O	1:E:631:MET:N	2.51	0.43
1:M:79:GLU:N	1:M:304:ALA:O	2.51	0.43
1:O:1341:TYR:HA	1:O:1348:HIS:CD2	2.53	0.43
1:S:799:ASN:HD21	1:S:802:LEU:HG	1.84	0.43
1:U:406:LEU:HD21	1:U:1191:PHE:CE2	2.53	0.43
1:U:540:PHE:O	1:U:559:ARG:NH1	2.51	0.43
1:W:501:TYR:OH	1:W:978:ASN:O	2.31	0.43
1:W:1067:SER:OG	1:W:1083:THR:OG1	2.36	0.43
1:4:514:GLN:HG3	1:4:531:LEU:HD11	1.99	0.43
1:4:993:SER:O	1:4:997:ALA:N	2.50	0.43
1:4:1176:THR:OG1	1:4:1178:GLU:OE2	2.35	0.43
4:6:287:HIS:N	4:6:300:CYS:SG	2.87	0.43
4:7:267:ARG:HA	4:7:270:PHE:HD2	1.84	0.43
4:9:109:THR:HG22	4:9:288:VAL:HB	1.99	0.43
3:e:94:LYS:NZ	4:g:106:ASP:OD1	2.49	0.43
4:i:110:GLN:HE22	4:i:287:HIS:CE1	2.37	0.43
4:i:179:THR:OG1	4:i:189:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ILE:HA	1:F:59:ASN:HD22	1.83	0.43
1:B:529:HIS:CE1	1:B:1223:SER:HB3	2.54	0.43
1:C:708:LEU:HD21	1:C:1022:PRO:HG2	1.98	0.43
1:D:451:LYS:HG2	1:D:1140:ALA:HB1	2.01	0.43
2:J:22:HIS:HB3	2:J:25:VAL:HG23	1.99	0.43
2:L:33:GLN:NE2	2:L:36:MET:O	2.46	0.43
1:M:145:THR:HG23	1:M:148:ASP:H	1.84	0.43
1:M:929:ASP:OD1	1:M:932:ARG:NH2	2.52	0.43
1:N:192:LEU:O	1:N:196:GLY:N	2.51	0.43
1:O:368:LYS:HG3	1:O:373:PHE:HE1	1.84	0.43
1:O:422:VAL:HG13	1:O:427:ILE:HG21	2.00	0.43
1:S:123:HIS:HB2	1:S:1086:ILE:HB	2.01	0.43
1:S:918:LEU:HB2	1:S:944:PHE:CZ	2.53	0.43
1:S:929:ASP:OD1	1:S:932:ARG:NH2	2.52	0.43
1:T:422:VAL:O	1:T:424:SER:N	2.51	0.43
1:T:959:PRO:O	1:T:963:ASN:N	2.47	0.43
1:U:701:GLY:HA3	1:U:1131:GLN:NE2	2.33	0.43
1:W:878:LEU:O	1:W:881:SER:OG	2.36	0.43
1:X:918:LEU:HB2	1:X:944:PHE:CE2	2.53	0.43
1:4:757:ILE:HA	1:4:788:LEU:HB3	1.99	0.43
3:b:199:LEU:HD22	3:b:245:PHE:CE2	2.52	0.43
1:A:1025:ILE:HG22	1:A:1029:LYS:HE2	1.99	0.43
1:D:10:PHE:HB2	1:D:12:TYR:CE1	2.54	0.43
1:D:436:ASN:OD1	1:D:437:LYS:N	2.49	0.43
1:D:927:VAL:HG21	1:D:957:LEU:HD11	2.00	0.43
1:E:1198:ARG:HG2	1:E:1239:ALA:HB1	2.01	0.43
1:F:1188:VAL:HG12	1:F:1192:GLN:HE22	1.82	0.43
1:M:831:LEU:HD22	2:P:9:PRO:HG2	2.00	0.43
1:M:947:LEU:HD21	1:M:995:VAL:HG12	2.00	0.43
1:O:124:HIS:ND1	1:O:1085:GLU:HG2	2.33	0.43
1:O:175:VAL:HG21	1:O:382:MET:HE1	1.99	0.43
1:S:76:VAL:HB	1:S:1060:SER:HA	1.99	0.43
1:S:404:VAL:HG23	1:S:432:THR:HG23	2.00	0.43
1:S:1200:ARG:HG3	1:S:1234:THR:HG23	1.99	0.43
1:T:960:LEU:O	1:T:964:TYR:N	2.51	0.43
1:U:342:SER:OG	1:U:343:VAL:N	2.51	0.43
1:X:380:GLN:HE21	1:X:393:ASN:HD21	1.67	0.43
1:4:707:HIS:HA	1:4:713:LEU:HD22	1.99	0.43
1:4:1077:ALA:HB3	4:6:83:ARG:HH22	1.84	0.43
4:c:114:LEU:HD11	4:c:145:GLY:HA2	1.99	0.43
4:c:235:HIS:CG	4:d:209:MET:HE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:110:GLN:HG2	4:d:287:HIS:CE1	2.54	0.43
4:g:97:ASN:HB3	4:g:105:TRP:HE1	1.83	0.43
1:A:992:LYS:HB2	1:A:994:PRO:HD2	2.00	0.43
1:B:197:ASP:HB3	1:B:199:VAL:HG12	2.00	0.43
1:C:1216:GLU:OE2	1:C:1242:ARG:NH2	2.52	0.43
1:D:658:ARG:HA	1:D:681:LEU:HD11	2.00	0.43
1:D:951:PRO:O	1:D:955:ALA:N	2.52	0.43
1:E:898:ARG:HE	1:E:913:VAL:HG23	1.83	0.43
1:F:404:VAL:HG23	1:F:432:THR:HG23	2.01	0.43
1:M:495:ARG:HH22	2:P:4:PHE:HB3	1.82	0.43
1:M:700:VAL:O	1:M:1131:GLN:NE2	2.52	0.43
1:M:713:LEU:HA	1:M:801:VAL:HG22	2.01	0.43
1:M:1109:THR:HG22	1:M:1111:MET:H	1.84	0.43
1:N:512:VAL:HG12	1:N:993:SER:HB3	2.00	0.43
1:O:1366:ARG:HD2	1:O:1368:LEU:HD21	2.00	0.43
1:S:71:LEU:N	1:S:377:GLU:OE2	2.52	0.43
1:S:236:ARG:HE	1:S:239:GLN:HB2	1.82	0.43
1:T:949:ALA:HB1	1:T:977:PHE:HD2	1.84	0.43
1:U:845:ASN:N	1:U:848:ASP:OD2	2.47	0.43
1:U:1247:ASP:OD1	1:U:1251:ASN:ND2	2.52	0.43
1:V:532:LEU:O	1:V:1241:GLN:NE2	2.52	0.43
1:W:496:THR:HG21	1:W:982:ASN:HD22	1.82	0.43
1:W:695:ALA:HB1	1:W:706:THR:HG22	2.01	0.43
1:X:90:LYS:HD2	1:X:117:MET:HE1	2.00	0.43
1:4:722:ALA:H	1:4:917:VAL:HG13	1.83	0.43
1:4:1183:PRO:HD2	1:4:1236:ASN:HD22	1.84	0.43
1:4:1199:GLY:HA2	1:4:1235:ASN:HB3	2.01	0.43
4:9:222:CYS:SG	4:a:215:SER:OG	2.65	0.43
1:B:560:THR:HG23	1:B:902:GLN:HE22	1.83	0.43
1:B:1342:MET:HA	1:B:1375:VAL:HG21	2.00	0.43
1:D:263:THR:HA	1:D:359:ARG:HH12	1.84	0.43
1:E:520:THR:HG22	1:E:568:PRO:HA	2.00	0.43
1:F:824:VAL:HG13	1:F:938:MET:HB3	2.01	0.43
1:F:926:ALA:HB2	1:F:953:VAL:HG22	2.00	0.43
1:O:75:CYS:SG	1:O:1059:THR:OG1	2.70	0.43
1:T:278:THR:HG22	1:T:1051:ILE:HG12	2.01	0.43
1:U:856:ASN:HB2	2:0:12:GLN:HE21	1.83	0.43
1:W:1364:MET:HE3	1:W:1364:MET:HB2	1.83	0.43
1:X:474:ASP:OD1	1:X:552:GLY:N	2.52	0.43
1:4:708:LEU:HD21	1:4:1020:SER:HB2	2.00	0.43
4:7:21:ALA:HA	4:7:24:GLN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:9:237:LEU:HD21	4:a:209:MET:HE3	2.01	0.43
4:f:66:LEU:HD11	4:f:113:VAL:HG12	2.01	0.43
4:f:87:MET:HE3	4:f:93:LEU:HD21	2.01	0.43
4:f:99:TYR:CE2	4:f:139:VAL:HG22	2.54	0.43
1:C:306:TYR:HA	1:C:324:ARG:HH12	1.82	0.43
1:D:438:ASN:HD22	1:D:1171:HIS:HD2	1.67	0.43
1:F:26:SER:HB3	1:F:31:LEU:HB2	2.01	0.43
1:F:744:ASP:H	1:F:786:HIS:CE1	2.37	0.43
1:F:1199:GLY:HA2	1:F:1235:ASN:HB3	2.00	0.43
1:M:402:PHE:HD2	1:M:1040:VAL:HB	1.83	0.43
1:N:678:ARG:HH22	1:O:608:ALA:HB3	1.83	0.43
1:O:71:LEU:N	1:O:377:GLU:OE2	2.52	0.43
1:O:898:ARG:HD2	1:O:903:SER:HA	2.01	0.43
1:S:244:MET:HE2	1:S:244:MET:HB2	1.92	0.43
1:S:578:ARG:NH1	1:S:1014:SER:O	2.39	0.43
1:T:224:HIS:CD2	1:T:244:MET:HE1	2.53	0.43
1:U:762:ARG:HB2	1:U:765:ASP:HB2	2.00	0.43
1:W:82:ASP:N	1:W:82:ASP:OD1	2.51	0.43
1:W:228:LEU:HD22	1:W:1103:HIS:HD2	1.84	0.43
1:W:1115:CYS:HA	1:W:1177:CYS:H	1.84	0.43
1:W:1308:VAL:HG21	1:W:1314:VAL:HG21	2.00	0.43
1:4:851:LEU:H	1:4:869:ARG:HE	1.67	0.43
3:e:89:PHE:HZ	3:e:161:PRO:HB3	1.83	0.43
4:g:125:ILE:HB	4:g:134:ILE:HD11	2.01	0.43
1:A:77:ASN:HA	1:A:1061:MET:HB2	2.00	0.42
1:A:545:HIS:CE1	1:A:555:ARG:HD2	2.52	0.42
1:A:1075:SER:N	4:j:92:ASN:O	2.52	0.42
1:A:1271:HIS:ND1	1:A:1274:ASP:OD2	2.50	0.42
1:C:1271:HIS:HB3	1:C:1274:ASP:HB2	2.00	0.42
1:E:620:ILE:HG22	1:E:623:GLN:H	1.84	0.42
1:E:777:ARG:NH2	1:E:886:PRO:O	2.52	0.42
1:F:1200:ARG:HG3	1:F:1234:THR:HG23	2.01	0.42
1:N:1190:TYR:OH	1:N:1196:ASN:O	2.26	0.42
1:T:1199:GLY:H	1:T:1240:SER:HG	1.66	0.42
1:X:831:LEU:HD23	2:3:11:ILE:HD12	2.01	0.42
3:5:201:CYS:HB2	3:5:313:PRO:HG2	2.01	0.42
4:9:220:ARG:HG2	4:9:265:ARG:HH12	1.83	0.42
4:a:26:LYS:HE2	4:a:98:VAL:HB	2.01	0.42
4:f:211:LEU:HG	4:g:222:CYS:HB2	1.99	0.42
3:h:129:ALA:HA	3:h:132:TRP:HD1	1.83	0.42
1:A:1348:HIS:CE1	1:A:1357:LEU:HD22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:849:ASP:HB2	1:B:869:ARG:HH21	1.85	0.42
1:C:436:ASN:HB3	1:C:440:VAL:H	1.83	0.42
1:C:1170:SER:OG	1:D:1227:PRO:O	2.37	0.42
1:E:826:TYR:HE2	1:E:886:PRO:HG2	1.83	0.42
1:F:1022:PRO:HD3	1:F:1136:ILE:HD11	2.00	0.42
1:N:494:PHE:CZ	2:Q:6:VAL:HG22	2.53	0.42
1:N:583:ASP:OD1	1:N:590:HIS:NE2	2.48	0.42
1:N:704:PRO:HD2	1:N:707:HIS:CE1	2.54	0.42
1:O:822:MET:SD	1:O:939:PHE:HB3	2.59	0.42
1:S:733:LYS:NZ	1:T:966:THR:O	2.42	0.42
1:T:133:ALA:HB2	1:T:1076:ASP:HA	2.01	0.42
1:U:560:THR:HG22	1:U:561:MET:HG3	2.01	0.42
1:U:674:HIS:HA	1:U:677:TYR:HD2	1.84	0.42
1:V:1251:ASN:HD21	1:V:1270:PHE:C	2.24	0.42
1:W:505:ASN:OD1	1:W:506:VAL:N	2.52	0.42
1:W:824:VAL:H	1:W:889:THR:HG21	1.84	0.42
1:X:255:ASP:HB3	1:X:1093:LEU:H	1.85	0.42
1:X:963:ASN:HA	1:X:966:THR:HG22	2.01	0.42
1:4:295:SER:HA	1:4:366:LEU:HD13	1.99	0.42
1:4:702:ARG:NH1	1:4:733:LYS:O	2.52	0.42
4:7:141:PRO:HG2	4:7:144:LEU:HD12	2.02	0.42
4:c:151:GLN:HE21	4:d:267:ARG:HH11	1.68	0.42
1:A:505:ASN:OD1	1:A:506:VAL:N	2.52	0.42
1:A:720:PRO:HD3	1:A:808:TYR:CZ	2.55	0.42
1:B:455:HIS:HA	1:B:1119:PHE:HE1	1.84	0.42
1:E:728:THR:HG21	1:E:753:ARG:HD3	2.01	0.42
1:F:494:PHE:HZ	2:L:6:VAL:HG22	1.83	0.42
1:F:1198:ARG:NH1	1:F:1201:ALA:O	2.52	0.42
2:I:73:HIS:O	2:I:76:THR:OG1	2.34	0.42
1:M:350:LEU:HD12	1:U:13:LEU:HB3	2.00	0.42
1:M:402:PHE:O	1:M:1040:VAL:N	2.52	0.42
1:M:918:LEU:HB2	1:M:944:PHE:CE2	2.54	0.42
1:S:402:PHE:O	1:S:1040:VAL:N	2.51	0.42
1:S:849:ASP:HB3	1:S:869:ARG:HB3	2.00	0.42
1:S:1278:TYR:HE2	1:S:1321:HIS:HB3	1.85	0.42
1:U:74:ALA:HB1	1:U:182:LYS:HE3	2.01	0.42
1:U:118:LYS:NZ	1:U:1091:THR:O	2.52	0.42
1:U:224:HIS:CD2	1:U:244:MET:HE1	2.54	0.42
1:U:518:VAL:HG13	1:U:522:ASP:HB3	2.00	0.42
1:U:543:PHE:CZ	1:U:555:ARG:HD3	2.54	0.42
1:V:76:VAL:HB	1:V:1060:SER:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:561:MET:HE2	1:V:711:ALA:HB1	2.01	0.42
1:W:507:ALA:HB1	1:W:978:ASN:HD21	1.84	0.42
1:X:71:LEU:N	1:X:377:GLU:OE2	2.53	0.42
1:X:613:CYS:HB3	1:X:637:VAL:HG11	2.00	0.42
1:X:720:PRO:HD2	1:X:807:TYR:HD2	1.84	0.42
1:X:777:ARG:HH12	1:X:882:PHE:HZ	1.67	0.42
3:5:143:ILE:HG22	3:5:145:ASN:H	1.85	0.42
3:8:285:PHE:HB2	3:8:331:LEU:HD13	2.01	0.42
4:9:144:LEU:HA	4:9:147:ALA:HB3	2.01	0.42
3:e:150:MET:HB3	3:e:239:PRO:HB2	2.01	0.42
4:f:261:ASP:O	4:f:264:THR:OG1	2.36	0.42
4:i:112:ALA:HB2	4:i:142:GLN:HG2	1.99	0.42
4:j:110:GLN:HG2	4:j:287:HIS:ND1	2.34	0.42
1:A:438:ASN:HB2	1:A:1171:HIS:HD2	1.85	0.42
1:A:856:ASN:HB2	2:G:12:GLN:HE21	1.84	0.42
1:B:524:LEU:O	1:B:1233:SER:N	2.41	0.42
1:B:586:THR:HA	1:B:693:LYS:HD2	2.00	0.42
1:C:331:ALA:HA	1:C:335:ASP:HB2	2.01	0.42
1:D:455:HIS:HE2	1:D:1122:PHE:HB2	1.84	0.42
1:D:842:ASP:O	1:D:844:VAL:N	2.53	0.42
1:D:1328:PRO:HB2	1:D:1358:ILE:HG21	2.01	0.42
1:E:1342:MET:HA	1:E:1375:VAL:HG21	2.00	0.42
1:F:133:ALA:N	1:F:1076:ASP:O	2.52	0.42
1:F:448:ASN:ND2	1:F:1113:VAL:HG12	2.34	0.42
1:M:1071:ARG:HH22	4:c:38:ARG:N	2.17	0.42
1:M:1366:ARG:HD2	1:M:1368:LEU:HD21	2.01	0.42
1:N:414:SER:OG	1:N:415:THR:N	2.52	0.42
1:O:850:ILE:HD11	1:O:872:VAL:HA	2.01	0.42
1:S:394:ARG:HD3	1:S:1315:PHE:HB3	2.01	0.42
1:S:851:LEU:HD22	1:S:854:LEU:HD11	2.02	0.42
1:T:1062:PHE:HB2	1:T:1087:ALA:HB3	2.01	0.42
1:U:192:LEU:HD22	1:U:251:ALA:HB1	2.02	0.42
1:U:650:PHE:HD2	1:U:660:ILE:HD11	1.85	0.42
1:V:1115:CYS:HA	1:V:1177:CYS:HB2	2.02	0.42
1:W:463:GLN:HB3	1:W:1248:VAL:HG13	2.01	0.42
1:4:835:TYR:OH	1:4:856:ASN:O	2.38	0.42
4:c:285:ARG:HH12	4:d:282:LEU:HD11	1.83	0.42
3:e:312:LEU:HD12	3:e:313:PRO:HD2	2.01	0.42
1:B:224:HIS:CD2	1:B:244:MET:HE1	2.54	0.42
1:C:545:HIS:N	1:C:553:SER:O	2.40	0.42
1:C:1328:PRO:HB2	1:C:1358:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:HIS:CE1	1:E:106:ARG:HD2	2.55	0.42
1:F:541:ASP:N	1:F:557:THR:O	2.49	0.42
1:M:51:GLU:HB3	1:N:87:ILE:HB	2.01	0.42
1:N:63:PHE:HZ	1:N:171:GLU:HG3	1.83	0.42
1:O:831:LEU:HD22	2:R:9:PRO:HG2	2.02	0.42
1:O:842:ASP:O	1:O:844:VAL:N	2.52	0.42
1:S:612:PHE:HD1	1:S:862:ILE:HG22	1.84	0.42
1:S:698:GLU:OE2	1:S:1135:TYR:OH	2.32	0.42
1:S:1344:ASN:ND2	1:S:1347:THR:OG1	2.52	0.42
1:U:773:ILE:O	1:U:776:THR:OG1	2.36	0.42
1:W:457:ARG:HH22	1:W:463:GLN:HB2	1.85	0.42
1:W:539:PHE:O	1:W:559:ARG:N	2.45	0.42
1:X:829:VAL:O	1:X:832:THR:OG1	2.31	0.42
1:X:987:TYR:O	1:X:992:LYS:NZ	2.49	0.42
1:X:1239:ALA:O	1:X:1244:SER:OG	2.31	0.42
1:X:1339:ASP:O	1:X:1343:SER:N	2.49	0.42
3:8:125:THR:O	3:8:129:ALA:N	2.47	0.42
3:8:205:VAL:HG21	3:8:262:HIS:CE1	2.55	0.42
3:b:228:ALA:HB2	3:b:291:LEU:HD11	2.01	0.42
4:f:151:GLN:NE2	4:f:178:THR:O	2.53	0.42
4:j:97:ASN:HB2	4:j:99:TYR:HD2	1.83	0.42
1:A:70:ALA:HB3	1:A:377:GLU:HG2	1.99	0.42
1:A:457:ARG:HH22	1:A:463:GLN:HB2	1.84	0.42
1:A:591:VAL:HG12	1:A:679:LYS:HG2	2.02	0.42
1:A:898:ARG:HD3	1:A:902:GLN:HG3	2.01	0.42
1:A:1115:CYS:HA	1:A:1177:CYS:HB2	2.01	0.42
1:A:1116:GLN:HE21	1:A:1262:MET:HG3	1.84	0.42
1:B:297:MET:HE3	1:B:364:ALA:HB3	2.02	0.42
1:B:472:PHE:HB3	1:B:475:PRO:HG3	2.02	0.42
1:E:658:ARG:NH2	1:F:929:ASP:OD2	2.52	0.42
1:E:717:LEU:HB2	1:E:990:TRP:CZ3	2.53	0.42
1:M:842:ASP:O	1:M:844:VAL:N	2.52	0.42
1:N:278:THR:HG22	1:N:1051:ILE:HG12	2.02	0.42
1:N:539:PHE:O	1:N:559:ARG:N	2.46	0.42
1:N:717:LEU:HD12	1:N:915:GLN:HE22	1.85	0.42
1:O:600:ILE:O	1:O:603:THR:OG1	2.34	0.42
1:T:107:ARG:HA	4:6:37:HIS:CE1	2.54	0.42
1:U:394:ARG:HD3	1:U:1315:PHE:HB3	2.00	0.42
1:V:709:VAL:HG13	1:V:1023:SER:HA	2.00	0.42
1:W:819:MET:N	1:W:950:ASP:OD2	2.46	0.42
1:X:958:HIS:HE1	1:X:960:LEU:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:402:PHE:O	1:4:1040:VAL:N	2.52	0.42
4:6:146:HIS:O	4:6:150:GLN:N	2.40	0.42
4:c:105:TRP:HB2	4:c:291:TYR:CZ	2.55	0.42
4:c:205:ASP:O	4:c:208:SER:OG	2.31	0.42
3:e:73:PHE:HD2	3:e:105:LEU:HD11	1.83	0.42
4:f:51:CYS:HB2	4:f:62:ILE:HD11	2.02	0.42
4:i:59:TYR:HA	4:i:62:ILE:HB	2.02	0.42
1:B:422:VAL:O	1:B:424:SER:N	2.53	0.42
1:C:297:MET:HE3	1:C:364:ALA:HB3	2.00	0.42
1:F:129:ILE:HD11	1:F:1082:ILE:HD11	2.01	0.42
1:F:687:LEU:HD23	1:F:805:LEU:HB3	2.02	0.42
1:N:9:PRO:HB3	1:N:45:GLU:HB3	2.02	0.42
1:N:674:HIS:HA	1:N:677:TYR:HD2	1.85	0.42
1:S:133:ALA:HA	1:S:136:ILE:HD12	2.00	0.42
1:S:413:TYR:HA	1:X:421:GLY:HA3	2.01	0.42
1:T:505:ASN:OD1	1:T:506:VAL:N	2.53	0.42
1:U:539:PHE:O	1:U:559:ARG:N	2.40	0.42
1:U:1334:HIS:HB2	1:U:1355:GLN:HG2	2.02	0.42
1:X:328:GLN:HG2	1:X:349:ALA:HB1	2.02	0.42
4:6:160:LYS:NZ	4:7:228:ALA:O	2.43	0.42
3:b:218:GLU:HA	3:b:219:PRO:HD3	1.87	0.42
4:d:33:LEU:N	4:d:69:CYS:SG	2.92	0.42
4:f:211:LEU:HD12	4:g:218:VAL:HG13	2.02	0.42
1:A:165:PHE:HE1	1:B:98:PRO:HA	1.85	0.42
1:B:191:ILE:HA	1:B:217:PHE:HE1	1.85	0.42
1:C:1188:VAL:HG12	1:C:1192:GLN:HE22	1.83	0.42
1:D:297:MET:HE3	1:D:364:ALA:HB3	2.02	0.42
1:E:861:ASP:HA	1:E:864:GLN:HB2	2.02	0.42
1:E:1169:LEU:O	1:F:1206:SER:OG	2.31	0.42
1:F:856:ASN:ND2	2:L:12:GLN:HE21	2.17	0.42
1:N:697:HIS:HB2	1:O:509:VAL:HG21	2.02	0.42
1:S:18:ASN:OD1	1:S:19:LEU:N	2.53	0.42
1:T:980:PRO:HD2	1:T:983:LEU:HD12	2.02	0.42
1:T:1170:SER:OG	1:U:1227:PRO:O	2.31	0.42
1:V:1200:ARG:HG3	1:V:1234:THR:HG23	2.02	0.42
1:W:452:SER:HB3	1:W:1118:LEU:H	1.85	0.42
1:W:1107:ILE:HD11	1:W:1364:MET:HE1	2.00	0.42
3:e:81:SER:OG	3:e:84:GLU:OE2	2.37	0.42
1:A:1169:LEU:HD12	1:B:211:SER:HB2	2.01	0.42
1:C:623:GLN:OE1	1:C:724:HIS:NE2	2.40	0.42
1:D:130:GLU:HG2	1:D:1079:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:820:CYS:O	1:D:924:ALA:N	2.53	0.42
1:D:1364:MET:HE3	1:D:1364:MET:HB2	1.92	0.42
1:E:509:VAL:HG22	1:E:976:VAL:HG13	2.02	0.42
1:E:538:PRO:HD3	1:E:1238:TRP:NE1	2.35	0.42
1:F:537:HIS:HA	1:F:1238:TRP:HE1	1.85	0.42
1:N:214:VAL:HA	1:N:217:PHE:CD2	2.55	0.42
1:N:1169:LEU:HD12	1:O:211:SER:HB2	2.02	0.42
1:O:102:HIS:CE1	1:O:106:ARG:HD2	2.55	0.42
1:O:777:ARG:HG2	1:O:782:HIS:CE1	2.55	0.42
1:S:537:HIS:HB3	1:S:1245:LEU:HB2	2.02	0.42
1:U:861:ASP:HB3	1:U:931:SER:HB2	2.01	0.42
1:W:78:THR:HG22	1:W:304:ALA:HB3	2.01	0.42
1:W:455:HIS:CE1	1:W:1122:PHE:HB2	2.55	0.42
1:W:1341:TYR:HB2	1:W:1357:LEU:HD11	2.00	0.42
1:X:1163:CYS:SG	1:X:1164:GLU:N	2.93	0.42
1:4:685:ILE:HA	1:4:688:GLU:HG2	2.01	0.42
4:6:209:MET:HG2	4:7:241:PHE:HE2	1.85	0.42
3:8:227:TYR:HD2	3:8:255:VAL:HG11	1.85	0.42
4:9:224:ARG:NH2	4:9:255:ASP:O	2.53	0.42
3:e:154:GLU:O	3:e:157:THR:OG1	2.36	0.42
4:f:179:THR:HB	4:f:190:LEU:HD12	2.02	0.42
4:i:241:PHE:HE2	4:j:213:ILE:HG23	1.84	0.42
1:B:278:THR:HG22	1:B:1051:ILE:HG12	2.01	0.42
1:C:236:ARG:HD2	1:C:239:GLN:HB3	2.02	0.42
1:E:780:GLU:HB3	1:E:785:ARG:HH12	1.85	0.42
1:F:163:LEU:HD12	3:e:34:PHE:CE1	2.55	0.42
1:M:1070:ARG:NH1	4:c:2:ALA:O	2.52	0.42
1:N:744:ASP:H	1:N:786:HIS:CE1	2.38	0.42
1:N:984:MET:HE2	1:N:984:MET:HB3	1.75	0.42
1:S:945:ASN:OD1	1:S:946:LYS:N	2.53	0.42
1:T:890:GLN:HB2	1:T:919:VAL:HB	2.01	0.42
1:U:455:HIS:HE2	1:U:1122:PHE:HB2	1.85	0.42
1:U:1250:TYR:HB2	1:U:1270:PHE:HD2	1.83	0.42
1:V:80:PHE:HE2	1:V:83:LEU:HD12	1.84	0.42
1:V:1109:THR:HG23	1:V:1173:GLN:HB3	2.02	0.42
1:W:438:ASN:HD22	1:W:1171:HIS:CD2	2.34	0.42
1:W:582:PHE:HA	1:W:1032:MET:HE1	2.01	0.42
1:X:1044:ASP:HA	1:X:1109:THR:HB	2.02	0.42
2:Y:33:GLN:NE2	2:Y:36:MET:O	2.46	0.42
3:8:165:MET:HE2	3:8:165:MET:HB3	1.85	0.42
3:b:253:ALA:HB2	4:c:281:ASN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:62:ILE:HG21	4:d:115:PRO:HB3	2.02	0.42
4:d:144:LEU:HD23	4:d:144:LEU:HA	1.86	0.42
4:d:288:VAL:HA	4:d:299:SER:O	2.20	0.42
1:A:401:PHE:N	1:A:1327:TYR:O	2.43	0.41
1:A:649:ALA:O	1:A:677:TYR:OH	2.30	0.41
1:A:822:MET:HE1	1:A:957:LEU:HD11	2.02	0.41
1:C:591:VAL:N	1:C:683:GLU:OE1	2.52	0.41
1:C:845:ASN:N	1:C:848:ASP:OD2	2.51	0.41
1:D:1295:GLY:H	1:D:1321:HIS:HE1	1.67	0.41
1:E:10:PHE:HB2	1:E:12:TYR:HE1	1.85	0.41
1:E:455:HIS:CE1	1:E:1122:PHE:HB2	2.54	0.41
1:E:538:PRO:HB2	1:E:565:ILE:HG12	2.02	0.41
1:E:918:LEU:HD13	1:E:944:PHE:HZ	1.84	0.41
1:F:177:THR:O	1:F:181:VAL:N	2.48	0.41
1:F:958:HIS:CE1	1:F:960:LEU:HB3	2.55	0.41
2:H:33:GLN:NE2	2:H:36:MET:O	2.46	0.41
1:M:273:ALA:HB3	1:M:372:LYS:HB3	2.01	0.41
1:M:1188:VAL:HG12	1:M:1192:GLN:HE22	1.84	0.41
1:O:76:VAL:O	1:O:1061:MET:N	2.50	0.41
1:O:78:THR:OG1	1:O:1061:MET:O	2.36	0.41
1:O:1116:GLN:HE21	1:O:1121:ILE:HD11	1.84	0.41
1:O:1225:PRO:HB2	1:O:1230:GLU:HA	2.01	0.41
1:S:402:PHE:HD2	1:S:1040:VAL:HB	1.85	0.41
1:S:623:GLN:HB2	1:S:626:LYS:HB2	2.02	0.41
1:S:649:ALA:O	1:S:677:TYR:OH	2.34	0.41
1:S:916:THR:OG1	1:S:984:MET:SD	2.71	0.41
1:U:138:LEU:HD21	1:U:151:GLU:HG3	2.02	0.41
1:U:826:TYR:HA	1:U:829:VAL:HG23	2.02	0.41
1:V:102:HIS:HE1	1:V:106:ARG:HD2	1.84	0.41
1:W:434:VAL:HG11	1:W:1042:ARG:HH22	1.85	0.41
1:W:1214:SER:HA	1:W:1217:ARG:HD3	2.01	0.41
1:X:582:PHE:HE1	1:X:694:LEU:HD11	1.85	0.41
2:1:73:HIS:O	2:1:76:THR:OG1	2.34	0.41
1:4:1073:VAL:HG22	1:4:1079:THR:H	1.84	0.41
3:5:224:VAL:HB	3:5:296:PHE:HB2	2.02	0.41
4:9:88:ASP:HB2	4:9:91:ASP:HB2	2.01	0.41
4:9:151:GLN:HB2	4:a:267:ARG:HH12	1.85	0.41
4:f:9:VAL:HB	4:f:82:LEU:HB2	2.01	0.41
4:f:213:ILE:HA	4:g:244:VAL:HG11	2.01	0.41
4:i:50:VAL:HG13	4:i:62:ILE:HG12	2.02	0.41
4:i:233:ASP:O	4:i:235:HIS:ND1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLN:HE22	1:A:115:ILE:HG23	1.84	0.41
1:A:851:LEU:HD23	1:A:851:LEU:HA	1.88	0.41
1:B:133:ALA:HB2	1:B:1076:ASP:HA	2.02	0.41
1:D:11:PRO:HB2	1:N:332:ARG:HG2	2.01	0.41
1:D:916:THR:OG1	1:D:984:MET:SD	2.72	0.41
1:E:725:ASP:OD2	1:E:728:THR:OG1	2.32	0.41
1:F:718:LEU:HD12	1:F:894:VAL:HG21	2.02	0.41
1:M:591:VAL:N	1:M:683:GLU:OE1	2.52	0.41
1:N:297:MET:HE3	1:N:364:ALA:HB3	2.02	0.41
1:O:394:ARG:HB2	1:O:1050:HIS:NE2	2.35	0.41
1:O:1294:ALA:HB1	1:O:1321:HIS:HE1	1.85	0.41
1:S:170:LEU:HD11	1:S:1084:HIS:HB2	2.01	0.41
1:S:512:VAL:HG12	1:S:993:SER:HB3	2.01	0.41
1:S:1210:TYR:HE1	1:S:1280:ARG:HG2	1.84	0.41
1:U:468:LEU:HD13	1:U:1243:GLY:HA3	2.02	0.41
1:V:963:ASN:HA	1:V:966:THR:HG22	2.02	0.41
1:W:1200:ARG:HG2	1:W:1226:ASP:OD2	2.20	0.41
1:X:946:LYS:HE2	1:X:993:SER:HA	2.02	0.41
1:4:124:HIS:HA	1:4:1085:GLU:HG2	2.00	0.41
3:b:207:LEU:HB3	3:b:248:SER:HB3	2.01	0.41
4:c:144:LEU:HD21	4:c:183:PHE:HB2	2.01	0.41
4:d:183:PHE:O	4:d:186:ARG:N	2.50	0.41
3:e:232:TYR:O	3:e:270:LYS:NZ	2.37	0.41
4:f:13:SER:OG	4:f:129:SER:OG	2.32	0.41
4:f:151:GLN:HB2	4:g:267:ARG:NH1	2.35	0.41
1:A:181:VAL:HG22	1:A:184:ARG:HD2	2.01	0.41
1:C:256:THR:HA	1:C:1092:ALA:HB2	2.02	0.41
1:D:95:ILE:HB	1:D:114:TYR:HB2	2.01	0.41
1:D:191:ILE:HA	1:D:217:PHE:CE1	2.55	0.41
1:E:538:PRO:HA	1:E:559:ARG:NH1	2.35	0.41
1:E:1178:GLU:OE2	1:E:1265:PRO:HD2	2.20	0.41
1:M:446:TYR:O	1:M:450:LEU:N	2.53	0.41
1:N:63:PHE:HE2	1:N:65:LYS:HE2	1.85	0.41
1:N:205:LEU:HD13	1:N:1282:LEU:HD22	2.01	0.41
1:N:692:LEU:HD23	1:N:692:LEU:HA	1.84	0.41
1:N:845:ASN:N	1:N:848:ASP:OD2	2.47	0.41
1:N:1067:SER:OG	1:N:1083:THR:OG1	2.35	0.41
1:N:1167:PRO:HD3	1:O:1224:ILE:HD13	2.01	0.41
1:O:759:LEU:HD22	1:O:792:PRO:HB3	2.03	0.41
1:O:1067:SER:OG	1:O:1083:THR:OG1	2.38	0.41
1:O:1198:ARG:NH1	1:O:1200:ARG:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1251:ASN:ND2	1:O:1271:HIS:HA	2.35	0.41
1:S:1071:ARG:HH22	4:6:38:ARG:N	2.18	0.41
1:T:1264:SER:HB2	1:T:1267:ARG:HB2	2.01	0.41
1:U:76:VAL:HB	1:U:1060:SER:HA	2.02	0.41
1:U:396:ILE:HD11	1:U:1050:HIS:CE1	2.55	0.41
1:V:284:ARG:O	1:V:288:ASN:ND2	2.54	0.41
1:V:582:PHE:HE1	1:V:694:LEU:HD11	1.85	0.41
1:V:1198:ARG:HB3	1:V:1240:SER:HG	1.85	0.41
1:V:1216:GLU:OE2	1:V:1242:ARG:NH2	2.53	0.41
1:W:736:ARG:HH22	1:W:899:ASP:HA	1.84	0.41
1:W:1107:ILE:HD13	1:W:1111:MET:HE3	2.02	0.41
3:5:111:LEU:HD12	3:5:114:LEU:HD22	2.02	0.41
4:7:75:GLU:HB3	4:7:83:ARG:HD3	2.03	0.41
4:a:5:LYS:HD2	4:a:86:ARG:HB3	2.02	0.41
4:a:110:GLN:HG2	4:a:287:HIS:CE1	2.55	0.41
4:c:241:PHE:HE2	4:d:213:ILE:HG23	1.85	0.41
4:i:32:PRO:HD3	4:i:137:PRO:HG3	2.02	0.41
1:A:1170:SER:OG	1:B:1227:PRO:O	2.32	0.41
1:A:1334:HIS:CD2	1:A:1335:ARG:H	2.38	0.41
1:C:396:ILE:HD11	1:C:1050:HIS:HE1	1.85	0.41
1:D:402:PHE:O	1:D:1040:VAL:N	2.48	0.41
1:D:957:LEU:HD23	1:D:957:LEU:HA	1.87	0.41
1:M:140:PHE:HZ	3:b:57:HIS:HB2	1.84	0.41
1:M:737:GLN:HB3	1:M:897:LYS:HE2	2.01	0.41
1:M:845:ASN:HB3	1:M:846:ALA:H	1.66	0.41
1:N:799:ASN:HD21	1:N:802:LEU:HG	1.86	0.41
1:S:191:ILE:HA	1:S:217:PHE:HE1	1.84	0.41
1:S:851:LEU:HD23	1:S:854:LEU:HD21	2.02	0.41
1:U:1200:ARG:HG3	1:U:1234:THR:HG23	2.01	0.41
1:V:252:VAL:HG11	1:V:1055:SER:HB3	2.02	0.41
1:X:75:CYS:HG	1:X:1059:THR:HG1	1.57	0.41
1:4:461:PRO:HB2	1:4:542:PHE:HE1	1.86	0.41
4:6:219:PRO:HA	4:6:265:ARG:HH11	1.85	0.41
3:8:228:ALA:HB2	3:8:291:LEU:HD11	2.02	0.41
3:e:305:LEU:HD12	3:e:312:LEU:HB3	2.02	0.41
3:h:227:TYR:HB2	3:h:246:PHE:HB2	2.02	0.41
4:j:223:LEU:HD13	4:j:252:ILE:HB	2.02	0.41
1:A:454:CYS:O	1:A:1127:TYR:OH	2.31	0.41
1:A:509:VAL:HG22	1:A:976:VAL:HG13	2.03	0.41
1:B:457:ARG:HH22	1:B:463:GLN:HB3	1.84	0.41
1:B:796:ASN:OD1	1:C:932:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1236:ASN:HB2	1:B:1238:TRP:HE3	1.86	0.41
1:D:740:ILE:HB	1:D:747:TYR:HB3	2.02	0.41
1:D:1017:GLN:HE22	1:D:1027:GLN:CD	2.29	0.41
1:E:1341:TYR:HA	1:E:1348:HIS:CD2	2.56	0.41
2:J:33:GLN:NE2	2:J:36:MET:O	2.46	0.41
1:M:868:ILE:HG22	1:M:870:PRO:HD3	2.02	0.41
1:M:958:HIS:CE1	1:M:960:LEU:HB3	2.56	0.41
1:M:1020:SER:O	1:M:1023:SER:OG	2.35	0.41
1:M:1335:ARG:HH22	1:M:1370:LEU:HD11	1.86	0.41
1:N:422:VAL:H	1:N:422:VAL:HG23	1.62	0.41
1:N:619:MET:HE1	1:N:833:LEU:HD12	2.02	0.41
1:O:736:ARG:HA	1:O:736:ARG:HD3	1.86	0.41
1:U:73:ALA:O	1:U:1057:ALA:N	2.45	0.41
1:U:712:LEU:HA	1:U:712:LEU:HD23	1.88	0.41
1:U:1210:TYR:CE1	1:U:1280:ARG:HG2	2.55	0.41
1:U:1302:THR:OG1	1:U:1304:LEU:O	2.33	0.41
1:X:245:LEU:HD22	1:X:369:ILE:HD13	2.01	0.41
1:X:831:LEU:HD22	2:3:9:PRO:HG2	2.03	0.41
1:A:608:ALA:HA	1:A:928:ALA:HB2	2.02	0.41
1:B:694:LEU:HD21	1:B:1032:MET:HE3	2.03	0.41
1:C:1115:CYS:HA	1:C:1177:CYS:HB2	2.03	0.41
1:D:290:LEU:HB3	1:D:367:VAL:HG21	2.02	0.41
1:E:45:GLU:OE1	1:T:158:THR:OG1	2.37	0.41
1:E:826:TYR:CE2	1:E:886:PRO:HG2	2.55	0.41
1:F:946:LYS:HE2	1:F:993:SER:HA	2.01	0.41
1:M:532:LEU:O	1:M:1241:GLN:NE2	2.53	0.41
1:O:145:THR:HG23	1:O:148:ASP:H	1.84	0.41
1:O:1109:THR:O	1:O:1111:MET:N	2.50	0.41
1:T:927:VAL:HG21	1:T:957:LEU:HD21	2.02	0.41
1:V:684:LEU:HD23	1:V:802:LEU:HD22	2.03	0.41
1:V:1341:TYR:HA	1:V:1348:HIS:HD2	1.86	0.41
1:W:172:ARG:NH1	1:W:382:MET:O	2.54	0.41
2:2:33:GLN:NE2	2:2:36:MET:O	2.46	0.41
4:c:258:SER:OG	4:c:261:ASP:OD2	2.37	0.41
1:A:1190:TYR:HD1	1:A:1229:TYR:HE2	1.68	0.41
1:B:436:ASN:HD21	1:B:442:LEU:HG	1.86	0.41
1:C:296:ALA:H	1:C:366:LEU:HD13	1.85	0.41
1:C:651:VAL:HG12	1:C:811:MET:HE1	2.02	0.41
1:D:1020:SER:N	1:D:1023:SER:OG	2.54	0.41
1:D:1312:THR:OG1	1:D:1313:ASP:N	2.53	0.41
1:D:1336:VAL:HG22	1:E:413:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:406:LEU:HB3	1:E:407:HIS:H	1.72	0.41
1:F:675:GLY:O	1:F:679:LYS:HG2	2.20	0.41
1:M:255:ASP:OD2	1:M:1094:GLY:N	2.41	0.41
1:M:537:HIS:HA	1:M:1238:TRP:CD1	2.50	0.41
1:O:493:LEU:HB2	1:O:940:TYR:HE2	1.85	0.41
2:R:33:GLN:NE2	2:R:36:MET:O	2.46	0.41
1:U:307:VAL:HG12	1:U:309:ARG:H	1.85	0.41
1:V:945:ASN:OD1	1:V:946:LYS:N	2.54	0.41
1:X:842:ASP:O	1:X:844:VAL:N	2.54	0.41
1:X:916:THR:OG1	1:X:984:MET:SD	2.64	0.41
4:9:120:ARG:O	4:9:124:THR:N	2.38	0.41
4:j:5:LYS:HD2	4:j:86:ARG:HB3	2.02	0.41
1:B:512:VAL:HG12	1:B:993:SER:HB3	2.02	0.41
1:B:706:THR:HB	1:B:713:LEU:HD13	2.03	0.41
1:C:572:ARG:HH21	1:C:1002:CYS:HA	1.84	0.41
1:D:612:PHE:O	1:D:616:ILE:HD12	2.19	0.41
1:E:83:LEU:HD21	1:E:122:LYS:HD2	2.02	0.41
1:E:153:ALA:HA	1:E:156:ILE:HG22	2.03	0.41
1:E:395:ARG:HD3	1:E:1045:GLU:HB3	2.02	0.41
1:E:538:PRO:HA	1:E:559:ARG:HH11	1.85	0.41
1:M:545:HIS:ND1	1:M:555:ARG:HG2	2.36	0.41
1:N:351:ALA:HB1	1:N:354:HIS:HB2	2.03	0.41
1:N:545:HIS:CD2	1:N:555:ARG:HD3	2.55	0.41
1:N:1070:ARG:HD3	3:8:67:GLN:HE22	1.85	0.41
1:O:76:VAL:HB	1:O:1060:SER:HA	2.03	0.41
1:O:123:HIS:HB2	1:O:1086:ILE:HB	2.03	0.41
1:T:1328:PRO:HB2	1:T:1358:ILE:HG21	2.03	0.41
1:V:105:GLY:HA2	4:d:40:GLN:HA	2.02	0.41
1:V:130:GLU:HG3	1:W:110:LYS:HD2	2.03	0.41
1:V:1171:HIS:HE1	1:W:1228:ALA:HA	1.85	0.41
1:W:1198:ARG:HH12	1:W:1200:ARG:HB2	1.85	0.41
3:8:206:ASP:OD1	3:8:207:LEU:N	2.52	0.41
3:b:38:VAL:HG13	3:b:41:LEU:HD13	2.02	0.41
3:b:206:ASP:OD1	3:b:207:LEU:N	2.54	0.41
4:c:212:CYS:N	4:d:222:CYS:SG	2.94	0.41
4:d:47:LEU:HB2	4:d:135:VAL:HB	2.02	0.41
4:j:60:ILE:HD11	4:j:210:TYR:HE2	1.85	0.41
1:A:780:GLU:HB3	1:A:785:ARG:HH12	1.86	0.41
1:B:680:ILE:O	1:B:684:LEU:N	2.54	0.41
1:C:184:ARG:HG2	1:C:1291:ALA:HA	2.03	0.41
1:C:248:MET:HE3	1:C:248:MET:HB2	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:TYR:HD2	1:N:94:LYS:HD2	1.86	0.41
1:D:127:ALA:HB3	1:D:1082:ILE:HB	2.03	0.41
1:D:274:GLY:H	1:D:1056:ARG:HB2	1.86	0.41
1:D:809:VAL:HG13	1:D:1012:MET:HB2	2.03	0.41
1:D:918:LEU:HB2	1:D:944:PHE:CE2	2.56	0.41
1:E:313:LEU:HD21	1:M:150:THR:HG21	2.03	0.41
1:E:1236:ASN:HB2	1:E:1238:TRP:HE3	1.85	0.41
1:F:368:LYS:HG2	1:F:373:PHE:CE1	2.55	0.41
1:F:422:VAL:HG13	1:F:427:ILE:HD13	2.02	0.41
1:F:620:ILE:HG22	1:F:622:GLY:H	1.86	0.41
1:F:731:MET:HG3	1:F:747:TYR:HE2	1.85	0.41
1:M:157:LYS:HD2	1:N:338:ASN:HA	2.02	0.41
1:M:829:VAL:O	1:M:832:THR:OG1	2.30	0.41
1:M:1080:PHE:HZ	3:b:60:LEU:HD21	1.86	0.41
1:N:612:PHE:O	1:N:616:ILE:HD12	2.20	0.41
1:O:83:LEU:HD22	1:O:1085:GLU:HB3	2.03	0.41
1:O:457:ARG:HH22	1:O:1254:PHE:HB3	1.85	0.41
1:O:458:MET:HE1	1:O:1181:PRO:HG3	2.03	0.41
1:O:1251:ASN:HB3	1:O:1252:ILE:H	1.67	0.41
1:O:1342:MET:HE1	1:O:1370:LEU:H	1.85	0.41
1:S:1003:GLN:NE2	1:X:587:ASN:OD1	2.53	0.41
1:S:1178:GLU:HB3	1:S:1179:ILE:H	1.68	0.41
1:S:1341:TYR:HB2	1:S:1357:LEU:HD11	2.03	0.41
1:T:692:LEU:HD23	1:T:692:LEU:HA	1.79	0.41
1:U:244:MET:HE2	1:U:244:MET:HB2	1.97	0.41
1:U:1190:TYR:OH	1:U:1196:ASN:O	2.31	0.41
1:V:165:PHE:HE1	1:W:98:PRO:HA	1.86	0.41
1:V:491:MET:HB2	1:V:783:ASP:HA	2.02	0.41
1:V:493:LEU:O	1:V:496:THR:OG1	2.34	0.41
1:W:189:VAL:HG21	1:W:248:MET:HE2	2.03	0.41
1:W:436:ASN:HB3	1:W:440:VAL:H	1.86	0.41
1:W:536:VAL:HG13	1:W:1244:SER:HA	2.01	0.41
1:W:1108:THR:O	1:W:1173:GLN:N	2.51	0.41
1:X:394:ARG:HB2	1:X:1050:HIS:NE2	2.35	0.41
1:X:569:LEU:HD23	1:X:569:LEU:HA	1.87	0.41
1:X:839:VAL:O	2:3:57:TYR:OH	2.27	0.41
2:Y:28:MET:HE2	2:Y:45:LYS:HG2	2.03	0.41
1:4:406:LEU:HD21	1:4:1191:PHE:HE2	1.85	0.41
1:4:636:LEU:HD21	1:4:871:THR:H	1.86	0.41
1:4:861:ASP:O	1:4:930:ARG:NH2	2.54	0.41
4:7:276:LEU:HD12	4:7:279:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:81:SER:N	3:8:133:TYR:OH	2.54	0.41
4:9:211:LEU:HD12	4:a:218:VAL:HG13	2.02	0.41
4:a:26:LYS:HE2	4:a:26:LYS:HB3	1.88	0.41
4:a:124:THR:OG1	4:a:134:ILE:O	2.26	0.41
4:d:217:LEU:HB3	4:d:269:MET:SD	2.60	0.41
4:g:144:LEU:HD23	4:g:144:LEU:HA	1.91	0.41
4:g:286:LEU:HD13	4:g:300:CYS:HB2	2.03	0.41
3:h:227:TYR:HE2	3:h:255:VAL:HG21	1.86	0.41
1:A:185:HIS:O	1:A:1097:SER:OG	2.39	0.41
1:A:889:THR:HA	1:A:920:ASN:HB3	2.03	0.41
1:B:307:VAL:HB	1:B:309:ARG:HH11	1.86	0.41
1:B:558:HIS:CE1	1:B:902:GLN:HG3	2.56	0.41
1:B:598:ASP:O	1:B:602:GLU:N	2.41	0.41
1:B:627:PHE:HE2	1:B:663:HIS:HB2	1.87	0.41
1:B:708:LEU:HD21	1:B:1022:PRO:HG2	2.02	0.41
1:B:717:LEU:HA	1:B:915:GLN:NE2	2.35	0.41
1:C:829:VAL:O	1:C:832:THR:OG1	2.32	0.41
1:D:494:PHE:HZ	2:J:6:VAL:HG22	1.86	0.41
1:E:397:GLN:HB3	1:E:1318:GLN:HB3	2.03	0.41
1:E:538:PRO:HD3	1:E:1238:TRP:HE1	1.85	0.41
1:M:61:VAL:HG11	1:N:98:PRO:HG3	2.02	0.41
1:M:793:LEU:HD12	1:M:798:TYR:HE1	1.86	0.41
1:N:146:PRO:HA	1:N:149:PHE:HD2	1.86	0.41
1:N:595:LEU:HD23	1:N:676:HIS:HE1	1.86	0.41
1:S:85:ARG:HH22	1:4:151:GLU:HB3	1.85	0.41
1:T:494:PHE:HZ	2:Z:6:VAL:HG22	1.86	0.41
1:U:436:ASN:HB3	1:U:440:VAL:H	1.86	0.41
1:U:889:THR:HB	1:U:918:LEU:HD11	2.03	0.41
1:V:1109:THR:O	1:V:1111:MET:N	2.54	0.41
1:W:736:ARG:NH2	1:W:899:ASP:OD1	2.54	0.41
1:X:780:GLU:OE1	1:X:785:ARG:NH1	2.39	0.41
1:X:1011:ALA:O	1:X:1015:MET:N	2.54	0.41
2:1:28:MET:HE2	2:1:45:LYS:HG2	2.03	0.41
1:4:156:ILE:HA	1:4:159:ILE:HG22	2.02	0.41
3:5:250:LYS:HA	4:6:68:LYS:HG2	2.03	0.41
4:a:269:MET:HE3	4:a:269:MET:HB3	1.88	0.41
4:c:272:TYR:O	4:c:275:SER:OG	2.30	0.41
4:d:47:LEU:O	4:d:51:CYS:N	2.47	0.41
4:i:124:THR:HG22	4:i:135:VAL:HG13	2.03	0.41
4:j:60:ILE:HD11	4:j:210:TYR:CE2	2.55	0.41
4:j:97:ASN:CG	4:j:105:TRP:HE1	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1250:TYR:CD2	1:B:1266:CYS:HB2	2.55	0.40
1:C:736:ARG:NH1	1:C:898:ARG:O	2.38	0.40
1:E:539:PHE:HE1	1:E:1019:LEU:HD22	1.85	0.40
1:E:898:ARG:HD3	1:E:902:GLN:HG3	2.03	0.40
1:F:226:PHE:HE2	1:F:1364:MET:HB3	1.86	0.40
2:G:28:MET:HE2	2:G:45:LYS:HG2	2.03	0.40
1:M:557:THR:HA	1:M:898:ARG:NH2	2.36	0.40
1:M:1065:LEU:HD23	1:M:1065:LEU:HA	1.93	0.40
1:N:326:PHE:O	1:N:330:MET:N	2.54	0.40
1:N:1043:THR:HG23	1:N:1265:PRO:HG3	2.02	0.40
1:O:1280:ARG:NH2	1:O:1288:GLU:OE1	2.54	0.40
1:S:447:GLN:HE22	1:T:521:GLU:CD	2.28	0.40
1:S:898:ARG:NH1	1:S:910:GLY:O	2.53	0.40
1:T:446:TYR:O	1:T:450:LEU:N	2.54	0.40
1:T:951:PRO:O	1:T:955:ALA:N	2.50	0.40
1:U:252:VAL:HG13	1:U:1096:SER:HA	2.03	0.40
1:V:127:ALA:HB3	1:V:1082:ILE:HB	2.03	0.40
1:V:455:HIS:ND1	1:V:457:ARG:HG2	2.36	0.40
1:W:165:PHE:HE1	1:X:98:PRO:HA	1.86	0.40
1:W:518:VAL:HG13	1:W:522:ASP:HB3	2.03	0.40
1:W:712:LEU:HD22	1:W:805:LEU:HD23	2.01	0.40
1:4:627:PHE:HE2	1:4:663:HIS:HB2	1.85	0.40
4:6:207:LEU:O	4:6:211:LEU:N	2.38	0.40
4:a:105:TRP:CZ3	4:a:141:PRO:HD3	2.57	0.40
4:c:5:LYS:HD2	4:c:86:ARG:HB3	2.04	0.40
4:d:183:PHE:CE2	4:d:184:MET:HE2	2.56	0.40
1:A:608:ALA:HB3	1:F:678:ARG:HH12	1.86	0.40
1:A:612:PHE:O	1:A:616:ILE:HD12	2.21	0.40
1:A:1178:GLU:CD	1:A:1265:PRO:HD2	2.46	0.40
1:B:540:PHE:HE1	1:B:558:HIS:HD2	1.68	0.40
1:B:675:GLY:O	1:B:679:LYS:HG2	2.22	0.40
1:B:1171:HIS:CE1	1:C:1228:ALA:HA	2.54	0.40
1:B:1210:TYR:HE1	1:B:1280:ARG:HG2	1.86	0.40
1:C:740:ILE:HB	1:C:747:TYR:HB3	2.03	0.40
1:E:191:ILE:HA	1:E:217:PHE:HE1	1.87	0.40
1:E:394:ARG:HB2	1:E:1050:HIS:NE2	2.35	0.40
1:F:627:PHE:HE2	1:F:663:HIS:HB2	1.86	0.40
2:I:28:MET:HE2	2:I:45:LYS:HG2	2.03	0.40
2:L:28:MET:HE2	2:L:45:LYS:HG2	2.03	0.40
1:M:406:LEU:HB3	1:M:407:HIS:H	1.79	0.40
1:M:1341:TYR:HA	1:M:1348:HIS:HD2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:847:GLN:HG2	1:N:871:THR:HG21	2.03	0.40
1:N:856:ASN:ND2	2:P:66:GLY:O	2.55	0.40
1:N:950:ASP:HA	1:N:951:PRO:HD3	1.92	0.40
1:O:279:THR:HB	1:O:380:GLN:HE21	1.86	0.40
1:O:562:VAL:HA	1:O:1019:LEU:HD11	2.04	0.40
2:Q:28:MET:HE2	2:Q:45:LYS:HG2	2.03	0.40
1:S:681:LEU:HD23	1:S:681:LEU:HA	1.92	0.40
1:U:10:PHE:HE1	1:V:318:SER:HA	1.86	0.40
1:U:932:ARG:O	1:U:936:GLU:N	2.54	0.40
1:U:1058:SER:OG	1:U:1059:THR:N	2.54	0.40
1:V:1190:TYR:OH	1:V:1196:ASN:O	2.37	0.40
1:W:854:LEU:HA	1:W:854:LEU:HD23	1.87	0.40
1:X:402:PHE:O	1:X:1040:VAL:N	2.47	0.40
1:4:469:ASN:HA	1:4:554:TYR:HE2	1.86	0.40
1:4:984:MET:HE1	1:4:989:GLU:HA	2.04	0.40
4:6:202:ARG:O	4:6:206:ASP:N	2.53	0.40
4:d:97:ASN:HD22	4:d:105:TRP:CD1	2.35	0.40
4:i:29:SER:HG	4:i:99:TYR:HH	1.63	0.40
1:A:294:GLU:HB2	1:A:366:LEU:HD22	2.03	0.40
1:A:697:HIS:CE1	1:B:509:VAL:HG11	2.56	0.40
1:B:53:LEU:HD23	1:C:90:LYS:HB3	2.03	0.40
1:B:592:ILE:HG13	1:B:683:GLU:HG2	2.03	0.40
1:B:736:ARG:NH2	1:B:899:ASP:OD1	2.29	0.40
1:B:945:ASN:H	1:B:984:MET:HE1	1.86	0.40
1:C:704:PRO:HD2	1:C:707:HIS:ND1	2.37	0.40
1:C:1295:GLY:H	1:C:1321:HIS:CE1	2.38	0.40
1:D:824:VAL:H	1:D:889:THR:HG21	1.85	0.40
1:E:744:ASP:H	1:E:786:HIS:HE1	1.69	0.40
2:K:73:HIS:O	2:K:76:THR:OG1	2.34	0.40
1:M:1341:TYR:HA	1:M:1348:HIS:CD2	2.56	0.40
1:N:822:MET:SD	1:N:939:PHE:HB3	2.61	0.40
1:O:191:ILE:HA	1:O:217:PHE:CE1	2.57	0.40
1:S:1366:ARG:HD2	1:S:1368:LEU:HD21	2.04	0.40
1:U:731:MET:HG2	1:U:738:PRO:HG2	2.04	0.40
1:V:175:VAL:HG11	1:V:382:MET:HE2	2.03	0.40
1:V:1211:SER:C	1:V:1279:ASN:HD21	2.30	0.40
1:W:297:MET:HE3	1:W:364:ALA:HB3	2.03	0.40
1:W:398:TYR:CZ	1:W:1363:PRO:HG3	2.56	0.40
1:W:459:HIS:NE2	1:W:1021:ALA:HB2	2.37	0.40
1:W:831:LEU:HD22	2:2:9:PRO:HG2	2.03	0.40
1:4:794:ASP:H	1:4:798:TYR:HE1	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:7:7:ILE:HB	4:7:84:LEU:HB2	2.03	0.40
4:9:9:VAL:HG21	4:9:45:LEU:HD21	2.01	0.40
4:9:59:TYR:OH	4:9:191:ASP:O	2.33	0.40
4:j:141:PRO:HG2	4:j:144:LEU:HD12	2.03	0.40
1:A:829:VAL:O	1:A:832:THR:OG1	2.32	0.40
1:A:868:ILE:HG22	1:A:870:PRO:HD3	2.03	0.40
1:B:929:ASP:OD1	1:B:932:ARG:NH2	2.55	0.40
1:C:243:THR:O	1:C:247:ASP:N	2.49	0.40
1:C:446:TYR:O	1:C:450:LEU:N	2.55	0.40
1:C:512:VAL:HG12	1:C:993:SER:HB3	2.04	0.40
1:C:1198:ARG:HA	1:C:1239:ALA:HB3	2.03	0.40
1:D:842:ASP:OD2	2:J:19:TYR:OH	2.39	0.40
1:D:979:VAL:HG11	1:D:984:MET:HB2	2.03	0.40
1:E:156:ILE:HA	1:E:159:ILE:HG22	2.03	0.40
1:E:325:ASN:HB3	1:E:328:GLN:HB3	2.04	0.40
1:E:680:ILE:O	1:E:684:LEU:N	2.50	0.40
1:E:883:LEU:HD11	2:K:55:HIS:HA	2.02	0.40
2:J:28:MET:HE2	2:J:45:LYS:HG2	2.03	0.40
1:M:148:ASP:O	1:M:152:TYR:N	2.48	0.40
1:M:436:ASN:HB3	1:M:440:VAL:H	1.86	0.40
1:M:1074:ARG:NE	3:b:295:PRO:HB3	2.36	0.40
1:N:515:LYS:NZ	1:N:535:GLU:HG3	2.37	0.40
1:O:494:PHE:HZ	2:R:6:VAL:HG22	1.87	0.40
1:T:78:THR:OG1	1:T:1061:MET:O	2.32	0.40
1:T:81:LYS:HD3	1:T:81:LYS:HA	1.89	0.40
1:W:515:LYS:NZ	1:W:534:LEU:O	2.51	0.40
2:Z:28:MET:HE2	2:Z:45:LYS:HG2	2.03	0.40
2:0:28:MET:HE2	2:0:45:LYS:HG2	2.03	0.40
3:5:255:VAL:O	3:5:259:ILE:N	2.42	0.40
3:b:159:LEU:O	3:b:327:TRP:NE1	2.41	0.40
4:g:89:PRO:HB3	4:g:304:PRO:HG3	2.02	0.40
4:j:60:ILE:HG21	4:j:60:ILE:HD13	1.91	0.40
4:j:253:ASP:HB3	4:j:255:ASP:H	1.86	0.40
1:B:1166:LEU:HD13	1:B:1169:LEU:HD23	2.04	0.40
1:C:312:ASN:O	1:C:315:THR:OG1	2.30	0.40
1:C:669:ILE:HD13	1:C:674:HIS:HB2	2.04	0.40
1:C:695:ALA:HB1	1:C:706:THR:HG22	2.03	0.40
1:C:822:MET:SD	1:C:939:PHE:HB3	2.61	0.40
1:D:380:GLN:HB3	1:D:384:ASN:ND2	2.37	0.40
1:D:507:ALA:HB1	1:D:978:ASN:HD22	1.87	0.40
1:D:702:ARG:NH1	1:D:735:SER:OG	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:851:LEU:HD23	1:D:854:LEU:HD11	2.03	0.40
1:D:1211:SER:H	1:D:1279:ASN:HD21	1.69	0.40
1:E:447:GLN:NE2	1:F:521:GLU:OE1	2.53	0.40
1:F:75:CYS:SG	1:F:1059:THR:OG1	2.60	0.40
1:F:457:ARG:HG3	1:F:1122:PHE:CD2	2.56	0.40
1:F:984:MET:HE2	1:F:984:MET:HB3	1.92	0.40
2:K:28:MET:HE2	2:K:45:LYS:HG2	2.03	0.40
1:M:443:CYS:N	1:N:1231:CYS:SG	2.95	0.40
1:M:539:PHE:HB3	1:M:558:HIS:CE1	2.56	0.40
1:M:1200:ARG:HG3	1:M:1234:THR:HG23	2.04	0.40
1:N:859:LEU:HD23	1:N:859:LEU:HA	1.84	0.40
1:N:1216:GLU:HG3	1:N:1220:TYR:HD2	1.86	0.40
1:O:63:PHE:HE2	1:O:65:LYS:HE2	1.87	0.40
1:O:188:PRO:HD2	1:O:191:ILE:HD12	2.04	0.40
1:O:301:ALA:HB2	1:O:360:THR:HB	2.03	0.40
1:O:492:ASN:ND2	2:R:4:PHE:O	2.54	0.40
2:Q:73:HIS:O	2:Q:76:THR:OG1	2.34	0.40
1:S:544:VAL:HG22	1:S:554:TYR:HE1	1.87	0.40
1:S:1001:SER:O	1:X:587:ASN:ND2	2.55	0.40
1:S:1073:VAL:HG13	1:S:1078:VAL:HG22	2.02	0.40
1:T:674:HIS:HA	1:T:677:TYR:HD2	1.86	0.40
1:U:741:LYS:HG2	1:U:746:ASN:ND2	2.37	0.40
1:V:394:ARG:HB2	1:V:1050:HIS:NE2	2.37	0.40
1:V:958:HIS:CE1	1:V:960:LEU:HB3	2.57	0.40
1:W:182:LYS:NZ	1:W:1058:SER:HG	2.20	0.40
1:W:457:ARG:NH1	1:W:462:THR:OG1	2.48	0.40
1:W:717:LEU:HB2	1:W:990:TRP:CZ3	2.56	0.40
1:X:545:HIS:N	1:X:553:SER:O	2.51	0.40
1:X:824:VAL:HG13	1:X:939:PHE:HE1	1.87	0.40
2:3:28:MET:HE2	2:3:45:LYS:HG2	2.03	0.40
1:4:82:ASP:OD1	1:4:82:ASP:N	2.51	0.40
1:4:400:TYR:N	1:4:1042:ARG:O	2.49	0.40
4:6:157:ILE:HG22	4:6:161:ILE:HD11	2.04	0.40
4:7:42:ILE:HG13	4:7:45:LEU:HD21	2.03	0.40
4:f:36:CYS:HB3	4:f:86:ARG:HH12	1.87	0.40
3:h:74:LEU:O	3:h:103:ASP:HB3	2.22	0.40
3:h:75:VAL:HG11	3:h:80:PHE:HB3	2.03	0.40
3:h:150:MET:HE1	3:h:241:MET:HB3	2.04	0.40
4:j:74:LEU:HA	4:j:84:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4	1200/1376 (87%)	1061 (88%)	136 (11%)	3 (0%)	36	71
1	A	1359/1376 (99%)	1204 (89%)	155 (11%)	0	100	100
1	B	1351/1376 (98%)	1192 (88%)	158 (12%)	1 (0%)	48	82
1	C	1350/1376 (98%)	1200 (89%)	148 (11%)	2 (0%)	48	82
1	D	1351/1376 (98%)	1186 (88%)	163 (12%)	2 (0%)	48	82
1	E	1359/1376 (99%)	1203 (88%)	155 (11%)	1 (0%)	48	82
1	F	1352/1376 (98%)	1197 (88%)	149 (11%)	6 (0%)	30	66
1	M	1351/1376 (98%)	1185 (88%)	163 (12%)	3 (0%)	43	77
1	N	1359/1376 (99%)	1189 (88%)	168 (12%)	2 (0%)	48	82
1	O	1351/1376 (98%)	1191 (88%)	155 (12%)	5 (0%)	30	66
1	S	1273/1376 (92%)	1126 (88%)	145 (11%)	2 (0%)	43	77
1	T	1354/1376 (98%)	1195 (88%)	154 (11%)	5 (0%)	30	66
1	U	1351/1376 (98%)	1199 (89%)	150 (11%)	2 (0%)	48	82
1	V	1348/1376 (98%)	1200 (89%)	146 (11%)	2 (0%)	48	82
1	W	1350/1376 (98%)	1211 (90%)	136 (10%)	3 (0%)	43	77
1	X	1339/1376 (97%)	1198 (90%)	140 (10%)	1 (0%)	48	82
2	0	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	1	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	2	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	3	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	G	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	H	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	I	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	J	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	K	76/170 (45%)	73 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	P	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	Q	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	R	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	Y	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
2	Z	76/170 (45%)	73 (96%)	3 (4%)	0	100	100
3	5	313/331 (95%)	279 (89%)	34 (11%)	0	100	100
3	8	315/331 (95%)	293 (93%)	22 (7%)	0	100	100
3	b	315/331 (95%)	288 (91%)	27 (9%)	0	100	100
3	e	311/331 (94%)	288 (93%)	23 (7%)	0	100	100
3	h	315/331 (95%)	288 (91%)	26 (8%)	1 (0%)	36	71
4	6	290/305 (95%)	263 (91%)	27 (9%)	0	100	100
4	7	296/305 (97%)	261 (88%)	35 (12%)	0	100	100
4	9	290/305 (95%)	264 (91%)	26 (9%)	0	100	100
4	a	296/305 (97%)	270 (91%)	26 (9%)	0	100	100
4	c	290/305 (95%)	265 (91%)	25 (9%)	0	100	100
4	d	296/305 (97%)	277 (94%)	19 (6%)	0	100	100
4	f	290/305 (95%)	263 (91%)	27 (9%)	0	100	100
4	g	296/305 (97%)	269 (91%)	27 (9%)	0	100	100
4	i	290/305 (95%)	264 (91%)	26 (9%)	0	100	100
4	j	296/305 (97%)	272 (92%)	24 (8%)	0	100	100
All	All	27037/29271 (92%)	24136 (89%)	2860 (11%)	41 (0%)	44	77

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1251	ASN
1	O	144	GLU
1	T	10	PHE
1	V	1251	ASN
1	B	843	VAL
1	D	843	VAL
1	E	843	VAL
1	F	843	VAL
1	M	843	VAL

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Mol	Chain	Res	Type
1	O	294	GLU
1	O	843	VAL
1	O	1251	ASN
1	S	843	VAL
1	T	843	VAL
1	T	945	ASN
1	U	843	VAL
1	V	843	VAL
1	W	423	GLU
1	W	843	VAL
1	X	843	VAL
1	D	842	ASP
1	F	294	GLU
1	F	423	GLU
1	M	352	ASP
1	O	279	THR
1	U	1252	ILE
1	C	843	VAL
1	F	945	ASN
1	M	842	ASP
1	N	843	VAL
1	N	945	ASN
1	W	842	ASP
1	4	842	ASP
1	4	843	VAL
1	F	842	ASP
1	S	842	ASP
1	T	842	ASP
1	4	849	ASP
1	T	11	PRO
3	h	297	ASP
1	F	738	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	4	1039/1166 (89%)	1038 (100%)	1 (0%)	88	88
1	A	1155/1166 (99%)	1155 (100%)	0	100	100
1	B	1151/1166 (99%)	1150 (100%)	1 (0%)	88	88
1	C	1150/1166 (99%)	1149 (100%)	1 (0%)	88	88
1	D	1151/1166 (99%)	1151 (100%)	0	100	100
1	E	1155/1166 (99%)	1153 (100%)	2 (0%)	87	85
1	F	1152/1166 (99%)	1151 (100%)	1 (0%)	88	88
1	M	1151/1166 (99%)	1149 (100%)	2 (0%)	87	85
1	N	1155/1166 (99%)	1154 (100%)	1 (0%)	88	88
1	O	1151/1166 (99%)	1149 (100%)	2 (0%)	87	85
1	S	1094/1166 (94%)	1092 (100%)	2 (0%)	87	85
1	T	1154/1166 (99%)	1153 (100%)	1 (0%)	88	88
1	U	1151/1166 (99%)	1149 (100%)	2 (0%)	87	85
1	V	1148/1166 (98%)	1147 (100%)	1 (0%)	88	88
1	W	1150/1166 (99%)	1150 (100%)	0	100	100
1	X	1143/1166 (98%)	1141 (100%)	2 (0%)	87	85
2	0	70/141 (50%)	70 (100%)	0	100	100
2	1	70/141 (50%)	70 (100%)	0	100	100
2	2	70/141 (50%)	70 (100%)	0	100	100
2	3	70/141 (50%)	70 (100%)	0	100	100
2	G	70/141 (50%)	70 (100%)	0	100	100
2	H	70/141 (50%)	70 (100%)	0	100	100
2	I	70/141 (50%)	70 (100%)	0	100	100
2	J	70/141 (50%)	70 (100%)	0	100	100
2	K	70/141 (50%)	70 (100%)	0	100	100
2	L	70/141 (50%)	70 (100%)	0	100	100
2	P	70/141 (50%)	70 (100%)	0	100	100
2	Q	70/141 (50%)	70 (100%)	0	100	100
2	R	70/141 (50%)	70 (100%)	0	100	100
2	Y	70/141 (50%)	70 (100%)	0	100	100
2	Z	70/141 (50%)	70 (100%)	0	100	100
3	5	271/281 (96%)	271 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	8	272/281 (97%)	272 (100%)	0	100	100
3	b	272/281 (97%)	272 (100%)	0	100	100
3	e	270/281 (96%)	270 (100%)	0	100	100
3	h	272/281 (97%)	272 (100%)	0	100	100
4	6	267/274 (97%)	267 (100%)	0	100	100
4	7	270/274 (98%)	270 (100%)	0	100	100
4	9	267/274 (97%)	267 (100%)	0	100	100
4	a	270/274 (98%)	270 (100%)	0	100	100
4	c	267/274 (97%)	267 (100%)	0	100	100
4	d	270/274 (98%)	270 (100%)	0	100	100
4	f	267/274 (97%)	267 (100%)	0	100	100
4	g	270/274 (98%)	270 (100%)	0	100	100
4	i	267/274 (97%)	267 (100%)	0	100	100
4	j	270/274 (98%)	270 (100%)	0	100	100
All	All	23342/24916 (94%)	23323 (100%)	19 (0%)	87	88

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	947	LEU
1	C	669	ILE
1	E	616	ILE
1	E	947	LEU
1	F	947	LEU
1	M	616	ILE
1	M	620	ILE
1	N	947	LEU
1	O	616	ILE
1	O	1249	LEU
1	S	616	ILE
1	S	947	LEU
1	T	947	LEU
1	U	616	ILE
1	U	961	LEU
1	V	947	LEU
1	X	616	ILE
1	X	669	ILE

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Mol	Chain	Res	Type
1	4	947	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (509) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	113	GLN
1	A	224	HIS
1	A	239	GLN
1	A	354	HIS
1	A	380	GLN
1	A	384	ASN
1	A	397	GLN
1	A	428	GLN
1	A	545	HIS
1	A	697	HIS
1	A	746	ASN
1	A	818	HIS
1	A	902	GLN
1	A	1003	GLN
1	A	1030	HIS
1	A	1103	HIS
1	A	1116	GLN
1	A	1131	GLN
1	A	1171	HIS
1	A	1173	GLN
1	A	1222	HIS
1	A	1241	GLN
1	A	1251	ASN
1	A	1268	GLN
1	A	1344	ASN
1	B	92	GLN
1	B	113	GLN
1	B	224	HIS
1	B	288	ASN
1	B	325	ASN
1	B	380	GLN
1	B	384	ASN
1	B	436	ASN
1	B	460	ASN
1	B	529	HIS
1	B	567	GLN

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Mol	Chain	Res	Type
1	B	587	ASN
1	B	674	HIS
1	B	689	GLN
1	B	697	HIS
1	B	716	HIS
1	B	724	HIS
1	B	752	ASN
1	B	902	GLN
1	B	915	GLN
1	B	958	HIS
1	B	991	HIS
1	B	1030	HIS
1	B	1114	HIS
1	B	1133	HIS
1	B	1171	HIS
1	B	1318	GLN
1	B	1321	HIS
1	B	1344	ASN
1	C	113	GLN
1	C	123	HIS
1	C	224	HIS
1	C	328	GLN
1	C	463	GLN
1	C	498	HIS
1	C	537	HIS
1	C	590	HIS
1	C	630	ASN
1	C	663	HIS
1	C	689	GLN
1	C	971	GLN
1	C	978	ASN
1	C	1003	GLN
1	C	1128	GLN
1	C	1171	HIS
1	C	1196	ASN
1	C	1241	GLN
1	C	1305	GLN
1	C	1321	HIS
1	C	1344	ASN
1	C	1348	HIS
1	D	22	GLN
1	D	102	HIS

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Mol	Chain	Res	Type
1	D	113	GLN
1	D	123	HIS
1	D	224	HIS
1	D	312	ASN
1	D	325	ASN
1	D	387	GLN
1	D	397	GLN
1	D	428	GLN
1	D	438	ASN
1	D	487	GLN
1	D	498	HIS
1	D	575	GLN
1	D	689	GLN
1	D	816	ASN
1	D	902	GLN
1	D	958	HIS
1	D	1027	GLN
1	D	1103	HIS
1	D	1171	HIS
1	D	1241	GLN
1	D	1279	ASN
1	D	1318	GLN
1	D	1321	HIS
1	D	1324	GLN
1	D	1334	HIS
1	E	92	GLN
1	E	102	HIS
1	E	224	HIS
1	E	328	GLN
1	E	354	HIS
1	E	428	GLN
1	E	439	ASN
1	E	448	ASN
1	E	463	GLN
1	E	590	HIS
1	E	644	ASN
1	E	663	HIS
1	E	697	HIS
1	E	902	GLN
1	E	971	GLN
1	E	1003	GLN
1	E	1084	HIS

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Mol	Chain	Res	Type
1	E	1116	GLN
1	E	1171	HIS
1	E	1196	ASN
1	E	1241	GLN
1	E	1251	ASN
1	E	1318	GLN
1	E	1324	GLN
1	E	1348	HIS
1	F	92	GLN
1	F	113	GLN
1	F	224	HIS
1	F	312	ASN
1	F	328	GLN
1	F	428	GLN
1	F	459	HIS
1	F	587	ASN
1	F	630	ASN
1	F	674	HIS
1	F	689	GLN
1	F	786	HIS
1	F	902	GLN
1	F	945	ASN
1	F	1050	HIS
1	F	1171	HIS
1	F	1241	GLN
1	F	1268	GLN
1	F	1279	ASN
1	F	1324	GLN
1	F	1344	ASN
2	G	12	GLN
2	G	55	HIS
2	G	75	GLN
2	H	75	GLN
2	I	12	GLN
2	I	75	GLN
2	J	22	HIS
2	J	75	GLN
2	K	12	GLN
2	K	73	HIS
2	K	75	GLN
2	L	12	GLN
2	L	22	HIS

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Mol	Chain	Res	Type
2	L	75	GLN
1	M	22	GLN
1	M	224	HIS
1	M	312	ASN
1	M	354	HIS
1	M	380	GLN
1	M	428	GLN
1	M	460	ASN
1	M	498	HIS
1	M	499	GLN
1	M	558	HIS
1	M	587	ASN
1	M	623	GLN
1	M	663	HIS
1	M	674	HIS
1	M	958	HIS
1	M	1030	HIS
1	M	1103	HIS
1	M	1131	GLN
1	M	1171	HIS
1	M	1173	GLN
1	M	1305	GLN
1	M	1324	GLN
1	M	1348	HIS
1	N	113	GLN
1	N	123	HIS
1	N	224	HIS
1	N	312	ASN
1	N	397	GLN
1	N	448	ASN
1	N	487	GLN
1	N	492	ASN
1	N	545	HIS
1	N	587	ASN
1	N	623	GLN
1	N	674	HIS
1	N	724	HIS
1	N	737	GLN
1	N	786	HIS
1	N	856	ASN
1	N	902	GLN
1	N	907	HIS

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Mol	Chain	Res	Type
1	N	915	GLN
1	N	1003	GLN
1	N	1017	GLN
1	N	1030	HIS
1	N	1133	HIS
1	N	1171	HIS
1	N	1173	GLN
1	N	1256	GLN
1	O	92	GLN
1	O	113	GLN
1	O	224	HIS
1	O	312	ASN
1	O	325	ASN
1	O	354	HIS
1	O	438	ASN
1	O	459	HIS
1	O	558	HIS
1	O	564	ASN
1	O	567	GLN
1	O	623	GLN
1	O	724	HIS
1	O	782	HIS
1	O	816	ASN
1	O	1003	GLN
1	O	1116	GLN
1	O	1131	GLN
1	O	1173	GLN
1	O	1196	ASN
1	O	1241	GLN
1	O	1251	ASN
1	O	1256	GLN
1	O	1268	GLN
1	O	1305	GLN
1	O	1318	GLN
1	O	1321	HIS
2	P	12	GLN
2	P	22	HIS
2	P	75	GLN
2	Q	75	GLN
2	R	75	GLN
1	S	113	GLN
1	S	224	HIS

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Mol	Chain	Res	Type
1	S	438	ASN
1	S	439	ASN
1	S	447	GLN
1	S	558	HIS
1	S	567	GLN
1	S	587	ASN
1	S	816	ASN
1	S	907	HIS
1	S	1003	GLN
1	S	1030	HIS
1	S	1133	HIS
1	S	1268	GLN
1	S	1279	ASN
1	S	1318	GLN
1	S	1321	HIS
1	S	1324	GLN
1	S	1344	ASN
1	T	36	GLN
1	T	59	ASN
1	T	92	GLN
1	T	113	GLN
1	T	224	HIS
1	T	328	GLN
1	T	380	GLN
1	T	384	ASN
1	T	479	HIS
1	T	537	HIS
1	T	623	GLN
1	T	737	GLN
1	T	786	HIS
1	T	978	ASN
1	T	1003	GLN
1	T	1133	HIS
1	T	1171	HIS
1	T	1173	GLN
1	T	1196	ASN
1	T	1334	HIS
1	T	1344	ASN
1	U	59	ASN
1	U	113	GLN
1	U	123	HIS
1	U	124	HIS

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Mol	Chain	Res	Type
1	U	224	HIS
1	U	312	ASN
1	U	328	GLN
1	U	438	ASN
1	U	537	HIS
1	U	545	HIS
1	U	564	ASN
1	U	666	ASN
1	U	716	HIS
1	U	737	GLN
1	U	746	ASN
1	U	786	HIS
1	U	816	ASN
1	U	1003	GLN
1	U	1128	GLN
1	U	1131	GLN
1	U	1133	HIS
1	U	1241	GLN
1	U	1318	GLN
1	U	1321	HIS
1	U	1324	GLN
1	U	1334	HIS
1	U	1344	ASN
1	U	1355	GLN
1	V	102	HIS
1	V	113	GLN
1	V	123	HIS
1	V	224	HIS
1	V	288	ASN
1	V	325	ASN
1	V	328	GLN
1	V	397	GLN
1	V	428	GLN
1	V	438	ASN
1	V	525	HIS
1	V	567	GLN
1	V	587	ASN
1	V	786	HIS
1	V	978	ASN
1	V	1003	GLN
1	V	1030	HIS
1	V	1171	HIS

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Mol	Chain	Res	Type
1	V	1173	GLN
1	V	1196	ASN
1	V	1222	HIS
1	W	92	GLN
1	W	102	HIS
1	W	113	GLN
1	W	123	HIS
1	W	224	HIS
1	W	380	GLN
1	W	428	GLN
1	W	438	ASN
1	W	460	ASN
1	W	463	GLN
1	W	487	GLN
1	W	623	GLN
1	W	689	GLN
1	W	746	ASN
1	W	786	HIS
1	W	816	ASN
1	W	970	ASN
1	W	978	ASN
1	W	1103	HIS
1	W	1131	GLN
1	W	1133	HIS
1	W	1196	ASN
1	W	1251	ASN
1	W	1318	GLN
1	W	1321	HIS
1	W	1324	GLN
1	W	1334	HIS
1	W	1344	ASN
1	X	7	GLN
1	X	18	ASN
1	X	113	GLN
1	X	123	HIS
1	X	288	ASN
1	X	354	HIS
1	X	380	GLN
1	X	387	GLN
1	X	428	GLN
1	X	438	ASN
1	X	439	ASN

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Mol	Chain	Res	Type
1	X	447	GLN
1	X	499	GLN
1	X	567	GLN
1	X	587	ASN
1	X	630	ASN
1	X	663	HIS
1	X	666	ASN
1	X	907	HIS
1	X	991	HIS
1	X	1003	GLN
1	X	1084	HIS
1	X	1131	GLN
1	X	1268	GLN
1	X	1318	GLN
1	X	1321	HIS
1	X	1324	GLN
1	X	1334	HIS
1	X	1344	ASN
2	Y	22	HIS
2	Y	75	GLN
2	Z	12	GLN
2	Z	75	GLN
2	0	12	GLN
2	0	22	HIS
2	0	55	HIS
2	0	75	GLN
2	1	12	GLN
2	1	55	HIS
2	1	75	GLN
2	2	22	HIS
2	2	73	HIS
2	2	75	GLN
2	3	55	HIS
2	3	75	GLN
1	4	380	GLN
1	4	397	GLN
1	4	498	HIS
1	4	514	GLN
1	4	558	HIS
1	4	564	ASN
1	4	567	GLN
1	4	581	GLN

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Mol	Chain	Res	Type
1	4	590	HIS
1	4	663	HIS
1	4	674	HIS
1	4	689	GLN
1	4	737	GLN
1	4	907	HIS
1	4	920	ASN
1	4	978	ASN
1	4	1131	GLN
1	4	1133	HIS
3	5	67	GLN
3	5	167	GLN
3	5	170	HIS
3	5	262	HIS
3	5	276	HIS
3	5	319	ASN
4	6	37	HIS
4	6	110	GLN
4	6	130	ASN
4	6	142	GLN
4	6	146	HIS
4	6	151	GLN
4	6	156	HIS
4	7	94	GLN
4	7	150	GLN
4	7	232	HIS
4	7	281	ASN
3	8	67	GLN
3	8	194	HIS
3	8	262	HIS
3	8	299	HIS
4	9	64	GLN
4	9	104	GLN
4	9	130	ASN
4	9	142	GLN
4	9	150	GLN
4	9	151	GLN
4	a	92	ASN
4	a	146	HIS
3	b	7	ASN
3	b	14	GLN
3	b	78	GLN

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Mol	Chain	Res	Type
3	b	95	GLN
3	b	262	HIS
3	b	276	HIS
4	c	24	GLN
4	c	40	GLN
4	c	110	GLN
4	c	130	ASN
4	c	146	HIS
4	c	150	GLN
4	c	151	GLN
4	c	180	ASN
4	d	24	GLN
4	d	41	ASN
4	d	104	GLN
4	d	146	HIS
4	d	232	HIS
3	e	7	ASN
3	e	98	ASN
3	e	194	HIS
3	e	262	HIS
4	f	24	GLN
4	f	37	HIS
4	f	40	GLN
4	f	104	GLN
4	f	110	GLN
4	f	151	GLN
4	f	156	HIS
4	f	180	ASN
4	f	281	ASN
4	g	37	HIS
4	g	92	ASN
4	g	104	GLN
4	g	108	ASN
4	g	150	GLN
4	g	156	HIS
4	g	256	GLN
4	g	274	GLN
4	g	281	ASN
3	h	4	GLN
3	h	14	GLN
3	h	95	GLN
3	h	302	HIS

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Mol	Chain	Res	Type
4	i	24	GLN
4	i	37	HIS
4	i	40	GLN
4	i	110	GLN
4	i	130	ASN
4	i	146	HIS
4	i	180	ASN
4	j	94	GLN
4	j	110	GLN
4	j	150	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	N	1
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	9:PRO	C	10:PHE	N	1.20
1	F	454:CYS	C	455:HIS	N	1.17

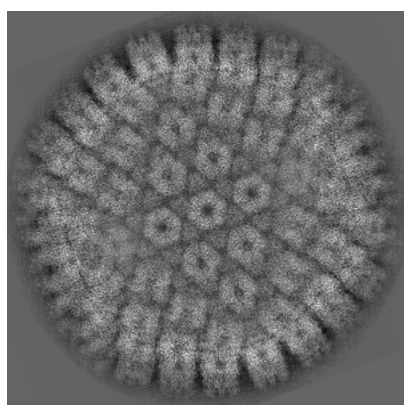
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7047. These allow visual inspection of the internal detail of the map and identification of artifacts.

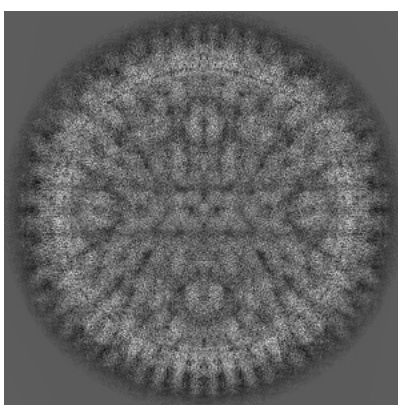
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

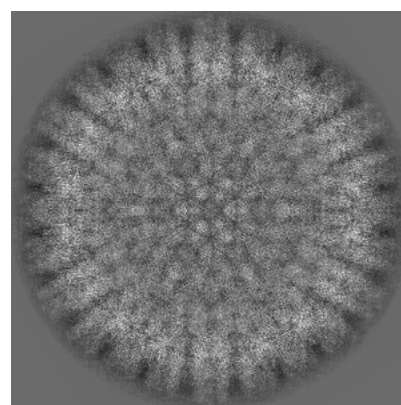
6.1.1 Primary map



X



Y

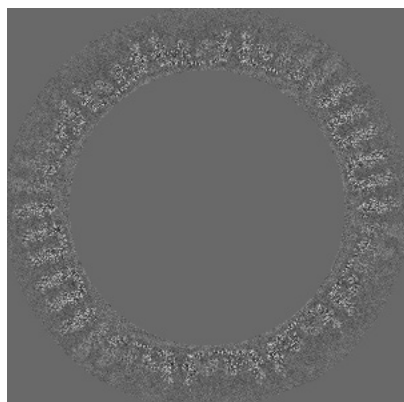


Z

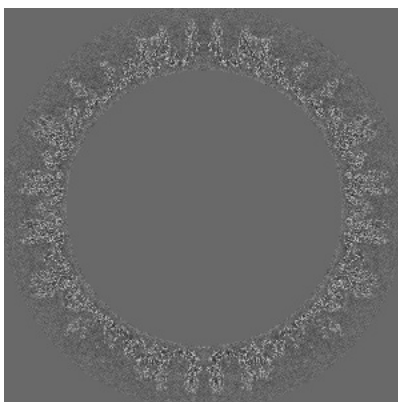
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

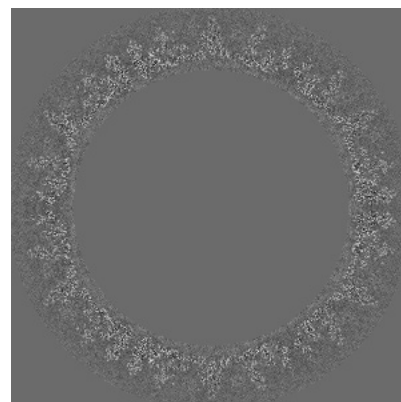
6.2.1 Primary map



X Index: 640



Y Index: 640

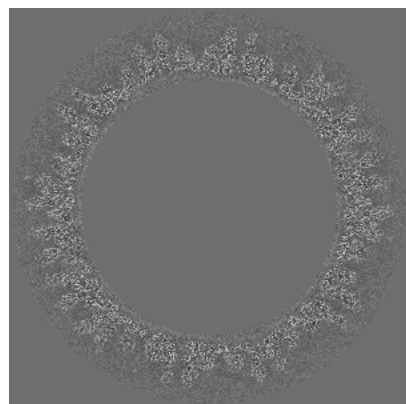


Z Index: 640

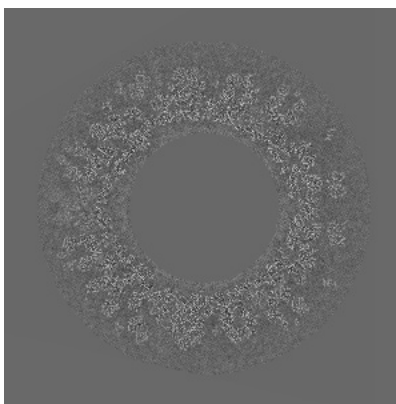
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

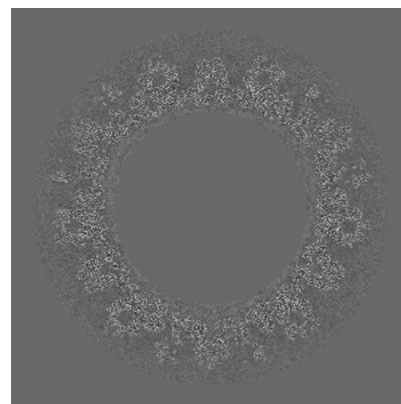
6.3.1 Primary map



X Index: 475



Y Index: 270

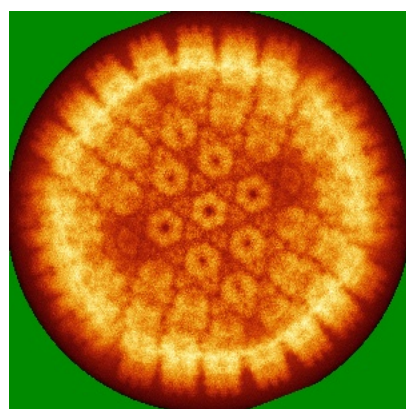


Z Index: 326

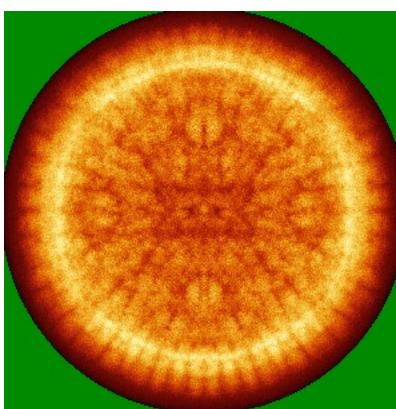
The images above show the largest variance slices of the map in three orthogonal directions.

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

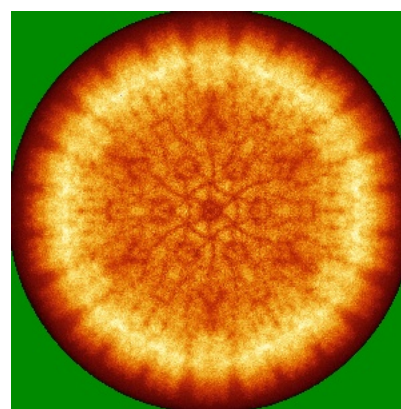
6.4.1 Primary map



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](#)

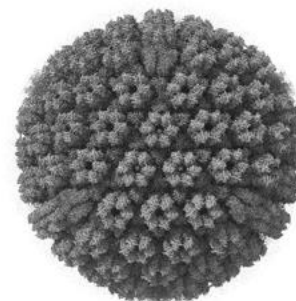
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

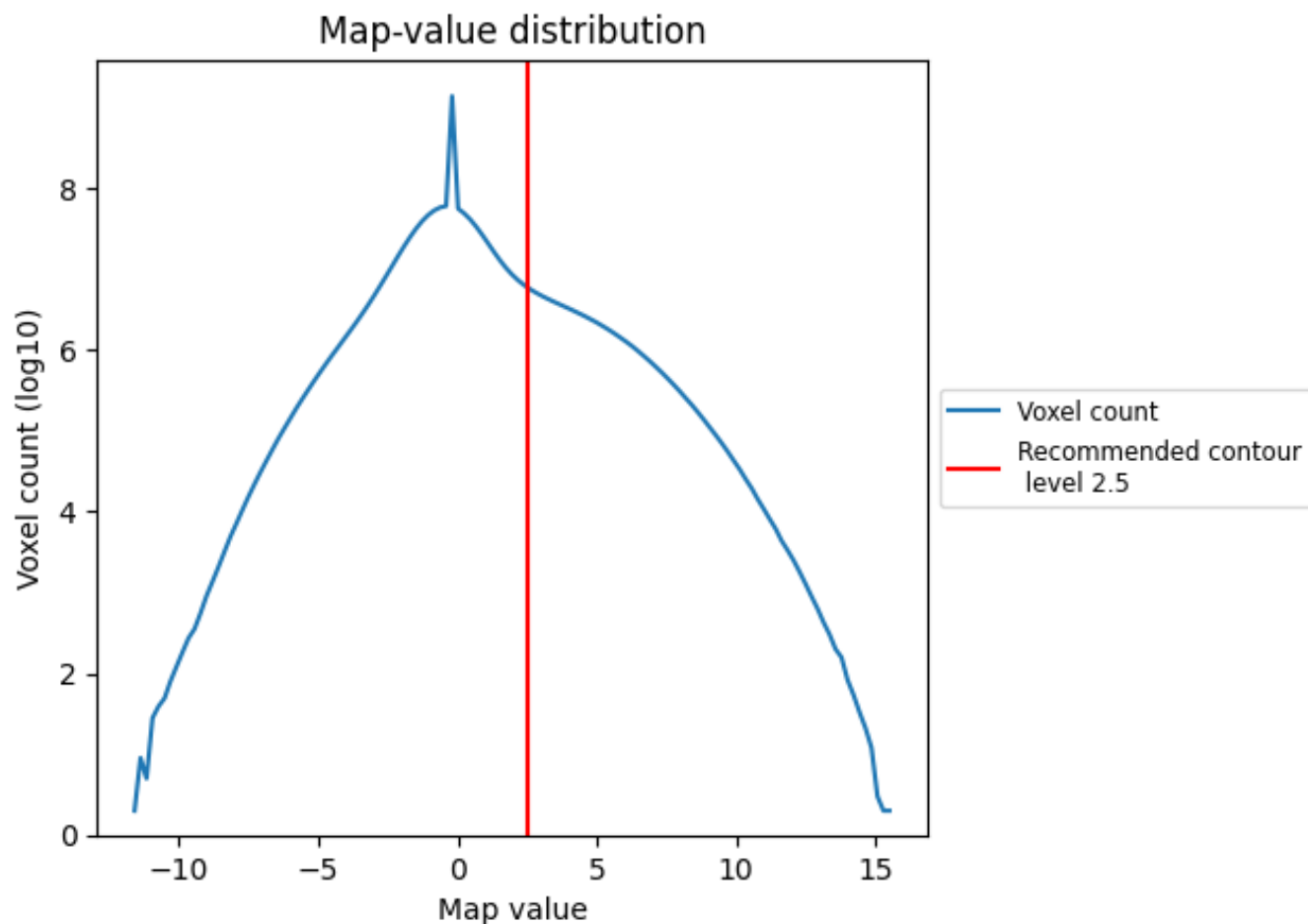
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

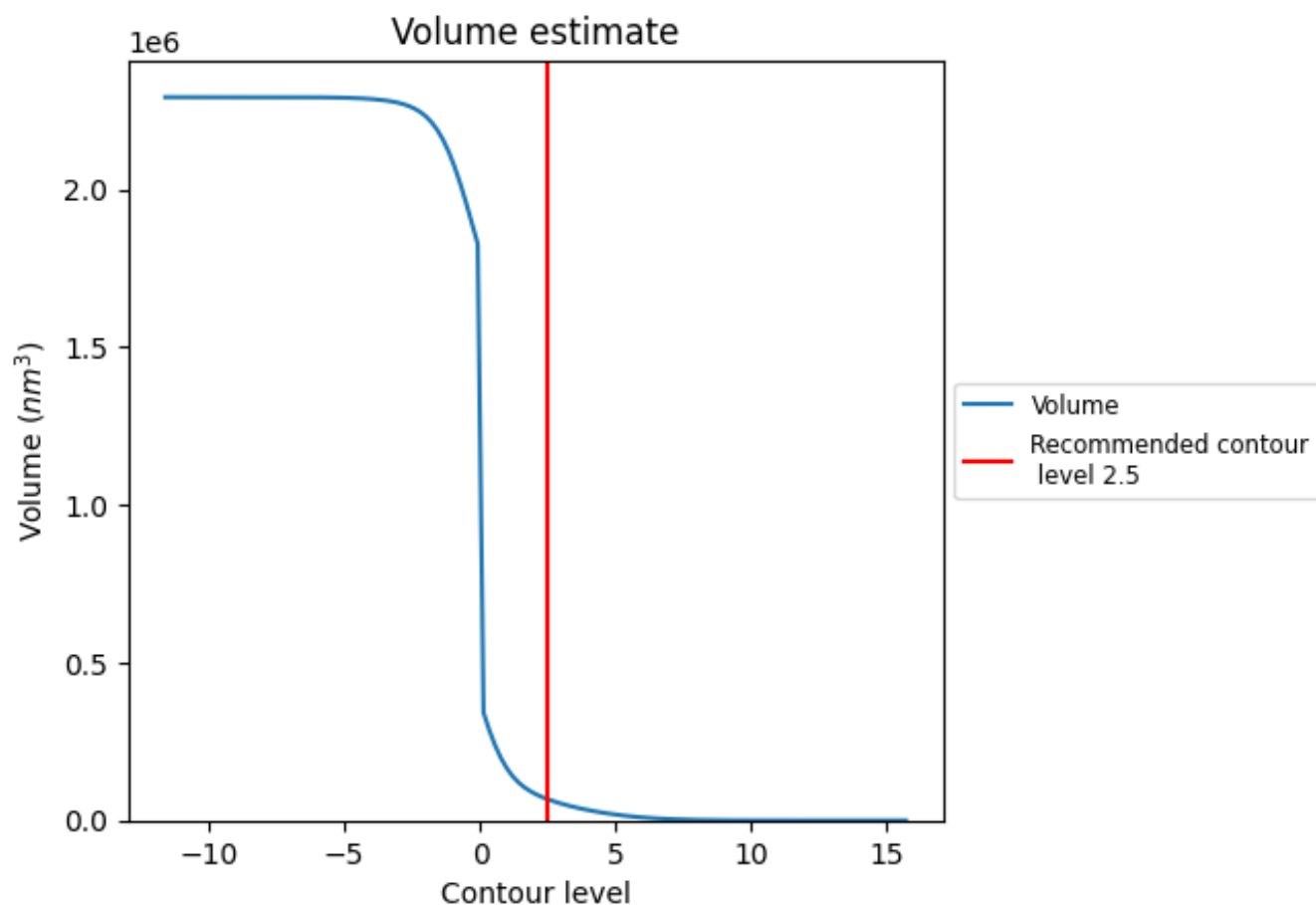
This section contains the results of statistical analysis of the map.

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.

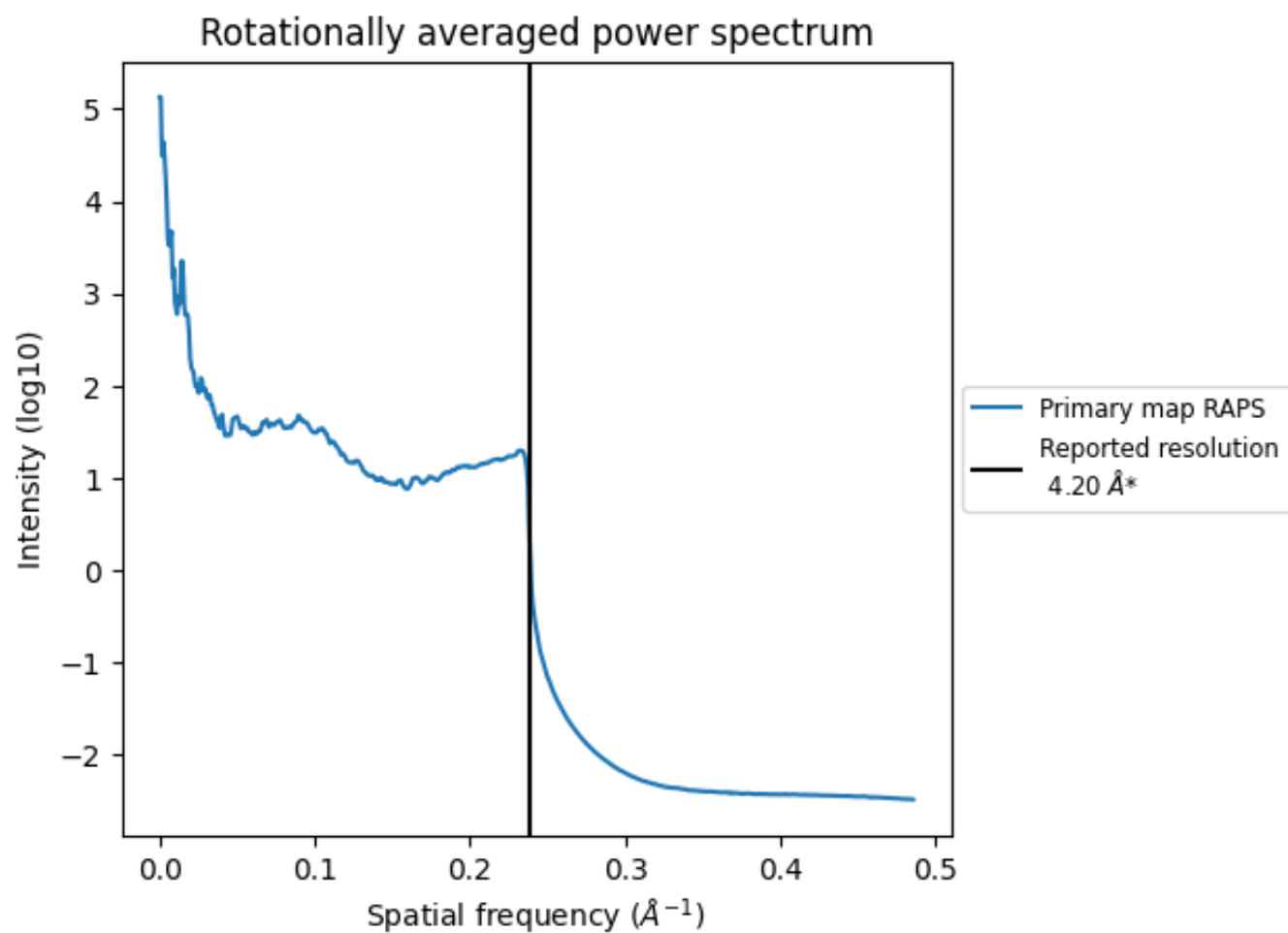
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 67318 nm³; this corresponds to an approximate mass of 60810 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 0.238 Å⁻¹

8 Fourier-Shell correlation

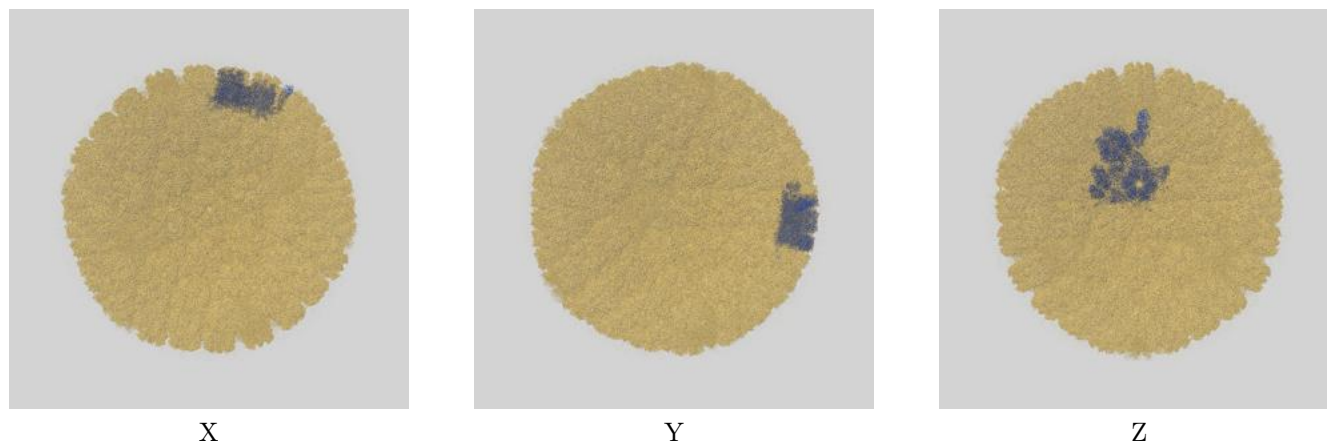
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7047 and PDB model 6B43. Per-residue inclusion information can be found in section [3](#) on page [8](#).

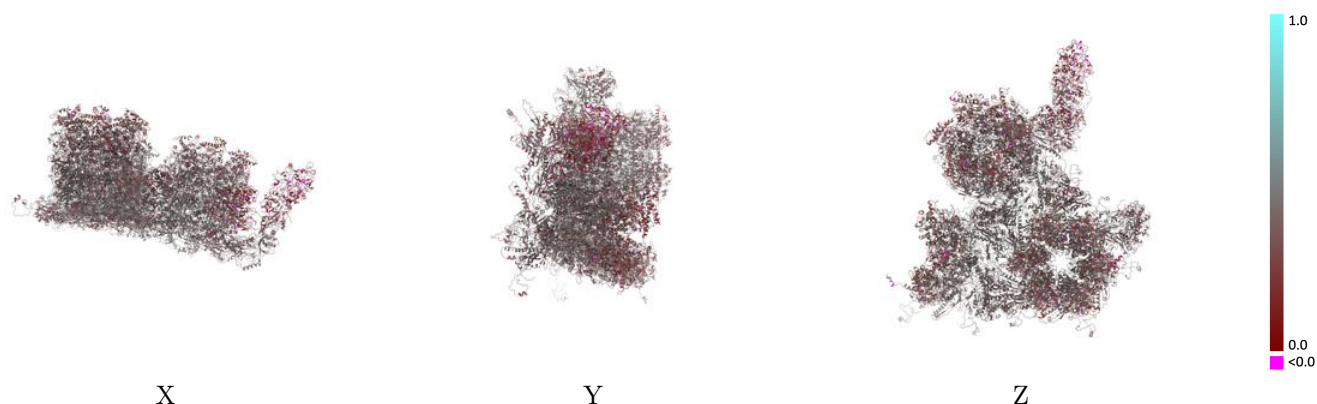
9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)



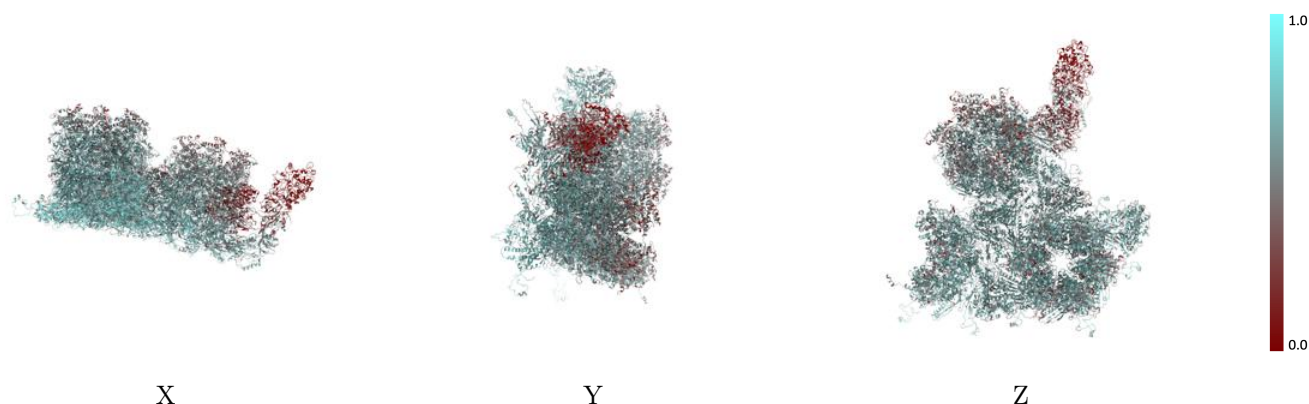
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



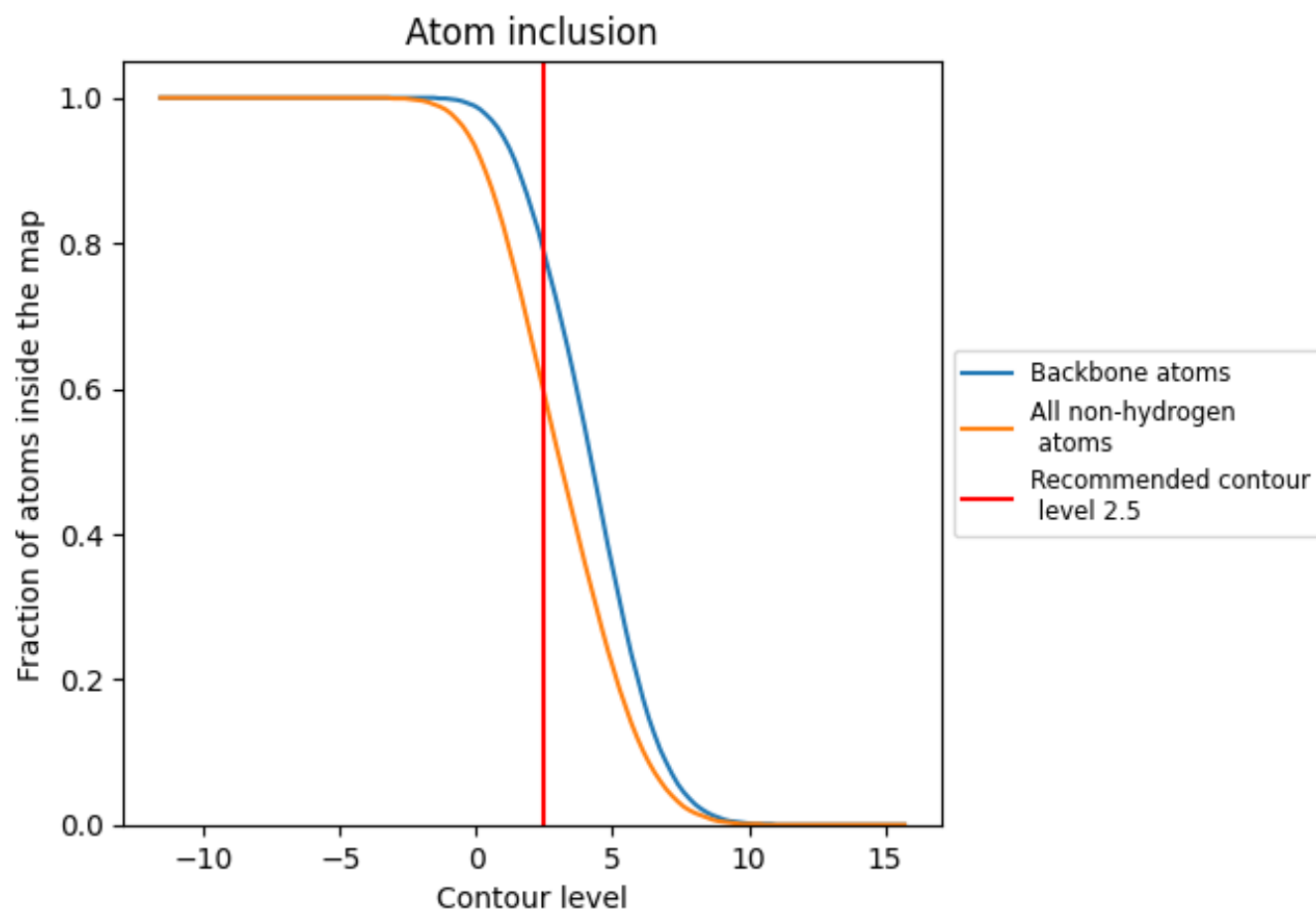
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 59% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5910	 0.3760
0	 0.4380	 0.2910
1	 0.4520	 0.3070
2	 0.3660	 0.2610
3	 0.3600	 0.2470
4	 0.2800	 0.2860
5	 0.3310	 0.3130
6	 0.3450	 0.2850
7	 0.1930	 0.2500
8	 0.6510	 0.3990
9	 0.6270	 0.3870
A	 0.6420	 0.3980
B	 0.6390	 0.3880
C	 0.6270	 0.3870
D	 0.6330	 0.3840
E	 0.6450	 0.3990
F	 0.6420	 0.3960
G	 0.4830	 0.3050
H	 0.4020	 0.2270
I	 0.5030	 0.3280
J	 0.4730	 0.2980
K	 0.4830	 0.2990
L	 0.4840	 0.3170
M	 0.6510	 0.3990
N	 0.6490	 0.3980
O	 0.6500	 0.3960
P	 0.5000	 0.3220
Q	 0.4840	 0.2840
R	 0.4950	 0.2980
S	 0.5690	 0.3780
T	 0.6080	 0.3870
U	 0.6240	 0.3890
V	 0.6210	 0.3830
W	 0.5950	 0.3780
X	 0.5730	 0.3720



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Chain	Atom inclusion	Q-score
Y	 0.3890	 0.2760
Z	 0.3520	 0.2410
a	 0.6350	 0.3950
b	 0.6460	 0.4070
c	 0.6560	 0.3980
d	 0.6500	 0.3980
e	 0.6140	 0.3910
f	 0.5620	 0.3680
g	 0.5930	 0.3790
h	 0.6380	 0.3950
i	 0.6420	 0.3950
j	 0.6410	 0.3940