



## Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 06:11 PM EST

PDB ID : 6W2D  
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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

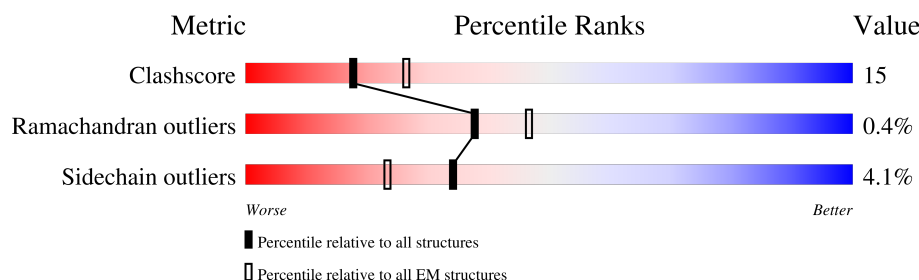
# 1 Overall quality at a glance

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.



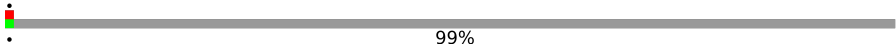
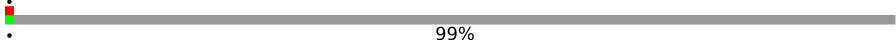




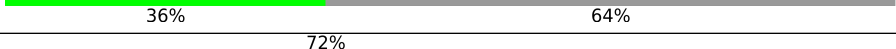


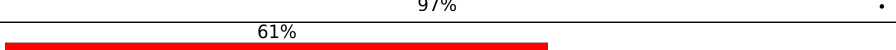
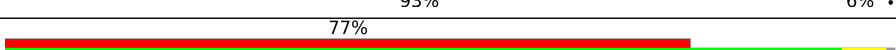
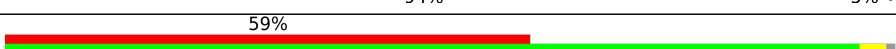
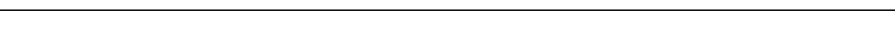
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	
1	K	1381	
1	N	1381	
1	O	1381	
1	P	1381	
2	v	507	
3	w	570	
3	x	570	

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Mol	Chain	Length	Quality of chain
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		

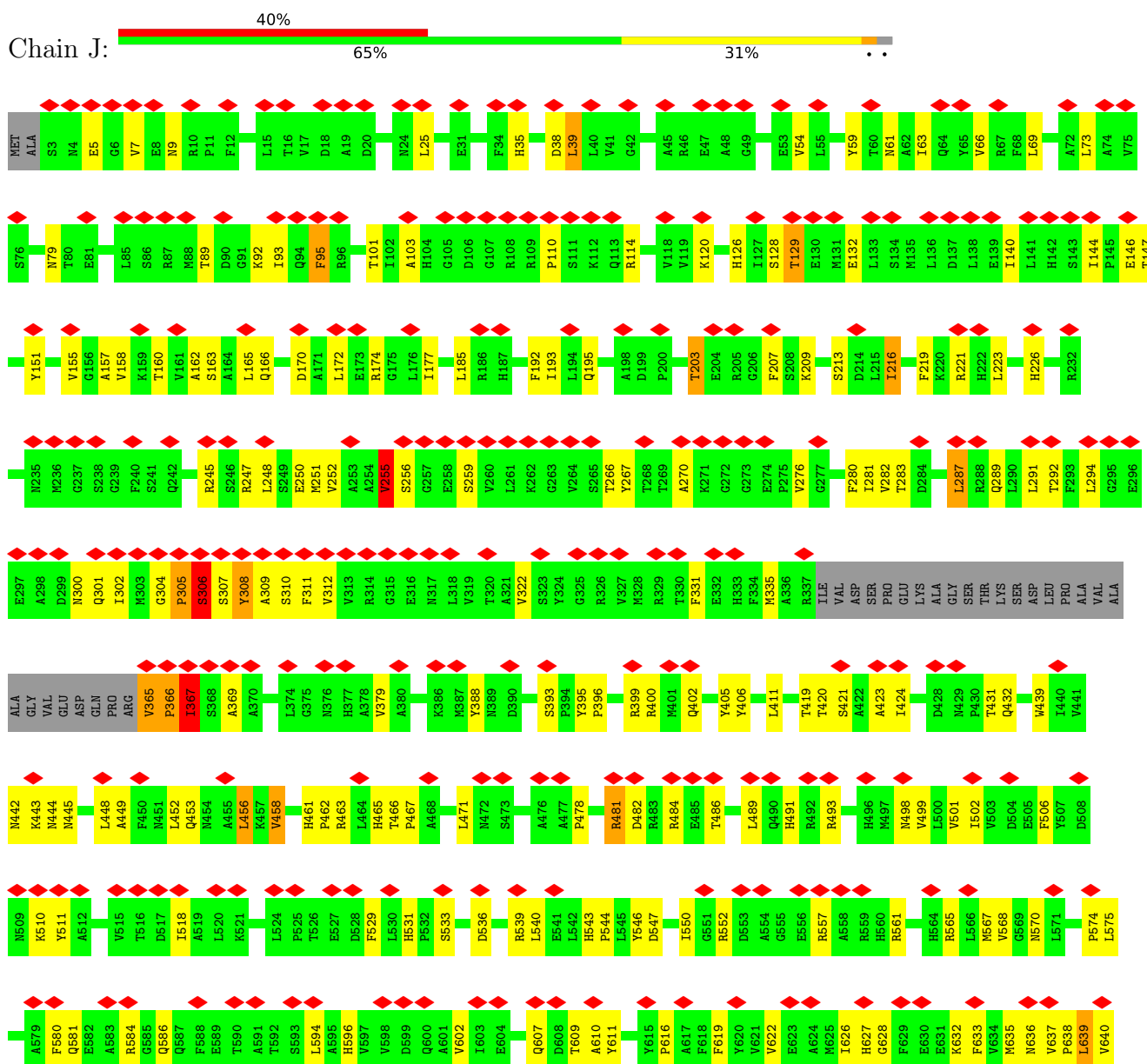
- Molecule 7 is a protein called Triplex capsid protein 2.

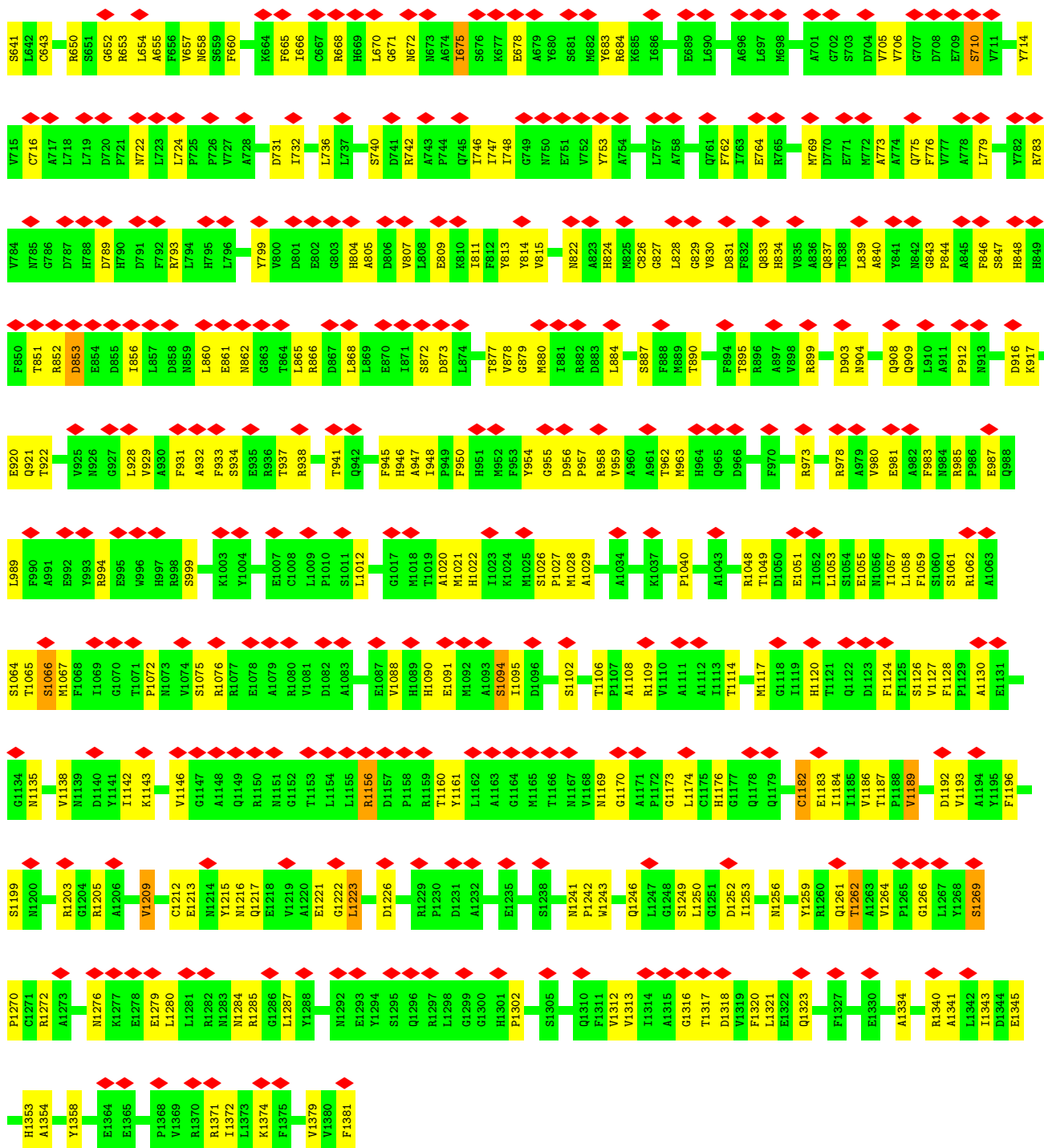
Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	m	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	p	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		
7	r	299	Total	C	N	O	S	0	0
			2338	1500	386	434	18		

### 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.

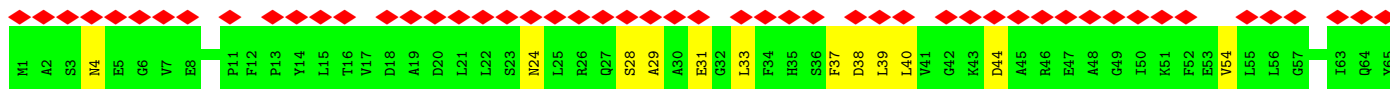
#### • Molecule 1: Major capsid protein



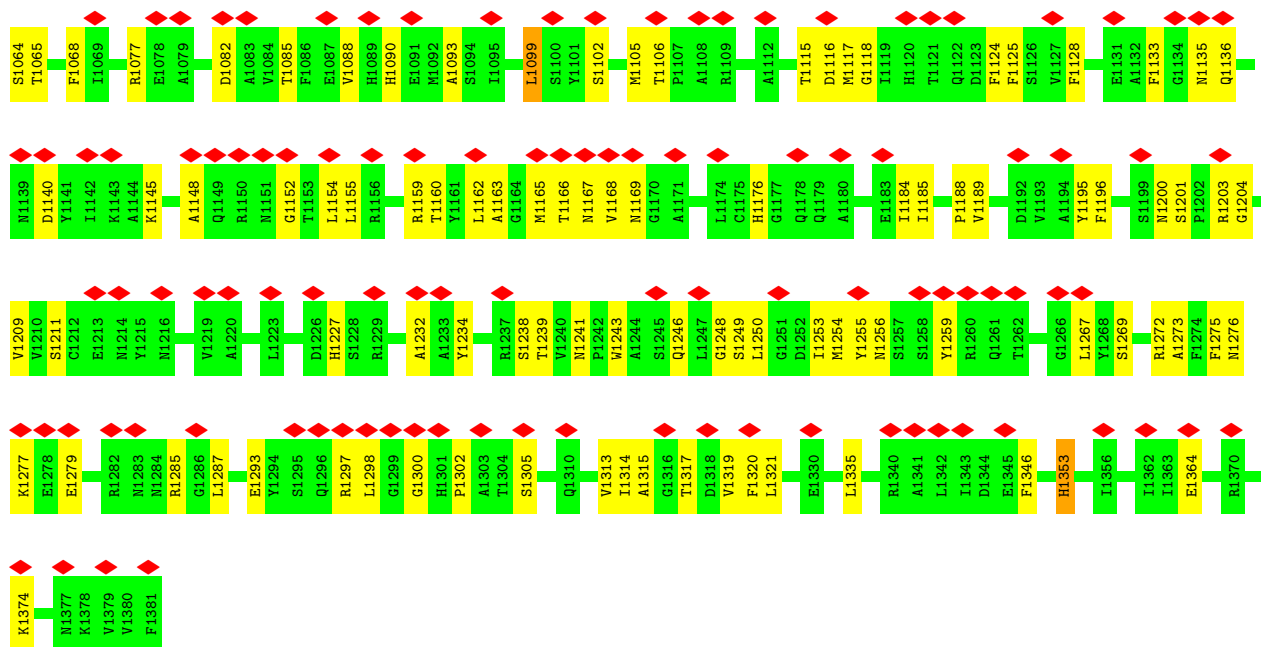


• Molecule 1: Major capsid protein

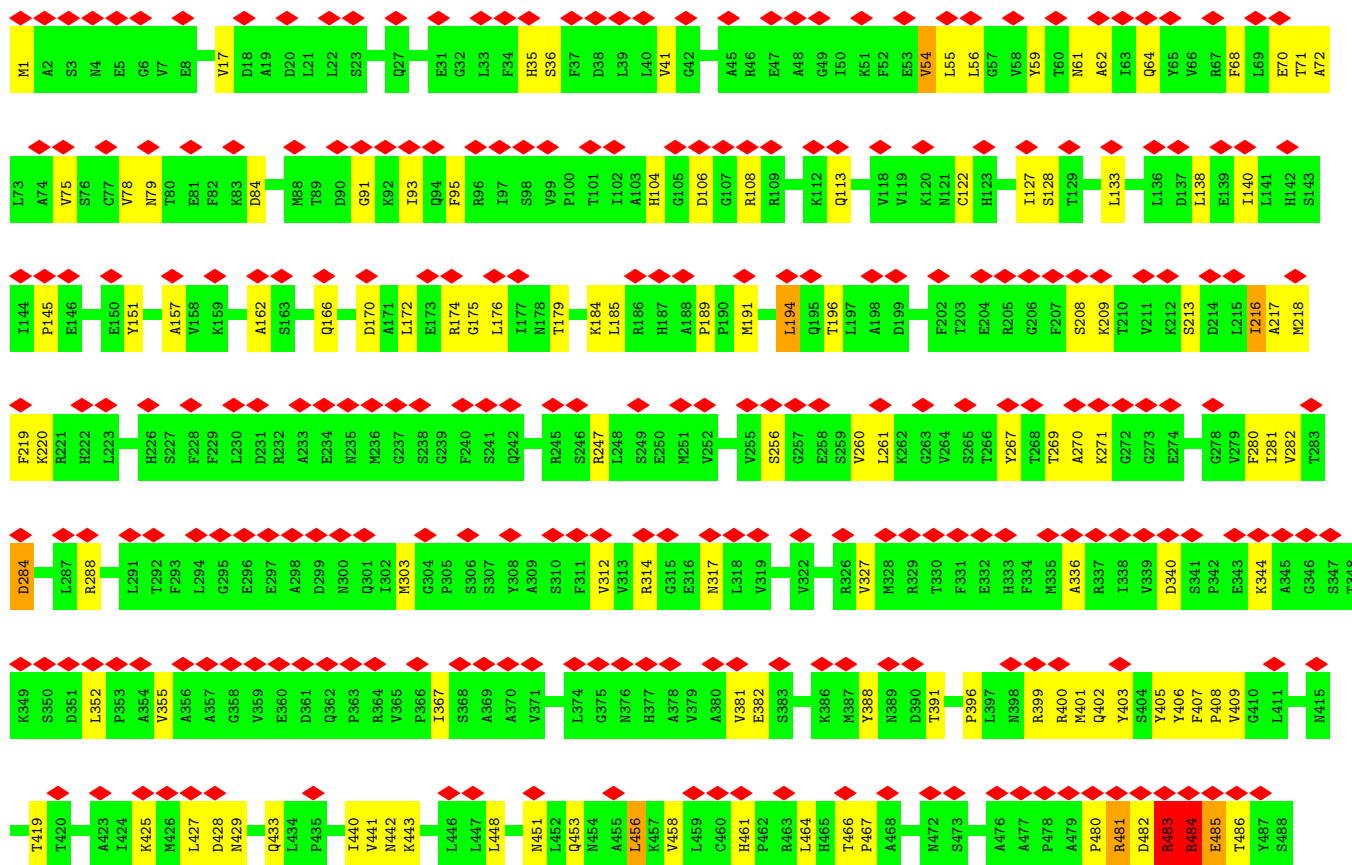
Chain K:



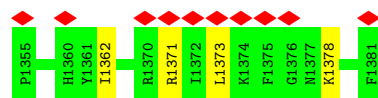




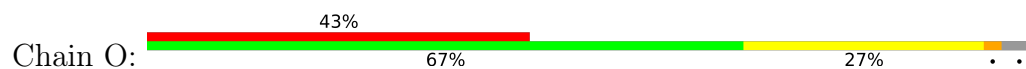
• Molecule 1: Major capsid protein

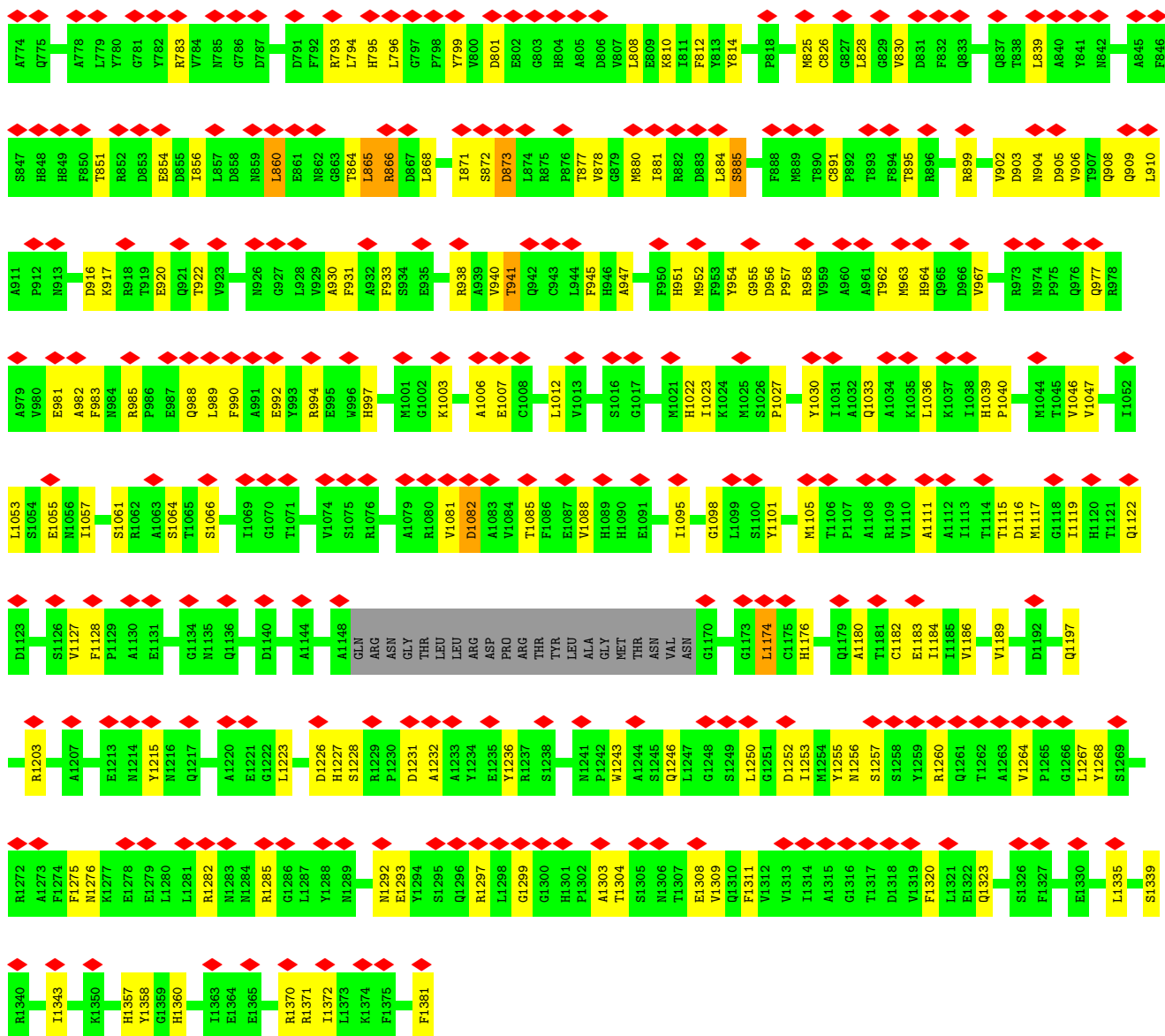


L1286	L1287	Y1288	M1289	E1293	Y1294	S1295	Q1296	R1297	L1298	G1299	G1300	H1301	P1302	A1303	T1304	S1305	M1306	T1307	E1308	F1311	V1312	V1313	L1314	A1315	G1316	T1317	D1318	L1321	E1322	F1327	L1328	Q1329	E1330	A1331	F1332	P1333	A1334	S1335	A1337	S1338	S1339	R1340	D1344	E1345	F1346	M1347	S1348	V1349	K1350	Q1351	T1352	H1353	A1354					
E1221	G1222	L1223	D1226	H1227	S1228	P1229	P1230	D1231	A1232	A1233	Y1236	R1237	S1238	A1239	V1240	N1241	A1244	L1247	L1260	G1261	D1262	I1263	M1264	Y1265	N1266	S1267	S1268	Y1269	R1260	Q1261	T1262	A1263	V1264	P1265	G1266	L1267	Y1268	S1269	P1270	C1271	R1272	A1273	F1274	N1275	K1277	E1278	A1279	L1280	L1281	R1282	N1283	N1284	R1285					
THR	LEU	ARG	ASP	PRO	ARG	THR	TYR	LEU	ALA	GLY	MET	THR	ASN	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	P1202	R1203	G1204	R1205	A1206	A1207	C1208	V1209	V1210	M1214	Y1215	M1216	Q1217	A1220						
D1082	A1083	V1084	T1085	V1088	H1089	H1090	E1091	A1092	A1093	S1094	I1095	D1096	T1097	G1098	L1099	S1100	Y1101	S1102	M1105	T1106	R1109	V1110	A1111	A1112	T1113	T1114	T1115	D1116	M1117	G1118	I1119	Q1122	D1123	F1124	V1127	F1128	P1129	A1130	E1131	G1134	D1140	K1143	A1144	K1145	V1146	G1147	A1148	Q1149	ARG	ASN	GLY							
S1016	G1017	M1018	T1019	V1088	A1020	M1021	I1022	T1023	K1024	M1025	M1028	V1036	T1031	A1032	Q1033	F1034	K1035	L1036	K1037	I1038	H1039	A1043	M1044	V1047	R1048	T1049	D1050	E1051	I1052	L1053	S1054	E1055	N1056	L1057	L1058	F1059	S1060	A1063	S1064	T1065	S1066	M1067	F1068	T1069	G1070	M1073	V1074	S1075	R1076	L1077	E1078	A1079	R1080	V1081				
F953	Y954	G955	R958	V959	A960	A961	T962	H963	H964	Q965	D966	V967	A968	T969	F970	V971	M972	N973	P974	Q975	Q976	Q977	R978	A979	V980	E981	A982	F983	N984	R985	P986	E987	Q988	L989	A990	A991	E992	Y993	R994	E995	W996	H997	R998	S999	M1000	G1002	K1003	Y1004	A1005	A1006	E1007	C1008	L1009	P1010	S1011	L1012	M1013	
T893	F894	T895	R896	A897	V898	R899	V900	S901	V902	D903	N904	V906	T907	Q908	Q909	L910	A911	P912	N913	A914	A915	D916	R917	R918	T919	E920	Q921	T922	V923	L924	N925	N926	Q927	L928	V929	A930	F931	A932	F933	S934	E935	R936	T937	R938	A939	V940	T941	Q942	C943	L944	F945	H946	A947	I948	P949	F950	H951	N952
G829	V830	D831	F832	R833	H834	V835	L839	A840	Y841	N842	G843	P844	A845	Q846	S847	H848	R849	F850	T851	R852	D853	E854	D855	L856	L857	D858	R859	L860	E861	T864	L865	R866	D867	L868	L869	E870	I871	S872	D873	L874	R875	P876	T877	V878	G879	M880	L881	R882	D883	L884	S885	A886	S887	T890	C891	P892		
R765	V766	G767	N768	M769	D770	E771	M772	A773	A774	Q775	A778	L779	Y780	G781	Y782	R783	V784	N785	G786	D787	H788	D789	H790	D791	F792	R793	Y794	H795	L796	Y799	V800	D801	E802	G803	H804	A805	D806	V807	L808	E809	K810	I811	F812	Y813	Y814	L817	P818	R882	T819	N822	A823	H824	M825	C826	L828			
R561	A562	R565	L566	M567	V568	Y569	N570	P574	L575	F580	Q581	E582	A583	R584	Q587	A591	A595	H596	V597	V598	D599	Q600	A601	V602	I603	V606	Q607	D608	T609	A610	Y611	D612	T613	A614	Y615	P616	A617	F618	F619	Y620	V621	V622	E623	A624	M625	H626	G627	G628	F629	E630	F633							
L489	Q490	H491	R492	R493	M494	M495	H496	M497	M498	V501	I502	E505	N509	K510	Y511	A512	A513	P514	D517	I518	K521	C522	G523	L524	P525	T526	E527	N534	Y535	D536	L537	L538	R539	L540	H543	P544	L545	Y546	D547	I548	Y549	I550	G551	R552	D553	A554	G555	E556	R557	A558	R559	H560						

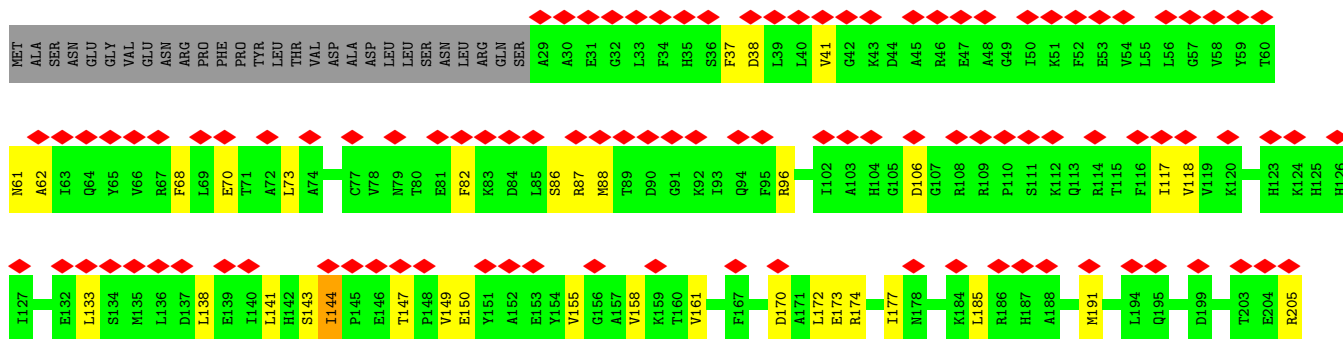


• Molecule 1: Major capsid protein

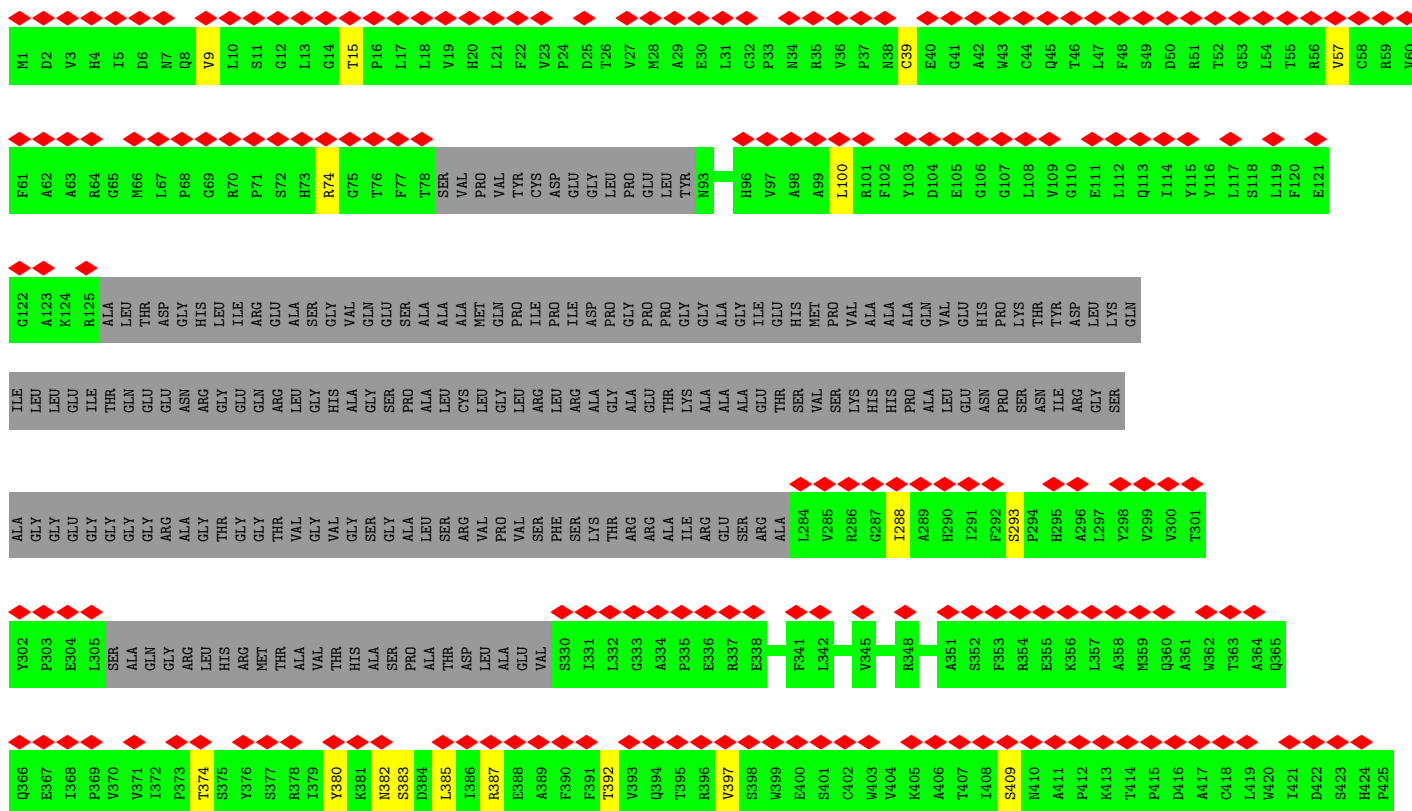




• Molecule 1: Major capsid protein



T969	Q909	H849	T666	V606	P544	R483	K417	LYS	G372	G206
F970	L910	D789	C667	Q607	L545	R484	Y418	ALA	G273	F207
R973	A911	T851	R668	D608	Y546	E485	T419	SER	E274	S208
Q976	N913	D791	H669	T609	D547	E486	T420	THR	T381	K209
Q977	N914	F792	L670	A610	T548	S488	S421	LVS	V282	T210
R978	A915	F793	L671	Y611	Y549	A487	A422	SER	T283	V211
A979	L916	T734	G671	D612	Y550	Q490	A423	LEU	D284	K212
A980	D916	H795	H672	T613	R551	H491	I424	PRO	N285	S213
V980	K917	L736	H673	A614	D553	R492	K425	ALA	V286	N286
E981	R918	L737	L674	T615	A554	R493	A426	VAL	L287	D214
E982	T919	L738	L675	Y616	G555	P494	L427	ALA	R288	L215
F983	E920	T738	S676	F616	E556	R495	D428	ALA	I216	I216
N984	E921	F738	K677	A617	E557	H496	N429	GLY	A217	A217
N985	Q921	D741	L678	F618	R557	H497	P430	VAL	M218	M218
R986	T922	R742	L679	Y619	A558	N498	N431	GLU	F219	F219
F987	E923	A743	S681	Y620	R559	N499	Q432	ASP	F293	K220
Q988	L924	H744	H682	V622	H560	L500	Q433		L294	R221
L989	Y925	Q745	H683	E623	R561	V501	L434		G295	H222
F990	N926	L746	R684	A624	A562	I502	P435		E296	E225
A991	G927	L747	K685	T626	V563	V503	Y436		E297	H226
Y992	L928	L748	L686	L626	H564	D504	E437		A298	H227
Y993	Y929	Q749	Y687	H627	R565	E505	A438		D299	F228
Y994	A930	N750	G688	G628	L566	F506	Y439		M303	F229
Y995	F931	E751	E689	F629	M567	Y507	N444		S306	D231
Y996	A932	Y752	L690	E630	V568	D508	L374		S307	R232
Y997	F933	Y753	L691	E631	G569	N509	G375		Y308	A233
Y998	S934	A754	A692	K632	N570	K510	N445		A309	E234
Y999	E935	D755	L693	F633	L571	Y511	L447		S310	N235
P1000	R936	T756	E694	V634	P572	A512	L448		F311	M236
M1001	T937	L757	Q695	M635	T573	A513	F450		V312	G237
G1002	R938	A758	L697	N636	P574	P514	N451		V313	S238
K1003	A939	L759	M698	V637	A576	V515	N452		R314	G239
Y1004	Y940	A759	M699	P638	P577	T516	N387		G315	F240
A1005	T941	F760	R699	L639	A578	D517	Y388		E316	Y243
A1006	N822	Q761	L700	V640	A579	I518	N389		N317	V244
E1007	A823	F762		S641	F680	A519	D390		L318	R245
C1008	H824	L763	S703	L642	R584	L520	P396		V319	S246
L1009	R825	E764	D704	C643	G585	C522	L397		T320	R247
	M826	V766	V705	T644	Q586	G523	N398		A321	L248
L1012	G827	W766	W706	N645	Q587	L524	P462		V322	S249
V1013	L828	G767	G707	T646	F588	P525	R400		S323	E250
S1014	G829	N768	D708	Y647	E589	T526	M401		Y324	M251
I1015	C830	H769	E709	L648	T590	E527	Y405		G325	V255
S1016	D831	D770	S710	E649	A591	L530	Y406		R326	SER
G1017	F832	E771	W711	R650	T592	H531	Y406		V327	GLY
M1018	Q833	M772	G712	S651	T592	P532	F407		M328	GLU
T1019	H834	A773	Q713	G652	S593	S333	P408		R329	SER
A1020	V835	A774	W714	R653	L594	N534	L411		T330	VAL
A1021	A836	Q775	W715	L654	A595	N534	F412		E332	LEU
M1022	Q837	F776	G716	A655	H596	Y535	M413		H333	GLY
H1023	T838	V777	A717	G655	V597	D536	P414		R337	S265
K1024	L839	L778	L718	F656	V598	L537	A476		D340	T269
M1025	Y841	L779	L719	V657	D599	L538	A477		S341	A270
S1026	N842	W780	D720	N658	Q600	R539	P478		PRO	K271
P1027	G843	T782	F721	S659	A601	L540	A479			
M1028	P844	R783	L723	F660	V602	E541	L542			
A1029	A845	W784	L724	M662	I603	L542	H543			
Y1030	F846	N785	L724	M663	E604	H543	D482			
I1031	S847	G786	V727	K664	T605	H543				
	H848	D787		F665						





[illegible]

- Molecule 4: Large tegument protein deneddylase

Chain v:  99%

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



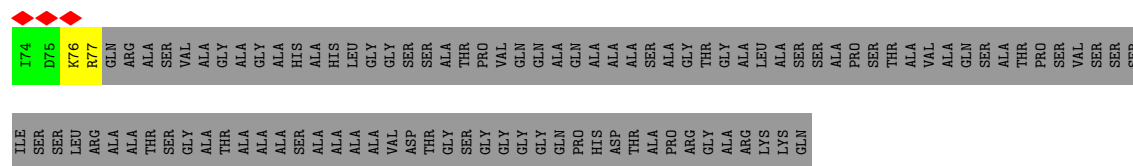




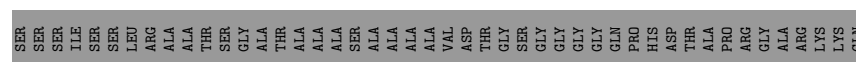
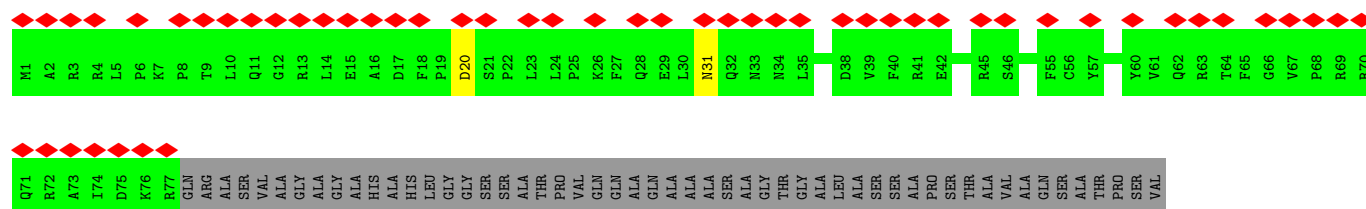


R3121	F3122	V3123	S3124	Q3125	L3126	R3127	R3128	S3129	L3130	E3131	S3132	S3133	T3134	H3135	R3136	T3137	T3138	A3139	D3140	L3141	E3142	R3143	L3144	K3145	F3146	T3147	V3148	L3149
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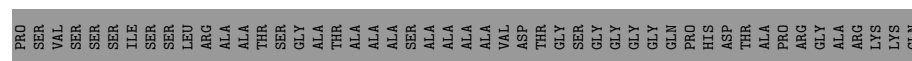
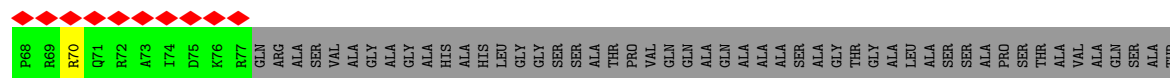
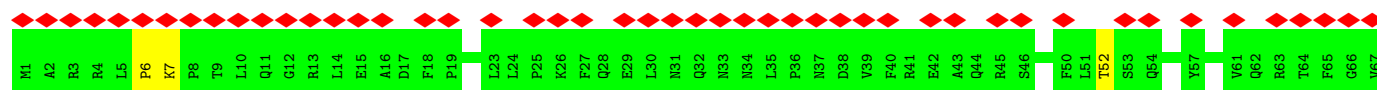
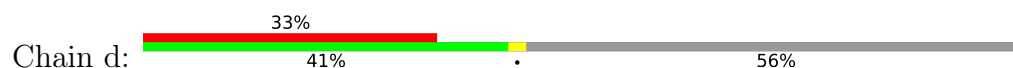
The chart displays 256 elements arranged in 16 groups of 16 elements each. The groups are labeled M1 through M16. Each group contains 16 elements, with some elements highlighted in red and others in green. The elements are labeled M1, A2, R3, P8, T9, L10, Q11, G12, R13, L14, E15, A16, D17, D20, S21, P22, L23, L24, P25, K26, F27, Q28, E29, L30, N31, Q32, N33, N34, L35, D38, R41, E42, S46, Y47, L48, V49, F50, C56, Y57, Y60, V61, Q62, R63, T64, F65, G66, V67, P68, R69, R70, Q71, R72, and so on. The chart shows a complex pattern of red and green elements across the groups.



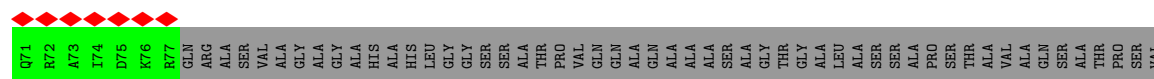
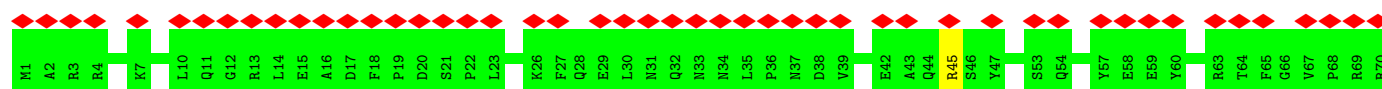
• Molecule 5: Small capsomere-interacting protein



• Molecule 5: Small capsomere-interacting protein

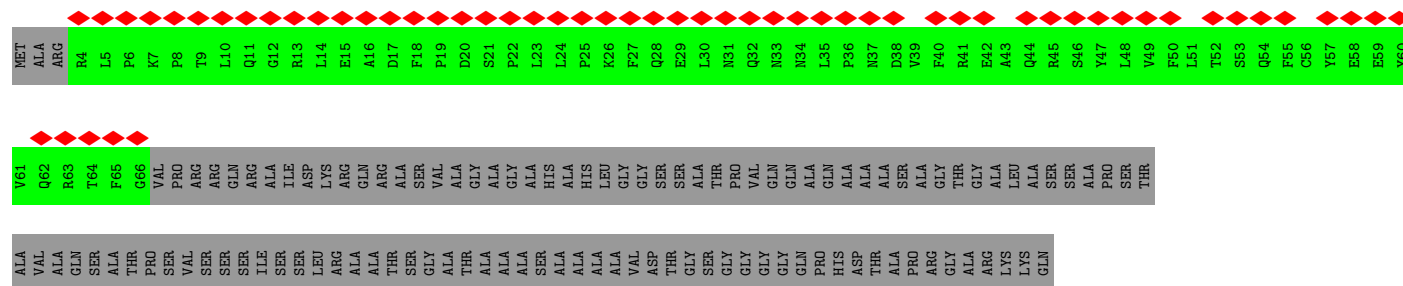


• Molecule 5: Small capsomere-interacting protein

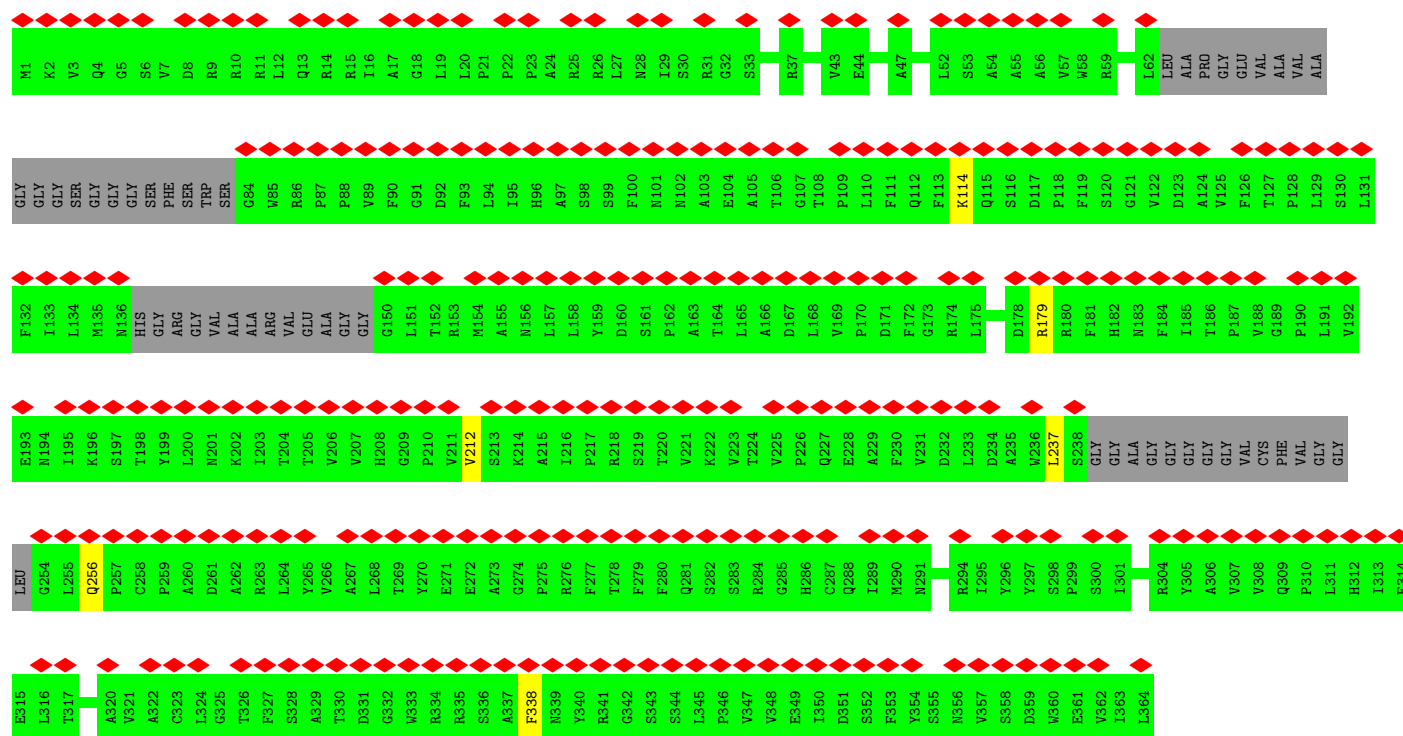
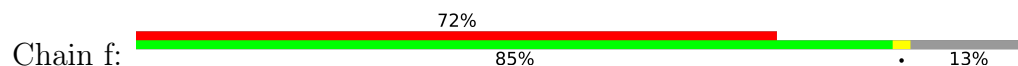


• Molecule 5: Small capsomere-interacting protein

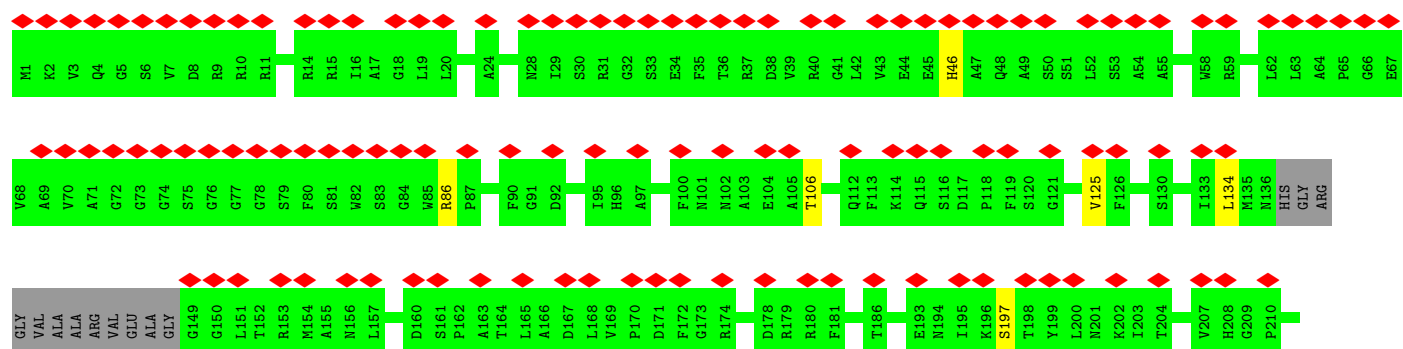
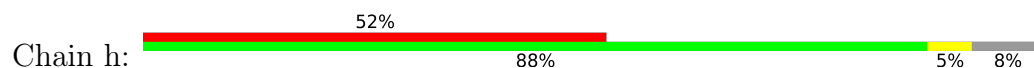


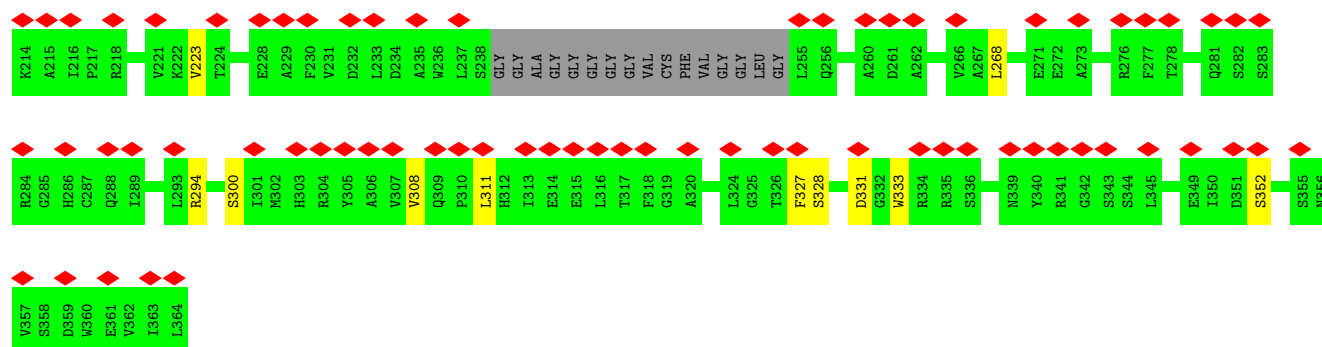


• Molecule 6: Triplex capsid protein 1

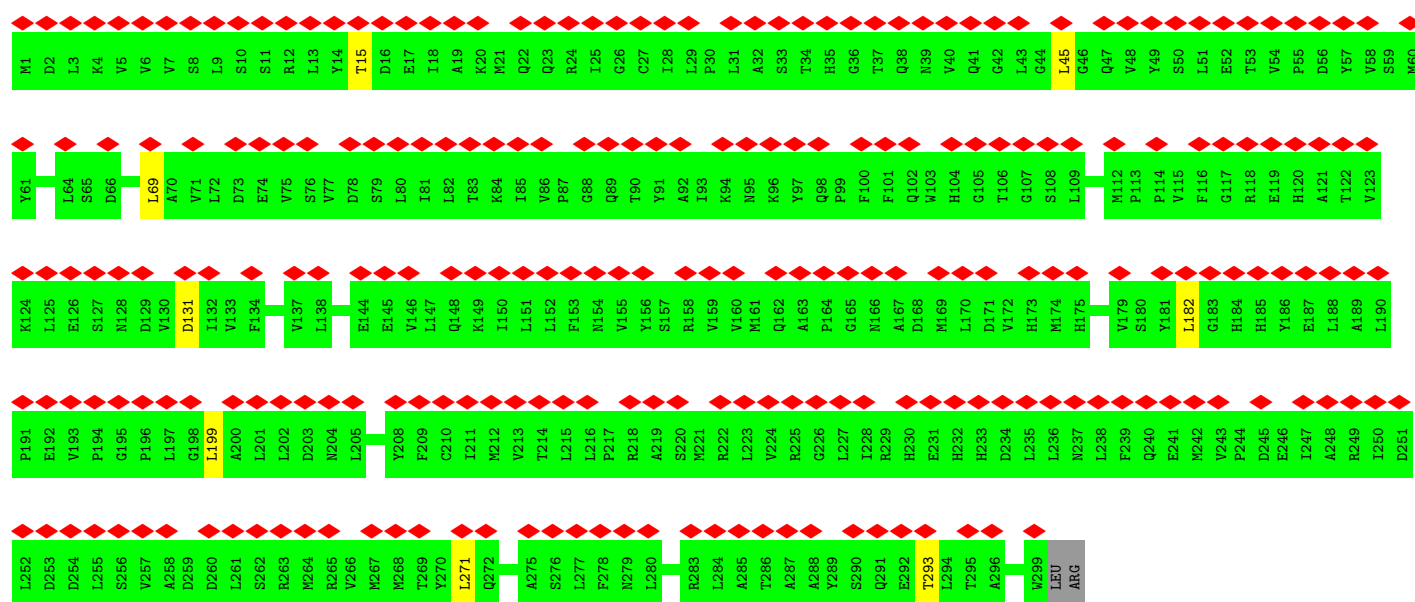
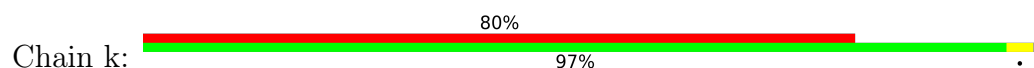


• Molecule 6: Triplex capsid protein 1

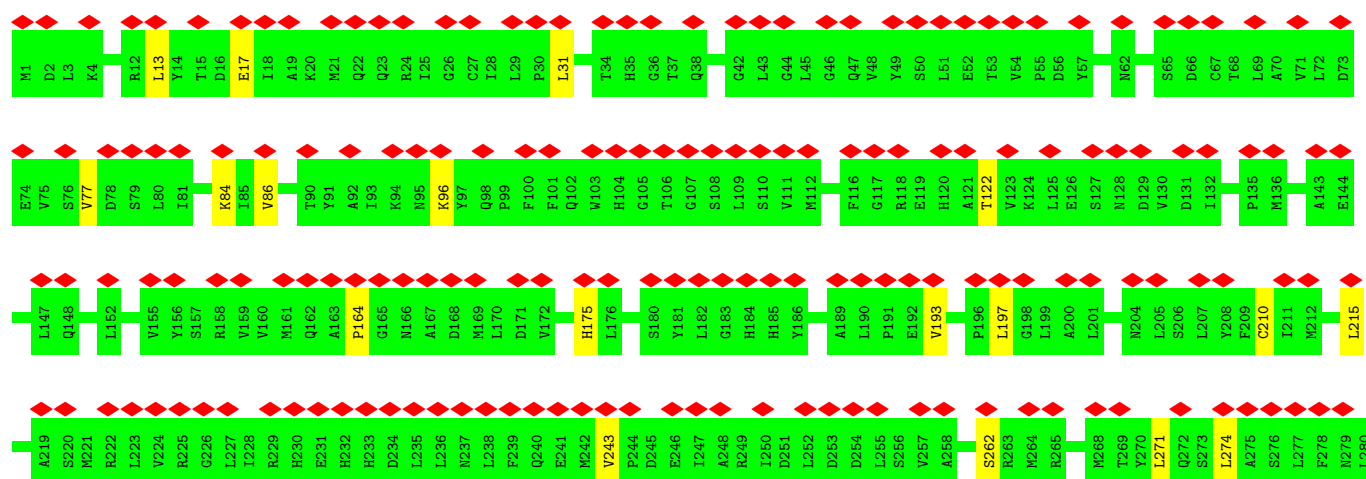




• Molecule 7: Triplex capsid protein 2



• Molecule 7: Triplex capsid protein 2





## 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 ( $\text{\AA}$ )	435.2, 435.2, 435.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.36, 1.36, 1.36	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	J	0.36	0/10877	0.49	0/14781
1	K	0.36	0/11085	0.47	0/15066
1	N	0.34	0/10933	0.47	0/14858
1	O	0.35	0/10693	0.47	0/14531
1	P	0.32	0/10349	0.47	0/14057
2	v	0.32	0/2341	0.48	0/3183
3	w	0.26	0/553	0.41	0/741
3	x	0.30	0/553	0.44	0/741
4	y	0.30	0/320	0.45	0/424
4	z	0.29	0/320	0.45	0/424
5	Z	0.30	0/664	0.42	0/896
5	a	0.31	0/664	0.44	0/896
5	d	0.30	0/664	0.48	0/896
5	e	0.29	0/664	0.45	0/896
5	u	0.30	0/542	0.47	0/735
6	f	0.30	0/2537	0.48	0/3450
6	h	0.34	0/2672	0.48	0/3635
7	k	0.30	0/2388	0.50	0/3254
7	m	0.32	0/2388	0.50	0/3254
7	p	0.29	0/2388	0.50	0/3254
7	r	0.33	0/2388	0.50	0/3254
All	All	0.34	0/75983	0.48	0/103226

There are no bond length outliers.

There are no bond angle outliers.

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	344	0
1	K	10832	0	10655	309	0
1	N	10683	0	10500	345	0
1	O	10447	0	10273	306	0
1	P	10113	0	9949	260	0
2	v	2283	0	2268	0	0
3	w	549	0	540	0	0
3	x	549	0	540	0	0
4	y	317	0	341	0	0
4	z	317	0	341	0	0
5	Z	649	0	649	45	0
5	a	649	0	649	0	0
5	d	649	0	649	0	0
5	e	649	0	649	0	0
5	u	528	0	510	0	0
6	f	2474	0	2459	0	0
6	h	2604	0	2577	0	0
7	k	2338	0	2364	0	0
7	m	2338	0	2364	0	0
7	p	2338	0	2364	0	0
7	r	2338	0	2364	0	0
All	All	74272	0	73453	1530	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 15.

All (1530) 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
1:N:483:ARG:NH1	1:N:485:GLU:HG2	1.25	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: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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:483:ARG:HH11	1:N:485:GLU:CG	1.59	1.15
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:N:484:ARG:NH2	1:N:558:ALA:CB	2.33	0.92
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
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
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
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:K:804:HIS:O	1:K:805:ALA:HB2	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:861:GLU:CB	5:Z:69:ARG:HD2	2.09	0.82
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: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
1:O:245:ARG:NH2	1:O:294:LEU:O	2.13	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
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:O:258:GLU:CG	1:O:262:LYS:HD3	1.93	0.79
1:K:861:GLU:HB2	5:Z:69:ARG:HD2	1.63	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:184:LYS:NZ	1:K:1064:SER:OG	2.14	0.78
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:N:674:ALA:O	1:N:675:ILE:HG12	1.86	0.76
1:O:436:VAL:HG11	1:O:587:GLN:HE22	1.50	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:P:1283:ASN:ND2	1:P:1326:SER:OG	2.19	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
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
1:N:480:PRO:C	1:N:481:ARG:HG2	2.08	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
1:N:674:ALA:C	1:N:675:ILE:HG12	2.08	0.73
1:N:484:ARG:CD	1:N:550:ILE:HG21	2.18	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: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
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
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
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
5:Z:68:PRO:CB	5:Z:71:GLN:HE21	1.98	0.71
1:P:727:VAL:HG22	1:P:924:LEU:HB2	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:941:THR:HA	1:P:944:LEU:O	1.89	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
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:O:401:MET:SD	1:O:403:TYR:OH	2.48	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
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
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: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
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
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
1:O:80:THR:HG22	1:O:309:ALA:HB3	1.75	0.69
1:N:905:ASP:OD1	1:N:905:ASP:N	2.25	0.69
1:J:1061:SER:HG	1:J:1064:SER:HG	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
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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1187:THR:OG1	1:P:1241:ASN:ND2	2.26	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
1:J:834:HIS:HD2	5:Z:8:PRO:HD3	1.60	0.67
1:N:281:ILE:HD12	1:N:1058:LEU:HD23	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
1:J:402:GLN:HG2	1:J:1051:GLU:HG2	1.77	0.67
1:O:475:ASN:HB3	1:O:560:HIS:HD2	1.58	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
1:N:650:ARG:CZ	1:N:873:ASP:OD2	2.43	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
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: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
1:O:630:GLU:OE2	1:O:669:HIS:NE2	2.28	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:743:ALA:HB3	1:K:918:ARG:HH12	1.61	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
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
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: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
1:P:639:LEU:HD13	1:P:880:MET:HB2	1.77	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
1:K:1188:PRO:HD2	1:K:1241:ASN:HB2	1.79	0.64
1:J:1264:VAL:HG12	1:J:1266:GLY:H	1.62	0.64
1:N:677:LYS:O	1:N:678:GLU:C	2.36	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:P:585:GLY:HA3	1:P:1017:GLY:HA2	1.80	0.63
1:K:1051:GLU:N	1:K:1115:THR:OG1	2.31	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
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:705:VAL:HG12	1:O:710:SER:HA	1.80	0.63
1:J:365:VAL:C	1:J:366:PRO:O	2.37	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:P:147:THR:OG1	1:P:150:GLU:OE1	2.16	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: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
1:K:1204:GLY:HA3	1:K:1239:THR:HG23	1.81	0.62
1:J:938:ARG:HA	1:J:941:THR:HG22	1.80	0.62
1:P:1122:GLN:NE2	1:P:1268:TYR:O	2.32	0.62
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
1:O:258:GLU:HA	1:O:262:LYS:HE3	1.82	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
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
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
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:1335:LEU:HD12	1:P:1373:LEU:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:N:480:PRO:O	1:N:481:ARG:CD	2.48	0.61
1:O:68:PHE:O	1:O:71:THR:OG1	2.19	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
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
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
1:O:39:LEU:HB2	1:O:52:PHE:HB2	1.82	0.60
1:O:443:LYS:NZ	1:O:1176:HIS:O	2.23	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
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
1:O:268:THR:OG1	1:O:364:ARG:NH1	2.35	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:288:ARG:NH2	1:O:250:GLU:OE2	2.31	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
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
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:O:184:LYS:HZ3	1:O:1064:SER:HB2	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
1:J:489:LEU:O	1:J:994:ARG:NH2	2.36	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: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
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
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
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
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
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
1:N:674:ALA:C	1:N:675:ILE:CG1	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:736:LEU:O	1:O:740:SER:OG	2.14	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
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
1:O:258:GLU:O	1:O:259:SER:C	2.42	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
1:J:501:VAL:HB	5:Z:1:MET:HE3	1.87	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
1:J:310:SER:O	1:J:311:PHE:CD1	2.57	0.57
1:J:1183:GLU:OE2	1:J:1269:SER:OG	2.17	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
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
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
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
1:O:952:MET:HE1	1:O:981:GLU:HA	1.85	0.57
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:68:PHE:N	1:P:173:GLU:OE1	2.37	0.56
1:J:185:LEU:HD13	1:J:399:ARG:HH21	1.70	0.56
1:J:310:SER:C	1:J:311:PHE:CD1	2.79	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:969:THR:O	1:N:973:ARG:HG2	2.06	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
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: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
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
1:J:922:THR:HG21	1:J:989:LEU:O	2.06	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
1:N:990:PHE:CE2	1:N:992:GLU:HG2	2.41	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
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
1:N:400:ARG:HH11	1:N:1305:SER:HB3	1.72	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
1:J:69:LEU:CD1	1:J:308:TYR:CG	2.90	0.55
1:O:576:ALA:HB1	1:O:580:PHE:HD2	1.72	0.55
1:O:667:CYS:O	1:O:680:TYR:OH	2.20	0.55
1:P:494:PRO:O	1:P:750:ASN:ND2	2.39	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: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
1:J:92:LYS:HD2	1:J:120:LYS:H	1.72	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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
1:N:72:ALA:HB3	1:N:382:GLU:HB2	1.90	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: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: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
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:P:251:MET:SD	1:P:1106:THR:OG1	2.66	0.53
1:J:388:TYR:CE2	1:J:396:PRO:HD3	2.43	0.53
1:J:805:ALA:HA	1:K:972:MET:HE1	1.89	0.53
1:K:951:HIS:O	1:K:955:GLY:N	2.42	0.53
1:O:825:MET:N	1:O:956:ASP:OD2	2.30	0.53
1:P:207:PHE:C	1:P:209:LYS:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:N:441:VAL:HG11	1:N:1373:LEU:HD22	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:399:ARG:HG3	1:N:1105:MET:HE1	1.90	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:P:906:VAL:HG11	1:P:1135:ASN:H	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:N:672:ASN:HD21	1:O:871:ILE:C	2.07	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
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:934:SER:HB3	1:K:937:THR:OG1	2.10	0.52
1:N:644:ILE:HG22	1:N:675:ILE:CG2	2.32	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: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
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
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
5:Z:68:PRO:C	5:Z:70:ARG:N	2.60	0.52
1:J:481:ARG:N	1:J:481:ARG:HD3	2.25	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
1:J:255:VAL:HG11	1:J:1102:SER:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:1013:VAL:O	1:N:1016:SER:OG	2.25	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
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: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
1:P:500:LEU:HD13	1:P:946:HIS:CG	2.45	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:937:THR:O	1:P:941:THR:HG23	2.10	0.51
1:J:419:THR:OG1	1:J:420:THR:N	2.44	0.51
1:K:461:HIS:CD2	1:K:1124:PHE:HB3	2.46	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
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:K:487:TYR:HH	1:K:985:ARG:H	1.59	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
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:P:225:GLU:O	1:P:1370:ARG:NH1	2.43	0.51
1:J:622:VAL:HG21	1:J:639:LEU:HD21	1.92	0.51
1:P:415:ASN:HD21	1:P:579:ALA:HB3	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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: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:271:LYS:HB3	1:K:299:ASP:CG	2.31	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
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:813:TYR:O	1:N:954:TYR:OH	2.12	0.50
1:N:1348:SER:OG	1:N:1349:VAL:N	2.45	0.50
1:O:258:GLU:C	1:O:259:SER:O	2.49	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:959:VAL:O	1:P:962:THR:OG1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:P:981:GLU:OE1	1:P:999:SER:HA	2.12	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: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
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:N:35:HIS:O	1:N:36:SER:OG	2.29	0.49
1:P:879:GLY:O	1:P:882:ARG:NE	2.44	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: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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:399:ARG:CD	1:O:1320:PHE:HB3	2.42	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: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: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
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
5:Z:68:PRO:O	5:Z:69:ARG:C	2.50	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
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
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:531:HIS:CG	1:P:532:PRO:HD2	2.48	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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:677:LYS:C	1:N:679:ALA:N	2.63	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
1:J:824:HIS:HD1	1:J:956:ASP:CG	2.15	0.48
1:K:548:ILE:HD12	1:K:561:ARG:O	2.13	0.48
1:K:861:GLU:CD	5:Z:67:VAL:HG11	2.34	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
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:P:61:ASN:OD1	1:P:62:ALA:N	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
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:560:HIS:HD1	1:K:560:HIS:H	1.60	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: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
1:J:69:LEU:HD13	1:J:308:TYR:CZ	2.47	0.47
1:O:483:ARG:HE	1:O:550:ILE:HG21	1.78	0.47
1:J:203:THR:HB	1:J:207:PHE:HE1	1.79	0.47
1:K:184:LYS:HZ3	1:K:1064:SER:HG	1.55	0.47
1:K:813:TYR:O	1:K:954:TYR:OH	2.22	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:884:LEU:O	1:K:887:SER:OG	2.20	0.47
1:O:854:GLU:O	1:O:878:VAL:HG23	2.15	0.47
1:P:723:LEU:HB3	1:P:810:LYS:HZ2	1.79	0.47
1:K:1045:THR:OG1	1:K:1185:ILE:HB	2.14	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
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
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
1:J:128:SER:HA	1:J:1088:VAL:O	2.15	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: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
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:N:176:LEU:O	1:N:179:THR:OG1	2.30	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
5:Z:68:PRO:C	5:Z:70:ARG:H	2.18	0.47
1:J:283:THR:HG22	1:J:395:TYR:HE2	1.79	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
1:N:1347:MET:HE2	1:N:1378:LYS:HG3	1.97	0.47
1:O:977:GLN:HE21	1:O:983:PHE:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:826:CYS:HA	1:N:954:TYR:O	2.15	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
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: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
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
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
1:J:877:THR:H	1:J:880:MET:HE2	1.80	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: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
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
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
5:Z:76:LYS:HD2	5:Z:77:ARG:H	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:636:ASN:O	1:O:640:VAL:HG13	2.16	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: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
1:J:289:GLN:O	1:J:292:THR:OG1	2.27	0.45
1:J:789:ASP:OD2	5:Z:1:MET:N	2.43	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:K:184:LYS:HZ3	1:K:1065:THR:HG23	1.81	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
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
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:P:1027:PRO:HG2	1:P:1133:PHE:CZ	2.50	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:843:GLY:O	1:P:846:PHE:N	2.49	0.45
1:J:978:ARG:HB3	1:O:698:MET:SD	2.56	0.45
1:J:978:ARG:H	1:O:698:MET:HE3	1.80	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: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

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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:828:LEU:HD13	1:J:963:MET:HE2	1.98	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
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
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
5:Z:68:PRO:HB2	5:Z:71:GLN:HB2	1.99	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:H	2.20	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
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:N:401:MET:HE3	1:N:403:TYR:HE1	1.82	0.44
1:N:481:ARG:HB3	1:N:550:ILE:HD13	1.98	0.44
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
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:K:806:ASP:O	1:K:807:VAL:C	2.55	0.44
1:N:55:LEU:HD23	1:N:55:LEU:HA	1.87	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
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: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: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
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

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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:P:586:GLN:HG2	1:P:1013:VAL:HG13	1.99	0.44
1:J:95:PHE:HD1	1:J:95:PHE:HA	1.59	0.44
1:J:266:THR:C	1:J:305:PRO:HG3	2.38	0.44
1:J:581:GLN:CB	1:J:1021:MET:HE2	2.48	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:409:VAL:HG11	1:N:1044:MET:HE2	1.99	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:488:SER:C	1:P:991:ALA:HB1	2.38	0.44
1:P:515:VAL:HG11	1:P:976:GLN:NE2	2.33	0.44
1:J:300:ASN:HB3	1:J:369:ALA:O	2.17	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
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
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:J:934:SER:O	1:J:937:THR:OG1	2.34	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
1:O:131:MET:HE3	1:O:1088:VAL:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:216:ILE:HA	1:J:219:PHE:CD2	2.53	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: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
5:Z:68:PRO:HB2	5:Z:71:GLN:NE2	2.19	0.44
1:J:209:LYS:NZ	1:O:1308:GLU:OE2	2.47	0.43
1:J:511:TYR:O	1:J:973:ARG:NH2	2.51	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
1:P:1132:ALA:HB1	1:P:1139:ASN:CG	2.39	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
1:N:612:ASP:C	1:N:614:ALA:H	2.22	0.43
1:N:1255:TYR:HB2	1:N:1275:PHE:CD2	2.50	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1378:LYS:H	1:P:1378:LYS:HD3	1.83	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
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
1:J:92:LYS:HB3	1:J:120:LYS:O	2.19	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: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
1:J:632:LYS:HZ1	1:J:887:SER:HB2	1.84	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:143:SER:OG	1:P:144:ILE:N	2.52	0.43
1:P:439:TRP:NE1	1:P:1340:ARG:HB2	2.34	0.43
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:K:711:VAL:HB	1:K:1028:MET:HE1	2.01	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
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:1353:HIS:CE1	1:K:1364:GLU:OE2	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:J:69:LEU:HD21	1:J:79:ASN:ND2	2.34	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
1:P:215:LEU:HD23	1:P:215:LEU:HA	1.98	0.42
1:P:723:LEU:O	1:P:810:LYS:NZ	2.40	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: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
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: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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
1:J:660:PHE:N	1:J:813:TYR:OH	2.40	0.42
1:J:824:HIS:HA	1:J:956:ASP:CG	2.39	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:P:1203:ARG:H	1:P:1203:ARG:HG3	1.52	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
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
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:539:ARG:O	1:K:540:LEU:HD23	2.20	0.42
1:J:471:LEU:HD12	1:J:912:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:630:GLU:CD	1:K:665:PHE:HE1	2.24	0.42
1:N:54:VAL:HA	1:O:327:VAL:O	2.20	0.42
1:N:602:VAL:O	1:N:606:VAL:HG23	2.20	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
5:Z:69:ARG:HG3	5:Z:69:ARG:O	2.20	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
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:652:GLY:C	1:K:653:ARG:HD3	2.41	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:758:ALA:HB1	1:P:762:PHE:CD1	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:482:ASP:CG	1:J:484:ARG:HE	2.23	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:542:LEU:HD23	1:P:1248:GLY:C	2.41	0.41
1:P:746:ILE:HG23	1:P:900:VAL:HG22	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
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: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: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:O:280:PHE:CE2	1:O:379:VAL:HG11	2.55	0.41
1:O:399:ARG:HG3	1:O:1105:MET:HE1	2.03	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1053:LEU:HA	1:J:1053:LEU:HD23	1.77	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:1119:ILE:H	1:N:1119:ILE:HG13	1.67	0.41
1:O:469:HIS:HB3	1:O:1253:ILE:HD12	2.02	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
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:N:987:GLU:H	1:N:987:GLU:HG3	1.72	0.41
1:O:616:PRO:HB3	1:O:872:SER:HB3	2.02	0.41
1:O:1267:LEU:HD23	1:O:1267:LEU:HA	1.81	0.41
1:J:38:ASP:OD1	1:J:39:LEU:N	2.54	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: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:1077:ARG:O	1:N:1085:THR:OG1	2.26	0.41
1:N:1188:PRO:HD2	1:N:1241:ASN:HB3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1292:ASN:HA	1:P:1295:SER:OG	2.20	0.41
1:J:453:GLN:HA	1:J:456:LEU:HD22	2.01	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:O:68:PHE:HA	1:O:177:ILE:HD11	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:J:73:LEU:HD13	1:J:177:ILE:HD11	2.03	0.40
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: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
1:J:245:ARG:HA	1:J:245:ARG:HD2	1.94	0.40
1:K:356:ALA:C	1:K:358:GLY:H	2.24	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:899:ARG:HH21	1:N:920:GLU:CD	2.24	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:43:LYS:C	1:P:314:ARG:HH12	2.25	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
1:J:251:MET:HE3	1:J:251:MET:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:432:GLN:CD	1:J:586:GLN:HG3	2.42	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: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: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: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:O:1257:SER:HB3	1:O:1276:ASN:CG	2.42	0.40
1:P:86:SER:OG	1:P:87:ARG:NH2	2.54	0.40
1:P:191:MET:HE2	1:P:251:MET:HA	2.04	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:Z:68:PRO:HB3	5:Z:71:GLN:CD	2.20	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:K:893:THR:OG1	1:K:894:PHE:N	2.54	0.40
1:N:352:LEU:HD23	1:N:352:LEU:HA	1.83	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
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: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

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	1348/1381 (98%)	1269 (94%)	72 (5%)	7 (0%)	29	67
1	K	1379/1381 (100%)	1310 (95%)	67 (5%)	2 (0%)	51	84
1	N	1358/1381 (98%)	1288 (95%)	62 (5%)	8 (1%)	25	63
1	O	1328/1381 (96%)	1259 (95%)	68 (5%)	1 (0%)	51	84
1	P	1273/1381 (92%)	1202 (94%)	69 (5%)	2 (0%)	47	79
2	v	282/507 (56%)	262 (93%)	19 (7%)	1 (0%)	34	71
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%)	5	34
5	a	75/176 (43%)	70 (93%)	5 (7%)	0	100	100
5	d	75/176 (43%)	69 (92%)	4 (5%)	2 (3%)	5	34
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	k	297/301 (99%)	282 (95%)	14 (5%)	1 (0%)	41	75
7	m	297/301 (99%)	282 (95%)	13 (4%)	2 (1%)	22	61
7	p	297/301 (99%)	282 (95%)	10 (3%)	5 (2%)	9	43
7	r	297/301 (99%)	288 (97%)	8 (3%)	1 (0%)	41	75
All	All	9356/17662 (53%)	8851 (95%)	471 (5%)	34 (0%)	38	71

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
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

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Mol	Chain	Res	Type
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%)	1092 (95%)	57 (5%)	24	52
1	K	1171/1171 (100%)	1126 (96%)	45 (4%)	33	59
1	N	1155/1171 (99%)	1102 (95%)	53 (5%)	27	54
1	O	1128/1171 (96%)	1080 (96%)	48 (4%)	29	56
1	P	1093/1171 (93%)	1058 (97%)	35 (3%)	39	62
2	v	243/400 (61%)	227 (93%)	16 (7%)	16	45
3	w	57/465 (12%)	57 (100%)	0	100	100
3	x	57/465 (12%)	57 (100%)	0	100	100
4	y	35/2539 (1%)	34 (97%)	1 (3%)	42	65
4	z	35/2539 (1%)	34 (97%)	1 (3%)	42	65
5	Z	71/128 (56%)	70 (99%)	1 (1%)	67	81
5	a	71/128 (56%)	69 (97%)	2 (3%)	43	65
5	d	71/128 (56%)	69 (97%)	2 (3%)	43	65
5	e	71/128 (56%)	70 (99%)	1 (1%)	67	81
5	u	59/128 (46%)	59 (100%)	0	100	100
6	f	267/289 (92%)	261 (98%)	6 (2%)	52	71
6	h	278/289 (96%)	261 (94%)	17 (6%)	18	47
7	k	265/267 (99%)	258 (97%)	7 (3%)	46	67
7	m	265/267 (99%)	248 (94%)	17 (6%)	17	45
7	p	265/267 (99%)	252 (95%)	13 (5%)	25	52
7	r	265/267 (99%)	256 (97%)	9 (3%)	37	61
All	All	8071/14549 (56%)	7740 (96%)	331 (4%)	34	57

All (331) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	5	GLU
1	J	39	LEU
1	J	66	VAL
1	J	89	THR
1	J	95	PHE
1	J	101	THR
1	J	129	THR
1	J	144	ILE
1	J	147	THR
1	J	165	LEU
1	J	203	THR
1	J	216	ILE
1	J	248	LEU
1	J	255	VAL
1	J	259	SER
1	J	287	LEU
1	J	306	SER
1	J	308	TYR
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
1	J	481	ARG
1	J	518	ILE
1	J	536	ASP
1	J	602	VAL
1	J	639	LEU
1	J	641	SER
1	J	657	VAL
1	J	675	ILE
1	J	706	VAL
1	J	710	SER
1	J	716	CYS
1	J	847	SER
1	J	851	THR
1	J	853	ASP
1	J	861	GLU
1	J	928	LEU
1	J	1065	THR

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Mol	Chain	Res	Type
1	J	1066	SER
1	J	1094	SER
1	J	1106	THR
1	J	1156	ARG
1	J	1161	TYR
1	J	1182	CYS
1	J	1189	VAL
1	J	1192	ASP
1	J	1199	SER
1	J	1209	VAL
1	J	1223	LEU
1	J	1262	THR
1	J	1269	SER
1	J	1312	VAL
1	J	1313	VAL
1	K	39	LEU
1	K	54	VAL
1	K	96	ARG
1	K	147	THR
1	K	179	THR
1	K	182	SER
1	K	232	ARG
1	K	291	LEU
1	K	314	ARG
1	K	361	ASP
1	K	381	VAL
1	K	440	ILE
1	K	451	ASN
1	K	486	THR
1	K	517	ASP
1	K	526	THR
1	K	589	GLU
1	K	602	VAL
1	K	637	VAL
1	K	653	ARG
1	K	654	LEU
1	K	690	LEU
1	K	693	LEU
1	K	697	LEU
1	K	711	VAL
1	K	742	ARG
1	K	794	LEU

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Mol	Chain	Res	Type
1	K	851	THR
1	K	874	LEU
1	K	905	ASP
1	K	907	THR
1	K	928	LEU
1	K	964	HIS
1	K	1018	MET
1	K	1048	ARG
1	K	1049	THR
1	K	1054	SER
1	K	1099	LEU
1	K	1168	VAL
1	K	1189	VAL
1	K	1209	VAL
1	K	1238	SER
1	K	1267	LEU
1	K	1305	SER
1	K	1353	HIS
1	N	17	VAL
1	N	41	VAL
1	N	54	VAL
1	N	113	GLN
1	N	194	LEU
1	N	213	SER
1	N	216	ILE
1	N	284	ASP
1	N	355	VAL
1	N	381	VAL
1	N	419	THR
1	N	425	LYS
1	N	456	LEU
1	N	482	ASP
1	N	483	ARG
1	N	484	ARG
1	N	485	GLU
1	N	486	THR
1	N	489	LEU
1	N	501	VAL
1	N	550	ILE
1	N	598	VAL
1	N	637	VAL
1	N	657	VAL

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Mol	Chain	Res	Type
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	736	LEU
1	N	740	SER
1	N	769	MET
1	N	813	TYR
1	N	853	ASP
1	N	905	ASP
1	N	925	VAL
1	N	933	PHE
1	N	938	ARG
1	N	950	PHE
1	N	1044	MET
1	N	1048	ARG
1	N	1099	LEU
1	N	1116	ASP
1	N	1124	PHE
1	N	1201	SER
1	N	1209	VAL
1	N	1256	ASN
1	N	1287	LEU
1	N	1336	SER
1	N	1347	MET
1	N	1352	THR
1	O	47	GLU
1	O	52	PHE
1	O	84	ASP
1	O	88	MET
1	O	104	HIS
1	O	136	LEU
1	O	137	ASP
1	O	147	THR
1	O	194	LEU
1	O	197	LEU
1	O	216	ILE
1	O	230	LEU
1	O	256	SER

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Mol	Chain	Res	Type
1	O	258	GLU
1	O	259	SER
1	O	260	VAL
1	O	261	LEU
1	O	279	VAL
1	O	294	LEU
1	O	313	VAL
1	O	466	THR
1	O	592	THR
1	O	598	VAL
1	O	602	VAL
1	O	637	VAL
1	O	653	ARG
1	O	654	LEU
1	O	657	VAL
1	O	681	SER
1	O	700	LEU
1	O	851	THR
1	O	860	LEU
1	O	865	LEU
1	O	866	ARG
1	O	873	ASP
1	O	885	SER
1	O	940	VAL
1	O	941	THR
1	O	1053	LEU
1	O	1082	ASP
1	O	1116	ASP
1	O	1174	LEU
1	O	1183	GLU
1	O	1189	VAL
1	O	1282	ARG
1	O	1309	VAL
1	O	1335	LEU
1	O	1343	ILE
1	P	144	ILE
1	P	149	VAL
1	P	210	THR
1	P	211	VAL
1	P	227	SER
1	P	247	ARG
1	P	284	ASP

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Mol	Chain	Res	Type
1	P	293	PHE
1	P	319	VAL
1	P	333	HIS
1	P	597	VAL
1	P	598	VAL
1	P	675	ILE
1	P	756	THR
1	P	769	MET
1	P	796	LEU
1	P	813	TYR
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	1058	LEU
1	P	1071	THR
1	P	1106	THR
1	P	1110	VAL
1	P	1189	VAL
1	P	1203	ARG
1	P	1210	VAL
1	P	1260	ARG
1	P	1349	VAL
1	P	1378	LYS
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	288	ILE
2	v	293	SER
2	v	374	THR
2	v	380	TYR
2	v	383	SER
2	v	385	LEU
2	v	387	ARG
2	v	392	THR

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Mol	Chain	Res	Type
2	v	397	VAL
2	v	409	SER
4	y	3137	LEU
4	z	3114	GLN
5	Z	69	ARG
5	a	20	ASP
5	a	31	ASN
5	d	52	THR
5	d	70	ARG
5	e	45	ARG
6	f	114	LYS
6	f	179	ARG
6	f	212	VAL
6	f	237	LEU
6	f	256	GLN
6	f	338	PHE
6	h	46	HIS
6	h	86	ARG
6	h	106	THR
6	h	125	VAL
6	h	134	LEU
6	h	197	SER
6	h	223	VAL
6	h	268	LEU
6	h	294	ARG
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	131	ASP
7	k	182	LEU
7	k	199	LEU
7	k	271	LEU
7	k	293	THR
7	m	13	LEU
7	m	17	GLU

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Mol	Chain	Res	Type
7	m	31	LEU
7	m	77	VAL
7	m	84	LYS
7	m	86	VAL
7	m	96	LYS
7	m	122	THR
7	m	175	HIS
7	m	193	VAL
7	m	210	CYS
7	m	215	LEU
7	m	243	VAL
7	m	262	SER
7	m	271	LEU
7	m	274	LEU
7	m	293	THR
7	p	3	LEU
7	p	21	MET
7	p	27	CYS
7	p	45	LEU
7	p	54	VAL
7	p	98	GLN
7	p	101	PHE
7	p	148	GLN
7	p	182	LEU
7	p	197	LEU
7	p	199	LEU
7	p	202	LEU
7	p	245	ASP
7	r	3	LEU
7	r	27	CYS
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	293	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (161) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	35	HIS

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Mol	Chain	Res	Type
1	J	79	ASN
1	J	121	ASN
1	J	126	HIS
1	J	195	GLN
1	J	285	ASN
1	J	389	ASN
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	859	ASN
1	J	862	ASN
1	J	921	GLN
1	J	984	ASN
1	J	997	HIS
1	J	1022	HIS
1	J	1090	HIS
1	J	1176	HIS
1	J	1241	ASN
1	J	1292	ASN
1	J	1301	HIS
1	K	79	ASN
1	K	94	GLN
1	K	104	HIS
1	K	126	HIS
1	K	142	HIS
1	K	289	GLN
1	K	301	GLN
1	K	317	ASN
1	K	385	GLN
1	K	398	ASN
1	K	444	ASN
1	K	496	HIS
1	K	531	HIS
1	K	543	HIS
1	K	564	HIS
1	K	570	ASN

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Mol	Chain	Res	Type
1	K	722	ASN
1	K	822	ASN
1	K	904	ASN
1	K	951	HIS
1	K	984	ASN
1	K	997	HIS
1	K	1137	GLN
1	K	1167	ASN
1	K	1256	ASN
1	K	1284	ASN
1	K	1289	ASN
1	N	79	ASN
1	N	104	HIS
1	N	126	HIS
1	N	317	ASN
1	N	402	GLN
1	N	444	ASN
1	N	491	HIS
1	N	496	HIS
1	N	531	HIS
1	N	534	ASN
1	N	543	HIS
1	N	587	GLN
1	N	596	HIS
1	N	824	HIS
1	N	834	HIS
1	N	908	GLN
1	N	926	ASN
1	N	965	GLN
1	N	974	ASN
1	N	997	HIS
1	N	1033	GLN
1	N	1169	ASN
1	N	1276	ASN
1	N	1310	GLN
1	N	1353	HIS
1	O	79	ASN
1	O	125	HIS
1	O	317	ASN
1	O	333	HIS
1	O	432	GLN
1	O	465	HIS

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Mol	Chain	Res	Type
1	O	496	HIS
1	O	531	HIS
1	O	581	GLN
1	O	587	GLN
1	O	695	GLN
1	O	824	HIS
1	O	909	GLN
1	O	977	GLN
1	O	997	HIS
1	O	1033	GLN
1	O	1176	HIS
1	O	1351	GLN
1	P	222	HIS
1	P	226	HIS
1	P	415	ASN
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	735	HIS
1	P	750	ASN
1	P	837	GLN
1	P	842	ASN
1	P	908	GLN
1	P	942	GLN
1	P	964	HIS
1	P	977	GLN
1	P	984	ASN
1	P	1120	HIS
1	P	1178	GLN
1	P	1241	ASN
1	P	1283	ASN
2	v	7	ASN
2	v	34	ASN
2	v	45	GLN
2	v	290	HIS
2	v	295	HIS
2	v	382	ASN
2	v	394	GLN
4	y	3114	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	z	3114	GLN
5	Z	11	GLN
5	Z	54	GLN
5	Z	71	GLN
5	a	44	GLN
5	e	31	ASN
5	e	54	GLN
5	u	11	GLN
6	f	102	ASN
6	f	303	HIS
6	h	13	GLN
6	h	28	ASN
6	h	46	HIS
6	h	182	HIS
6	h	288	GLN
6	h	291	ASN
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	230	HIS
7	m	233	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	r	128	ASN
7	r	162	GLN
7	r	184	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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.

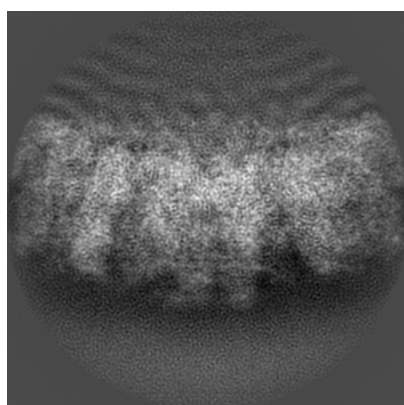
## 6 Map visualisation [i](#)

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.

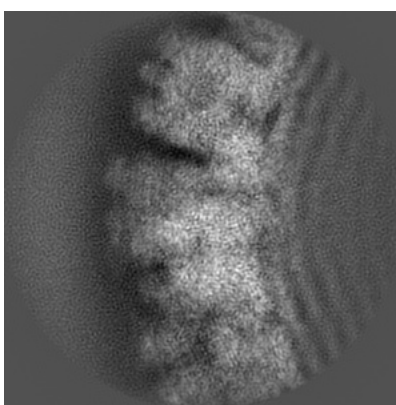
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

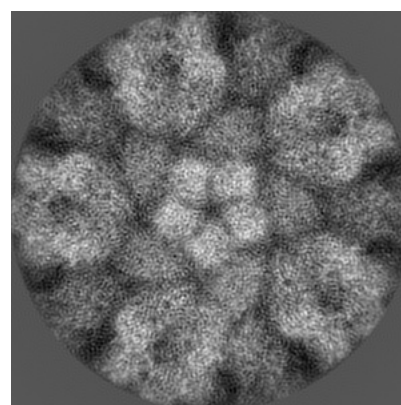
#### 6.1.1 Primary map



X



Y

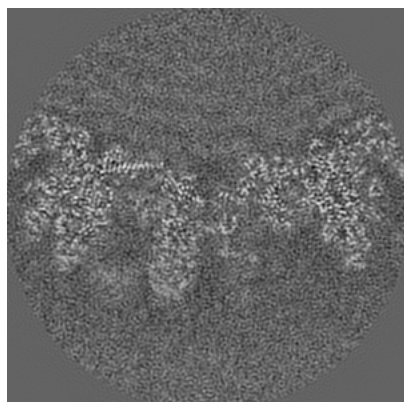


Z

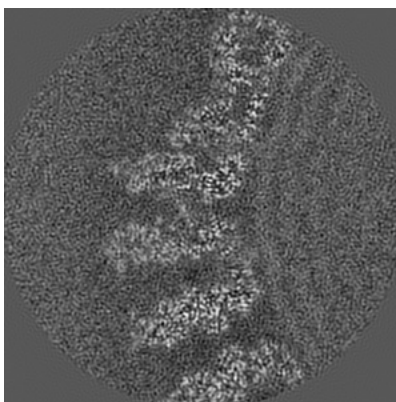
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

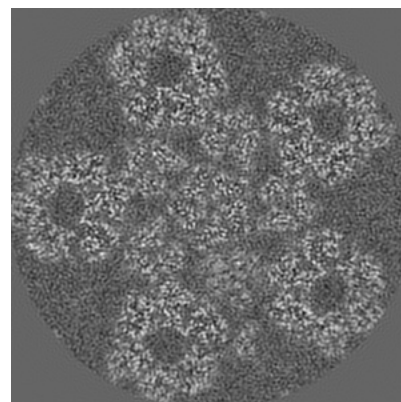
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

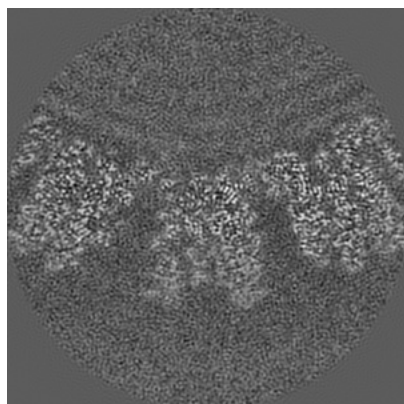


Z Index: 160

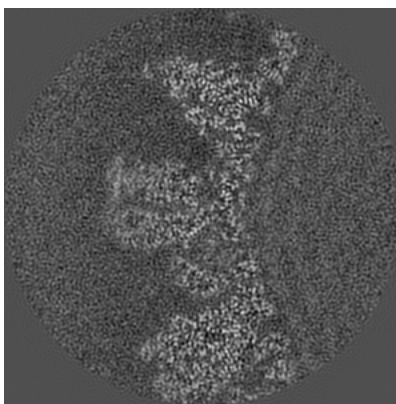
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

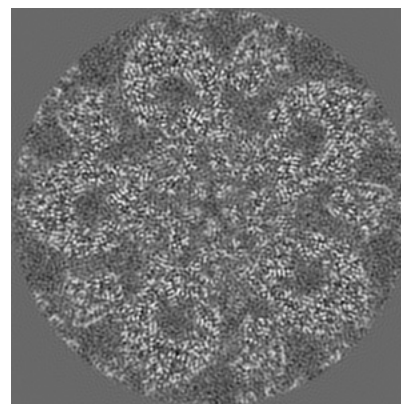
### 6.3.1 Primary map



X Index: 147



Y Index: 189



Z Index: 185

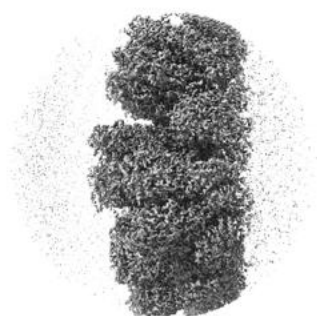
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

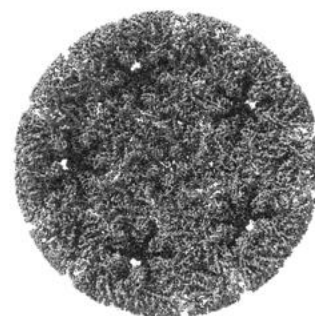
### 6.4.1 Primary map



X



Y



Z

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.

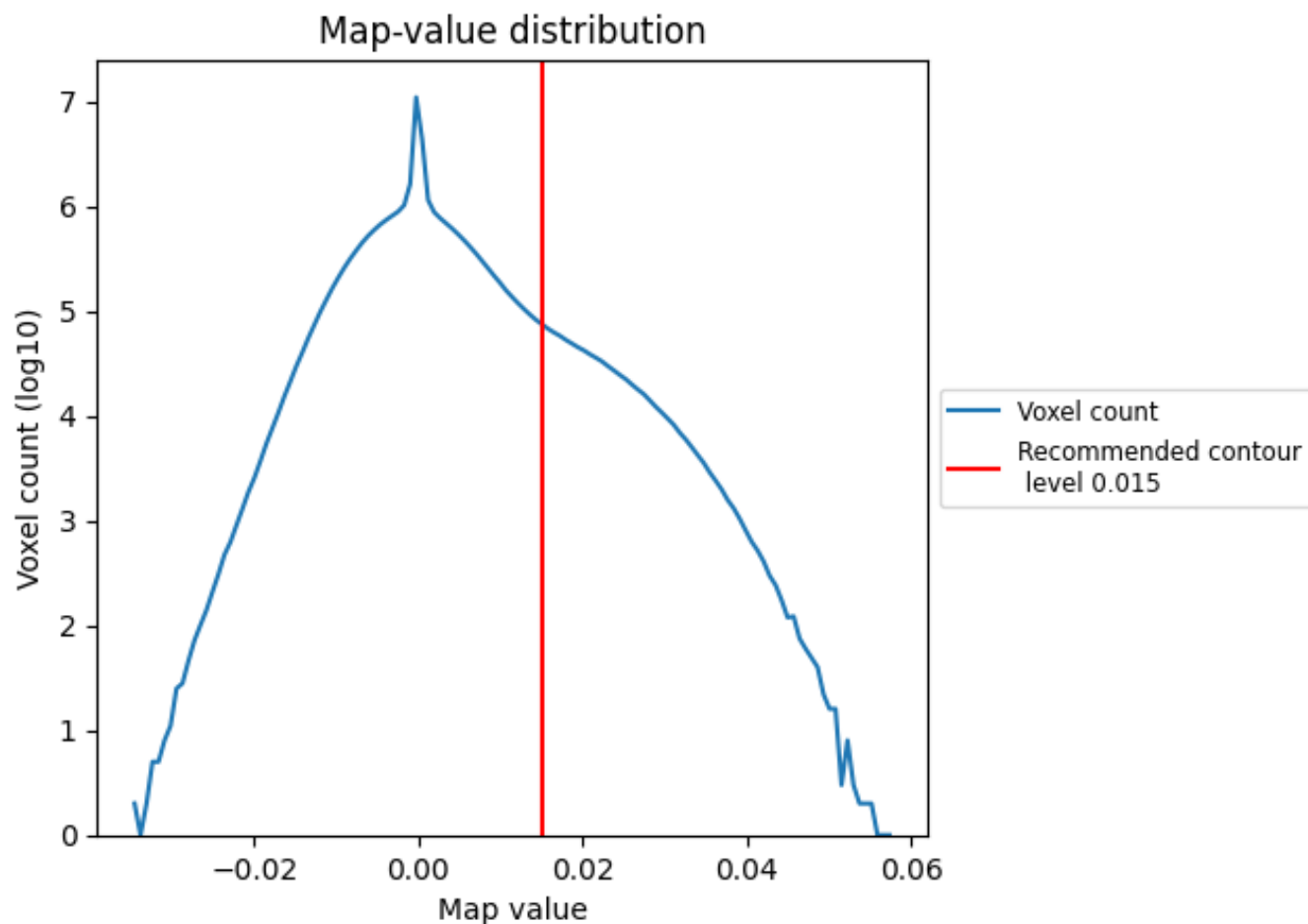
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

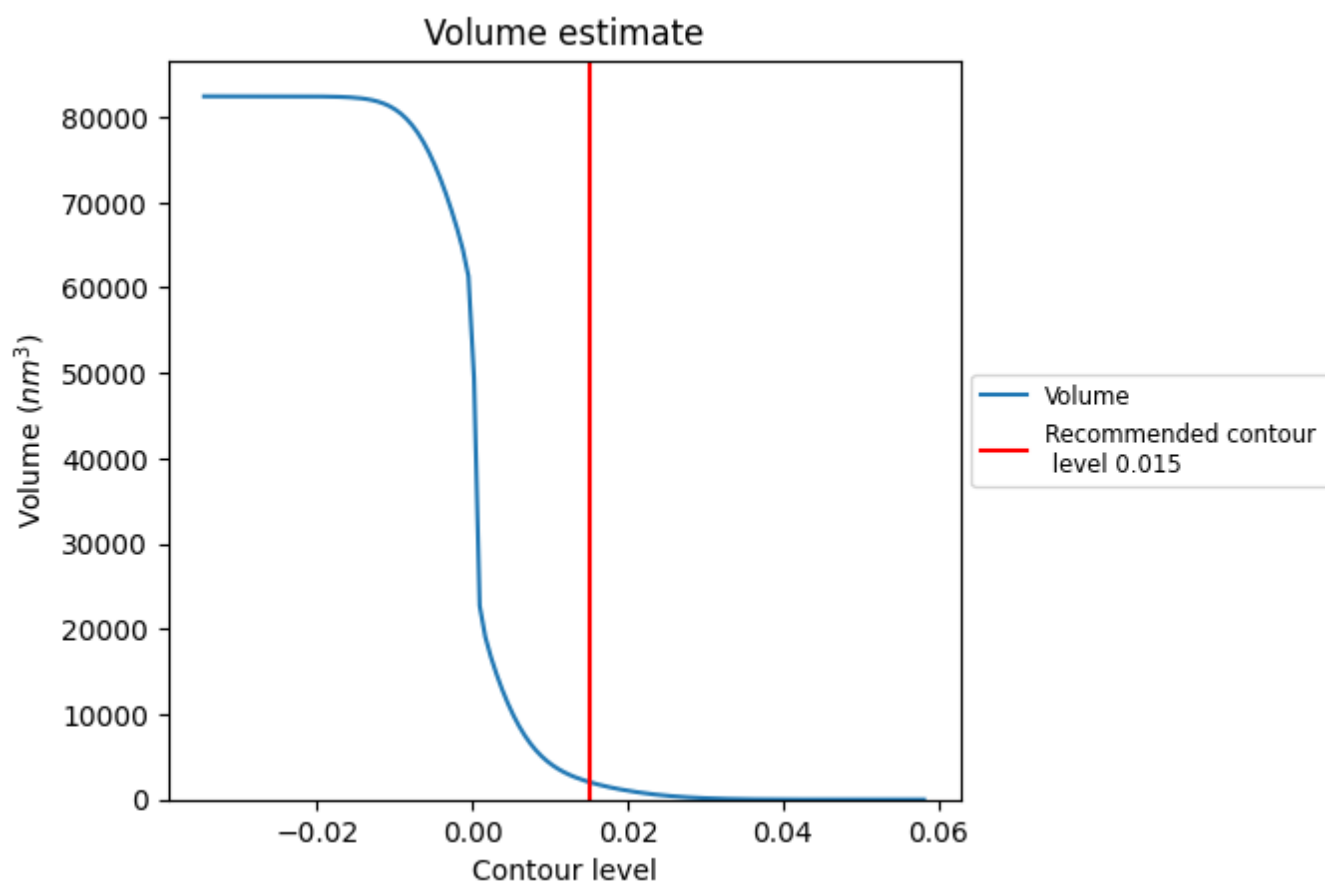
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

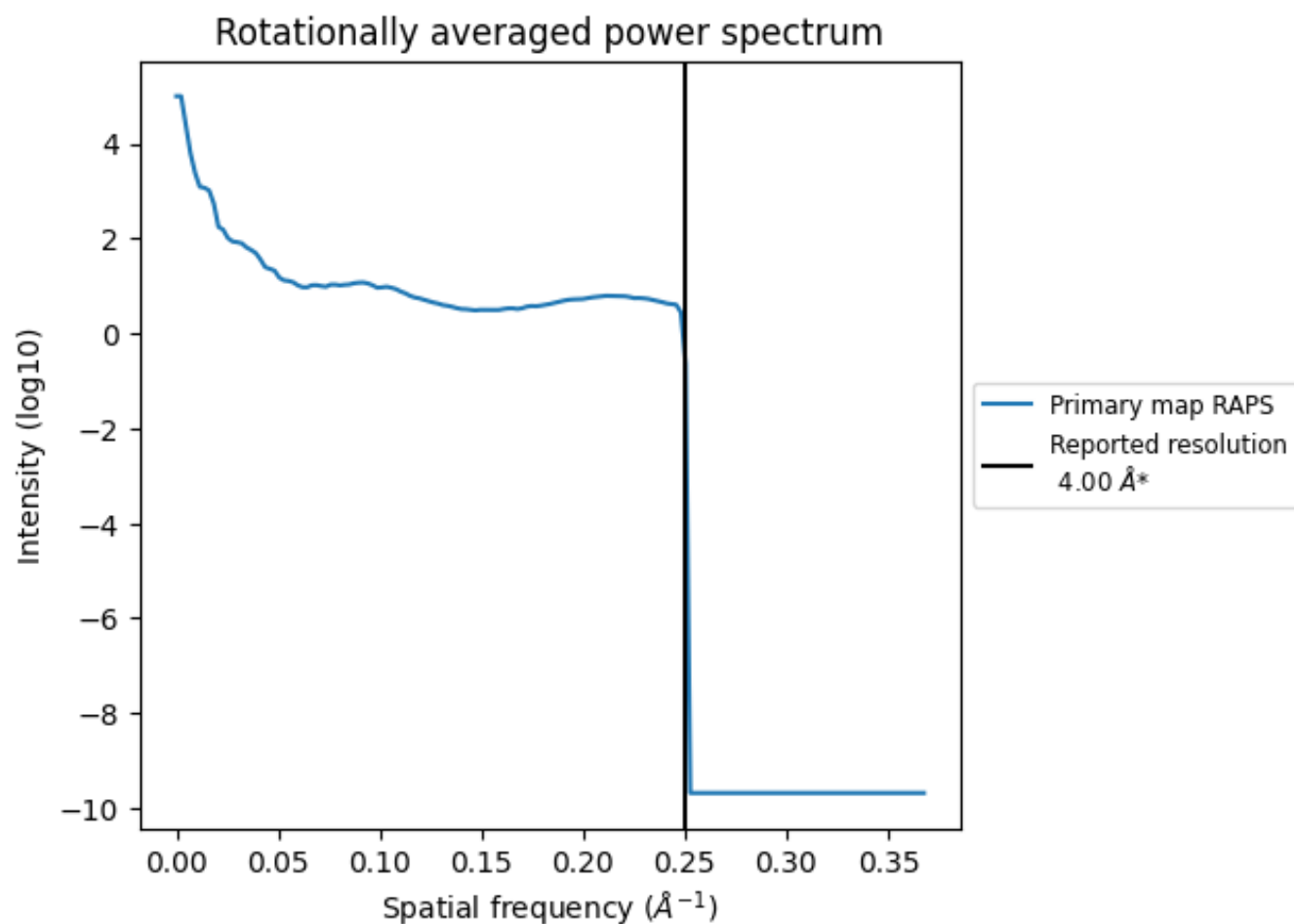
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2067 nm<sup>3</sup>; 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  $\text{\AA}^{-1}$

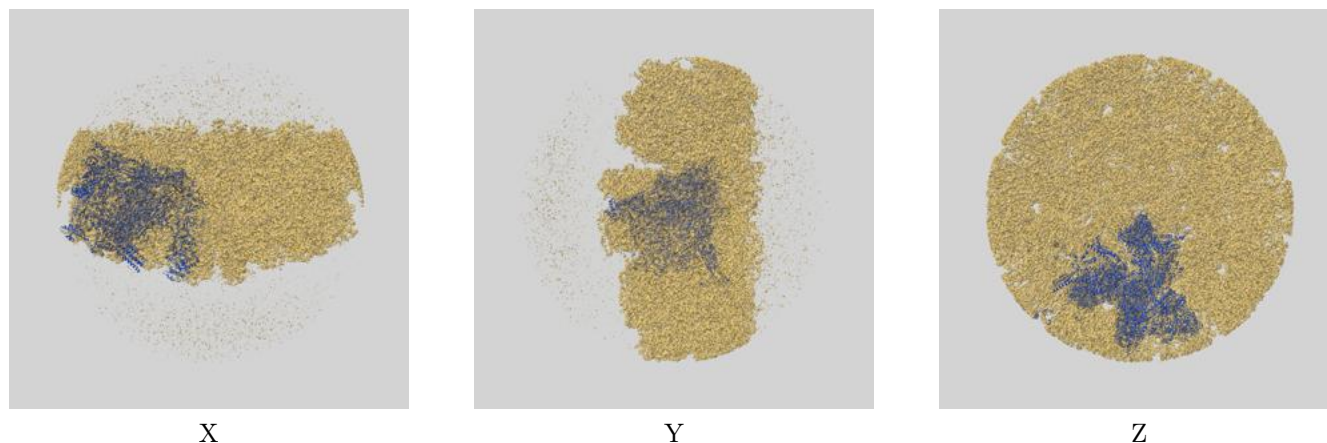
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

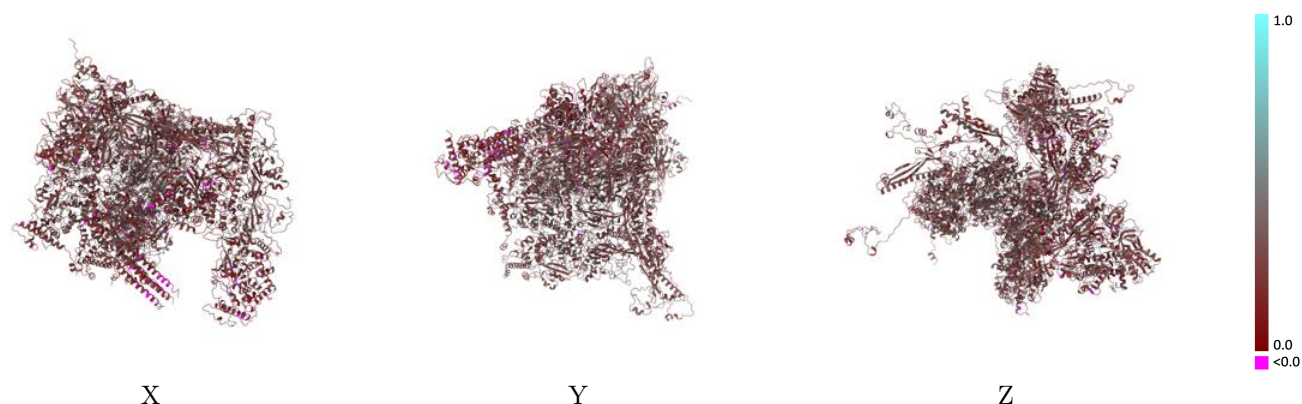
This section contains information regarding the fit between EMDB map EMD-21525 and PDB model 6W2D. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

### 9.1 Map-model overlay [i](#)



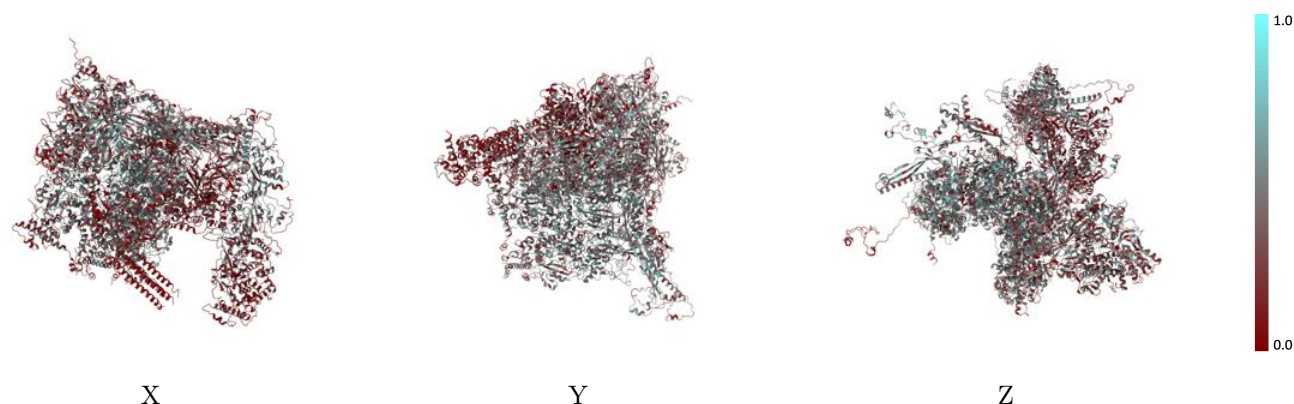
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



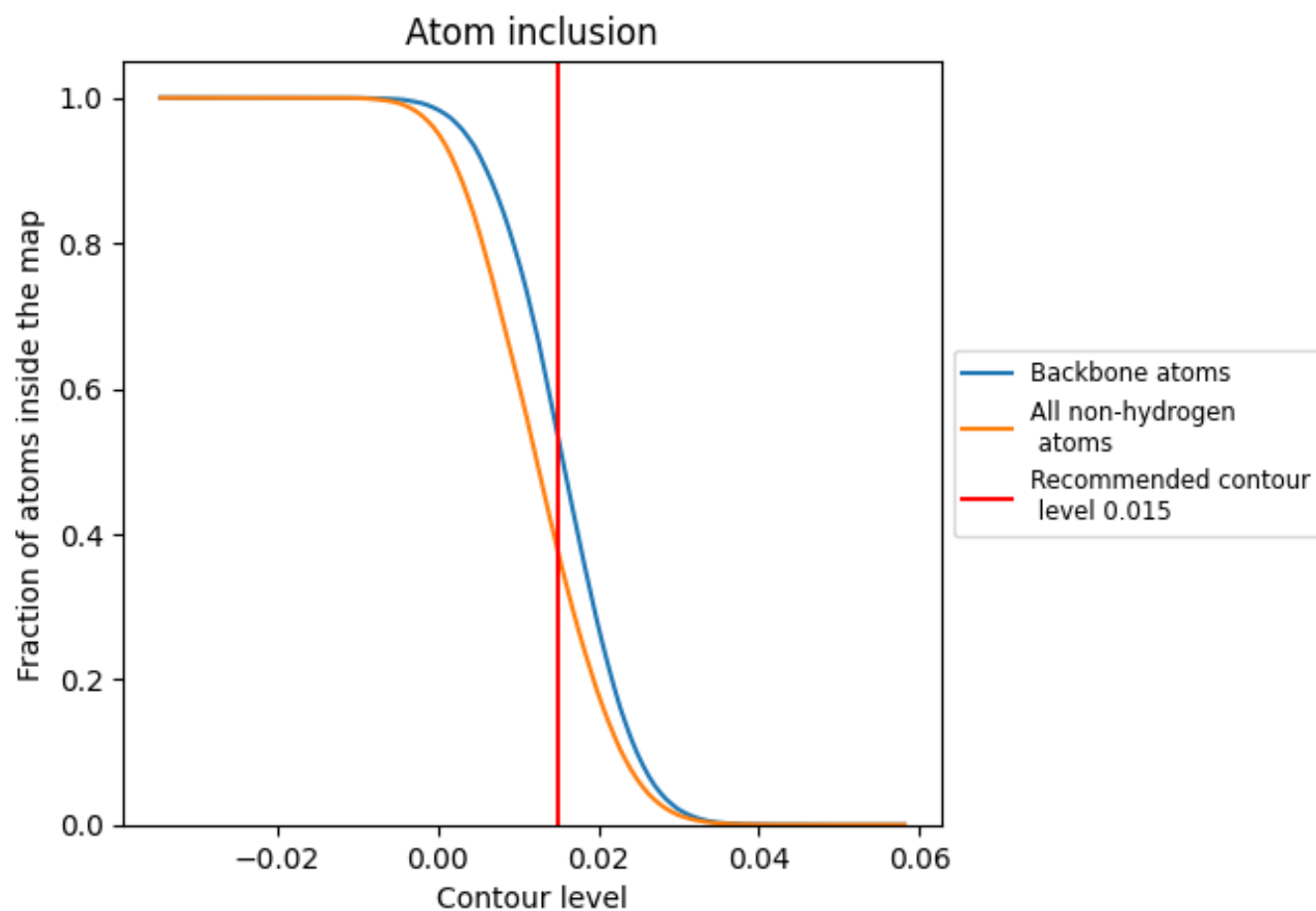
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.4584	 0.3060
K	 0.4469	 0.3030
N	 0.4054	 0.2910
O	 0.4403	 0.3030
P	 0.3244	 0.2580
Z	 0.3450	 0.2420
a	 0.3083	 0.2810
d	 0.2428	 0.2360
e	 0.2955	 0.2580
f	 0.2000	 0.2340
h	 0.3765	 0.2720
k	 0.2458	 0.2530
m	 0.3428	 0.2700
p	 0.2388	 0.2550
r	 0.3662	 0.2810
u	 0.1379	 0.1670
v	 0.2224	 0.2410
w	 0.1004	 0.1640
x	 0.1875	 0.1900
y	 0.1093	 0.1880
z	 0.0960	 0.1620

