



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 02:17 AM UTC

PDB ID : 6W2D / pdb_00006w2d
EMDB ID : EMD-21525
Title : Structures of Capsid and Capsid-Associated Tegument Complex inside the Epstein-Barr Virus
Authors : Liu, W.; Cui, Y.X.; Wang, C.Y.; Li, Z.H.; Gong, D.Y.; Dai, X.H.; Bi, G.Q.; Sun, R.; Zhou, Z.H.
Deposited on : 2020-03-05
Resolution : 4.00 Å(reported)

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

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

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:

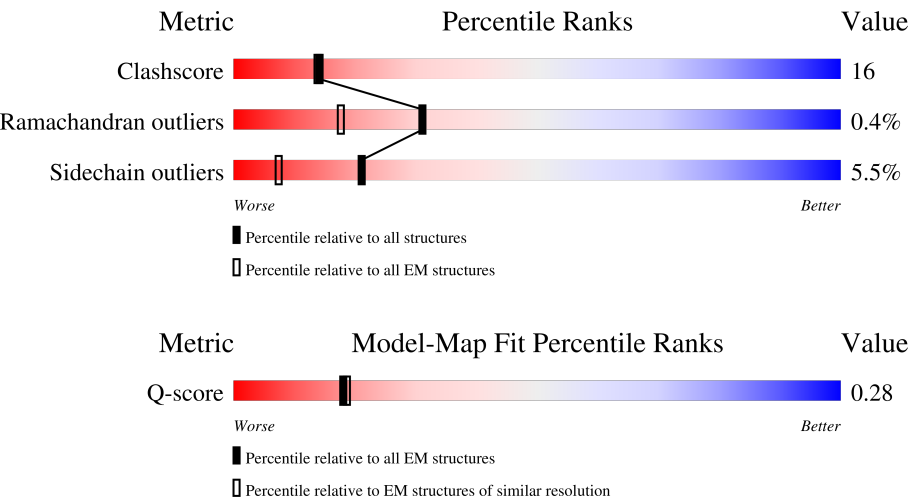
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	J	1381	40% 62% 33% ..
1	K	1381	42% 68% 31% .
1	N	1381	51% 66% 30% ..
1	O	1381	43% 64% 30% ..

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Mol	Chain	Length	Quality of chain
1	P	1381	
2	v	507	
3	w	570	
3	x	570	
4	y	3149	
4	z	3149	
5	Z	176	
5	a	176	
5	d	176	
5	e	176	
5	u	176	
6	f	364	
6	h	364	
7	k	301	
7	m	301	
7	p	301	
7	r	301	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 74272 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	1352	Total	C	N	O	S	0	0
			10628	6744	1849	1974	61		
1	K	1381	Total	C	N	O	S	0	0
			10832	6868	1884	2018	62		
1	N	1362	Total	C	N	O	S	0	0
			10683	6777	1854	1991	61		
1	O	1332	Total	C	N	O	S	0	0
			10447	6633	1812	1942	60		
1	P	1283	Total	C	N	O	S	0	0
			10113	6429	1754	1871	59		

- Molecule 2 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	v	292	Total	C	N	O	S	0	0
			2283	1469	397	406	11		

- Molecule 3 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	w	68	Total	C	N	O	S	0	0
			549	332	106	108	3		
3	x	68	Total	C	N	O	S	0	0
			549	332	106	108	3		

- Molecule 4 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	y	37	Total	C	N	O	0	0
			317	200	64	53		
4	z	37	Total	C	N	O	0	0
			317	200	64	53		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Z	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
5	a	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
5	d	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
5	e	77	Total	C	N	O	S	0	0
			649	411	121	115	2		
5	u	63	Total	C	N	O	S	0	0
			528	339	90	98	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	315	Total	C	N	O	S	0	0
			2474	1586	436	444	8		
6	h	336	Total	C	N	O	S	0	0
			2604	1667	458	471	8		

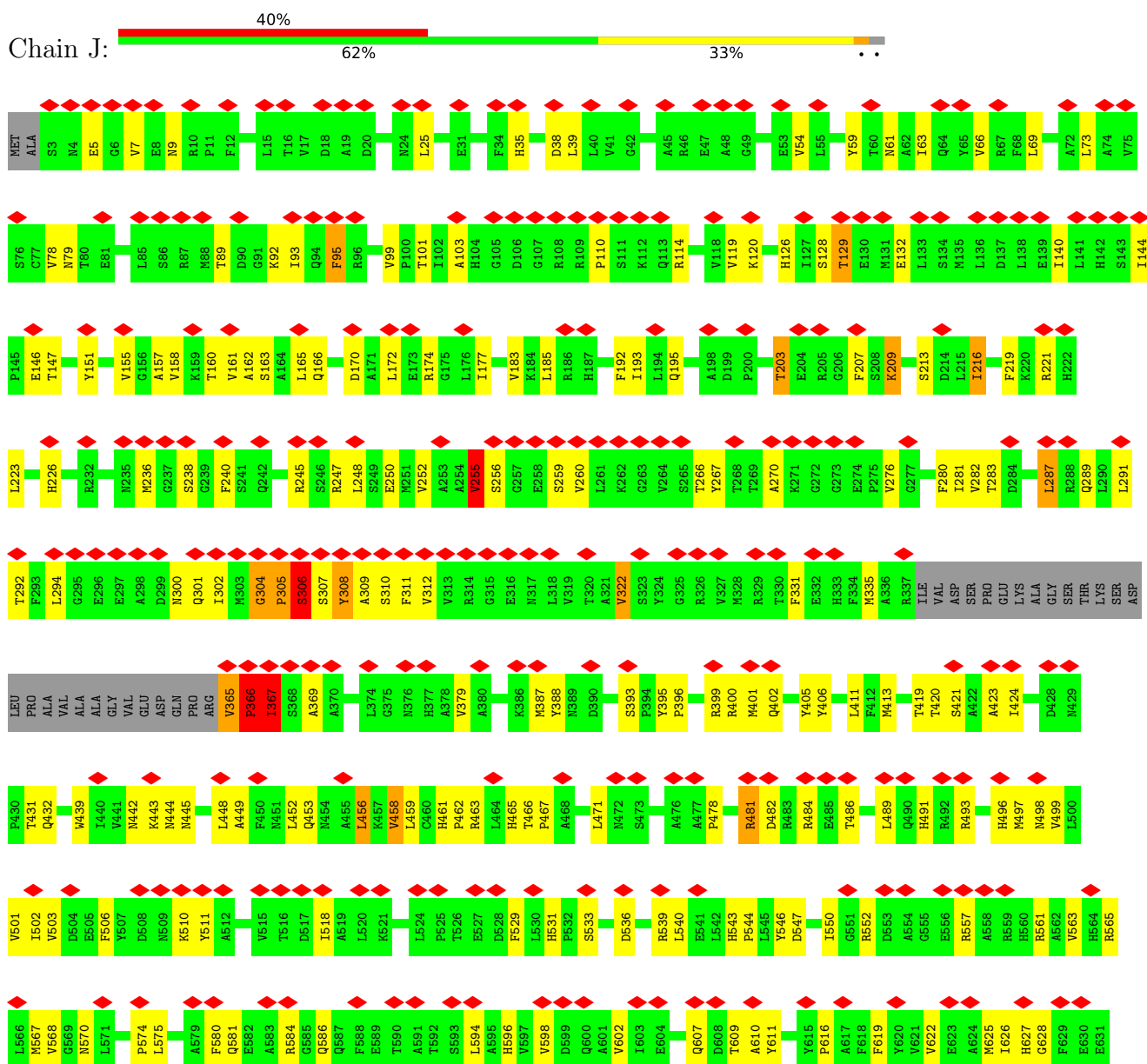
- Molecule 7 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	m	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	p	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	r	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		

3 Residue-property plots

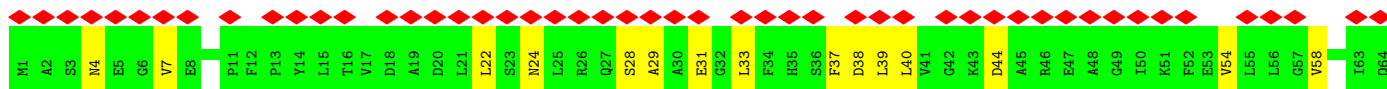
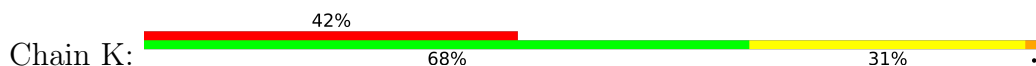
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

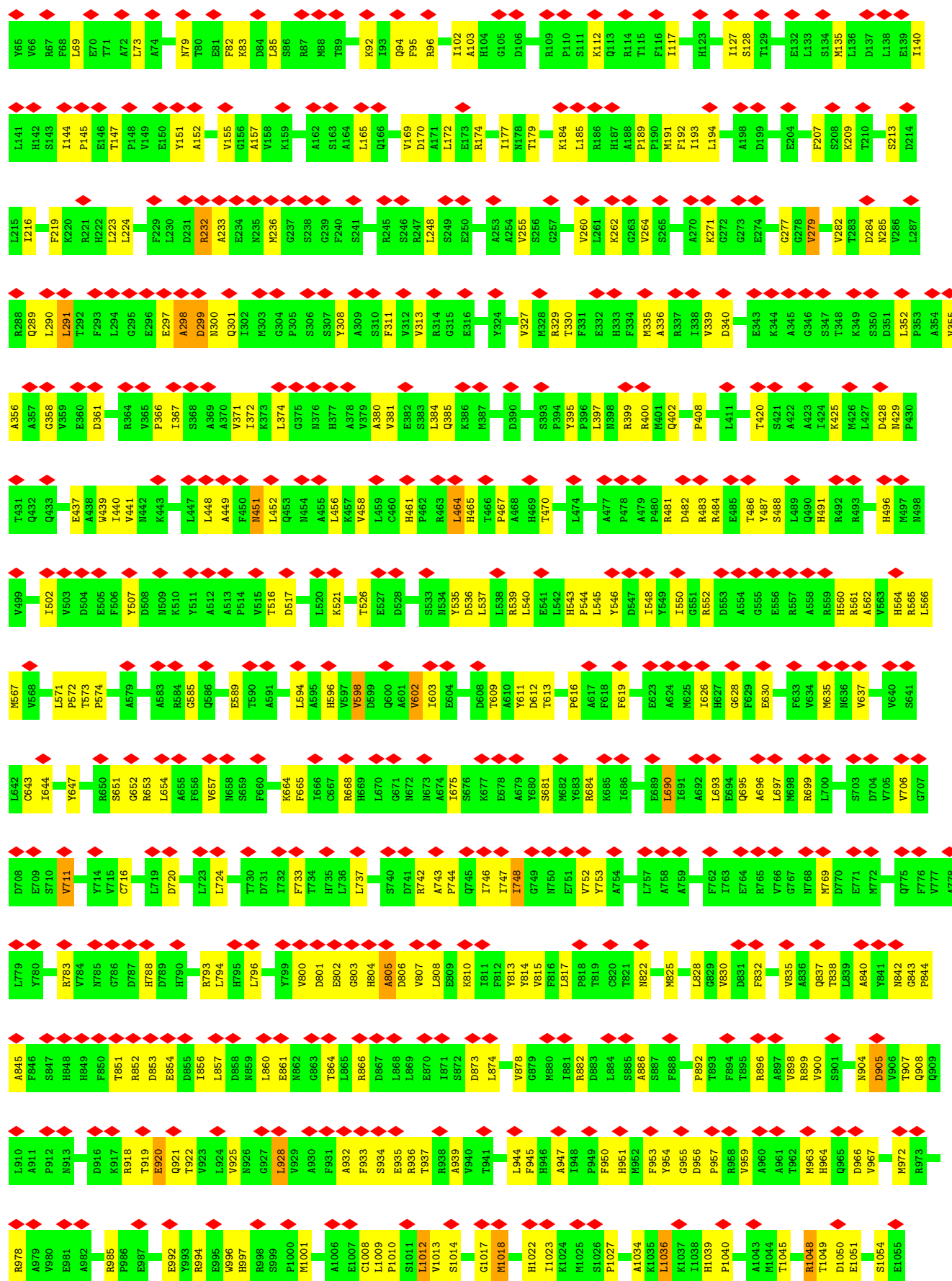
• Molecule 1: Major capsid protein

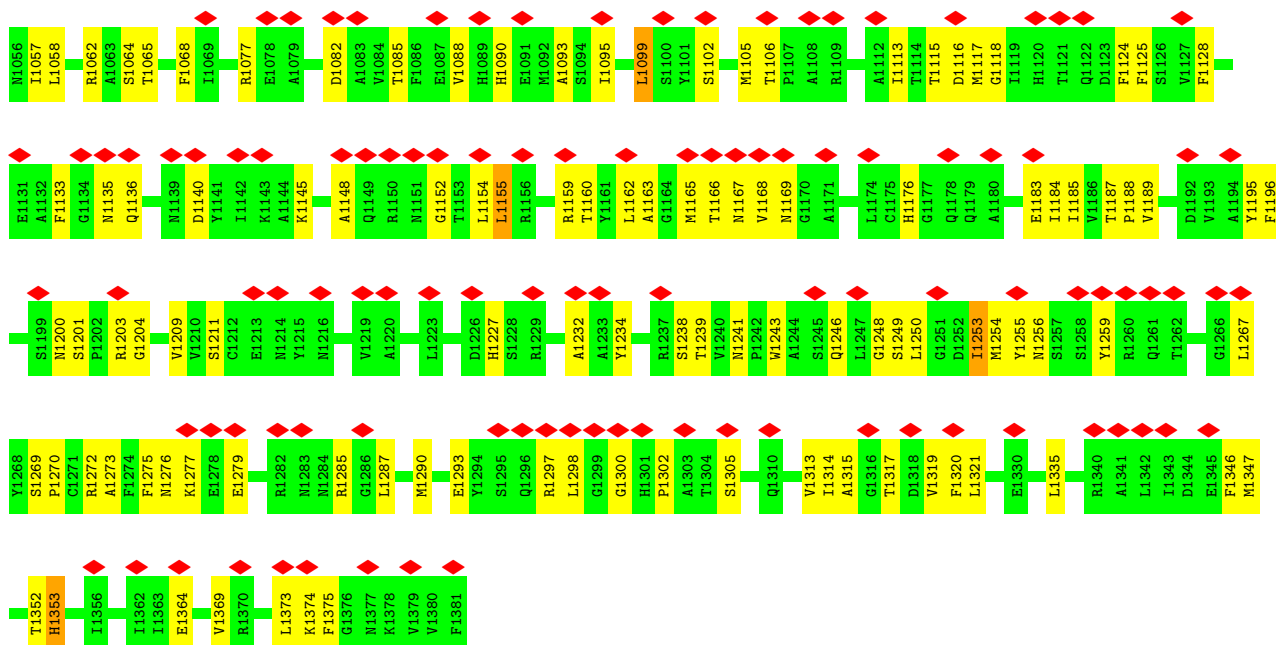




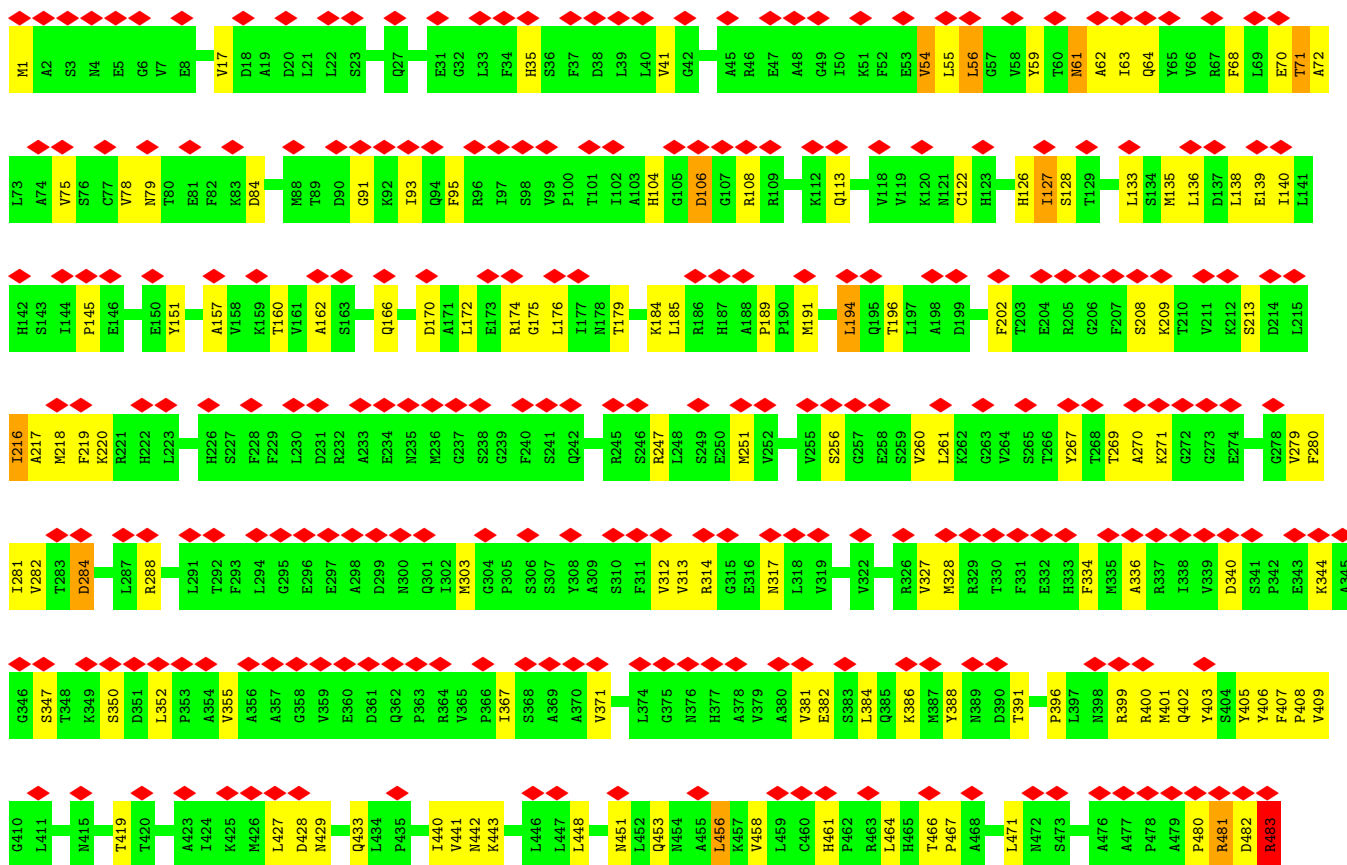
• Molecule 1: Major capsid protein



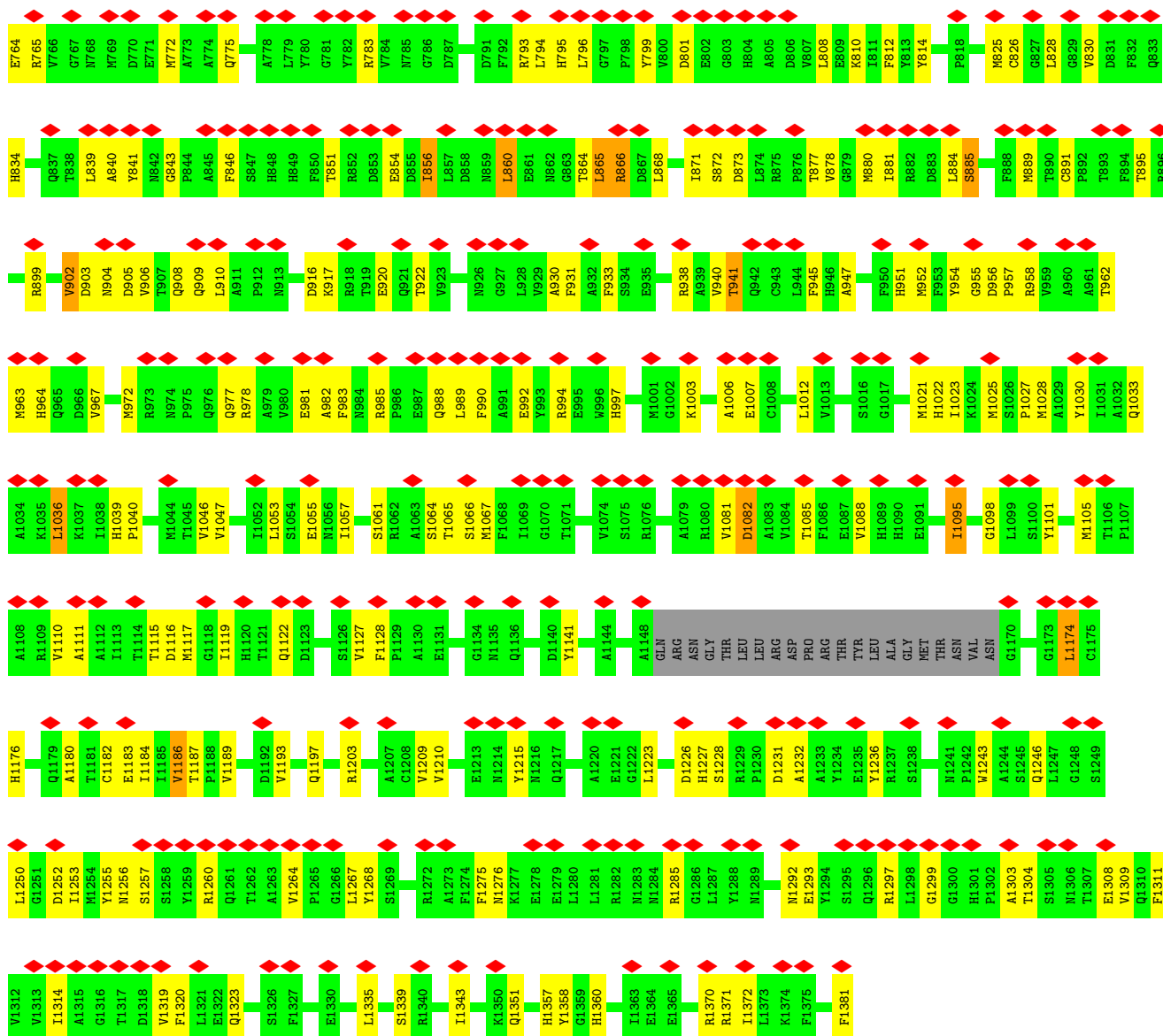




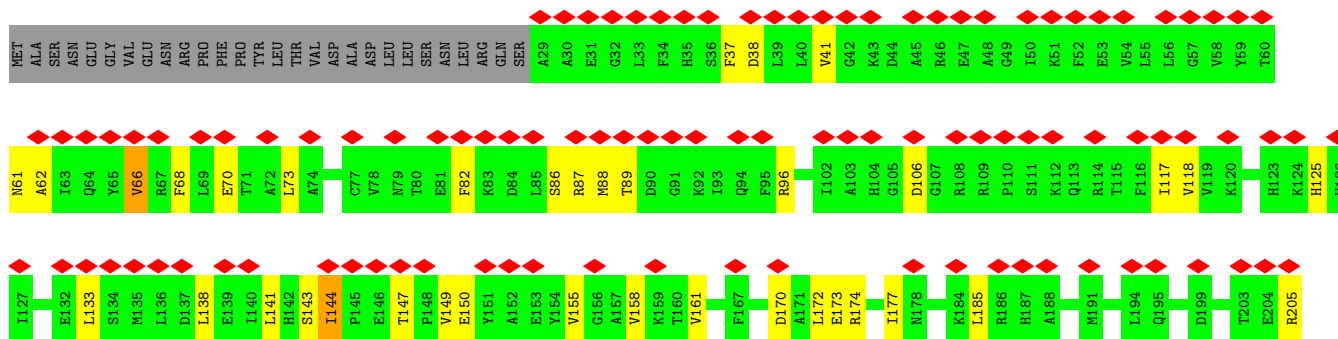
• Molecule 1: Major capsid protein



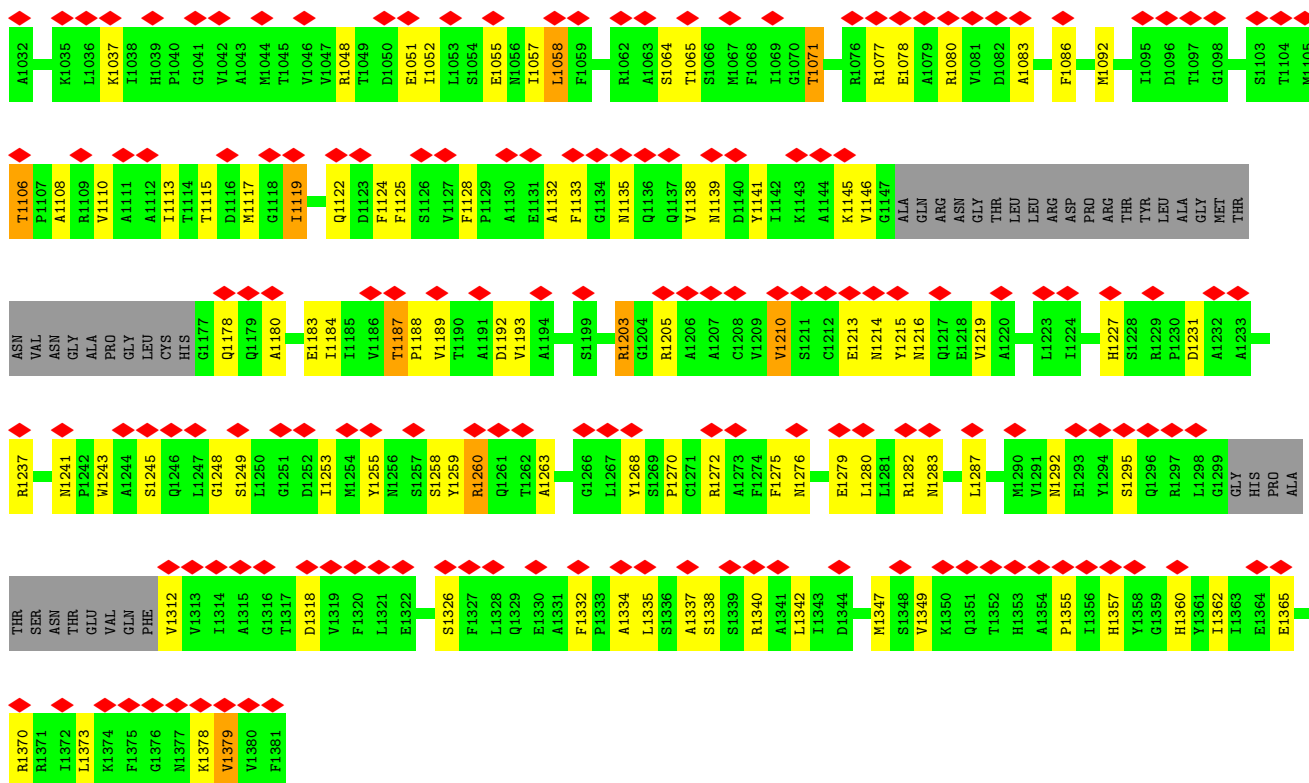
E1278	E1279	L1280	L1281	N1282	N1283	N1284	R1285	G1286	L1287	Y1288	N1289	E1293	Y1294	S1295	Q1296	R1297	L1298	G1299	G1300	H1301	P1302	A1303	T1304	S1305	N1306	T1307	E1308	F1311	V1312	I1313	A1314	A1315	G1316	T1317	D1318	L1321	E1322	F1327	L1328	Q1329	A1330	A1331	F1332	F1333	A1334	L1335	S1336	A1337	S1338	S1339	R1340	D1344	E1345	F1346				
V1210	N1214	N1215	N1216	Q1217	A1220	E1221	G1222	L1223	D1226	H1227	S1228	R1229	P1230	D1231	A1232	A1233	Y1236	R1237	S1238	T1239	V1240	N1241	A1244	L1247	L1250	G1251	D1252	I1253	M1254	Y1255	N1256	S1257	S1258	R1259	Q1261	T1262	A1263	V1264	P1265	G1266	L1267	Y1268	S1269	G1271	R1272	A1273	F1274	F1275	N1276	K1277								
K1145	V1146	G1147	A1148	Q1149	ARG	ASN	GLY	THR	LEU	ARG	ASP	PRO	ARG	THR	TYR	LEU	ALA	GLY	MET	THR	ASN	VAL	M1169	G1170	A1171	P1172	G1173	L1174	C1175	H1176	G1177	Q1178	Q1179	A1180	T1181	I1184	T1187	P1188	A1191	D1192	Y1195	F1196	S1199	M1200	S1201	F1202	R1203	G1204	H1205	A1206	A1207	C1208	V1209					
N1073	V1074	S1075	R1076	R1077	E1078	A1079	R1080	V1081	A1083	V1084	V1088	H1089	H1090	E1091	H1092	A1093	ASN	I1095	D1096	T1097	G1098	L1099	S1100	Y1101	S1102	M1105	T1106	R1109	V1110	A1111	A1112	I1113	T1114	T1115	D1116	G1117	G1118	I1119	Q1122	D1123	F1124	V1127	F1128	P1129	A1130	E1131	G1134	D1140	K1143	A1144								
A1005	A1006	E1007	C1008	P1010	S1011	V1013	S1016	G1017	M1018	T1019	A1020	M1021	H1022	Y1023	K1024	M1025	H1028	I1031	A1032	Q1033	A1034	K1035	L1036	I1038	H1039	A1043	M1044	V1047	R1048	T1049	D1050	F1051	N1052	L1053	S1054	E1055	N1056	I1057	L1058	F1059	S1060	A1063	S1064	T1065	S1066	M1067	I1069	G1070										
L944	F945	H946	A947	I948	N899	P949	F950	H951	M952	F953	Y954	G955	R958	V959	A961	T962	M963	H964	Q965	D966	V967	A968	T969	F970	V971	M972	R973	N974	P975	Q976	Q977	R978	A979	V980	E981	A982	F983	R984	R985	F986	E987	Q988	L989	F990	A991	E992	Y993	R994	E995	W996	H997	R998	S999	P1000	M1001	K1002	K1003	Y1004
L884	S885	A886	S887	F888	N889	T890	C891	P892	T893	F894	T895	R896	A897	V898	R899	V900	S901	Y902	D903	N904	D905	V906	Q908	Q909	L910	A911	P912	N913	P914	A915	D916	K917	R918	T919	E920	Q921	T922	L923	V925	N926	G927	L928	V929	A930	F931	A932	F933	S934	E935	R936	R938	A939	T941	Q942	C943			
A823	H824	N825	C826	G827	L828	G829	V830	D831	F832	Q833	H834	V835	A836	Q837	T838	L839	A840	Y841	N842	G843	P844	A845	F846	S847	H848	H849	F850	T851	R852	D853	E854	D855	L856	L857	D858	N859	L860	E861	T864	L865	R866	D867	L868	L869	E870	T871	S872	D873	L874	R875	F876	T877	V878	N880	I881	R882	D883	
A758	Q761	F762	I763	E764	R765	V766	G767	N768	M769	D770	E771	M772	A773	A774	Q775	A778	L779	Y780	G781	Y782	R783	V784	N785	G786	F787	N788	H789	Y790	D791	F792	R793	L794	H795	L796	Y799	V800	D801	E802	G803	H804	A805	D806	V807	L808	E809	K810	I811	F812	Y813	Y814	L817	P818	T819	N822				
L690	I691	A692	L693	E694	Q695	A696	L697	M698	R699	L700	A701	G702	C569	D704	T644	N645	T646	Y647	E648	R650	S651	G652	L654	A655	F656	V657	N658	S659	F660	S661	M662	I663	K664	F665	I666	C667	R668	H669	L670	G671	N672	N673	A674	T675	S676	K677	E678	A679	Y680	S681	M682	Y683	R684	K685	I686	Y687	G688	E689
E556	R557	A558	R559	H560	R561	A562	R565	L566	M567	V568	C569	N570	L571	P574	L575	F580	Q581	E582	A583	R584	Q587	A591	A595	H596	V597	V598	D599	G523	A601	V602	T526	E527	N534	Y535	D536	L537	L538	R539	L540	H543	P544	L545	Y546	D547	I548	Y549	I550	G551	R552	D553	A554	G555						



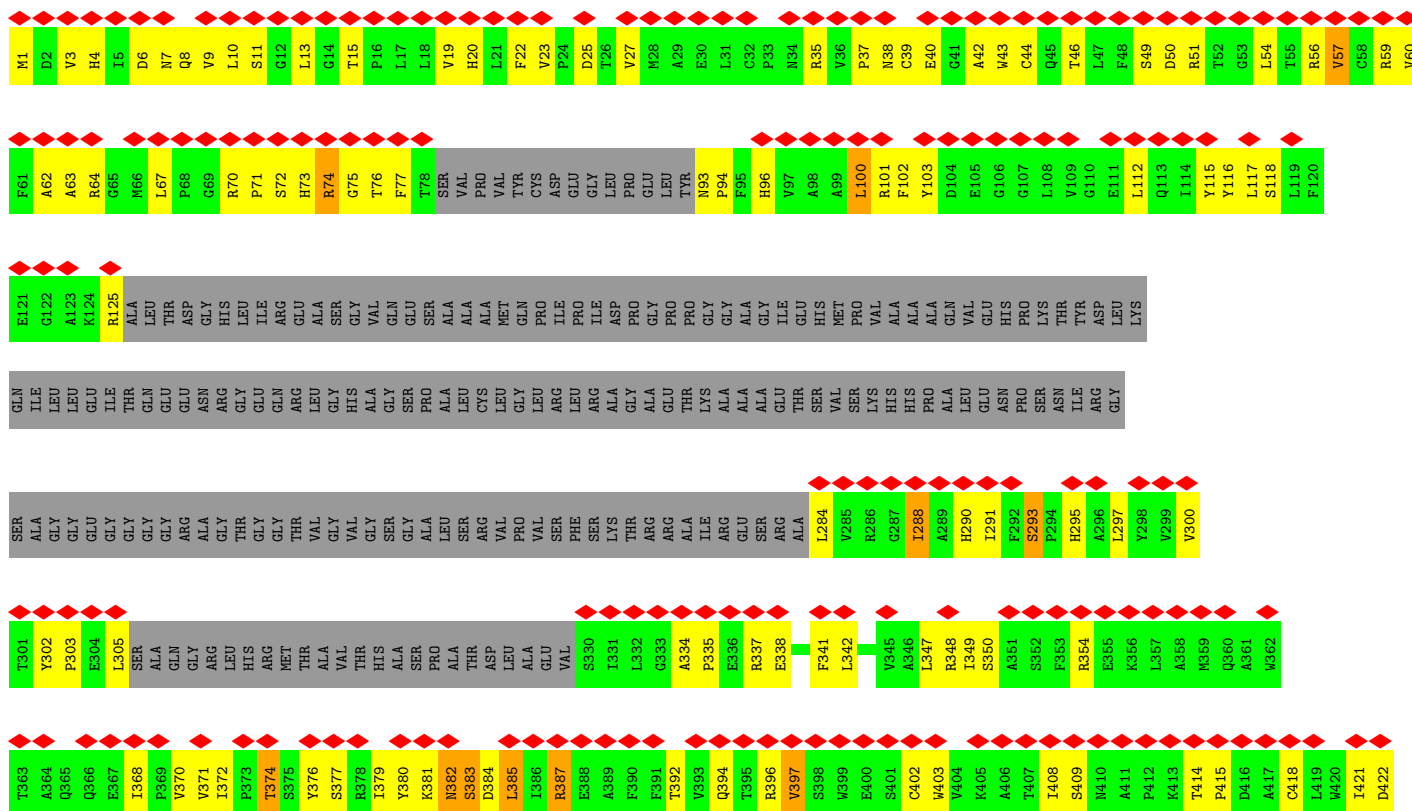
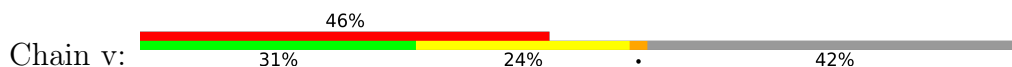
• Molecule 1: Major capsid protein







• Molecule 2: Capsid vertex component 1



[illegible]

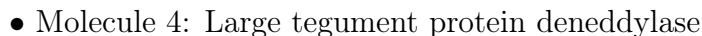
- Molecule 4: Large tegument protein deneddylase

Chain v: 99%

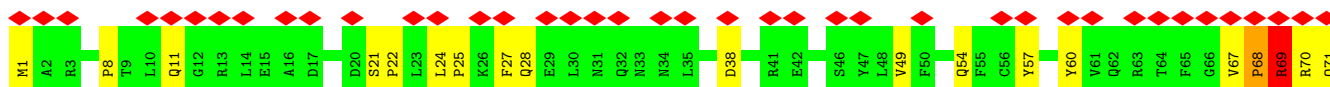
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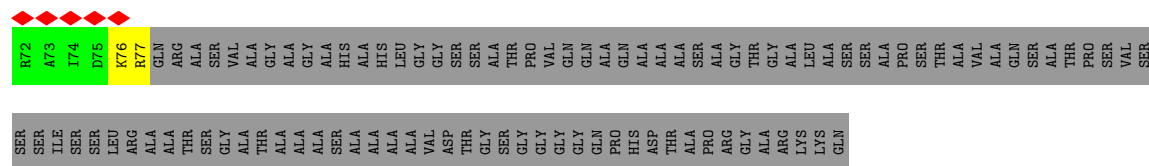




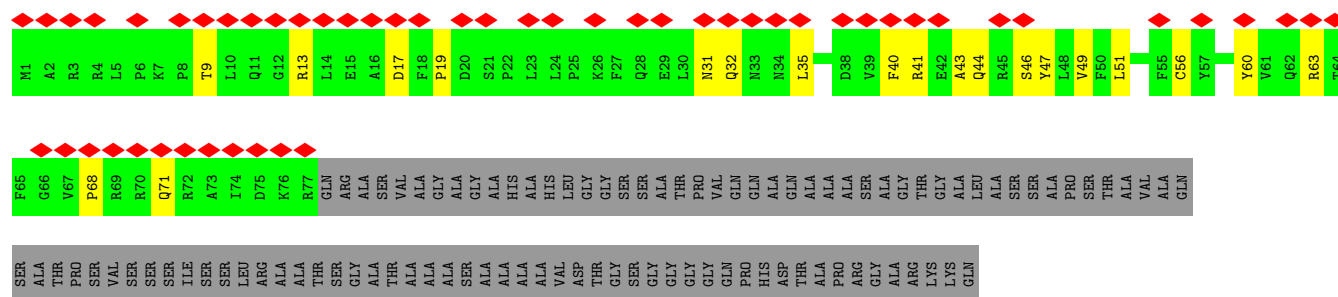
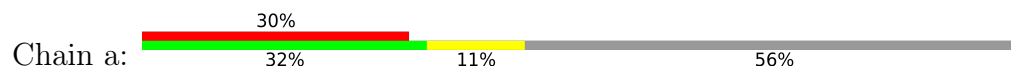
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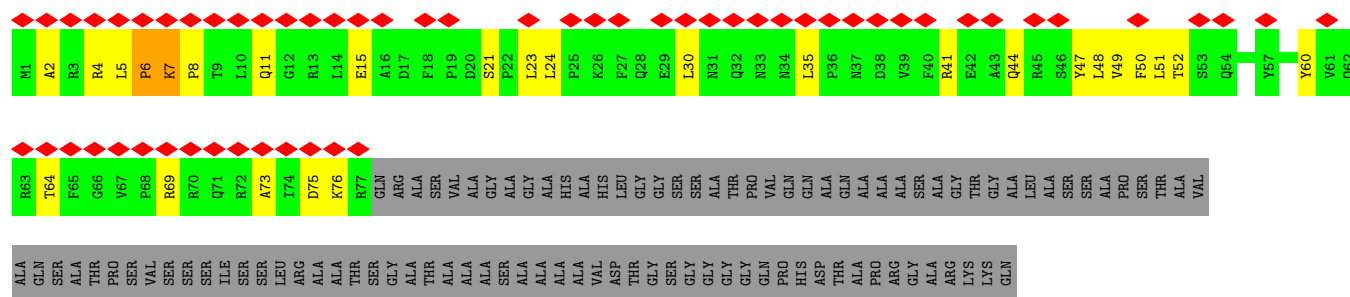
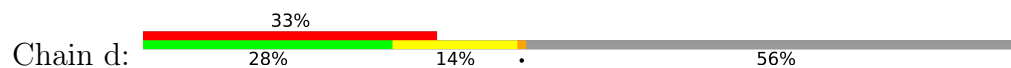
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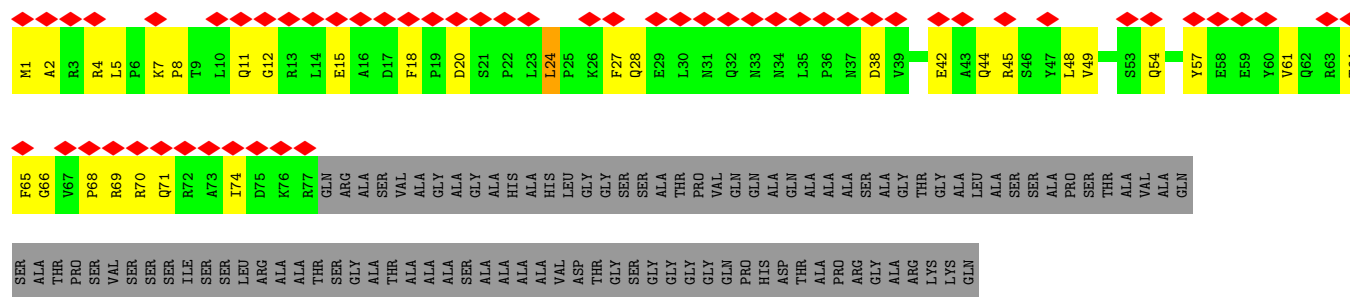
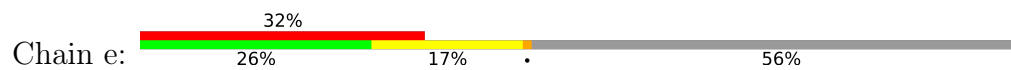
• Molecule 5: Small capsomere-interacting protein



• Molecule 5: Small capsomere-interacting protein

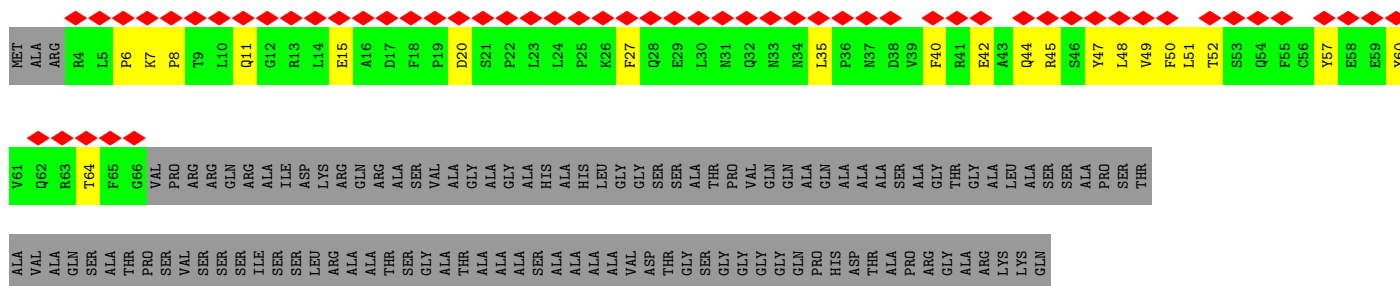


• Molecule 5: Small capsomere-interacting protein

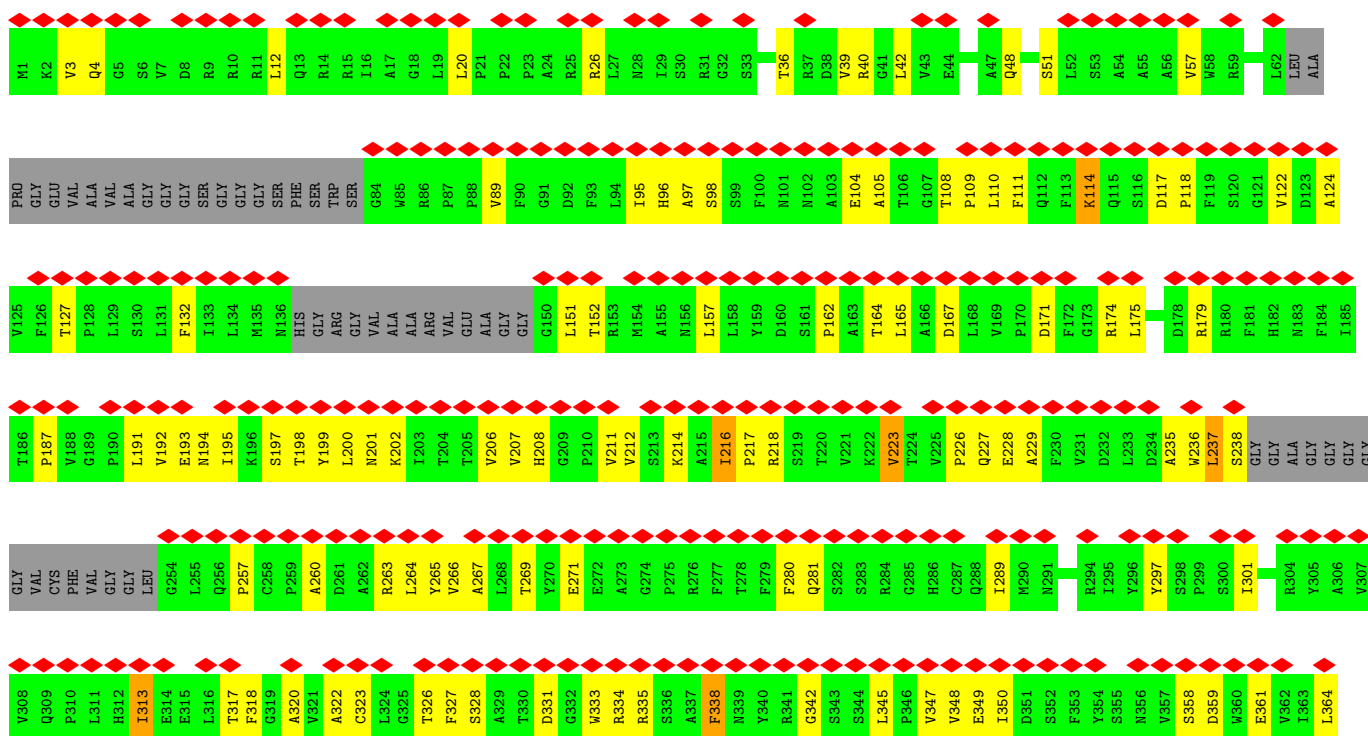


• Molecule 5: Small capsomere-interacting protein

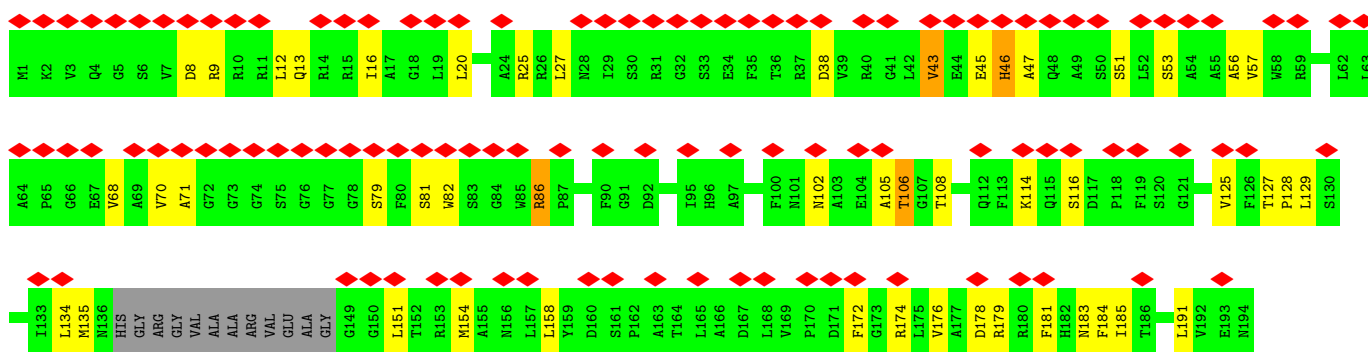


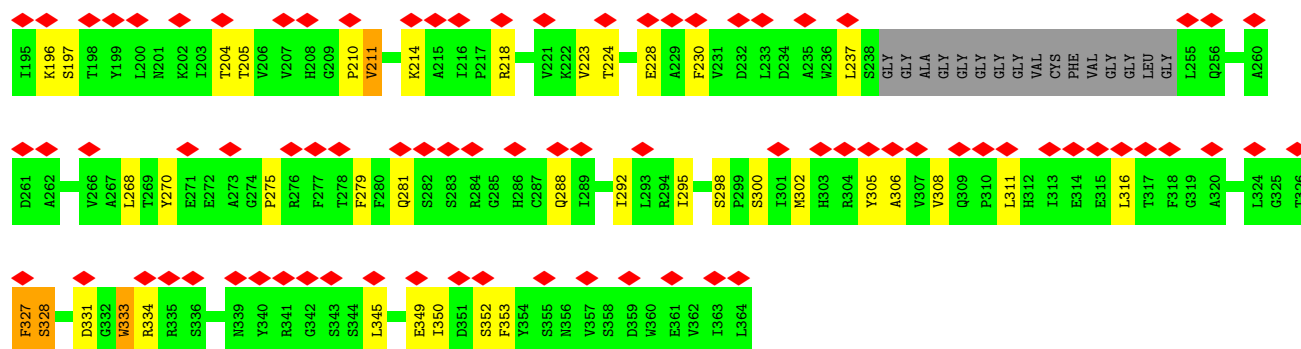


• Molecule 6: Triplex capsid protein 1

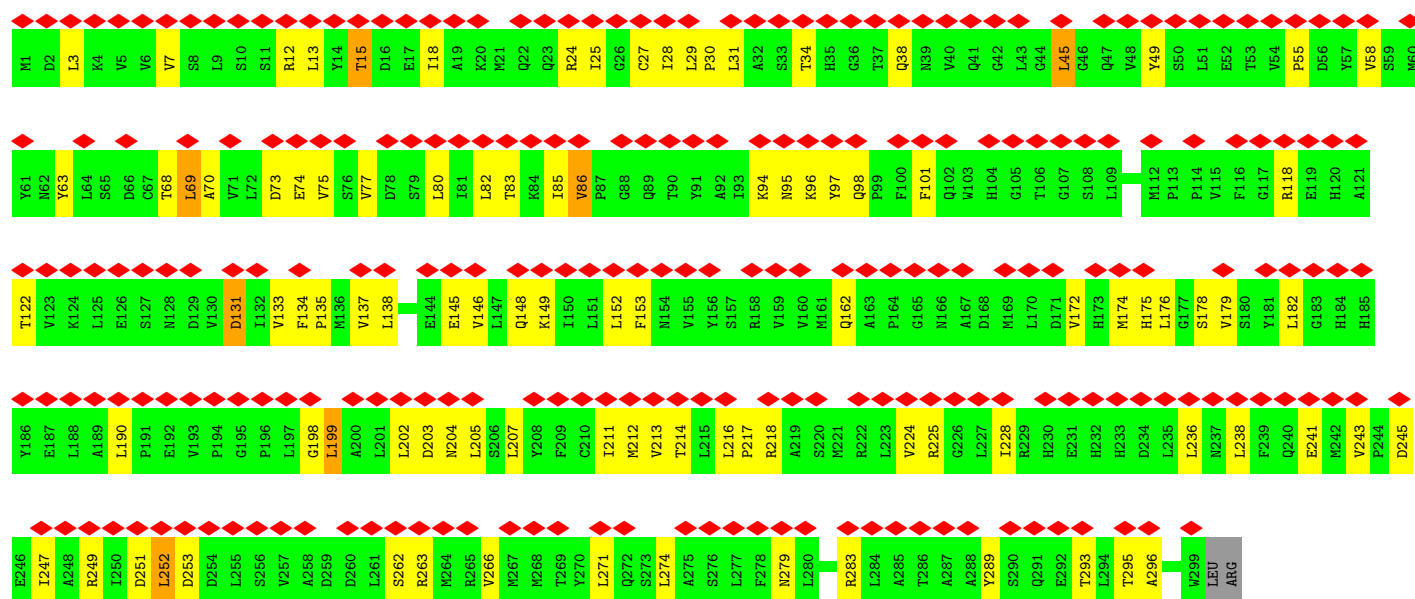
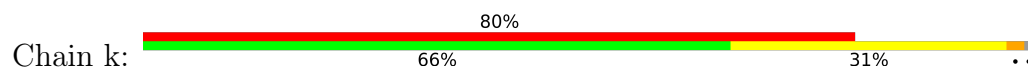


• Molecule 6: Triplex capsid protein 1

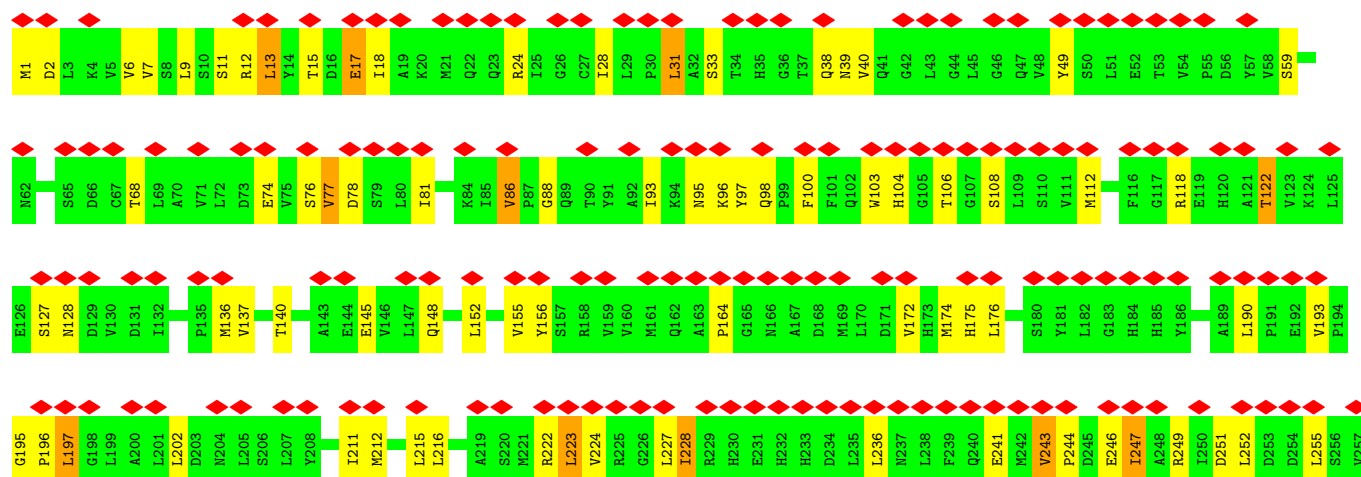


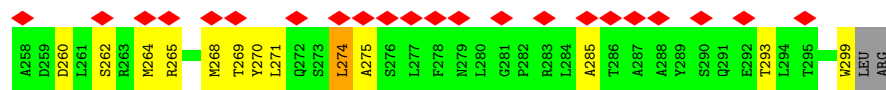


• Molecule 7: Triplex capsid protein 2

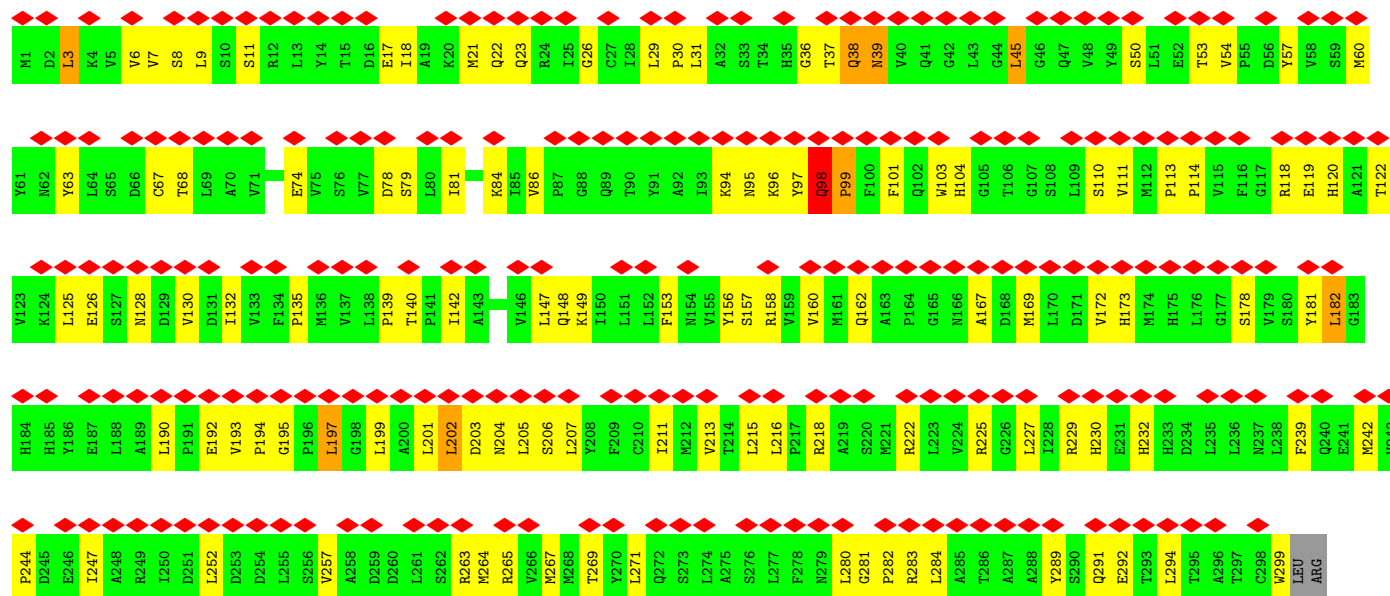
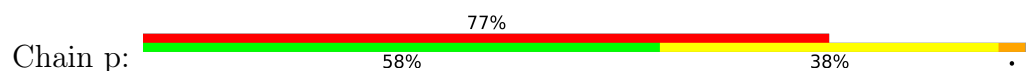


• Molecule 7: Triplex capsid protein 2

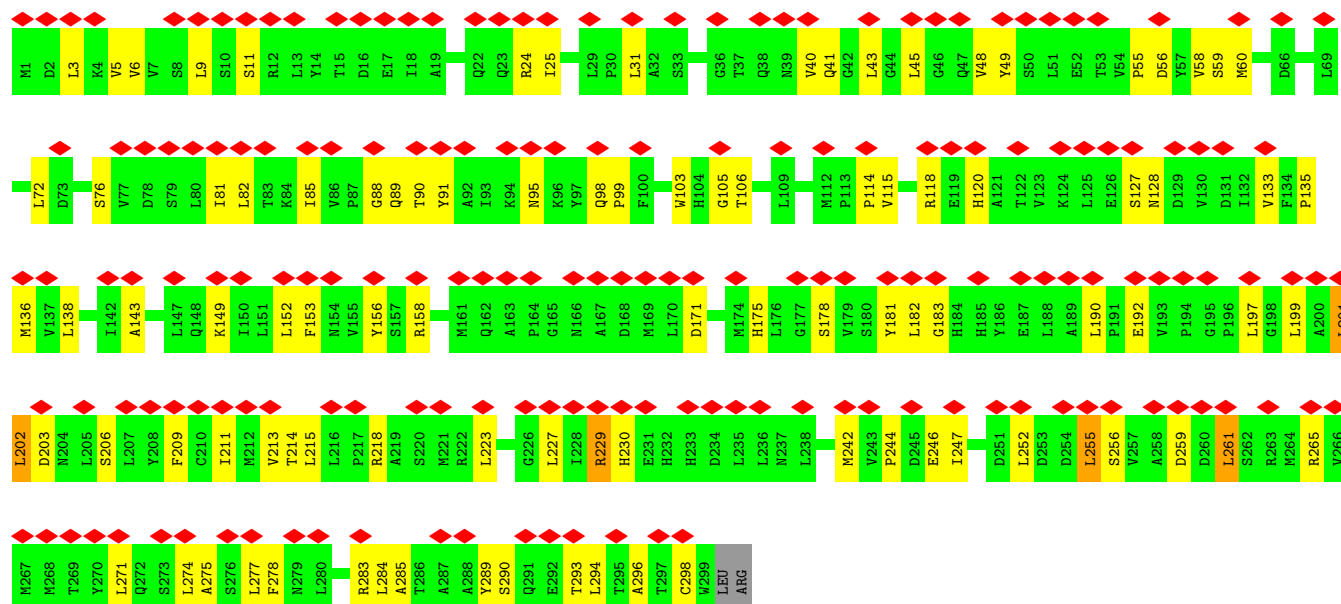




• Molecule 7: Triplex capsid protein 2



• Molecule 7: Triplex capsid protein 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21085	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 ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.058	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	J	0.28	0/10877	0.47	3/14781 (0.0%)
1	K	0.27	0/11085	0.44	1/15066 (0.0%)
1	N	0.26	0/10933	0.42	0/14858
1	O	0.26	0/10693	0.42	0/14531
1	P	0.23	0/10349	0.43	1/14057 (0.0%)
2	v	0.23	0/2341	0.43	0/3183
3	w	0.19	0/553	0.39	0/741
3	x	0.22	0/553	0.44	0/741
4	y	0.21	0/320	0.45	0/424
4	z	0.22	0/320	0.42	0/424
5	Z	0.20	0/664	0.44	0/896
5	a	0.22	0/664	0.43	0/896
5	d	0.21	0/664	0.51	0/896
5	e	0.21	0/664	0.42	0/896
5	u	0.20	0/542	0.44	0/735
6	f	0.22	0/2537	0.45	0/3450
6	h	0.26	0/2672	0.46	0/3635
7	k	0.22	0/2388	0.44	0/3254
7	m	0.24	0/2388	0.45	0/3254
7	p	0.21	0/2388	0.45	0/3254
7	r	0.24	0/2388	0.42	0/3254
All	All	0.25	0/75983	0.44	5/103226 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	304	GLY	CA-C-N	7.65	129.40	119.84
1	J	304	GLY	C-N-CA	7.65	129.40	119.84
1	P	319	VAL	N-CA-C	-5.84	107.60	113.20
1	J	366	PRO	N-CA-C	-5.58	100.97	112.47
1	K	299	ASP	N-CA-C	-5.36	105.44	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	10628	0	10448	366	0
1	K	10832	0	10655	323	0
1	N	10683	0	10500	379	0
1	O	10447	0	10273	357	0
1	P	10113	0	9949	290	0
2	v	2283	0	2268	132	0
3	w	549	0	540	19	0
3	x	549	0	540	32	0
4	y	317	0	341	17	0
4	z	317	0	341	16	0
5	Z	649	0	649	51	0
5	a	649	0	649	19	0
5	d	649	0	649	32	0
5	e	649	0	649	28	0
5	u	528	0	510	27	0
6	f	2474	0	2459	78	0
6	h	2604	0	2577	62	0
7	k	2338	0	2364	75	0
7	m	2338	0	2364	65	0
7	p	2338	0	2364	110	0
7	r	2338	0	2364	70	0
All	All	74272	0	73453	2308	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 16.

All (2308) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:258:GLU:CG	1:O:262:LYS:CD	1.74	1.55
1:O:258:GLU:HG2	1:O:262:LYS:CD	1.28	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:483:ARG:NH1	1:N:485:GLU:HG2	1.25	1.40
1:O:743:ALA:HB2	2:v:73:HIS:NE2	1.21	1.40
1:O:258:GLU:CG	1:O:262:LYS:HD2	0.91	1.39
5:Z:68:PRO:HB3	5:Z:71:GLN:NE2	1.29	1.38
1:O:743:ALA:HB2	2:v:73:HIS:CD2	1.60	1.37
1:O:258:GLU:CB	1:O:262:LYS:HD2	1.63	1.29
1:N:672:ASN:ND2	1:O:871:ILE:O	1.67	1.28
1:O:743:ALA:CB	2:v:73:HIS:NE2	1.98	1.24
1:N:484:ARG:HB3	1:N:551:GLY:O	1.36	1.22
5:Z:68:PRO:CB	5:Z:71:GLN:NE2	2.03	1.21
1:N:484:ARG:NH2	1:N:558:ALA:HA	1.58	1.18
1:N:483:ARG:HH11	1:N:485:GLU:CG	1.59	1.15
7:p:97:TYR:O	7:p:98:GLN:HB2	1.35	1.12
1:J:69:LEU:HD13	1:J:308:TYR:CD2	1.84	1.11
1:N:483:ARG:NH1	1:N:485:GLU:CG	2.13	1.10
1:O:258:GLU:HG2	1:O:262:LYS:HD3	1.31	1.09
1:N:480:PRO:O	1:N:481:ARG:HG2	1.50	1.08
1:N:484:ARG:HH21	1:N:558:ALA:HA	0.94	1.06
1:N:484:ARG:CB	1:N:551:GLY:O	2.06	1.04
1:N:484:ARG:HD2	1:N:550:ILE:CG2	1.86	1.03
1:N:484:ARG:HH21	1:N:558:ALA:CA	1.71	1.03
1:J:365:VAL:O	1:J:366:PRO:O	1.77	1.02
1:N:484:ARG:NH2	1:N:558:ALA:CA	2.23	1.01
1:O:258:GLU:HG3	1:O:262:LYS:HD2	1.10	1.00
1:O:258:GLU:HG3	1:O:262:LYS:CD	1.62	0.98
1:K:464:LEU:HD11	1:K:1254:MET:CG	1.94	0.98
1:N:670:LEU:O	1:N:674:ALA:HB3	1.64	0.97
5:Z:68:PRO:HB3	5:Z:71:GLN:HE22	1.17	0.96
1:N:480:PRO:O	1:N:481:ARG:NE	1.99	0.95
1:O:258:GLU:O	1:O:259:SER:O	1.85	0.94
1:N:483:ARG:HH12	1:N:485:GLU:HG2	1.23	0.94
1:J:69:LEU:HD13	1:J:308:TYR:CE2	2.02	0.92
1:O:743:ALA:CB	2:v:73:HIS:CD2	2.44	0.92
1:N:484:ARG:NH2	1:N:558:ALA:CB	2.33	0.92
1:N:834:HIS:HD2	5:d:8:PRO:HD3	1.34	0.91
2:v:35:ARG:HE	2:v:37:PRO:HB3	1.35	0.90
1:N:677:LYS:O	1:N:679:ALA:N	2.03	0.90
1:J:308:TYR:HB3	1:J:312:VAL:HG23	1.52	0.90
1:O:258:GLU:HG3	1:O:262:LYS:HZ2	1.34	0.89
1:N:480:PRO:O	1:N:481:ARG:CG	2.20	0.89
1:J:308:TYR:O	1:J:312:VAL:N	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:831:ASP:HB3	5:d:5:LEU:HD22	1.56	0.88
1:J:1205:ARG:NH2	1:J:1223:LEU:O	2.07	0.88
1:N:677:LYS:O	1:N:680:TYR:N	2.07	0.88
1:K:271:LYS:HD3	1:K:299:ASP:HB2	1.54	0.87
1:O:258:GLU:O	1:O:262:LYS:HB3	1.73	0.87
1:K:465:HIS:CE1	1:K:1027:PRO:HD3	2.10	0.86
1:N:565:ARG:HA	1:N:998:ARG:HH12	1.40	0.86
1:K:464:LEU:HD11	1:K:1254:MET:SD	2.16	0.86
1:K:861:GLU:OE2	5:Z:67:VAL:HG11	1.74	0.86
1:N:644:ILE:HG22	1:N:675:ILE:HG21	1.57	0.85
2:v:464:HIS:HB3	2:v:476:VAL:HB	1.58	0.84
1:O:488:SER:HB2	1:O:992:GLU:H	1.43	0.84
1:N:59:TYR:CD1	1:O:260:VAL:HG21	2.11	0.84
2:v:67:LEU:HB2	2:v:72:SER:OG	1.76	0.84
6:h:16:ILE:O	6:h:20:LEU:HB2	1.77	0.84
2:v:354:ARG:HH11	2:v:394:GLN:HE22	1.26	0.83
7:p:98:GLN:HG3	7:p:120:HIS:CE1	2.13	0.83
1:O:258:GLU:HG3	1:O:262:LYS:NZ	1.94	0.82
1:O:258:GLU:HG3	1:O:262:LYS:CE	2.08	0.82
1:N:677:LYS:HG2	1:N:678:GLU:N	1.95	0.82
1:O:568:VAL:HA	1:O:1025:MET:HE3	1.62	0.82
1:K:804:HIS:O	1:K:805:ALA:HB2	1.80	0.82
1:K:861:GLU:CB	5:Z:69:ARG:HD2	2.09	0.82
1:O:303:MET:HE2	1:O:366:PRO:HG3	1.59	0.81
1:J:463:ARG:NH2	1:J:1253:ILE:O	2.13	0.81
1:N:484:ARG:HD2	1:N:550:ILE:HG22	1.61	0.81
1:J:301:GLN:HB3	1:J:366:PRO:HB2	1.61	0.81
1:O:303:MET:SD	1:O:364:ARG:NH2	2.53	0.81
1:O:258:GLU:O	1:O:262:LYS:CB	2.29	0.81
1:P:568:VAL:HA	1:P:1025:MET:HE3	1.62	0.80
1:K:185:LEU:HD13	1:K:399:ARG:HH21	1.47	0.80
1:K:399:ARG:NH1	1:K:1320:PHE:O	2.14	0.80
1:N:974:ASN:HD21	1:N:976:GLN:HE21	1.27	0.80
1:N:670:LEU:O	1:N:674:ALA:CB	2.30	0.80
7:p:60:MET:SD	7:p:118:ARG:NH2	2.55	0.80
1:K:184:LYS:NZ	1:K:1064:SER:OG	2.14	0.80
1:O:245:ARG:NH2	1:O:294:LEU:O	2.13	0.80
1:O:743:ALA:CA	2:v:73:HIS:NE2	2.44	0.80
1:J:848:HIS:HE2	5:Z:21:SER:HG	1.24	0.80
1:P:776:PHE:O	1:P:780:TYR:CB	2.29	0.80
1:O:591:ALA:HB1	1:O:1036:LEU:HD12	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:740:SER:HB2	1:N:744:PRO:HG3	1.64	0.79
1:O:1372:ILE:HG23	1:O:1381:PHE:HB3	1.62	0.79
1:N:483:ARG:HH11	1:N:485:GLU:HG2	0.99	0.79
1:N:672:ASN:OD1	1:O:873:ASP:HB2	1.82	0.79
1:P:205:ARG:HH21	1:P:209:LYS:HG2	1.47	0.79
1:K:544:PRO:O	1:K:565:ARG:NH1	2.15	0.79
1:N:480:PRO:C	1:N:481:ARG:HG2	2.08	0.79
1:O:258:GLU:CG	1:O:262:LYS:HD3	1.93	0.79
7:k:24:ARG:HH12	7:k:97:TYR:HE1	1.27	0.79
1:K:861:GLU:HB2	5:Z:69:ARG:HD2	1.63	0.79
1:P:1282:ARG:HD3	6:f:98:SER:HB3	1.64	0.79
1:K:861:GLU:HG3	5:Z:69:ARG:HD2	1.65	0.79
1:N:484:ARG:HD2	1:N:550:ILE:HG21	1.65	0.79
1:K:804:HIS:O	1:K:805:ALA:CB	2.29	0.78
1:P:776:PHE:O	1:P:780:TYR:HB3	1.83	0.78
1:K:997:HIS:HE1	1:K:1022:HIS:HE1	1.32	0.78
1:N:56:LEU:HA	1:O:329:ARG:HB2	1.64	0.78
1:N:674:ALA:C	1:N:675:ILE:HG12	2.08	0.78
1:O:690:LEU:HD21	1:O:812:PHE:HB2	1.65	0.78
1:J:69:LEU:HD13	1:J:308:TYR:CG	2.18	0.78
1:N:442:ASN:OD1	1:N:443:LYS:N	2.16	0.78
1:J:955:GLY:HA3	1:J:985:ARG:HE	1.47	0.78
1:K:861:GLU:CG	5:Z:69:ARG:HD2	2.14	0.78
1:N:737:LEU:HD23	1:N:744:PRO:HG2	1.64	0.78
5:Z:68:PRO:O	5:Z:70:ARG:N	2.17	0.78
1:N:844:PRO:HG2	1:N:856:ILE:HG23	1.67	0.77
7:p:38:GLN:O	7:p:39:ASN:O	2.01	0.77
6:f:216:ILE:HG13	6:f:217:PRO:HD2	1.65	0.77
1:J:195:GLN:NE2	1:J:250:GLU:OE2	2.17	0.77
1:O:185:LEU:HD13	1:O:399:ARG:HH21	1.50	0.77
1:N:484:ARG:CD	1:N:550:ILE:CG2	2.62	0.77
1:O:258:GLU:HG2	1:O:262:LYS:CG	2.14	0.77
1:J:769:MET:HG2	1:J:890:THR:HG21	1.67	0.77
1:N:391:THR:HG21	1:O:102:ILE:HG13	1.65	0.77
1:N:722:ASN:HB3	1:N:902:VAL:HG11	1.67	0.77
1:N:842:ASN:HD21	1:N:860:LEU:HD21	1.50	0.77
3:x:85:ARG:HD3	4:z:3130:LEU:HD13	1.67	0.77
1:N:856:ILE:HG22	1:N:860:LEU:HG	1.67	0.76
1:P:491:HIS:O	1:P:899:ARG:NH2	2.17	0.76
3:x:102:GLN:HA	4:y:3114:GLN:HG3	1.65	0.76
1:N:674:ALA:O	1:N:675:ILE:HG12	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:436:VAL:HG11	1:O:587:GLN:HE22	1.50	0.76
1:P:1272:ARG:NH2	6:f:167:ASP:OD2	2.19	0.76
1:O:1117:MET:SD	1:O:1371:ARG:NH1	2.59	0.76
1:N:924:LEU:HB2	1:N:950:PHE:HZ	1.51	0.76
1:J:166:GLN:HG2	1:J:322:VAL:HG13	1.66	0.76
1:O:1252:ASP:OD1	1:O:1256:ASN:ND2	2.19	0.76
1:O:743:ALA:N	2:v:73:HIS:NE2	2.35	0.75
1:P:1283:ASN:ND2	1:P:1326:SER:OG	2.19	0.75
2:v:67:LEU:HB2	2:v:72:SER:CB	2.16	0.75
7:r:49:TYR:HD2	7:r:60:MET:HE1	1.51	0.75
1:J:481:ARG:HD2	1:J:539:ARG:HD2	1.68	0.75
1:J:670:LEU:HD11	1:J:675:ILE:HG13	1.67	0.75
7:m:222:ARG:NH1	7:m:251:ASP:OD1	2.20	0.75
2:v:67:LEU:HD12	2:v:72:SER:HB2	1.68	0.75
1:N:860:LEU:O	1:N:866:ARG:NH1	2.20	0.75
1:O:764:GLU:HB2	1:O:795:HIS:HA	1.66	0.74
6:f:223:VAL:HG13	6:f:350:ILE:HG13	1.70	0.74
1:O:78:VAL:HG21	1:O:261:LEU:HD13	1.70	0.74
1:J:565:ARG:O	1:J:570:ASN:ND2	2.20	0.73
7:p:119:GLU:HA	7:p:122:THR:HG22	1.70	0.73
7:m:145:GLU:OE2	7:r:265:ARG:NH1	2.21	0.73
1:N:484:ARG:CD	1:N:550:ILE:HG21	2.18	0.73
2:v:426:LEU:HD12	2:v:461:HIS:HA	1.70	0.73
7:k:49:TYR:HE2	7:k:118:ARG:HD3	1.52	0.73
1:J:498:ASN:ND2	5:Z:1:MET:O	2.20	0.73
1:N:493:ARG:HH12	1:N:747:ILE:HG12	1.54	0.73
1:P:594:LEU:HD13	1:P:696:ALA:HB2	1.70	0.73
1:J:862:ASN:HD21	5:e:66:GLY:HA3	1.54	0.72
6:f:323:CYS:H	6:f:358:SER:HB3	1.54	0.72
1:J:1061:SER:HG	1:J:1064:SER:HG	1.36	0.72
1:P:655:ALA:O	1:P:683:TYR:OH	2.08	0.72
1:P:1378:LYS:HG2	1:P:1379:VAL:HG23	1.70	0.72
1:J:626:ILE:HG22	1:J:628:GLY:H	1.54	0.72
2:v:376:TYR:HA	2:v:379:ILE:HG12	1.71	0.72
1:K:329:ARG:HG2	1:K:330:THR:HG23	1.72	0.72
1:K:737:LEU:HD23	1:K:744:PRO:HG2	1.70	0.72
2:v:428:GLU:HB2	3:w:50:ARG:HG2	1.71	0.72
1:K:483:ARG:NH2	1:K:536:ASP:OD2	2.23	0.72
1:J:452:LEU:HD11	1:J:1040:PRO:HD3	1.70	0.72
1:J:140:ILE:HD11	1:J:157:ALA:HB2	1.71	0.72
1:K:1068:PHE:HB2	1:K:1093:ALA:HB3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:258:GLU:HG2	1:O:262:LYS:HD2	0.92	0.72
1:K:609:THR:HG22	1:K:653:ARG:HB3	1.72	0.71
7:m:9:LEU:HD13	7:m:40:VAL:HG11	1.72	0.71
7:p:21:MET:N	7:p:21:MET:SD	2.62	0.71
5:Z:68:PRO:CB	5:Z:71:GLN:HE21	1.98	0.71
3:w:85:ARG:NH1	4:y:3130:LEU:O	2.24	0.71
1:P:727:VAL:HG22	1:P:924:LEU:HB2	1.72	0.71
2:v:1:MET:HA	2:v:77:PHE:HZ	1.55	0.71
1:N:743:ALA:O	1:N:918:ARG:NH2	2.23	0.71
1:O:612:ASP:OD2	1:O:647:TYR:OH	2.08	0.71
1:O:1299:GLY:O	1:O:1323:GLN:NE2	2.23	0.71
1:P:941:THR:HA	1:P:944:LEU:O	1.89	0.71
6:f:226:PRO:HA	6:f:347:VAL:HG22	1.72	0.71
1:N:484:ARG:NH2	1:N:558:ALA:HB2	2.06	0.71
1:N:658:ASN:ND2	1:N:929:VAL:O	2.23	0.71
2:v:372:ILE:HG13	2:v:374:THR:H	1.53	0.71
1:O:947:ALA:HB2	1:O:963:MET:HB2	1.71	0.70
1:J:478:PRO:O	1:J:557:ARG:NH2	2.24	0.70
1:K:852:ARG:HD3	5:a:63:ARG:HH11	1.56	0.70
1:O:401:MET:SD	1:O:403:TYR:OH	2.48	0.70
7:p:3:LEU:HB2	7:p:84:LYS:HB3	1.73	0.70
1:J:1187:THR:OG1	1:J:1241:ASN:ND2	2.24	0.70
1:P:499:VAL:H	1:P:894:PHE:HE2	1.39	0.70
4:z:3127:ARG:HA	4:z:3130:LEU:HD12	1.72	0.70
7:p:118:ARG:O	7:p:122:THR:N	2.23	0.70
1:K:535:TYR:HE2	1:K:539:ARG:HH21	1.37	0.70
1:J:213:SER:OG	1:O:1174:LEU:O	2.08	0.70
1:J:611:TYR:OH	1:J:822:ASN:ND2	2.25	0.70
1:J:722:ASN:ND2	1:J:740:SER:OG	2.23	0.70
1:K:464:LEU:HD21	1:K:1254:MET:SD	2.32	0.70
7:p:38:GLN:O	7:p:39:ASN:C	2.34	0.70
1:J:146:GLU:OE1	1:J:146:GLU:N	2.25	0.70
1:P:609:THR:HG22	1:P:653:ARG:HB2	1.72	0.70
1:O:443:LYS:NZ	1:O:1176:HIS:O	2.23	0.70
1:N:495:ASN:OD1	1:N:496:HIS:N	2.25	0.69
1:N:832:PHE:HE2	1:N:892:PRO:HG2	1.56	0.69
7:r:158:ARG:NH2	7:r:206:SER:OG	2.25	0.69
7:k:101:PHE:HD2	7:k:138:LEU:HD22	1.56	0.69
1:N:625:MET:SD	1:N:887:SER:OG	2.51	0.69
1:O:133:LEU:HB3	1:O:138:LEU:HD21	1.74	0.69
6:h:86:ARG:NH1	7:r:90:THR:OG1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:k:238:LEU:HD11	7:p:263:ARG:HE	1.57	0.69
1:J:226:HIS:HB3	1:J:247:ARG:HH22	1.57	0.69
1:K:464:LEU:HD11	1:K:1254:MET:HG3	1.75	0.69
1:O:731:ASP:OD2	1:O:765:ARG:NH1	2.25	0.69
1:P:492:ARG:HD3	1:P:987:GLU:HB3	1.72	0.69
1:K:172:LEU:HD11	1:K:1090:HIS:HB2	1.73	0.69
1:N:544:PRO:O	1:N:565:ARG:NH1	2.25	0.69
6:f:194:ASN:HA	6:f:202:LYS:O	1.91	0.69
6:f:260:ALA:HB2	7:k:34:THR:HG21	1.74	0.69
1:O:80:THR:HG22	1:O:309:ALA:HB3	1.75	0.69
6:f:114:LYS:HZ2	7:p:182:LEU:HD12	1.56	0.69
1:N:677:LYS:O	1:N:678:GLU:C	2.36	0.69
1:N:905:ASP:OD1	1:N:905:ASP:N	2.25	0.69
7:k:97:TYR:HE2	7:k:137:VAL:H	1.41	0.69
1:N:938:ARG:HH22	1:N:965:GLN:HE21	1.39	0.69
1:P:465:HIS:O	1:P:546:TYR:OH	2.07	0.69
5:Z:68:PRO:O	5:Z:71:GLN:N	2.25	0.69
1:K:1255:TYR:HB2	1:K:1275:PHE:HD2	1.57	0.69
1:O:877:THR:OG1	1:O:880:MET:SD	2.50	0.69
2:v:43:TRP:HZ3	2:v:56:ARG:HA	1.59	0.68
5:d:41:ARG:NH1	5:d:44:GLN:OE1	2.26	0.68
6:f:157:LEU:HD13	6:f:342:GLY:HA3	1.74	0.68
1:J:302:ILE:HB	1:J:367:ILE:HG21	1.76	0.68
1:N:622:VAL:HG21	1:N:639:LEU:HD21	1.75	0.68
1:O:793:ARG:NH1	4:z:3146:PHE:O	2.26	0.68
2:v:115:TYR:O	2:v:118:SER:OG	2.12	0.68
1:O:1128:PHE:HZ	1:O:1260:ARG:HD2	1.57	0.68
1:O:1285:ARG:NH2	1:O:1293:GLU:OE1	2.27	0.68
5:d:15:GLU:HB2	5:d:48:LEU:HD21	1.73	0.68
7:r:99:PRO:HD3	7:r:120:HIS:HB3	1.74	0.68
1:K:828:LEU:HD11	1:K:945:PHE:HB3	1.74	0.68
1:O:399:ARG:HD3	1:O:1320:PHE:HB3	1.75	0.68
6:h:114:LYS:HB3	7:r:182:LEU:HD11	1.75	0.68
1:K:585:GLY:HA3	1:K:1017:GLY:HA2	1.74	0.68
1:P:534:ASN:HD21	1:P:537:LEU:HD22	1.59	0.68
1:P:1187:THR:OG1	1:P:1241:ASN:ND2	2.26	0.68
1:P:1318:ASP:O	6:f:198:THR:OG1	2.11	0.68
1:K:860:LEU:O	1:K:866:ARG:NH1	2.27	0.68
1:N:312:VAL:HG12	1:N:314:ARG:H	1.59	0.68
1:P:729:TYR:OH	1:P:927:GLY:O	2.09	0.68
7:m:228:ILE:HD11	7:m:243:VAL:HB	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:46:HIS:CE1	6:h:71:ALA:H	2.12	0.67
1:J:365:VAL:C	1:J:366:PRO:O	2.37	0.67
1:J:834:HIS:HD2	5:Z:8:PRO:HD3	1.60	0.67
7:m:118:ARG:HE	7:m:122:THR:HG21	1.60	0.67
1:N:281:ILE:HD12	1:N:1058:LEU:HD23	1.77	0.67
7:k:7:VAL:HG22	7:k:38:GLN:HB2	1.75	0.67
1:N:135:MET:HG3	6:h:45:GLU:HG2	1.77	0.67
1:N:1204:GLY:HA3	1:N:1239:THR:HG23	1.76	0.67
1:O:450:PHE:HD2	1:O:1119:ILE:HD12	1.59	0.67
1:K:1297:ARG:NH2	1:K:1298:LEU:O	2.27	0.67
1:N:172:LEU:HD11	1:N:1090:HIS:HB2	1.75	0.67
1:O:317:ASN:HB3	1:O:327:VAL:HG13	1.75	0.67
5:Z:67:VAL:O	5:Z:69:ARG:N	2.26	0.67
1:P:903:ASP:OD2	1:P:909:GLN:NE2	2.27	0.67
6:h:25:ARG:HD3	7:m:1:MET:HG3	1.76	0.67
1:J:402:GLN:HG2	1:J:1051:GLU:HG2	1.77	0.67
1:K:1347:MET:HE2	1:K:1375:PHE:HB2	1.76	0.67
7:m:49:TYR:HE2	7:m:118:ARG:HD3	1.59	0.67
1:O:475:ASN:HB3	1:O:560:HIS:HD2	1.58	0.67
7:r:9:LEU:HD13	7:r:128:ASN:HD21	1.60	0.67
7:r:229:ARG:HD2	7:r:230:HIS:H	1.59	0.67
1:K:1246:GLN:HB2	1:K:1249:SER:HB3	1.76	0.67
1:O:1293:GLU:OE2	1:O:1297:ARG:NH1	2.27	0.67
1:P:764:GLU:HG2	1:P:795:HIS:HA	1.77	0.66
2:v:8:GLN:HA	2:v:11:SER:HB3	1.76	0.66
1:K:817:LEU:HB3	1:K:825:MET:HE1	1.75	0.66
1:N:650:ARG:CZ	1:N:873:ASP:OD2	2.43	0.66
3:x:67:ARG:NH1	4:z:3149:LEU:OXT	2.28	0.66
1:N:336:ALA:HA	1:N:340:ASP:HB2	1.76	0.66
1:O:1226:ASP:OD1	1:O:1228:SER:N	2.21	0.66
1:P:484:ARG:HG3	1:P:552:ARG:HG2	1.75	0.66
1:P:944:LEU:HD22	1:P:945:PHE:H	1.58	0.66
7:p:30:PRO:HD3	7:p:135:PRO:HD3	1.77	0.66
1:J:1124:PHE:HA	1:J:1127:VAL:HG12	1.77	0.66
1:K:484:ARG:HG2	1:K:552:ARG:HA	1.76	0.66
1:N:924:LEU:HB2	1:N:950:PHE:CZ	2.30	0.66
1:N:899:ARG:NE	1:N:920:GLU:OE2	2.28	0.66
1:O:180:VAL:HG22	1:O:1067:MET:HE2	1.76	0.66
1:O:644:ILE:HG21	1:O:675:ILE:HD11	1.78	0.66
1:P:742:ARG:NH1	1:P:903:ASP:O	2.22	0.66
1:N:543:HIS:HD2	1:N:546:TYR:H	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:630:GLU:OE2	1:O:669:HIS:NE2	2.28	0.66
1:J:877:THR:H	1:J:880:MET:HE2	1.60	0.66
1:J:899:ARG:NH2	1:J:920:GLU:OE1	2.26	0.66
1:P:536:ASP:OD1	1:P:539:ARG:NH2	2.28	0.66
1:P:899:ARG:NH2	1:P:988:GLN:O	2.29	0.66
2:v:38:ASN:OD1	2:v:64:ARG:NH1	2.28	0.66
7:k:45:LEU:HB3	7:k:133:VAL:HB	1.77	0.66
1:J:1374:LYS:HG2	1:J:1379:VAL:HG22	1.78	0.66
1:N:407:PHE:CZ	1:N:440:ILE:HD11	2.31	0.66
1:N:706:VAL:HG23	1:N:711:VAL:HG12	1.78	0.66
1:O:843:GLY:HA3	5:d:69:ARG:HH22	1.61	0.66
3:w:57:CYS:SG	3:w:58:ALA:N	2.68	0.66
7:k:202:LEU:HD23	7:k:205:LEU:HD12	1.78	0.66
1:J:952:MET:HE2	1:J:999:SER:HA	1.77	0.66
1:O:442:ASN:OD1	1:O:443:LYS:N	2.29	0.66
1:O:899:ARG:HH12	1:O:990:PHE:HA	1.61	0.65
1:N:483:ARG:O	1:N:485:GLU:N	2.29	0.65
1:J:7:VAL:HG11	1:J:38:ASP:HB2	1.79	0.65
1:N:184:LYS:NZ	1:N:1064:SER:OG	2.28	0.65
1:O:258:GLU:HA	1:O:262:LYS:CE	2.26	0.65
7:k:149:LYS:NZ	7:k:178:SER:O	2.28	0.65
7:p:97:TYR:O	7:p:98:GLN:CB	2.23	0.65
1:K:743:ALA:HB3	1:K:918:ARG:HH12	1.61	0.65
5:u:27:PHE:O	5:u:44:GLN:NE2	2.21	0.65
7:r:136:MET:HE2	7:r:138:LEU:HD13	1.78	0.65
1:J:853:ASP:OD1	1:J:853:ASP:N	2.27	0.65
1:O:1215:TYR:HE1	1:O:1285:ARG:HG2	1.61	0.65
1:J:266:THR:HG21	1:J:1062:ARG:HE	1.61	0.65
1:J:1272:ARG:NH2	1:J:1279:GLU:OE2	2.29	0.65
2:v:381:LYS:O	2:v:384:ASP:N	2.30	0.65
3:w:63:ASN:HB3	4:y:3149:LEU:HD11	1.77	0.65
1:K:297:GLU:O	1:K:298:ALA:HB2	1.96	0.65
1:O:388:TYR:CE2	1:O:396:PRO:HD3	2.32	0.65
1:O:1203:ARG:HG2	1:O:1275:PHE:HE1	1.61	0.65
6:h:27:LEU:HD11	6:h:38:ASP:HB3	1.79	0.65
1:K:825:MET:N	1:K:956:ASP:OD2	2.29	0.65
1:N:456:LEU:HD23	1:N:1146:VAL:HG23	1.78	0.65
1:N:675:ILE:HD13	1:N:675:ILE:N	2.12	0.65
1:P:840:ALA:HB3	5:u:49:VAL:HG13	1.79	0.65
1:J:267:TYR:HA	1:J:305:PRO:HD3	1.79	0.65
1:K:452:LEU:HD23	1:K:1034:ALA:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:639:LEU:HD13	1:P:880:MET:HB2	1.77	0.65
7:k:145:GLU:OE1	7:p:265:ARG:NH2	2.29	0.65
1:J:658:ASN:ND2	1:J:929:VAL:O	2.26	0.65
1:J:1242:PRO:O	1:J:1246:GLN:NE2	2.30	0.65
1:K:861:GLU:HB2	5:Z:69:ARG:CD	2.26	0.65
1:P:1192:ASP:OD2	1:P:1237:ARG:NH2	2.30	0.65
1:J:129:THR:HG23	1:K:103:ALA:HB2	1.79	0.64
1:P:1357:HIS:ND1	1:P:1357:HIS:O	2.30	0.64
1:J:302:ILE:O	1:J:367:ILE:HB	1.98	0.64
1:J:958:ARG:HH11	1:O:695:GLN:HG3	1.62	0.64
1:O:951:HIS:O	1:O:955:GLY:N	2.30	0.64
1:P:587:GLN:NE2	1:P:1037:LYS:O	2.29	0.64
1:P:776:PHE:O	1:P:780:TYR:HB2	1.96	0.64
2:v:74:ARG:HG3	2:v:74:ARG:NH1	2.11	0.64
6:f:171:ASP:HB3	6:f:174:ARG:HB3	1.79	0.64
7:m:11:SER:OG	7:m:128:ASN:ND2	2.30	0.64
1:K:1188:PRO:HD2	1:K:1241:ASN:HB2	1.79	0.64
7:k:131:ASP:OD1	7:k:131:ASP:N	2.30	0.64
7:k:153:PHE:HA	7:k:176:LEU:HD13	1.80	0.64
1:J:979:ALA:H	1:O:698:MET:HE1	1.62	0.64
1:J:1264:VAL:HG12	1:J:1266:GLY:H	1.62	0.64
1:P:1203:ARG:NH1	1:P:1205:ARG:O	2.31	0.64
1:K:664:LYS:NZ	1:K:802:GLU:OE1	2.30	0.64
1:O:68:PHE:HD1	1:O:177:ILE:HG12	1.61	0.64
7:m:174:MET:O	7:m:175:HIS:ND1	2.31	0.64
1:K:400:ARG:NH2	1:K:1051:GLU:OE2	2.30	0.64
1:N:1068:PHE:HB2	1:N:1093:ALA:HB3	1.79	0.64
1:O:938:ARG:NH2	1:O:962:THR:O	2.30	0.64
2:v:43:TRP:HE1	2:v:101:ARG:HD2	1.63	0.64
7:m:274:LEU:HD13	7:r:271:LEU:HD21	1.78	0.64
1:K:1353:HIS:NE2	1:K:1364:GLU:OE2	2.31	0.64
1:N:451:ASN:ND2	1:O:527:GLU:OE2	2.31	0.64
1:P:150:GLU:OE1	1:P:150:GLU:N	2.31	0.64
1:K:298:ALA:HB2	1:K:371:VAL:O	1.98	0.64
1:N:1195:TYR:O	1:N:1200:ASN:ND2	2.31	0.64
7:p:97:TYR:C	7:p:99:PRO:HD2	2.22	0.64
1:J:804:HIS:O	1:K:978:ARG:NH1	2.28	0.64
1:K:1203:ARG:HG2	1:K:1275:PHE:HE1	1.63	0.64
6:f:89:VAL:HG23	6:f:207:VAL:HB	1.79	0.63
1:J:908:GLN:NE2	1:J:1026:SER:OG	2.30	0.63
1:K:1008:CYS:SG	1:K:1014:SER:HB3	2.37	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:585:GLY:HA3	1:P:1017:GLY:HA2	1.80	0.63
1:P:1071:THR:HB	6:f:26:ARG:HD2	1.81	0.63
2:v:44:CYS:SG	2:v:57:VAL:HG23	2.38	0.63
1:K:1051:GLU:N	1:K:1115:THR:OG1	2.31	0.63
5:u:15:GLU:HG3	5:u:48:LEU:HD22	1.80	0.63
1:K:128:SER:HA	1:K:1088:VAL:O	1.97	0.63
1:K:951:HIS:HD2	1:K:953:PHE:H	1.47	0.63
1:N:70:GLU:HA	1:N:367:ILE:HD12	1.79	0.63
6:f:334:ARG:NH2	6:f:349:GLU:OE2	2.31	0.63
2:v:415:PRO:HA	2:v:418:CYS:HB3	1.80	0.63
1:P:958:ARG:NH1	1:P:978:ARG:O	2.31	0.63
1:J:402:GLN:HG3	1:J:1321:LEU:HD11	1.79	0.63
1:J:561:ARG:NH2	1:J:916:ASP:OD1	2.31	0.63
1:O:131:MET:HE2	1:O:168:GLY:HA3	1.81	0.63
7:k:69:LEU:HB2	7:k:85:ILE:HD12	1.80	0.63
1:O:705:VAL:HG12	1:O:710:SER:HA	1.80	0.63
6:h:46:HIS:HE1	6:h:71:ALA:H	1.46	0.63
7:k:73:ASP:OD2	7:k:83:THR:N	2.30	0.63
1:K:482:ASP:N	1:K:482:ASP:OD1	2.31	0.63
1:N:481:ARG:HB2	1:N:484:ARG:HD3	1.80	0.63
1:N:674:ALA:C	1:N:675:ILE:CG1	2.72	0.63
5:e:24:LEU:O	5:e:28:GLN:HG2	1.99	0.63
1:O:539:ARG:HG2	1:O:540:LEU:HD22	1.79	0.62
1:P:1283:ASN:HD21	1:P:1326:SER:HG	1.46	0.62
1:O:174:ARG:HD2	1:O:387:MET:HE3	1.81	0.62
7:p:26:GLY:HA3	7:p:94:LYS:HB2	1.80	0.62
7:p:147:LEU:HD21	7:p:205:LEU:HD13	1.81	0.62
1:K:491:HIS:CD2	1:K:899:ARG:HD2	2.34	0.62
1:O:1101:TYR:OH	1:O:1292:ASN:OD1	2.12	0.62
2:v:354:ARG:NH1	2:v:394:GLN:HE22	1.94	0.62
7:k:13:LEU:HD22	7:k:77:VAL:HA	1.81	0.62
1:J:401:MET:HE3	1:J:1324:PRO:HG3	1.82	0.62
1:J:817:LEU:HD13	1:J:825:MET:HE2	1.81	0.62
1:K:1204:GLY:HA3	1:K:1239:THR:HG23	1.81	0.62
5:a:32:GLN:NE2	5:a:35:LEU:O	2.33	0.62
7:p:149:LYS:NZ	7:p:178:SER:O	2.33	0.62
1:J:568:VAL:HA	1:J:1025:MET:HE3	1.82	0.62
1:J:938:ARG:HA	1:J:941:THR:HG22	1.80	0.62
1:O:258:GLU:O	1:O:259:SER:C	2.42	0.62
1:P:1122:GLN:NE2	1:P:1268:TYR:O	2.32	0.62
7:m:275:ALA:HB2	7:r:275:ALA:HB1	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:531:HIS:HD2	1:O:533:SER:H	1.47	0.62
1:O:535:TYR:HE1	1:O:1227:HIS:HB2	1.64	0.62
1:K:465:HIS:NE2	1:K:1027:PRO:HD3	2.14	0.62
1:N:609:THR:HG22	1:N:653:ARG:HB3	1.82	0.62
1:K:950:PHE:CD1	1:K:951:HIS:HB2	2.34	0.62
2:v:74:ARG:O	2:v:74:ARG:HG2	1.99	0.62
1:O:258:GLU:HA	1:O:262:LYS:HE3	1.82	0.62
3:x:101:MET:HE3	4:y:3117:ARG:HH12	1.65	0.62
1:J:170:ASP:OD1	1:J:174:ARG:NE	2.33	0.62
1:O:495:ASN:OD1	1:O:496:HIS:N	2.33	0.62
7:r:45:LEU:HB2	7:r:133:VAL:HB	1.80	0.62
1:K:428:ASP:OD1	1:K:429:ASN:N	2.32	0.61
1:O:565:ARG:NH1	1:O:572:PRO:HD3	2.15	0.61
2:v:396:ARG:NH1	2:v:422:ASP:OD2	2.28	0.61
1:N:1255:TYR:HB2	1:N:1275:PHE:HD2	1.64	0.61
1:P:546:TYR:O	1:P:565:ARG:NH2	2.33	0.61
6:f:97:ALA:N	6:f:199:TYR:O	2.33	0.61
1:N:704:ASP:OD1	1:N:704:ASP:N	2.33	0.61
1:N:1043:ALA:HB3	1:N:1187:THR:O	2.00	0.61
1:O:39:LEU:HD11	1:O:149:VAL:HG21	1.80	0.61
1:O:388:TYR:HE2	1:O:396:PRO:HD3	1.65	0.61
1:P:147:THR:OG1	1:P:150:GLU:OE1	2.16	0.61
1:P:1335:LEU:HD12	1:P:1373:LEU:HD13	1.82	0.61
7:m:49:TYR:CE2	7:m:118:ARG:HD3	2.34	0.61
7:r:5:VAL:HG11	7:r:31:LEU:HD21	1.82	0.61
2:v:489:LEU:HB3	2:v:493:GLU:HG3	1.83	0.61
7:k:49:TYR:HE1	7:k:55:PRO:HB3	1.65	0.61
1:J:92:LYS:HB2	1:J:1095:ILE:HD11	1.83	0.61
1:J:547:ASP:HB2	1:J:565:ARG:HE	1.66	0.61
1:K:451:ASN:OD1	1:K:451:ASN:N	2.29	0.61
1:K:1057:ILE:O	1:K:1105:MET:HA	2.00	0.61
1:N:1231:ASP:N	1:N:1231:ASP:OD1	2.33	0.61
7:m:24:ARG:HH22	7:m:98:GLN:HE22	1.49	0.61
1:J:310:SER:C	1:J:311:PHE:CD1	2.79	0.61
1:J:1142:ILE:O	1:J:1146:VAL:HG12	1.99	0.61
1:K:73:LEU:HD13	1:K:177:ILE:HD11	1.82	0.61
1:K:311:PHE:HE2	1:K:329:ARG:HG3	1.64	0.61
1:J:132:GLU:HG3	1:K:112:LYS:HD3	1.82	0.61
1:J:308:TYR:HB3	1:J:312:VAL:CG2	2.29	0.61
1:O:1122:GLN:HE21	1:O:1127:VAL:HG21	1.65	0.61
7:k:279:ASN:OD1	7:k:283:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:m:241:GLU:N	7:m:241:GLU:OE1	2.32	0.61
2:v:74:ARG:HH11	2:v:74:ARG:CG	2.14	0.61
1:N:480:PRO:O	1:N:481:ARG:CD	2.48	0.61
1:N:834:HIS:CD2	5:d:8:PRO:HD3	2.26	0.61
2:v:49:SER:H	2:v:96:HIS:CD2	2.18	0.61
5:d:11:GLN:OE1	5:d:11:GLN:N	2.29	0.61
7:m:33:SER:HB2	7:m:38:GLN:HE22	1.65	0.61
7:r:95:ASN:HD21	7:r:294:LEU:HD22	1.66	0.61
1:O:68:PHE:O	1:O:71:THR:OG1	2.19	0.61
1:O:761:GLN:HE22	3:x:67:ARG:HD3	1.65	0.61
1:J:308:TYR:O	1:J:312:VAL:HG23	2.01	0.60
1:J:501:VAL:HG21	5:Z:1:MET:HB3	1.82	0.60
1:N:684:ARG:HH22	1:O:612:ASP:HA	1.66	0.60
1:N:947:ALA:HB2	1:N:963:MET:HB2	1.83	0.60
6:f:132:PHE:HE2	6:f:152:THR:HA	1.66	0.60
1:N:484:ARG:HB2	1:N:551:GLY:O	2.01	0.60
1:P:611:TYR:OH	1:P:822:ASN:ND2	2.29	0.60
1:P:1213:GLU:N	1:P:1213:GLU:OE1	2.34	0.60
7:p:140:THR:HG21	7:p:283:ARG:HH22	1.64	0.60
6:f:111:PHE:HD1	6:f:187:PRO:HA	1.67	0.60
6:h:8:ASP:HA	6:h:12:LEU:HD13	1.82	0.60
6:h:176:VAL:O	6:h:179:ARG:NH2	2.34	0.60
1:J:92:LYS:HG2	1:J:93:ILE:N	2.16	0.60
1:J:481:ARG:CD	1:J:481:ARG:H	2.12	0.60
1:K:566:LEU:HD21	1:K:904:ASN:ND2	2.16	0.60
7:k:241:GLU:OE1	7:k:241:GLU:N	2.29	0.60
7:r:149:LYS:NZ	7:r:178:SER:O	2.31	0.60
1:J:1183:GLU:OE2	1:J:1269:SER:OG	2.17	0.60
7:k:289:TYR:CD2	7:k:296:ALA:HB2	2.35	0.60
1:O:39:LEU:HB2	1:O:52:PHE:HB2	1.82	0.60
1:O:184:LYS:HZ3	1:O:1064:SER:HB2	1.66	0.60
1:P:1283:ASN:ND2	1:P:1326:SER:O	2.34	0.60
1:P:1334:ALA:HA	1:P:1365:GLU:HG3	1.82	0.60
2:v:74:ARG:HG3	2:v:74:ARG:HH11	1.65	0.60
6:f:263:ARG:HG2	6:f:326:THR:HG22	1.82	0.60
1:J:805:ALA:HA	1:K:972:MET:HE1	1.82	0.60
1:J:1259:TYR:HE2	1:J:1262:THR:HB	1.65	0.60
1:J:1323:GLN:OE1	1:J:1323:GLN:N	2.34	0.60
1:O:480:PRO:O	1:O:539:ARG:NH1	2.34	0.60
1:N:405:TYR:HD2	1:N:1334:ALA:HB2	1.66	0.60
2:v:40:GLU:HB3	7:p:230:HIS:NE2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:68:PRO:HB3	5:Z:71:GLN:CD	2.20	0.60
1:O:268:THR:OG1	1:O:364:ARG:NH1	2.35	0.60
4:y:3131:GLU:O	4:y:3135:HIS:ND1	2.30	0.60
1:J:814:TYR:OH	1:J:921:GLN:NE2	2.34	0.59
1:J:830:VAL:H	1:J:895:THR:HG21	1.67	0.59
1:N:813:TYR:O	1:N:954:TYR:OH	2.12	0.59
1:N:828:LEU:HD21	1:N:945:PHE:CG	2.37	0.59
1:N:1023:ILE:HG21	1:N:1033:GLN:HE21	1.67	0.59
1:P:680:TYR:OH	1:P:684:ARG:NH2	2.33	0.59
1:N:513:ALA:HB1	1:N:984:ASN:HD22	1.67	0.59
1:N:746:ILE:HB	1:N:753:TYR:HB3	1.83	0.59
1:O:667:CYS:O	1:O:680:TYR:OH	2.20	0.59
1:O:846:PHE:HE1	5:e:48:LEU:HD11	1.67	0.59
1:K:248:LEU:HB3	1:K:374:LEU:HD21	1.84	0.59
1:K:746:ILE:HB	1:K:753:TYR:HB3	1.84	0.59
1:N:288:ARG:NH2	1:O:250:GLU:OE2	2.31	0.59
5:e:70:ARG:O	5:e:74:ILE:HG13	2.02	0.59
6:h:129:LEU:HD23	6:h:158:LEU:HD12	1.83	0.59
1:J:310:SER:O	1:J:311:PHE:HD1	1.85	0.59
1:J:1216:ASN:O	1:J:1284:ASN:ND2	2.35	0.59
1:K:596:HIS:NE2	1:K:1012:LEU:HB3	2.18	0.59
1:O:70:GLU:HA	1:O:367:ILE:HD12	1.83	0.59
2:v:349:ILE:HD11	2:v:487:LEU:HD13	1.84	0.59
6:f:328:SER:OG	6:f:331:ASP:OD2	2.18	0.59
7:k:13:LEU:HD21	7:k:18:ILE:HG12	1.83	0.59
1:J:544:PRO:HG3	1:J:1243:TRP:CD2	2.37	0.59
1:K:845:ALA:O	1:K:882:ARG:NE	2.34	0.59
1:K:1285:ARG:NH2	1:K:1293:GLU:OE1	2.35	0.59
7:p:18:ILE:HG22	7:p:22:GLN:HE21	1.67	0.59
1:J:824:HIS:ND1	1:J:956:ASP:OD1	2.31	0.59
1:K:861:GLU:HG3	5:Z:69:ARG:CD	2.32	0.59
1:K:1195:TYR:O	1:K:1200:ASN:ND2	2.30	0.59
1:P:807:VAL:O	1:P:810:LYS:N	2.36	0.59
1:K:546:TYR:HA	1:K:564:HIS:HA	1.85	0.59
1:N:847:SER:HB2	1:N:850:PHE:HD2	1.68	0.59
1:K:630:GLU:OE2	1:K:668:ARG:NH2	2.36	0.59
1:N:804:HIS:CD2	1:N:808:LEU:HG	2.38	0.59
1:O:720:ASP:O	1:O:810:LYS:NZ	2.36	0.59
1:P:1080:ARG:HD2	1:P:1083:ALA:HB3	1.84	0.59
7:k:95:ASN:OD1	7:k:96:LYS:N	2.36	0.59
1:J:489:LEU:O	1:J:994:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:136:LEU:HD22	6:h:218:ARG:HG2	1.85	0.59
1:P:491:HIS:HB2	1:P:899:ARG:NH1	2.18	0.58
1:J:266:THR:O	1:J:305:PRO:HG3	2.03	0.58
1:J:301:GLN:HB3	1:J:366:PRO:CB	2.33	0.58
1:O:736:LEU:O	1:O:740:SER:OG	2.14	0.58
1:O:864:THR:O	1:O:868:LEU:HB2	2.03	0.58
1:P:718:LEU:HD13	1:P:811:ILE:HG12	1.83	0.58
7:m:108:SER:O	7:m:140:THR:OG1	2.19	0.58
1:J:1302:PRO:HB2	1:J:1321:LEU:HD23	1.84	0.58
1:K:1050:ASP:HA	1:K:1115:THR:HG21	1.85	0.58
1:N:1128:PHE:HZ	1:N:1260:ARG:HG3	1.68	0.58
6:h:305:TYR:OH	7:r:242:MET:SD	2.52	0.58
7:p:101:PHE:HZ	7:p:142:ILE:HG21	1.67	0.58
1:J:748:ILE:HD12	1:J:762:PHE:HD2	1.69	0.58
1:N:484:ARG:CD	1:N:550:ILE:HG22	2.29	0.58
1:N:720:ASP:O	1:N:810:LYS:NZ	2.36	0.58
6:h:154:MET:HE2	6:h:345:LEU:HD22	1.84	0.58
1:J:909:GLN:NE2	1:J:917:LYS:HD3	2.17	0.58
1:K:611:TYR:OH	1:K:822:ASN:ND2	2.36	0.58
7:k:13:LEU:HD11	7:k:18:ILE:HD13	1.84	0.58
7:k:28:ILE:HD12	7:k:137:VAL:HG21	1.86	0.58
7:r:25:ILE:O	7:r:72:LEU:HB2	2.03	0.58
1:K:644:ILE:HG21	1:K:675:ILE:HD11	1.85	0.58
1:K:793:ARG:O	1:K:896:ARG:NH2	2.36	0.58
1:O:1039:HIS:ND1	1:O:1040:PRO:O	2.30	0.58
5:d:75:ASP:OD1	5:d:76:LYS:N	2.37	0.58
1:J:904:ASN:HB2	1:J:917:LYS:O	2.04	0.58
1:K:1077:ARG:O	1:K:1085:THR:OG1	2.15	0.58
2:v:49:SER:H	2:v:96:HIS:HD2	1.48	0.58
7:k:212:MET:HE1	7:k:274:LEU:HD11	1.86	0.58
7:p:94:LYS:HB3	7:p:96:LYS:HZ3	1.69	0.58
1:K:619:PHE:CE1	1:K:643:CYS:HB3	2.38	0.58
1:K:950:PHE:HD1	1:K:951:HIS:HB2	1.66	0.58
1:N:402:GLN:HA	1:N:1050:ASP:O	2.04	0.58
1:O:417:LYS:NZ	1:O:431:THR:O	2.37	0.58
1:P:207:PHE:C	1:P:209:LYS:H	2.12	0.58
6:h:129:LEU:HD21	6:h:154:MET:HE1	1.86	0.58
1:J:209:LYS:HB3	1:O:1174:LEU:HD11	1.85	0.57
1:P:170:ASP:O	1:P:174:ARG:HG2	2.04	0.57
2:v:43:TRP:CZ3	2:v:56:ARG:HA	2.39	0.57
7:p:6:VAL:O	7:p:37:THR:HG23	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:4:ASN:ND2	1:K:38:ASP:HB2	2.18	0.57
1:K:40:LEU:HB3	1:K:44:ASP:HB3	1.85	0.57
1:K:282:VAL:HG12	1:K:1057:ILE:HG12	1.86	0.57
1:K:905:ASP:N	1:K:905:ASP:OD1	2.37	0.57
1:N:591:ALA:HB1	1:N:1036:LEU:HD12	1.86	0.57
7:m:223:LEU:O	7:m:227:LEU:HG	2.03	0.57
7:p:11:SER:OG	7:p:128:ASN:OD1	2.21	0.57
1:J:979:ALA:N	1:O:698:MET:HE1	2.18	0.57
1:J:1169:ASN:OD1	1:J:1170:GLY:N	2.37	0.57
1:K:828:LEU:HB3	1:K:928:LEU:O	2.04	0.57
1:O:828:LEU:HD11	1:O:945:PHE:HB3	1.85	0.57
1:J:170:ASP:O	1:J:174:ARG:HG2	2.03	0.57
1:N:1117:MET:SD	1:N:1371:ARG:NH2	2.77	0.57
1:O:258:GLU:CA	1:O:262:LYS:HD2	2.32	0.57
1:O:561:ARG:NH2	1:O:916:ASP:OD1	2.36	0.57
7:p:160:VAL:HG23	7:p:167:ALA:HB1	1.87	0.57
1:N:672:ASN:HD21	1:O:871:ILE:C	2.07	0.57
1:O:977:GLN:NE2	1:O:982:ALA:O	2.38	0.57
1:P:475:ASN:OD1	1:P:560:HIS:N	2.35	0.57
7:p:23:GLN:NE2	7:p:23:GLN:O	2.37	0.57
1:J:310:SER:O	1:J:311:PHE:CD1	2.57	0.57
1:K:947:ALA:HB2	1:K:963:MET:HB2	1.87	0.57
1:O:170:ASP:O	1:O:174:ARG:HG2	2.04	0.57
1:O:565:ARG:HH12	1:O:572:PRO:HD3	1.68	0.57
7:p:74:GLU:HB3	7:p:81:ILE:HD12	1.87	0.57
1:J:731:ASP:HB3	1:J:799:TYR:HB2	1.87	0.57
1:J:1372:ILE:HG12	1:J:1381:PHE:HD2	1.69	0.57
2:v:13:LEU:HD11	7:p:252:LEU:H	1.68	0.57
2:v:44:CYS:HB3	2:v:59:ARG:HG2	1.87	0.57
2:v:96:HIS:HB2	2:v:116:TYR:CE2	2.40	0.57
5:a:13:ARG:HH11	5:a:41:ARG:HH22	1.51	0.57
1:J:742:ARG:HB3	1:J:903:ASP:HB2	1.86	0.57
1:K:140:ILE:HD11	1:K:157:ALA:HB2	1.86	0.57
1:N:832:PHE:CE2	1:N:892:PRO:HG2	2.38	0.57
1:O:43:LYS:HA	1:P:314:ARG:HH22	1.70	0.57
2:v:4:HIS:CE1	2:v:20:HIS:HB3	2.38	0.57
1:N:282:VAL:HG12	1:N:1057:ILE:HG12	1.86	0.57
1:O:881:ILE:O	1:O:885:SER:OG	2.23	0.57
3:x:74:MET:HE3	3:x:78:LEU:HD11	1.86	0.57
5:Z:68:PRO:C	5:Z:70:ARG:N	2.60	0.57
7:k:146:VAL:HG22	7:k:179:VAL:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:255:VAL:HG11	1:J:1102:SER:C	2.30	0.56
1:K:864:THR:HG23	5:a:9:THR:HB	1.87	0.56
1:N:758:ALA:HB1	1:N:761:GLN:HG2	1.86	0.56
1:N:1174:LEU:O	1:O:213:SER:OG	2.15	0.56
3:w:59:GLN:O	3:w:62:LYS:NZ	2.37	0.56
6:f:195:ILE:HB	6:f:202:LYS:HB3	1.86	0.56
7:r:56:ASP:O	7:r:59:SER:OG	2.19	0.56
1:J:844:PRO:HG2	1:J:860:LEU:HD23	1.87	0.56
1:J:1135:ASN:HB3	1:J:1138:VAL:HG12	1.87	0.56
1:K:184:LYS:HZ3	1:K:1065:THR:HG23	1.70	0.56
1:K:285:ASN:O	1:K:289:GLN:NE2	2.38	0.56
1:N:736:LEU:O	1:N:740:SER:OG	2.17	0.56
1:P:68:PHE:N	1:P:173:GLU:OE1	2.37	0.56
6:h:191:LEU:HD23	6:h:205:THR:HG22	1.87	0.56
7:k:204:ASN:HA	7:k:207:LEU:HD12	1.85	0.56
1:J:174:ARG:HD2	1:J:387:MET:HE3	1.87	0.56
1:J:185:LEU:HD13	1:J:399:ARG:HH21	1.70	0.56
1:J:655:ALA:O	1:J:683:TYR:OH	2.16	0.56
1:J:1072:PRO:HB3	1:J:1090:HIS:HD2	1.69	0.56
1:N:138:LEU:HB2	6:h:45:GLU:HB2	1.86	0.56
1:N:969:THR:O	1:N:973:ARG:HG2	2.06	0.56
1:O:741:ASP:O	2:v:73:HIS:HE1	1.88	0.56
1:O:856:ILE:HD11	1:O:878:VAL:HA	1.87	0.56
1:P:861:GLU:OE1	1:P:861:GLU:N	2.38	0.56
1:P:899:ARG:HG2	1:P:922:THR:HG22	1.86	0.56
1:P:913:ASN:HD21	1:P:915:ALA:HB3	1.70	0.56
2:v:342:LEU:HD12	2:v:397:VAL:HG23	1.87	0.56
6:f:122:VAL:HG12	6:f:124:ALA:H	1.70	0.56
6:f:318:PHE:HB2	6:f:364:LEU:HD13	1.87	0.56
7:k:49:TYR:CE2	7:k:118:ARG:HD3	2.36	0.56
7:k:274:LEU:HD13	7:p:271:LEU:HD21	1.86	0.56
7:m:39:ASN:OD1	7:m:40:VAL:N	2.37	0.56
1:J:302:ILE:HB	1:J:367:ILE:CG2	2.36	0.56
1:K:626:ILE:HG22	1:K:628:GLY:H	1.69	0.56
1:N:485:GLU:OE2	1:N:993:TYR:OH	2.23	0.56
1:N:997:HIS:HE1	1:N:1022:HIS:NE2	2.04	0.56
1:O:1231:ASP:OD1	1:O:1231:ASP:N	2.39	0.56
1:P:571:LEU:HD21	1:P:1025:MET:HE1	1.88	0.56
6:h:9:ARG:HH22	6:h:13:GLN:NE2	2.03	0.56
1:N:145:PRO:HG3	1:N:151:TYR:HD1	1.70	0.56
1:N:535:TYR:CE1	1:N:1227:HIS:HB2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:596:HIS:CD2	1:N:1012:LEU:HB2	2.40	0.56
1:O:73:LEU:HD12	1:O:281:ILE:HD11	1.88	0.56
1:P:434:LEU:HD12	1:P:435:PRO:HD2	1.87	0.56
5:d:7:LYS:HE2	5:d:8:PRO:HD2	1.87	0.56
7:m:260:ASP:OD2	7:r:156:TYR:OH	2.23	0.56
1:J:922:THR:HG21	1:J:989:LEU:O	2.06	0.56
1:N:138:LEU:HD22	6:h:43:VAL:HG13	1.87	0.56
1:N:461:HIS:CD2	1:N:1124:PHE:HB3	2.40	0.56
1:O:947:ALA:HB3	1:O:964:HIS:CE1	2.41	0.56
1:O:1252:ASP:O	1:O:1256:ASN:HB2	2.06	0.56
1:P:869:LEU:HD13	1:P:876:PRO:HG2	1.88	0.56
1:P:1027:PRO:HG2	1:P:1133:PHE:HZ	1.69	0.56
2:v:1:MET:HA	2:v:77:PHE:CZ	2.38	0.56
7:p:103:TRP:HB2	7:p:289:TYR:CD2	2.41	0.56
1:N:620:TYR:HE1	1:N:828:LEU:HD22	1.71	0.56
1:P:856:ILE:HD11	1:P:878:VAL:HA	1.88	0.56
1:J:226:HIS:HB3	1:J:247:ARG:NH2	2.21	0.56
1:J:652:GLY:H	1:O:677:LYS:NZ	2.04	0.56
1:K:612:ASP:OD2	1:K:647:TYR:OH	2.22	0.56
1:N:483:ARG:NH1	1:N:485:GLU:CB	2.68	0.56
1:N:543:HIS:CD2	1:N:545:LEU:H	2.23	0.56
1:N:607:GLN:HE21	1:N:611:TYR:HE2	1.53	0.56
1:O:280:PHE:HB2	1:O:381:VAL:HG22	1.87	0.56
1:K:1255:TYR:HB2	1:K:1275:PHE:CD2	2.41	0.56
1:O:1226:ASP:OD1	1:O:1227:HIS:N	2.38	0.56
1:P:612:ASP:OD2	1:P:653:ARG:NH1	2.39	0.56
1:P:667:CYS:O	1:P:684:ARG:NH2	2.28	0.56
7:p:17:GLU:OE2	7:p:126:GLU:N	2.38	0.56
1:J:61:ASN:HD21	1:J:63:ILE:HG12	1.71	0.56
1:J:724:LEU:HD21	1:J:736:LEU:HD12	1.88	0.56
1:P:515:VAL:HG11	1:P:976:GLN:HE22	1.70	0.56
1:P:932:ALA:HA	1:P:959:VAL:HG13	1.88	0.56
4:y:3122:PHE:O	4:y:3126:LEU:HG	2.06	0.56
6:f:226:PRO:HB3	6:f:345:LEU:HD11	1.88	0.56
7:p:157:SER:HB2	7:p:194:PRO:HD3	1.87	0.56
1:O:1197:GLN:NE2	1:O:1197:GLN:O	2.39	0.55
1:P:222:HIS:HE1	1:P:247:ARG:HH12	1.51	0.55
6:f:281:GLN:HG3	6:f:327:PHE:HZ	1.71	0.55
7:m:212:MET:HE2	7:m:270:TYR:HB3	1.88	0.55
1:N:650:ARG:NH1	1:N:873:ASP:OD2	2.39	0.55
1:N:718:LEU:HD13	1:N:811:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1057:ILE:HG13	1:P:1108:ALA:HB2	1.86	0.55
1:J:444:ASN:HD22	1:J:1176:HIS:CD2	2.24	0.55
1:J:746:ILE:HB	1:J:753:TYR:HB3	1.88	0.55
1:O:1061:SER:O	1:O:1064:SER:OG	2.23	0.55
1:P:605:THR:O	1:P:609:THR:HG23	2.06	0.55
1:P:705:VAL:HA	1:P:710:SER:HA	1.86	0.55
7:k:211:ILE:O	7:k:214:THR:OG1	2.24	0.55
7:p:84:LYS:HE3	7:p:86:VAL:HG22	1.88	0.55
1:N:990:PHE:CE2	1:N:992:GLU:HG2	2.41	0.55
1:O:889:MET:HE2	5:e:54:GLN:HE22	1.71	0.55
1:O:1203:ARG:HG2	1:O:1275:PHE:CE1	2.42	0.55
1:P:1342:LEU:HB3	1:P:1362:ILE:HD12	1.89	0.55
7:p:215:LEU:HD21	7:p:263:ARG:HD2	1.88	0.55
1:K:566:LEU:HD21	1:K:904:ASN:HD21	1.71	0.55
1:N:175:GLY:HA3	1:O:103:ALA:HB3	1.88	0.55
1:N:764:GLU:HB2	1:N:793:ARG:HD3	1.89	0.55
2:v:46:THR:OG1	2:v:54:LEU:O	2.18	0.55
5:u:42:GLU:HG3	5:u:45:ARG:HH12	1.72	0.55
6:h:86:ARG:HH22	7:r:89:GLN:HA	1.71	0.55
7:p:67:CYS:SG	7:p:68:THR:N	2.79	0.55
1:K:271:LYS:HB3	1:K:299:ASP:CG	2.31	0.55
1:N:400:ARG:HH11	1:N:1305:SER:HB3	1.72	0.55
7:r:256:SER:OG	7:r:259:ASP:OD2	2.24	0.55
1:N:483:ARG:HH11	1:N:485:GLU:CB	2.20	0.55
1:N:998:ARG:HB3	1:N:1000:PRO:HD2	1.89	0.55
2:v:354:ARG:HH12	3:x:43:GLU:HB2	1.71	0.55
5:e:20:ASP:OD1	5:e:20:ASP:N	2.40	0.55
1:J:69:LEU:CD1	1:J:308:TYR:CG	2.90	0.55
1:O:258:GLU:C	1:O:259:SER:O	2.49	0.55
1:O:576:ALA:HB1	1:O:580:PHE:HD2	1.72	0.55
1:P:494:PRO:O	1:P:750:ASN:ND2	2.39	0.55
3:x:80:ARG:O	3:x:84:ILE:HG12	2.06	0.55
1:J:110:PRO:HB2	1:O:130:GLU:HG3	1.87	0.55
1:N:208:SER:OG	1:N:209:LYS:N	2.39	0.55
1:N:944:LEU:HA	5:d:5:LEU:HD21	1.88	0.55
1:P:1028:MET:HE2	1:P:1138:VAL:HG13	1.88	0.55
7:r:6:VAL:HG22	7:r:81:ILE:HG12	1.88	0.55
1:N:535:TYR:HE1	1:N:1227:HIS:HB2	1.71	0.55
1:N:842:ASN:ND2	1:N:860:LEU:HD21	2.21	0.55
1:J:670:LEU:HG	1:J:671:GLY:H	1.72	0.54
3:w:56:ARG:CZ	3:x:56:ARG:HG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:92:LYS:HD2	1:J:120:LYS:H	1.72	0.54
1:J:862:ASN:ND2	5:e:65:PHE:O	2.40	0.54
1:K:886:ALA:HB2	5:a:56:CYS:HB2	1.89	0.54
1:O:111:SER:OG	1:O:114:ARG:NH2	2.39	0.54
1:O:938:ARG:HA	1:O:941:THR:HG22	1.89	0.54
1:P:607:GLN:HE21	1:P:611:TYR:HE2	1.55	0.54
3:w:43:GLU:O	3:w:47:GLU:HG3	2.06	0.54
5:u:47:TYR:HA	5:u:50:PHE:CZ	2.43	0.54
1:K:298:ALA:CB	1:K:371:VAL:O	2.55	0.54
1:O:762:PHE:O	1:O:793:ARG:HG3	2.07	0.54
7:k:98:GLN:N	7:k:98:GLN:OE1	2.39	0.54
7:p:128:ASN:HB2	7:p:130:VAL:HG22	1.90	0.54
1:J:114:ARG:NH2	1:O:392:GLN:OE1	2.36	0.54
1:J:856:ILE:HD11	1:J:878:VAL:HA	1.88	0.54
1:N:1128:PHE:CE1	1:N:1263:ALA:HB2	2.43	0.54
1:O:846:PHE:CE1	5:e:48:LEU:HD11	2.42	0.54
1:J:465:HIS:CE1	1:J:1027:PRO:HD3	2.43	0.54
1:J:607:GLN:HE21	1:J:611:TYR:HE2	1.56	0.54
1:J:684:ARG:HH22	1:K:653:ARG:HH22	1.56	0.54
1:N:453:GLN:HB2	1:N:1034:ALA:HB1	1.89	0.54
1:P:70:GLU:HA	1:P:367:ILE:HD12	1.89	0.54
1:P:491:HIS:HD2	1:P:493:ARG:HG3	1.72	0.54
1:N:481:ARG:CG	1:N:550:ILE:HD13	2.37	0.54
1:N:1081:VAL:HB	6:h:210:PRO:HB3	1.89	0.54
1:P:89:THR:HA	6:f:216:ILE:HD11	1.88	0.54
2:v:402:CYS:SG	2:v:467:THR:OG1	2.52	0.54
1:K:546:TYR:HB3	1:K:562:ALA:HB1	1.90	0.54
1:K:1165:MET:SD	1:K:1166:THR:N	2.81	0.54
1:O:905:ASP:O	1:O:909:GLN:HG2	2.08	0.54
1:O:1003:LYS:NZ	1:O:1007:GLU:OE2	2.38	0.54
1:P:744:PRO:HB3	1:P:902:VAL:HG22	1.88	0.54
2:v:37:PRO:C	2:v:64:ARG:HH22	2.16	0.54
5:e:61:VAL:O	5:e:64:THR:OG1	2.22	0.54
6:h:230:PHE:HA	6:h:279:PHE:HB2	1.88	0.54
1:N:690:LEU:HD21	1:N:812:PHE:HB2	1.89	0.54
1:N:857:LEU:HD23	1:N:860:LEU:HD12	1.89	0.54
1:O:90:ASP:OD1	1:O:91:GLY:N	2.41	0.54
7:k:24:ARG:NH2	7:k:27:CYS:SG	2.81	0.54
1:J:1186:VAL:HG22	1:J:1250:LEU:HD22	1.89	0.54
1:K:262:LYS:HD2	1:K:1062:ARG:HH21	1.73	0.54
1:K:481:ARG:HG2	1:K:550:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:462:PRO:HG2	1:P:1132:ALA:HA	1.90	0.54
1:P:732:ILE:HG22	1:P:799:TYR:CE2	2.43	0.54
3:x:88:LEU:HD13	4:z:3130:LEU:HD11	1.89	0.54
5:Z:68:PRO:O	5:Z:69:ARG:C	2.50	0.54
7:p:95:ASN:HD21	7:p:294:LEU:HD22	1.72	0.54
1:N:72:ALA:HB3	1:N:382:GLU:HB2	1.90	0.53
1:N:625:MET:HE1	1:N:839:LEU:HD12	1.91	0.53
1:P:841:TYR:CD1	5:u:45:ARG:HG3	2.43	0.53
3:w:50:ARG:HG3	3:w:53:ARG:HD2	1.89	0.53
5:u:35:LEU:HB2	5:u:40:PHE:CZ	2.43	0.53
7:p:122:THR:OG1	7:p:132:ILE:O	2.18	0.53
1:J:827:GLY:HA3	1:J:950:PHE:HE1	1.73	0.53
1:N:78:VAL:HG21	1:N:261:LEU:HD12	1.90	0.53
1:P:829:GLY:HA3	1:P:946:HIS:CE1	2.44	0.53
1:P:841:TYR:CD1	5:u:48:LEU:HD11	2.44	0.53
2:v:3:VAL:O	2:v:7:ASN:ND2	2.41	0.53
1:K:461:HIS:NE2	1:K:1128:PHE:HB2	2.23	0.53
1:K:1250:LEU:O	1:K:1253:ILE:HG22	2.08	0.53
1:N:543:HIS:CE1	1:N:1250:LEU:HD12	2.43	0.53
1:N:1195:TYR:OH	1:N:1203:ARG:O	2.25	0.53
1:O:131:MET:HE3	1:O:1088:VAL:HG21	1.90	0.53
1:O:741:ASP:O	2:v:73:HIS:CE1	2.62	0.53
1:J:575:LEU:HD21	1:J:1243:TRP:CZ2	2.44	0.53
1:J:668:ARG:HD2	1:K:935:GLU:HB3	1.91	0.53
1:K:1195:TYR:OH	1:K:1201:SER:O	2.26	0.53
1:O:258:GLU:CB	1:O:262:LYS:CD	2.55	0.53
1:P:789:ASP:OD1	1:P:790:HIS:N	2.41	0.53
1:P:881:ILE:O	1:P:885:SER:OG	2.25	0.53
7:m:249:ARG:NE	7:r:246:GLU:OE1	2.41	0.53
7:p:94:LYS:HD3	7:p:96:LYS:NZ	2.24	0.53
1:K:840:ALA:HB3	5:a:49:VAL:HG22	1.90	0.53
1:N:401:MET:HE3	1:N:403:TYR:HE1	1.74	0.53
2:v:464:HIS:HE1	2:v:466:ALA:HB2	1.73	0.53
6:f:171:ASP:O	6:f:175:LEU:N	2.38	0.53
6:f:320:ALA:HA	6:f:361:GLU:O	2.09	0.53
6:h:179:ARG:HG3	6:h:270:TYR:CD2	2.43	0.53
1:J:59:TYR:HB2	1:K:95:PHE:HD1	1.72	0.53
1:K:861:GLU:CG	5:Z:69:ARG:CD	2.86	0.53
1:N:853:ASP:OD1	1:N:853:ASP:N	2.37	0.53
1:O:952:MET:HE1	1:O:981:GLU:HA	1.89	0.53
1:P:251:MET:SD	1:P:1106:THR:OG1	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:w:65:LEU:O	3:w:69:GLU:HG2	2.09	0.53
7:r:40:VAL:HA	7:r:43:LEU:HD23	1.91	0.53
1:J:388:TYR:CE2	1:J:396:PRO:HD3	2.43	0.53
1:K:951:HIS:O	1:K:955:GLY:N	2.42	0.53
1:N:677:LYS:C	1:N:679:ALA:N	2.63	0.53
1:O:825:MET:N	1:O:956:ASP:OD2	2.30	0.53
1:P:1214:ASN:OD1	1:P:1215:TYR:N	2.36	0.53
5:Z:38:ASP:OD1	5:Z:38:ASP:N	2.40	0.53
7:m:195:GLY:H	7:m:196:PRO:HD2	1.74	0.53
7:p:98:GLN:OE1	7:p:98:GLN:HA	2.08	0.53
1:J:824:HIS:HD1	1:J:956:ASP:CG	2.15	0.53
1:K:861:GLU:CD	5:Z:67:VAL:HG11	2.34	0.53
1:N:441:VAL:HG11	1:N:1373:LEU:HD22	1.91	0.53
6:f:151:LEU:HG	6:f:345:LEU:HD13	1.91	0.53
1:J:399:ARG:HD3	1:J:1320:PHE:HB3	1.91	0.53
1:J:568:VAL:HG21	1:J:584:ARG:NH2	2.24	0.53
1:N:646:THR:HG21	1:N:874:LEU:HD13	1.90	0.53
1:P:510:LYS:O	1:P:973:ARG:NH2	2.42	0.53
1:K:543:HIS:CE1	1:K:1250:LEU:HD12	2.44	0.53
1:N:837:GLN:HA	5:d:49:VAL:HG21	1.90	0.53
1:P:834:HIS:HD2	5:u:8:PRO:HD3	1.74	0.53
1:P:906:VAL:HG11	1:P:1135:ASN:H	1.73	0.53
2:v:93:ASN:HB3	2:v:96:HIS:HE1	1.73	0.53
5:Z:24:LEU:HA	5:Z:27:PHE:HB3	1.90	0.53
1:J:852:ARG:HD2	1:J:879:GLY:HA3	1.90	0.52
1:P:68:PHE:HA	1:P:177:ILE:HD11	1.90	0.52
1:N:91:GLY:HA3	1:N:122:CYS:SG	2.49	0.52
1:N:677:LYS:CG	1:N:678:GLU:N	2.69	0.52
1:P:1210:VAL:HG21	1:P:1287:LEU:HD22	1.91	0.52
7:p:244:PRO:HD2	7:p:247:ILE:HD12	1.91	0.52
1:J:309:ALA:HA	1:J:312:VAL:HB	1.91	0.52
1:J:1217:GLN:O	1:J:1221:GLU:HG2	2.09	0.52
1:J:1340:ARG:HA	1:J:1343:ILE:HG22	1.89	0.52
1:K:852:ARG:HD3	5:a:63:ARG:NH1	2.23	0.52
1:K:934:SER:HB3	1:K:937:THR:OG1	2.10	0.52
1:K:1113:ILE:HG21	1:K:1117:MET:HE3	1.91	0.52
1:N:644:ILE:HG22	1:N:675:ILE:CG2	2.32	0.52
1:O:745:GLN:HE22	2:v:295:HIS:HE1	1.58	0.52
1:O:1227:HIS:CE1	1:O:1246:GLN:HG2	2.45	0.52
1:P:732:ILE:HG22	1:P:799:TYR:HE2	1.75	0.52
1:P:841:TYR:HD1	5:u:48:LEU:HD11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:p:110:SER:OG	7:p:280:LEU:O	2.28	0.52
1:J:478:PRO:HA	1:J:557:ARG:HH22	1.74	0.52
1:K:170:ASP:O	1:K:174:ARG:HG2	2.10	0.52
1:K:408:PRO:HB3	1:K:1196:PHE:CD2	2.44	0.52
1:K:957:PRO:HG2	1:K:978:ARG:O	2.10	0.52
1:N:481:ARG:HG3	1:N:550:ILE:HD13	1.90	0.52
1:N:543:HIS:CD2	1:N:546:TYR:HD1	2.27	0.52
3:x:98:LEU:HD13	4:y:3118:VAL:HG21	1.91	0.52
7:p:7:VAL:HA	7:p:37:THR:HG23	1.90	0.52
1:K:297:GLU:O	1:K:298:ALA:CB	2.57	0.52
1:K:918:ARG:O	1:K:994:ARG:NH1	2.39	0.52
6:f:333:TRP:CZ3	6:f:335:ARG:HG2	2.45	0.52
1:K:857:LEU:HD22	1:K:866:ARG:NH2	2.25	0.52
1:N:269:THR:HG22	1:N:271:LYS:H	1.75	0.52
1:O:232:ARG:HH12	1:O:1370:ARG:NH2	2.07	0.52
1:P:1355:PRO:HG2	1:P:1357:HIS:HD2	1.75	0.52
6:h:53:SER:HB2	6:h:56:ALA:HB3	1.91	0.52
7:p:18:ILE:O	7:p:22:GLN:HG2	2.10	0.52
1:J:481:ARG:N	1:J:481:ARG:HD3	2.25	0.52
1:J:789:ASP:OD2	5:Z:1:MET:N	2.43	0.52
1:K:835:VAL:HG22	1:K:944:LEU:HD13	1.91	0.52
1:P:980:VAL:HG11	1:P:1006:ALA:HB2	1.91	0.52
3:x:65:LEU:HB3	4:y:3148:TYR:CE2	2.45	0.52
5:e:27:PHE:HZ	5:e:44:GLN:HG3	1.74	0.52
7:r:197:LEU:O	7:r:199:LEU:N	2.40	0.52
1:J:459:LEU:HD11	1:J:1044:MET:HE1	1.91	0.52
3:w:91:VAL:HG22	4:z:3122:PHE:HD1	1.75	0.52
7:p:192:GLU:H	7:p:192:GLU:CD	2.18	0.52
1:J:103:ALA:HB1	1:O:127:ILE:HG23	1.92	0.52
1:J:424:ILE:HD11	1:J:1345:GLU:HB2	1.90	0.52
1:K:402:GLN:HG3	1:K:1321:LEU:HD13	1.92	0.52
1:N:1304:THR:HG22	1:N:1313:VAL:HB	1.91	0.52
1:O:290:LEU:O	1:O:294:LEU:HB2	2.09	0.52
2:v:42:ALA:HB1	2:v:102:PHE:HD1	1.73	0.52
3:x:88:LEU:O	3:x:92:VAL:HG23	2.10	0.52
7:p:158:ARG:HH22	7:p:197:LEU:HD22	1.75	0.52
1:K:284:ASP:H	1:K:385:GLN:NE2	2.08	0.52
1:N:742:ARG:HB3	1:N:903:ASP:HB2	1.91	0.52
1:N:1113:ILE:HG21	1:N:1117:MET:HE3	1.92	0.52
1:O:216:ILE:HA	1:O:219:PHE:CD2	2.45	0.52
1:O:997:HIS:HE1	1:O:1022:HIS:NE2	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:500:LEU:HD13	1:P:946:HIS:CG	2.45	0.52
3:w:76:ASP:C	4:z:3136:ARG:HH22	2.18	0.52
7:k:12:ARG:HG2	7:k:13:LEU:H	1.75	0.52
1:J:252:VAL:HG23	1:J:1059:PHE:CZ	2.44	0.51
1:N:133:LEU:HD13	1:N:138:LEU:HD21	1.92	0.51
1:P:862:ASN:HB2	5:u:11:GLN:HE21	1.75	0.51
1:P:937:THR:O	1:P:941:THR:HG23	2.10	0.51
3:x:77:HIS:HA	4:y:3136:ARG:NH2	2.25	0.51
5:Z:68:PRO:C	5:Z:70:ARG:H	2.18	0.51
7:k:101:PHE:CD2	7:k:138:LEU:HD22	2.41	0.51
7:k:122:THR:HG22	7:k:133:VAL:HG13	1.91	0.51
1:J:419:THR:OG1	1:J:420:THR:N	2.44	0.51
1:J:889:MET:HE1	5:Z:57:TYR:HD2	1.76	0.51
1:K:461:HIS:CD2	1:K:1124:PHE:HB3	2.46	0.51
1:K:813:TYR:O	1:K:954:TYR:OH	2.22	0.51
1:K:955:GLY:O	1:K:985:ARG:NH2	2.32	0.51
1:K:1159:ARG:NH2	1:K:1317:THR:OG1	2.43	0.51
1:P:724:LEU:HD11	1:P:736:LEU:HD22	1.92	0.51
1:P:1004:TYR:O	1:P:1008:CYS:HB2	2.11	0.51
5:a:47:TYR:O	5:a:51:LEU:HG	2.11	0.51
7:k:49:TYR:CE1	7:k:55:PRO:HB3	2.45	0.51
7:m:228:ILE:HG22	7:m:236:LEU:HD22	1.90	0.51
1:J:642:LEU:HD22	1:J:880:MET:HE1	1.92	0.51
1:J:848:HIS:CD2	5:Z:22:PRO:HD2	2.45	0.51
1:K:311:PHE:CE2	1:K:329:ARG:HG3	2.44	0.51
1:N:216:ILE:HD12	1:N:219:PHE:HD2	1.76	0.51
1:O:258:GLU:O	1:O:262:LYS:HB2	2.10	0.51
1:O:1055:GLU:HG3	1:O:1111:ALA:HB2	1.93	0.51
1:P:858:ASP:OD1	1:P:858:ASP:N	2.37	0.51
1:P:908:GLN:NE2	1:P:1026:SER:OG	2.44	0.51
6:h:281:GLN:CD	6:h:333:TRP:HE1	2.19	0.51
1:K:543:HIS:CD2	1:K:545:LEU:H	2.29	0.51
1:N:443:LYS:HD2	1:N:1113:ILE:HB	1.92	0.51
1:N:1353:HIS:HE1	1:N:1362:ILE:HD13	1.73	0.51
1:P:1253:ILE:HD12	1:P:1259:TYR:HD2	1.75	0.51
1:J:481:ARG:CD	1:J:481:ARG:N	2.73	0.51
1:J:1126:SER:HB2	1:J:1156:ARG:HB2	1.93	0.51
1:K:189:PRO:HG2	1:K:194:LEU:HD12	1.93	0.51
1:N:126:HIS:CE1	7:m:6:VAL:HG21	2.45	0.51
1:P:225:GLU:O	1:P:1370:ARG:NH1	2.43	0.51
6:f:117:ASP:HB3	6:f:118:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:25:ARG:HD2	7:m:2:ASP:HB2	1.93	0.51
1:J:622:VAL:HG21	1:J:639:LEU:HD21	1.92	0.51
1:N:952:MET:HE2	1:N:999:SER:HA	1.91	0.51
1:P:415:ASN:HD21	1:P:579:ALA:HB3	1.76	0.51
2:v:338:GLU:OE2	2:v:496:TYR:OH	2.23	0.51
2:v:382:ASN:HA	2:v:385:LEU:HD23	1.93	0.51
2:v:384:ASP:OD1	2:v:387:ARG:NH1	2.37	0.51
5:e:27:PHE:CZ	5:e:44:GLN:HG3	2.45	0.51
5:e:38:ASP:O	5:e:42:GLU:HG2	2.11	0.51
6:f:105:ALA:HB2	6:f:338:PHE:HE1	1.75	0.51
7:m:7:VAL:HG22	7:m:38:GLN:HB2	1.93	0.51
1:J:486:THR:OG1	1:J:552:ARG:NH1	2.42	0.51
1:O:230:LEU:HD21	1:O:289:GLN:HG2	1.92	0.51
1:O:988:GLN:OE1	1:O:988:GLN:N	2.44	0.51
1:P:133:LEU:HD12	1:P:1086:PHE:HE2	1.76	0.51
1:P:531:HIS:CD2	1:P:533:SER:H	2.29	0.51
2:v:43:TRP:NE1	2:v:101:ARG:HD2	2.25	0.51
7:r:171:ASP:O	7:r:175:HIS:ND1	2.36	0.51
1:J:1049:THR:HG23	1:J:1270:PRO:HB3	1.92	0.51
1:K:284:ASP:OD1	1:K:385:GLN:HB2	2.10	0.51
1:K:484:ARG:HG2	1:K:552:ARG:CA	2.40	0.51
1:K:716:CYS:SG	1:K:1023:ILE:HG12	2.50	0.51
1:N:498:ASN:HB3	1:N:501:VAL:HG12	1.93	0.51
1:N:753:TYR:HE1	1:N:762:PHE:HB2	1.75	0.51
1:O:501:VAL:HG21	5:e:2:ALA:HB3	1.93	0.51
2:v:460:GLY:HA2	2:v:478:PRO:HB3	1.93	0.51
4:z:3145:LYS:HA	4:z:3149:LEU:HD23	1.93	0.51
5:d:23:LEU:HD22	5:d:51:LEU:HB3	1.93	0.51
5:u:35:LEU:HB2	5:u:40:PHE:CE1	2.46	0.51
7:k:289:TYR:HD2	7:k:296:ALA:HB2	1.72	0.51
1:J:367:ILE:HG22	1:J:367:ILE:O	2.11	0.51
1:N:317:ASN:HB3	1:N:327:VAL:HG13	1.92	0.51
3:x:41:LEU:O	3:x:45:GLU:HG2	2.11	0.51
5:a:41:ARG:HA	5:a:44:GLN:HG2	1.91	0.51
5:a:41:ARG:HA	5:a:44:GLN:HE21	1.76	0.51
1:K:191:MET:HB2	1:K:1106:THR:HB	1.93	0.50
1:O:783:ARG:NH2	1:O:891:CYS:O	2.43	0.50
1:P:997:HIS:HA	1:P:1001:MET:HE1	1.93	0.50
2:v:51:ARG:HA	2:v:51:ARG:HE	1.75	0.50
7:m:155:VAL:HG12	7:m:156:TYR:CD1	2.46	0.50
7:p:142:ILE:HD11	7:p:181:TYR:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:632:LYS:NZ	1:J:887:SER:HB2	2.26	0.50
1:J:1067:MET:SD	1:J:1094:SER:HB3	2.52	0.50
1:K:594:LEU:HD13	1:K:696:ALA:HB2	1.93	0.50
1:K:955:GLY:HA3	1:K:985:ARG:HE	1.75	0.50
1:N:620:TYR:OH	1:N:930:ALA:HB2	2.10	0.50
1:J:331:PHE:O	1:J:335:MET:HG2	2.12	0.50
1:J:1213:GLU:OE1	1:J:1213:GLU:N	2.36	0.50
1:N:782:TYR:CE1	1:N:786:GLY:HA3	2.46	0.50
1:P:832:PHE:CE2	1:P:891:CYS:HB3	2.46	0.50
2:v:354:ARG:HG2	3:x:39:LEU:HD11	1.93	0.50
6:f:297:TYR:O	6:f:301:ILE:HG13	2.11	0.50
1:P:841:TYR:CE1	5:u:45:ARG:HG3	2.47	0.50
2:v:63:ALA:O	2:v:77:PHE:HB3	2.11	0.50
1:J:283:THR:HG22	1:J:395:TYR:CE2	2.47	0.50
1:J:411:LEU:HD23	1:J:1193:VAL:HG22	1.94	0.50
1:K:706:VAL:HG23	1:K:711:VAL:HG12	1.94	0.50
1:N:127:ILE:HG23	1:O:103:ALA:HB1	1.94	0.50
1:N:481:ARG:CB	1:N:550:ILE:HD13	2.42	0.50
1:N:1348:SER:OG	1:N:1349:VAL:N	2.45	0.50
2:v:43:TRP:HD1	2:v:103:TYR:CE1	2.29	0.50
2:v:455:ALA:O	2:v:458:THR:OG1	2.28	0.50
5:Z:24:LEU:O	5:Z:28:GLN:HG2	2.12	0.50
1:J:567:MET:HB2	1:J:570:ASN:ND2	2.26	0.50
1:K:800:VAL:HB	1:K:802:GLU:HG3	1.92	0.50
1:K:815:VAL:HG13	1:K:1018:MET:HG2	1.93	0.50
1:N:140:ILE:HD11	1:N:157:ALA:HB2	1.93	0.50
1:N:481:ARG:HG3	1:N:550:ILE:HG21	1.92	0.50
1:N:990:PHE:HE2	1:N:992:GLU:HG2	1.75	0.50
1:P:155:VAL:HA	1:P:158:VAL:HG22	1.93	0.50
1:P:282:VAL:HG12	1:P:1057:ILE:HG12	1.92	0.50
1:P:913:ASN:ND2	1:P:915:ALA:HB3	2.26	0.50
1:P:942:GLN:HE21	5:u:6:PRO:HD2	1.76	0.50
1:P:959:VAL:O	1:P:962:THR:OG1	2.27	0.50
7:m:86:VAL:HG12	7:m:88:GLY:H	1.76	0.50
7:p:110:SER:HA	7:p:282:PRO:O	2.12	0.50
1:K:482:ASP:O	1:K:484:ARG:NH1	2.44	0.50
1:K:507:TYR:CD1	1:K:967:VAL:HG22	2.47	0.50
1:O:529:PHE:HZ	1:O:541:GLU:HG3	1.77	0.50
1:O:572:PRO:HB2	1:O:574:PRO:HD2	1.93	0.50
1:P:522:CYS:SG	1:P:1000:PRO:HG3	2.51	0.50
1:P:876:PRO:HB3	1:P:880:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:981:GLU:OE1	1:P:999:SER:HA	2.12	0.50
4:z:3122:PHE:O	4:z:3126:LEU:HG	2.11	0.50
7:p:103:TRP:HB2	7:p:289:TYR:CE2	2.47	0.50
1:J:856:ILE:HG23	1:J:860:LEU:HD21	1.94	0.50
1:K:461:HIS:HE2	1:K:1128:PHE:HB2	1.76	0.50
1:N:170:ASP:O	1:N:174:ARG:HG2	2.12	0.50
1:O:658:ASN:HD21	1:O:930:ALA:HA	1.77	0.50
1:O:834:HIS:HD2	5:e:8:PRO:HD3	1.77	0.50
5:u:42:GLU:HA	5:u:45:ARG:NH1	2.27	0.50
1:K:550:ILE:HG12	1:K:560:HIS:CD2	2.46	0.50
1:K:616:PRO:HG2	1:K:619:PHE:CE2	2.47	0.50
1:O:1128:PHE:CZ	1:O:1260:ARG:HD2	2.42	0.50
1:P:769:MET:SD	1:P:769:MET:N	2.76	0.50
5:u:48:LEU:O	5:u:52:THR:HG23	2.12	0.50
1:J:458:VAL:HG11	1:J:1184:ILE:HB	1.93	0.49
1:J:957:PRO:HG3	1:J:983:PHE:CG	2.47	0.49
1:P:879:GLY:O	1:P:882:ARG:NE	2.44	0.49
1:P:1001:MET:HB3	1:P:1018:MET:HE1	1.93	0.49
1:J:1130:ALA:HB3	1:J:1261:GLN:HE21	1.76	0.49
1:K:79:ASN:HB3	1:K:308:TYR:HD1	1.77	0.49
1:K:437:GLU:OE2	1:K:439:TRP:NE1	2.42	0.49
1:K:1256:ASN:HD21	1:K:1277:LYS:H	1.61	0.49
1:N:1353:HIS:HE1	1:N:1362:ILE:HG21	1.77	0.49
1:O:465:HIS:CE1	1:O:1027:PRO:HD3	2.47	0.49
1:O:677:LYS:O	1:O:681:SER:OG	2.28	0.49
1:P:484:ARG:NH1	1:P:550:ILE:HD12	2.26	0.49
1:P:487:TYR:OH	1:P:984:ASN:HB3	2.12	0.49
1:P:780:TYR:CE2	5:u:50:PHE:HB2	2.47	0.49
5:d:7:LYS:HG3	5:d:8:PRO:HD2	1.94	0.49
7:p:57:TYR:HB3	7:p:204:ASN:HD22	1.76	0.49
1:J:625:MET:HE2	1:J:835:VAL:HG12	1.93	0.49
1:K:548:ILE:HD11	1:K:560:HIS:HB3	1.95	0.49
1:N:657:VAL:HA	1:N:663:ILE:HD11	1.94	0.49
1:O:69:LEU:HD12	6:f:3:VAL:HG23	1.94	0.49
1:O:639:LEU:HD12	1:O:880:MET:HE2	1.93	0.49
1:P:886:ALA:HB1	5:u:57:TYR:HB2	1.93	0.49
7:k:94:LYS:HB2	7:k:295:THR:HG23	1.93	0.49
1:N:75:VAL:HA	1:N:267:TYR:CE1	2.48	0.49
1:N:196:THR:HG21	1:N:218:MET:HB3	1.94	0.49
1:N:559:ARG:HH22	1:N:561:ARG:HE	1.58	0.49
1:O:480:PRO:HG2	1:O:483:ARG:NH2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:229:PHE:HB2	1:P:243:TYR:HE2	1.77	0.49
1:P:824:HIS:ND1	1:P:956:ASP:OD2	2.44	0.49
1:P:901:SER:OG	1:P:918:ARG:NH2	2.45	0.49
5:Z:68:PRO:CG	5:Z:71:GLN:HE21	2.25	0.49
5:d:11:GLN:H	5:d:11:GLN:CD	2.18	0.49
7:p:203:ASP:OD1	7:p:204:ASN:N	2.44	0.49
7:r:95:ASN:OD1	7:r:294:LEU:HB3	2.11	0.49
1:K:467:PRO:HD3	1:K:546:TYR:CZ	2.48	0.49
1:N:1252:ASP:O	1:N:1256:ASN:HB2	2.11	0.49
1:N:1260:ARG:NH1	1:N:1269:SER:OG	2.40	0.49
1:O:399:ARG:CD	1:O:1320:PHE:HB3	2.42	0.49
2:v:51:ARG:NH2	2:v:337:ARG:HD3	2.28	0.49
1:N:526:THR:HG22	1:N:574:PRO:HA	1.94	0.49
1:N:1272:ARG:HH21	1:N:1276:ASN:ND2	2.11	0.49
1:O:731:ASP:HA	1:O:796:LEU:HD13	1.95	0.49
1:O:860:LEU:HD11	1:O:865:LEU:HB3	1.94	0.49
1:P:805:ALA:C	1:P:807:VAL:H	2.20	0.49
6:f:235:ALA:O	6:f:238:SER:OG	2.27	0.49
1:J:764:GLU:HB2	1:J:793:ARG:HH11	1.78	0.49
1:J:840:ALA:HB3	5:Z:49:VAL:HG22	1.95	0.49
1:K:806:ASP:O	1:K:807:VAL:C	2.55	0.49
1:O:933:PHE:HD2	1:O:963:MET:HG2	1.78	0.49
1:P:439:TRP:N	1:P:1337:ALA:O	2.45	0.49
1:P:675:ILE:HD13	1:P:680:TYR:HB2	1.95	0.49
2:v:10:LEU:HD23	7:p:225:ARG:HD3	1.95	0.49
2:v:59:ARG:HG3	2:v:60:VAL:N	2.27	0.49
3:x:101:MET:O	4:y:3114:GLN:NE2	2.45	0.49
6:h:135:MET:HG2	6:h:172:PHE:HZ	1.78	0.49
7:m:12:ARG:O	7:m:127:SER:OG	2.27	0.49
7:p:95:ASN:HD22	7:p:103:TRP:HE1	1.59	0.49
1:J:203:THR:O	1:J:203:THR:OG1	2.24	0.49
1:J:932:ALA:HB2	1:J:959:VAL:HG22	1.95	0.49
1:K:932:ALA:HA	1:K:959:VAL:HG13	1.95	0.49
1:N:93:ILE:HD12	1:N:1095:ILE:HG21	1.94	0.49
1:N:667:CYS:SG	1:N:683:TYR:HB3	2.52	0.49
1:O:655:ALA:O	1:O:683:TYR:OH	2.28	0.49
6:f:109:PRO:HD3	6:f:223:VAL:HG23	1.95	0.49
1:J:266:THR:C	1:J:305:PRO:HG3	2.38	0.49
1:J:406:TYR:HE2	1:J:1196:PHE:HD1	1.61	0.49
1:N:847:SER:HB2	1:N:850:PHE:CD2	2.46	0.49
1:O:690:LEU:HB3	1:O:808:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:947:ALA:HB3	1:O:964:HIS:ND1	2.28	0.49
1:P:800:VAL:HG23	1:P:802:GLU:HG2	1.94	0.49
5:d:6:PRO:O	5:d:7:LYS:HB2	2.13	0.49
7:p:101:PHE:HE2	7:p:139:PRO:HD2	1.77	0.49
1:J:103:ALA:HB3	1:O:175:GLY:HA3	1.94	0.49
1:J:155:VAL:HA	1:J:158:VAL:HG22	1.94	0.49
1:J:421:SER:HB3	1:J:1354:ALA:HB2	1.94	0.49
1:J:714:TYR:HD2	1:J:1028:MET:HG3	1.77	0.49
1:J:934:SER:HB3	1:J:937:THR:HG23	1.95	0.49
1:N:467:PRO:HG2	1:N:912:PRO:HD3	1.94	0.49
1:N:1353:HIS:CE1	1:N:1362:ILE:HD13	2.48	0.49
1:P:488:SER:C	1:P:991:ALA:HB1	2.38	0.49
1:P:531:HIS:CG	1:P:532:PRO:HD2	2.48	0.49
7:r:255:LEU:H	7:r:255:LEU:HD23	1.78	0.49
1:J:93:ILE:HA	1:O:32:GLY:O	2.13	0.48
1:K:1313:VAL:HG21	1:K:1319:VAL:HG21	1.93	0.48
1:N:466:THR:HG22	1:N:910:LEU:HB3	1.94	0.48
1:N:606:VAL:O	1:N:609:THR:OG1	2.22	0.48
1:N:620:TYR:CE1	1:N:828:LEU:HD22	2.47	0.48
1:O:843:GLY:HA3	5:d:69:ARG:HH12	1.77	0.48
1:O:906:VAL:HA	1:O:909:GLN:CG	2.43	0.48
1:O:906:VAL:HA	1:O:909:GLN:HG2	1.94	0.48
2:v:118:SER:HB2	2:v:288:ILE:HD12	1.95	0.48
2:v:350:SER:O	2:v:354:ARG:HG3	2.12	0.48
6:f:236:TRP:CE3	6:f:237:LEU:HD23	2.48	0.48
7:m:28:ILE:HD12	7:m:137:VAL:HG11	1.94	0.48
1:K:1152:GLY:O	1:K:1167:ASN:ND2	2.46	0.48
1:N:64:GLN:OE1	1:N:64:GLN:N	2.28	0.48
1:N:645:ASN:HA	1:N:675:ILE:CG2	2.43	0.48
1:N:1353:HIS:CE1	1:N:1362:ILE:HG21	2.48	0.48
1:O:406:TYR:HA	1:O:1046:VAL:O	2.13	0.48
1:O:596:HIS:CG	1:O:1012:LEU:HD11	2.47	0.48
1:O:1255:TYR:HA	1:O:1260:ARG:NH1	2.28	0.48
1:P:724:LEU:HD22	1:P:732:ILE:HD12	1.95	0.48
2:v:43:TRP:CD1	2:v:103:TYR:CE1	3.01	0.48
7:p:111:VAL:HB	7:p:282:PRO:HB2	1.95	0.48
7:r:49:TYR:CE1	7:r:118:ARG:HD3	2.48	0.48
1:J:266:THR:HG21	1:J:1062:ARG:NE	2.26	0.48
1:J:1252:ASP:O	1:J:1256:ASN:HB2	2.13	0.48
1:K:1195:TYR:OH	1:K:1203:ARG:O	2.32	0.48
1:N:217:ALA:HA	1:N:220:LYS:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:832:PHE:HD2	1:N:892:PRO:O	1.97	0.48
1:O:30:ALA:HB1	1:O:33:LEU:HD13	1.95	0.48
1:O:670:LEU:O	1:O:672:ASN:N	2.46	0.48
1:P:586:GLN:HE21	1:P:1013:VAL:HG13	1.79	0.48
1:P:734:THR:HG22	1:P:753:TYR:OH	2.13	0.48
1:P:863:GLY:HA2	1:P:866:ARG:HB3	1.95	0.48
6:f:110:LEU:HD22	6:f:191:LEU:HD21	1.95	0.48
6:f:206:VAL:HG11	6:f:211:VAL:HG12	1.95	0.48
6:f:228:GLU:OE1	6:f:229:ALA:N	2.47	0.48
6:h:116:SER:O	7:r:183:GLY:HA3	2.13	0.48
1:J:192:PHE:CE2	1:J:193:ILE:HG13	2.48	0.48
1:K:352:LEU:O	1:K:355:VAL:HG12	2.13	0.48
1:N:191:MET:HB2	1:N:1106:THR:HB	1.96	0.48
1:N:388:TYR:CE2	1:N:396:PRO:HD3	2.48	0.48
1:N:1023:ILE:HG21	1:N:1033:GLN:NE2	2.28	0.48
1:N:1128:PHE:CZ	1:N:1260:ARG:HG3	2.47	0.48
1:O:726:PRO:HD3	1:O:814:TYR:CE1	2.49	0.48
1:P:37:PHE:O	1:P:41:VAL:HG13	2.14	0.48
1:P:1132:ALA:HB1	1:P:1139:ASN:CG	2.39	0.48
2:v:377:SER:C	2:v:379:ILE:H	2.20	0.48
7:m:104:HIS:HB3	7:m:106:THR:HG23	1.94	0.48
7:p:38:GLN:C	7:p:39:ASN:O	2.56	0.48
7:r:274:LEU:HG	7:r:278:PHE:HE2	1.77	0.48
1:J:442:ASN:OD1	1:J:443:LYS:N	2.43	0.48
1:K:135:MET:N	1:K:1082:ASP:O	2.37	0.48
1:N:840:ALA:HB3	5:d:49:VAL:HG22	1.95	0.48
1:O:826:CYS:HA	1:O:954:TYR:O	2.13	0.48
1:P:226:HIS:HD2	1:P:243:TYR:OH	1.96	0.48
1:P:842:ASN:HD22	1:P:865:LEU:HD12	1.79	0.48
1:P:1205:ARG:HG3	1:P:1231:ASP:HB3	1.95	0.48
2:v:49:SER:N	2:v:96:HIS:HD2	2.10	0.48
2:v:290:HIS:CD2	2:v:293:SER:H	2.32	0.48
6:f:266:VAL:HG13	6:f:322:ALA:HB3	1.95	0.48
6:h:46:HIS:HE1	6:h:70:VAL:HA	1.78	0.48
7:m:216:LEU:HD22	7:r:213:VAL:HG23	1.96	0.48
7:m:222:ARG:HD3	7:m:255:LEU:HD11	1.96	0.48
7:r:138:LEU:HD23	7:r:143:ALA:HA	1.96	0.48
1:J:889:MET:HE3	5:Z:54:GLN:NE2	2.29	0.48
1:K:548:ILE:HD12	1:K:561:ARG:O	2.13	0.48
1:O:904:ASN:ND2	1:O:908:GLN:O	2.47	0.48
1:P:933:PHE:CD2	1:P:963:MET:HG2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:267:TYR:O	1:J:276:VAL:HG23	2.14	0.48
1:J:461:HIS:CG	1:J:462:PRO:HD2	2.49	0.48
1:K:921:GLN:HB2	1:K:996:TRP:HD1	1.77	0.48
1:K:1188:PRO:HD2	1:K:1241:ASN:CB	2.43	0.48
1:O:413:MET:HE1	1:O:1193:VAL:HG21	1.96	0.48
1:P:61:ASN:OD1	1:P:62:ALA:N	2.46	0.48
2:v:115:TYR:HB2	2:v:291:ILE:HD12	1.95	0.48
2:v:490:THR:N	2:v:493:GLU:OE2	2.32	0.48
1:N:104:HIS:CD2	1:N:108:ARG:HH11	2.31	0.48
1:N:162:ALA:O	1:N:166:GLN:HG2	2.13	0.48
1:N:1053:LEU:HD22	1:N:1111:ALA:HB3	1.96	0.48
1:N:1297:ARG:NH2	1:N:1298:LEU:O	2.47	0.48
1:O:489:LEU:H	1:O:489:LEU:HD12	1.79	0.48
1:O:764:GLU:OE2	1:O:793:ARG:NE	2.28	0.48
1:P:481:ARG:NH2	1:P:540:LEU:HD11	2.28	0.48
6:f:267:ALA:HA	6:f:320:ALA:O	2.13	0.48
1:J:830:VAL:HG22	1:J:945:PHE:HD1	1.78	0.48
1:N:559:ARG:NH2	1:N:561:ARG:HE	2.12	0.48
1:N:619:PHE:HE2	1:N:647:TYR:HB2	1.79	0.48
1:N:794:LEU:HD21	1:N:925:VAL:HG11	1.96	0.48
1:N:1378:LYS:NZ	1:O:1351:GLN:O	2.35	0.48
1:O:524:LEU:O	1:O:574:PRO:HG3	2.14	0.48
1:O:633:PHE:CE2	1:O:665:PHE:HB3	2.49	0.48
1:O:889:MET:HE2	5:e:54:GLN:NE2	2.29	0.48
1:P:544:PRO:HG3	1:P:1243:TRP:CD2	2.49	0.48
1:P:861:GLU:HB3	1:P:866:ARG:NH1	2.28	0.48
7:m:155:VAL:HG12	7:m:156:TYR:HD1	1.79	0.48
1:J:59:TYR:HB2	1:K:95:PHE:CD1	2.48	0.48
1:J:543:HIS:CE1	1:J:1250:LEU:HD12	2.48	0.48
1:J:831:ASP:OD2	1:J:834:HIS:ND1	2.47	0.48
1:K:384:LEU:O	1:K:395:TYR:HE2	1.96	0.48
1:K:842:ASN:OD1	1:K:843:GLY:N	2.47	0.48
1:K:1136:GLN:NE2	1:K:1140:ASP:OD2	2.46	0.48
1:K:1346:PHE:HD1	1:K:1353:HIS:CD2	2.32	0.48
1:N:467:PRO:HD3	1:N:546:TYR:CZ	2.49	0.48
1:N:484:ARG:HG3	1:N:484:ARG:NH1	2.28	0.48
1:P:413:MET:HE1	1:P:1193:VAL:HG11	1.94	0.48
1:P:437:GLU:OE1	1:P:437:GLU:N	2.47	0.48
1:P:843:GLY:O	1:P:847:SER:N	2.29	0.48
5:d:21:SER:HB3	5:d:24:LEU:HD23	1.96	0.48
1:J:69:LEU:HD13	1:J:308:TYR:CZ	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:483:ARG:HE	1:O:550:ILE:HG21	1.78	0.47
5:d:15:GLU:OE1	5:d:48:LEU:HD11	2.15	0.47
6:f:95:ILE:O	6:f:201:ASN:N	2.44	0.47
1:J:203:THR:HB	1:J:207:PHE:HE1	1.79	0.47
1:N:639:LEU:HD12	1:N:880:MET:HB3	1.96	0.47
1:O:388:TYR:HD2	1:O:395:TYR:HA	1.80	0.47
5:Z:68:PRO:CG	5:Z:71:GLN:NE2	2.73	0.47
5:d:30:LEU:HD23	5:d:44:GLN:HG2	1.95	0.47
7:k:225:ARG:NH2	7:k:243:VAL:HG11	2.28	0.47
7:p:50:SER:OG	7:p:53:THR:N	2.28	0.47
1:J:783:ARG:HG2	1:J:833:GLN:HE21	1.79	0.47
1:K:452:LEU:HD13	1:K:1040:PRO:HG2	1.96	0.47
1:K:543:HIS:CD2	1:K:546:TYR:HD1	2.31	0.47
1:N:269:THR:HG22	1:N:271:LYS:N	2.29	0.47
1:O:154:TYR:O	1:O:158:VAL:HG13	2.14	0.47
1:P:658:ASN:HB2	1:P:931:PHE:CE2	2.50	0.47
2:v:372:ILE:HG13	2:v:374:THR:N	2.25	0.47
6:f:197:SER:HB2	6:f:200:LEU:O	2.15	0.47
6:h:237:LEU:HG	6:h:292:ILE:HD12	1.96	0.47
7:m:265:ARG:O	7:m:269:THR:HG23	2.15	0.47
1:J:848:HIS:NE2	5:Z:21:SER:OG	2.29	0.47
1:J:1075:SER:OG	1:J:1076:ARG:N	2.47	0.47
1:O:854:GLU:O	1:O:878:VAL:HG23	2.15	0.47
3:w:76:ASP:HB3	4:z:3136:ARG:NH1	2.29	0.47
3:x:69:GLU:CD	4:y:3143:ARG:HH12	2.21	0.47
3:x:80:ARG:HE	4:y:3136:ARG:HD3	1.78	0.47
6:f:110:LEU:HD22	6:f:191:LEU:HD11	1.96	0.47
7:r:48:VAL:HG12	7:r:60:MET:HE2	1.96	0.47
7:r:55:PRO:HB2	7:r:201:LEU:HD23	1.95	0.47
1:K:1045:THR:OG1	1:K:1185:ILE:HB	2.14	0.47
1:N:612:ASP:C	1:N:614:ALA:H	2.22	0.47
1:O:436:VAL:CG1	1:O:587:GLN:HE22	2.24	0.47
1:P:641:SER:O	1:P:645:ASN:ND2	2.47	0.47
1:P:863:GLY:O	1:P:867:ASP:N	2.35	0.47
2:v:43:TRP:CD1	7:k:162:GLN:HE22	2.33	0.47
3:x:77:HIS:HA	4:y:3136:ARG:HH22	1.79	0.47
3:x:80:ARG:HD2	4:y:3136:ARG:CZ	2.44	0.47
3:x:88:LEU:HG	4:y:3126:LEU:HD22	1.97	0.47
6:h:51:SER:HB3	6:h:56:ALA:HB1	1.97	0.47
1:N:644:ILE:HG21	1:N:675:ILE:HG13	1.95	0.47
1:N:790:HIS:ND1	1:N:790:HIS:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:543:HIS:CE1	1:O:545:LEU:HB2	2.49	0.47
1:O:724:LEU:O	1:O:814:TYR:OH	2.29	0.47
1:P:549:TYR:CZ	1:P:561:ARG:HB3	2.49	0.47
1:P:1255:TYR:HB2	1:P:1275:PHE:HD2	1.79	0.47
2:v:464:HIS:CE1	2:v:466:ALA:HB2	2.49	0.47
3:x:71:ASP:O	3:x:75:ARG:HG3	2.14	0.47
6:f:162:PRO:O	6:f:165:LEU:HB2	2.13	0.47
1:J:128:SER:HA	1:J:1088:VAL:O	2.15	0.47
1:J:413:MET:HE1	1:J:1193:VAL:HG21	1.96	0.47
1:J:493:ARG:HE	1:J:747:ILE:HD13	1.80	0.47
1:J:584:ARG:NH1	1:J:1020:ALA:O	2.33	0.47
1:J:1117:MET:SD	1:J:1371:ARG:NH1	2.88	0.47
1:K:546:TYR:CD2	1:K:564:HIS:HB3	2.50	0.47
1:K:1159:ARG:HD3	1:K:1315:ALA:HB3	1.97	0.47
1:N:176:LEU:O	1:N:179:THR:OG1	2.30	0.47
1:N:344:LYS:HB3	1:N:344:LYS:HE2	1.73	0.47
1:N:699:ARG:HH22	1:O:1006:ALA:HB1	1.79	0.47
1:N:950:PHE:HD1	1:N:950:PHE:HA	1.61	0.47
1:N:1215:TYR:CE1	1:N:1285:ARG:HG2	2.50	0.47
1:O:951:HIS:HE2	1:O:997:HIS:HD2	1.61	0.47
1:P:481:ARG:HH22	1:P:540:LEU:HD11	1.80	0.47
2:v:402:CYS:SG	2:v:403:TRP:N	2.88	0.47
4:z:3131:GLU:O	4:z:3135:HIS:ND1	2.47	0.47
7:k:148:GLN:HE22	7:p:269:THR:HG23	1.79	0.47
7:m:11:SER:H	7:m:128:ASN:HD21	1.61	0.47
7:m:176:LEU:HD23	7:m:176:LEU:HA	1.65	0.47
1:J:1287:LEU:HD12	1:J:1287:LEU:HA	1.80	0.47
1:K:1048:ARG:NH2	1:K:1117:MET:O	2.48	0.47
1:O:93:ILE:HD11	1:O:1095:ILE:HG21	1.96	0.47
1:O:388:TYR:CD2	1:O:395:TYR:HA	2.50	0.47
1:P:133:LEU:HD22	1:P:161:VAL:HG12	1.96	0.47
1:P:630:GLU:O	1:P:634:VAL:HG23	2.14	0.47
1:P:830:VAL:HG13	1:P:944:LEU:HD11	1.97	0.47
1:P:1342:LEU:HD13	1:P:1362:ILE:HB	1.96	0.47
6:f:313:ILE:HD11	7:k:263:ARG:HG2	1.97	0.47
1:J:209:LYS:NZ	1:O:1308:GLU:OE2	2.47	0.47
1:J:283:THR:HG22	1:J:395:TYR:HE2	1.79	0.47
1:J:824:HIS:HA	1:J:956:ASP:CG	2.39	0.47
1:K:1154:LEU:HD23	1:K:1167:ASN:HB2	1.97	0.47
1:N:483:ARG:NH1	1:N:485:GLU:HB3	2.29	0.47
1:N:557:ARG:HG2	1:N:558:ALA:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:552:ARG:HH22	3:w:42:ALA:HB1	1.79	0.47
1:O:933:PHE:CE2	1:O:963:MET:HE2	2.50	0.47
1:O:977:GLN:HE21	1:O:983:PHE:HA	1.79	0.47
1:O:1081:VAL:HG23	1:O:1082:ASP:OD1	2.15	0.47
1:P:405:TYR:HA	1:P:1332:PHE:O	2.15	0.47
5:Z:11:GLN:HB2	5:e:69:ARG:HH12	1.80	0.47
6:h:45:GLU:OE2	6:h:82:TRP:NE1	2.48	0.47
6:h:135:MET:HB3	6:h:275:PRO:HG2	1.97	0.47
7:m:74:GLU:HB3	7:m:81:ILE:HB	1.96	0.47
7:p:289:TYR:HE2	7:p:291:GLN:HG2	1.80	0.47
7:r:41:GLN:OE1	7:r:41:GLN:N	2.40	0.47
1:J:162:ALA:O	1:J:166:GLN:HG3	2.15	0.47
1:J:431:THR:HG23	1:J:432:GLN:HG3	1.97	0.47
1:J:635:MET:HG2	5:Z:60:TYR:CE2	2.50	0.47
1:J:637:VAL:HA	1:J:640:VAL:HG22	1.97	0.47
1:J:1174:LEU:O	1:K:213:SER:OG	2.31	0.47
1:K:1160:THR:HG21	1:K:1314:ILE:HD11	1.97	0.47
1:N:347:SER:O	1:N:350:SER:OG	2.28	0.47
1:N:826:CYS:HA	1:N:954:TYR:O	2.15	0.47
3:w:49:ALA:O	3:w:53:ARG:HG3	2.14	0.47
5:d:5:LEU:HG	5:d:6:PRO:HD2	1.97	0.47
1:J:420:THR:O	1:J:420:THR:OG1	2.33	0.46
1:J:423:ALA:HB1	1:K:420:THR:O	2.15	0.46
1:J:609:THR:HG22	1:J:653:ARG:HB3	1.97	0.46
1:K:832:PHE:CE2	1:K:892:PRO:HG2	2.49	0.46
1:K:861:GLU:CG	5:Z:69:ARG:HE	2.28	0.46
1:K:933:PHE:CD2	1:K:963:MET:HG2	2.50	0.46
1:O:526:THR:OG1	1:O:527:GLU:N	2.47	0.46
1:O:860:LEU:HB3	1:O:866:ARG:HD3	1.98	0.46
1:P:736:LEU:O	1:P:740:SER:OG	2.30	0.46
7:k:247:ILE:O	7:k:251:ASP:HB2	2.14	0.46
7:p:95:ASN:HB3	7:p:103:TRP:CZ2	2.51	0.46
7:p:98:GLN:CB	7:p:99:PRO:CD	2.92	0.46
1:J:126:HIS:CD2	1:J:1091:GLU:HG2	2.49	0.46
1:J:482:ASP:N	1:J:482:ASP:OD1	2.42	0.46
1:J:1259:TYR:CE2	1:J:1262:THR:HB	2.47	0.46
1:K:441:VAL:HG11	1:K:1373:LEU:HD22	1.98	0.46
1:K:630:GLU:CD	1:K:665:PHE:HE1	2.24	0.46
1:K:1152:GLY:HA2	1:K:1169:ASN:O	2.16	0.46
1:N:955:GLY:HA3	1:N:985:ARG:HH21	1.81	0.46
1:O:397:LEU:O	1:O:399:ARG:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:605:THR:O	1:O:609:THR:HG23	2.15	0.46
1:O:922:THR:HG21	1:O:989:LEU:O	2.15	0.46
1:P:269:THR:OG1	1:P:273:GLY:HA2	2.14	0.46
1:P:542:LEU:HB3	1:P:1249:SER:HA	1.95	0.46
1:P:1227:HIS:NE2	1:P:1245:SER:O	2.49	0.46
5:Z:22:PRO:O	5:Z:25:PRO:HD2	2.15	0.46
5:e:57:TYR:O	5:e:61:VAL:HG23	2.15	0.46
7:k:153:PHE:HE1	7:k:172:VAL:HG13	1.80	0.46
7:p:158:ARG:O	7:p:162:GLN:HG2	2.15	0.46
1:J:400:ARG:HH22	1:J:1114:THR:HG21	1.79	0.46
1:J:633:PHE:CE2	1:J:665:PHE:HB3	2.50	0.46
1:J:1092:MET:HE3	1:J:1092:MET:HB2	1.77	0.46
1:K:997:HIS:HE1	1:K:1022:HIS:CE1	2.22	0.46
1:N:84:ASP:OD1	1:N:84:ASP:N	2.37	0.46
1:N:536:ASP:OD1	1:N:536:ASP:N	2.47	0.46
1:O:964:HIS:HB3	1:O:967:VAL:H	1.80	0.46
6:f:95:ILE:HA	6:f:122:VAL:HG13	1.97	0.46
1:J:306:SER:HB2	1:J:307:SER:H	1.54	0.46
1:J:666:ILE:O	1:J:670:LEU:HB3	2.16	0.46
1:K:652:GLY:C	1:K:653:ARG:HD3	2.41	0.46
1:K:1269:SER:HB2	1:K:1272:ARG:HB2	1.97	0.46
1:N:428:ASP:OD1	1:N:429:ASN:N	2.49	0.46
1:N:513:ALA:HB1	1:N:984:ASN:ND2	2.30	0.46
1:O:193:ILE:HG22	1:O:197:LEU:HD22	1.97	0.46
1:O:734:THR:HG23	1:O:763:ILE:HD12	1.98	0.46
1:O:841:TYR:HB2	5:e:45:ARG:NH1	2.30	0.46
1:O:933:PHE:CD2	1:O:963:MET:HG2	2.51	0.46
1:O:1268:TYR:CG	1:O:1303:ALA:HB2	2.50	0.46
1:P:872:SER:O	1:P:874:LEU:HG	2.16	0.46
5:e:4:ARG:HH22	5:e:7:LYS:HG2	1.79	0.46
6:h:179:ARG:HG3	6:h:270:TYR:CE2	2.51	0.46
7:p:9:LEU:HD13	7:p:128:ASN:HD21	1.79	0.46
7:p:284:LEU:HG	7:p:299:TRP:O	2.16	0.46
1:J:172:LEU:HD23	1:J:172:LEU:HA	1.71	0.46
1:J:267:TYR:CD2	1:J:304:GLY:HA2	2.51	0.46
1:K:336:ALA:HA	1:K:340:ASP:HB3	1.98	0.46
1:K:861:GLU:HG2	5:Z:69:ARG:HE	1.81	0.46
1:N:399:ARG:HG3	1:N:1105:MET:HE1	1.96	0.46
1:N:484:ARG:HH11	1:N:484:ARG:CG	2.29	0.46
1:P:461:HIS:CD2	1:P:1124:PHE:HB3	2.50	0.46
1:P:831:ASP:H	1:P:944:LEU:HD21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:122:VAL:HG12	6:f:124:ALA:N	2.30	0.46
1:J:482:ASP:CG	1:J:484:ARG:HE	2.23	0.46
1:K:172:LEU:HD21	1:K:1090:HIS:ND1	2.31	0.46
1:K:835:VAL:O	1:K:838:THR:OG1	2.25	0.46
1:K:1039:HIS:ND1	1:K:1040:PRO:O	2.49	0.46
1:N:217:ALA:O	1:N:220:LYS:HG2	2.15	0.46
1:N:658:ASN:HD21	1:N:930:ALA:HA	1.80	0.46
1:N:818:PRO:HB3	1:N:953:PHE:HB3	1.98	0.46
1:O:184:LYS:NZ	1:O:1064:SER:HB2	2.30	0.46
1:O:487:TYR:OH	1:O:985:ARG:O	2.23	0.46
1:O:609:THR:HG22	1:O:653:ARG:HB3	1.98	0.46
1:O:660:PHE:HB2	1:O:812:PHE:CD2	2.51	0.46
1:O:668:ARG:HD2	1:O:669:HIS:CE1	2.50	0.46
1:P:542:LEU:HD23	1:P:1248:GLY:C	2.41	0.46
1:P:731:ASP:HB2	1:P:797:GLY:HA3	1.98	0.46
1:P:1008:CYS:SG	1:P:1014:SER:HB2	2.55	0.46
2:v:125:ARG:HH22	2:v:303:PRO:HA	1.79	0.46
5:a:68:PRO:HG2	5:a:71:GLN:HB3	1.96	0.46
7:k:25:ILE:HD11	7:k:74:GLU:HA	1.98	0.46
7:p:169:MET:HE3	7:p:173:HIS:HE1	1.81	0.46
1:K:4:ASN:HD22	1:K:38:ASP:HB2	1.81	0.46
1:K:216:ILE:HD12	1:K:219:PHE:HD2	1.80	0.46
1:K:899:ARG:HH21	1:K:920:GLU:HG3	1.81	0.46
1:N:1070:GLY:O	1:N:1090:HIS:NE2	2.49	0.46
1:O:386:LYS:HD2	1:O:386:LYS:HA	1.73	0.46
1:P:488:SER:O	1:P:991:ALA:HB1	2.15	0.46
1:P:491:HIS:CD2	1:P:493:ARG:HG3	2.50	0.46
2:v:43:TRP:CZ3	2:v:56:ARG:HG2	2.51	0.46
2:v:368:ILE:HG22	2:v:370:VAL:HG23	1.98	0.46
5:e:1:MET:SD	5:e:4:ARG:HG2	2.56	0.46
6:f:179:ARG:NE	6:f:317:THR:HB	2.30	0.46
1:J:1120:HIS:N	1:J:1182:CYS:SG	2.80	0.46
1:K:783:ARG:O	1:K:788:HIS:NE2	2.47	0.46
1:N:680:TYR:O	1:N:684:ARG:HG3	2.16	0.46
2:v:7:ASN:ND2	2:v:60:VAL:HG22	2.31	0.46
2:v:414:THR:HB	2:v:415:PRO:HD3	1.97	0.46
5:Z:76:LYS:HD2	5:Z:77:ARG:H	1.80	0.46
6:h:151:LEU:HB2	6:h:228:GLU:HG3	1.98	0.46
6:h:302:MET:O	6:h:306:ALA:HB2	2.16	0.46
7:k:174:MET:HG3	7:k:175:HIS:ND1	2.31	0.46
7:k:199:LEU:HA	7:k:202:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:k:238:LEU:HD11	7:p:263:ARG:NE	2.28	0.46
1:N:1174:LEU:HD13	1:O:209:LYS:HD2	1.97	0.46
1:N:1322:GLU:OE1	1:N:1322:GLU:N	2.49	0.46
1:O:610:ALA:HA	1:O:931:PHE:CD2	2.51	0.46
1:O:636:ASN:O	1:O:640:VAL:HG13	2.16	0.46
2:v:381:LYS:O	2:v:383:SER:N	2.49	0.46
5:e:15:GLU:OE1	5:e:44:GLN:NE2	2.48	0.46
6:f:236:TRP:HE3	6:f:237:LEU:HD23	1.80	0.46
6:f:359:ASP:OD2	7:p:283:ARG:NH2	2.49	0.46
7:m:17:GLU:H	7:m:17:GLU:HG2	1.58	0.46
1:J:287:LEU:O	1:J:291:LEU:HG	2.16	0.46
1:J:402:GLN:NE2	1:J:1051:GLU:OE2	2.44	0.46
1:J:497:MET:HE1	1:J:748:ILE:HG22	1.98	0.46
1:J:724:LEU:HD22	1:J:732:ILE:HD11	1.98	0.46
1:P:627:HIS:CE1	1:P:629:PHE:HB2	2.51	0.46
1:P:1077:ARG:HD3	1:P:1078:GLU:O	2.16	0.46
2:v:23:VAL:HG23	2:v:76:THR:HB	1.98	0.46
6:f:162:PRO:HB2	6:f:165:LEU:HD22	1.99	0.46
7:m:15:THR:O	7:m:18:ILE:HG22	2.16	0.46
7:p:29:LEU:HD23	7:p:30:PRO:HD2	1.97	0.46
7:p:153:PHE:CD1	7:p:190:LEU:HD23	2.50	0.46
7:r:244:PRO:HD2	7:r:247:ILE:HD12	1.98	0.46
1:J:289:GLN:O	1:J:292:THR:OG1	2.27	0.45
1:J:933:PHE:CE2	1:J:963:MET:HG2	2.51	0.45
1:J:1215:TYR:HE1	1:J:1285:ARG:HG2	1.80	0.45
1:N:189:PRO:HG2	1:N:194:LEU:HD21	1.97	0.45
1:O:1023:ILE:HG21	1:O:1033:GLN:NE2	2.31	0.45
1:P:73:LEU:HD13	1:P:281:ILE:HD11	1.99	0.45
1:P:96:ARG:HA	1:P:117:ILE:HG13	1.97	0.45
7:m:97:TYR:O	7:m:100:PHE:HB3	2.16	0.45
7:p:222:ARG:HA	7:p:252:LEU:HD21	1.98	0.45
1:J:531:HIS:HD2	1:J:533:SER:H	1.65	0.45
1:J:619:PHE:CE1	1:J:643:CYS:HB3	2.51	0.45
1:K:496:HIS:HE1	1:K:502:ILE:HG12	1.81	0.45
1:K:690:LEU:HD23	1:K:808:LEU:HB3	1.98	0.45
1:N:128:SER:HA	1:N:1088:VAL:O	2.15	0.45
1:N:172:LEU:HD21	1:N:1090:HIS:ND1	2.31	0.45
1:N:830:VAL:HB	1:N:832:PHE:CE1	2.51	0.45
1:O:529:PHE:HE2	1:O:575:LEU:HD21	1.80	0.45
1:P:735:HIS:CE1	1:P:739:VAL:HG21	2.52	0.45
3:w:56:ARG:NH1	3:x:56:ARG:HG2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:k:118:ARG:HD2	7:k:122:THR:HG21	1.97	0.45
7:m:28:ILE:HD11	7:m:93:ILE:HD11	1.98	0.45
7:m:59:SER:HB2	7:m:197:LEU:HD12	1.98	0.45
7:r:105:GLY:O	7:r:106:THR:OG1	2.34	0.45
1:K:301:GLN:HE21	1:K:366:PRO:HB2	1.81	0.45
1:K:856:ILE:HG13	1:K:878:VAL:HG22	1.98	0.45
1:O:460:CYS:HB3	1:O:1027:PRO:HB3	1.98	0.45
1:O:743:ALA:N	2:v:73:HIS:CE1	2.84	0.45
1:O:745:GLN:HE22	2:v:295:HIS:CE1	2.35	0.45
1:P:1027:PRO:HG2	1:P:1133:PHE:CZ	2.50	0.45
7:k:31:LEU:HG	7:k:68:THR:HG23	1.99	0.45
7:r:229:ARG:HD2	7:r:230:HIS:N	2.26	0.45
1:J:270:ALA:HB3	1:J:301:GLN:HB2	1.98	0.45
1:J:1243:TRP:O	1:J:1249:SER:HB2	2.16	0.45
1:K:165:LEU:O	1:K:169:VAL:HG23	2.15	0.45
1:O:488:SER:HB2	1:O:992:GLU:N	2.21	0.45
1:P:172:LEU:HD23	1:P:172:LEU:HA	1.74	0.45
1:P:463:ARG:HD2	1:P:463:ARG:HA	1.80	0.45
1:P:834:HIS:CD2	5:u:7:LYS:HA	2.51	0.45
1:P:843:GLY:O	1:P:846:PHE:N	2.49	0.45
2:v:348:ARG:HH12	2:v:493:GLU:CD	2.24	0.45
3:w:88:LEU:O	3:w:91:VAL:HB	2.17	0.45
5:a:13:ARG:HH11	5:a:41:ARG:NH2	2.13	0.45
5:d:47:TYR:O	5:d:51:LEU:HG	2.16	0.45
6:f:48:GLN:C	6:f:57:VAL:HG13	2.42	0.45
6:f:257:PRO:HG3	7:k:63:TYR:CE2	2.52	0.45
7:m:95:ASN:HB2	7:m:103:TRP:CH2	2.50	0.45
1:J:978:ARG:HB3	1:O:698:MET:SD	2.56	0.45
1:K:395:TYR:HD1	1:K:397:LEU:H	1.62	0.45
1:N:428:ASP:HB3	1:N:433:GLN:HE21	1.81	0.45
1:N:899:ARG:HH21	1:N:920:GLU:CD	2.24	0.45
1:O:43:LYS:C	1:P:314:ARG:HH12	2.25	0.45
1:O:258:GLU:HB3	1:O:262:LYS:HB3	1.98	0.45
1:P:718:LEU:HD21	1:P:1022:HIS:CD2	2.51	0.45
2:v:37:PRO:O	2:v:64:ARG:NH2	2.41	0.45
2:v:116:TYR:O	2:v:117:LEU:HB2	2.16	0.45
2:v:354:ARG:HD3	3:x:39:LEU:HD21	1.98	0.45
5:Z:68:PRO:CB	5:Z:71:GLN:CD	2.82	0.45
5:e:24:LEU:HD12	5:e:28:GLN:NE2	2.31	0.45
7:k:153:PHE:CE1	7:k:190:LEU:HD23	2.52	0.45
7:r:252:LEU:H	7:r:252:LEU:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:69:LEU:HD22	1:J:308:TYR:CE2	2.52	0.45
1:J:424:ILE:HD13	1:J:1341:ALA:HB1	1.98	0.45
1:J:432:GLN:CD	1:J:586:GLN:HG3	2.42	0.45
1:J:1056:ASN:HD22	1:J:1105:MET:HE2	1.81	0.45
1:K:82:PHE:CE2	1:K:85:LEU:HA	2.52	0.45
1:K:936:ARG:HH11	1:K:939:ALA:HB3	1.81	0.45
1:N:1336:SER:O	1:N:1362:ILE:HA	2.17	0.45
1:O:451:ASN:OD1	1:O:452:LEU:N	2.49	0.45
1:O:550:ILE:HG12	1:O:560:HIS:ND1	2.31	0.45
1:O:608:ASP:HB3	1:O:653:ARG:HD2	1.99	0.45
1:O:1339:SER:HB3	1:O:1360:HIS:ND1	2.31	0.45
7:p:21:MET:HE1	7:p:125:LEU:HD21	1.98	0.45
7:r:85:ILE:HA	7:r:91:TYR:OH	2.17	0.45
1:J:174:ARG:HB2	1:K:102:ILE:HG23	1.98	0.45
1:J:773:ALA:HA	1:J:776:PHE:CE2	2.51	0.45
1:J:789:ASP:OD1	1:J:789:ASP:N	2.49	0.45
1:J:837:GLN:HG3	5:Z:49:VAL:HG21	1.99	0.45
1:K:543:HIS:CG	1:K:544:PRO:HD2	2.51	0.45
1:N:145:PRO:HG3	1:N:151:TYR:CD1	2.50	0.45
1:N:524:LEU:HD13	1:N:534:ASN:HD22	1.80	0.45
1:N:819:THR:HG23	1:N:1008:CYS:SG	2.57	0.45
1:O:637:VAL:HG13	1:O:638:PRO:HD3	1.97	0.45
7:k:217:PRO:HD2	7:p:213:VAL:HG21	1.98	0.45
7:k:252:LEU:HD12	7:k:253:ASP:N	2.31	0.45
7:r:11:SER:OG	7:r:127:SER:O	2.29	0.45
1:J:93:ILE:HG21	1:O:34:PHE:CE1	2.52	0.45
1:J:151:TYR:O	1:J:155:VAL:HG13	2.16	0.45
1:J:192:PHE:CE2	1:J:223:LEU:HD12	2.52	0.45
1:K:29:ALA:HB1	1:K:37:PHE:CE2	2.52	0.45
1:K:335:MET:HG2	1:K:339:VAL:HG12	1.98	0.45
1:K:452:LEU:HD22	1:K:1040:PRO:HG3	1.98	0.45
1:O:1257:SER:HB3	1:O:1276:ASN:CG	2.42	0.45
5:Z:68:PRO:HB2	5:Z:71:GLN:HB2	1.99	0.45
6:h:288:GLN:NE2	6:h:288:GLN:H	2.13	0.45
7:k:218:ARG:HH12	7:k:253:ASP:HB2	1.82	0.45
7:m:224:VAL:HG11	7:r:214:THR:HG21	1.99	0.45
7:p:142:ILE:HD12	7:p:142:ILE:H	1.82	0.45
7:p:289:TYR:CE2	7:p:291:GLN:HG2	2.51	0.45
1:N:514:PRO:O	1:N:984:ASN:ND2	2.47	0.45
1:N:736:LEU:HA	1:N:739:VAL:HG22	1.98	0.45
1:N:846:PHE:CE1	5:d:48:LEU:HD23	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:938:ARG:HH12	1:N:965:GLN:NE2	2.15	0.45
1:O:439:TRP:CZ3	1:O:449:ALA:HB2	2.51	0.45
1:P:291:LEU:HA	1:P:291:LEU:HD23	1.73	0.45
1:P:507:TYR:OH	1:P:984:ASN:O	2.31	0.45
1:P:979:ALA:HB3	1:P:982:ALA:HB3	1.99	0.45
2:v:70:ARG:N	2:v:71:PRO:CD	2.80	0.45
3:w:64:ARG:O	3:w:68:VAL:HG23	2.17	0.45
7:k:15:THR:O	7:k:18:ILE:HG22	2.17	0.45
7:r:285:ALA:O	7:r:298:CYS:HB2	2.16	0.45
1:J:491:HIS:ND1	1:J:987:GLU:O	2.50	0.45
1:J:575:LEU:HD21	1:J:1243:TRP:CH2	2.52	0.45
1:J:1066:SER:OG	1:J:1095:ILE:HG22	2.17	0.45
1:K:546:TYR:CE2	1:K:564:HIS:HB3	2.52	0.45
1:K:748:ILE:HG13	1:K:898:VAL:HG13	1.99	0.45
1:K:1290:MET:HE3	1:K:1290:MET:HB3	1.73	0.45
1:N:139:GLU:HB3	6:h:47:ALA:HB2	1.99	0.45
1:N:427:LEU:HG	1:O:417:LYS:O	2.17	0.45
1:N:867:ASP:HB2	1:N:940:VAL:HG11	1.97	0.45
1:P:1258:SER:OG	1:P:1259:TYR:N	2.49	0.45
2:v:376:TYR:HB3	2:v:382:ASN:HD21	1.82	0.45
6:h:316:LEU:HD23	7:m:211:ILE:HD12	1.98	0.45
7:p:7:VAL:HA	7:p:37:THR:CG2	2.47	0.45
1:J:862:ASN:HA	1:J:866:ARG:HD3	1.98	0.44
1:J:1345:GLU:OE2	1:J:1353:HIS:HA	2.16	0.44
1:K:255:VAL:HG13	1:K:1102:SER:HA	1.99	0.44
1:K:402:GLN:HA	1:K:1050:ASP:O	2.17	0.44
1:K:635:MET:HE2	5:a:60:TYR:HE2	1.82	0.44
1:N:860:LEU:HA	1:N:860:LEU:HD23	1.71	0.44
1:O:535:TYR:CE1	1:O:1227:HIS:HB2	2.47	0.44
1:O:737:LEU:HD23	1:O:744:PRO:HG2	1.99	0.44
1:O:843:GLY:HA3	5:d:69:ARG:NH2	2.31	0.44
1:P:222:HIS:CE1	1:P:247:ARG:HH12	2.32	0.44
1:P:759:ALA:O	1:P:763:ILE:HG12	2.17	0.44
1:P:805:ALA:C	1:P:807:VAL:N	2.75	0.44
1:P:1048:ARG:NH2	1:P:1117:MET:O	2.50	0.44
1:P:1178:GLN:HE21	1:P:1180:ALA:HB3	1.81	0.44
5:u:20:ASP:OD1	5:u:20:ASP:N	2.50	0.44
1:J:529:PHE:CD2	1:J:574:PRO:HB2	2.52	0.44
1:K:31:GLU:O	1:K:33:LEU:HG	2.18	0.44
1:K:1045:THR:HG1	1:K:1185:ILE:HB	1.82	0.44
1:N:481:ARG:HB3	1:N:550:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:627:HIS:O	1:N:627:HIS:ND1	2.47	0.44
1:N:699:ARG:NH1	1:O:1007:GLU:OE2	2.50	0.44
1:P:619:PHE:CE1	1:P:643:CYS:HB3	2.53	0.44
1:P:830:VAL:O	1:P:894:PHE:HA	2.17	0.44
2:v:291:ILE:HD13	3:x:65:LEU:HD21	1.98	0.44
6:h:204:THR:HG21	6:h:214:LYS:NZ	2.33	0.44
7:k:218:ARG:HG2	7:k:263:ARG:HH12	1.81	0.44
7:p:30:PRO:HG2	7:p:45:LEU:HD12	1.98	0.44
7:p:60:MET:HB3	7:p:113:PRO:HB3	2.00	0.44
1:J:255:VAL:HG12	1:J:1102:SER:HA	1.98	0.44
1:J:811:ILE:O	1:J:815:VAL:HB	2.17	0.44
1:N:55:LEU:HD23	1:N:55:LEU:HA	1.87	0.44
1:N:1080:ARG:NE	6:h:328:SER:OG	2.48	0.44
1:N:1260:ARG:HH22	1:N:1269:SER:HB2	1.81	0.44
1:O:106:ASP:HB2	1:O:108:ARG:HG2	1.99	0.44
1:P:82:PHE:CE2	1:P:88:MET:HG3	2.52	0.44
1:P:1338:SER:O	1:P:1360:HIS:ND1	2.47	0.44
2:v:408:ILE:HD11	2:v:497:ILE:HG22	2.00	0.44
4:z:3118:VAL:HG13	4:z:3122:PHE:CD2	2.52	0.44
7:m:285:ALA:HB3	7:m:299:TRP:HE3	1.81	0.44
7:p:218:ARG:NH2	7:p:252:LEU:HA	2.31	0.44
1:K:470:THR:HG23	1:K:1248:GLY:O	2.18	0.44
1:K:743:ALA:CB	1:K:918:ARG:HH12	2.29	0.44
1:K:886:ALA:HB2	5:a:56:CYS:CB	2.47	0.44
1:K:1135:ASN:OD1	1:K:1136:GLN:N	2.50	0.44
1:K:1188:PRO:HD3	1:K:1243:TRP:CE3	2.52	0.44
1:N:1236:TYR:HD1	1:N:1236:TYR:H	1.65	0.44
1:N:1347:MET:HE3	1:N:1380:VAL:HG23	2.00	0.44
1:O:748:ILE:HD13	1:O:794:LEU:HD22	1.99	0.44
1:O:830:VAL:H	1:O:895:THR:CG2	2.29	0.44
1:P:118:VAL:HG12	1:P:1312:VAL:HB	1.99	0.44
1:P:170:ASP:OD1	1:P:174:ARG:NE	2.50	0.44
6:f:51:SER:HB2	6:f:57:VAL:HG11	2.00	0.44
6:f:227:GLN:HA	6:f:348:VAL:HG13	2.00	0.44
6:h:86:ARG:NH2	7:r:88:GLY:O	2.50	0.44
7:m:224:VAL:O	7:m:228:ILE:HG23	2.17	0.44
1:J:567:MET:SD	1:J:1022:HIS:HA	2.58	0.44
1:J:705:VAL:HG12	1:J:710:SER:HA	1.99	0.44
1:J:805:ALA:HB3	1:J:807:VAL:H	1.83	0.44
1:K:291:LEU:HD13	1:K:291:LEU:HA	1.78	0.44
1:K:356:ALA:C	1:K:358:GLY:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:400:ARG:NH1	1:N:1305:SER:HB3	2.32	0.44
1:N:903:ASP:OD1	1:N:918:ARG:HD3	2.18	0.44
1:O:279:VAL:HA	1:O:380:ALA:O	2.18	0.44
1:O:387:MET:HE2	1:O:388:TYR:CE1	2.52	0.44
1:P:586:GLN:HG2	1:P:1013:VAL:HG13	1.99	0.44
2:v:421:ILE:HB	2:v:464:HIS:NE2	2.33	0.44
6:f:216:ILE:O	6:f:218:ARG:N	2.47	0.44
6:h:154:MET:HE3	6:h:154:MET:HB3	1.58	0.44
7:k:29:LEU:HD11	7:k:82:LEU:HD21	1.99	0.44
7:k:30:PRO:HD3	7:k:135:PRO:HG3	2.00	0.44
7:k:216:LEU:HD21	7:p:216:LEU:HD23	1.99	0.44
7:k:262:SER:O	7:k:266:VAL:HG23	2.17	0.44
7:m:244:PRO:HG2	7:m:247:ILE:HG13	1.99	0.44
7:p:160:VAL:HG11	7:p:169:MET:SD	2.57	0.44
1:J:95:PHE:HD1	1:J:95:PHE:HA	1.59	0.44
1:J:627:HIS:NE2	1:J:632:LYS:HE2	2.33	0.44
1:J:868:LEU:HD23	1:J:868:LEU:HA	1.69	0.44
1:J:1055:GLU:OE2	1:J:1109:ARG:NH2	2.51	0.44
1:K:279:VAL:HA	1:K:380:ALA:O	2.18	0.44
1:K:297:GLU:OE2	1:K:300:ASN:ND2	2.50	0.44
1:K:461:HIS:CD2	1:K:1125:PHE:CD1	3.06	0.44
1:K:464:LEU:HD11	1:K:1254:MET:HG2	1.93	0.44
1:K:921:GLN:HB2	1:K:996:TRP:CD1	2.52	0.44
1:N:867:ASP:CB	1:N:940:VAL:HG11	2.48	0.44
1:N:1050:ASP:OD2	1:N:1117:MET:HG2	2.17	0.44
1:O:282:VAL:HG12	1:O:1057:ILE:HG12	1.98	0.44
1:O:742:ARG:HD3	1:O:903:ASP:O	2.17	0.44
1:P:448:LEU:HB3	1:P:1119:ILE:HD12	1.98	0.44
1:P:515:VAL:HG11	1:P:976:GLN:NE2	2.33	0.44
2:v:44:CYS:SG	2:v:59:ARG:N	2.88	0.44
3:x:89:ASP:OD1	4:z:3127:ARG:NH1	2.50	0.44
6:f:216:ILE:HD12	6:f:216:ILE:HA	1.89	0.44
6:f:358:SER:OG	6:f:359:ASP:N	2.50	0.44
6:h:79:SER:C	6:h:81:SER:H	2.25	0.44
7:m:156:TYR:CE2	7:r:261:LEU:HD23	2.53	0.44
7:p:21:MET:CE	7:p:125:LEU:HD21	2.48	0.44
1:J:300:ASN:HB3	1:J:369:ALA:O	2.17	0.44
1:J:496:HIS:CG	5:Z:1:MET:HE2	2.53	0.44
1:J:828:LEU:HD12	1:J:946:HIS:O	2.18	0.44
1:J:829:GLY:O	1:J:946:HIS:ND1	2.50	0.44
1:J:1048:ARG:HD3	1:J:1182:CYS:SG	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:193:ILE:HA	1:K:219:PHE:CE1	2.52	0.44
1:K:400:ARG:HD3	1:K:1051:GLU:OE2	2.18	0.44
1:N:68:PHE:HE2	1:N:79:ASN:HD21	1.65	0.44
1:N:491:HIS:HB2	1:N:899:ARG:NH2	2.33	0.44
1:N:831:ASP:OD1	1:N:833:GLN:HG2	2.18	0.44
1:P:531:HIS:ND1	1:P:532:PRO:HD2	2.33	0.44
1:P:830:VAL:H	1:P:895:THR:HG23	1.83	0.44
2:v:25:ASP:CG	2:v:75:GLY:HA2	2.43	0.44
6:f:269:THR:HG22	6:f:271:GLU:HG3	2.00	0.44
6:f:333:TRP:CZ3	6:f:348:VAL:HG12	2.52	0.44
7:k:96:LYS:HE2	7:k:96:LYS:HB2	1.70	0.44
7:p:94:LYS:HD3	7:p:96:LYS:HZ3	1.83	0.44
1:J:388:TYR:HD2	1:J:395:TYR:CD1	2.36	0.44
1:J:616:PRO:HB3	1:J:872:SER:HB2	2.00	0.44
1:K:458:VAL:HG21	1:K:1184:ILE:HD13	2.00	0.44
1:K:507:TYR:O	1:K:966:ASP:HB3	2.17	0.44
1:K:1374:LYS:HB2	1:K:1374:LYS:HE3	1.77	0.44
6:f:216:ILE:HG23	6:f:217:PRO:N	2.33	0.44
7:p:229:ARG:O	7:p:232:HIS:HD2	2.01	0.44
1:J:216:ILE:HA	1:J:219:PHE:CD2	2.53	0.44
1:K:1018:MET:HE3	1:K:1018:MET:HB2	1.70	0.44
1:N:448:LEU:HD22	1:O:1236:TYR:HE1	1.83	0.44
1:N:951:HIS:NE2	1:N:997:HIS:CD2	2.86	0.44
1:O:185:LEU:HD11	1:O:397:LEU:HD23	1.99	0.44
1:O:399:ARG:HG3	1:O:1105:MET:HE1	2.00	0.44
1:P:461:HIS:CE1	1:P:1128:PHE:HB2	2.53	0.44
1:P:1125:PHE:HE2	1:P:1146:VAL:HG11	1.82	0.44
2:v:70:ARG:N	2:v:71:PRO:HD2	2.32	0.44
5:Z:68:PRO:HB2	5:Z:71:GLN:NE2	2.19	0.44
5:u:47:TYR:O	5:u:51:LEU:HG	2.18	0.44
1:J:511:TYR:O	1:J:973:ARG:NH2	2.51	0.43
1:J:934:SER:O	1:J:937:THR:OG1	2.34	0.43
1:J:1321:LEU:HD12	1:J:1321:LEU:HA	1.78	0.43
1:K:564:HIS:CE1	1:K:908:GLN:HB3	2.52	0.43
1:N:1050:ASP:OD1	1:N:1115:THR:OG1	2.34	0.43
1:O:121:ASN:OD1	1:O:121:ASN:N	2.49	0.43
2:v:421:ILE:HD13	2:v:438:ILE:HD11	2.00	0.43
7:m:76:SER:OG	7:m:77:VAL:N	2.51	0.43
7:m:236:LEU:HD23	7:r:211:ILE:HD11	2.00	0.43
1:K:733:PHE:N	1:K:733:PHE:CD1	2.85	0.43
1:N:569:GLY:HA3	1:N:1001:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1255:TYR:HB2	1:N:1275:PHE:CD2	2.50	0.43
1:O:889:MET:HE3	1:O:889:MET:HB2	1.80	0.43
1:P:588:PHE:HE1	1:P:700:LEU:HD22	1.83	0.43
1:P:1052:ILE:HD12	1:P:1113:ILE:HG12	2.00	0.43
1:P:1216:ASN:HB2	1:P:1219:VAL:HG22	1.99	0.43
2:v:100:LEU:HD11	2:v:112:LEU:HB3	2.00	0.43
5:d:35:LEU:HD23	5:d:35:LEU:HA	1.88	0.43
1:J:467:PRO:HD3	1:J:546:TYR:CZ	2.53	0.43
1:J:594:LEU:HD23	1:J:594:LEU:HA	1.86	0.43
1:J:826:CYS:HA	1:J:954:TYR:O	2.18	0.43
1:J:830:VAL:H	1:J:895:THR:CG2	2.31	0.43
1:K:448:LEU:HD23	1:K:448:LEU:HA	1.84	0.43
1:K:1125:PHE:HD2	1:K:1148:ALA:HB3	1.83	0.43
1:N:1:MET:HG2	1:N:35:HIS:ND1	2.33	0.43
1:N:106:ASP:N	1:N:106:ASP:OD1	2.50	0.43
1:N:903:ASP:HB3	1:N:909:GLN:NE2	2.33	0.43
3:x:85:ARG:NH1	4:z:3131:GLU:HG2	2.33	0.43
4:z:3143:ARG:O	4:z:3147:LEU:HB2	2.17	0.43
7:m:172:VAL:O	7:m:176:LEU:HB2	2.18	0.43
7:r:182:LEU:HD12	7:r:182:LEU:HA	1.82	0.43
1:J:1026:SER:O	1:J:1029:ALA:N	2.50	0.43
1:K:465:HIS:CD2	1:K:1133:PHE:HZ	2.36	0.43
1:K:796:LEU:HD21	1:K:925:VAL:HG13	2.01	0.43
1:K:1273:ALA:HA	1:K:1279:GLU:OE1	2.17	0.43
1:N:540:LEU:HD11	1:N:550:ILE:HD11	2.01	0.43
1:N:830:VAL:H	1:N:895:THR:CG2	2.31	0.43
1:N:943:CYS:O	1:N:944:LEU:HD23	2.17	0.43
1:O:956:ASP:HA	1:O:957:PRO:HD3	1.89	0.43
1:O:1127:VAL:O	1:O:1264:VAL:HG23	2.18	0.43
1:P:38:ASP:O	1:P:41:VAL:HG22	2.18	0.43
1:P:648:TRP:CZ3	1:P:682:MET:HE1	2.54	0.43
1:P:1378:LYS:H	1:P:1378:LYS:HD3	1.83	0.43
2:v:489:LEU:O	2:v:494:ARG:NE	2.51	0.43
5:e:68:PRO:HG2	5:e:71:GLN:HB3	2.00	0.43
6:h:102:ASN:HD21	6:h:196:LYS:HD3	1.83	0.43
6:h:183:ASN:OD1	6:h:184:PHE:N	2.52	0.43
7:p:18:ILE:CG2	7:p:22:GLN:HE21	2.31	0.43
1:J:59:TYR:CD2	1:K:260:VAL:HG11	2.54	0.43
1:J:281:ILE:HD12	1:J:1058:LEU:HD23	2.01	0.43
1:J:282:VAL:HG12	1:J:1057:ILE:HG12	1.99	0.43
1:K:1048:ARG:NH2	1:K:1118:GLY:O	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:406:TYR:HD1	1:N:1047:VAL:HG22	1.84	0.43
1:N:722:ASN:CB	1:N:902:VAL:HG11	2.43	0.43
1:O:463:ARG:NH2	1:O:1253:ILE:O	2.51	0.43
1:O:634:VAL:O	1:O:637:VAL:HG12	2.18	0.43
1:O:1186:VAL:HG22	1:O:1250:LEU:HD22	2.01	0.43
2:v:20:HIS:HA	2:v:59:ARG:HH12	1.84	0.43
5:u:47:TYR:HA	5:u:50:PHE:CE1	2.54	0.43
1:J:92:LYS:HB3	1:J:120:LYS:O	2.19	0.43
1:J:236:MET:HE2	1:J:236:MET:HB3	1.83	0.43
1:J:399:ARG:CD	1:J:1320:PHE:HB3	2.48	0.43
1:J:439:TRP:CZ3	1:J:449:ALA:HB2	2.53	0.43
1:J:843:GLY:HA2	1:J:846:PHE:HB3	2.01	0.43
1:J:848:HIS:NE2	5:Z:22:PRO:HD2	2.34	0.43
1:J:1317:THR:OG1	1:J:1318:ASP:N	2.51	0.43
1:K:922:THR:HG23	1:K:950:PHE:CZ	2.53	0.43
1:N:664:LYS:HE2	1:N:668:ARG:HH21	1.83	0.43
1:N:1024:LYS:HE2	1:N:1024:LYS:HB3	1.84	0.43
1:N:1195:TYR:CG	1:N:1240:VAL:HG21	2.54	0.43
1:O:299:ASP:HB3	1:O:371:VAL:CG2	2.49	0.43
1:O:507:TYR:OH	1:O:985:ARG:HA	2.18	0.43
1:O:1028:MET:HE1	1:O:1141:TYR:CE2	2.53	0.43
1:O:1357:HIS:CG	1:O:1358:TYR:H	2.36	0.43
1:P:496:HIS:CE1	1:P:501:VAL:HB	2.54	0.43
1:P:874:LEU:O	1:P:876:PRO:HD3	2.18	0.43
2:v:7:ASN:O	2:v:11:SER:N	2.50	0.43
2:v:385:LEU:HD13	2:v:385:LEU:HA	1.76	0.43
6:f:36:THR:O	6:f:40:ARG:HG2	2.19	0.43
6:f:264:LEU:HD12	6:f:280:PHE:O	2.18	0.43
6:h:46:HIS:CE1	6:h:70:VAL:HA	2.53	0.43
7:k:148:GLN:O	7:k:152:LEU:HG	2.19	0.43
7:r:152:LEU:HD23	7:r:152:LEU:HA	1.79	0.43
1:J:1246:GLN:H	1:J:1246:GLN:HG3	1.57	0.43
1:K:144:ILE:HA	1:K:145:PRO:HD3	1.91	0.43
1:K:801:ASP:OD1	1:K:801:ASP:N	2.42	0.43
1:K:853:ASP:O	1:K:854:GLU:HG3	2.18	0.43
1:N:903:ASP:HB3	1:N:909:GLN:HE21	1.83	0.43
1:N:1172:PRO:HB2	1:O:1223:LEU:HB2	2.00	0.43
1:N:1346:PHE:HB2	1:N:1353:HIS:CE1	2.53	0.43
1:O:531:HIS:CD2	1:O:533:SER:H	2.33	0.43
1:O:619:PHE:CE1	1:O:643:CYS:HB3	2.54	0.43
1:P:439:TRP:NE1	1:P:1340:ARG:HB2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:544:PRO:HG3	1:P:1243:TRP:CE3	2.53	0.43
1:P:1260:ARG:HG2	1:P:1263:ALA:HB2	2.00	0.43
5:a:41:ARG:HA	5:a:44:GLN:NE2	2.33	0.43
6:f:333:TRP:HZ3	6:f:335:ARG:HG2	1.82	0.43
7:k:29:LEU:HD23	7:k:134:PHE:CE1	2.53	0.43
7:m:148:GLN:O	7:m:152:LEU:HG	2.18	0.43
1:J:567:MET:HE2	1:J:717:ALA:HB3	2.00	0.43
1:K:301:GLN:HE21	1:K:366:PRO:CB	2.32	0.43
1:K:481:ARG:HB3	1:K:539:ARG:HD2	2.01	0.43
1:K:572:PRO:HB2	1:K:574:PRO:HD2	2.01	0.43
1:K:810:LYS:O	1:K:814:TYR:HB2	2.19	0.43
1:K:1256:ASN:HD22	1:K:1276:ASN:HA	1.83	0.43
1:N:68:PHE:O	1:N:71:THR:OG1	2.35	0.43
1:O:75:VAL:HG23	1:O:267:TYR:CG	2.53	0.43
1:O:247:ARG:HD2	1:O:247:ARG:HA	1.74	0.43
1:O:335:MET:O	1:O:339:VAL:HG12	2.19	0.43
1:O:761:GLN:NE2	3:x:67:ARG:HD3	2.31	0.43
1:O:933:PHE:O	1:O:962:THR:HG21	2.19	0.43
1:O:1066:SER:HB3	1:O:1095:ILE:HG13	2.00	0.43
1:P:141:LEU:HA	1:P:141:LEU:HD23	1.85	0.43
2:v:13:LEU:HD11	7:p:252:LEU:HB2	2.00	0.43
5:u:45:ARG:HA	5:u:48:LEU:CD2	2.49	0.43
7:p:98:GLN:HG3	7:p:120:HIS:NE2	2.34	0.43
1:J:805:ALA:CB	1:J:807:VAL:H	2.32	0.43
1:K:695:GLN:O	1:K:699:ARG:HG3	2.19	0.43
1:K:1099:LEU:H	1:K:1099:LEU:HG	1.44	0.43
1:N:280:PHE:CE1	1:N:1059:PHE:HB2	2.54	0.43
1:N:498:ASN:ND2	5:d:2:ALA:HB1	2.34	0.43
1:N:1073:ASN:HB2	1:N:1089:HIS:HB2	2.01	0.43
1:N:1124:PHE:HD1	1:N:1124:PHE:HA	1.68	0.43
1:O:132:GLU:HG2	1:O:1085:THR:HG22	2.01	0.43
1:P:133:LEU:HD13	1:P:138:LEU:HD21	2.00	0.43
1:P:491:HIS:HB2	1:P:899:ARG:CZ	2.48	0.43
1:P:543:HIS:HE1	1:P:545:LEU:HD12	1.84	0.43
1:P:638:PRO:HG2	1:P:882:ARG:HH22	1.84	0.43
1:P:1282:ARG:CD	6:f:96:HIS:HE1	2.31	0.43
3:w:98:LEU:O	4:z:3114:GLN:NE2	2.51	0.43
6:h:86:ARG:HH12	7:r:90:THR:N	2.17	0.43
7:k:7:VAL:HB	7:k:80:LEU:HB2	2.01	0.43
7:k:31:LEU:HD23	7:k:70:ALA:HB2	2.00	0.43
7:p:31:LEU:HD12	7:p:31:LEU:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:p:114:PRO:HD2	7:p:118:ARG:CZ	2.49	0.43
1:J:839:LEU:HD23	1:J:865:LEU:HD11	2.01	0.43
1:J:933:PHE:N	1:J:962:THR:HG21	2.34	0.43
1:J:1276:ASN:O	1:J:1280:LEU:HB2	2.19	0.43
1:K:24:ASN:HB3	1:K:28:SER:HB3	2.00	0.43
1:N:694:GLU:HG3	1:N:807:VAL:HG11	2.01	0.43
1:N:924:LEU:HD22	1:N:950:PHE:CE2	2.54	0.43
1:N:961:ALA:HB1	1:N:968:ALA:HA	2.00	0.43
1:O:549:TYR:CE1	1:O:561:ARG:HB2	2.53	0.43
1:O:742:ARG:O	1:O:744:PRO:HD3	2.19	0.43
1:P:439:TRP:CE2	1:P:449:ALA:HB2	2.54	0.43
1:P:1188:PRO:HD3	1:P:1243:TRP:CE3	2.54	0.43
2:v:94:PRO:O	2:v:116:TYR:HB2	2.19	0.43
2:v:341:PHE:HD2	2:v:342:LEU:HD23	1.83	0.43
3:x:99:GLU:HG2	3:x:102:GLN:NE2	2.34	0.43
6:f:313:ILE:H	6:f:313:ILE:HG12	1.64	0.43
1:K:83:LYS:HE3	1:K:83:LYS:HB3	1.85	0.42
1:K:152:ALA:O	1:K:155:VAL:HG22	2.19	0.42
1:K:192:PHE:CZ	1:K:223:LEU:HD12	2.54	0.42
1:K:458:VAL:HG21	1:K:1184:ILE:HB	2.01	0.42
1:K:598:VAL:HG13	1:K:602:VAL:HG22	2.00	0.42
1:K:613:THR:O	1:K:934:SER:HB2	2.18	0.42
1:K:783:ARG:HA	1:K:788:HIS:CE1	2.54	0.42
1:K:837:GLN:HA	5:a:49:VAL:HG21	2.00	0.42
1:K:1353:HIS:CE1	1:K:1364:GLU:OE2	2.72	0.42
1:N:484:ARG:HH22	1:N:558:ALA:CA	2.26	0.42
1:O:456:LEU:HD22	1:O:1030:TYR:HB3	2.01	0.42
1:O:487:TYR:CD2	1:O:488:SER:HB3	2.54	0.42
1:P:763:ILE:HA	1:P:794:LEU:HB3	2.01	0.42
1:P:837:GLN:NE2	5:u:45:ARG:HH21	2.17	0.42
1:P:980:VAL:HG22	1:P:981:GLU:OE2	2.19	0.42
1:P:1064:SER:OG	1:P:1065:THR:N	2.52	0.42
2:v:302:TYR:HD2	2:v:305:LEU:H	1.66	0.42
6:h:174:ARG:NE	6:h:178:ASP:OD2	2.52	0.42
7:m:222:ARG:HG2	7:m:251:ASP:OD1	2.19	0.42
1:J:69:LEU:HD21	1:J:79:ASN:ND2	2.34	0.42
1:J:496:HIS:HB2	5:Z:1:MET:HE2	2.01	0.42
1:J:1222:GLY:O	1:J:1226:ASP:HB3	2.19	0.42
1:K:1259:TYR:O	1:K:1259:TYR:CG	2.72	0.42
1:N:61:ASN:OD1	1:N:62:ALA:N	2.52	0.42
1:N:122:CYS:HA	1:N:1094:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:889:MET:HE1	5:d:50:PHE:CE1	2.54	0.42
6:h:135:MET:HG2	6:h:172:PHE:CZ	2.54	0.42
7:m:9:LEU:HD12	7:m:128:ASN:OD1	2.19	0.42
7:p:215:LEU:HD23	7:p:215:LEU:HA	1.74	0.42
1:J:280:PHE:CE2	1:J:379:VAL:HG11	2.55	0.42
1:J:388:TYR:CD2	1:J:396:PRO:HD3	2.53	0.42
1:J:660:PHE:CD2	1:J:809:GLU:HG2	2.53	0.42
1:J:678:GLU:OE1	1:J:678:GLU:N	2.38	0.42
1:K:567:MET:SD	1:K:1022:HIS:ND1	2.91	0.42
1:N:202:PHE:CE1	1:N:218:MET:HE1	2.55	0.42
1:N:443:LYS:NZ	1:N:1113:ILE:O	2.52	0.42
1:N:484:ARG:HH22	1:N:558:ALA:HB2	1.81	0.42
1:N:769:MET:HB2	1:N:890:THR:HG21	2.00	0.42
1:P:458:VAL:HG21	1:P:1184:ILE:HD13	2.00	0.42
2:v:379:ILE:O	2:v:379:ILE:HG13	2.18	0.42
7:p:193:VAL:HG22	7:p:195:GLY:H	1.84	0.42
7:p:264:MET:HE3	7:p:264:MET:HB3	1.91	0.42
7:r:58:VAL:HG12	7:r:277:LEU:HD11	2.01	0.42
7:r:114:PRO:HD3	7:r:135:PRO:HA	2.01	0.42
7:r:223:LEU:O	7:r:227:LEU:HG	2.18	0.42
1:J:255:VAL:HB	1:J:256:SER:H	1.52	0.42
1:J:388:TYR:HD2	1:J:395:TYR:HD1	1.68	0.42
1:J:626:ILE:HD11	1:J:636:ASN:HD22	1.84	0.42
1:K:507:TYR:CG	1:K:967:VAL:HG22	2.54	0.42
1:K:681:SER:HA	1:K:684:ARG:NH1	2.33	0.42
1:K:842:ASN:ND2	1:K:844:PRO:HD2	2.35	0.42
1:N:401:MET:HE3	1:N:403:TYR:CE1	2.53	0.42
1:N:587:GLN:NE2	1:N:1038:ILE:HA	2.35	0.42
1:N:615:TYR:CD1	1:N:616:PRO:HD2	2.54	0.42
1:N:829:GLY:HA3	1:N:946:HIS:NE2	2.34	0.42
1:N:1001:MET:HE3	1:N:1001:MET:HB3	1.87	0.42
1:N:1048:ARG:NH2	1:N:1118:GLY:O	2.53	0.42
1:N:1049:THR:HG23	1:N:1270:PRO:HB3	2.02	0.42
1:O:466:THR:HB	1:O:910:LEU:HB3	2.02	0.42
1:O:507:TYR:CD2	1:O:967:VAL:HG22	2.54	0.42
1:O:1184:ILE:O	1:O:1255:TYR:OH	2.26	0.42
1:P:66:VAL:HG11	1:P:387:MET:HE2	2.02	0.42
2:v:27:VAL:HG11	2:v:297:LEU:HD11	2.00	0.42
2:v:423:SER:HA	2:v:463:VAL:O	2.19	0.42
1:J:221:ARG:HE	1:J:221:ARG:HB3	1.72	0.42
1:J:531:HIS:HD2	1:J:533:SER:HB3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:580:PHE:CE1	1:J:1189:VAL:HG11	2.54	0.42
1:J:610:ALA:HA	1:J:931:PHE:CE1	2.55	0.42
1:J:930:ALA:HB3	1:J:963:MET:HE1	2.02	0.42
1:J:1127:VAL:HG13	1:J:1128:PHE:CD2	2.55	0.42
1:J:1203:ARG:H	1:J:1203:ARG:HG3	1.71	0.42
1:J:1209:VAL:HG12	1:J:1212:CYS:SG	2.59	0.42
1:K:209:LYS:HG3	1:K:1211:SER:O	2.19	0.42
1:K:1183:GLU:CD	1:K:1270:PRO:HD2	2.44	0.42
1:O:259:SER:OG	1:O:1098:GLY:HA2	2.19	0.42
1:P:1141:TYR:CZ	1:P:1145:LYS:HG3	2.54	0.42
2:v:22:PHE:HD1	2:v:77:PHE:HA	1.85	0.42
7:p:202:LEU:O	7:p:206:SER:OG	2.27	0.42
1:J:160:THR:O	1:J:163:SER:OG	2.32	0.42
1:J:448:LEU:HD23	1:J:448:LEU:HA	1.90	0.42
1:J:653:ARG:HH22	1:O:684:ARG:CZ	2.33	0.42
1:J:947:ALA:HB2	1:J:963:MET:HB2	2.02	0.42
1:K:277:GLY:O	1:K:1062:ARG:HB2	2.19	0.42
1:K:439:TRP:CZ3	1:K:449:ALA:HB2	2.54	0.42
1:N:247:ARG:HD2	1:N:247:ARG:HA	1.77	0.42
1:O:507:TYR:CG	1:O:967:VAL:HG22	2.54	0.42
1:O:617:ALA:O	1:O:620:TYR:HD1	2.03	0.42
1:P:143:SER:OG	1:P:144:ILE:N	2.52	0.42
1:P:185:LEU:HD23	1:P:1058:LEU:HD13	2.00	0.42
1:P:293:PHE:HD1	1:P:293:PHE:HA	1.66	0.42
1:P:636:ASN:O	1:P:640:VAL:HG13	2.19	0.42
1:P:724:LEU:O	1:P:921:GLN:NE2	2.41	0.42
1:P:1051:GLU:N	1:P:1115:THR:OG1	2.38	0.42
5:Z:67:VAL:O	5:Z:67:VAL:HG12	2.19	0.42
6:h:127:THR:HB	6:h:128:PRO:HD2	2.01	0.42
7:p:114:PRO:HB2	7:p:118:ARG:HE	1.84	0.42
7:r:192:GLU:H	7:r:192:GLU:HG2	1.63	0.42
7:r:290:SER:O	7:r:294:LEU:N	2.53	0.42
1:J:660:PHE:N	1:J:813:TYR:OH	2.40	0.42
1:K:603:ILE:HG21	1:K:1010:PRO:O	2.20	0.42
1:N:566:LEU:HD23	1:N:566:LEU:HA	1.93	0.42
1:O:1021:MET:HE3	1:O:1021:MET:HB2	1.89	0.42
1:P:1203:ARG:H	1:P:1203:ARG:HG3	1.52	0.42
6:f:265:TYR:CZ	6:f:289:ILE:HG21	2.55	0.42
1:J:35:HIS:CD2	1:J:35:HIS:H	2.36	0.42
1:J:499:VAL:HA	1:J:502:ILE:HD12	2.02	0.42
1:J:637:VAL:HG13	1:J:638:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:980:VAL:HG23	1:J:981:GLU:OE2	2.19	0.42
1:K:207:PHE:CE2	1:K:1287:LEU:HD21	2.55	0.42
1:K:1300:GLY:O	1:K:1302:PRO:HD3	2.20	0.42
1:K:1353:HIS:ND1	1:K:1353:HIS:O	2.52	0.42
1:N:1075:SER:OG	1:N:1076:ARG:N	2.52	0.42
1:O:687:TYR:CE2	1:O:691:ILE:HD11	2.54	0.42
1:O:884:LEU:HD23	1:O:884:LEU:HA	1.94	0.42
1:P:232:ARG:HB3	1:P:1370:ARG:HD2	2.02	0.42
2:v:35:ARG:NE	2:v:37:PRO:HB3	2.17	0.42
5:a:43:ALA:O	5:a:46:SER:OG	2.27	0.42
5:u:15:GLU:CG	5:u:48:LEU:HD22	2.49	0.42
7:k:212:MET:HE1	7:k:274:LEU:HD21	2.02	0.42
7:p:104:HIS:NE2	7:p:182:LEU:HD13	2.34	0.42
1:J:650:ARG:NH2	1:J:873:ASP:HB3	2.35	0.42
1:J:1057:ILE:HG13	1:J:1108:ALA:HB2	2.02	0.42
1:J:1173:GLY:O	1:K:1232:ALA:HB2	2.20	0.42
1:K:92:LYS:HB2	1:K:92:LYS:HE3	1.80	0.42
1:K:233:ALA:HA	1:K:236:MET:HE2	2.02	0.42
1:K:539:ARG:O	1:K:540:LEU:HD23	2.20	0.42
1:N:328:MET:HE2	1:N:334:PHE:CZ	2.55	0.42
3:x:94:PHE:HB2	4:y:3122:PHE:CZ	2.54	0.42
6:f:208:HIS:HB2	7:p:299:TRP:CZ2	2.55	0.42
7:k:3:LEU:HD12	7:k:86:VAL:HG22	2.02	0.42
7:k:228:ILE:HG22	7:k:236:LEU:HD22	2.01	0.42
7:m:31:LEU:O	7:m:68:THR:HG22	2.20	0.42
1:J:471:LEU:HD12	1:J:912:PRO:HG2	2.01	0.42
1:J:506:PHE:CE2	1:J:510:LYS:HE3	2.55	0.42
1:K:491:HIS:CG	1:K:899:ARG:HD2	2.55	0.42
1:K:521:LYS:HG2	1:K:537:LEU:HD13	2.01	0.42
1:K:573:THR:N	1:K:574:PRO:HD2	2.34	0.42
1:N:54:VAL:HA	1:O:327:VAL:O	2.20	0.42
1:N:484:ARG:O	1:N:485:GLU:C	2.63	0.42
1:N:602:VAL:O	1:N:606:VAL:HG23	2.20	0.42
1:N:1013:VAL:O	1:N:1016:SER:OG	2.25	0.42
1:O:917:LYS:HB2	1:O:917:LYS:HE3	1.63	0.42
1:P:245:ARG:NH2	1:P:294:LEU:HB3	2.35	0.42
1:P:904:ASN:HB3	1:P:908:GLN:HB2	2.01	0.42
1:P:1086:PHE:CZ	6:f:42:LEU:HD11	2.55	0.42
5:Z:69:ARG:HG3	5:Z:69:ARG:O	2.20	0.42
5:u:48:LEU:HA	5:u:51:LEU:HD12	2.02	0.42
7:k:58:VAL:HG21	7:k:198:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:m:155:VAL:HG23	7:m:202:LEU:HD13	2.02	0.42
1:J:294:LEU:HD23	1:J:294:LEU:HA	1.84	0.41
1:J:852:ARG:O	1:J:879:GLY:N	2.53	0.41
1:K:720:ASP:O	1:K:810:LYS:NZ	2.53	0.41
1:N:408:PRO:HG3	1:N:1196:PHE:CD2	2.54	0.41
1:N:543:HIS:HD2	1:N:546:TYR:N	2.14	0.41
1:N:842:ASN:ND2	1:N:865:LEU:HD23	2.34	0.41
1:N:961:ALA:O	1:N:968:ALA:HB2	2.20	0.41
1:N:1298:LEU:HA	1:N:1298:LEU:HD13	1.74	0.41
1:O:78:VAL:HG21	1:O:261:LEU:CD1	2.46	0.41
1:P:573:THR:N	1:P:574:PRO:HD2	2.35	0.41
1:P:658:ASN:OD1	1:P:929:VAL:HG23	2.20	0.41
2:v:67:LEU:HB2	2:v:72:SER:HB2	2.01	0.41
2:v:427:TYR:CE2	3:w:47:GLU:HG2	2.55	0.41
5:a:17:ASP:O	5:a:19:PRO:HD3	2.20	0.41
6:f:104:GLU:OE1	6:f:127:THR:HG21	2.20	0.41
6:h:295:ILE:HA	6:h:298:SER:OG	2.20	0.41
7:k:118:ARG:O	7:k:122:THR:OG1	2.25	0.41
7:m:112:MET:HG2	7:m:136:MET:O	2.19	0.41
1:J:174:ARG:CB	1:K:102:ILE:HG12	2.50	0.41
1:K:290:LEU:HD23	1:K:290:LEU:HA	1.88	0.41
1:K:1036:LEU:HD13	1:K:1036:LEU:HA	1.90	0.41
1:N:672:ASN:HB3	1:N:673:ASN:H	1.61	0.41
1:N:1146:VAL:HG13	1:N:1148:ALA:H	1.84	0.41
1:O:735:HIS:O	1:O:739:VAL:HG22	2.21	0.41
1:O:765:ARG:HA	1:O:765:ARG:HD3	1.91	0.41
1:O:799:TYR:CE2	1:O:801:ASP:HB3	2.55	0.41
1:P:125:HIS:HB2	1:P:1092:MET:HE2	2.02	0.41
1:P:758:ALA:HB1	1:P:762:PHE:CD1	2.54	0.41
1:P:861:GLU:H	1:P:861:GLU:CD	2.29	0.41
2:v:3:VAL:HG22	2:v:77:PHE:HE2	1.85	0.41
5:u:60:TYR:CZ	5:u:64:THR:HG21	2.55	0.41
6:f:208:HIS:HB2	7:p:299:TRP:CH2	2.55	0.41
6:h:211:VAL:HG11	6:h:353:PHE:HB3	2.02	0.41
7:k:245:ASP:O	7:k:249:ARG:HG2	2.20	0.41
7:r:85:ILE:HD13	7:r:91:TYR:CZ	2.54	0.41
1:K:69:LEU:HA	1:K:69:LEU:HD12	1.80	0.41
1:K:151:TYR:O	1:K:155:VAL:HG13	2.19	0.41
1:K:279:VAL:HG22	1:K:380:ALA:HB3	2.02	0.41
1:K:724:LEU:HD12	1:K:900:VAL:HG21	2.01	0.41
1:K:803:GLY:O	1:K:805:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1001:MET:HE3	1:K:1001:MET:HB3	1.89	0.41
1:O:258:GLU:HA	1:O:262:LYS:CD	2.50	0.41
1:O:632:LYS:HA	1:O:635:MET:SD	2.60	0.41
1:P:1347:MET:HE3	1:P:1347:MET:HB3	1.91	0.41
2:v:60:VAL:HG12	2:v:62:ALA:HB2	2.01	0.41
2:v:347:LEU:HD23	2:v:347:LEU:HA	1.78	0.41
6:f:192:VAL:HG12	6:f:193:GLU:HG3	2.03	0.41
7:p:97:TYR:O	7:p:99:PRO:HD2	2.20	0.41
7:p:156:TYR:O	7:p:160:VAL:HG12	2.20	0.41
7:p:207:LEU:O	7:p:211:ILE:HG13	2.20	0.41
7:r:24:ARG:HH11	7:r:98:GLN:CG	2.33	0.41
7:r:138:LEU:HD12	7:r:138:LEU:HA	1.86	0.41
1:J:255:VAL:CG1	1:J:1102:SER:HA	2.50	0.41
1:J:304:GLY:HA2	1:J:305:PRO:HD3	1.87	0.41
1:J:539:ARG:O	1:J:540:LEU:HD23	2.20	0.41
1:J:654:LEU:HB2	1:J:683:TYR:CE2	2.55	0.41
1:J:684:ARG:NH2	1:K:653:ARG:HH22	2.18	0.41
1:K:232:ARG:HE	1:K:232:ARG:HB2	1.32	0.41
1:K:1115:THR:O	1:K:1116:ASP:HB3	2.20	0.41
1:N:484:ARG:NE	1:N:550:ILE:HG22	2.36	0.41
1:N:1175:CYS:H	1:O:1232:ALA:HB1	1.86	0.41
1:O:332:GLU:OE1	1:O:333:HIS:HD2	2.04	0.41
1:O:467:PRO:HG3	1:O:546:TYR:CD1	2.55	0.41
1:P:746:ILE:HG23	1:P:900:VAL:HG22	2.02	0.41
6:h:181:PHE:CE2	6:h:185:ILE:HD11	2.54	0.41
7:m:9:LEU:HB2	7:m:78:ASP:O	2.20	0.41
7:m:13:LEU:HD11	7:m:18:ILE:HD13	2.02	0.41
7:m:246:GLU:OE1	7:r:218:ARG:HG2	2.19	0.41
7:r:60:MET:HE3	7:r:60:MET:HB2	1.85	0.41
1:J:501:VAL:HB	5:Z:1:MET:HE3	2.02	0.41
1:J:722:ASN:OD1	1:J:742:ARG:NH2	2.54	0.41
1:J:775:GLN:O	1:J:779:LEU:HG	2.20	0.41
1:J:884:LEU:HD23	1:J:884:LEU:HA	1.84	0.41
1:J:981:GLU:OE1	1:J:999:SER:HB3	2.21	0.41
1:J:1160:THR:O	1:J:1160:THR:OG1	2.36	0.41
1:K:395:TYR:CE1	1:K:397:LEU:HB2	2.55	0.41
1:K:488:SER:O	1:K:488:SER:OG	2.38	0.41
1:N:884:LEU:HD23	1:N:884:LEU:HA	1.80	0.41
1:O:618:PHE:O	1:O:621:VAL:HB	2.21	0.41
1:O:631:GLU:O	1:O:635:MET:HG3	2.21	0.41
1:O:920:GLU:HG2	1:O:994:ARG:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1047:VAL:O	1:O:1182:CYS:HA	2.20	0.41
1:P:647:TYR:CE2	1:P:653:ARG:HG3	2.55	0.41
1:P:770:ASP:HA	1:P:776:PHE:CE1	2.55	0.41
1:P:807:VAL:O	1:P:808:LEU:C	2.64	0.41
1:P:831:ASP:H	1:P:944:LEU:CD2	2.33	0.41
1:P:981:GLU:HB3	1:P:999:SER:HB3	2.02	0.41
1:P:1183:GLU:CD	1:P:1270:PRO:HD2	2.46	0.41
7:r:215:LEU:HA	7:r:215:LEU:HD23	1.77	0.41
1:J:672:ASN:OD1	1:K:873:ASP:HB2	2.21	0.41
1:K:488:SER:OG	1:K:992:GLU:HB3	2.21	0.41
1:K:1145:LYS:HD2	1:K:1145:LYS:HA	1.84	0.41
1:N:889:MET:HE1	5:d:50:PHE:HE1	1.85	0.41
1:O:280:PHE:CE2	1:O:379:VAL:HG11	2.55	0.41
1:O:475:ASN:HB3	1:O:560:HIS:CD2	2.47	0.41
1:O:985:ARG:HD3	1:O:990:PHE:HE2	1.84	0.41
1:P:462:PRO:O	1:P:466:THR:HG23	2.20	0.41
1:P:658:ASN:HB2	1:P:931:PHE:HE2	1.85	0.41
1:P:682:MET:HE3	1:P:682:MET:HB2	1.87	0.41
1:P:832:PHE:CD2	1:P:891:CYS:HB3	2.55	0.41
1:P:899:ARG:HH21	1:P:988:GLN:C	2.26	0.41
2:v:3:VAL:HA	2:v:6:ASP:HB2	2.02	0.41
2:v:19:VAL:O	2:v:59:ARG:NH1	2.48	0.41
6:f:216:ILE:C	6:f:218:ARG:H	2.27	0.41
6:h:288:GLN:O	6:h:292:ILE:HG12	2.21	0.41
6:h:327:PHE:CD1	6:h:350:ILE:HG23	2.55	0.41
7:r:283:ARG:C	7:r:284:LEU:HD12	2.45	0.41
7:r:289:TYR:HD1	7:r:296:ALA:HB2	1.86	0.41
1:J:544:PRO:HG3	1:J:1243:TRP:CE3	2.56	0.41
1:J:568:VAL:HG12	1:J:581:GLN:HE22	1.86	0.41
1:J:1053:LEU:HA	1:J:1053:LEU:HD23	1.77	0.41
1:K:635:MET:HE1	1:K:769:MET:SD	2.61	0.41
1:N:95:PHE:HE1	1:N:260:VAL:HG21	1.85	0.41
1:N:284:ASP:N	1:N:284:ASP:OD1	2.50	0.41
1:N:429:ASN:O	1:N:433:GLN:HG3	2.20	0.41
1:N:697:LEU:HD23	1:N:697:LEU:HA	1.91	0.41
1:N:1105:MET:HE3	1:N:1105:MET:HB2	1.84	0.41
1:N:1119:ILE:H	1:N:1119:ILE:HG13	1.67	0.41
1:N:1351:GLN:C	1:N:1353:HIS:H	2.29	0.41
1:O:469:HIS:HB3	1:O:1253:ILE:HD12	2.02	0.41
1:O:772:MET:HE1	1:O:775:GLN:OE1	2.21	0.41
1:O:840:ALA:HB3	5:e:49:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:841:TYR:HD1	5:e:45:ARG:CZ	2.33	0.41
1:O:902:VAL:HG23	1:O:903:ASP:O	2.20	0.41
1:P:722:ASN:OD1	1:P:742:ARG:NH2	2.54	0.41
1:P:807:VAL:HG12	1:P:811:ILE:HG13	2.03	0.41
2:v:377:SER:C	2:v:379:ILE:N	2.78	0.41
5:d:76:LYS:HA	5:d:76:LYS:HD3	1.82	0.41
5:e:11:GLN:HG3	5:e:12:GLY:N	2.36	0.41
6:f:20:LEU:HA	6:f:20:LEU:HD23	1.82	0.41
6:h:135:MET:HE3	6:h:135:MET:HB2	1.96	0.41
7:m:264:MET:HE1	7:r:209:PHE:CE2	2.55	0.41
7:p:78:ASP:OD1	7:p:79:SER:N	2.53	0.41
7:p:142:ILE:HD11	7:p:181:TYR:CE2	2.55	0.41
1:J:596:HIS:HD2	1:J:1012:LEU:HD22	1.86	0.41
1:J:616:PRO:HB3	1:J:872:SER:CB	2.50	0.41
1:K:1116:ASP:CG	1:K:1176:HIS:HB3	2.45	0.41
1:N:136:LEU:HD22	6:h:218:ARG:CG	2.50	0.41
1:N:384:LEU:C	1:N:386:LYS:H	2.28	0.41
1:N:987:GLU:H	1:N:987:GLU:HG3	1.72	0.41
1:O:131:MET:HE1	6:f:12:LEU:HD21	2.03	0.41
1:O:616:PRO:HB3	1:O:872:SER:HB3	2.02	0.41
1:O:722:ASN:CG	1:O:742:ARG:HD2	2.45	0.41
1:O:1267:LEU:HD23	1:O:1267:LEU:HA	1.81	0.41
2:v:1:MET:HA	2:v:4:HIS:HD2	1.86	0.41
2:v:290:HIS:HB2	2:v:297:LEU:HD13	2.03	0.41
7:r:40:VAL:HG23	7:r:43:LEU:HD21	2.02	0.41
1:J:38:ASP:OD1	1:J:39:LEU:N	2.54	0.41
1:J:309:ALA:C	1:J:311:PHE:N	2.76	0.41
1:J:400:ARG:O	1:J:1321:LEU:HD12	2.21	0.41
1:J:544:PRO:HG3	1:J:1243:TRP:CE2	2.56	0.41
1:J:596:HIS:CD2	1:J:1012:LEU:HD22	2.56	0.41
1:J:637:VAL:N	1:J:638:PRO:HD2	2.35	0.41
1:J:670:LEU:HD21	1:J:675:ILE:CG1	2.51	0.41
1:J:1261:GLN:O	1:J:1261:GLN:HG2	2.21	0.41
1:K:94:GLN:HE21	1:K:117:ILE:HG21	1.85	0.41
1:K:747:ILE:HB	1:K:899:ARG:HB2	2.02	0.41
1:K:814:TYR:OH	1:K:921:GLN:NE2	2.53	0.41
1:K:947:ALA:HB2	1:K:963:MET:CB	2.51	0.41
1:K:1154:LEU:O	1:K:1155:LEU:HD13	2.20	0.41
1:K:1335:LEU:HD23	1:K:1335:LEU:HA	1.88	0.41
1:N:216:ILE:HD12	1:N:216:ILE:HA	1.82	0.41
1:N:251:MET:HE3	1:N:251:MET:HB2	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:256:SER:OG	1:N:1100:SER:HB2	2.21	0.41
1:N:458:VAL:HG21	1:N:1184:ILE:HB	2.03	0.41
1:N:633:PHE:CE2	1:N:665:PHE:HB3	2.56	0.41
1:N:736:LEU:HG	1:N:740:SER:OG	2.21	0.41
1:N:753:TYR:CE1	1:N:762:PHE:HB2	2.55	0.41
1:N:1188:PRO:HD2	1:N:1241:ASN:HB3	2.01	0.41
1:O:581:GLN:HE21	1:O:1021:MET:HE2	1.86	0.41
1:O:1304:THR:HG22	1:O:1311:PHE:O	2.21	0.41
1:P:328:MET:O	1:P:332:GLU:HG2	2.21	0.41
1:P:408:PRO:HB2	1:P:411:LEU:HD13	2.02	0.41
1:P:863:GLY:CA	1:P:866:ARG:HB3	2.50	0.41
1:P:1276:ASN:O	1:P:1280:LEU:HG	2.20	0.41
1:P:1292:ASN:HA	1:P:1295:SER:OG	2.20	0.41
2:v:426:LEU:O	2:v:429:GLU:HG3	2.21	0.41
3:x:76:ASP:O	4:y:3136:ARG:NH2	2.54	0.41
6:h:105:ALA:O	6:h:106:THR:HG22	2.20	0.41
6:h:334:ARG:HB3	6:h:349:GLU:HG3	2.03	0.41
7:k:203:ASP:O	7:k:207:LEU:HG	2.21	0.41
7:r:103:TRP:HB2	7:r:289:TYR:CE1	2.55	0.41
7:r:202:LEU:HD13	7:r:202:LEU:HA	1.91	0.41
1:J:453:GLN:HA	1:J:456:LEU:HD22	2.01	0.41
1:J:972:MET:HE3	1:O:801:ASP:HB2	2.03	0.41
1:K:1116:ASP:OD1	1:K:1176:HIS:HB3	2.21	0.41
1:K:1162:LEU:HD12	1:K:1163:ALA:N	2.36	0.41
1:N:464:LEU:HD11	1:N:1254:MET:SD	2.61	0.41
1:N:484:ARG:HD2	1:N:550:ILE:CB	2.45	0.41
1:N:549:TYR:CZ	1:N:561:ARG:HB2	2.55	0.41
1:N:817:LEU:HA	1:N:817:LEU:HD23	1.84	0.41
1:N:1004:TYR:CE2	1:N:1021:MET:HE1	2.57	0.41
1:O:68:PHE:HA	1:O:177:ILE:HD11	2.02	0.41
1:O:191:MET:HE3	1:O:195:GLN:HB2	2.02	0.41
1:O:598:VAL:HG13	1:O:599:ASP:O	2.21	0.41
1:O:985:ARG:HD3	1:O:990:PHE:CE2	2.56	0.41
1:P:285:ASN:ND2	1:P:1055:GLU:OE2	2.51	0.41
1:P:717:ALA:HA	1:P:1024:LYS:HE3	2.03	0.41
1:P:854:GLU:O	1:P:878:VAL:HG23	2.21	0.41
1:P:1279:GLU:CD	1:P:1282:ARG:HH12	2.29	0.41
7:m:13:LEU:HA	7:m:127:SER:CB	2.51	0.41
7:p:281:GLY:HA3	7:p:282:PRO:HD3	1.91	0.41
1:J:73:LEU:HD13	1:J:177:ILE:HD11	2.03	0.40
1:J:238:SER:C	1:J:240:PHE:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:282:VAL:HG23	1:J:283:THR:O	2.21	0.40
1:J:540:LEU:HD11	1:J:550:ILE:HD11	2.03	0.40
1:K:535:TYR:CE1	1:K:1227:HIS:HB2	2.56	0.40
1:N:59:TYR:CE1	1:O:260:VAL:HG21	2.51	0.40
1:N:270:ALA:HA	1:N:303:MET:HG2	2.03	0.40
1:N:1215:TYR:HE1	1:N:1285:ARG:HG2	1.86	0.40
1:O:483:ARG:HD3	1:O:551:GLY:O	2.20	0.40
1:O:544:PRO:HG3	1:O:1243:TRP:CD2	2.57	0.40
1:O:972:MET:HE1	1:O:978:ARG:NH2	2.36	0.40
1:P:70:GLU:O	1:P:367:ILE:HG23	2.21	0.40
1:P:783:ARG:NH1	1:P:888:PHE:O	2.46	0.40
5:d:73:ALA:HB2	5:e:18:PHE:CD2	2.55	0.40
7:k:218:ARG:HG2	7:k:263:ARG:NH1	2.36	0.40
7:p:158:ARG:HH21	7:p:202:LEU:HB3	1.85	0.40
7:r:153:PHE:CD1	7:r:190:LEU:HG	2.55	0.40
1:J:245:ARG:HA	1:J:245:ARG:HD2	1.94	0.40
1:J:567:MET:HE2	1:J:717:ALA:CB	2.51	0.40
1:K:367:ILE:HD13	1:K:367:ILE:HA	1.87	0.40
1:K:487:TYR:HD1	1:K:516:THR:HG23	1.86	0.40
1:K:487:TYR:OH	1:K:985:ARG:N	2.44	0.40
1:K:1250:LEU:HA	1:K:1253:ILE:HG22	2.03	0.40
1:N:999:SER:N	1:N:1000:PRO:HD2	2.35	0.40
1:N:1217:GLN:OE1	1:N:1281:LEU:HD13	2.21	0.40
1:O:481:ARG:NH2	1:O:540:LEU:HD23	2.36	0.40
1:O:839:LEU:HD23	1:O:839:LEU:HA	1.88	0.40
1:P:271:LYS:H	1:P:299:ASP:HB3	1.85	0.40
1:P:534:ASN:OD1	1:P:537:LEU:HB2	2.21	0.40
1:P:777:VAL:HA	1:P:780:TYR:HB3	2.03	0.40
2:v:42:ALA:HB1	2:v:102:PHE:CD1	2.53	0.40
2:v:50:ASP:C	2:v:337:ARG:HH12	2.29	0.40
2:v:334:ALA:HB3	2:v:335:PRO:HD3	2.02	0.40
2:v:379:ILE:C	2:v:381:LYS:H	2.30	0.40
5:a:32:GLN:HG3	5:a:40:PHE:CG	2.56	0.40
7:p:239:PHE:HD1	7:p:242:MET:HG3	1.86	0.40
1:J:456:LEU:HA	1:J:456:LEU:HD12	1.82	0.40
1:J:714:TYR:N	1:J:714:TYR:CD1	2.89	0.40
1:J:1143:LYS:HE3	1:J:1143:LYS:HB2	1.94	0.40
1:N:138:LEU:CB	6:h:45:GLU:HB2	2.51	0.40
1:N:185:LEU:HD13	1:N:399:ARG:HH21	1.87	0.40
1:N:830:VAL:H	1:N:895:THR:HG23	1.86	0.40
1:N:833:GLN:NE2	5:d:4:ARG:HD3	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:474:LEU:HG	1:O:560:HIS:NE2	2.37	0.40
1:O:545:LEU:HD23	1:O:545:LEU:HA	1.91	0.40
1:O:576:ALA:HB1	1:O:580:PHE:CD2	2.55	0.40
1:O:639:LEU:HA	1:O:880:MET:HE3	2.03	0.40
1:O:746:ILE:HB	1:O:753:TYR:HB3	2.03	0.40
1:O:951:HIS:NE2	1:O:997:HIS:HD2	2.18	0.40
1:P:86:SER:OG	1:P:87:ARG:NH2	2.54	0.40
1:P:388:TYR:HE2	1:P:396:PRO:HD3	1.86	0.40
1:P:679:ALA:O	1:P:683:TYR:HD1	2.03	0.40
1:P:759:ALA:HB1	1:P:763:ILE:HD13	2.03	0.40
1:P:1007:GLU:H	1:P:1007:GLU:HG2	1.73	0.40
5:d:60:TYR:O	5:d:64:THR:HG23	2.20	0.40
5:e:4:ARG:HD2	5:e:5:LEU:O	2.20	0.40
7:k:213:VAL:HA	7:k:216:LEU:HG	2.02	0.40
7:p:227:LEU:HD12	7:p:227:LEU:HA	1.90	0.40
1:J:405:TYR:CD1	1:J:1334:ALA:HB2	2.56	0.40
1:J:948:ILE:HG22	1:J:950:PHE:HD1	1.86	0.40
1:J:1358:TYR:CZ	1:O:427:LEU:HD11	2.57	0.40
1:K:224:LEU:HD23	1:K:224:LEU:HA	1.90	0.40
1:N:352:LEU:HD23	1:N:352:LEU:HA	1.83	0.40
1:O:335:MET:HE2	1:O:335:MET:HB3	1.78	0.40
1:O:989:LEU:HD23	1:O:989:LEU:HA	1.95	0.40
1:O:1115:THR:CG2	1:O:1180:ALA:HB2	2.52	0.40
1:O:1122:GLN:NE2	1:O:1127:VAL:HG21	2.32	0.40
2:v:43:TRP:HZ3	2:v:56:ARG:HG2	1.87	0.40
6:h:105:ALA:HB3	6:h:108:THR:HG23	2.03	0.40
7:r:181:TYR:CD2	7:r:182:LEU:HB2	2.56	0.40
1:J:25:LEU:HA	1:J:25:LEU:HD23	1.89	0.40
1:J:54:VAL:HG12	1:K:327:VAL:HB	2.04	0.40
1:J:955:GLY:HA3	1:J:985:ARG:NE	2.25	0.40
1:K:399:ARG:HD2	1:K:1320:PHE:HB3	2.04	0.40
1:K:651:SER:HB2	1:K:653:ARG:HE	1.86	0.40
1:K:1009:LEU:HA	1:K:1010:PRO:HD3	1.92	0.40
1:K:1195:TYR:HD1	1:K:1234:TYR:HE2	1.69	0.40
1:K:1254:MET:HE3	1:K:1255:TYR:CE2	2.56	0.40
1:N:603:ILE:HG21	1:N:1010:PRO:O	2.21	0.40
1:N:671:GLY:O	1:N:672:ASN:O	2.40	0.40
1:N:695:GLN:HG2	1:O:958:ARG:CZ	2.51	0.40
1:N:966:ASP:O	1:N:969:THR:OG1	2.31	0.40
1:N:1005:ALA:HA	1:N:1008:CYS:HB2	2.04	0.40
1:O:430:PRO:O	1:O:433:GLN:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:670:LEU:HD22	1:O:680:TYR:CD1	2.57	0.40
1:O:947:ALA:HB2	1:O:963:MET:CB	2.45	0.40
1:P:494:PRO:HG2	1:P:749:GLY:HA2	2.04	0.40
2:v:93:ASN:HB3	2:v:96:HIS:CE1	2.55	0.40
6:f:334:ARG:HB2	6:f:349:GLU:HG3	2.03	0.40
7:m:268:MET:HG3	7:r:278:PHE:CD1	2.57	0.40
7:p:8:SER:H	7:p:37:THR:CG2	2.34	0.40
7:p:63:TYR:CE1	7:p:67:CYS:HB2	2.57	0.40
7:p:216:LEU:HD13	7:p:267:MET:HE3	2.04	0.40
7:p:292:GLU:H	7:p:292:GLU:HG2	1.58	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	1348/1381 (98%)	1269 (94%)	72 (5%)	7 (0%)	24	60
1	K	1379/1381 (100%)	1310 (95%)	67 (5%)	2 (0%)	48	81
1	N	1358/1381 (98%)	1288 (95%)	62 (5%)	8 (1%)	21	57
1	O	1328/1381 (96%)	1259 (95%)	68 (5%)	1 (0%)	48	81
1	P	1273/1381 (92%)	1202 (94%)	69 (5%)	2 (0%)	43	75
2	v	282/507 (56%)	262 (93%)	19 (7%)	1 (0%)	30	65
3	w	66/570 (12%)	65 (98%)	1 (2%)	0	100	100
3	x	66/570 (12%)	66 (100%)	0	0	100	100
4	y	35/3149 (1%)	34 (97%)	1 (3%)	0	100	100
4	z	35/3149 (1%)	34 (97%)	1 (3%)	0	100	100
5	Z	75/176 (43%)	67 (89%)	6 (8%)	2 (3%)	4	28
5	a	75/176 (43%)	70 (93%)	5 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	d	75/176 (43%)	69 (92%)	4 (5%)	2 (3%)	4	28
5	e	75/176 (43%)	72 (96%)	3 (4%)	0	100	100
5	u	61/176 (35%)	56 (92%)	5 (8%)	0	100	100
6	f	307/364 (84%)	289 (94%)	18 (6%)	0	100	100
6	h	330/364 (91%)	305 (92%)	25 (8%)	0	100	100
7	k	297/301 (99%)	282 (95%)	14 (5%)	1 (0%)	36	70
7	m	297/301 (99%)	282 (95%)	13 (4%)	2 (1%)	18	54
7	p	297/301 (99%)	282 (95%)	10 (3%)	5 (2%)	7	36
7	r	297/301 (99%)	288 (97%)	8 (3%)	1 (0%)	36	70
All	All	9356/17662 (53%)	8851 (95%)	471 (5%)	34 (0%)	31	65

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	305	PRO
1	J	366	PRO
1	K	298	ALA
1	K	805	ALA
1	N	483	ARG
1	N	484	ARG
1	N	672	ASN
1	N	675	ILE
1	N	678	GLU
1	O	259	SER
5	Z	69	ARG
5	d	7	LYS
7	p	39	ASN
7	p	98	GLN
1	J	255	VAL
1	N	481	ARG
1	N	677	LYS
7	k	15	THR
1	J	9	ASN
1	N	873	ASP
1	P	806	ASP
7	p	36	GLY
1	J	306	SER
1	J	1316	GLY
2	v	382	ASN

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Mol	Chain	Res	Type
5	Z	68	PRO
7	r	202	LEU
1	P	106	ASP
7	m	197	LEU
7	p	38	GLN
5	d	6	PRO
1	J	367	ILE
7	m	164	PRO
7	p	99	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	1149/1171 (98%)	1073 (93%)	76 (7%)	15	40
1	K	1171/1171 (100%)	1100 (94%)	71 (6%)	17	41
1	N	1155/1171 (99%)	1080 (94%)	75 (6%)	15	40
1	O	1128/1171 (96%)	1064 (94%)	64 (6%)	18	43
1	P	1093/1171 (93%)	1047 (96%)	46 (4%)	26	49
2	v	243/400 (61%)	222 (91%)	21 (9%)	10	33
3	w	57/465 (12%)	56 (98%)	1 (2%)	51	68
3	x	57/465 (12%)	56 (98%)	1 (2%)	51	68
4	y	35/2539 (1%)	34 (97%)	1 (3%)	37	58
4	z	35/2539 (1%)	35 (100%)	0	100	100
5	Z	71/128 (56%)	70 (99%)	1 (1%)	59	71
5	a	71/128 (56%)	70 (99%)	1 (1%)	59	71
5	d	71/128 (56%)	70 (99%)	1 (1%)	59	71
5	e	71/128 (56%)	70 (99%)	1 (1%)	59	71
5	u	59/128 (46%)	59 (100%)	0	100	100
6	f	267/289 (92%)	255 (96%)	12 (4%)	24	47
6	h	278/289 (96%)	257 (92%)	21 (8%)	12	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	k	265/267 (99%)	254 (96%)	11 (4%)	26	49
7	m	265/267 (99%)	246 (93%)	19 (7%)	13	37
7	p	265/267 (99%)	253 (96%)	12 (4%)	24	47
7	r	265/267 (99%)	255 (96%)	10 (4%)	29	51
All	All	8071/14549 (56%)	7626 (94%)	445 (6%)	21	44

All (445) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	5	GLU
1	J	66	VAL
1	J	78	VAL
1	J	89	THR
1	J	95	PHE
1	J	99	VAL
1	J	101	THR
1	J	119	VAL
1	J	129	THR
1	J	144	ILE
1	J	147	THR
1	J	161	VAL
1	J	165	LEU
1	J	183	VAL
1	J	203	THR
1	J	209	LYS
1	J	216	ILE
1	J	248	LEU
1	J	255	VAL
1	J	259	SER
1	J	260	VAL
1	J	287	LEU
1	J	306	SER
1	J	308	TYR
1	J	322	VAL
1	J	365	VAL
1	J	367	ILE
1	J	393	SER
1	J	445	ASN
1	J	456	LEU
1	J	458	VAL
1	J	466	THR

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Mol	Chain	Res	Type
1	J	481	ARG
1	J	503	VAL
1	J	518	ILE
1	J	536	ASP
1	J	563	VAL
1	J	598	VAL
1	J	602	VAL
1	J	642	LEU
1	J	657	VAL
1	J	675	ILE
1	J	690	LEU
1	J	706	VAL
1	J	716	CYS
1	J	847	SER
1	J	851	THR
1	J	853	ASP
1	J	861	GLU
1	J	871	ILE
1	J	928	LEU
1	J	969	THR
1	J	1042	VAL
1	J	1058	LEU
1	J	1065	THR
1	J	1094	SER
1	J	1095	ILE
1	J	1106	THR
1	J	1110	VAL
1	J	1156	ARG
1	J	1161	TYR
1	J	1174	LEU
1	J	1182	CYS
1	J	1187	THR
1	J	1189	VAL
1	J	1192	ASP
1	J	1199	SER
1	J	1209	VAL
1	J	1223	LEU
1	J	1246	GLN
1	J	1262	THR
1	J	1264	VAL
1	J	1269	SER
1	J	1312	VAL

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Mol	Chain	Res	Type
1	J	1313	VAL
1	J	1349	VAL
1	K	7	VAL
1	K	22	LEU
1	K	39	LEU
1	K	54	VAL
1	K	58	VAL
1	K	96	ARG
1	K	127	ILE
1	K	147	THR
1	K	179	THR
1	K	232	ARG
1	K	264	VAL
1	K	279	VAL
1	K	291	LEU
1	K	313	VAL
1	K	361	ASP
1	K	372	ILE
1	K	381	VAL
1	K	425	LYS
1	K	440	ILE
1	K	451	ASN
1	K	456	LEU
1	K	464	LEU
1	K	486	THR
1	K	517	ASP
1	K	526	THR
1	K	571	LEU
1	K	589	GLU
1	K	598	VAL
1	K	602	VAL
1	K	637	VAL
1	K	654	LEU
1	K	657	VAL
1	K	690	LEU
1	K	693	LEU
1	K	697	LEU
1	K	711	VAL
1	K	742	ARG
1	K	748	ILE
1	K	752	VAL
1	K	794	LEU

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Mol	Chain	Res	Type
1	K	830	VAL
1	K	851	THR
1	K	874	LEU
1	K	905	ASP
1	K	907	THR
1	K	919	THR
1	K	920	GLU
1	K	928	LEU
1	K	964	HIS
1	K	1012	LEU
1	K	1013	VAL
1	K	1018	MET
1	K	1036	LEU
1	K	1048	ARG
1	K	1049	THR
1	K	1054	SER
1	K	1058	LEU
1	K	1095	ILE
1	K	1099	LEU
1	K	1155	LEU
1	K	1168	VAL
1	K	1187	THR
1	K	1189	VAL
1	K	1209	VAL
1	K	1238	SER
1	K	1253	ILE
1	K	1267	LEU
1	K	1305	SER
1	K	1352	THR
1	K	1353	HIS
1	K	1369	VAL
1	N	17	VAL
1	N	41	VAL
1	N	54	VAL
1	N	56	LEU
1	N	61	ASN
1	N	63	ILE
1	N	71	THR
1	N	106	ASP
1	N	113	GLN
1	N	127	ILE
1	N	160	THR

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Mol	Chain	Res	Type
1	N	194	LEU
1	N	213	SER
1	N	216	ILE
1	N	279	VAL
1	N	284	ASP
1	N	313	VAL
1	N	355	VAL
1	N	371	VAL
1	N	381	VAL
1	N	409	VAL
1	N	419	THR
1	N	456	LEU
1	N	471	LEU
1	N	482	ASP
1	N	483	ARG
1	N	484	ARG
1	N	485	GLU
1	N	486	THR
1	N	501	VAL
1	N	538	LEU
1	N	550	ILE
1	N	571	LEU
1	N	582	GLU
1	N	598	VAL
1	N	602	VAL
1	N	637	VAL
1	N	657	VAL
1	N	670	LEU
1	N	672	ASN
1	N	673	ASN
1	N	675	ILE
1	N	676	SER
1	N	700	LEU
1	N	704	ASP
1	N	719	LEU
1	N	736	LEU
1	N	740	SER
1	N	769	MET
1	N	828	LEU
1	N	902	VAL
1	N	905	ASP
1	N	919	THR

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Mol	Chain	Res	Type
1	N	925	VAL
1	N	933	PHE
1	N	938	ARG
1	N	950	PHE
1	N	981	GLU
1	N	1035	LYS
1	N	1044	MET
1	N	1048	ARG
1	N	1081	VAL
1	N	1099	LEU
1	N	1110	VAL
1	N	1116	ASP
1	N	1124	PHE
1	N	1201	SER
1	N	1209	VAL
1	N	1210	VAL
1	N	1256	ASN
1	N	1287	LEU
1	N	1313	VAL
1	N	1336	SER
1	N	1347	MET
1	N	1352	THR
1	O	47	GLU
1	O	84	ASP
1	O	88	MET
1	O	89	THR
1	O	98	SER
1	O	104	HIS
1	O	121	ASN
1	O	136	LEU
1	O	137	ASP
1	O	147	THR
1	O	177	ILE
1	O	194	LEU
1	O	197	LEU
1	O	216	ILE
1	O	230	LEU
1	O	256	SER
1	O	258	GLU
1	O	259	SER
1	O	260	VAL
1	O	261	LEU

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Mol	Chain	Res	Type
1	O	269	THR
1	O	279	VAL
1	O	313	VAL
1	O	338	ILE
1	O	466	THR
1	O	518	ILE
1	O	540	LEU
1	O	592	THR
1	O	597	VAL
1	O	598	VAL
1	O	602	VAL
1	O	637	VAL
1	O	654	LEU
1	O	657	VAL
1	O	681	SER
1	O	700	LEU
1	O	851	THR
1	O	856	ILE
1	O	860	LEU
1	O	865	LEU
1	O	866	ARG
1	O	885	SER
1	O	902	VAL
1	O	940	VAL
1	O	941	THR
1	O	1036	LEU
1	O	1053	LEU
1	O	1065	THR
1	O	1082	ASP
1	O	1095	ILE
1	O	1110	VAL
1	O	1116	ASP
1	O	1174	LEU
1	O	1183	GLU
1	O	1186	VAL
1	O	1187	THR
1	O	1189	VAL
1	O	1209	VAL
1	O	1210	VAL
1	O	1309	VAL
1	O	1314	ILE
1	O	1319	VAL

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Mol	Chain	Res	Type
1	O	1335	LEU
1	O	1343	ILE
1	P	66	VAL
1	P	144	ILE
1	P	149	VAL
1	P	210	THR
1	P	211	VAL
1	P	227	SER
1	P	293	PHE
1	P	319	VAL
1	P	327	VAL
1	P	333	HIS
1	P	474	LEU
1	P	524	LEU
1	P	597	VAL
1	P	598	VAL
1	P	632	LYS
1	P	640	VAL
1	P	675	ILE
1	P	689	GLU
1	P	752	VAL
1	P	756	THR
1	P	796	LEU
1	P	813	TYR
1	P	830	VAL
1	P	838	THR
1	P	860	LEU
1	P	880	MET
1	P	881	ILE
1	P	895	THR
1	P	901	SER
1	P	928	LEU
1	P	929	VAL
1	P	944	LEU
1	P	980	VAL
1	P	1007	GLU
1	P	1058	LEU
1	P	1071	THR
1	P	1106	THR
1	P	1110	VAL
1	P	1119	ILE
1	P	1187	THR

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Mol	Chain	Res	Type
1	P	1189	VAL
1	P	1203	ARG
1	P	1210	VAL
1	P	1260	ARG
1	P	1349	VAL
1	P	1379	VAL
2	v	9	VAL
2	v	15	THR
2	v	39	CYS
2	v	57	VAL
2	v	74	ARG
2	v	100	LEU
2	v	284	LEU
2	v	288	ILE
2	v	293	SER
2	v	300	VAL
2	v	371	VAL
2	v	374	THR
2	v	380	TYR
2	v	383	SER
2	v	385	LEU
2	v	387	ARG
2	v	392	THR
2	v	397	VAL
2	v	409	SER
2	v	437	VAL
2	v	469	SER
3	w	91	VAL
3	x	88	LEU
4	y	3137	LEU
5	Z	69	ARG
5	a	31	ASN
5	d	52	THR
5	e	24	LEU
6	f	4	GLN
6	f	39	VAL
6	f	108	THR
6	f	114	LYS
6	f	164	THR
6	f	212	VAL
6	f	214	LYS
6	f	216	ILE

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Mol	Chain	Res	Type
6	f	223	VAL
6	f	237	LEU
6	f	313	ILE
6	f	338	PHE
6	h	43	VAL
6	h	46	HIS
6	h	57	VAL
6	h	68	VAL
6	h	86	ARG
6	h	106	THR
6	h	125	VAL
6	h	134	LEU
6	h	197	SER
6	h	211	VAL
6	h	223	VAL
6	h	224	THR
6	h	268	LEU
6	h	300	SER
6	h	308	VAL
6	h	311	LEU
6	h	327	PHE
6	h	328	SER
6	h	331	ASP
6	h	333	TRP
6	h	352	SER
7	k	45	LEU
7	k	69	LEU
7	k	75	VAL
7	k	86	VAL
7	k	131	ASP
7	k	182	LEU
7	k	199	LEU
7	k	224	VAL
7	k	252	LEU
7	k	271	LEU
7	k	293	THR
7	m	13	LEU
7	m	17	GLU
7	m	31	LEU
7	m	77	VAL
7	m	86	VAL
7	m	96	LYS

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Mol	Chain	Res	Type
7	m	122	THR
7	m	190	LEU
7	m	193	VAL
7	m	215	LEU
7	m	223	LEU
7	m	228	ILE
7	m	243	VAL
7	m	247	ILE
7	m	252	LEU
7	m	262	SER
7	m	271	LEU
7	m	274	LEU
7	m	293	THR
7	p	3	LEU
7	p	45	LEU
7	p	54	VAL
7	p	98	GLN
7	p	148	GLN
7	p	172	VAL
7	p	182	LEU
7	p	197	LEU
7	p	199	LEU
7	p	201	LEU
7	p	202	LEU
7	p	257	VAL
7	r	3	LEU
7	r	76	SER
7	r	82	LEU
7	r	115	VAL
7	r	201	LEU
7	r	203	ASP
7	r	229	ARG
7	r	255	LEU
7	r	261	LEU
7	r	293	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (195) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	35	HIS
1	J	61	ASN
1	J	79	ASN

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Mol	Chain	Res	Type
1	J	121	ASN
1	J	126	HIS
1	J	195	GLN
1	J	285	ASN
1	J	389	ASN
1	J	392	GLN
1	J	444	ASN
1	J	491	HIS
1	J	531	HIS
1	J	564	HIS
1	J	581	GLN
1	J	596	HIS
1	J	600	GLN
1	J	636	ASN
1	J	695	GLN
1	J	722	ASN
1	J	822	ASN
1	J	833	GLN
1	J	834	HIS
1	J	862	ASN
1	J	921	GLN
1	J	984	ASN
1	J	1090	HIS
1	J	1122	GLN
1	J	1176	HIS
1	J	1241	ASN
1	J	1301	HIS
1	K	27	GLN
1	K	79	ASN
1	K	94	GLN
1	K	104	HIS
1	K	123	HIS
1	K	126	HIS
1	K	222	HIS
1	K	226	HIS
1	K	289	GLN
1	K	301	GLN
1	K	376	ASN
1	K	377	HIS
1	K	385	GLN
1	K	398	ASN
1	K	402	GLN

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Mol	Chain	Res	Type
1	K	444	ASN
1	K	496	HIS
1	K	531	HIS
1	K	543	HIS
1	K	570	ASN
1	K	596	HIS
1	K	722	ASN
1	K	735	HIS
1	K	822	ASN
1	K	951	HIS
1	K	977	GLN
1	K	997	HIS
1	K	1122	GLN
1	K	1137	GLN
1	K	1178	GLN
1	K	1256	ASN
1	K	1360	HIS
1	N	79	ASN
1	N	104	HIS
1	N	121	ASN
1	N	126	HIS
1	N	178	ASN
1	N	402	GLN
1	N	444	ASN
1	N	469	HIS
1	N	491	HIS
1	N	496	HIS
1	N	531	HIS
1	N	543	HIS
1	N	596	HIS
1	N	645	ASN
1	N	788	HIS
1	N	804	HIS
1	N	824	HIS
1	N	833	GLN
1	N	834	HIS
1	N	908	GLN
1	N	921	GLN
1	N	926	ASN
1	N	965	GLN
1	N	974	ASN
1	N	997	HIS

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Mol	Chain	Res	Type
1	N	1033	GLN
1	N	1169	ASN
1	N	1276	ASN
1	N	1353	HIS
1	O	125	HIS
1	O	226	HIS
1	O	289	GLN
1	O	301	GLN
1	O	333	HIS
1	O	398	ASN
1	O	415	ASN
1	O	444	ASN
1	O	445	ASN
1	O	465	HIS
1	O	469	HIS
1	O	496	HIS
1	O	531	HIS
1	O	581	GLN
1	O	587	GLN
1	O	636	ASN
1	O	673	ASN
1	O	695	GLN
1	O	849	HIS
1	O	908	GLN
1	O	909	GLN
1	O	974	ASN
1	O	977	GLN
1	O	997	HIS
1	O	1033	GLN
1	O	1351	GLN
1	P	166	GLN
1	P	222	HIS
1	P	226	HIS
1	P	415	ASN
1	P	432	GLN
1	P	472	ASN
1	P	509	ASN
1	P	531	HIS
1	P	586	GLN
1	P	596	HIS
1	P	627	HIS
1	P	713	GLN

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Mol	Chain	Res	Type
1	P	735	HIS
1	P	750	ASN
1	P	842	ASN
1	P	848	HIS
1	P	849	HIS
1	P	908	GLN
1	P	942	GLN
1	P	977	GLN
1	P	984	ASN
1	P	1120	HIS
1	P	1122	GLN
1	P	1137	GLN
1	P	1178	GLN
1	P	1241	ASN
1	P	1283	ASN
1	P	1329	GLN
2	v	7	ASN
2	v	8	GLN
2	v	34	ASN
2	v	45	GLN
2	v	290	HIS
2	v	295	HIS
2	v	382	ASN
2	v	394	GLN
3	x	77	HIS
3	x	102	GLN
4	z	3114	GLN
5	Z	11	GLN
5	Z	54	GLN
5	Z	71	GLN
5	a	44	GLN
5	a	71	GLN
5	d	54	GLN
5	e	31	ASN
5	e	33	ASN
5	e	54	GLN
5	u	11	GLN
6	f	46	HIS
6	f	303	HIS
6	f	309	GLN
6	h	13	GLN
6	h	28	ASN

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Mol	Chain	Res	Type
6	h	46	HIS
6	h	182	HIS
6	h	201	ASN
6	h	256	GLN
6	h	288	GLN
6	h	291	ASN
7	k	102	GLN
7	k	148	GLN
7	k	184	HIS
7	m	38	GLN
7	m	62	ASN
7	m	98	GLN
7	m	128	ASN
7	m	148	GLN
7	m	184	HIS
7	p	22	GLN
7	p	23	GLN
7	p	89	GLN
7	p	184	HIS
7	p	185	HIS
7	p	204	ASN
7	p	237	ASN
7	r	128	ASN
7	r	184	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

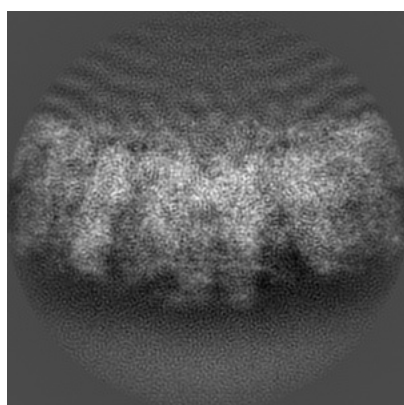
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21525. These allow visual inspection of the internal detail of the map and identification of artifacts.

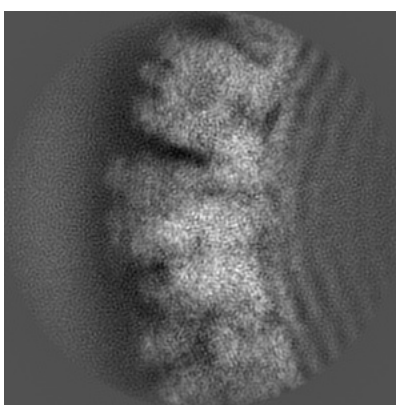
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

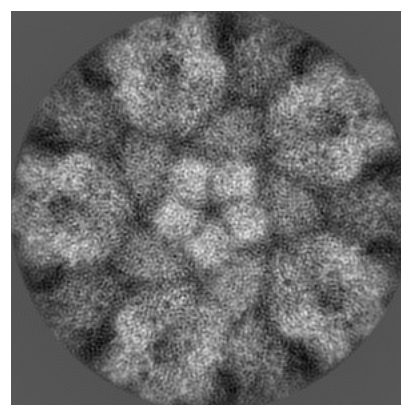
6.1.1 Primary map



X



Y

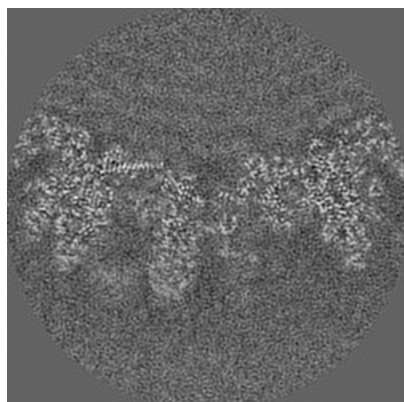


Z

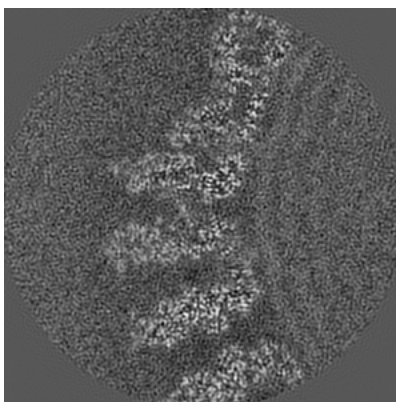
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

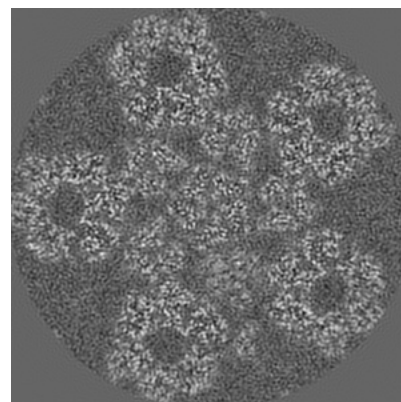
6.2.1 Primary map



X Index: 160



Y Index: 160

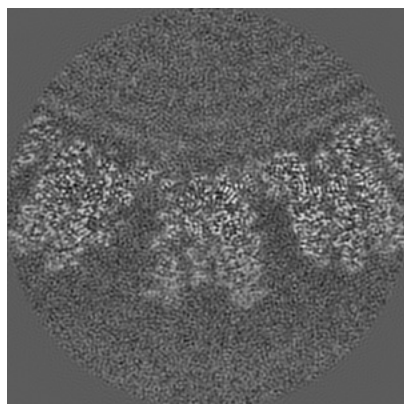


Z Index: 160

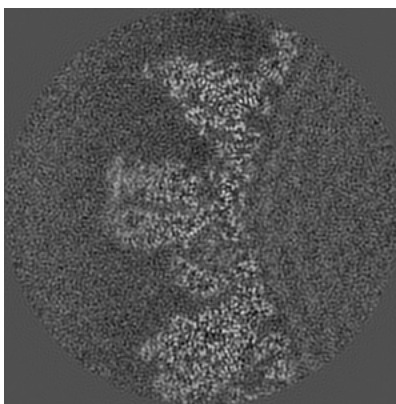
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

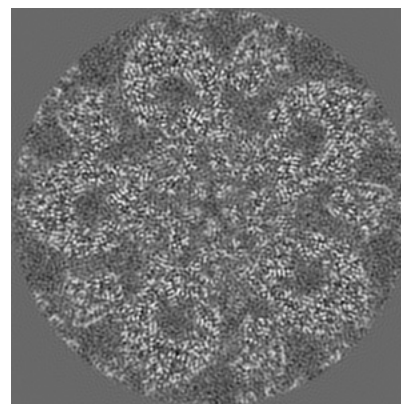
6.3.1 Primary map



X Index: 147



Y Index: 189

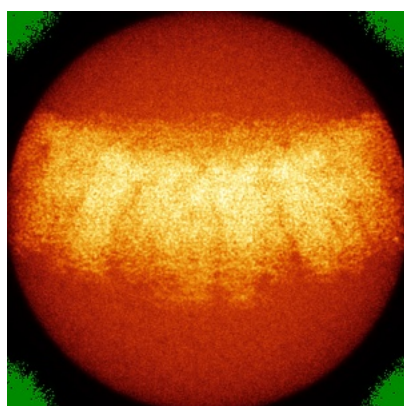


Z Index: 185

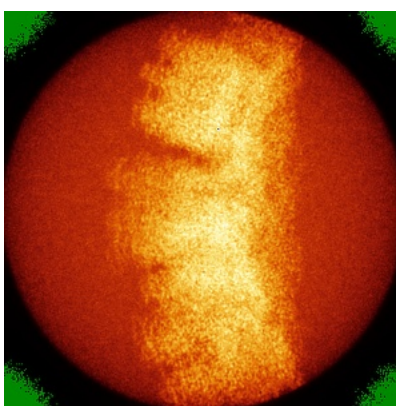
The images above show the largest variance slices of the map in three orthogonal directions.

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

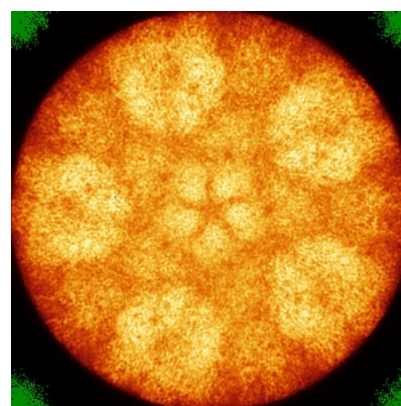
6.4.1 Primary map



X



Y

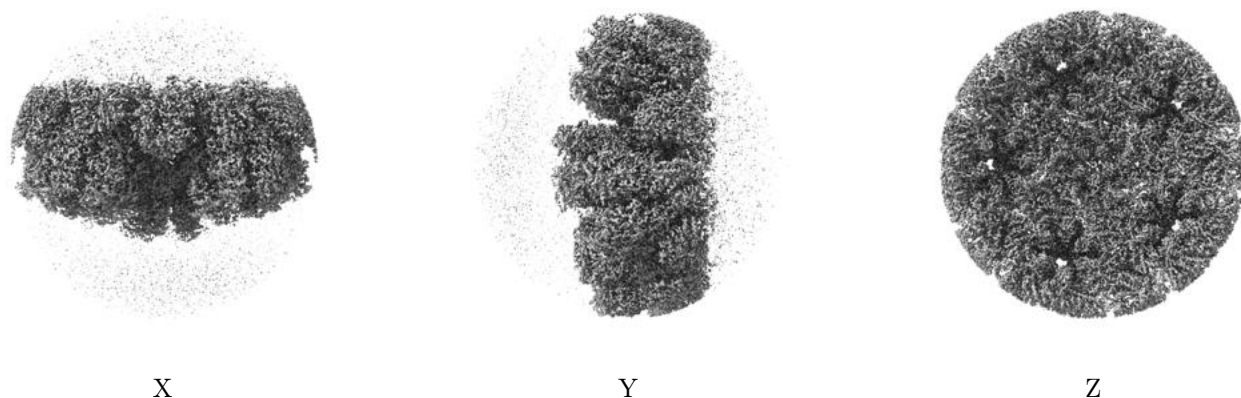


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

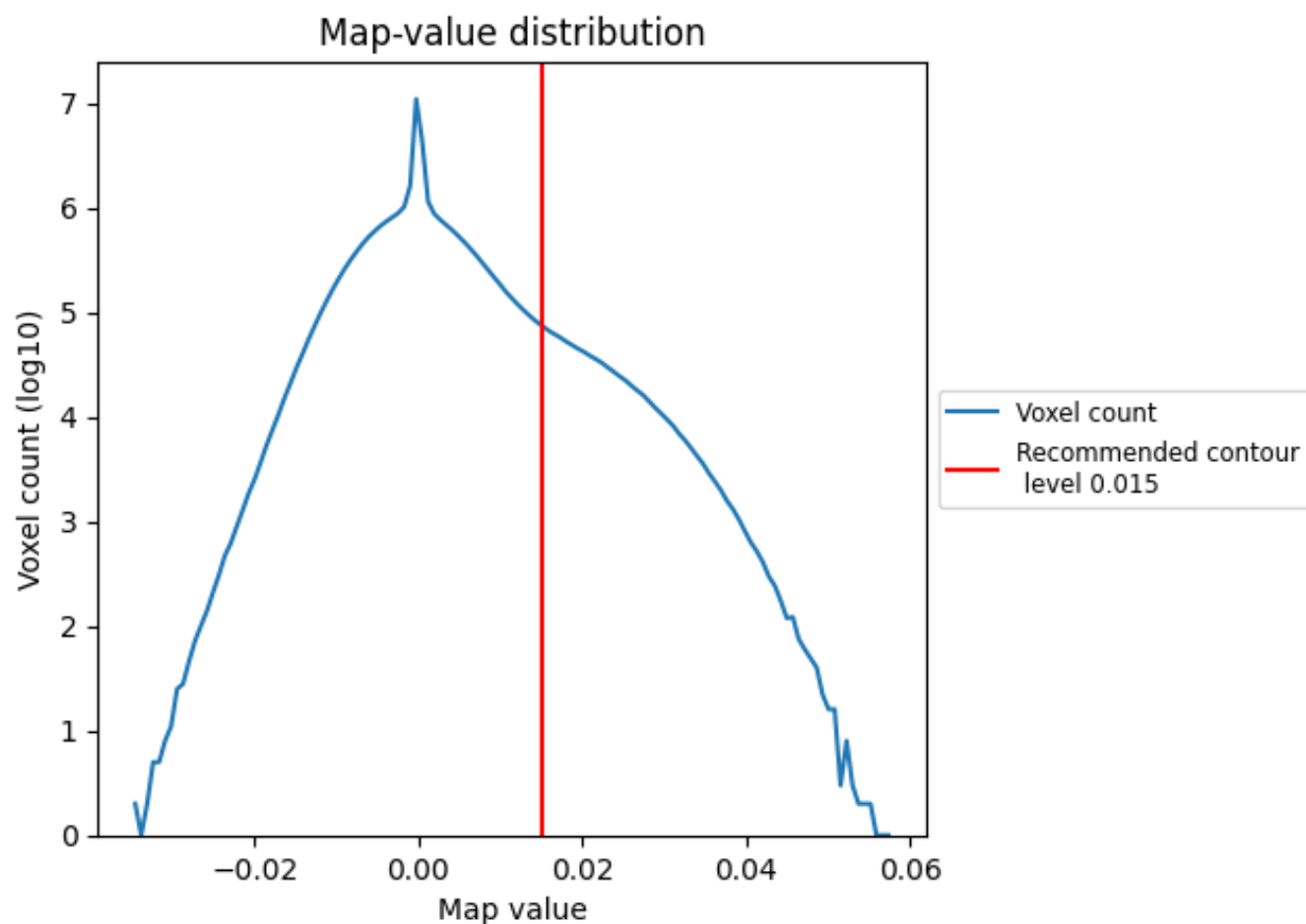
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

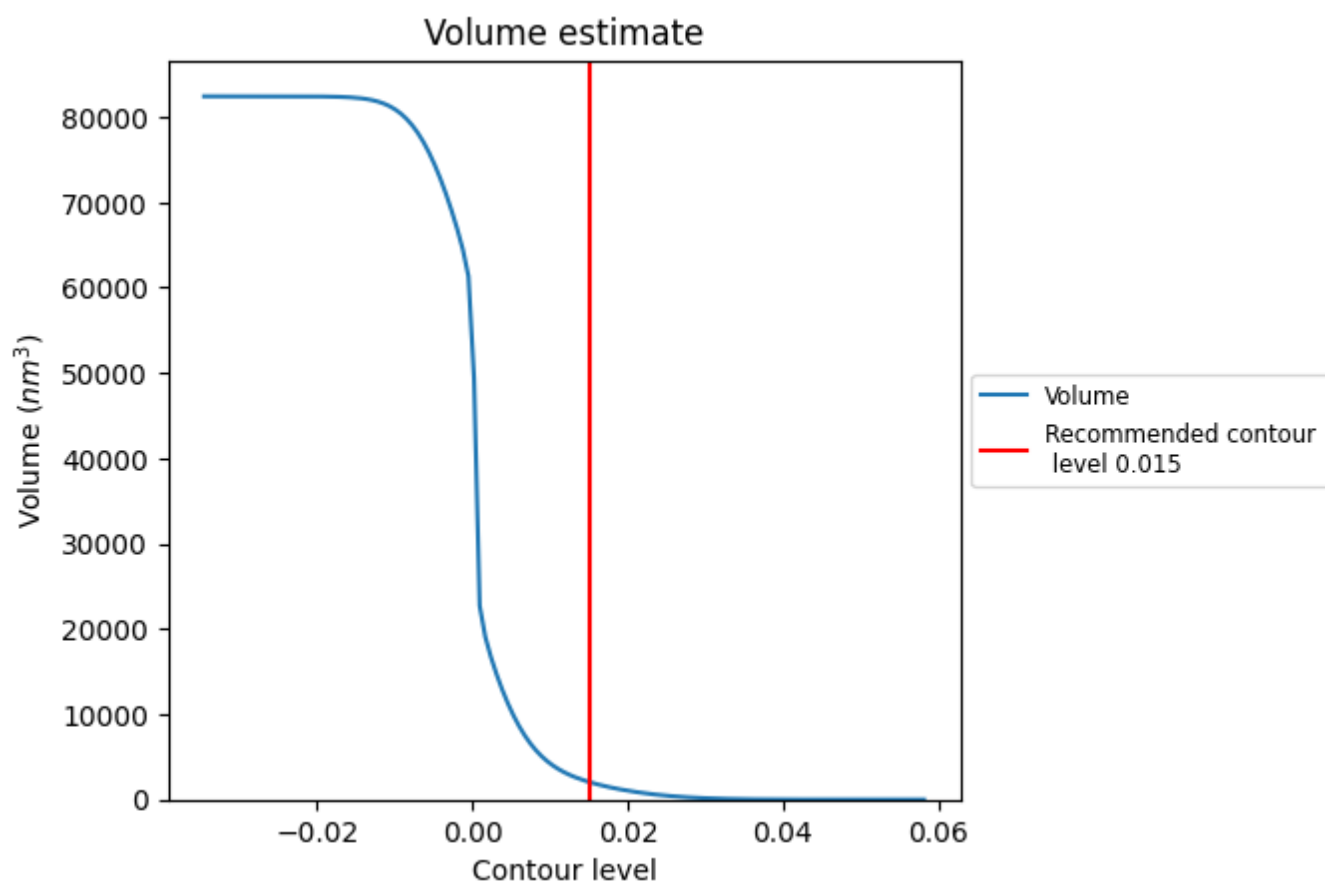
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

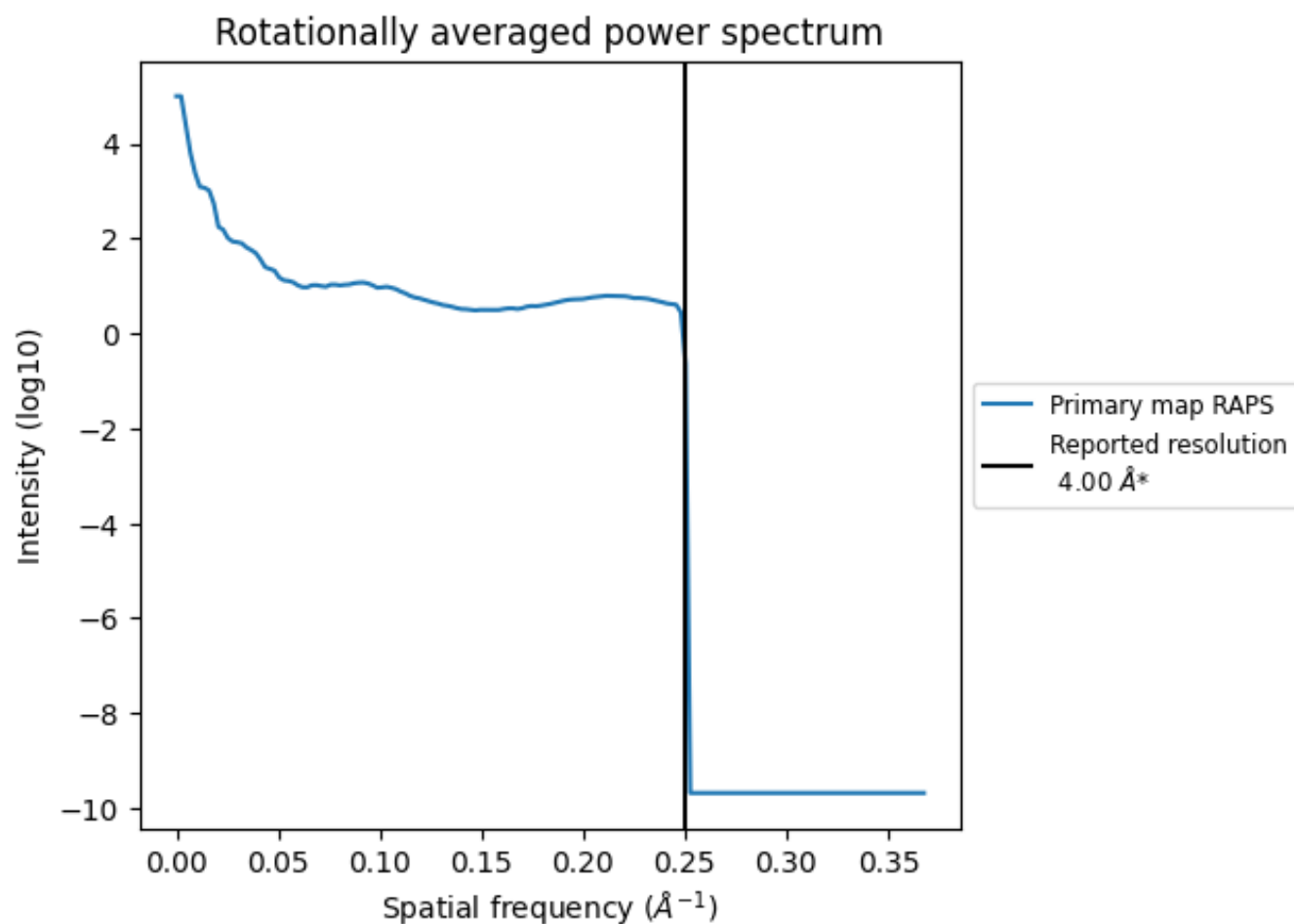
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2067 nm³; this corresponds to an approximate mass of 1867 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 0.250 $\text{\AA}^{-1}$

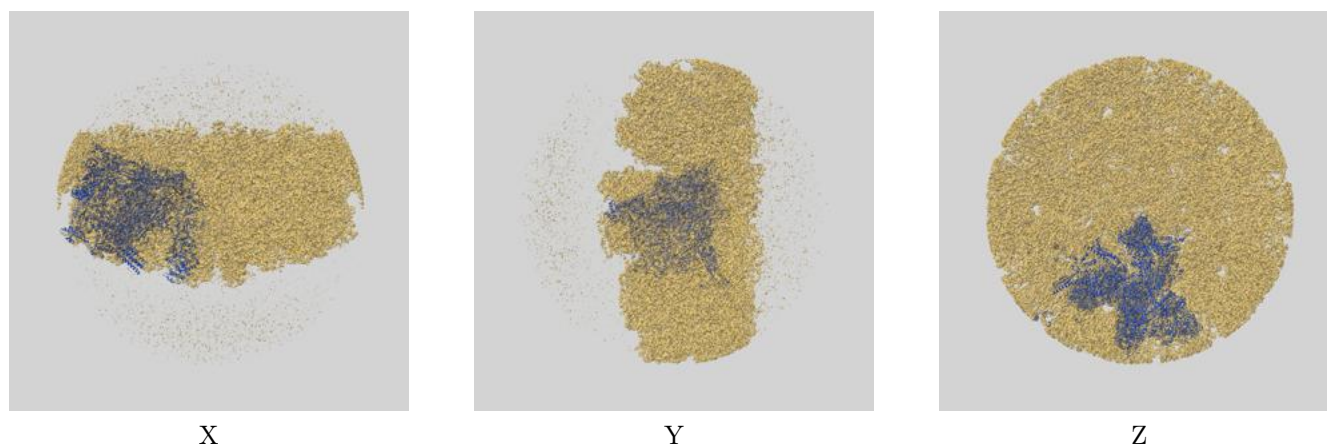
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

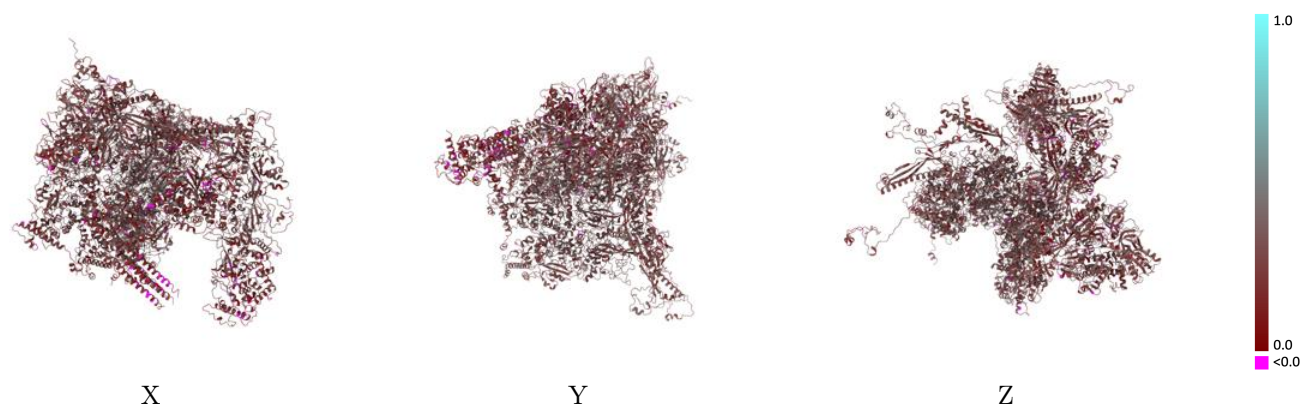
This section contains information regarding the fit between EMDB map EMD-21525 and PDB model 6W2D. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



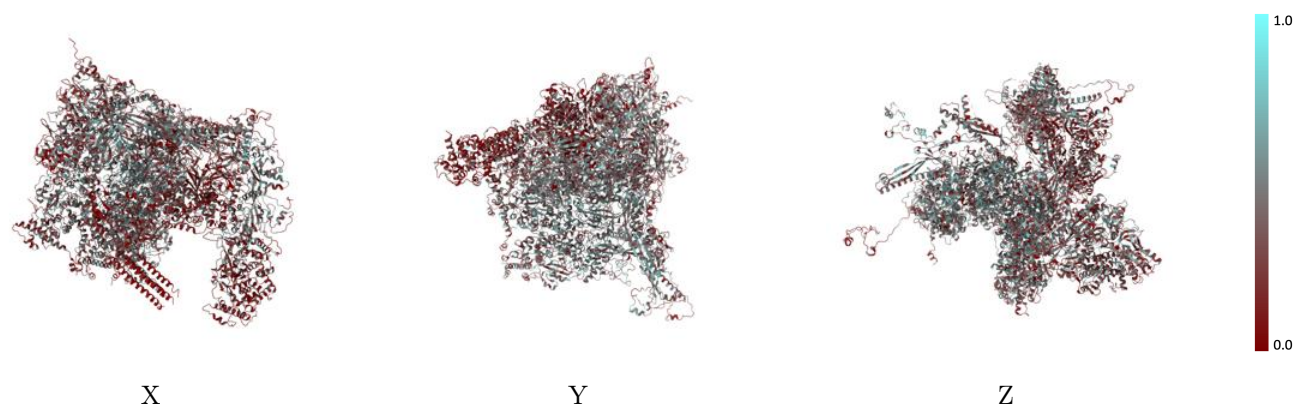
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



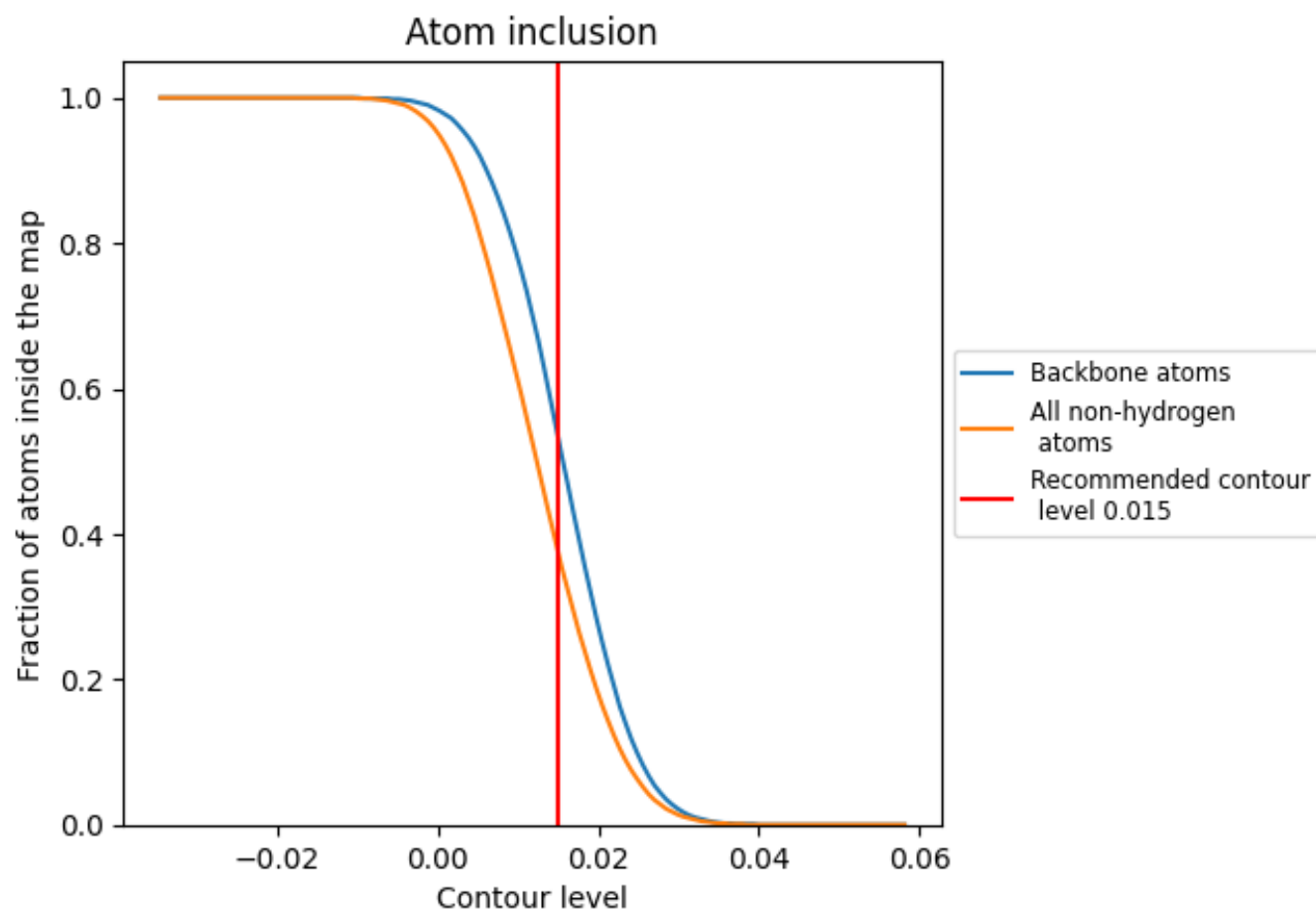
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 37% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3740	 0.2800
J	 0.4580	 0.3060
K	 0.4470	 0.3030
N	 0.4050	 0.2910
O	 0.4400	 0.3030
P	 0.3240	 0.2580
Z	 0.3450	 0.2420
a	 0.3080	 0.2810
d	 0.2430	 0.2360
e	 0.2950	 0.2580
f	 0.2000	 0.2340
h	 0.3770	 0.2720
k	 0.2460	 0.2530
m	 0.3430	 0.2700
p	 0.2390	 0.2550
r	 0.3660	 0.2810
u	 0.1380	 0.1670
v	 0.2220	 0.2410
w	 0.1000	 0.1630
x	 0.1880	 0.1900
y	 0.1090	 0.1880
z	 0.0960	 0.1620

