



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 04:49 AM UTC

PDB ID : 8TEU / pdb_00008teu
EMDB ID : EMD-41202
Title : Human cytomegalovirus portal vertex, non-infectious enveloped particle
(NIEP) configuration 2 - inverted (NC2-inv)
Authors : Jih, J.; Liu, Y.T.; Liu, W.; Zhou, H.
Deposited on : 2023-07-07
Resolution : 4.01 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:

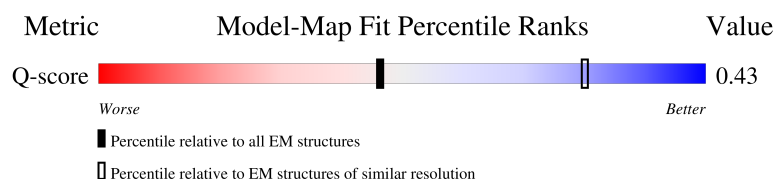
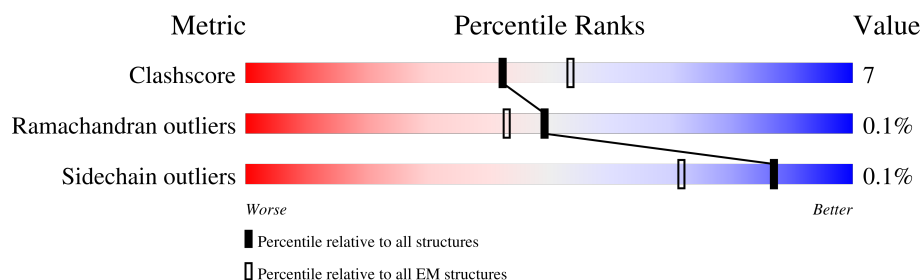
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.01 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	6765 (3.51 - 4.51)

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

Mol	Chain	Length	Quality of chain
1	A	2241	
1	C	2241	
2	E	642	
2	F	642	

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Mol	Chain	Length	Quality of chain
3	G	594	
4	H	1370	
4	I	1370	
4	J	1370	
4	K	1370	
4	L	1370	
4	M	1370	
5	N	75	
5	O	75	
5	P	75	
5	Q	75	
5	R	75	
5	S	75	
6	T	290	
6	W	290	
7	U	306	
7	V	306	
7	X	306	
7	Y	306	
8	Z	1048	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 96759 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 Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	722	Total	C	N	O	S	0	0
			5830	3723	1027	1058	22		
1	C	40	Total	C	N	O	S	0	0
			332	213	60	58	1		

- Molecule 2 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	495	Total	C	N	O	S	0	0
			3992	2559	706	715	12		
2	F	85	Total	C	N	O	S	0	0
			710	442	138	126	4		

- Molecule 3 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	471	Total	C	N	O	S	0	0
			3862	2416	740	692	14		

- Molecule 4 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	1309	Total	C	N	O	S	0	0
			10391	6619	1800	1911	61		
4	I	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		
4	J	1317	Total	C	N	O	S	0	0
			10433	6641	1814	1919	59		
4	K	1296	Total	C	N	O	S	0	0
			10259	6529	1787	1884	59		
4	L	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		

- Molecule 5 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	O	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	P	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	Q	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	R	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	S	63	Total	C	N	O	S	0	0
			513	321	97	91	4		

- Molecule 6 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	242	Total	C	N	O	S	0	0
			1939	1248	338	342	11		
6	W	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

- Molecule 7 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	292	Total	C	N	O	S	0	0
			2317	1489	399	411	18		
7	V	288	Total	C	N	O	S	0	0
			2292	1471	397	407	17		
7	X	295	Total	C	N	O	S	0	0
			2334	1501	402	412	19		
7	Y	285	Total	C	N	O	S	0	0
			2266	1456	387	405	18		

- Molecule 8 is a protein called Large structural phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	284	Total	C	N	O	S	0	0
			2320	1463	425	420	12		

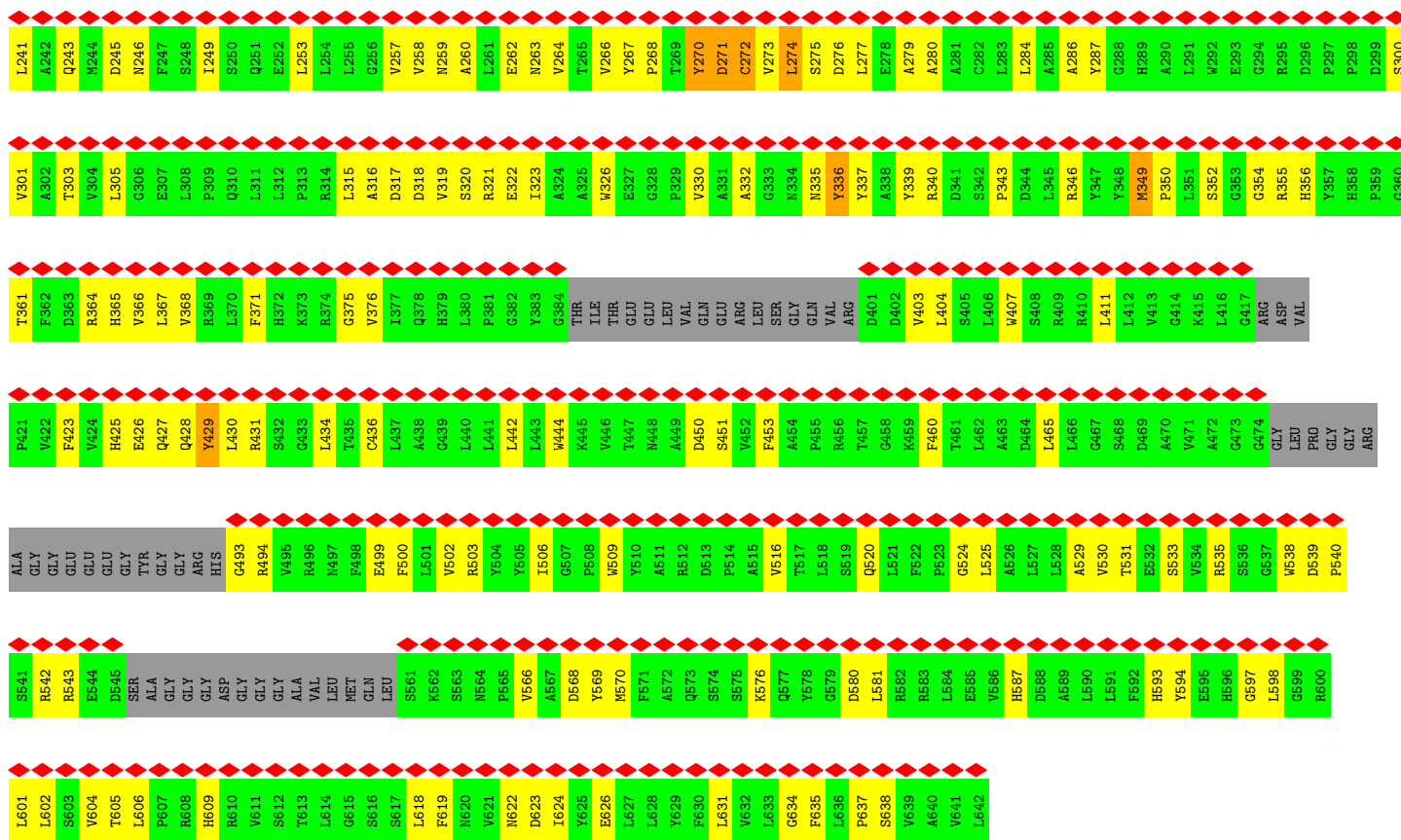


WORLDWIDE
PDB
PROTEIN DATA BANK

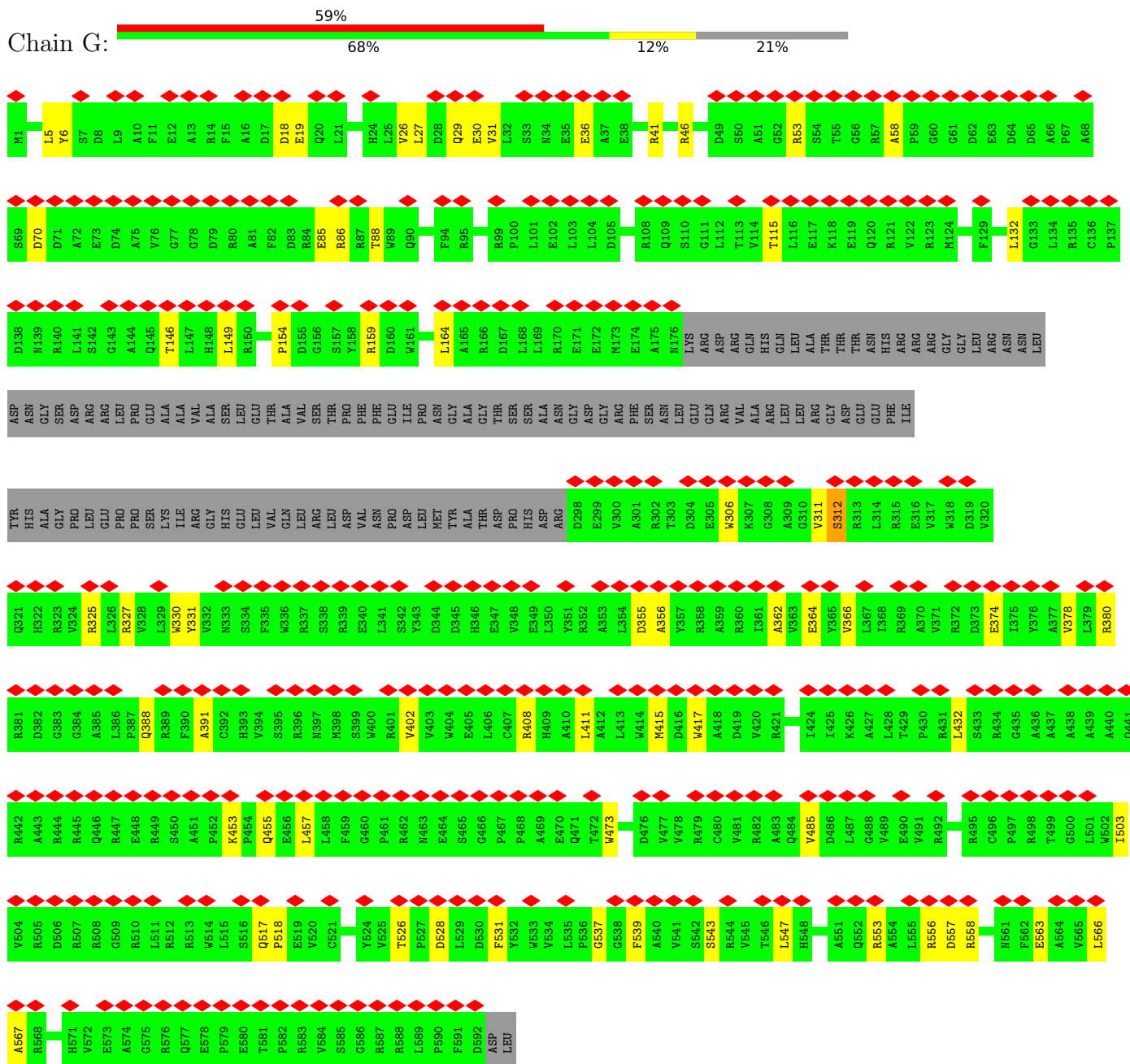
L2221	R2222	Q2223	L2224	A2225	Q2226	S2227	V2228	Q2229	D2230	T2231	L2232	Q2233	H2234	M2235	R2236	F2237	L2238	Y2239	L2240	L2241
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Chain E: 76% 52% 24% 23%

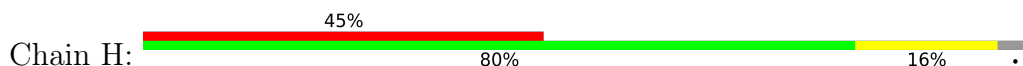
P181	S182	Y183	F184	G185	I186	T187	Q188	N189	D190	P191	F192	I193	R194	F195	H196	T197	D198	F199	R200	G201	F202	V203	V204	N205	T206	M207	F208	E209	N210	A211	S212	T213	W214	T215	F216	S217	F218	G219	T220	W221	Y222	Y223	R224	L225	K226	R227	G228	L229	Y230	T231	Q232	P233	R234	W235	K236	R237	V238	Y239	H240
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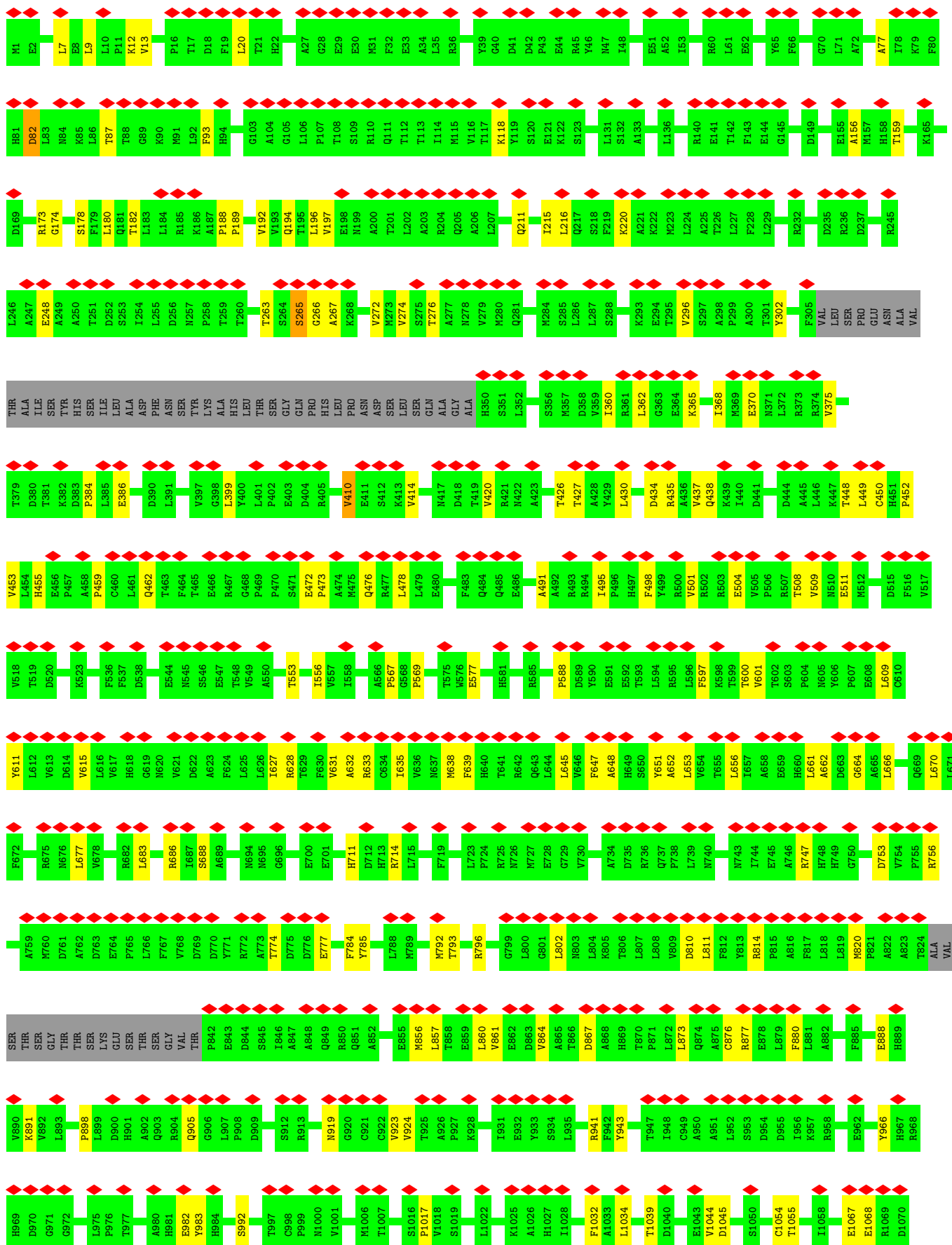


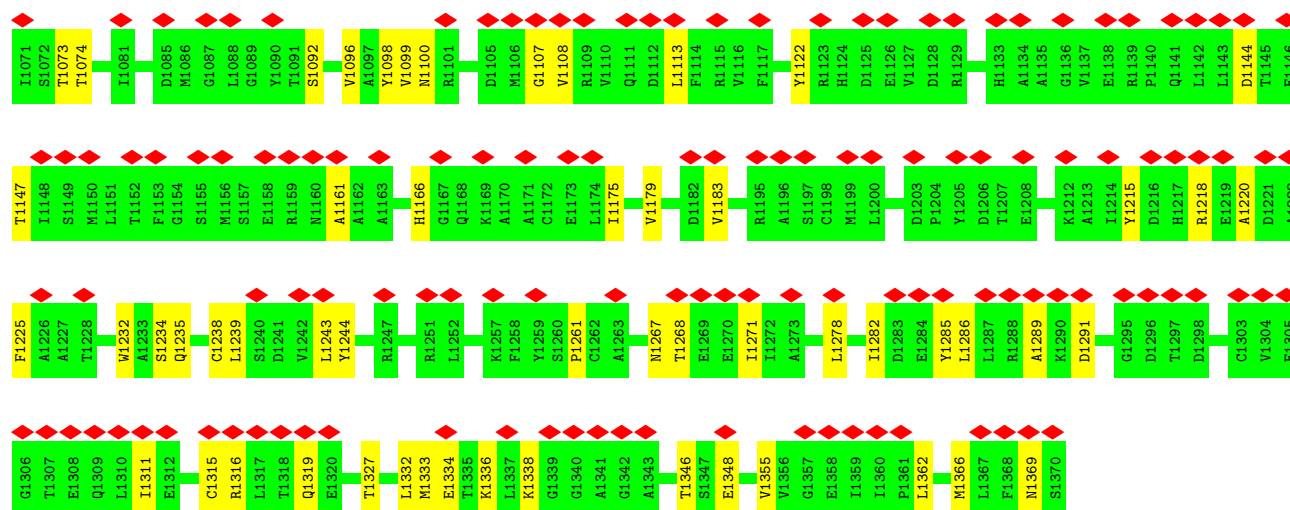
- Molecule 3: Capsid vertex component 1



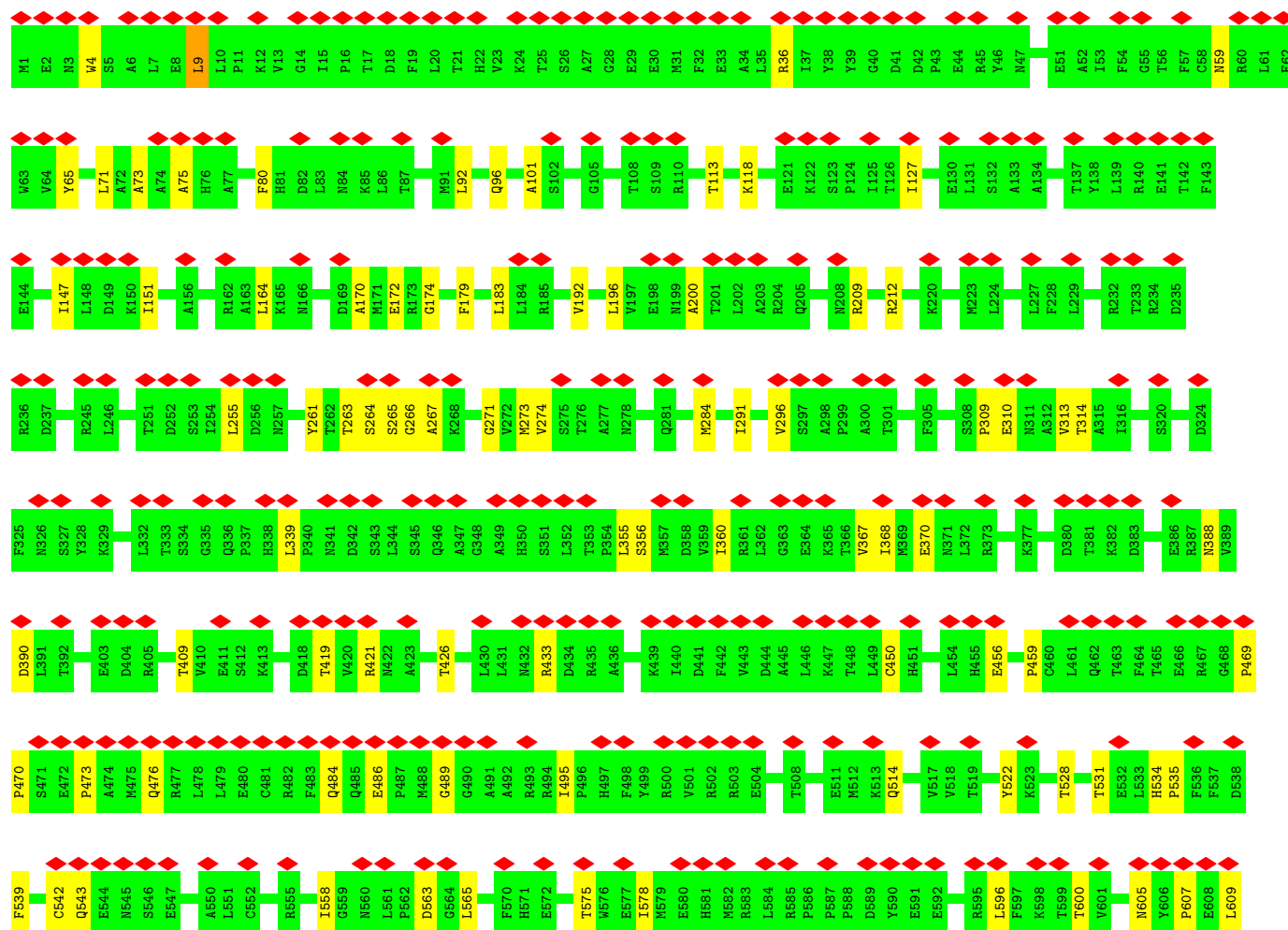
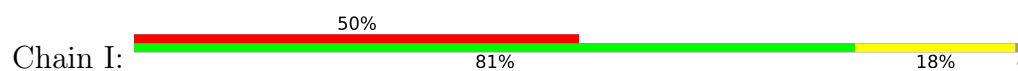
- Molecule 4: Major capsid protein

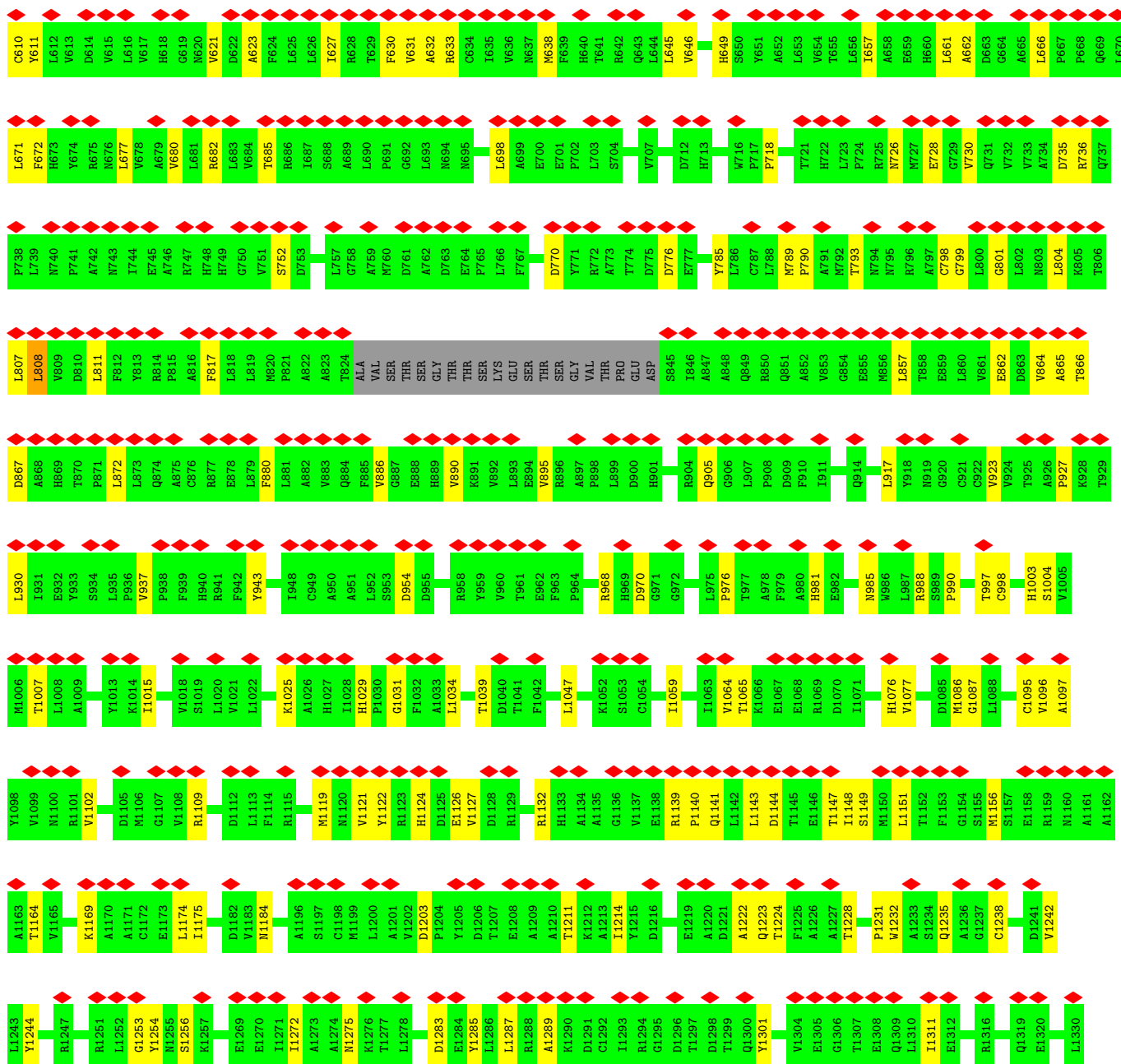




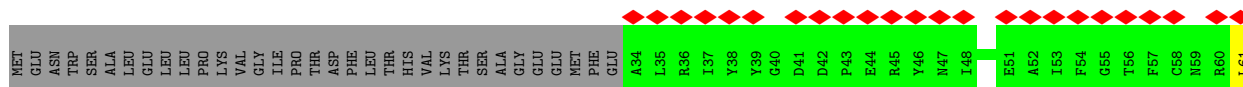
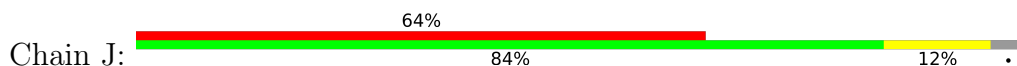


• Molecule 4: Major capsid protein

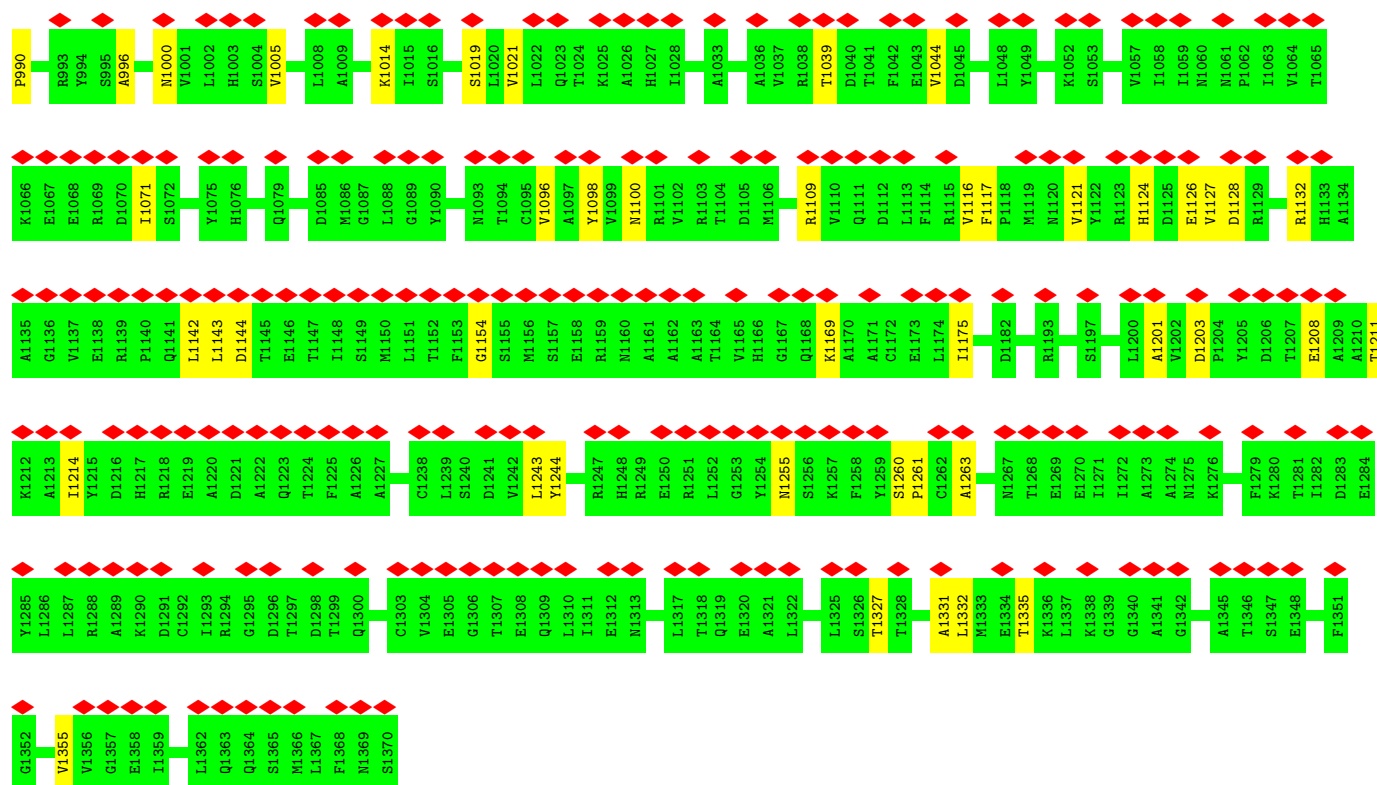




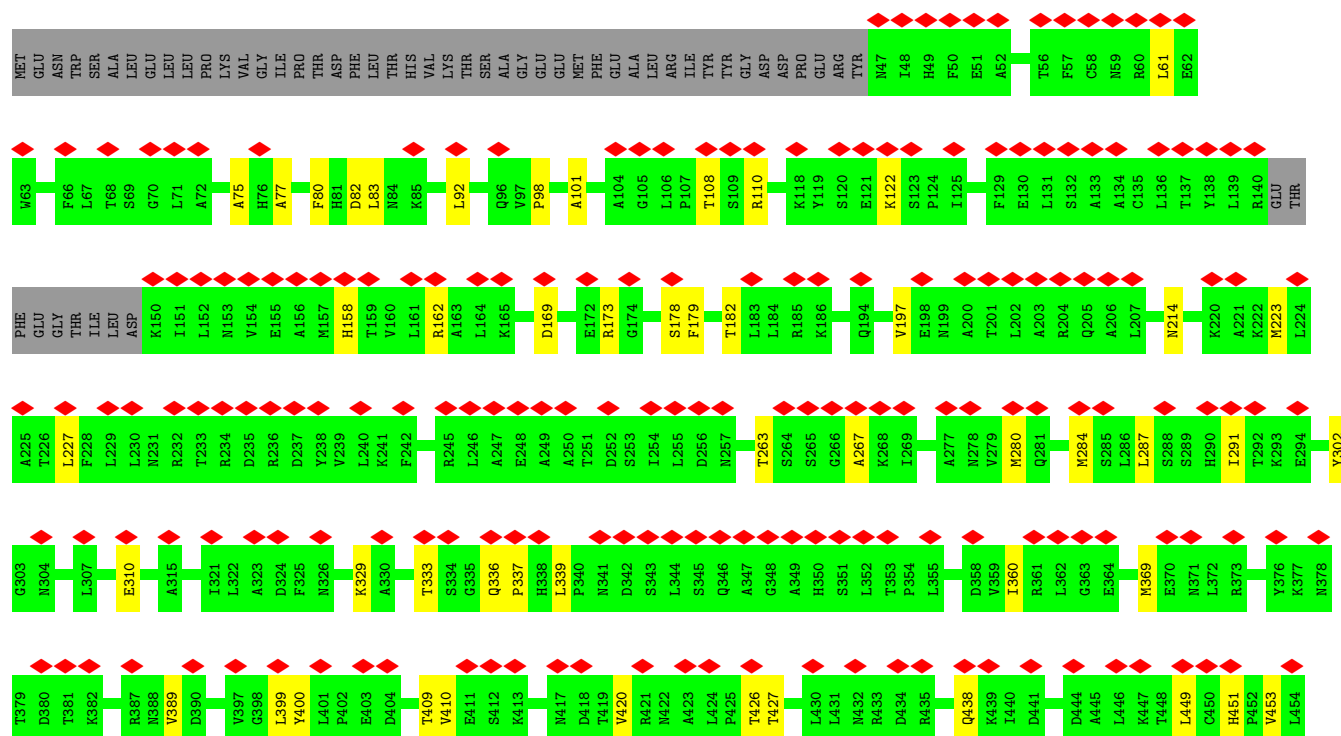
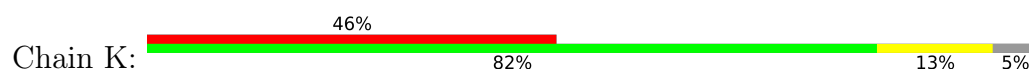
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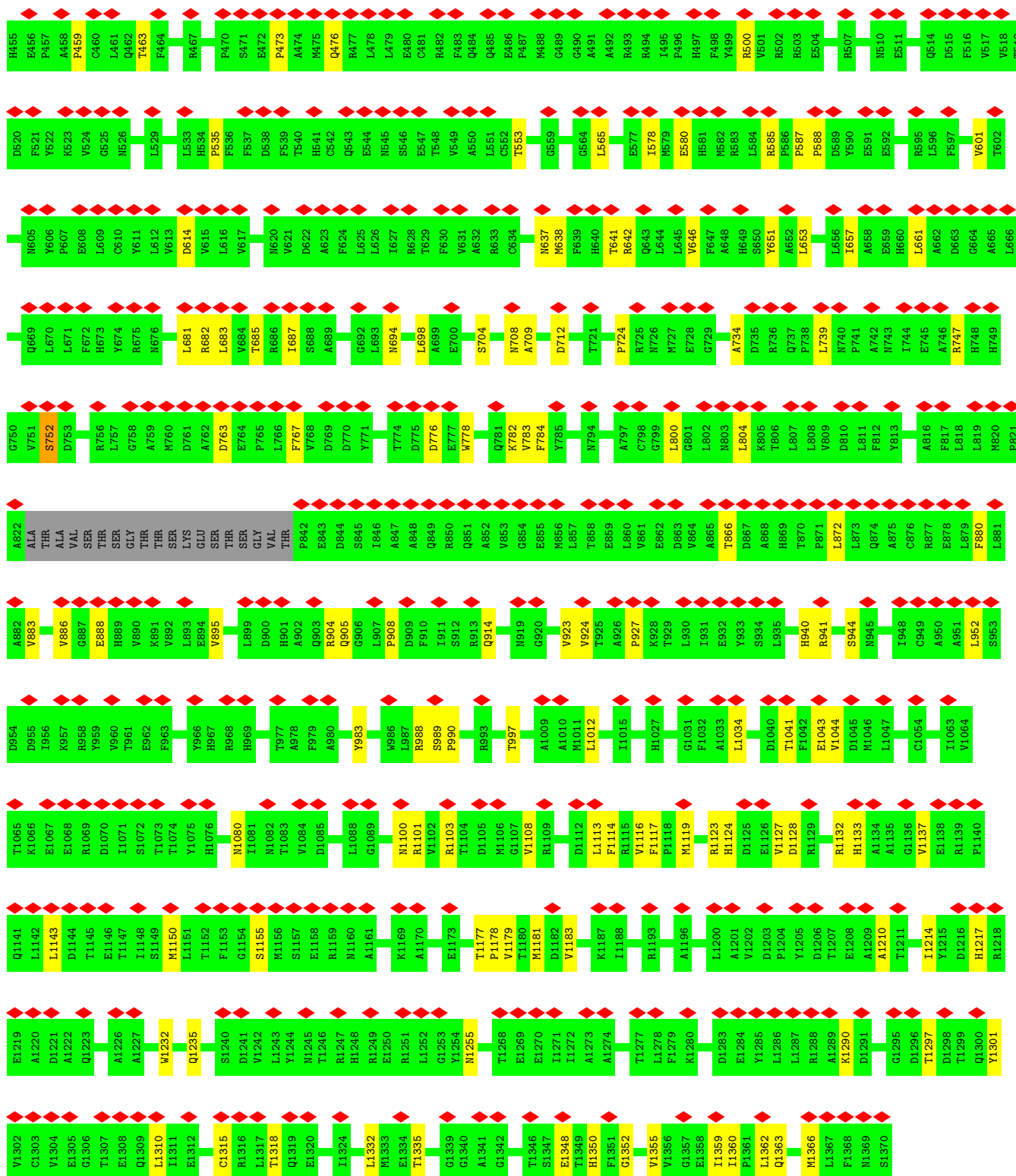


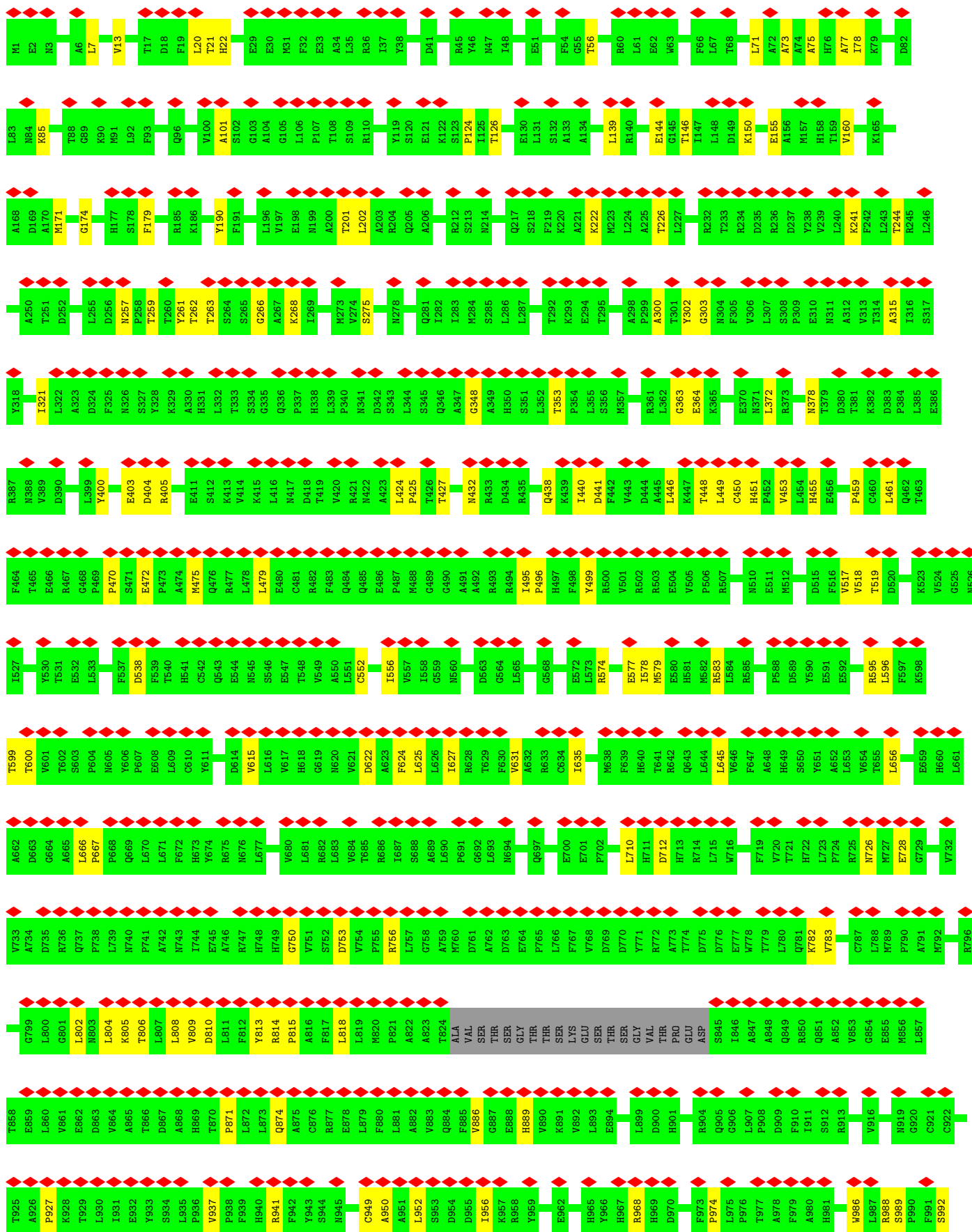


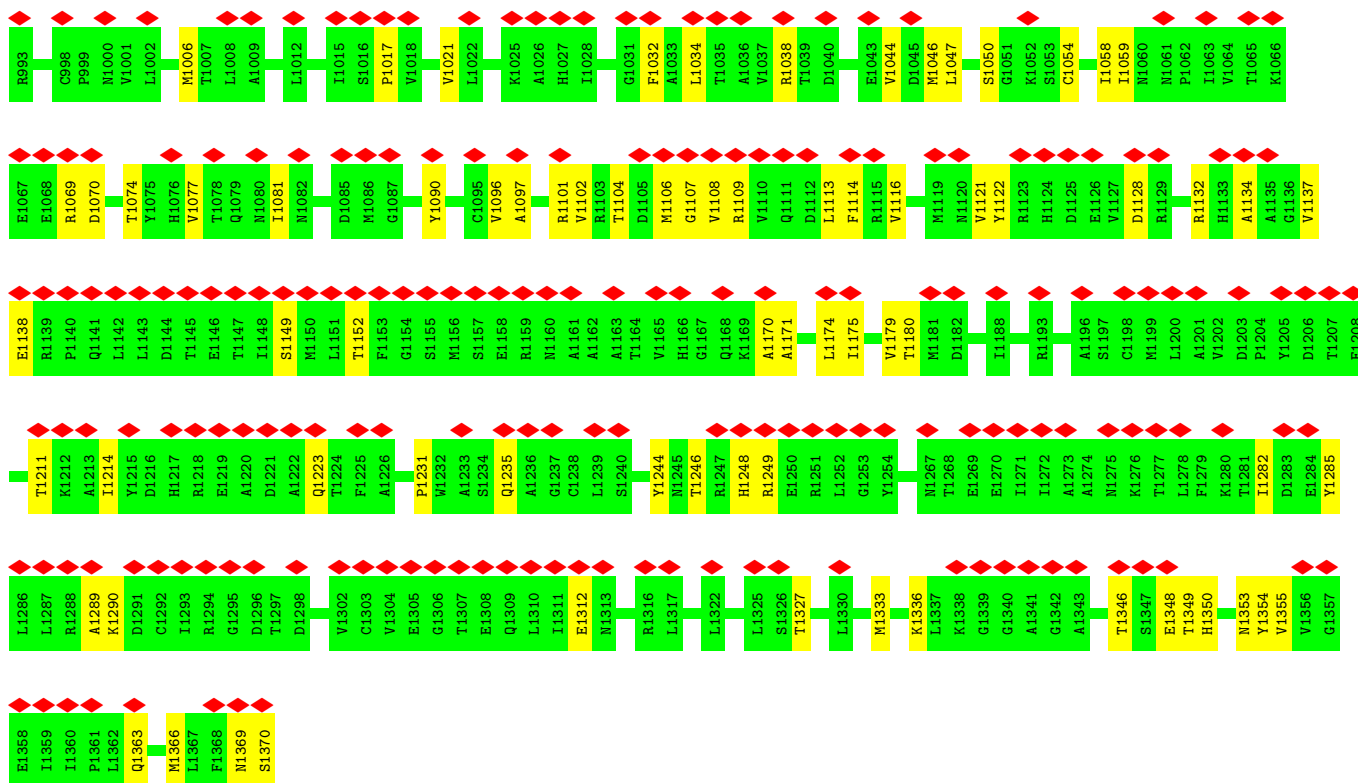


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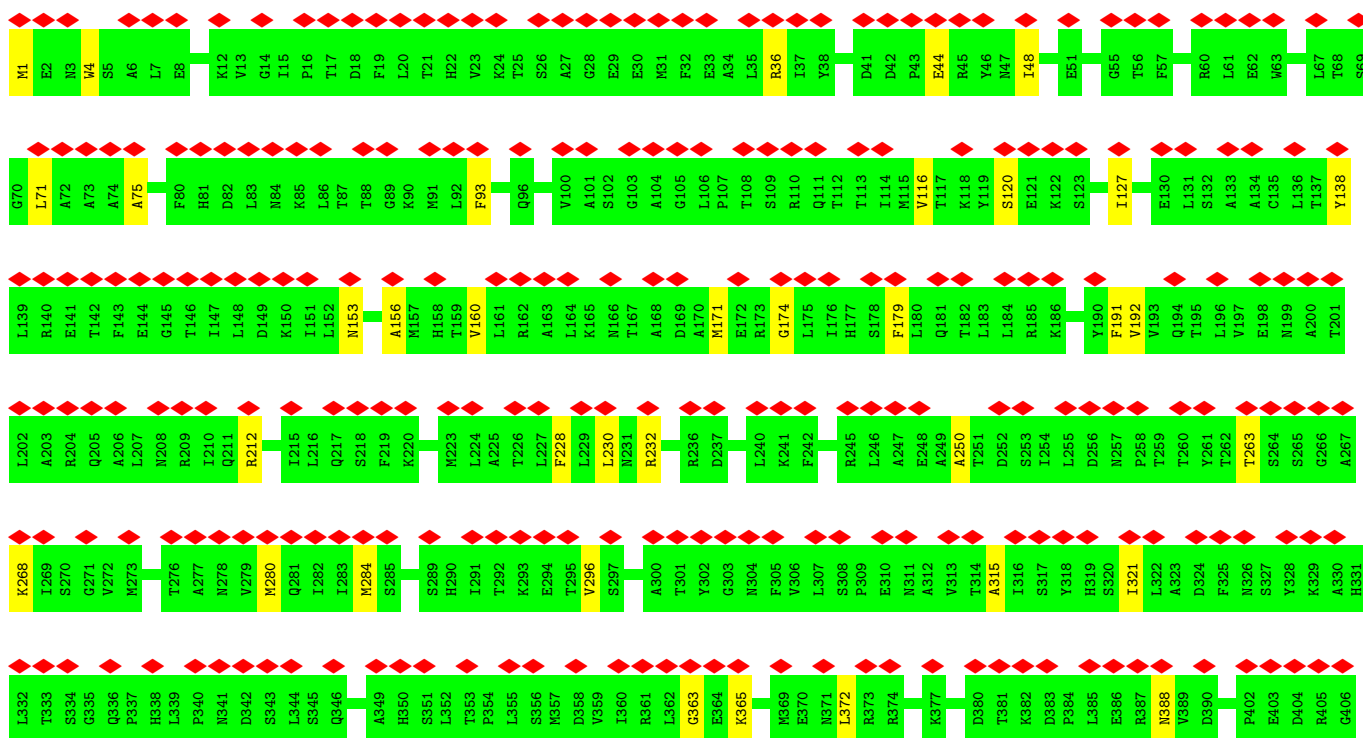
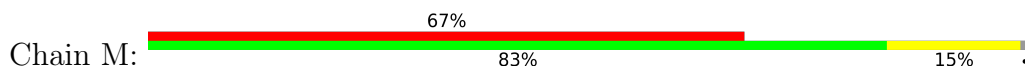




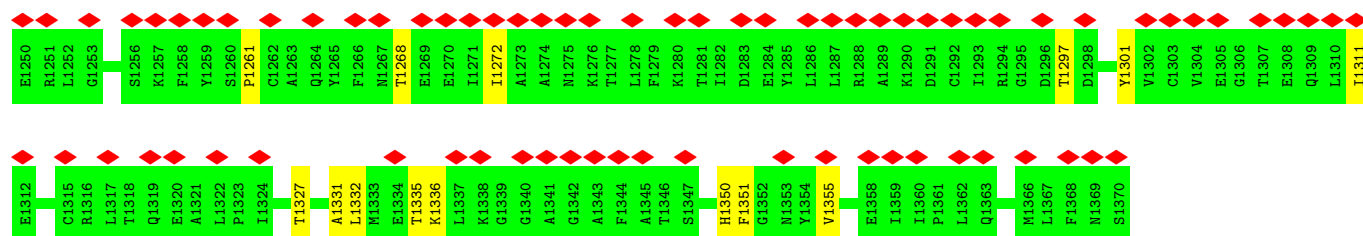




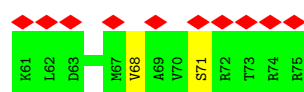
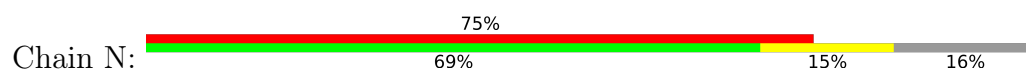
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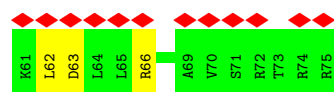
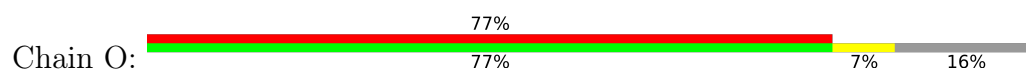
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K413	A474	F539	E809	P668	D736	N796	H856	A980	M1046	P1118	
L416	M475	C542	C610	Q669	L737	C798	L857	H981	L1047	M1119	K1187
M417	Q476	Q543	Y611	L670	P738	G799	E859	E982	L1048	N1120	I1188
D418	R477	Q544	L612	L671	L739	L800	H860	H984	Y1049	V1121	P1189
T419	L478	E544	H673	F672	N740	G801	Y861	H985	C1054	R1123	N1190
V420	L479	N545	V613	Y674	P741	L802	E862	N985	I1058	H1124	A1196
R421	E480	S546	D614	Y674	N742	N803	D863	W986	I1059	D1125	S1197
M422	C481	E547	V615	R675	A742	L804	H864	L987	M1060	L1128	C1198
A423	R482	T548	L616	L677	N743	R805	Y865	R988	M1061	D1129	M1199
L424	F483	V549	H617	V678	I744	T806	T866	H989		R1130	L1200
P425	Q484	A550	G619	A679	A746	L807	D867	L990	V1064	I1131	V1202
T426	Q485	L551	N620	V680	R747	L808	A868	I991	T1065	R1132	D1203
T427	E486	C552	V621	L681	H748	W809	H869	E992	K1066	A1133	P1204
L430	M488	P554	D622	L682	H749	L810	T870	C993	E1067	A1134	Y1205
L431	Q489	R555	A623	L683	G750	L811	L872	S994	E1068	A1135	D1206
M432	G490	I556	F624	V684	T751	F812	L873	L995	R1069	G1136	T1207
R433	A491		L625	T685	S752	R813	Q874	P996	D1070	V1137	E1208
D434	A492	L561	L626	R686	D753	R814	C876	A997	I1071	E1138	A1209
R435	R493	P562	I627	S688	V754	R815	R877	P998	T1074	R1139	A1210
A436	R494	D563	R628	A689	P755	R816	E878	P999	Y1075	P1140	T1211
V437	I495	G564	T629	L690	R756	L817	R879	H1003	H1076	Q1141	K1212
Q438	P496	L565	F630	P691	L757	L818	F880		H1077	L1142	I1214
K439	H497	A566	V631	G996	G758	L819	L881		Y1078	L1143	D1144
I440	F498	G568	A632	Q997	A759	M820	F882		V1079	M1010	Y1215
D441	Y499		R633	L698	W760	R821	H883		Q1079	A1009	D1216
F442	R500	H571	C634	L699	D761	A822	Y884		M1080	P946	H1217
V443	V501	E572	I635	A699	A762	A823	Q884		M1081	T947	R1218
D444	R502	L573	V636	E700	D763	T824	F885		M1082	L1012	E1219
A445	R503	R574	N637	E701	E764	ALA	Y886		C949	Y1013	A1220
L446	E504	T575	M638	E702	T765	VAL	G887		A950	K1014	D1221
K447	V505	W576	F639	P702	L766	SER	E888		A951	S1019	A1222
T448	P506	E577	H640	L703	L767	THR	H889		L952	L1020	D1223
L449	R507		T641	S704	F767	SER	Y890		S953	V1021	Q1224
C450	T508	E580	Q642	A705	V768	THR	H891		D954	L1022	F1225
H451	V509		Q643	Y706	D769	THR	Y892		I956	Q1023	A1226
P452	N510		L644	W708	D770	SER	E894		T1024	A1097	A1227
V453	E511		L645	A709	Y771	LVS	H895		K957	K1025	M1230
L454	M512		V646	L710	A772	GLU	L893		R958	A1026	P1231
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E456	Q514		D648	D712	T773	SER	R896		Y960	I1028	Q1235
P457	D515		H649	H713	T774	GLY	A897		T961	H1029	C1238
A458	D516		S650	R714	D775	VAL	P898		E962	I1030	S1240
P459	V517		E592	F719	E777	THR	L899		F964	G1031	V1241
C460	V518		T593	V720		PRD	D900		P964	F1032	V1242
L461	D520		L594	T721	L780	ASP	H901		H965	A1033	L1243
Q462	G525		R595	H722	Q781		A902		Y966	L1034	A1170
F464	N526		L596	H723	K782		Q903		H967	T1035	A1171
T465	I527		K598	L724	Y783		R904		R968	A1036	C1172
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P469	L533		T602	H728	C787		P908		Q972	D1040	L1176
P470	H534		S603	E728	L788		D909		F973	T1041	P1177
S471	P535		P604	G729	W789		F910		P974	F1042	H1248
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					T793						



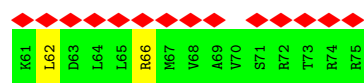
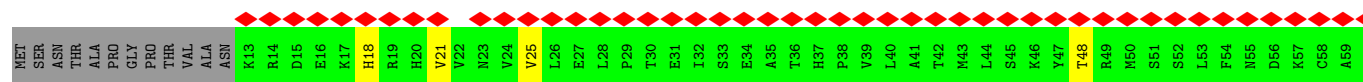
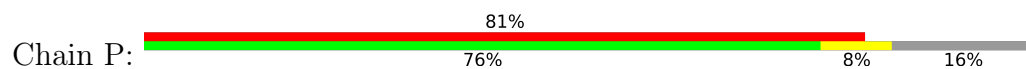
• Molecule 5: Small capsomere-interacting protein



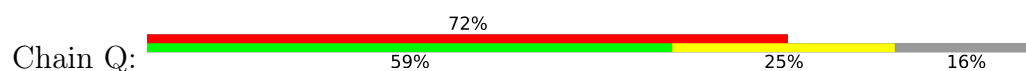
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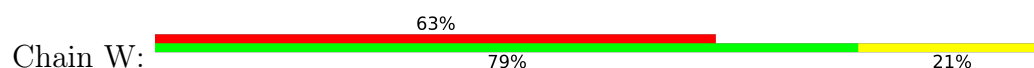


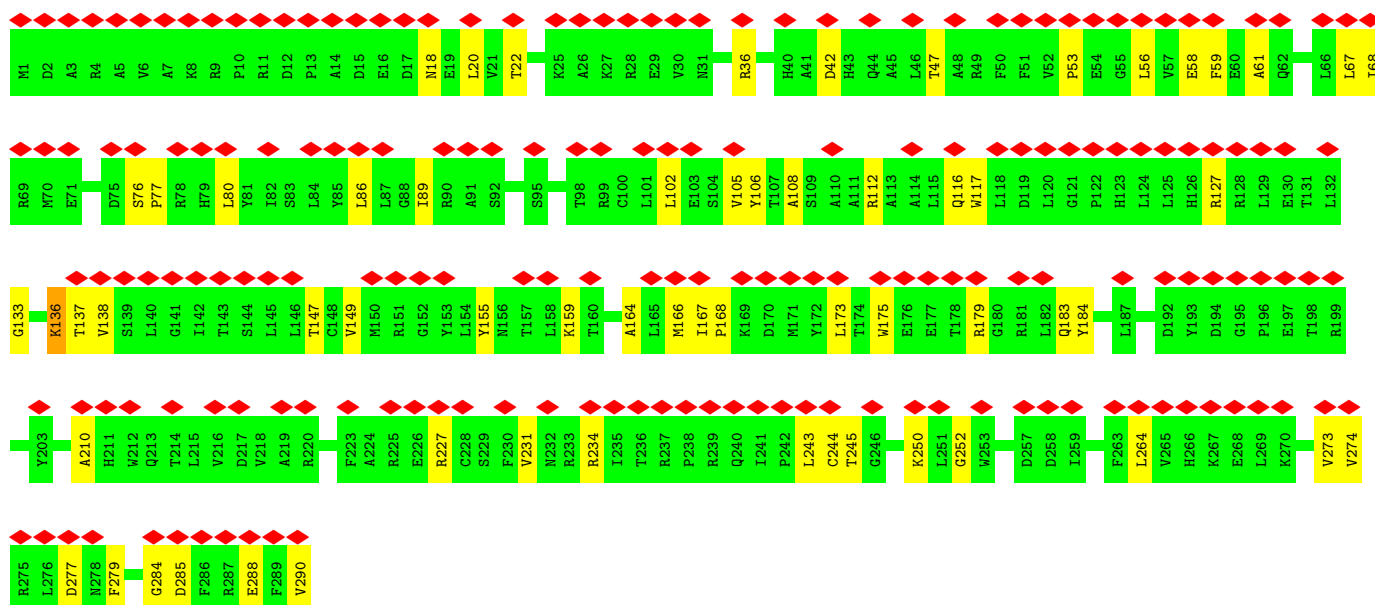
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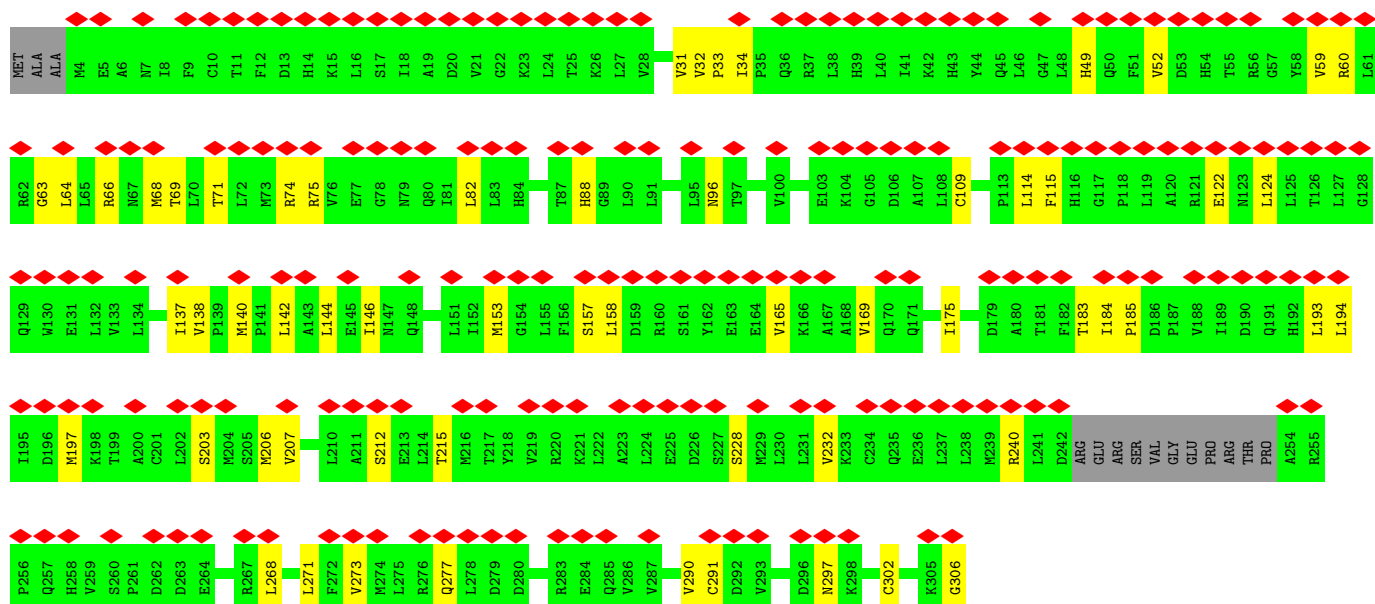
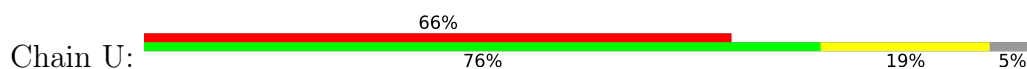
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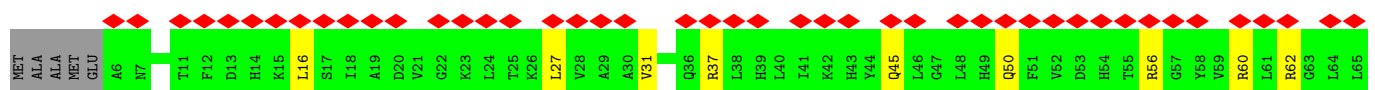


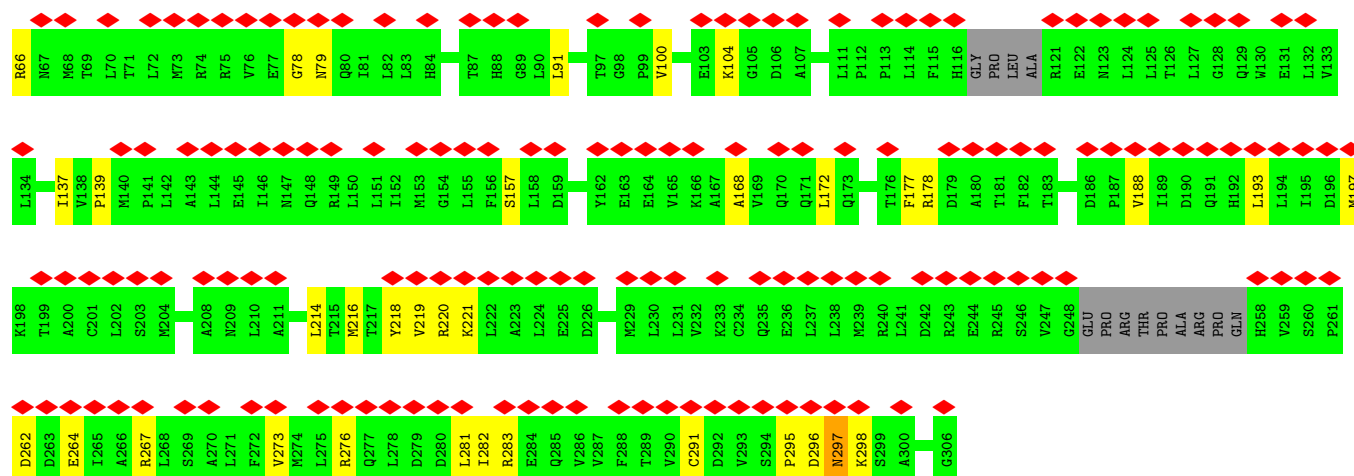


• Molecule 7: Triplex capsid protein 2

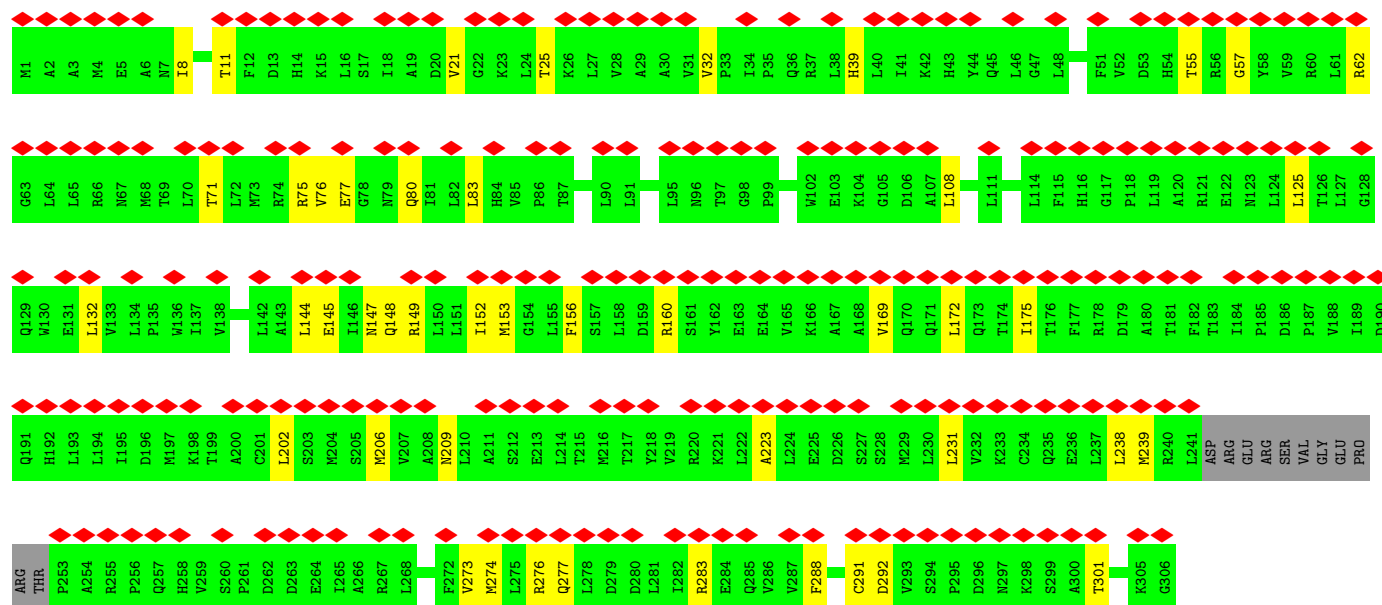
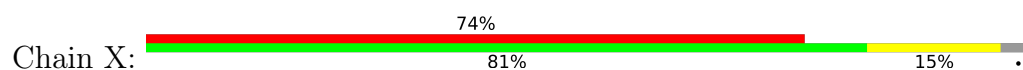


• Molecule 7: Triplex capsid protein 2

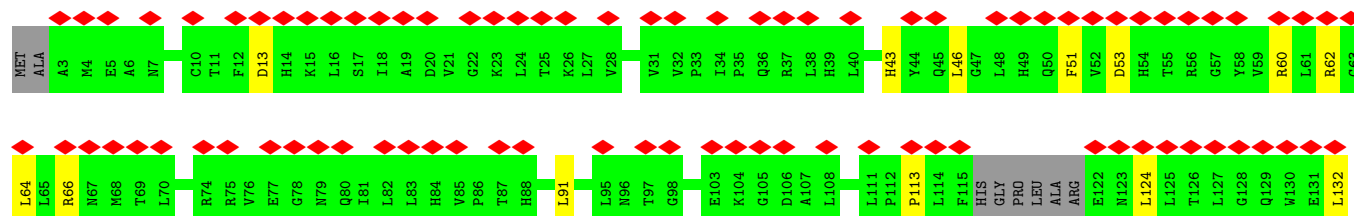
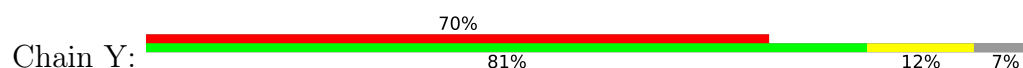


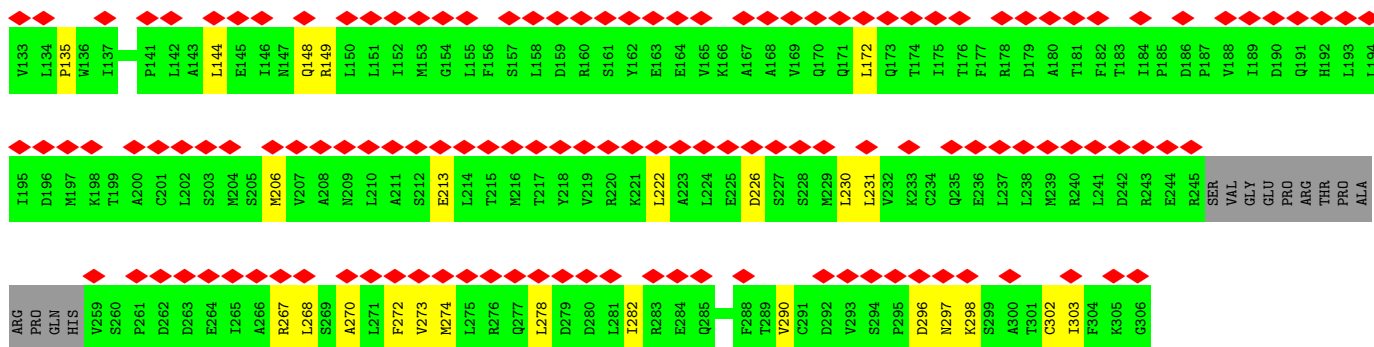


• Molecule 7: Triplex capsid protein 2

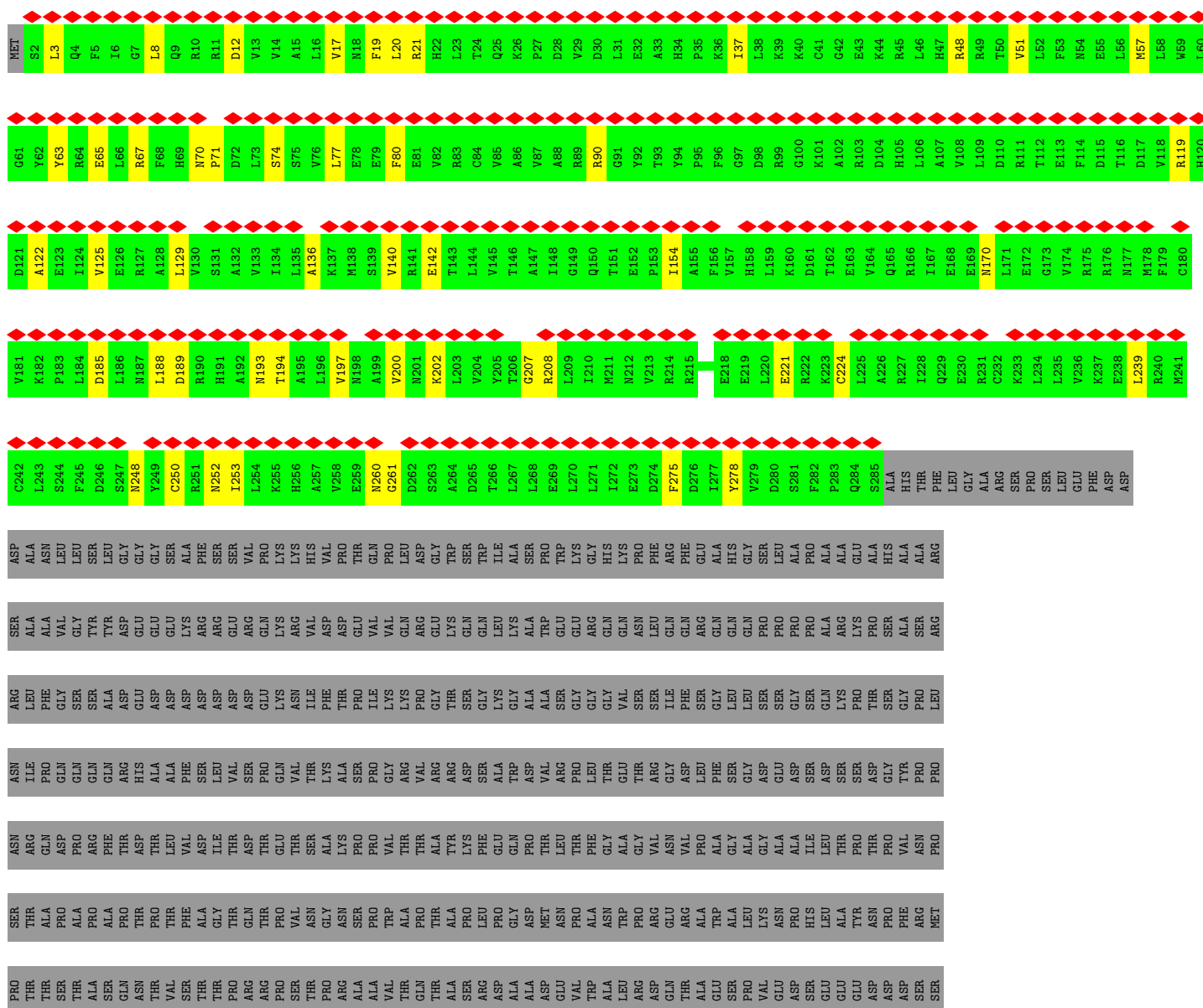


• Molecule 7: Triplex capsid protein 2





• Molecule 8: Large structural phosphoprotein



GLY	PRO	LEU	SER	VAL	ASP
MET	PRO	LYS	ALA	ALA	THR
GLY	VAL	PRO	SER	THR	SER
ALA	ALA	THR	ALA	HIS	VAL
LYS	PRO	GLY	ARG	ALA	SER
THR	SER	GLY	GLN	ALA	ASP
PRO	ILE	LYS	VAL	ALA	LEU
SER	LEU	VAL	SER	ARG	GLY
ASP	LYS	ALA	ALA	ALA	HIS
ALA	PRO	VAL	SER	GLN	THR
VAL	GLY	GLY	ALA	THR	THR
GLN	ALA	ARG	SER	VAL	PRO
ASN	SER	PRO	VAL	THR	SER
ILE	ALA	ARG	VAL	THR	SER
GLY	ALA	PRO	LEU	SER	ASP
LEU	LEU	SER	SER	THR	THR
LYS	GLN	VAL	PRO	PRO	TVR
ILE	SER	VAL	THR	VAL	ASN
GLY	ARG	SER	ASP	GLY	ASN
LYS	ARG	GLY	VAL	LEU	ASP
ILE	SER	SER	VAL	ARG	VAL
LYS	THR	ALA	VAL	GLY	SER
ASN	GLY	PRO	SER	LYS	PRO
THR	THR	GLY	PRO	GLN	PRO
GLY	ALA	ARG	ALA	VAL	SER
GLU	VAL	LEU	THR	SER	GLN
	VAL	GLY	SER	GLY	THR
	GLY	GLY	PRO	THR	PRO
	SER	SER	LEU	PRO	GLY
	PRO	SER	SER	SER	GLN
	VAL	ARG	MET	THR	SER
	LYS	ALA	LEU	VAL	THR
	SER	ALA	SER	PRO	PRO
	THR	SER	SER	ALA	SER
	THR	THR	ALA	THR	ARG
	GLY	THR	SER	LEU	ILE
	MET	PRO	PRO	LEU	ARG
	LYS	THR	SER	GLN	LYS
	THR	TVR	PRO	PRO	ALA
	VAL	PRO	ALA	GLN	LYS
	ALA	ALA	LYS	PRO	LEU
	PHE	VAL	SER	ALA	SER
	ASP	THR	ALA	SER	SER
	LEU	THR	PRO	SER	PRO
	SER	VAL	PRO	LYS	THR
	SER	TVR	SER	THR	THR
	PRO	PRO	PRO	THR	THR
	GLN	PRO	VAL	SER	THR
	LYS	SER	LYS	ARG	THR
	THR	SER	GLY	ASN	SER
	THR	ALA	GLY	VAL	GLN
	GLY	LYS	SER	THR	LYS
	PRO	SER	ARG	THR	PRO
	GLN	SER	VAL	SER	VAL
	PRO	VAL	GLY	ALA	LEU
	GLY	VAL	VAL	GLY	GLY
	PRO	ASN	PRO	THR	THR
	ALA	ALA	SER	SER	ARG

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	16225	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 ($e^-/\text{\AA}^2$)	47.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	489.6, 489.6, 489.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/5969	0.37	0/8139
1	C	0.17	0/334	0.36	0/450
2	E	0.16	0/4094	0.42	1/5558 (0.0%)
2	F	0.14	0/721	0.38	0/969
3	G	0.13	0/3951	0.36	0/5357
4	H	0.13	0/10638	0.39	0/14487
4	I	0.13	0/10949	0.39	0/14916
4	J	0.14	0/10682	0.38	0/14553
4	K	0.13	0/10503	0.37	2/14307 (0.0%)
4	L	0.14	0/10949	0.37	2/14916 (0.0%)
4	M	0.13	0/10949	0.38	2/14916 (0.0%)
5	N	0.10	0/520	0.32	0/697
5	O	0.09	0/520	0.28	0/697
5	P	0.12	0/520	0.32	0/697
5	Q	0.11	0/520	0.31	0/697
5	R	0.11	0/520	0.33	0/697
5	S	0.10	0/520	0.29	0/697
6	T	0.16	0/1981	0.44	0/2687
6	W	0.15	0/2374	0.43	0/3221
7	U	0.16	0/2361	0.41	0/3206
7	V	0.18	0/2333	0.45	0/3164
7	X	0.15	0/2379	0.41	2/3230 (0.1%)
7	Y	0.15	0/2305	0.43	0/3126
8	Z	0.15	0/2358	0.41	0/3182
All	All	0.14	0/98950	0.39	9/134566 (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
3	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	H	0	2
4	I	0	1
4	J	0	1
4	K	0	2
4	M	0	1
6	W	0	1
All	All	0	9

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	270	TYR	N-CA-C	-8.96	102.50	112.72
4	M	753	ASP	CA-C-N	6.52	124.35	120.24
4	M	753	ASP	C-N-CA	6.52	124.35	120.24
4	K	752	SER	CA-C-N	6.19	133.37	121.54
4	K	752	SER	C-N-CA	6.19	133.37	121.54
4	L	988	ARG	CA-C-N	5.68	127.19	120.09
4	L	988	ARG	C-N-CA	5.68	127.19	120.09
7	X	291	CYS	CA-C-N	5.50	132.06	121.54
7	X	291	CYS	C-N-CA	5.50	132.06	121.54

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	312	SER	Peptide
4	H	1100	ASN	Peptide
4	H	265	SER	Peptide
4	I	1143	LEU	Peptide
4	J	794	ASN	Peptide
4	K	1100	ASN	Peptide
4	K	941	ARG	Peptide
4	M	1097	ALA	Peptide
6	W	136	LYS	Peptide

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5830	0	5830	164	0
1	C	332	0	358	15	0
2	E	3992	0	3913	142	0
2	F	710	0	711	12	0
3	G	3862	0	3779	46	0
4	H	10391	0	10342	128	0
4	I	10693	0	10635	153	0
4	J	10433	0	10379	103	0
4	K	10259	0	10216	103	0
4	L	10693	0	10635	135	0
4	M	10693	0	10635	124	0
5	N	513	0	539	7	0
5	O	513	0	539	3	0
5	P	513	0	539	5	0
5	Q	513	0	539	12	0
5	R	513	0	539	11	0
5	S	513	0	539	10	0
6	T	1939	0	1972	20	0
6	W	2325	0	2363	44	0
7	U	2317	0	2405	36	0
7	V	2292	0	2379	27	0
7	X	2334	0	2431	29	0
7	Y	2266	0	2355	24	0
8	Z	2320	0	2351	30	0
All	All	96759	0	96923	1289	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 7.

All (1289) 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)
2:E:267:TYR:HE1	2:E:270:TYR:HB3	1.35	0.90
4:J:795:ASN:ND2	4:J:969:HIS:O	2.09	0.84
7:U:240:ARG:HB2	7:V:267:ARG:HH21	1.43	0.84
2:E:267:TYR:CE1	2:E:270:TYR:HB3	2.15	0.81
2:E:371:PHE:HB3	2:E:376:VAL:HB	1.64	0.80
4:M:575:THR:HG21	4:M:1007:THR:HA	1.63	0.78
3:G:53:ARG:NH2	3:G:58:ALA:O	2.17	0.77
4:L:1044:VAL:HG11	4:L:1096:VAL:HG13	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:337:TYR:HE2	2:E:431:ARG:HG3	1.51	0.75
2:E:207:MET:HE1	2:E:465:LEU:HD22	1.67	0.74
6:W:290:VAL:HG22	7:X:277:GLN:HG3	1.70	0.74
4:L:432:ASN:OD1	4:L:438:GLN:NE2	2.21	0.74
4:H:248:GLU:OE2	4:H:365:LYS:NZ	2.21	0.73
4:L:600:THR:HG21	4:L:645:LEU:HD23	1.70	0.73
4:L:1038:ARG:HH22	4:L:1106:MET:HG2	1.54	0.73
4:L:1047:LEU:HD22	4:L:1097:ALA:HB2	1.69	0.73
1:A:1765:PRO:HG2	1:A:1768:MET:HB2	1.72	0.72
4:M:710:LEU:HD21	4:M:783:VAL:HG23	1.73	0.71
4:L:144:GLU:H	6:W:36:ARG:HH22	1.38	0.71
8:Z:136:ALA:HB2	8:Z:200:VAL:HG21	1.72	0.70
6:W:167:ILE:HD12	6:W:168:PRO:HD2	1.74	0.70
4:H:263:THR:HG22	4:H:296:VAL:HG22	1.74	0.70
4:H:553:THR:HG21	4:H:983:TYR:HB3	1.72	0.70
4:M:600:THR:HG22	4:M:644:LEU:HB2	1.74	0.70
3:G:432:LEU:O	3:G:556:ARG:NH1	2.25	0.69
2:F:35:LEU:HB2	3:G:402:VAL:HG23	1.75	0.69
4:M:433:ARG:HD2	4:M:1105:ASP:HA	1.72	0.69
2:E:339:TYR:HB2	2:E:364:ARG:HD2	1.75	0.69
1:A:1859:LEU:HB3	1:A:1877:VAL:HG21	1.74	0.69
2:E:263:ASN:HA	2:E:266:VAL:HG22	1.74	0.69
4:H:820:MET:HG3	4:H:877:ARG:HD3	1.74	0.69
4:M:230:LEU:H	4:M:1097:ALA:HB1	1.58	0.69
4:I:212:ARG:NH2	4:I:1203:ASP:OD1	2.25	0.68
4:I:484:GLN:NE2	4:I:486:GLU:OE2	2.26	0.68
2:E:268:PRO:C	2:E:271:ASP:H	2.02	0.68
1:A:1483:ARG:NH1	1:A:1526:GLU:OE1	2.27	0.68
4:L:450:CYS:O	4:L:1122:TYR:OH	2.11	0.68
1:A:2217:VAL:HG22	2:E:82:ARG:HD3	1.76	0.68
4:M:574:ARG:NH2	4:M:1023:GLN:OE1	2.27	0.68
4:H:272:VAL:HG12	4:H:368:ILE:HB	1.76	0.67
1:A:1520:ARG:NH2	1:A:1905:PRO:O	2.28	0.67
4:J:601:VAL:HG11	4:J:793:THR:HG22	1.76	0.67
1:A:1754:TYR:HB2	1:A:1757:TYR:CE2	2.30	0.67
2:E:423:PHE:HB2	2:E:426:GLU:HG2	1.74	0.67
4:K:420:VAL:HB	4:K:580:GLU:HG3	1.76	0.67
4:L:470:PRO:HB2	4:L:475:MET:HG3	1.78	0.66
4:M:753:ASP:OD1	5:S:66:ARG:NH1	2.29	0.66
2:E:263:ASN:O	2:E:587:HIS:NE2	2.28	0.66
4:J:757:LEU:HD11	5:P:62:LEU:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:274:VAL:HG13	4:I:370:GLU:HB3	1.78	0.66
4:K:927:PRO:HD2	4:K:952:LEU:HD21	1.78	0.66
4:K:399:LEU:HD23	4:K:1183:VAL:HG22	1.78	0.66
4:M:989:SER:OG	4:M:993:ARG:NH2	2.29	0.66
1:A:2211:LEU:HD23	1:A:2214:LEU:HD12	1.77	0.66
4:K:657:ILE:HG23	4:K:661:LEU:HD12	1.78	0.66
2:E:500:PHE:HD1	2:E:503:ARG:HH12	1.44	0.66
4:H:1044:VAL:HG22	4:H:1099:VAL:HG22	1.78	0.66
2:E:268:PRO:HA	2:E:271:ASP:HA	1.78	0.65
4:M:759:ALA:O	4:M:761:ASP:N	2.29	0.65
4:K:553:THR:HG21	4:K:983:TYR:HB3	1.77	0.65
1:A:1476:LEU:HD22	1:A:1480:ARG:HH21	1.62	0.65
1:A:1867:LYS:HE3	1:A:1872:GLU:HA	1.77	0.64
7:Y:222:LEU:O	7:Y:226:ASP:N	2.31	0.64
1:A:1689:THR:OG1	1:A:2113:ARG:NH2	2.30	0.64
1:A:2206:ASN:OD1	2:E:93:GLN:NE2	2.31	0.64
4:K:709:ALA:HB3	4:K:1012:LEU:HD23	1.78	0.64
4:L:124:PRO:HG3	7:X:11:THR:HG21	1.79	0.64
4:H:1285:TYR:HA	4:H:1289:ALA:HB3	1.80	0.64
4:J:212:ARG:NH2	4:J:1203:ASP:OD1	2.30	0.64
4:H:87:THR:HG23	7:V:79:ASN:HA	1.80	0.63
4:L:139:LEU:HD22	4:L:160:VAL:HG21	1.79	0.63
4:L:596:LEU:O	4:L:600:THR:HG23	1.99	0.63
2:E:407:TRP:O	2:E:411:LEU:HD12	1.98	0.63
6:W:168:PRO:HA	6:W:273:VAL:HA	1.79	0.63
1:A:2221:LEU:HD23	1:A:2224:LEU:HD21	1.81	0.63
4:H:888:GLU:O	4:H:919:ASN:ND2	2.32	0.63
1:A:1984:ARG:HD2	2:E:493:GLY:HA3	1.79	0.63
4:K:694:ASN:HD22	4:K:704:SER:HB3	1.64	0.63
1:A:2228:VAL:HG11	2:F:72:VAL:HG11	1.81	0.63
2:E:365:HIS:O	2:E:368:VAL:HG12	1.99	0.63
3:G:146:THR:HA	3:G:164:LEU:HA	1.81	0.63
4:I:1235:GLN:HB2	4:I:1238:CYS:HB3	1.81	0.63
1:A:1527:ARG:HH11	1:A:1531:LEU:HD12	1.63	0.62
1:C:2211:LEU:O	1:C:2214:LEU:HG	1.99	0.62
4:L:315:ALA:HB2	4:L:321:ILE:HD11	1.80	0.62
7:U:290:VAL:HG12	7:U:302:CYS:SG	2.39	0.62
4:I:390:ASP:OD1	4:I:1039:THR:OG1	2.18	0.62
5:Q:28:LEU:HD12	5:Q:29:PRO:HD2	1.81	0.62
1:A:1792:MET:HE3	1:A:2039:LEU:HB2	1.82	0.62
3:G:374:GLU:O	3:G:378:VAL:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:638:MET:HE3	4:H:864:VAL:HA	1.80	0.62
4:I:1272:ILE:O	4:I:1275:ASN:ND2	2.33	0.62
4:K:101:ALA:HB3	4:L:174:GLY:HA3	1.82	0.62
6:W:61:ALA:HA	6:W:138:VAL:HG21	1.80	0.62
2:F:60:TYR:O	2:F:64:GLU:HG2	2.00	0.62
4:J:821:PRO:HD3	4:J:877:ARG:HH21	1.65	0.62
4:L:615:VAL:HG11	4:L:802:LEU:HD12	1.81	0.62
4:K:280:MET:O	4:K:284:MET:HG2	2.00	0.61
4:L:574:ARG:O	4:L:578:ILE:HG13	2.00	0.61
1:A:1806:ILE:HD12	1:A:1975:VAL:HG21	1.80	0.61
2:E:499:GLU:O	2:E:503:ARG:NH1	2.33	0.61
4:H:437:VAL:HG21	4:I:1184:ASN:HD22	1.64	0.61
1:A:1453:ALA:HA	1:A:1456:TYR:CD2	2.36	0.61
1:A:2051:ARG:HD2	1:A:2052:VAL:H	1.66	0.61
2:E:509:TRP:HE1	2:E:516:VAL:HG21	1.65	0.61
4:H:1161:ALA:O	4:I:209:ARG:NH2	2.34	0.61
4:H:1336:LYS:NZ	4:H:1346:THR:OG1	2.33	0.61
1:A:1702:THR:HA	1:A:1705:HIS:HD1	1.66	0.61
4:M:1297:THR:HG21	4:M:1301:TYR:HD2	1.64	0.61
7:U:74:ARG:HB2	7:U:82:LEU:O	2.01	0.61
2:E:230:TYR:HB2	2:E:241:LEU:HD23	1.83	0.61
2:E:539:ASP:HB3	2:E:542:ARG:HG3	1.80	0.61
4:J:705:ALA:HB1	4:J:712:ASP:HB3	1.82	0.61
4:M:672:PHE:HA	4:M:675:ARG:HG2	1.83	0.61
1:A:1476:LEU:O	1:A:1480:ARG:HG2	2.01	0.61
1:A:1486:PHE:CE2	1:A:1519:THR:HG22	2.36	0.61
2:E:367:LEU:O	2:E:371:PHE:HD1	1.83	0.61
7:Y:290:VAL:HG22	7:Y:302:CYS:SG	2.41	0.61
1:A:1473:ARG:HA	1:A:1476:LEU:HD12	1.81	0.61
1:A:1971:GLN:HG3	1:A:1972:ARG:HG3	1.83	0.61
1:A:1573:ARG:NH1	1:A:1619:ALA:O	2.33	0.60
4:H:688:SER:OG	4:H:711:HIS:NE2	2.31	0.60
4:L:1175:ILE:HG22	4:L:1244:TYR:HE2	1.66	0.60
2:E:576:LYS:HE3	2:E:576:LYS:HA	1.82	0.60
1:C:2236:ARG:HA	1:C:2240:LEU:HD12	1.84	0.60
4:I:1047:LEU:HD22	4:I:1097:ALA:HB2	1.83	0.60
4:J:697:GLN:NE2	4:J:699:ALA:O	2.35	0.60
2:E:286:ALA:HB2	2:E:404:LEU:HD13	1.83	0.60
7:V:100:VAL:HG11	7:V:139:PRO:HD3	1.84	0.60
4:J:804:LEU:HA	4:J:807:LEU:HB3	1.84	0.60
4:M:757:LEU:HA	4:M:760:MET:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:102:LEU:HA	6:W:105:VAL:HG12	1.84	0.60
3:G:566:LEU:HD12	7:U:165:VAL:HG21	1.84	0.59
4:L:949:CYS:SG	4:L:956:ILE:HG21	2.42	0.59
7:X:25:THR:HA	7:X:76:VAL:HG11	1.82	0.59
4:M:657:ILE:HG12	4:M:661:LEU:HD12	1.84	0.59
1:A:1786:VAL:O	1:A:1972:ARG:NH1	2.35	0.59
1:A:1817:ASN:OD1	1:A:1818:LYS:N	2.35	0.59
4:H:856:MET:O	4:H:860:LEU:HG	2.02	0.59
1:A:1612:ASN:HB2	1:A:1615:PHE:HB2	1.84	0.59
2:E:355:ARG:O	2:E:355:ARG:NH1	2.32	0.59
4:K:1128:ASP:O	4:K:1132:ARG:HG2	2.03	0.59
5:P:18:HIS:HA	5:P:48:THR:HG21	1.85	0.59
4:M:120:SER:HB3	4:M:1084:VAL:HG12	1.83	0.59
4:M:430:LEU:HD12	4:M:1108:VAL:HG12	1.84	0.59
4:I:804:LEU:HA	4:I:807:LEU:HB3	1.84	0.59
1:A:1481:ASP:O	1:A:1485:ARG:HG2	2.02	0.59
7:V:104:LYS:HG3	7:V:291:CYS:HA	1.85	0.59
4:I:662:ALA:HA	4:I:671:LEU:HD11	1.85	0.58
4:M:250:ALA:HB3	4:M:1049:TYR:HE2	1.67	0.58
7:Y:144:LEU:O	7:Y:148:GLN:HG2	2.03	0.58
2:E:349:MET:HB3	2:E:428:GLN:NE2	2.18	0.58
2:E:350:PRO:HD2	2:E:428:GLN:HG3	1.84	0.58
4:M:1217:HIS:NE2	4:M:1235:GLN:HG3	2.18	0.58
4:K:866:THR:HG22	4:K:872:LEU:HA	1.85	0.58
2:E:243:GLN:HE21	2:E:246:ASN:HB3	1.68	0.58
4:L:303:GLY:HA3	4:L:348:GLY:HA2	1.86	0.58
4:K:904:ARG:NH1	4:K:908:PRO:O	2.36	0.58
4:M:806:THR:HA	4:M:809:VAL:HG12	1.85	0.58
1:A:1779:GLN:OE1	1:A:2065:ARG:NH1	2.37	0.58
2:E:205:ASN:HA	2:E:208:PHE:CE1	2.37	0.58
4:I:65:TYR:HA	4:I:172:GLU:HG2	1.85	0.58
4:L:459:PRO:HB3	4:L:1248:HIS:CE1	2.38	0.58
4:M:75:ALA:HB2	4:M:179:PHE:CZ	2.38	0.58
4:M:617:VAL:HG13	4:M:619:GLY:H	1.69	0.58
4:M:785:TYR:O	4:M:943:TYR:OH	2.21	0.58
6:T:46:LEU:HD22	7:V:91:LEU:HD23	1.84	0.58
2:E:287:TYR:HB2	2:E:371:PHE:HE2	1.68	0.58
4:H:20:LEU:HD11	4:K:197:VAL:HG22	1.85	0.58
4:I:1336:LYS:NZ	4:I:1346:THR:OG1	2.37	0.58
7:U:122:GLU:O	7:U:124:LEU:N	2.37	0.58
4:M:895:VAL:HB	4:M:914:GLN:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:89:ILE:HG23	6:T:115:LEU:HD11	1.86	0.58
2:E:606:LEU:HB2	2:E:609:HIS:HB2	1.86	0.58
4:H:747:ARG:NH2	4:H:888:GLU:OE1	2.36	0.58
4:K:1043:GLU:OE1	4:K:1101:ARG:NH1	2.34	0.58
4:L:144:GLU:H	6:W:36:ARG:NH2	2.02	0.57
4:I:627:ILE:HG22	4:I:631:VAL:HG23	1.85	0.57
4:M:571:HIS:O	4:M:575:THR:HG23	2.04	0.57
1:A:1574:ARG:HE	1:A:1604:ILE:HG22	1.70	0.57
2:E:203:VAL:O	2:E:207:MET:HG2	2.03	0.57
4:H:426:THR:HG23	4:H:427:THR:HG23	1.87	0.57
4:I:118:LYS:NZ	4:I:1087:GLY:O	2.31	0.57
2:E:32:ARG:O	2:E:36:GLU:HG3	2.04	0.57
1:A:1587:VAL:HG12	1:A:1910:VAL:HA	1.85	0.57
2:E:316:ALA:HB2	2:E:444:TRP:HZ3	1.67	0.57
4:K:214:ASN:HB3	4:L:1101:ARG:HD2	1.86	0.57
2:E:538:TRP:HE1	2:E:543:ARG:HA	1.69	0.57
4:L:101:ALA:HB3	4:M:174:GLY:HA3	1.87	0.57
4:I:633:ARG:NH1	4:I:867:ASP:OD2	2.36	0.57
4:L:1348:GLU:O	4:L:1355:VAL:N	2.34	0.57
4:L:1369:ASN:OD1	4:L:1370:SER:N	2.38	0.57
7:U:59:VAL:HG21	7:U:193:LEU:HD12	1.85	0.57
7:V:56:ARG:HD2	7:V:60:ARG:HD3	1.86	0.57
2:E:568:ASP:OD1	2:E:569:TYR:N	2.38	0.57
2:E:346:ARG:HH22	2:E:540:PRO:HB2	1.69	0.56
4:K:158:HIS:HB3	4:K:162:ARG:HH21	1.70	0.56
6:W:136:LYS:O	6:W:137:THR:HG23	2.05	0.56
4:H:652:ALA:O	4:H:656:LEU:HD12	2.04	0.56
4:I:265:SER:O	4:I:267:ALA:N	2.38	0.56
4:J:595:ARG:HA	4:J:598:LYS:HG2	1.87	0.56
4:J:970:ASP:HA	4:J:996:ALA:HB2	1.86	0.56
2:E:21:GLU:HB2	2:F:7:PHE:HB2	1.88	0.56
4:L:1327:THR:HG22	4:L:1333:MET:HE2	1.86	0.56
2:E:201:GLY:O	2:E:205:ASN:ND2	2.35	0.56
7:Y:226:ASP:HB2	7:Y:231:LEU:HD12	1.87	0.56
2:E:34:LEU:HD12	3:G:408:ARG:HD3	1.88	0.56
4:H:1068:GLU:HA	4:H:1073:THR:HG23	1.85	0.56
2:E:200:ARG:NH2	2:E:520:GLN:OE1	2.39	0.56
1:A:1452:LEU:HA	1:A:1455:GLU:HG2	1.88	0.56
3:G:132:LEU:HD11	3:G:149:LEU:HD13	1.88	0.56
4:I:623:ALA:O	4:I:627:ILE:HG12	2.05	0.56
4:J:625:LEU:HD13	4:J:628:ARG:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:635:ILE:HG22	4:J:670:LEU:HD13	1.87	0.56
4:I:1025:LYS:NZ	4:J:520:ASP:OD2	2.33	0.56
6:W:67:LEU:C	6:W:68:ILE:HD13	2.31	0.56
7:Y:149:ARG:HD3	7:Y:172:LEU:O	2.06	0.56
2:E:500:PHE:HA	2:E:503:ARG:NH1	2.21	0.56
4:H:632:ALA:HB2	4:H:661:LEU:HD11	1.88	0.56
4:H:880:PHE:HZ	5:N:68:VAL:HG23	1.71	0.56
4:K:588:PRO:HD2	4:K:683:LEU:HD11	1.87	0.56
4:L:438:GLN:HE22	4:L:1107:GLY:HA2	1.71	0.56
4:L:499:TYR:OH	4:L:974:PRO:O	2.18	0.56
4:I:633:ARG:NH1	4:I:865:ALA:O	2.39	0.55
1:A:1671:LEU:HD11	1:A:1694:LYS:HG2	1.88	0.55
4:H:1098:TYR:OH	4:H:1369:ASN:OD1	2.17	0.55
4:I:531:THR:OG1	4:I:539:PHE:O	2.23	0.55
4:L:806:THR:HA	4:L:809:VAL:HG12	1.89	0.55
4:M:533:LEU:HG	4:M:1238:CYS:HA	1.88	0.55
1:A:1778:HIS:HB3	2:E:609:HIS:CE1	2.41	0.55
4:I:798:CYS:SG	4:I:799:GLY:N	2.79	0.55
4:J:1039:THR:HG23	4:J:1261:PRO:HB3	1.89	0.55
2:E:530:VAL:HG13	2:E:593:HIS:HE1	1.69	0.55
4:H:265:SER:O	4:H:267:ALA:N	2.39	0.55
4:I:1003:HIS:O	4:I:1007:THR:HG23	2.07	0.55
4:K:169:ASP:OD2	4:K:173:ARG:NH1	2.39	0.55
4:K:800:LEU:HD23	4:K:923:VAL:HG21	1.89	0.55
2:E:365:HIS:HE2	2:E:434:LEU:HB3	1.72	0.55
3:G:115:THR:HB	3:G:312:SER:HB3	1.88	0.55
4:I:535:PRO:HD3	4:I:1232:TRP:CG	2.41	0.55
4:M:1069:ARG:HH22	4:M:1074:THR:HB	1.71	0.55
7:U:142:LEU:O	7:U:146:ILE:HG12	2.06	0.55
7:U:158:LEU:HB2	7:V:221:LYS:HE3	1.89	0.55
1:A:1607:VAL:HG13	1:A:1608:THR:HG23	1.89	0.55
1:A:1851:THR:HG22	1:A:1877:VAL:HG12	1.89	0.55
4:H:448:THR:HG23	4:H:1113:LEU:HD22	1.88	0.55
4:K:1150:MET:HE1	7:U:64:LEU:HB3	1.89	0.55
5:O:62:LEU:O	5:O:66:ARG:HG2	2.07	0.55
4:I:426:THR:HG22	4:I:1029:HIS:HD2	1.72	0.55
4:K:1041:THR:HG23	4:K:1103:ARG:HB3	1.89	0.55
4:K:1119:MET:HE2	4:K:1143:LEU:HB2	1.88	0.55
4:K:1332:LEU:HA	4:K:1335:THR:HG22	1.89	0.55
4:L:666:LEU:HD12	4:L:667:PRO:HD2	1.88	0.55
4:L:726:ASN:HB2	4:L:728:GLU:OE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:1124:HIS:HB3	4:K:1127:VAL:HG12	1.88	0.55
4:M:538:ASP:OD1	4:M:555:ARG:NE	2.38	0.55
4:J:588:PRO:HD2	4:J:683:LEU:HD11	1.90	0.54
4:K:638:MET:HG2	4:K:646:VAL:HG11	1.88	0.54
4:M:726:ASN:ND2	4:M:775:ASP:OD1	2.39	0.54
8:Z:260:ASN:OD1	8:Z:261:GLY:N	2.40	0.54
1:A:1867:LYS:NZ	1:A:1874:TYR:O	2.40	0.54
2:E:365:HIS:CE1	2:E:367:LEU:HB2	2.43	0.54
3:G:30:GLU:HG2	3:G:325:ARG:HB3	1.88	0.54
4:K:601:VAL:HG13	4:K:924:VAL:HG11	1.88	0.54
5:Q:62:LEU:O	5:Q:66:ARG:HG2	2.07	0.54
6:W:86:LEU:HD12	6:W:89:ILE:HD12	1.90	0.54
8:Z:119:ARG:H	8:Z:119:ARG:HD2	1.72	0.54
4:H:615:VAL:HG11	4:H:802:LEU:HD12	1.88	0.54
4:K:284:MET:HE1	4:K:369:MET:SD	2.48	0.54
4:L:1336:LYS:NZ	4:L:1346:THR:OG1	2.40	0.54
4:M:627:ILE:HG22	4:M:631:VAL:HG23	1.89	0.54
7:X:144:LEU:HD21	7:X:283:ARG:HE	1.71	0.54
7:V:66:ARG:NH1	7:V:283:ARG:O	2.35	0.54
1:A:1834:PRO:HG2	1:A:1838:THR:HG21	1.90	0.54
4:I:388:ASN:HB2	4:I:1311:ILE:HG12	1.89	0.54
4:I:1124:HIS:ND1	4:I:1127:VAL:HG23	2.23	0.54
4:L:440:ILE:HD12	4:L:1108:VAL:HB	1.89	0.54
2:E:259:ASN:OD1	2:E:260:ALA:N	2.41	0.54
2:E:337:TYR:CE2	2:E:431:ARG:HG3	2.39	0.54
2:E:428:GLN:CD	2:E:428:GLN:H	2.15	0.54
4:I:164:LEU:HD21	6:W:20:LEU:HD22	1.90	0.54
4:I:1211:THR:HA	4:I:1214:ILE:HG22	1.88	0.54
4:J:624:PHE:HA	4:J:627:ILE:HG22	1.87	0.54
4:M:263:THR:HB	4:M:296:VAL:HG12	1.90	0.54
7:U:140:MET:HG3	7:U:144:LEU:HD23	1.88	0.54
1:A:1856:GLN:H	1:A:2181:ASP:HB3	1.73	0.54
1:A:2037:ILE:N	1:A:2038:PRO:HD3	2.22	0.54
3:G:355:ASP:OD1	3:G:356:ALA:N	2.40	0.54
4:I:575:THR:HA	4:I:578:ILE:HD12	1.89	0.54
4:J:1331:ALA:O	4:J:1335:THR:HG23	2.06	0.54
1:A:1527:ARG:NH1	1:A:1531:LEU:HD12	2.23	0.54
3:G:311:VAL:HG23	3:G:330:TRP:O	2.08	0.54
4:H:276:THR:HG21	4:H:386:GLU:HG2	1.90	0.54
4:J:1144:ASP:OD1	4:J:1144:ASP:N	2.37	0.54
4:M:545:ASN:O	4:M:545:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:631:VAL:HG13	4:J:647:PHE:CE2	2.43	0.54
5:R:19:ARG:HA	5:R:22:VAL:HG22	1.88	0.54
7:U:228:SER:O	7:U:232:VAL:N	2.36	0.54
1:A:1783:HIS:HA	1:A:1786:VAL:HG12	1.90	0.54
1:A:1786:VAL:HG11	1:A:2066:LEU:HD11	1.89	0.54
1:A:2051:ARG:HD2	1:A:2052:VAL:N	2.23	0.54
2:E:270:TYR:CZ	2:E:273:VAL:HB	2.43	0.54
4:L:1109:ARG:O	4:L:1171:ALA:HA	2.08	0.54
4:M:565:LEU:HG	4:M:1178:PRO:HB3	1.89	0.54
2:E:287:TYR:HB2	2:E:371:PHE:CE2	2.42	0.53
4:K:712:ASP:O	4:K:782:LYS:NZ	2.40	0.53
7:X:223:ALA:HA	7:X:231:LEU:HD21	1.90	0.53
8:Z:140:VAL:HG13	8:Z:142:GLU:H	1.73	0.53
1:A:1486:PHE:HE2	1:A:1519:THR:HG22	1.73	0.53
4:J:133:ALA:HB3	4:J:1071:ILE:HD12	1.90	0.53
5:S:17:LYS:O	5:S:21:VAL:HG23	2.07	0.53
1:A:1689:THR:HG23	1:A:2112:LEU:HD22	1.89	0.53
4:K:451:HIS:HB3	4:K:1113:LEU:HD23	1.91	0.53
4:K:940:HIS:O	4:K:944:SER:OG	2.23	0.53
1:A:1653:VAL:HG21	1:A:1962:VAL:HG11	1.90	0.53
1:A:1969:LYS:O	1:A:1969:LYS:HD3	2.09	0.53
1:A:2211:LEU:HD21	2:F:90:LEU:HD12	1.91	0.53
2:E:428:GLN:O	2:E:430:LEU:N	2.41	0.53
4:H:215:ILE:HG21	4:H:1278:LEU:HD11	1.90	0.53
4:K:698:LEU:HD21	4:K:1127:VAL:HG23	1.90	0.53
4:K:1348:GLU:H	4:K:1355:VAL:HG13	1.74	0.53
4:L:201:THR:HG23	4:L:202:LEU:HD22	1.91	0.53
4:M:689:ALA:HB2	4:M:711:HIS:CE1	2.43	0.53
5:O:19:ARG:O	5:O:23:ASN:ND2	2.42	0.53
1:A:1548:ARG:NH2	1:A:1550:GLU:HB3	2.23	0.53
4:H:811:LEU:HD22	4:H:857:LEU:HD13	1.89	0.53
4:I:661:LEU:HB3	4:I:666:LEU:HD12	1.91	0.53
4:J:203:ALA:HB2	4:J:211:GLN:HE22	1.73	0.53
4:L:517:VAL:HG13	4:L:519:THR:H	1.74	0.53
3:G:566:LEU:HD13	7:U:157:SER:HB3	1.91	0.53
4:K:1362:LEU:O	4:K:1366:MET:HG3	2.08	0.53
6:T:76:SER:HB2	6:T:77:PRO:HD3	1.91	0.53
6:T:231:VAL:O	6:T:235:ILE:HG22	2.09	0.53
6:W:80:LEU:HD12	6:W:117:TRP:HZ3	1.74	0.53
7:Y:62:ARG:O	7:Y:66:ARG:HG2	2.08	0.53
1:A:1982:THR:HG22	1:A:1984:ARG:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:284:LEU:HD13	2:E:315:LEU:HD22	1.90	0.53
4:H:567:PRO:HB2	4:H:569:PRO:HD2	1.90	0.53
4:I:255:LEU:HD13	4:I:1086:MET:HE1	1.90	0.53
4:J:148:LEU:HA	4:J:151:ILE:HD12	1.90	0.53
4:K:80:PHE:CZ	4:K:82:ASP:HB2	2.44	0.53
6:W:179:ARG:HB3	6:W:183:GLN:HE22	1.74	0.53
4:I:677:LEU:O	4:I:680:VAL:HG12	2.08	0.53
4:J:138:TYR:O	4:J:153:ASN:ND2	2.35	0.53
5:Q:25:VAL:HA	5:Q:57:LYS:HE2	1.89	0.53
4:I:1147:THR:O	4:I:1151:LEU:HG	2.09	0.53
4:L:624:PHE:HB2	4:L:656:LEU:HD23	1.91	0.53
4:L:1246:THR:HA	4:L:1249:ARG:HB3	1.90	0.53
5:Q:18:HIS:O	5:Q:22:VAL:HG23	2.08	0.53
6:W:166:MET:HE3	6:W:264:LEU:HD21	1.91	0.53
4:J:794:ASN:OD1	4:J:1000:ASN:ND2	2.35	0.52
2:E:403:VAL:HG22	2:E:407:TRP:CD1	2.44	0.52
4:I:672:PHE:CZ	4:J:643:GLN:HB2	2.44	0.52
4:L:1070:ASP:OD2	6:W:155:TYR:OH	2.17	0.52
4:H:508:THR:HG23	4:H:511:GLU:H	1.75	0.52
8:Z:129:LEU:HD21	8:Z:207:GLY:HA3	1.91	0.52
4:I:981:HIS:O	4:I:985:ASN:ND2	2.41	0.52
7:U:32:VAL:HG23	7:U:71:THR:HG23	1.91	0.52
2:E:270:TYR:HE2	2:E:274:LEU:H	1.57	0.52
4:M:592:GLU:O	4:M:595:ARG:HG2	2.09	0.52
3:G:41:ARG:HH21	3:G:567:ALA:HB3	1.73	0.52
4:M:1039:THR:HG23	4:M:1261:PRO:HB3	1.91	0.52
6:T:251:LEU:HA	6:T:282:GLU:O	2.10	0.52
1:A:1987:ASP:OD1	1:A:1988:PHE:N	2.43	0.52
1:C:2220:ASP:OD2	2:F:79:LEU:HD13	2.10	0.52
2:E:343:PRO:HG3	2:E:543:ARG:HD2	1.91	0.52
5:N:37:HIS:ND1	5:N:40:LEU:HB2	2.24	0.52
5:S:33:SER:OG	5:S:34:GLU:N	2.42	0.52
1:A:1602:GLU:HB3	1:A:1607:VAL:HB	1.91	0.52
1:A:1857:ASP:H	1:A:2181:ASP:HB2	1.74	0.52
2:E:280:ALA:HB2	2:E:436:CYS:SG	2.50	0.52
3:G:26:VAL:HG23	3:G:327:ARG:HB2	1.91	0.52
4:I:1034:LEU:HD21	4:I:1174:LEU:HD22	1.92	0.52
4:J:1327:THR:HG22	4:J:1355:VAL:HG13	1.92	0.52
4:L:446:LEU:HD13	4:L:1021:VAL:HG23	1.92	0.52
2:E:580:ASP:OD1	2:E:581:LEU:N	2.42	0.52
4:I:1164:THR:H	4:J:1201:ALA:HB1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:1069:ARG:HH22	4:L:1074:THR:HG22	1.75	0.52
7:Y:296:ASP:O	7:Y:298:LYS:N	2.43	0.52
1:A:1570:ASP:OD2	1:A:1574:ARG:NH1	2.42	0.52
1:A:1699:LEU:HD21	1:A:1766:VAL:HG13	1.92	0.52
2:E:530:VAL:HG13	2:E:593:HIS:CE1	2.44	0.52
4:H:9:LEU:HD13	4:L:155:GLU:HG3	1.91	0.52
4:K:1297:THR:HG21	4:K:1301:TYR:HD2	1.75	0.52
6:W:288:GLU:OE2	7:X:276:ARG:NH2	2.36	0.52
7:Y:91:LEU:HA	7:Y:303:ILE:HA	1.92	0.52
1:A:2099:PRO:HB3	2:E:605:THR:HG22	1.91	0.51
4:H:810:ASP:O	4:H:814:ARG:NH1	2.43	0.51
4:K:223:MET:O	4:K:227:LEU:HG	2.09	0.51
4:K:1114:PHE:CD1	4:K:1137:VAL:HG11	2.44	0.51
7:Y:43:HIS:HA	7:Y:46:LEU:HD23	1.92	0.51
1:A:1767:GLN:NE2	1:A:2080:GLN:OE1	2.35	0.51
4:L:710:LEU:HD21	4:L:783:VAL:HG22	1.90	0.51
6:W:155:TYR:CG	6:W:159:LYS:HG2	2.44	0.51
3:G:362:ALA:O	3:G:366:VAL:HG12	2.10	0.51
4:H:7:LEU:HD13	4:K:92:LEU:HG	1.92	0.51
4:H:414:VAL:HG12	4:I:409:THR:HG22	1.93	0.51
4:J:295:THR:HA	4:J:356:SER:HA	1.93	0.51
4:J:1124:HIS:CD2	4:J:1126:GLU:HB3	2.45	0.51
4:J:1128:ASP:O	4:J:1132:ARG:HG2	2.11	0.51
4:L:75:ALA:HB2	4:L:179:PHE:CE2	2.45	0.51
4:L:78:ILE:HB	4:L:1058:ILE:HG22	1.91	0.51
4:L:363:GLY:O	4:L:364:GLU:HG2	2.11	0.51
5:R:21:VAL:HA	5:R:25:VAL:HG22	1.93	0.51
7:V:27:LEU:HD23	7:V:27:LEU:H	1.75	0.51
3:G:86:ARG:NH1	3:G:563:GLU:OE1	2.33	0.51
4:L:1363:GLN:HA	4:L:1366:MET:HE2	1.92	0.51
1:A:1915:ARG:NH1	1:A:1916:VAL:O	2.44	0.51
2:E:635:PHE:HD2	2:E:637:PRO:HD3	1.76	0.51
4:I:1065:THR:N	4:I:1076:HIS:O	2.37	0.51
4:J:138:TYR:CZ	4:J:152:LEU:HD13	2.45	0.51
7:V:177:PHE:CD2	7:V:178:ARG:HG2	2.46	0.51
1:A:1480:ARG:O	1:A:1484:THR:HG23	2.10	0.51
3:G:18:ASP:OD1	3:G:19:GLU:N	2.44	0.51
4:H:1327:THR:HG21	4:H:1333:MET:HB2	1.91	0.51
1:A:1888:PHE:HA	1:A:1891:GLN:NE2	2.26	0.51
2:E:594:TYR:CZ	2:E:598:LEU:HD11	2.45	0.51
4:H:1362:LEU:HG	4:H:1366:MET:SD	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:638:MET:HG3	4:I:646:VAL:HG11	1.93	0.51
4:J:985:ASN:O	4:J:988:ARG:NH1	2.44	0.51
4:L:475:MET:O	4:L:479:LEU:HG	2.10	0.51
4:L:1349:THR:HA	4:L:1354:TYR:HA	1.93	0.51
4:I:954:ASP:N	4:I:954:ASP:OD1	2.44	0.51
4:K:451:HIS:CE1	4:K:1117:PHE:HB2	2.45	0.51
4:M:534:HIS:HD2	4:M:536:PHE:H	1.58	0.51
4:M:861:VAL:HG21	4:M:876:CYS:SG	2.51	0.51
5:Q:42:THR:O	5:Q:45:SER:OG	2.21	0.51
7:U:63:GLY:HA2	7:U:66:ARG:HE	1.75	0.51
3:G:411:LEU:O	3:G:415:MET:HG2	2.11	0.51
4:J:775:ASP:O	4:J:779:THR:HG23	2.11	0.51
4:L:805:LYS:HE2	5:R:58:CYS:HB2	1.93	0.51
6:W:53:PRO:HG2	6:W:56:LEU:HD12	1.92	0.51
1:A:1645:ARG:HA	1:A:2163:PHE:HE1	1.76	0.51
4:I:735:ASP:OD1	4:I:736:ARG:N	2.38	0.51
4:K:747:ARG:NH1	4:K:888:GLU:OE2	2.32	0.51
7:X:11:THR:HG22	7:X:80:GLN:HG2	1.93	0.51
4:I:291:ILE:HG12	4:I:360:ILE:HG22	1.91	0.50
4:I:862:GLU:O	4:I:866:THR:OG1	2.23	0.50
4:J:798:CYS:SG	4:J:799:GLY:N	2.84	0.50
4:M:690:LEU:HD12	4:M:707:VAL:HG21	1.92	0.50
1:A:1663:TRP:CE2	1:A:1744:GLN:HB3	2.46	0.50
2:E:337:TYR:CG	2:E:365:HIS:HD2	2.30	0.50
2:E:350:PRO:HG2	2:E:354:GLY:HA2	1.93	0.50
4:K:1363:GLN:HA	4:K:1366:MET:HE2	1.94	0.50
4:L:400:TYR:HB2	4:L:1179:VAL:HG12	1.93	0.50
4:M:1350:HIS:CD2	4:M:1351:PHE:H	2.29	0.50
4:M:1332:LEU:O	4:M:1336:LYS:HG2	2.12	0.50
1:A:1855:PRO:HB3	1:A:2181:ASP:HA	1.93	0.50
4:I:1121:VAL:HG12	4:I:1132:ARG:HH21	1.76	0.50
4:J:488:MET:HG3	4:J:894:GLU:HB2	1.92	0.50
4:K:291:ILE:HA	4:K:360:ILE:HG22	1.93	0.50
4:L:404:ASP:OD1	4:L:405:ARG:N	2.44	0.50
4:L:1113:LEU:HA	4:L:1116:VAL:HG12	1.93	0.50
1:A:1853:VAL:HG12	1:A:1995:ARG:HB2	1.94	0.50
4:M:138:TYR:O	4:M:153:ASN:ND2	2.44	0.50
7:Y:213:GLU:OE1	7:Y:267:ARG:NH1	2.44	0.50
1:A:2149:ASP:OD1	1:A:2150:THR:N	2.45	0.50
4:I:1175:ILE:HG22	4:I:1244:TYR:CE2	2.47	0.50
1:C:2228:VAL:HG11	2:E:72:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:27:LEU:HB3	3:G:31:VAL:HG11	1.93	0.50
4:L:190:TYR:CD1	4:L:226:THR:HG21	2.47	0.50
4:L:518:VAL:HG22	4:L:1180:THR:HG21	1.93	0.50
4:M:1122:TYR:HB2	4:M:1128:ASP:HB2	1.94	0.50
5:N:39:VAL:HG11	5:N:71:SER:HB3	1.94	0.50
7:Y:53:ASP:OD2	7:Y:60:ARG:NH1	2.44	0.50
2:E:263:ASN:HA	2:E:266:VAL:CG2	2.40	0.50
4:I:785:TYR:O	4:I:943:TYR:OH	2.28	0.50
4:K:681:LEU:O	4:K:685:THR:HG23	2.11	0.50
6:T:136:LYS:O	6:T:137:THR:HG23	2.12	0.50
1:A:1572:LEU:HA	1:A:1575:LEU:HD12	1.93	0.49
1:A:1651:VAL:HG22	1:A:2109:ILE:HD11	1.92	0.49
4:I:450:CYS:O	4:I:1122:TYR:OH	2.25	0.49
4:L:440:ILE:HB	4:L:1108:VAL:HG21	1.94	0.49
4:M:1175:ILE:HG22	4:M:1244:TYR:CE2	2.47	0.49
1:A:1552:ILE:HA	1:A:2022:ARG:HH22	1.76	0.49
4:K:1290:LYS:HE2	4:K:1310:LEU:HB3	1.95	0.49
4:L:538:ASP:OD1	4:L:538:ASP:N	2.41	0.49
4:L:941:ARG:HG2	4:L:992:SER:HB3	1.94	0.49
4:M:517:VAL:HG22	4:M:518:VAL:H	1.77	0.49
4:M:857:LEU:O	4:M:861:VAL:HG22	2.11	0.49
1:A:1850:ALA:HB1	1:A:1949:LEU:HD22	1.94	0.49
1:A:1958:VAL:H	1:A:1981:TYR:HB3	1.76	0.49
2:E:337:TYR:HB2	2:E:365:HIS:HD2	1.77	0.49
2:E:502:VAL:O	2:E:506:ILE:HB	2.12	0.49
4:L:886:VAL:HG11	5:R:62:LEU:HD21	1.93	0.49
4:L:1175:ILE:HG22	4:L:1244:TYR:CE2	2.47	0.49
6:T:116:GLN:O	6:T:120:LEU:HB2	2.13	0.49
1:A:1943:THR:HB	1:A:2047:HIS:CE1	2.47	0.49
2:E:349:MET:HB3	2:E:428:GLN:HE21	1.76	0.49
4:J:61:LEU:HD12	4:J:61:LEU:H	1.76	0.49
4:J:1044:VAL:HG21	4:J:1096:VAL:HG13	1.94	0.49
4:L:126:THR:HG21	7:X:39:HIS:HD2	1.76	0.49
4:H:941:ARG:NH1	4:H:982:GLU:OE2	2.46	0.49
4:I:596:LEU:HD21	4:I:645:LEU:HB2	1.95	0.49
4:L:448:THR:HG23	4:L:1113:LEU:HD22	1.95	0.49
4:L:1122:TYR:HB2	4:L:1128:ASP:HB2	1.93	0.49
4:L:1285:TYR:HA	4:L:1289:ALA:HB3	1.93	0.49
4:M:495:ILE:HG22	4:M:496:PRO:HD3	1.93	0.49
4:M:534:HIS:CE1	4:M:1239:LEU:HD12	2.47	0.49
1:C:2214:LEU:HD23	2:E:87:GLU:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:682:ARG:HA	4:I:685:THR:HG22	1.95	0.49
4:K:77:ALA:HB1	4:K:302:TYR:CD2	2.48	0.49
4:L:400:TYR:OH	4:L:403:GLU:OE2	2.23	0.49
5:N:34:GLU:CD	5:N:34:GLU:H	2.21	0.49
8:Z:19:PHE:CE2	8:Z:37:ILE:HG13	2.48	0.49
1:A:1684:PRO:O	1:A:1687:THR:OG1	2.29	0.49
2:E:460:PHE:CE1	2:E:465:LEU:HD11	2.47	0.49
4:H:498:PHE:O	4:H:501:VAL:HG22	2.12	0.49
4:H:1291:ASP:OD1	4:H:1316:ARG:NH2	2.40	0.49
4:I:426:THR:HG22	4:I:1029:HIS:CD2	2.47	0.49
4:J:689:ALA:HB2	4:J:711:HIS:NE2	2.28	0.49
5:R:64:LEU:O	5:R:68:VAL:HG23	2.12	0.49
7:V:193:LEU:HD11	7:V:197:MET:HB3	1.95	0.49
1:A:1474:SER:O	1:A:1478:LYS:HG2	2.13	0.49
4:H:638:MET:SD	4:H:864:VAL:HG23	2.53	0.49
4:J:592:GLU:O	4:J:595:ARG:HG2	2.13	0.49
4:K:641:THR:HG23	4:K:642:ARG:HG3	1.94	0.49
5:S:47:TYR:OH	5:S:63:ASP:OD2	2.23	0.49
1:A:1839:PRO:HG3	1:A:1939:ILE:HG21	1.94	0.49
2:E:260:ALA:O	2:E:264:VAL:HG23	2.13	0.49
3:G:85:GLU:HG3	3:G:556:ARG:HG3	1.94	0.49
4:H:211:GLN:O	4:H:215:ILE:HG12	2.13	0.49
4:I:273:MET:N	4:I:368:ILE:O	2.40	0.49
4:J:1124:HIS:O	4:J:1127:VAL:HG12	2.13	0.49
4:L:750:GLY:HA2	5:R:70:VAL:HG11	1.94	0.49
7:X:149:ARG:HH21	7:X:172:LEU:HA	1.77	0.49
1:A:1613:VAL:HG21	1:A:2021:ILE:HD11	1.95	0.48
1:A:1693:LEU:O	1:A:1696:PHE:HB3	2.13	0.48
2:E:337:TYR:HB2	2:E:365:HIS:CD2	2.48	0.48
4:H:438:GLN:HE22	4:H:1107:GLY:HA2	1.78	0.48
4:H:941:ARG:HG2	4:H:992:SER:HB3	1.95	0.48
4:K:1359:ILE:HG23	4:K:1360:ILE:HG13	1.95	0.48
4:L:1034:LEU:HD12	4:L:1174:LEU:HD13	1.95	0.48
4:L:1290:LYS:NZ	4:L:1312:GLU:OE2	2.40	0.48
1:A:1526:GLU:HB2	1:A:1530:GLN:NE2	2.28	0.48
1:A:1589:ASP:OD1	1:A:1593:MET:N	2.32	0.48
1:C:2235:MET:HE3	1:C:2235:MET:HB3	1.77	0.48
2:E:276:ASP:O	2:E:279:ALA:N	2.46	0.48
4:I:862:GLU:HA	4:I:872:LEU:HG	1.94	0.48
7:U:212:SER:O	7:U:215:THR:HG22	2.13	0.48
1:A:1526:GLU:HB2	1:A:1530:GLN:HE22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:428:GLN:C	2:E:430:LEU:N	2.70	0.48
4:L:262:THR:HG22	4:L:268:LYS:HD3	1.95	0.48
4:M:594:LEU:HD21	4:M:680:VAL:HG21	1.95	0.48
1:C:2215:ARG:HA	1:C:2215:ARG:HE	1.78	0.48
2:E:300:SER:O	2:E:303:THR:OG1	2.31	0.48
2:E:365:HIS:HB3	2:E:368:VAL:HG12	1.95	0.48
2:E:425:HIS:NE2	2:E:426:GLU:OE2	2.46	0.48
8:Z:189:ASP:OD1	8:Z:189:ASP:N	2.41	0.48
2:E:460:PHE:CE1	2:E:465:LEU:HD21	2.49	0.48
4:H:82:ASP:OD1	4:H:82:ASP:N	2.35	0.48
4:H:588:PRO:HD2	4:H:683:LEU:HD21	1.96	0.48
4:H:753:ASP:OD2	4:H:756:ARG:HD3	2.13	0.48
4:I:514:GLN:HE21	4:I:563:ASP:HB2	1.78	0.48
4:M:626:LEU:HD21	4:M:881:LEU:HB2	1.96	0.48
5:Q:63:ASP:OD1	5:Q:66:ARG:NH1	2.47	0.48
5:R:14:ARG:HH12	5:R:48:THR:HG21	1.78	0.48
6:W:59:PHE:CE2	6:W:105:VAL:HG11	2.48	0.48
2:E:219:GLY:HA3	2:E:619:PHE:HA	1.96	0.48
4:M:535:PRO:HG3	4:M:1232:TRP:CD2	2.49	0.48
1:A:2106:PRO:HA	1:A:2157:ALA:HA	1.95	0.48
1:C:2230:ASP:O	1:C:2233:GLN:HG3	2.13	0.48
2:E:428:GLN:O	2:E:429:TYR:C	2.55	0.48
4:H:627:ILE:HG22	4:H:631:VAL:HG23	1.95	0.48
4:K:585:ARG:O	4:K:587:PRO:HD3	2.13	0.48
4:L:77:ALA:HB1	4:L:302:TYR:CD1	2.47	0.48
1:A:1491:LYS:HE2	1:A:1491:LYS:HA	1.95	0.48
1:A:1790:HIS:CD2	1:A:2056:PRO:HG2	2.48	0.48
1:A:1934:LEU:O	1:A:1938:PHE:HB2	2.13	0.48
1:A:2019:ALA:O	1:A:2023:ARG:HG2	2.14	0.48
4:J:1116:VAL:HG13	4:J:1117:PHE:CD2	2.49	0.48
7:U:49:HIS:HA	7:U:52:VAL:HG12	1.94	0.48
1:A:1663:TRP:CD1	1:A:1744:GLN:HB3	2.48	0.48
4:H:1332:LEU:HD13	4:H:1355:VAL:HG13	1.96	0.48
4:I:271:GLY:C	4:I:367:VAL:HG23	2.38	0.48
4:I:355:LEU:HD12	4:I:356:SER:H	1.78	0.48
4:I:698:LEU:HD21	4:I:1127:VAL:HG22	1.96	0.48
4:I:730:VAL:HG13	4:I:895:VAL:HG13	1.96	0.48
4:I:1331:ALA:O	4:I:1335:THR:HG23	2.14	0.48
4:J:886:VAL:HG11	5:P:62:LEU:HD11	1.96	0.48
4:J:1109:ARG:HG2	4:J:1169:LYS:HE3	1.96	0.48
4:M:542:CYS:SG	4:M:543:GLN:N	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:455:GLN:HE21	4:I:1253:GLY:N	2.12	0.48
5:S:40:LEU:HD21	5:S:64:LEU:HD11	1.95	0.48
7:U:203:SER:O	7:U:207:VAL:HG13	2.14	0.48
4:H:77:ALA:HB1	4:H:302:TYR:HD2	1.79	0.47
7:X:206:MET:HB2	7:X:274:MET:HE2	1.95	0.47
2:E:249:ILE:HG23	2:E:253:LEU:HD23	1.96	0.47
4:I:558:ILE:HD11	4:I:1031:GLY:HA3	1.96	0.47
4:J:1211:THR:HA	4:J:1214:ILE:HG22	1.96	0.47
1:C:2224:LEU:HD11	2:F:79:LEU:HD22	1.97	0.47
2:E:28:GLU:O	2:E:32:ARG:HG2	2.15	0.47
3:G:41:ARG:HG2	3:G:154:PRO:HD3	1.95	0.47
4:M:1038:ARG:NH1	4:M:1040:ASP:OD2	2.46	0.47
8:Z:63:TYR:HE1	8:Z:221:GLU:HG2	1.79	0.47
2:E:525:LEU:HD13	2:E:598:LEU:HD21	1.95	0.47
4:I:1156:MET:HG3	4:I:1301:TYR:CZ	2.49	0.47
4:L:927:PRO:HD2	4:L:952:LEU:HD21	1.96	0.47
4:M:1:MET:HE3	4:M:4:TRP:HD1	1.79	0.47
8:Z:3:LEU:HD22	8:Z:57:MET:HE2	1.95	0.47
1:A:1510:GLN:O	1:A:1513:THR:OG1	2.31	0.47
1:A:1875:ALA:N	1:A:1879:GLU:OE1	2.40	0.47
2:E:355:ARG:HH11	2:E:355:ARG:C	2.22	0.47
4:I:1139:ARG:HD2	4:I:1140:PRO:HD2	1.97	0.47
4:J:194:GLN:NE2	4:J:245:ARG:HD2	2.29	0.47
4:M:652:ALA:O	4:M:656:LEU:HG	2.15	0.47
5:P:21:VAL:HG23	5:P:25:VAL:HB	1.97	0.47
4:H:1267:ASN:O	4:H:1271:ILE:HG12	2.13	0.47
4:I:284:MET:HA	4:I:291:ILE:CD1	2.44	0.47
4:I:726:ASN:ND2	4:I:728:GLU:OE1	2.47	0.47
4:K:451:HIS:CE1	4:K:453:VAL:HG23	2.50	0.47
4:K:905:GLN:O	4:K:1123:ARG:NH1	2.48	0.47
4:M:1331:ALA:O	4:M:1335:THR:HG23	2.15	0.47
7:U:33:PRO:HB2	7:U:68:MET:SD	2.54	0.47
3:G:53:ARG:HH11	3:G:553:ARG:HH12	1.62	0.47
4:I:71:LEU:N	4:I:370:GLU:OE2	2.47	0.47
4:J:655:THR:O	4:J:659:GLU:HG2	2.14	0.47
4:J:747:ARG:HG2	4:J:767:PHE:HB3	1.95	0.47
4:L:424:LEU:HD12	4:L:425:PRO:HD2	1.95	0.47
4:L:556:ILE:HG21	4:L:986:TRP:CE2	2.50	0.47
4:L:712:ASP:O	4:L:782:LYS:NZ	2.47	0.47
4:M:460:CYS:HB3	4:M:533:LEU:HD23	1.97	0.47
4:M:862:GLU:HG2	4:M:863:ASP:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:364:GLU:OE1	3:G:558:ARG:NH1	2.48	0.47
4:H:611:TYR:CD1	4:H:923:VAL:HG22	2.50	0.47
4:I:263:THR:HB	4:I:296:VAL:HG12	1.96	0.47
4:I:718:PRO:HG2	4:I:943:TYR:HE2	1.79	0.47
4:J:75:ALA:HB2	4:J:179:PHE:CE2	2.50	0.47
4:L:77:ALA:HB1	4:L:302:TYR:HD1	1.80	0.47
4:L:813:TYR:HA	5:R:65:LEU:HD21	1.97	0.47
6:T:185:VAL:HG12	6:T:206:THR:HG22	1.96	0.47
6:T:251:LEU:HD12	6:T:251:LEU:O	2.15	0.47
7:X:273:VAL:O	7:X:277:GLN:HG2	2.15	0.47
8:Z:248:ASN:O	8:Z:252:ASN:ND2	2.47	0.47
2:E:323:ILE:HD12	2:E:335:ASN:ND2	2.30	0.47
4:I:310:GLU:O	4:I:314:THR:HG23	2.15	0.47
4:I:1350:HIS:CG	4:I:1351:PHE:H	2.32	0.47
6:W:112:ARG:O	6:W:116:GLN:HG2	2.15	0.47
1:A:1645:ARG:HA	1:A:2163:PHE:CE1	2.50	0.47
1:A:1795:ASP:HB3	2:E:453:PHE:HB2	1.96	0.47
4:I:263:THR:OG1	4:I:264:SER:N	2.47	0.47
4:J:669:GLN:O	4:J:673:HIS:ND1	2.46	0.47
4:K:685:THR:HG22	4:K:783:VAL:HG21	1.97	0.47
4:L:1149:SER:O	4:L:1152:THR:OG1	2.26	0.47
4:M:790:PRO:HA	4:M:793:THR:HG22	1.96	0.47
1:A:1549:LEU:O	1:A:1552:ILE:HG12	2.14	0.46
1:A:1754:TYR:HE1	1:A:1800:GLN:O	1.97	0.46
2:E:460:PHE:CZ	2:E:465:LEU:HD11	2.50	0.46
2:E:635:PHE:CD2	2:E:637:PRO:HD3	2.50	0.46
1:A:1504:PRO:HD3	1:A:1517:ALA:O	2.15	0.46
4:I:92:LEU:HB3	4:L:7:LEU:HD22	1.96	0.46
4:J:715:LEU:HG	4:J:782:LYS:HD3	1.97	0.46
4:K:389:VAL:HG12	4:K:1044:VAL:HG11	1.95	0.46
5:Q:37:HIS:CD2	5:Q:40:LEU:HB2	2.50	0.46
4:K:287:LEU:O	4:K:291:ILE:HG23	2.15	0.46
4:L:451:HIS:ND1	4:L:453:VAL:HG12	2.30	0.46
4:L:1090:TYR:CZ	4:L:1282:ILE:HD11	2.50	0.46
6:T:230:PHE:HE1	7:U:206:MET:HE2	1.81	0.46
2:E:270:TYR:C	2:E:272:CYS:N	2.72	0.46
2:E:271:ASP:O	2:E:272:CYS:C	2.57	0.46
2:E:352:SER:HB2	2:E:356:HIS:ND1	2.31	0.46
4:H:452:PRO:HB3	4:H:905:GLN:HE22	1.80	0.46
4:H:473:PRO:HA	4:H:476:GLN:HG2	1.97	0.46
4:H:1234:SER:OG	4:H:1235:GLN:OE1	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1095:CYS:SG	4:I:1096:VAL:N	2.88	0.46
4:J:861:VAL:HG13	4:J:865:ALA:HB3	1.96	0.46
1:A:1979:LEU:HD11	1:A:1988:PHE:HZ	1.80	0.46
4:H:472:GLU:OE1	4:H:1218:ARG:NH1	2.48	0.46
4:H:639:PHE:CD2	4:H:670:LEU:HD21	2.51	0.46
4:H:686:ARG:NH2	4:I:997:THR:HA	2.30	0.46
4:H:1166:HIS:CD2	4:I:1223:GLN:HA	2.51	0.46
4:I:1238:CYS:O	4:I:1242:VAL:HG12	2.16	0.46
4:J:499:TYR:O	4:J:502:ARG:NH2	2.48	0.46
4:K:804:LEU:HD21	4:K:886:VAL:HG22	1.97	0.46
4:L:871:PRO:HD2	4:L:874:GLN:HE22	1.81	0.46
4:L:941:ARG:HD3	4:L:989:SER:HA	1.97	0.46
4:M:534:HIS:CD2	4:M:536:PHE:H	2.32	0.46
1:A:1585:LEU:HA	1:A:1913:MET:HA	1.98	0.46
2:E:350:PRO:HD2	2:E:428:GLN:HE21	1.80	0.46
2:E:606:LEU:HD12	2:E:606:LEU:O	2.14	0.46
4:H:597:PHE:CD2	4:H:792:MET:HG2	2.50	0.46
4:H:601:VAL:HG13	4:H:924:VAL:HG11	1.98	0.46
4:H:1039:THR:OG1	4:H:1261:PRO:HB3	2.16	0.46
4:I:770:ASP:OD1	4:I:770:ASP:N	2.48	0.46
4:I:917:LEU:HD21	4:I:937:VAL:HG21	1.98	0.46
4:K:1133:HIS:HD1	4:K:1133:HIS:C	2.24	0.46
4:L:810:ASP:O	4:L:814:ARG:NH1	2.48	0.46
4:M:156:ALA:O	4:M:160:VAL:HG23	2.15	0.46
4:M:1111:GLN:HB3	4:M:1171:ALA:HB1	1.98	0.46
1:A:1957:PRO:O	1:A:2038:PRO:HG2	2.15	0.46
2:E:326:TRP:HE1	2:E:332:ALA:HB1	1.81	0.46
2:E:524:GLY:HA3	2:E:631:LEU:HA	1.97	0.46
4:H:662:ALA:HB1	4:I:605:ASN:HD22	1.81	0.46
4:H:1067:GLU:HB3	4:H:1074:THR:HG23	1.97	0.46
4:H:1215:TYR:CE2	4:H:1268:THR:HG21	2.51	0.46
4:I:1222:ALA:C	4:I:1224:THR:H	2.24	0.46
5:R:49:ARG:HA	5:R:49:ARG:NE	2.30	0.46
7:U:60:ARG:O	7:U:64:LEU:HG	2.16	0.46
7:Y:270:ALA:O	7:Y:274:MET:HG2	2.16	0.46
2:E:442:LEU:HD21	2:E:601:LEU:HB2	1.98	0.46
4:H:174:GLY:HA3	4:I:101:ALA:HB3	1.97	0.46
4:I:968:ARG:NH2	4:I:970:ASP:OD2	2.49	0.46
4:J:420:VAL:HG22	4:J:577:GLU:HG2	1.98	0.46
4:J:446:LEU:HD13	4:J:1021:VAL:HG23	1.96	0.46
4:J:651:TYR:HB2	4:J:784:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:867:ASP:HB2	4:J:870:THR:HG22	1.98	0.46
4:J:1332:LEU:HD13	4:J:1355:VAL:HG23	1.98	0.46
4:K:1315:CYS:HA	4:K:1318:THR:HG22	1.98	0.46
6:W:245:THR:HG22	6:W:290:VAL:HG12	1.97	0.46
1:A:1813:ALA:O	1:A:1814:MET:HE2	2.16	0.46
4:J:787:CYS:HB3	4:J:1005:VAL:HG13	1.98	0.46
4:L:1211:THR:HA	4:L:1214:ILE:HG22	1.97	0.46
4:L:1350:HIS:N	4:L:1353:ASN:O	2.37	0.46
5:S:37:HIS:ND1	5:S:40:LEU:HD23	2.31	0.46
7:U:153:MET:SD	7:U:169:VAL:HG12	2.56	0.46
7:U:175:ILE:HD11	7:U:184:ILE:HD11	1.97	0.46
1:A:1663:TRP:HA	1:A:1666:ILE:HG22	1.97	0.46
1:A:1839:PRO:HG3	1:A:1939:ILE:HD13	1.97	0.46
1:A:2103:ASN:ND2	2:E:317:ASP:HA	2.31	0.46
4:I:1064:VAL:HG22	4:I:1077:VAL:HG12	1.98	0.46
1:A:1981:TYR:CZ	1:A:1988:PHE:HB3	2.51	0.45
1:A:2001:GLN:N	1:A:2001:GLN:OE1	2.47	0.45
1:C:2235:MET:HA	1:C:2239:TYR:HD1	1.81	0.45
1:C:2239:TYR:HB3	2:F:57:ARG:HH22	1.81	0.45
2:E:226:LYS:NZ	2:E:243:GLN:O	2.44	0.45
4:H:194:GLN:HA	4:H:197:VAL:HG12	1.98	0.45
4:I:522:TYR:HB3	4:I:1228:THR:O	2.16	0.45
4:J:420:VAL:HG11	4:J:577:GLU:HA	1.97	0.45
4:K:895:VAL:N	4:K:914:GLN:O	2.32	0.45
7:X:153:MET:HE2	7:X:169:VAL:HG22	1.98	0.45
1:A:1516:GLY:HA2	1:A:1519:THR:HG23	1.98	0.45
1:A:1643:THR:HG22	1:A:2186:VAL:HG11	1.98	0.45
4:K:473:PRO:HA	4:K:476:GLN:HG2	1.98	0.45
4:L:1114:PHE:CD2	4:L:1137:VAL:HG21	2.51	0.45
7:X:238:LEU:HG	7:X:239:MET:H	1.82	0.45
1:A:1799:GLU:HG3	1:A:2164:GLY:HA3	1.99	0.45
1:A:1913:MET:HE1	1:A:1915:ARG:HB2	1.99	0.45
1:C:2238:LEU:HD23	1:C:2239:TYR:CZ	2.51	0.45
2:E:318:ASP:HA	2:E:321:ARG:HG2	1.97	0.45
4:H:1239:LEU:O	4:H:1243:LEU:HD23	2.16	0.45
4:K:983:TYR:O	4:K:988:ARG:NH2	2.49	0.45
6:W:67:LEU:O	6:W:68:ILE:HD13	2.17	0.45
6:W:234:ARG:NH2	7:X:209:ASN:OD1	2.49	0.45
8:Z:48:ARG:O	8:Z:51:VAL:HG12	2.17	0.45
8:Z:67:ARG:HG2	8:Z:67:ARG:HH11	1.81	0.45
1:A:1456:TYR:CD1	1:A:1482:LEU:HD11	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:274:VAL:HG12	4:H:370:GLU:HB3	1.97	0.45
4:J:600:THR:HG23	4:J:644:LEU:HG	1.99	0.45
4:J:988:ARG:HB2	4:J:990:PRO:HD2	1.98	0.45
5:R:47:TYR:OH	5:R:63:ASP:OD2	2.29	0.45
6:T:244:CYS:HB3	7:U:273:VAL:HG11	1.97	0.45
7:X:152:ILE:HD12	7:Y:268:LEU:HD23	1.97	0.45
7:X:202:LEU:HD22	7:Y:230:LEU:HD13	1.97	0.45
1:A:2236:ARG:HH12	2:F:66:ARG:HB2	1.81	0.45
4:H:178:SER:O	4:H:182:THR:HG23	2.17	0.45
4:I:542:CYS:SG	4:I:543:GLN:N	2.89	0.45
4:J:315:ALA:HB2	4:J:321:ILE:HG22	1.98	0.45
4:K:178:SER:O	4:K:182:THR:HG23	2.16	0.45
4:M:1046:MET:SD	4:M:1096:VAL:HG22	2.57	0.45
5:R:63:ASP:HA	5:R:66:ARG:HG2	1.98	0.45
4:H:785:TYR:O	4:H:943:TYR:OH	2.33	0.45
4:I:649:HIS:HA	4:I:789:MET:HE1	1.99	0.45
4:I:662:ALA:HB1	4:J:605:ASN:HB3	1.98	0.45
4:M:575:THR:HG22	4:M:1010:ALA:HB3	1.98	0.45
4:M:1222:ALA:C	4:M:1224:THR:H	2.24	0.45
8:Z:80:PHE:CZ	8:Z:125:VAL:HG23	2.51	0.45
1:A:2019:ALA:HA	1:A:2022:ARG:CZ	2.47	0.45
4:H:93:PHE:HE2	4:H:118:LYS:HG3	1.82	0.45
4:H:189:PRO:HD3	4:H:1286:LEU:HD21	1.97	0.45
4:H:1044:VAL:HG11	4:H:1096:VAL:HG13	1.98	0.45
4:K:400:TYR:HB3	4:K:1179:VAL:HG12	1.97	0.45
4:K:409:THR:HG23	4:K:410:VAL:HG13	1.99	0.45
4:M:315:ALA:HB2	4:M:321:ILE:HD11	1.99	0.45
4:M:811:LEU:HD23	4:M:812:PHE:CE2	2.52	0.45
4:M:1029:HIS:ND1	4:M:1030:PRO:O	2.44	0.45
5:P:62:LEU:O	5:P:66:ARG:HG2	2.17	0.45
6:W:252:GLY:HA3	6:W:279:PHE:CE1	2.52	0.45
2:E:442:LEU:HB2	2:E:602:LEU:HD22	1.99	0.45
2:E:529:ALA:O	2:E:597:GLY:HA3	2.17	0.45
4:H:478:LEU:HD11	4:H:509:VAL:HG23	1.98	0.45
4:H:597:PHE:HA	4:H:600:THR:HG22	1.98	0.45
6:T:290:VAL:OXT	7:U:277:GLN:NE2	2.50	0.45
4:I:339:LEU:HB2	4:L:13:VAL:HG22	1.99	0.45
4:J:633:ARG:HD3	4:J:870:THR:HG21	1.98	0.45
4:J:1142:LEU:HD12	4:J:1143:LEU:O	2.17	0.45
4:M:127:ILE:HG22	4:M:171:MET:HE2	1.99	0.45
4:M:280:MET:O	4:M:284:MET:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:214:LEU:HB3	7:V:218:TYR:CE2	2.52	0.45
7:Y:113:PRO:HG3	7:Y:135:PRO:HA	1.99	0.45
2:E:257:VAL:HG22	2:E:570:MET:HE1	1.98	0.45
2:E:533:SER:HB3	2:E:597:GLY:CA	2.46	0.45
4:J:684:VAL:HG21	4:J:1005:VAL:HG12	1.99	0.45
4:J:706:TYR:CE1	4:J:900:ASP:HB2	2.52	0.45
4:J:874:GLN:HA	4:J:877:ARG:HB2	1.99	0.45
4:L:241:LYS:O	4:L:244:THR:HG22	2.16	0.45
5:S:63:ASP:HA	5:S:66:ARG:HD2	1.99	0.45
7:U:34:ILE:O	7:U:69:THR:HG22	2.17	0.45
1:A:1456:TYR:CE1	1:A:1482:LEU:HD11	2.52	0.44
1:A:1526:GLU:O	1:A:1529:VAL:HG12	2.17	0.44
2:E:31:LEU:HD22	2:E:32:ARG:NH2	2.32	0.44
2:E:217:SER:N	2:E:638:SER:O	2.48	0.44
3:G:115:THR:HG22	3:G:115:THR:O	2.17	0.44
4:J:895:VAL:HB	4:J:914:GLN:HB2	1.99	0.44
4:K:1155:SER:OG	4:K:1255:ASN:ND2	2.49	0.44
4:M:1121:VAL:HG12	4:M:1132:ARG:HH21	1.81	0.44
5:S:22:VAL:HA	5:S:26:LEU:HD12	1.99	0.44
6:T:84:LEU:O	6:T:171:MET:HE1	2.18	0.44
6:W:250:LYS:O	6:W:284:GLY:N	2.48	0.44
4:I:92:LEU:HB3	4:L:7:LEU:HD13	1.99	0.44
4:K:426:THR:HG23	4:K:427:THR:HG23	2.00	0.44
4:K:1177:THR:OG1	4:K:1181:MET:SD	2.70	0.44
4:M:388:ASN:HB2	4:M:1311:ILE:HD12	1.98	0.44
4:M:424:LEU:HD12	4:M:425:PRO:HD2	1.99	0.44
4:M:1034:LEU:HD13	4:M:1174:LEU:HD22	1.99	0.44
5:Q:31:GLU:HG2	5:Q:32:ILE:HD12	1.99	0.44
6:T:134:CYS:O	6:T:149:VAL:HG22	2.18	0.44
6:T:252:GLY:HA3	6:T:279:PHE:CE2	2.53	0.44
8:Z:17:VAL:O	8:Z:21:ARG:HG3	2.17	0.44
8:Z:90:ARG:HH11	8:Z:90:ARG:HG2	1.81	0.44
4:H:459:PRO:HA	4:H:462:GLN:HG2	1.99	0.44
4:I:127:ILE:HD13	4:I:170:ALA:HB1	1.99	0.44
4:I:1349:THR:HA	4:I:1354:TYR:HA	1.98	0.44
4:I:1365:SER:O	4:I:1369:ASN:OD1	2.35	0.44
4:M:228:PHE:O	4:M:232:ARG:HG3	2.18	0.44
4:M:1113:LEU:HA	4:M:1116:VAL:HG12	1.99	0.44
7:U:63:GLY:HA2	7:U:66:ARG:NE	2.32	0.44
8:Z:74:SER:HA	8:Z:77:LEU:HB3	2.00	0.44
4:H:93:PHE:CE2	4:H:118:LYS:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:774:THR:OG1	4:H:777:GLU:OE1	2.31	0.44
4:J:601:VAL:HG13	4:J:924:VAL:HG11	2.00	0.44
4:L:73:ALA:HA	4:L:261:TYR:CZ	2.52	0.44
4:M:451:HIS:CE1	4:M:453:VAL:HG23	2.52	0.44
4:M:970:ASP:O	4:M:993:ARG:NH1	2.50	0.44
7:V:295:PRO:C	7:V:297:ASN:H	2.25	0.44
6:W:76:SER:OG	6:W:77:PRO:HD3	2.17	0.44
1:A:1657:GLN:OE1	1:A:2045:GLN:NE2	2.40	0.44
1:A:1756:GLU:HG2	1:A:2104:ARG:H	1.83	0.44
2:E:53:MET:HA	2:E:56:VAL:HG12	2.00	0.44
2:E:622:ASN:HB2	2:E:626:GLU:OE1	2.18	0.44
4:H:891:LYS:HB3	4:H:891:LYS:HE2	1.78	0.44
4:I:73:ALA:HA	4:I:261:TYR:CE2	2.52	0.44
4:I:96:GLN:HB3	4:I:113:THR:HG22	1.99	0.44
4:I:1254:TYR:CZ	4:I:1256:SER:HA	2.52	0.44
4:L:300:ALA:HB2	4:L:353:THR:HG23	2.00	0.44
4:L:805:LYS:HB2	4:L:889:HIS:NE2	2.31	0.44
4:M:898:PRO:HB2	4:M:904:ARG:NH2	2.32	0.44
7:V:157:SER:OG	7:V:188:VAL:HG11	2.18	0.44
7:V:218:TYR:OH	7:V:264:GLU:OE2	2.32	0.44
2:E:336:TYR:O	2:E:365:HIS:HA	2.17	0.44
4:H:188:PRO:HD2	4:H:1092:SER:O	2.17	0.44
4:H:430:LEU:O	4:H:438:GLN:N	2.51	0.44
4:K:752:SER:O	5:Q:66:ARG:NH1	2.51	0.44
4:L:631:VAL:O	4:L:635:ILE:HG12	2.17	0.44
4:M:763:ASP:OD1	4:M:763:ASP:N	2.50	0.44
4:M:1332:LEU:HD13	4:M:1355:VAL:HG23	1.99	0.44
7:X:75:ARG:HH12	7:X:77:GLU:CD	2.26	0.44
7:Y:124:LEU:HD23	7:Y:124:LEU:H	1.83	0.44
1:A:1753:LEU:HD21	1:A:1785:VAL:HG11	2.00	0.44
2:E:322:GLU:OE1	2:E:366:VAL:HG22	2.18	0.44
2:E:623:ASP:OD1	2:E:624:ILE:N	2.50	0.44
3:G:391:ALA:HB3	3:G:503:ILE:HD11	2.00	0.44
4:I:433:ARG:HB2	4:I:1102:VAL:HG21	2.00	0.44
4:I:611:TYR:CZ	4:I:923:VAL:HG23	2.53	0.44
4:I:927:PRO:HB2	4:I:930:LEU:HB3	1.99	0.44
4:I:1121:VAL:HG12	4:I:1132:ARG:NH2	2.33	0.44
4:I:1231:PRO:O	4:I:1235:GLN:HG2	2.18	0.44
4:K:682:ARG:NH2	4:K:776:ASP:OD2	2.44	0.44
4:K:880:PHE:O	4:K:883:VAL:HG12	2.17	0.44
4:L:71:LEU:HD13	4:L:372:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:862:GLU:O	4:M:864:VAL:N	2.50	0.44
5:N:18:HIS:CE1	5:N:44:LEU:HB3	2.53	0.44
5:S:33:SER:OG	5:S:34:GLU:OE1	2.35	0.44
6:W:167:ILE:O	6:W:274:VAL:N	2.37	0.44
6:W:227:ARG:O	6:W:231:VAL:HG23	2.17	0.44
4:I:801:GLY:HA3	4:I:890:VAL:HB	2.00	0.44
4:K:108:THR:O	4:K:110:ARG:NH1	2.51	0.44
4:K:651:TYR:HB2	4:K:784:PHE:CD1	2.52	0.44
7:X:145:GLU:OE1	7:X:175:ILE:HG23	2.18	0.44
7:Y:270:ALA:HA	7:Y:273:VAL:HG12	2.00	0.44
1:A:1486:PHE:CZ	1:A:1515:LEU:HG	2.53	0.44
1:C:2203:LEU:HD23	1:C:2203:LEU:HA	1.81	0.44
2:E:566:VAL:HG12	2:E:570:MET:HE3	1.99	0.44
4:H:216:LEU:O	4:H:220:LYS:HG3	2.18	0.44
4:H:628:ARG:HG3	4:H:661:LEU:HD13	2.00	0.44
4:H:664:GLY:O	4:H:666:LEU:N	2.50	0.44
4:H:1282:ILE:O	4:H:1286:LEU:HG	2.18	0.44
4:I:309:PRO:O	4:I:313:VAL:HG23	2.18	0.44
4:I:456:GLU:OE2	4:I:905:GLN:NE2	2.51	0.44
4:I:459:PRO:HB2	4:I:1242:VAL:HG21	2.00	0.44
4:L:427:THR:HG22	4:L:441:ASP:HB3	1.99	0.44
4:L:574:ARG:O	4:L:577:GLU:HG2	2.18	0.44
7:U:31:VAL:HG21	7:U:137:ILE:HG13	2.00	0.44
7:U:193:LEU:HD22	7:U:197:MET:HE2	1.98	0.44
7:V:273:VAL:HA	7:V:276:ARG:HD3	1.98	0.44
1:A:1698:TYR:HD1	1:A:1699:LEU:HD12	1.82	0.43
2:E:330:VAL:HG11	2:E:364:ARG:HG2	2.00	0.43
2:E:531:THR:O	2:E:535:ARG:HG2	2.18	0.43
3:G:46:ARG:NH2	3:G:557:ASP:OD1	2.49	0.43
3:G:388:GLN:HA	3:G:539:PHE:HA	2.00	0.43
4:H:631:VAL:O	4:H:635:ILE:HG22	2.18	0.43
4:H:651:TYR:HB2	4:H:784:PHE:CD1	2.53	0.43
4:I:9:LEU:HD13	4:J:316:ILE:HD11	1.99	0.43
4:I:80:PHE:N	4:I:1059:ILE:O	2.43	0.43
4:I:419:THR:HG22	4:I:421:ARG:H	1.82	0.43
4:K:1043:GLU:OE1	4:K:1101:ARG:HD2	2.18	0.43
5:Q:43:MET:HB3	5:Q:47:TYR:CZ	2.52	0.43
7:X:8:ILE:HB	7:X:83:LEU:HB2	2.00	0.43
8:Z:63:TYR:HB2	8:Z:224:CYS:SG	2.58	0.43
1:A:1548:ARG:HG3	1:A:1551:ASP:OD2	2.18	0.43
3:G:453:LYS:HB3	3:G:455:GLN:OE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:600:THR:HG21	4:I:645:LEU:O	2.18	0.43
4:I:807:LEU:HD23	4:I:808:LEU:HD22	1.99	0.43
8:Z:239:LEU:HD21	8:Z:250:CYS:HB3	1.99	0.43
4:H:192:VAL:O	4:H:196:LEU:HG	2.18	0.43
4:H:1166:HIS:NE2	4:I:1223:GLN:HA	2.33	0.43
4:J:900:ASP:OD1	4:J:1014:LYS:NZ	2.37	0.43
4:M:1066:LYS:NZ	4:M:1068:GLU:OE2	2.34	0.43
4:M:1297:THR:HG21	4:M:1301:TYR:CD2	2.51	0.43
6:T:252:GLY:HA3	6:T:279:PHE:HE2	1.83	0.43
8:Z:188:LEU:HD22	8:Z:202:LYS:HG3	2.00	0.43
1:A:2065:ARG:HD3	1:A:2065:ARG:HA	1.88	0.43
1:C:2235:MET:HA	1:C:2239:TYR:CD1	2.53	0.43
4:H:173:ARG:NH1	4:H:375:VAL:O	2.48	0.43
4:H:449:LEU:HD21	4:H:1034:LEU:HD21	1.99	0.43
4:I:528:THR:O	4:I:531:THR:HG22	2.17	0.43
4:I:1109:ARG:CZ	4:I:1169:LYS:HG3	2.48	0.43
4:M:1327:THR:HG22	4:M:1355:VAL:HG13	2.01	0.43
7:U:194:LEU:HA	7:U:197:MET:HE3	2.00	0.43
6:W:164:ALA:HB2	6:W:277:ASP:HA	1.98	0.43
1:A:1765:PRO:HB3	1:A:2118:PRO:O	2.19	0.43
2:E:350:PRO:HD2	2:E:428:GLN:CG	2.48	0.43
4:H:399:LEU:HD23	4:H:1183:VAL:HG22	2.01	0.43
4:J:461:LEU:O	4:J:465:THR:HG23	2.18	0.43
4:L:472:GLU:HB2	4:L:475:MET:HG2	2.01	0.43
4:L:595:ARG:O	4:L:599:THR:HG23	2.18	0.43
4:M:701:GLU:OE1	4:M:714:ARG:NH2	2.42	0.43
4:M:1235:GLN:N	4:M:1235:GLN:OE1	2.51	0.43
7:X:32:VAL:O	7:X:71:THR:OG1	2.34	0.43
1:A:1503:LEU:HD13	1:A:1590:VAL:HB	1.99	0.43
1:A:1609:ASP:O	1:A:1832:VAL:HG11	2.19	0.43
4:I:192:VAL:O	4:I:196:LEU:HG	2.19	0.43
4:I:209:ARG:HG2	4:I:212:ARG:HH22	1.84	0.43
4:I:718:PRO:HD2	4:I:785:TYR:HB3	2.01	0.43
4:K:535:PRO:HB3	4:K:1232:TRP:CZ2	2.53	0.43
7:X:62:ARG:NH1	7:X:147:ASN:OD1	2.52	0.43
7:Y:278:LEU:O	7:Y:282:ILE:HG12	2.18	0.43
1:A:1814:MET:HG2	1:A:2054:ARG:HB2	2.01	0.43
1:A:1957:PRO:HG3	1:A:2036:PHE:HA	1.99	0.43
2:E:223:TYR:OH	2:E:245:ASP:O	2.25	0.43
4:I:565:LEU:HD23	4:I:1232:TRP:CZ2	2.53	0.43
4:K:565:LEU:HG	4:K:1178:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:1116:VAL:HG13	4:K:1117:PHE:CD2	2.52	0.43
4:L:1121:VAL:HG12	4:L:1132:ARG:NH2	2.33	0.43
1:A:1526:GLU:HA	1:A:1529:VAL:HG12	2.01	0.43
1:A:1802:LYS:HZ3	1:A:2163:PHE:HZ	1.67	0.43
3:G:29:GLN:CD	3:G:29:GLN:H	2.27	0.43
4:J:600:THR:HA	4:J:644:LEU:HD12	2.00	0.43
4:L:441:ASP:OD1	4:L:441:ASP:N	2.49	0.43
4:L:950:ALA:HA	4:L:956:ILE:HB	2.00	0.43
7:V:31:VAL:HG12	7:V:137:ILE:HD11	2.01	0.43
7:V:62:ARG:O	7:V:66:ARG:HG3	2.18	0.43
7:Y:222:LEU:HB3	7:Y:231:LEU:HD13	2.00	0.43
1:A:1796:HIS:HA	2:E:451:SER:HB2	2.00	0.43
1:A:2104:ARG:NE	1:A:2153:THR:HB	2.33	0.43
1:A:2236:ARG:HH22	2:F:66:ARG:HB2	1.84	0.43
4:H:12:LYS:HG2	4:L:56:THR:HB	2.00	0.43
4:L:579:MET:HE3	4:L:1006:MET:HG3	2.01	0.43
4:L:627:ILE:O	4:L:627:ILE:HG22	2.19	0.43
4:L:815:PRO:HA	4:L:818:LEU:HG	2.01	0.43
1:A:1813:ALA:HB2	1:A:2051:ARG:HH12	1.84	0.43
1:A:1863:TRP:HH2	1:A:1880:LEU:HG	1.84	0.43
3:G:85:GLU:O	3:G:88:THR:HG22	2.18	0.43
4:H:410:VAL:CG1	4:H:414:VAL:HG22	2.49	0.43
4:H:1220:ALA:HB1	4:H:1225:PHE:HA	2.01	0.43
4:I:147:ILE:O	4:I:151:ILE:HG12	2.19	0.43
4:J:661:LEU:HD13	4:J:666:LEU:HD11	2.00	0.43
4:K:614:ASP:HA	4:K:653:LEU:HD21	2.00	0.43
6:W:173:LEU:HD21	6:W:175:TRP:NE1	2.34	0.43
7:X:21:VAL:O	7:X:25:THR:HG23	2.18	0.43
8:Z:250:CYS:O	8:Z:253:ILE:HG12	2.19	0.43
1:A:1835:GLN:HG2	1:A:1838:THR:HG23	2.00	0.42
4:H:87:THR:HG21	7:V:16:LEU:HD12	2.00	0.42
4:H:1175:ILE:HG22	4:H:1244:TYR:CE2	2.55	0.42
4:J:1098:TYR:HD2	4:J:1100:ASN:HD22	1.67	0.42
4:K:459:PRO:O	4:K:463:THR:HG23	2.18	0.42
4:L:495:ILE:HB	4:L:496:PRO:HD3	2.01	0.42
4:M:171:MET:HE3	4:M:1077:VAL:HG23	2.00	0.42
4:M:556:ILE:HD12	4:M:899:LEU:HD11	2.01	0.42
4:M:1002:LEU:HD13	4:M:1006:MET:HE3	2.00	0.42
6:W:58:GLU:HB2	6:W:106:TYR:CE1	2.54	0.42
8:Z:275:PHE:HA	8:Z:278:TYR:CE2	2.54	0.42
1:A:1596:ILE:O	1:A:1604:ILE:HG12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:301:VAL:O	2:E:305:LEU:HG	2.18	0.42
2:E:339:TYR:CB	2:E:364:ARG:HD2	2.47	0.42
2:E:604:VAL:HG22	2:E:606:LEU:H	1.84	0.42
4:I:638:MET:SD	4:I:864:VAL:HG13	2.59	0.42
4:I:752:SER:HA	5:O:63:ASP:OD1	2.19	0.42
4:K:310:GLU:H	4:K:310:GLU:HG2	1.64	0.42
4:L:449:LEU:HD21	4:L:1032:PHE:CE1	2.54	0.42
4:L:1180:THR:O	4:L:1180:THR:HG22	2.19	0.42
4:M:594:LEU:HD13	4:M:594:LEU:HA	1.93	0.42
4:M:646:VAL:HG23	4:M:647:PHE:CD2	2.54	0.42
6:T:227:ARG:O	6:T:231:VAL:HG23	2.19	0.42
7:V:216:MET:O	7:V:219:VAL:HG12	2.18	0.42
6:W:184:TYR:CE1	6:W:210:ALA:HB2	2.53	0.42
1:A:1800:GLN:NE2	2:E:450:ASP:HA	2.34	0.42
1:A:1999:LEU:HB2	1:A:2021:ILE:CG2	2.50	0.42
2:E:450:ASP:OD1	2:E:451:SER:N	2.52	0.42
3:G:417:TRP:HE3	3:G:485:VAL:HG13	1.85	0.42
3:G:517:GLN:HA	3:G:518:PRO:HD3	1.93	0.42
4:I:489:GLY:HA2	4:I:735:ASP:HA	2.01	0.42
4:J:495:ILE:HG21	4:J:938:PRO:HD2	2.01	0.42
4:K:75:ALA:HB2	4:K:179:PHE:CE2	2.54	0.42
4:M:698:LEU:HD11	4:M:1130:TRP:CG	2.54	0.42
6:W:243:LEU:HD12	6:W:244:CYS:SG	2.60	0.42
1:A:1604:ILE:O	1:A:1608:THR:OG1	2.27	0.42
1:A:1794:PRO:HG2	1:A:1977:ARG:NH2	2.35	0.42
4:H:645:LEU:HD12	4:H:648:ALA:HB2	2.01	0.42
4:J:706:TYR:O	4:J:1019:SER:HB2	2.19	0.42
4:J:1208:GLU:O	4:J:1211:THR:HG22	2.19	0.42
4:K:122:LYS:NZ	4:K:1080:ASN:OD1	2.32	0.42
4:K:329:LYS:O	4:K:333:THR:HG23	2.19	0.42
4:K:763:ASP:OD1	4:K:763:ASP:N	2.51	0.42
6:W:137:THR:HG1	6:W:147:THR:HG1	1.67	0.42
8:Z:20:LEU:HD12	8:Z:65:GLU:CD	2.45	0.42
1:A:1793:PRO:HG2	2:E:494:ARG:NH1	2.33	0.42
1:A:1863:TRP:CE3	1:A:1877:VAL:HA	2.55	0.42
2:E:224:ARG:HH22	2:E:618:LEU:HD22	1.83	0.42
2:E:226:LYS:HE3	2:E:246:ASN:O	2.18	0.42
2:E:258:VAL:HG12	2:E:262:GLU:OE2	2.18	0.42
4:I:776:ASP:OD1	4:I:776:ASP:N	2.50	0.42
4:I:917:LEU:HD23	4:I:917:LEU:HA	1.91	0.42
4:J:276:THR:HG21	4:J:386:GLU:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:222:LYS:O	4:L:226:THR:HG22	2.20	0.42
4:L:804:LEU:O	4:L:808:LEU:HB2	2.20	0.42
4:M:1221:ASP:OD1	4:M:1222:ALA:N	2.52	0.42
5:S:28:LEU:HG	5:S:29:PRO:HD2	2.01	0.42
1:A:1552:ILE:HA	1:A:2022:ARG:NH2	2.34	0.42
1:A:1579:ARG:HG3	1:A:1580:HIS:CE1	2.55	0.42
4:I:657:ILE:O	4:I:661:LEU:HB2	2.20	0.42
4:J:611:TYR:CZ	4:J:923:VAL:HG23	2.55	0.42
4:K:80:PHE:CE1	4:K:82:ASP:HB2	2.55	0.42
7:U:109:CYS:N	7:U:138:VAL:O	2.47	0.42
1:A:1698:TYR:HE2	1:A:2074:THR:HA	1.85	0.42
3:G:6:TYR:OH	7:V:220:ARG:HA	2.20	0.42
3:G:36:GLU:CD	3:G:159:ARG:HH12	2.28	0.42
3:G:457:LEU:HD23	6:W:116:GLN:OE1	2.20	0.42
4:H:156:ALA:O	4:H:159:THR:HG22	2.20	0.42
4:J:478:LEU:HB2	4:J:509:VAL:HG22	2.02	0.42
4:L:455:HIS:CD2	4:L:1017:PRO:HG3	2.53	0.42
4:L:461:LEU:HD13	4:L:552:CYS:HB2	2.02	0.42
4:M:849:GLN:OE1	4:M:871:PRO:HB2	2.20	0.42
1:A:1806:ILE:HG21	1:A:2053:LEU:HD13	2.00	0.42
1:A:1995:ARG:HE	1:A:1997:LEU:HD21	1.84	0.42
2:E:35:LEU:HD13	3:G:380:ARG:NH1	2.35	0.42
2:E:316:ALA:HA	2:E:319:VAL:HG22	2.02	0.42
2:E:428:GLN:C	2:E:430:LEU:H	2.28	0.42
3:G:531:PHE:CZ	3:G:543:SER:HB3	2.55	0.42
4:J:147:ILE:O	4:J:151:ILE:HG13	2.20	0.42
4:J:657:ILE:HG12	4:J:661:LEU:HD12	2.01	0.42
4:K:1210:ALA:O	4:K:1214:ILE:HG23	2.19	0.42
4:L:1059:ILE:HG22	4:L:1081:ILE:HG22	2.02	0.42
4:L:1336:LYS:NZ	4:L:1346:THR:O	2.42	0.42
4:M:611:TYR:CZ	4:M:923:VAL:HG23	2.55	0.42
5:Q:57:LYS:H	5:Q:57:LYS:HG2	1.62	0.42
6:T:61:ALA:HB3	6:T:266:HIS:NE2	2.34	0.42
1:A:1959:CYS:O	1:A:2040:VAL:N	2.49	0.42
2:E:366:VAL:HG13	2:E:367:LEU:HD13	2.02	0.42
4:H:438:GLN:NE2	4:H:1108:VAL:HG13	2.34	0.42
4:H:453:VAL:HG13	4:H:1243:LEU:HD11	2.02	0.42
4:I:988:ARG:HB2	4:I:990:PRO:HD2	2.02	0.42
4:J:597:PHE:CE1	4:J:648:ALA:HB1	2.54	0.42
4:J:723:LEU:HD13	4:J:768:VAL:HG11	2.02	0.42
4:K:263:THR:HB	4:K:267:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:44:LEU:O	5:N:48:THR:HG23	2.20	0.42
6:W:133:GLY:HA3	6:W:149:VAL:O	2.19	0.42
7:X:108:LEU:HD12	7:X:288:PHE:HB2	2.01	0.42
7:X:152:ILE:HD11	7:Y:272:PHE:CD2	2.55	0.42
8:Z:19:PHE:CD2	8:Z:20:LEU:HD22	2.55	0.42
3:G:311:VAL:HB	3:G:331:TYR:CD1	2.55	0.42
4:H:360:ILE:HG23	4:H:362:LEU:HD22	2.00	0.42
4:K:438:GLN:OE1	4:K:1108:VAL:HG22	2.20	0.42
4:M:212:ARG:NH2	4:M:1203:ASP:OD1	2.50	0.42
4:M:731:GLN:HB3	4:M:738:PRO:HB3	2.02	0.42
7:V:45:GLN:O	7:V:50:GLN:NE2	2.49	0.42
7:V:168:ALA:O	7:V:172:LEU:HD23	2.20	0.42
7:V:281:LEU:HD12	7:V:282:ILE:HG23	2.02	0.42
1:A:1675:LEU:HD21	1:A:2078:TYR:CD1	2.54	0.41
2:E:337:TYR:HD1	2:E:365:HIS:HB2	1.85	0.41
4:H:491:ALA:O	4:H:495:ILE:HG13	2.20	0.41
4:H:1144:ASP:H	4:H:1147:THR:HG22	1.85	0.41
4:I:469:PRO:HA	4:I:470:PRO:HD3	1.96	0.41
4:J:798:CYS:HA	4:J:943:TYR:HB3	2.01	0.41
4:L:275:SER:OG	4:L:1046:MET:O	2.34	0.41
7:Y:13:ASP:H	7:Y:43:HIS:CD2	2.38	0.41
1:A:1880:LEU:HD23	1:A:1880:LEU:HA	1.92	0.41
1:A:2207:VAL:O	1:A:2211:LEU:HG	2.19	0.41
4:I:632:ALA:HB2	4:I:661:LEU:HD11	2.02	0.41
4:M:647:PHE:CD1	4:M:653:LEU:HD13	2.55	0.41
4:M:1040:ASP:OD1	4:M:1106:MET:HG2	2.19	0.41
7:U:88:HIS:CE1	7:U:306:GLY:H	2.38	0.41
7:Y:51:PHE:CG	7:Y:64:LEU:HD13	2.54	0.41
2:E:365:HIS:ND1	2:E:368:VAL:N	2.68	0.41
4:I:607:PRO:HG2	4:I:610:CYS:SG	2.60	0.41
4:I:1065:THR:HB	4:I:1076:HIS:HB2	2.02	0.41
4:I:1124:HIS:CE1	4:I:1126:GLU:HB2	2.55	0.41
4:L:622:ASP:HA	4:L:625:LEU:HD23	2.03	0.41
4:L:968:ARG:NH2	4:M:691:PRO:O	2.52	0.41
4:M:426:THR:HG23	4:M:427:THR:HG23	2.01	0.41
4:M:651:TYR:CZ	4:M:655:THR:HG21	2.55	0.41
4:M:1043:GLU:OE2	4:M:1101:ARG:HB2	2.19	0.41
6:W:18:ASN:O	6:W:22:THR:HG23	2.20	0.41
6:W:42:ASP:OD2	6:W:159:LYS:NZ	2.42	0.41
7:X:55:THR:HG22	7:X:57:GLY:H	1.85	0.41
1:A:1456:TYR:OH	1:A:1486:PHE:HD1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1663:TRP:NE1	1:A:1744:GLN:HB3	2.36	0.41
1:A:1685:ALA:HA	1:A:1688:HIS:CE1	2.55	0.41
2:E:538:TRP:CH2	2:E:540:PRO:HA	2.56	0.41
3:G:473:TRP:CZ2	3:G:526:THR:HG22	2.55	0.41
4:I:4:TRP:CD1	4:I:36:ARG:HG3	2.55	0.41
4:I:59:ASN:HB2	4:J:95:VAL:HA	2.02	0.41
4:I:534:HIS:ND1	4:I:535:PRO:HD2	2.35	0.41
4:J:133:ALA:N	4:J:1071:ILE:O	2.43	0.41
4:K:637:ASN:O	4:K:641:THR:HG22	2.21	0.41
4:L:495:ILE:HD12	4:L:937:VAL:HG12	2.01	0.41
4:M:230:LEU:HD12	4:M:1097:ALA:O	2.20	0.41
4:M:798:CYS:SG	4:M:799:GLY:N	2.93	0.41
4:M:817:PHE:O	4:M:820:MET:HG2	2.19	0.41
7:V:296:ASP:O	7:V:298:LYS:N	2.54	0.41
1:A:1939:ILE:HG13	1:A:1940:GLN:N	2.34	0.41
1:A:2101:PRO:HB3	2:E:320:SER:HB2	2.02	0.41
1:A:2181:ASP:OD1	1:A:2182:GLU:N	2.54	0.41
4:H:1334:GLU:O	4:H:1338:LYS:HG3	2.20	0.41
4:I:1285:TYR:HA	4:I:1289:ALA:HB2	2.03	0.41
4:J:178:SER:O	4:J:182:THR:HG23	2.20	0.41
4:K:734:ALA:HB2	4:K:739:LEU:HD11	2.02	0.41
7:U:268:LEU:HD23	7:U:271:LEU:HD23	2.02	0.41
7:X:148:GLN:O	7:X:152:ILE:HG12	2.21	0.41
1:A:2019:ALA:HA	1:A:2022:ARG:NE	2.36	0.41
2:F:91:ASN:HB3	2:F:93:GLN:HG3	2.03	0.41
3:G:41:ARG:NH2	3:G:567:ALA:HB3	2.36	0.41
3:G:388:GLN:NE2	3:G:537:GLY:O	2.53	0.41
4:J:1243:LEU:HD23	4:J:1244:TYR:CE2	2.55	0.41
4:K:449:LEU:HD21	4:K:1034:LEU:HD21	2.02	0.41
4:L:21:THR:OG1	4:L:22:HIS:N	2.48	0.41
4:L:263:THR:HG23	4:L:266:GLY:H	1.85	0.41
4:L:1090:TYR:CE2	4:L:1282:ILE:HD11	2.56	0.41
4:M:71:LEU:HD22	4:M:372:LEU:HD11	2.02	0.41
4:M:704:SER:HA	4:M:707:VAL:HG12	2.02	0.41
7:X:156:PHE:CE1	7:X:160:ARG:HG3	2.55	0.41
1:A:1880:LEU:O	1:A:1884:LEU:HG	2.21	0.41
2:E:276:ASP:O	2:E:277:LEU:C	2.62	0.41
2:E:319:VAL:O	2:E:323:ILE:HG12	2.21	0.41
2:E:371:PHE:O	2:E:375:GLY:N	2.54	0.41
4:H:13:VAL:HG23	4:K:339:LEU:O	2.21	0.41
4:H:1232:TRP:O	4:H:1238:CYS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1315:CYS:O	4:H:1319:GLN:N	2.48	0.41
4:I:473:PRO:HA	4:I:476:GLN:HB3	2.03	0.41
4:J:344:LEU:H	4:J:344:LEU:HD22	1.85	0.41
4:J:1121:VAL:HG23	4:J:1128:ASP:OD2	2.21	0.41
4:K:61:LEU:H	4:K:61:LEU:HD12	1.86	0.41
4:K:708:ASN:OD1	4:K:709:ALA:N	2.52	0.41
4:M:363:GLY:C	4:M:365:LYS:H	2.29	0.41
4:M:710:LEU:HD12	4:M:1012:LEU:HD12	2.02	0.41
4:M:1190:ASN:OD1	4:M:1223:GLN:NE2	2.53	0.41
7:U:96:ASN:ND2	7:U:297:ASN:O	2.45	0.41
8:Z:119:ARG:HD2	8:Z:119:ARG:N	2.35	0.41
8:Z:154:ILE:HG21	8:Z:208:ARG:HD3	2.03	0.41
1:A:1585:LEU:HD11	1:A:1904:LEU:HD11	2.02	0.41
1:A:1960:LEU:HB2	1:A:1978:HIS:HD2	1.85	0.41
2:E:270:TYR:O	2:E:273:VAL:HG23	2.21	0.41
2:E:340:ARG:HB3	2:E:361:THR:HA	2.03	0.41
2:E:499:GLU:O	2:E:502:VAL:HG12	2.21	0.41
3:G:5:LEU:HD13	3:G:306:TRP:CD2	2.55	0.41
4:H:647:PHE:HB3	4:H:653:LEU:HB3	2.03	0.41
4:H:714:ARG:NH1	4:H:898:PRO:O	2.52	0.41
4:H:1032:PHE:HA	4:H:1179:VAL:HG22	2.02	0.41
4:I:1119:MET:HG2	4:I:1148:ILE:HD12	2.03	0.41
4:I:1149:SER:OG	6:W:117:TRP:NE1	2.41	0.41
4:J:1175:ILE:HG22	4:J:1244:TYR:CE2	2.56	0.41
4:L:171:MET:HE2	4:L:1077:VAL:HG23	2.02	0.41
4:M:610:CYS:SG	4:M:646:VAL:HB	2.61	0.41
4:M:970:ASP:HB2	4:M:993:ARG:HD3	2.01	0.41
4:M:1121:VAL:HG12	4:M:1132:ARG:NH2	2.36	0.41
8:Z:194:THR:HG23	8:Z:197:VAL:H	1.86	0.41
1:A:1574:ARG:NE	1:A:1604:ILE:HG22	2.34	0.41
2:E:354:GLY:O	2:E:427:GLN:HA	2.20	0.41
2:F:41:THR:HA	4:K:500:ARG:HH22	1.86	0.41
3:G:70:ASP:OD1	3:G:547:LEU:N	2.54	0.41
4:H:434:ASP:OD1	4:H:435:ARG:N	2.54	0.41
4:H:450:CYS:O	4:H:1122:TYR:OH	2.36	0.41
4:H:455:HIS:NE2	4:H:1017:PRO:HG3	2.36	0.41
4:H:556:ILE:H	4:H:556:ILE:HG12	1.69	0.41
4:H:633:ARG:NH1	4:H:867:ASP:OD2	2.51	0.41
4:H:1291:ASP:O	4:H:1311:ILE:N	2.48	0.41
4:H:1366:MET:HE2	4:H:1366:MET:HB2	1.86	0.41
4:I:75:ALA:HB2	4:I:179:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:558:ILE:HD12	4:I:1015:ILE:HD11	2.03	0.41
4:I:998:CYS:SG	4:I:1004:SER:HB2	2.61	0.41
4:K:694:ASN:ND2	4:K:704:SER:HB3	2.32	0.41
4:K:989:SER:N	4:K:990:PRO:HD2	2.36	0.41
4:K:997:THR:HG23	4:L:583:ARG:HD3	2.02	0.41
4:K:1350:HIS:C	4:K:1352:GLY:H	2.29	0.41
4:L:1104:THR:HB	4:L:1170:ALA:HB2	2.03	0.41
4:L:1231:PRO:O	4:L:1235:GLN:HG2	2.21	0.41
6:T:47:THR:HG22	6:T:149:VAL:HG12	2.03	0.41
6:T:69:ARG:HH21	6:T:79:HIS:CE1	2.38	0.41
7:U:115:PHE:HB2	7:U:183:THR:HG23	2.03	0.41
7:U:291:CYS:SG	7:V:37:ARG:HD3	2.61	0.41
6:W:108:ALA:O	6:W:112:ARG:HG2	2.21	0.41
6:W:127:ARG:HH22	6:W:243:LEU:HD11	1.85	0.41
6:W:285:ASP:OD1	6:W:285:ASP:N	2.47	0.41
7:X:292:ASP:HB3	7:X:301:THR:OG1	2.19	0.41
1:A:2220:ASP:O	1:A:2223:GLN:HG3	2.21	0.41
2:E:524:GLY:HA2	2:E:634:GLY:HA2	2.03	0.41
4:H:386:GLU:HA	4:H:1045:ASP:HA	2.03	0.41
4:H:504:GLU:HG3	4:H:966:TYR:OH	2.21	0.41
4:I:174:GLY:HA3	4:J:101:ALA:HB3	2.02	0.41
4:I:790:PRO:HA	4:I:793:THR:HG22	2.02	0.41
4:I:1139:ARG:O	4:I:1141:GLN:N	2.53	0.41
4:I:1283:ASP:O	4:I:1287:LEU:HD23	2.21	0.41
4:J:1154:GLY:O	4:J:1255:ASN:ND2	2.53	0.41
4:K:83:LEU:HD23	4:K:83:LEU:HA	1.87	0.41
4:L:1021:VAL:HG21	4:L:1134:ALA:HB1	2.03	0.41
4:L:1102:VAL:HG12	4:L:1104:THR:H	1.86	0.41
4:M:807:LEU:O	4:M:811:LEU:HB2	2.21	0.41
4:M:1119:MET:HE1	4:M:1151:LEU:HG	2.03	0.41
1:A:1955:GLY:HA2	1:A:1992:GLN:HE22	1.86	0.40
4:H:1054:CYS:SG	4:H:1055:THR:HG22	2.60	0.40
4:I:179:PHE:CE2	4:I:183:LEU:HD11	2.56	0.40
4:I:495:ILE:HD12	4:I:976:PRO:HG2	2.04	0.40
4:J:224:LEU:HD23	4:J:224:LEU:HA	1.85	0.40
4:J:1260:SER:HB2	4:J:1263:ALA:HB2	2.02	0.40
4:L:624:PHE:CB	4:L:656:LEU:HD23	2.51	0.40
4:M:93:PHE:HB2	4:M:116:VAL:HG22	2.02	0.40
4:M:191:PHE:CE1	4:M:192:VAL:HG13	2.55	0.40
4:M:419:THR:HG23	4:M:580:GLU:OE2	2.21	0.40
7:V:262:ASP:N	7:V:262:ASP:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:8:LEU:HD21	8:Z:12:ASP:HB2	2.02	0.40
8:Z:70:ASN:HA	8:Z:71:PRO:HD3	1.92	0.40
1:A:1473:ARG:O	1:A:1477:GLU:OE1	2.39	0.40
4:H:793:THR:O	4:H:796:ARG:HG2	2.21	0.40
4:I:200:ALA:HB1	4:L:20:LEU:O	2.21	0.40
4:I:811:LEU:HD21	4:I:857:LEU:HD21	2.03	0.40
4:I:817:PHE:HB3	4:I:880:PHE:CE2	2.55	0.40
4:J:118:LYS:HE2	4:J:118:LYS:HB2	1.95	0.40
4:K:336:GLN:HA	4:K:337:PRO:HD3	1.93	0.40
4:L:1050:SER:HG	4:L:1054:CYS:HG	1.65	0.40
5:N:21:VAL:O	5:N:25:VAL:HB	2.21	0.40
6:W:179:ARG:HB3	6:W:183:GLN:NE2	2.36	0.40
7:Y:46:LEU:HD11	7:Y:132:LEU:HD11	2.02	0.40
7:Y:206:MET:HE2	7:Y:206:MET:HB2	1.91	0.40
8:Z:122:ALA:HA	8:Z:125:VAL:HG12	2.03	0.40
1:A:1876:SER:OG	1:A:1879:GLU:HG3	2.21	0.40
1:A:2001:GLN:HA	1:A:2004:GLN:CD	2.46	0.40
1:C:2209:SER:O	1:C:2213:ILE:HG12	2.21	0.40
3:G:526:THR:OG1	3:G:528:ASP:OD1	2.34	0.40
4:H:180:LEU:HD23	4:H:384:PRO:HG2	2.03	0.40
4:H:420:VAL:HG21	4:H:577:GLU:HA	2.04	0.40
4:H:873:LEU:HA	4:H:876:CYS:SG	2.61	0.40
4:H:1348:GLU:O	4:H:1355:VAL:HG22	2.21	0.40
4:I:970:ASP:OD1	4:I:970:ASP:N	2.40	0.40
4:I:1144:ASP:OD1	4:I:1144:ASP:N	2.53	0.40
4:I:1333:MET:HE3	4:I:1337:LEU:HD21	2.03	0.40
4:J:704:SER:HA	4:J:707:VAL:HG12	2.03	0.40
4:J:760:MET:SD	4:J:888:GLU:HA	2.61	0.40
4:K:98:PRO:HD2	4:L:378:ASN:HB2	2.04	0.40
4:K:578:ILE:HG21	4:K:687:ILE:HG23	2.03	0.40
4:K:1217:HIS:NE2	4:K:1235:GLN:HB3	2.36	0.40
4:L:257:ASN:OD1	4:L:259:THR:HG22	2.22	0.40
4:M:709:ALA:HA	4:M:1014:LYS:HE3	2.01	0.40
4:M:1268:THR:O	4:M:1272:ILE:HG12	2.22	0.40
6:W:47:THR:HG22	6:W:149:VAL:HG12	2.03	0.40
7:X:125:LEU:HD12	7:X:132:LEU:HB2	2.03	0.40
4:H:609:LEU:HD11	4:H:861:VAL:HG22	2.03	0.40
4:I:609:LEU:HD21	4:I:630:PHE:HE2	1.87	0.40
4:J:209:ARG:HA	4:J:212:ARG:HG2	2.03	0.40
4:K:724:PRO:HB3	4:K:778:TRP:CE2	2.57	0.40
4:K:767:PHE:HB2	4:K:888:GLU:CD	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:85:LYS:HG2	4:M:48:ILE:O	2.21	0.40
4:L:146:THR:O	4:L:150:LYS:HG3	2.21	0.40
4:L:753:ASP:OD2	4:L:756:ARG:NH2	2.53	0.40
4:M:36:ARG:NH2	4:M:44:GLU:OE1	2.53	0.40
4:J:926:ALA:HB2	4:J:948:ILE:HG13	2.02	0.40
4:L:1138:GLU:CD	4:L:1138:GLU:H	2.30	0.40
4:M:446:LEU:HD21	4:M:1021:VAL:HG13	2.04	0.40
5:Q:17:LYS:O	5:Q:21:VAL:HG12	2.21	0.40
7:U:114:LEU:HD23	7:U:185:PRO:HD3	2.02	0.40
8:Z:170:ASN:ND2	8:Z:185:ASP:OD1	2.38	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	710/2241 (32%)	695 (98%)	15 (2%)	0	100	100
1	C	38/2241 (2%)	38 (100%)	0	0	100	100
2	E	483/642 (75%)	459 (95%)	22 (5%)	2 (0%)	30	65
2	F	81/642 (13%)	80 (99%)	1 (1%)	0	100	100
3	G	467/594 (79%)	451 (97%)	16 (3%)	0	100	100
4	H	1303/1370 (95%)	1241 (95%)	61 (5%)	1 (0%)	48	81
4	I	1346/1370 (98%)	1281 (95%)	64 (5%)	1 (0%)	48	81
4	J	1313/1370 (96%)	1251 (95%)	61 (5%)	1 (0%)	48	81
4	K	1290/1370 (94%)	1235 (96%)	55 (4%)	0	100	100
4	L	1346/1370 (98%)	1290 (96%)	55 (4%)	1 (0%)	48	81
4	M	1346/1370 (98%)	1288 (96%)	55 (4%)	3 (0%)	43	75
5	N	61/75 (81%)	60 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	O	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
5	P	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
5	Q	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
5	R	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
5	S	61/75 (81%)	61 (100%)	0	0	100	100
6	T	238/290 (82%)	228 (96%)	10 (4%)	0	100	100
6	W	288/290 (99%)	277 (96%)	11 (4%)	0	100	100
7	U	288/306 (94%)	270 (94%)	17 (6%)	1 (0%)	36	70
7	V	282/306 (92%)	265 (94%)	15 (5%)	2 (1%)	18	54
7	X	291/306 (95%)	275 (94%)	16 (6%)	0	100	100
7	Y	279/306 (91%)	268 (96%)	10 (4%)	1 (0%)	30	65
8	Z	282/1048 (27%)	275 (98%)	6 (2%)	1 (0%)	30	65
All	All	12037/17882 (67%)	11527 (96%)	496 (4%)	14 (0%)	49	81

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	266	GLY
4	I	266	GLY
4	M	760	MET
4	M	886	VAL
7	Y	297	ASN
2	E	336	TYR
2	E	429	TYR
7	U	75	ARG
4	L	1223	GLN
8	Z	193	ASN
7	V	297	ASN
4	J	795	ASN
4	M	268	LYS
7	V	78	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	647/1941 (33%)	647 (100%)	0	100	100
1	C	38/1941 (2%)	38 (100%)	0	100	100
2	E	422/526 (80%)	417 (99%)	5 (1%)	63	73
2	F	76/526 (14%)	76 (100%)	0	100	100
3	G	397/500 (79%)	397 (100%)	0	100	100
4	H	1142/1192 (96%)	1139 (100%)	3 (0%)	86	85
4	I	1175/1192 (99%)	1171 (100%)	4 (0%)	86	85
4	J	1146/1192 (96%)	1146 (100%)	0	100	100
4	K	1129/1192 (95%)	1129 (100%)	0	100	100
4	L	1175/1192 (99%)	1175 (100%)	0	100	100
4	M	1175/1192 (99%)	1175 (100%)	0	100	100
5	N	59/68 (87%)	59 (100%)	0	100	100
5	O	59/68 (87%)	59 (100%)	0	100	100
5	P	59/68 (87%)	59 (100%)	0	100	100
5	Q	59/68 (87%)	59 (100%)	0	100	100
5	R	59/68 (87%)	59 (100%)	0	100	100
5	S	59/68 (87%)	59 (100%)	0	100	100
6	T	211/252 (84%)	211 (100%)	0	100	100
6	W	252/252 (100%)	252 (100%)	0	100	100
7	U	262/273 (96%)	262 (100%)	0	100	100
7	V	260/273 (95%)	260 (100%)	0	100	100
7	X	263/273 (96%)	263 (100%)	0	100	100
7	Y	257/273 (94%)	257 (100%)	0	100	100
8	Z	255/883 (29%)	255 (100%)	0	100	100
All	All	10636/15473 (69%)	10624 (100%)	12 (0%)	87	89

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	271	ASP
2	E	272	CYS
2	E	274	LEU

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Mol	Chain	Res	Type
2	E	275	SER
2	E	349	MET
4	H	82	ASP
4	H	410	VAL
4	H	677	LEU
4	I	9	LEU
4	I	621	VAL
4	I	808	LEU
4	I	886	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1499	ASN
1	A	1691	HIS
1	A	1744	GLN
1	A	1796	HIS
1	A	1828	GLN
1	A	2047	HIS
1	A	2063	HIS
1	A	2206	ASN
1	C	2206	ASN
2	E	93	GLN
2	E	334	ASN
2	E	358	HIS
2	E	365	HIS
2	E	620	ASN
2	F	5	HIS
2	F	92	GLN
3	G	20	GLN
3	G	34	ASN
3	G	90	GLN
3	G	517	GLN
4	H	59	ASN
4	H	111	GLN
4	H	432	ASN
4	H	497	HIS
4	H	543	GLN
4	H	571	HIS
4	H	660	HIS
4	H	749	HIS
4	H	903	GLN

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Mol	Chain	Res	Type
4	H	1023	GLN
4	H	1124	HIS
4	I	181	GLN
4	I	455	HIS
4	I	669	GLN
4	I	697	GLN
4	I	722	HIS
4	I	795	ASN
4	I	915	HIS
4	I	969	HIS
4	I	1061	ASN
4	I	1079	GLN
4	I	1120	ASN
4	I	1184	ASN
4	I	1235	GLN
4	J	194	GLN
4	J	336	GLN
4	J	378	ASN
4	J	432	ASN
4	J	438	GLN
4	J	451	HIS
4	J	545	ASN
4	J	571	HIS
4	J	649	HIS
4	J	731	GLN
4	J	749	HIS
4	J	1166	HIS
4	K	211	GLN
4	K	217	GLN
4	K	304	ASN
4	K	319	HIS
4	K	451	HIS
4	K	722	HIS
4	K	849	GLN
4	K	889	HIS
4	K	981	HIS
4	K	1184	ASN
4	K	1248	HIS
4	K	1300	GLN
4	L	304	ASN
4	L	485	GLN
4	L	605	ASN

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Mol	Chain	Res	Type
4	L	620	ASN
4	L	849	GLN
4	L	965	HIS
4	L	969	HIS
4	L	1023	GLN
4	L	1079	GLN
4	L	1111	GLN
4	L	1248	HIS
4	L	1267	ASN
4	M	84	ASN
4	M	371	ASN
4	M	534	HIS
4	M	543	GLN
4	M	915	HIS
4	M	965	HIS
4	M	984	HIS
4	M	1060	ASN
4	M	1120	ASN
4	M	1184	ASN
4	M	1264	GLN
4	M	1350	HIS
5	N	18	HIS
5	R	20	HIS
6	T	249	GLN
7	U	67	ASN
7	U	209	ASN
7	V	7	ASN
7	V	39	HIS
7	V	88	HIS
6	W	18	ASN
6	W	43	HIS
7	X	49	HIS
7	X	173	GLN
7	Y	49	HIS
7	Y	67	ASN
8	Z	252	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

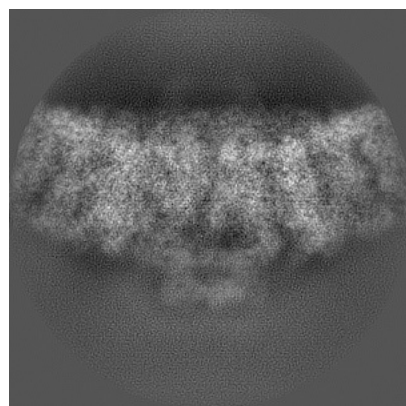
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41202. These allow visual inspection of the internal detail of the map and identification of artifacts.

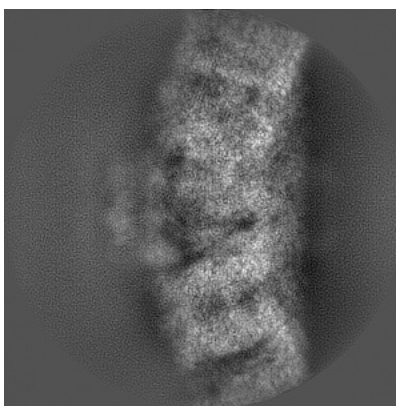
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

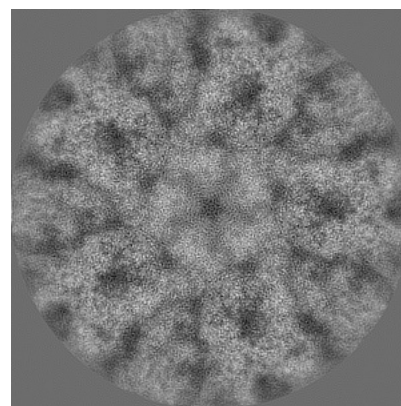
6.1.1 Primary map



X

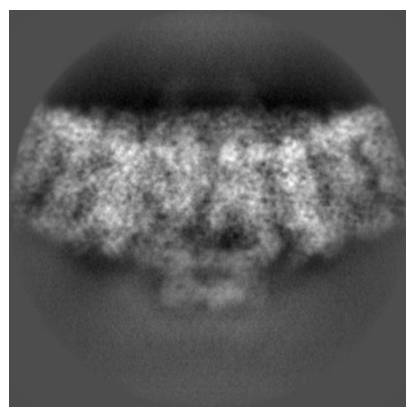


Y

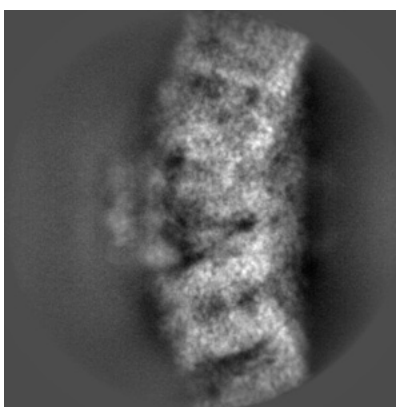


Z

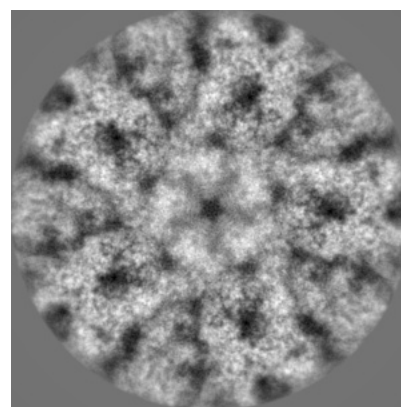
6.1.2 Raw map



X



Y

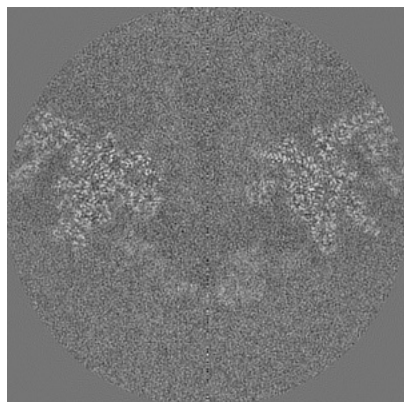


Z

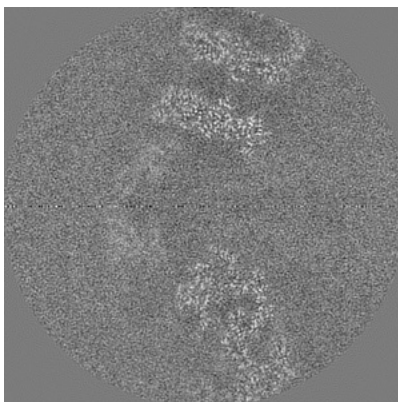
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

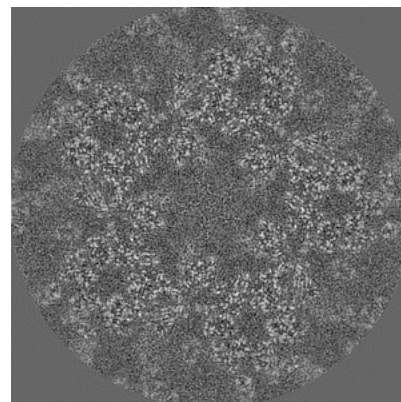
6.2.1 Primary map



X Index: 180

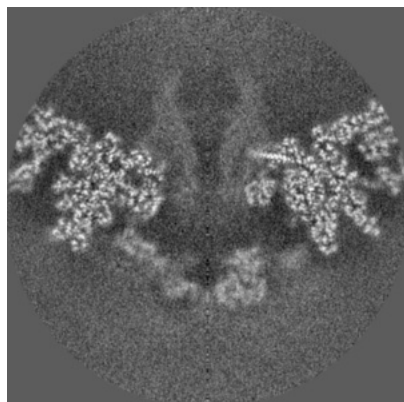


Y Index: 180

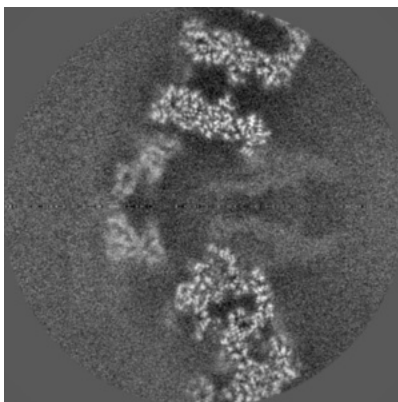


Z Index: 180

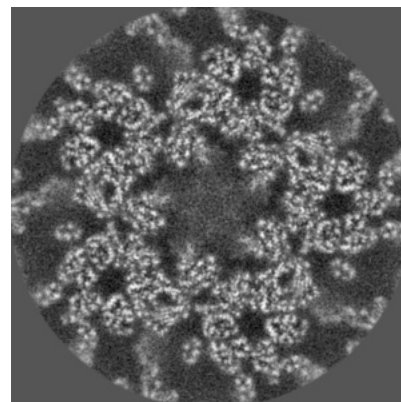
6.2.2 Raw map



X Index: 180



Y Index: 180

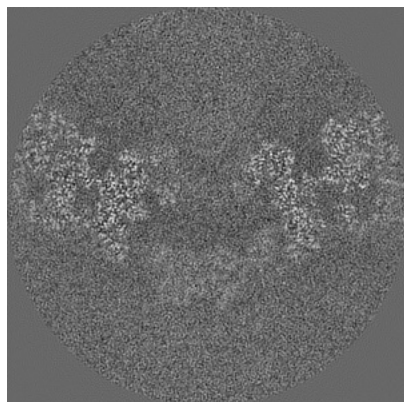


Z Index: 180

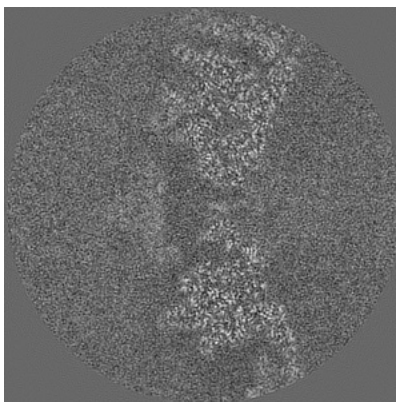
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

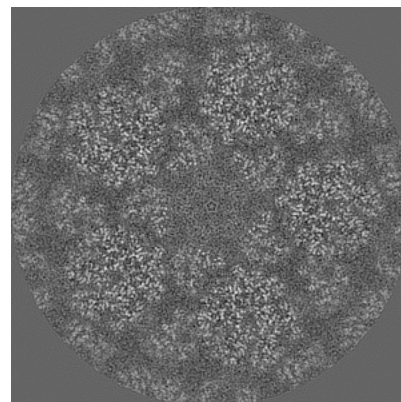
6.3.1 Primary map



X Index: 204

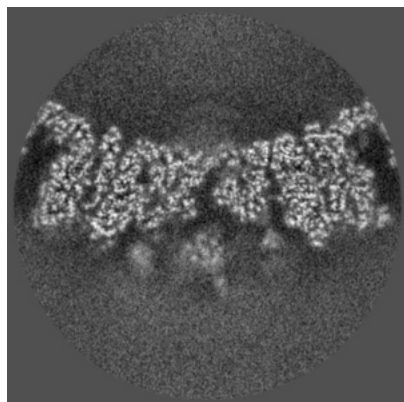


Y Index: 217

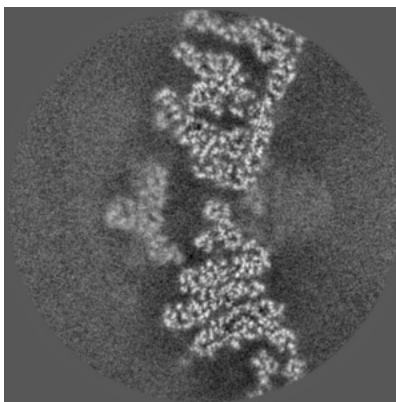


Z Index: 203

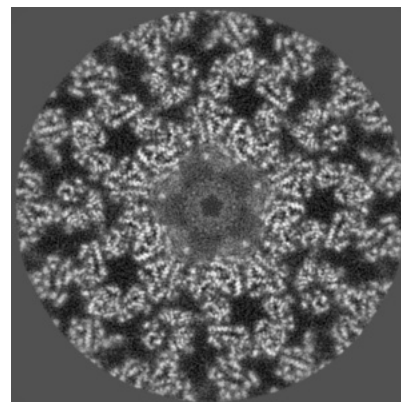
6.3.2 Raw map



X Index: 230



Y Index: 220

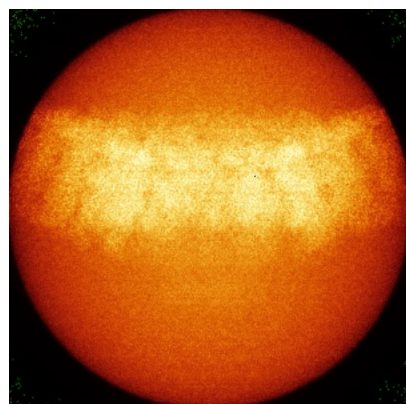


Z Index: 223

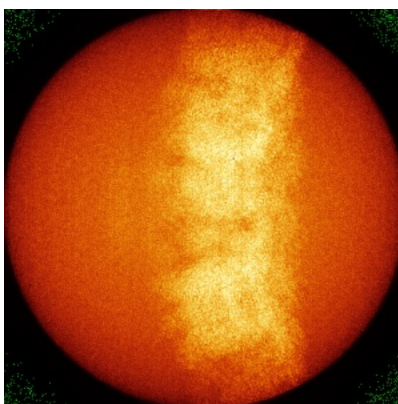
The images above show the largest variance slices of the map in three orthogonal directions.

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

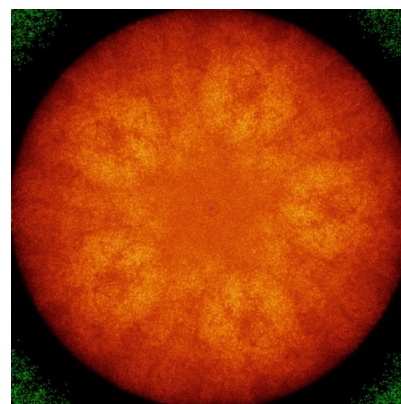
6.4.1 Primary map



X

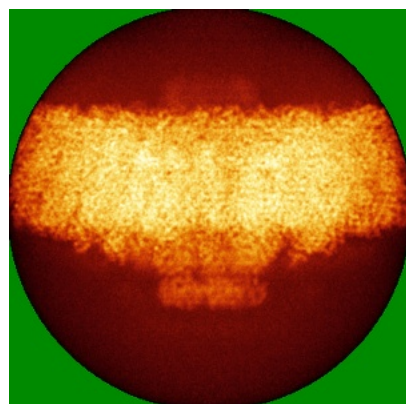


Y

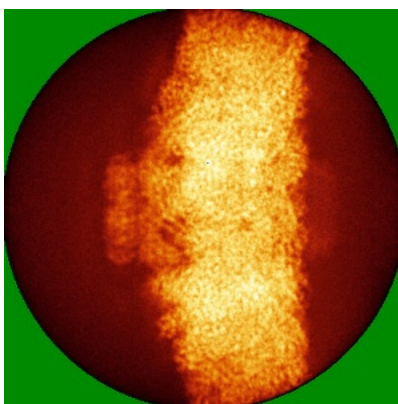


Z

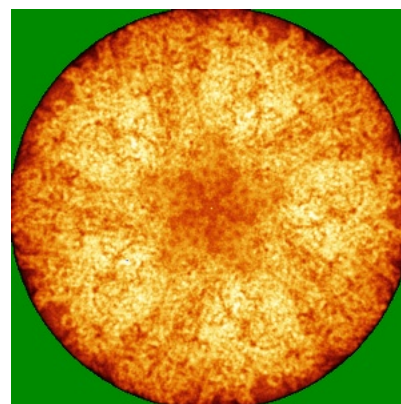
6.4.2 Raw map



X



Y

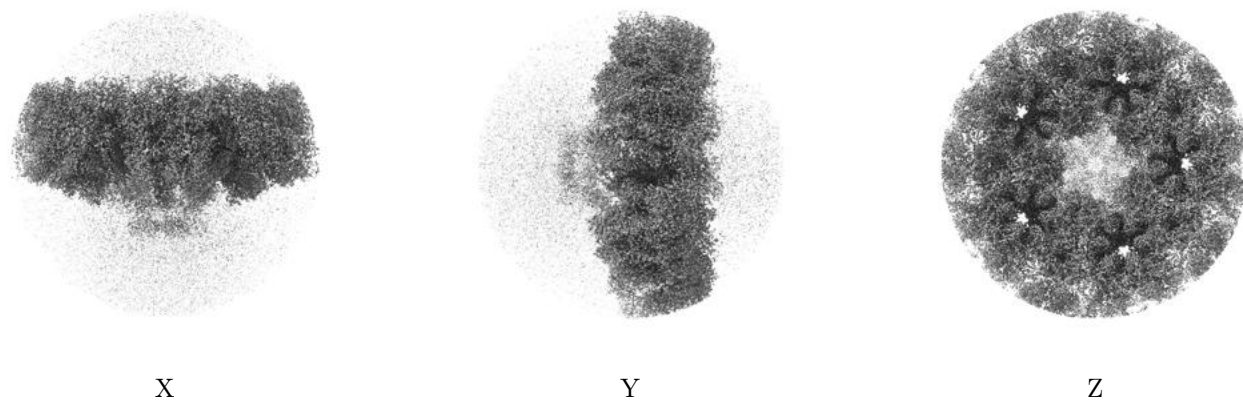


Z

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

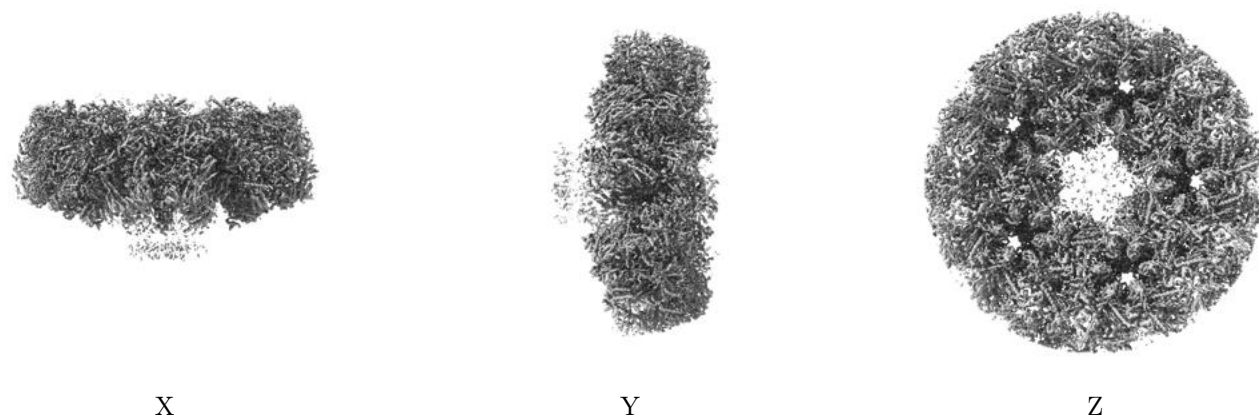
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

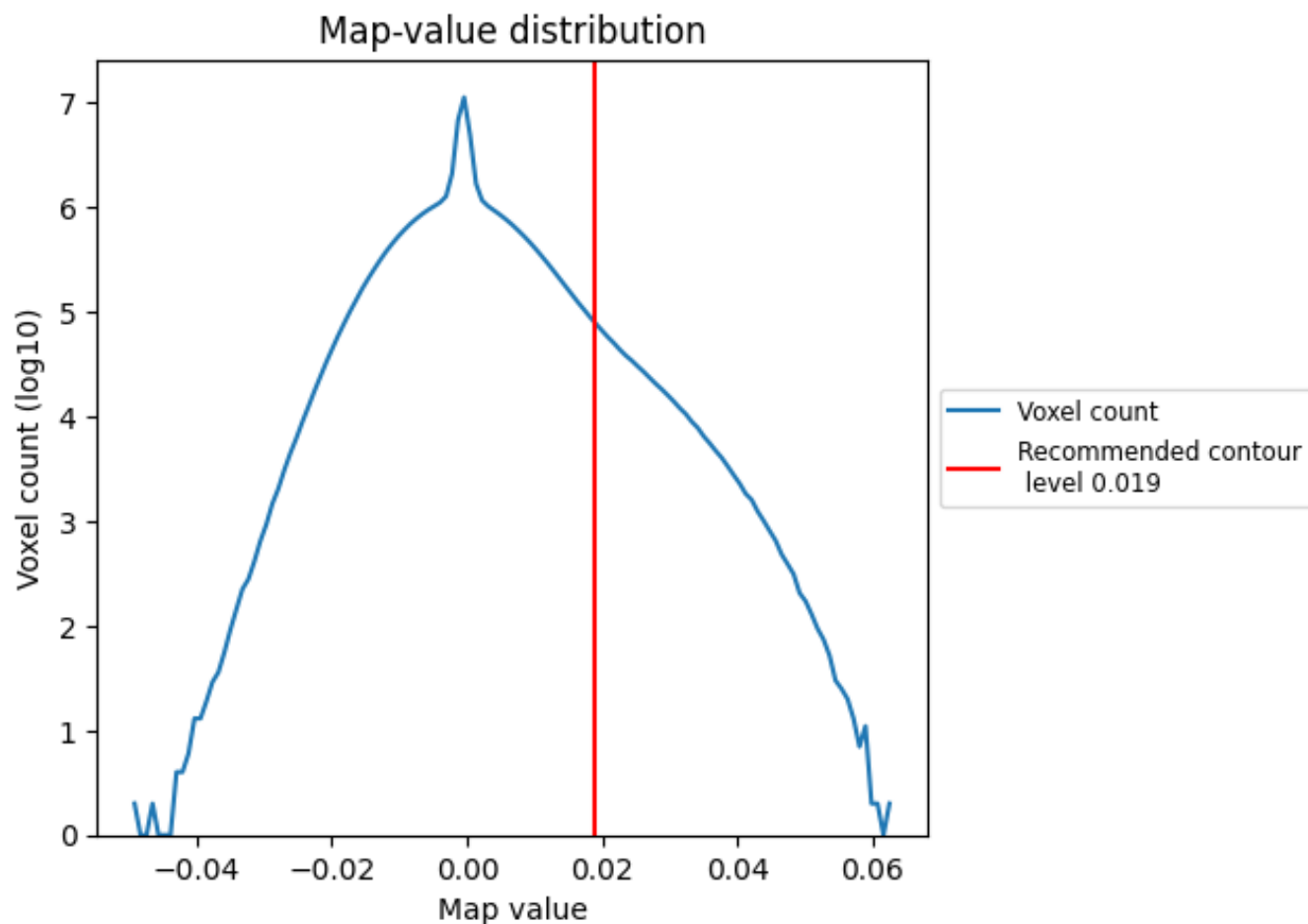
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

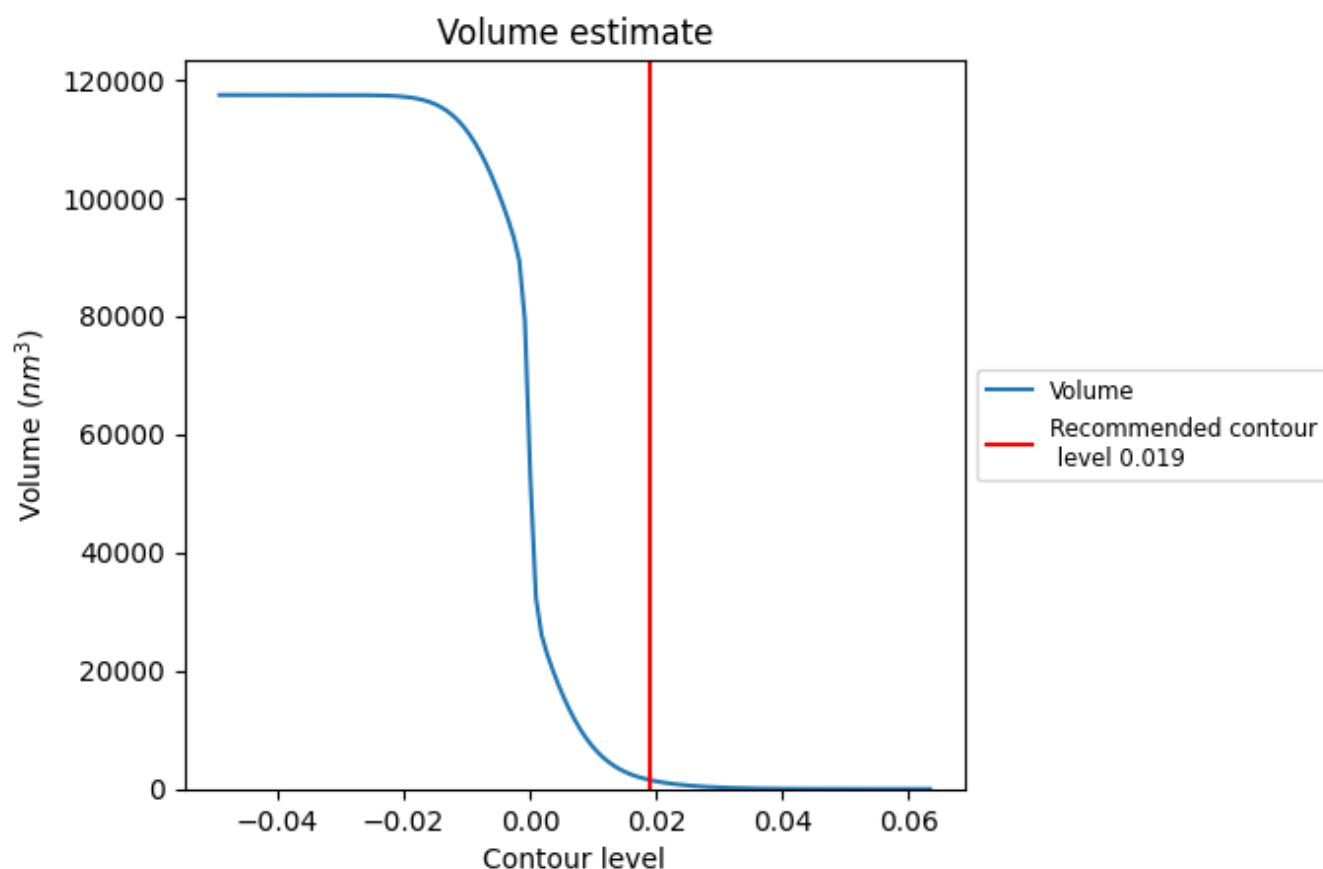
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

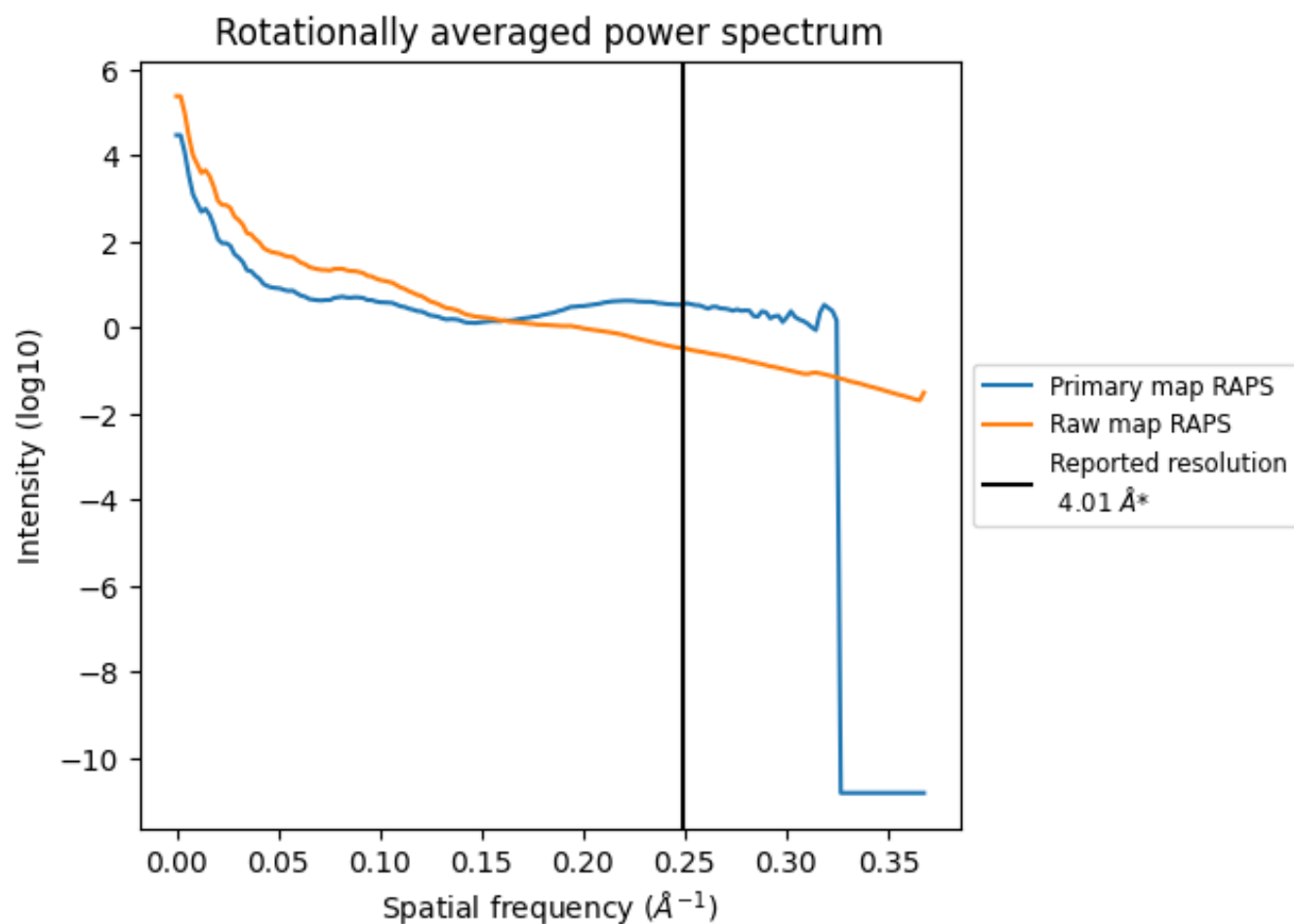
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1523 nm³; this corresponds to an approximate mass of 1376 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 ⓘ

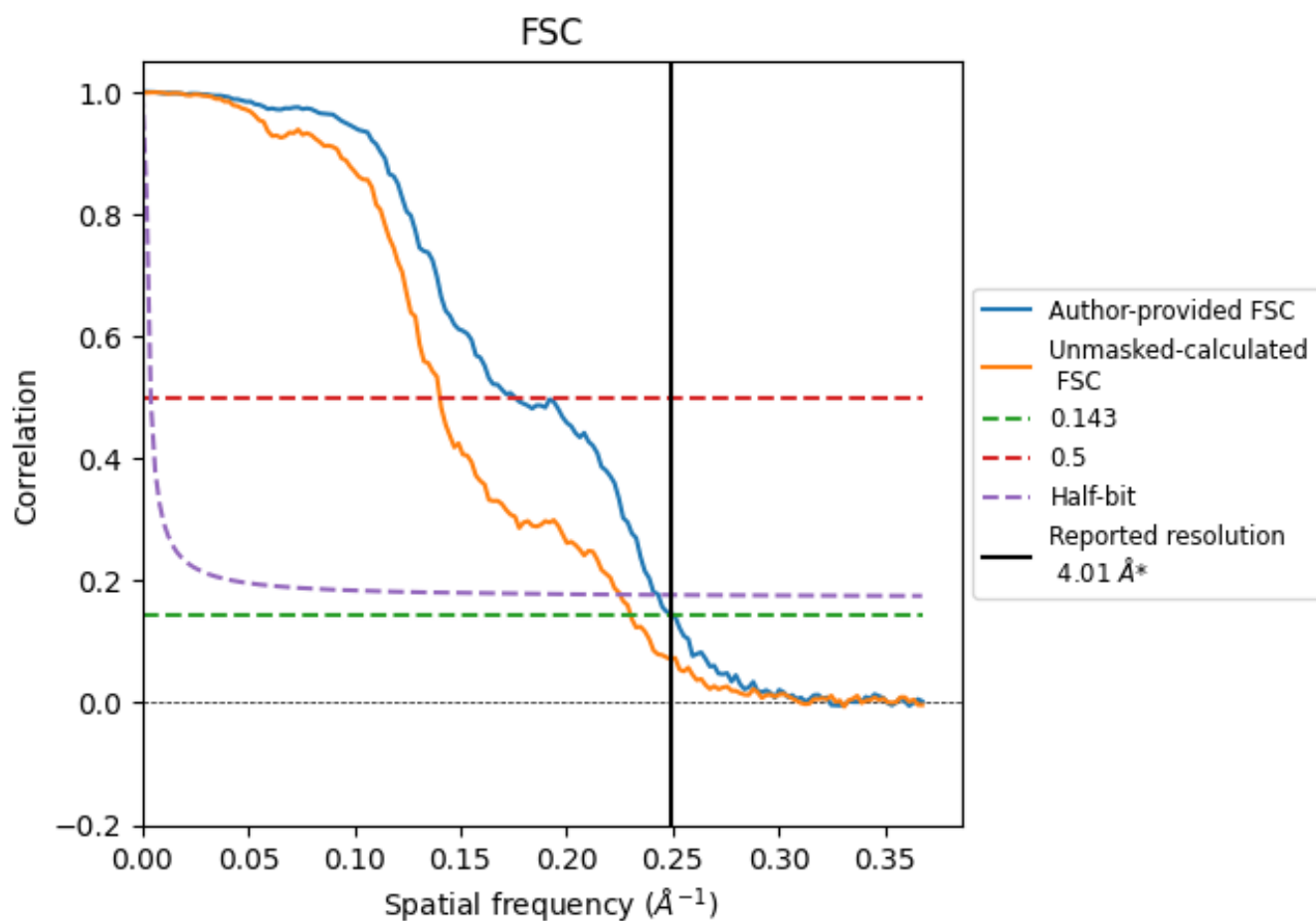


*Reported resolution corresponds to spatial frequency of 0.249 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.249 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

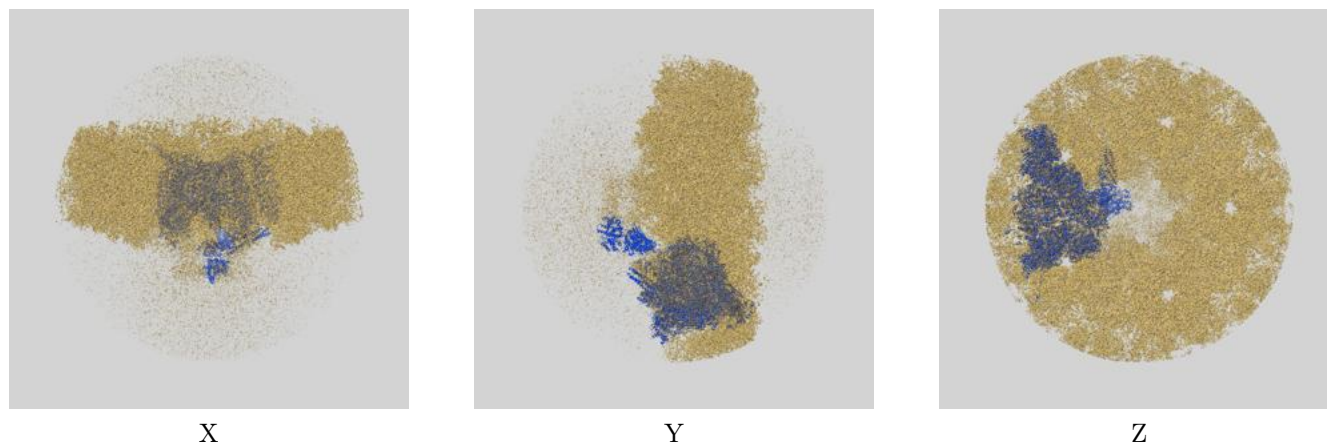
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.01	-	-
Author-provided FSC curve	3.99	5.69	4.11
Unmasked-calculated*	4.34	7.13	4.44

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

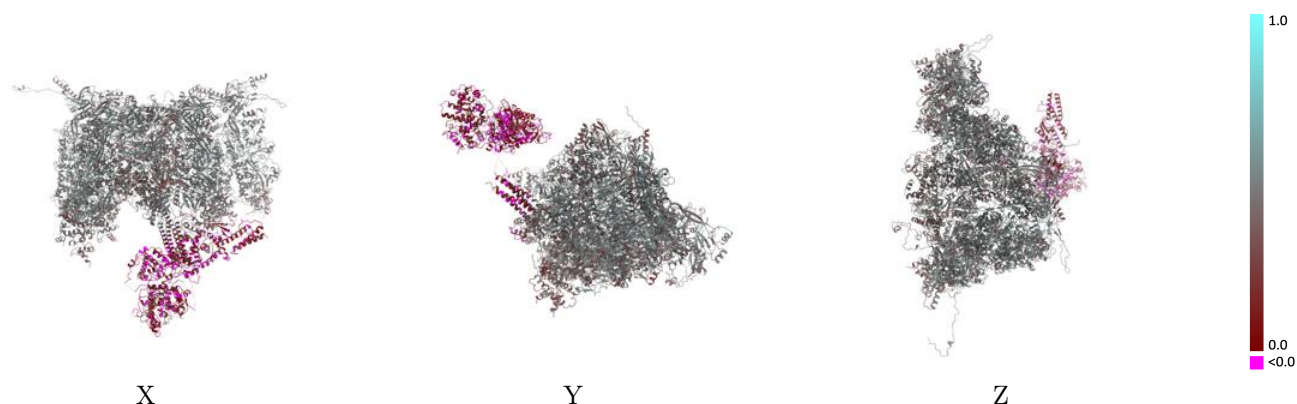
This section contains information regarding the fit between EMDB map EMD-41202 and PDB model 8TEU. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



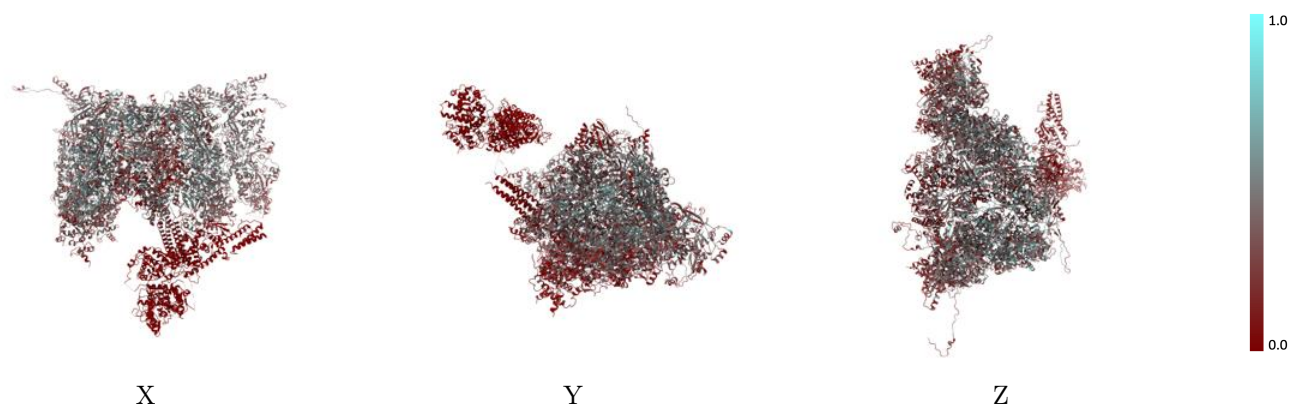
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



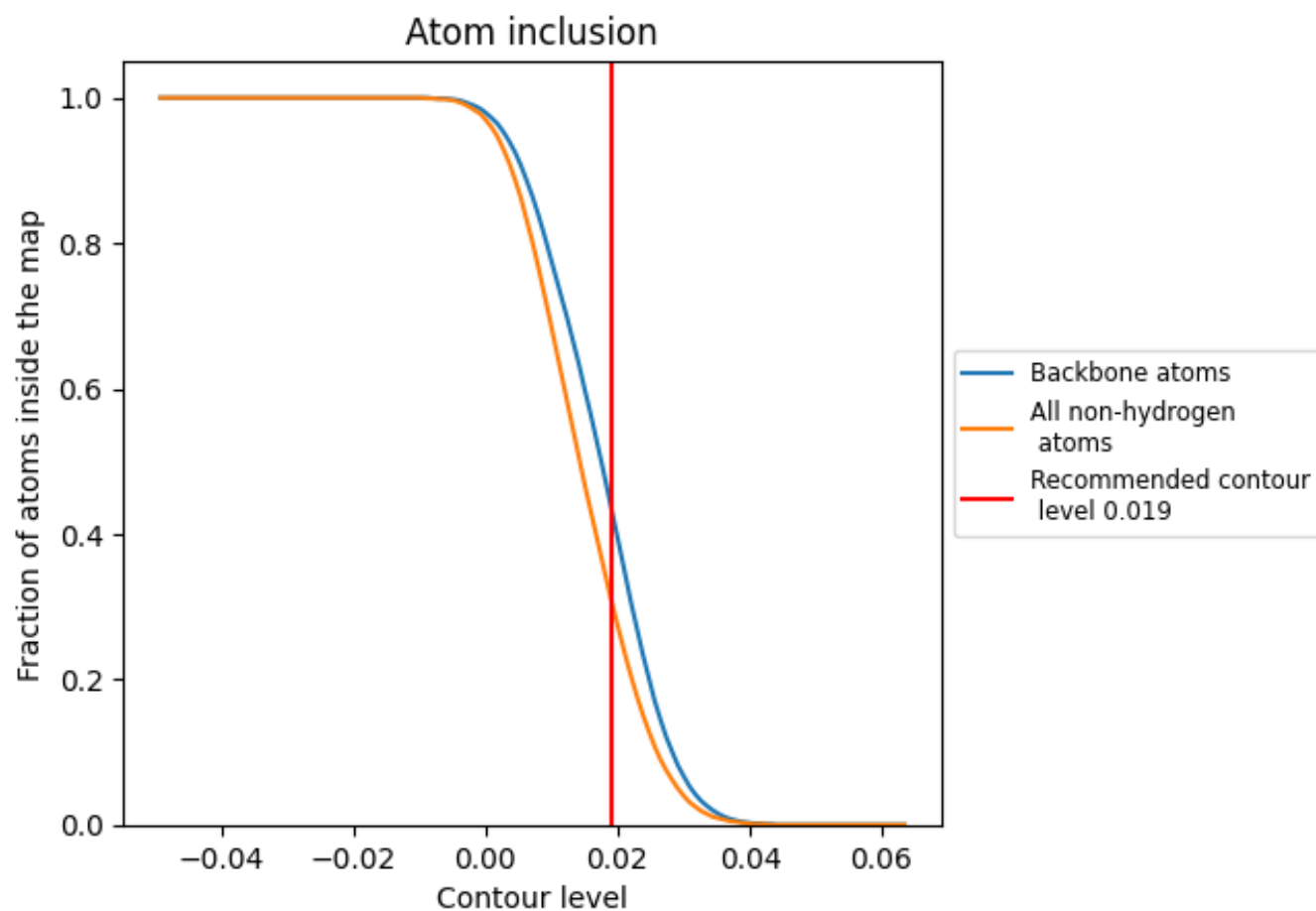
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.019).

9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 31% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3100	 0.4300
A	 0.0170	 0.1030
C	 0.0190	 0.1850
E	 0.0350	 0.1650
F	 0.1000	 0.3010
G	 0.3070	 0.4630
H	 0.4230	 0.4860
I	 0.4030	 0.4820
J	 0.3360	 0.4690
K	 0.4120	 0.4810
L	 0.3660	 0.4750
M	 0.3180	 0.4690
N	 0.1870	 0.3950
O	 0.1990	 0.3710
P	 0.1270	 0.3470
Q	 0.1950	 0.3570
R	 0.1290	 0.3740
S	 0.1120	 0.3710
T	 0.2090	 0.4150
U	 0.3140	 0.4590
V	 0.3100	 0.4470
W	 0.3340	 0.4730
X	 0.2610	 0.4490
Y	 0.2850	 0.4550
Z	 0.1620	 0.4000

