



Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 06:00 PM JST

PDB ID : 7VVZ
EMDB ID : EMD-32150
Title : NuA4 bound to the nucleosome
Authors : Qu, K.; Chen, Z.
Deposited on : 2021-11-09
Resolution : 8.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

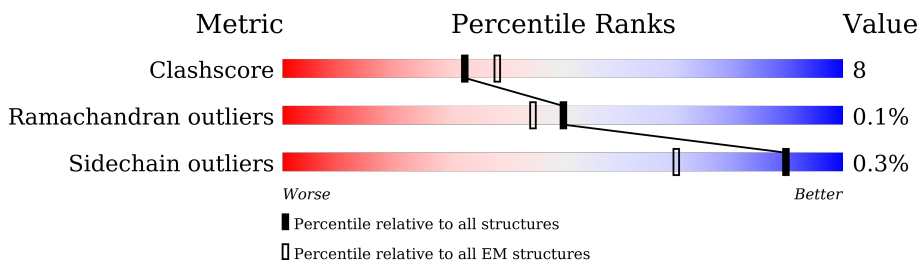
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	Y	113	
2	V	282	
3	H	832	
3	T	832	
4	A	136	
4	O	136	
5	B	103	
5	Q	103	

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Mol	Chain	Length	Quality of chain
6	N	130	
6	S	130	
7	D	126	
7	U	126	
8	P	445	
9	W	207	
10	I	207	
11	X	9	
12	E	1168	
13	F	489	
14	G	375	
15	K	476	
16	L	3744	

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 61920 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 Chromatin modification-related protein EAF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Y	46	Total	C	N	O	S	0	0
			396	245	64	86	1		

- Molecule 2 is a protein called Chromatin modification-related protein YNG2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	113	Total	C	N	O	S	0	0
			923	583	158	179	3		

- Molecule 3 is a protein called Enhancer of polycomb-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	274	Total	C	N	O	S	0	0
			2294	1441	403	441	9		
3	H	269	Total	C	N	O	S	0	0
			2250	1427	380	438	5		

- Molecule 4 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	96	Total	C	N	O	S	0	0
			791	500	151	137	3		
4	A	94	Total	C	N	O	S	0	0
			774	489	147	135	3		

- Molecule 5 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	80	Total	C	N	O	S	0	0
			641	405	125	110	1		
5	B	87	Total	C	N	O	S	0	0
			703	442	142	118	1		

- Molecule 6 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	S	106	Total	C	N	O	0	0
			814	513	159	142		
6	N	106	Total	C	N	O	0	0
			814	513	159	142		

- Molecule 7 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
7	D	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

- Molecule 8 is a protein called Histone acetyltransferase ESA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	270	Total	C	N	O	S	0	0
			2286	1481	380	415	10		

- Molecule 9 is a DNA chain called DNA (207-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	180	Total	C	N	O	P	0	0
			3666	1739	667	1080	180		

- Molecule 10 is a DNA chain called DNA (207-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	179	Total	C	N	O	P	0	0
			3695	1746	696	1074	179		

- Molecule 11 is a protein called Epl1 arginine anchor.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	X	9	Total	C	N	O	0	0
			82	53	19	10		

- Molecule 12 is a protein called Chromatin modification-related protein EAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	415	Total	C	N	O	S	0	0
			3448	2193	619	622	14		

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	983	ARG	-	expression tag	UNP Q06337
E	984	THR	-	expression tag	UNP Q06337
E	985	LEU	-	expression tag	UNP Q06337
E	986	GLN	-	expression tag	UNP Q06337
E	987	VAL	-	expression tag	UNP Q06337
E	988	ASP	-	expression tag	UNP Q06337
E	989	TRP	-	expression tag	UNP Q06337
E	990	SER	-	expression tag	UNP Q06337
E	991	HIS	-	expression tag	UNP Q06337
E	992	PRO	-	expression tag	UNP Q06337
E	993	GLN	-	expression tag	UNP Q06337
E	994	PHE	-	expression tag	UNP Q06337
E	995	GLU	-	expression tag	UNP Q06337
E	996	LYS	-	expression tag	UNP Q06337
E	997	HIS	-	expression tag	UNP Q06337
E	998	HIS	-	expression tag	UNP Q06337
E	999	HIS	-	expression tag	UNP Q06337
E	1000	HIS	-	expression tag	UNP Q06337
E	1001	HIS	-	expression tag	UNP Q06337
E	1002	HIS	-	expression tag	UNP Q06337
E	1003	HIS	-	expression tag	UNP Q06337
E	1004	HIS	-	expression tag	UNP Q06337
E	1005	HIS	-	expression tag	UNP Q06337
E	1006	HIS	-	expression tag	UNP Q06337
E	1007	HIS	-	expression tag	UNP Q06337
E	1008	HIS	-	expression tag	UNP Q06337
E	1009	ASP	-	expression tag	UNP Q06337
E	1010	TYR	-	expression tag	UNP Q06337
E	1011	ASP	-	expression tag	UNP Q06337
E	1012	ILE	-	expression tag	UNP Q06337
E	1013	PRO	-	expression tag	UNP Q06337
E	1014	THR	-	expression tag	UNP Q06337
E	1015	THR	-	expression tag	UNP Q06337
E	1016	ALA	-	expression tag	UNP Q06337
E	1017	SER	-	expression tag	UNP Q06337
E	1018	VAL	-	expression tag	UNP Q06337
E	1019	ASP	-	expression tag	UNP Q06337

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1020	GLY	-	expression tag	UNP Q06337
E	1021	SER	-	expression tag	UNP Q06337
E	1022	GLU	-	expression tag	UNP Q06337
E	1023	ASN	-	expression tag	UNP Q06337
E	1024	LEU	-	expression tag	UNP Q06337
E	1025	TYR	-	expression tag	UNP Q06337
E	1026	PHE	-	expression tag	UNP Q06337
E	1027	GLN	-	expression tag	UNP Q06337
E	1028	GLY	-	expression tag	UNP Q06337
E	1029	SER	-	expression tag	UNP Q06337
E	1030	PRO	-	expression tag	UNP Q06337
E	1031	GLN	-	expression tag	UNP Q06337
E	1032	GLN	-	expression tag	UNP Q06337
E	1033	ASN	-	expression tag	UNP Q06337
E	1034	LYS	-	expression tag	UNP Q06337
E	1035	THR	-	expression tag	UNP Q06337
E	1036	ALA	-	expression tag	UNP Q06337
E	1037	ALA	-	expression tag	UNP Q06337
E	1038	LEU	-	expression tag	UNP Q06337
E	1039	ALA	-	expression tag	UNP Q06337
E	1040	GLN	-	expression tag	UNP Q06337
E	1041	HIS	-	expression tag	UNP Q06337
E	1042	ASP	-	expression tag	UNP Q06337
E	1043	GLU	-	expression tag	UNP Q06337
E	1044	ALA	-	expression tag	UNP Q06337
E	1045	VAL	-	expression tag	UNP Q06337
E	1046	ASP	-	expression tag	UNP Q06337
E	1047	ASN	-	expression tag	UNP Q06337
E	1048	LYS	-	expression tag	UNP Q06337
E	1049	PHE	-	expression tag	UNP Q06337
E	1050	ASN	-	expression tag	UNP Q06337
E	1051	LYS	-	expression tag	UNP Q06337
E	1052	GLU	-	expression tag	UNP Q06337
E	1053	GLN	-	expression tag	UNP Q06337
E	1054	GLN	-	expression tag	UNP Q06337
E	1055	ASN	-	expression tag	UNP Q06337
E	1056	ALA	-	expression tag	UNP Q06337
E	1057	PHE	-	expression tag	UNP Q06337
E	1058	TYR	-	expression tag	UNP Q06337
E	1059	GLU	-	expression tag	UNP Q06337
E	1060	ILE	-	expression tag	UNP Q06337
E	1061	LEU	-	expression tag	UNP Q06337

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1062	HIS	-	expression tag	UNP Q06337
E	1063	LEU	-	expression tag	UNP Q06337
E	1064	PRO	-	expression tag	UNP Q06337
E	1065	ASN	-	expression tag	UNP Q06337
E	1066	LEU	-	expression tag	UNP Q06337
E	1067	ASN	-	expression tag	UNP Q06337
E	1068	GLU	-	expression tag	UNP Q06337
E	1069	GLU	-	expression tag	UNP Q06337
E	1070	GLN	-	expression tag	UNP Q06337
E	1071	ARG	-	expression tag	UNP Q06337
E	1072	ASN	-	expression tag	UNP Q06337
E	1073	ALA	-	expression tag	UNP Q06337
E	1074	PHE	-	expression tag	UNP Q06337
E	1075	ILE	-	expression tag	UNP Q06337
E	1076	GLN	-	expression tag	UNP Q06337
E	1077	SER	-	expression tag	UNP Q06337
E	1078	LEU	-	expression tag	UNP Q06337
E	1079	LYS	-	expression tag	UNP Q06337
E	1080	ASP	-	expression tag	UNP Q06337
E	1081	ASP	-	expression tag	UNP Q06337
E	1082	PRO	-	expression tag	UNP Q06337
E	1083	SER	-	expression tag	UNP Q06337
E	1084	GLN	-	expression tag	UNP Q06337
E	1085	SER	-	expression tag	UNP Q06337
E	1086	ALA	-	expression tag	UNP Q06337
E	1087	ASN	-	expression tag	UNP Q06337
E	1088	LEU	-	expression tag	UNP Q06337
E	1089	LEU	-	expression tag	UNP Q06337
E	1090	ALA	-	expression tag	UNP Q06337
E	1091	GLU	-	expression tag	UNP Q06337
E	1092	ALA	-	expression tag	UNP Q06337
E	1093	LYS	-	expression tag	UNP Q06337
E	1094	LYS	-	expression tag	UNP Q06337
E	1095	LEU	-	expression tag	UNP Q06337
E	1096	ASN	-	expression tag	UNP Q06337
E	1097	ASP	-	expression tag	UNP Q06337
E	1098	ALA	-	expression tag	UNP Q06337
E	1099	GLN	-	expression tag	UNP Q06337
E	1100	ALA	-	expression tag	UNP Q06337
E	1101	PRO	-	expression tag	UNP Q06337
E	1102	LYS	-	expression tag	UNP Q06337
E	1103	VAL	-	expression tag	UNP Q06337

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1104	ASP	-	expression tag	UNP Q06337
E	1105	ASN	-	expression tag	UNP Q06337
E	1106	LYS	-	expression tag	UNP Q06337
E	1107	PHE	-	expression tag	UNP Q06337
E	1108	ASN	-	expression tag	UNP Q06337
E	1109	LYS	-	expression tag	UNP Q06337
E	1110	GLU	-	expression tag	UNP Q06337
E	1111	GLN	-	expression tag	UNP Q06337
E	1112	GLN	-	expression tag	UNP Q06337
E	1113	ASN	-	expression tag	UNP Q06337
E	1114	ALA	-	expression tag	UNP Q06337
E	1115	PHE	-	expression tag	UNP Q06337
E	1116	TYR	-	expression tag	UNP Q06337
E	1117	GLU	-	expression tag	UNP Q06337
E	1118	ILE	-	expression tag	UNP Q06337
E	1119	LEU	-	expression tag	UNP Q06337
E	1120	HIS	-	expression tag	UNP Q06337
E	1121	LEU	-	expression tag	UNP Q06337
E	1122	PRO	-	expression tag	UNP Q06337
E	1123	ASN	-	expression tag	UNP Q06337
E	1124	LEU	-	expression tag	UNP Q06337
E	1125	ASN	-	expression tag	UNP Q06337
E	1126	GLU	-	expression tag	UNP Q06337
E	1127	GLU	-	expression tag	UNP Q06337
E	1128	GLN	-	expression tag	UNP Q06337
E	1129	ARG	-	expression tag	UNP Q06337
E	1130	ASN	-	expression tag	UNP Q06337
E	1131	ALA	-	expression tag	UNP Q06337
E	1132	PHE	-	expression tag	UNP Q06337
E	1133	ILE	-	expression tag	UNP Q06337
E	1134	GLN	-	expression tag	UNP Q06337
E	1135	SER	-	expression tag	UNP Q06337
E	1136	LEU	-	expression tag	UNP Q06337
E	1137	LYS	-	expression tag	UNP Q06337
E	1138	ASP	-	expression tag	UNP Q06337
E	1139	ASP	-	expression tag	UNP Q06337
E	1140	PRO	-	expression tag	UNP Q06337
E	1141	SER	-	expression tag	UNP Q06337
E	1142	GLN	-	expression tag	UNP Q06337
E	1143	SER	-	expression tag	UNP Q06337
E	1144	ALA	-	expression tag	UNP Q06337
E	1145	ASN	-	expression tag	UNP Q06337

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1146	LEU	-	expression tag	UNP Q06337
E	1147	LEU	-	expression tag	UNP Q06337
E	1148	ALA	-	expression tag	UNP Q06337
E	1149	GLU	-	expression tag	UNP Q06337
E	1150	ALA	-	expression tag	UNP Q06337
E	1151	LYS	-	expression tag	UNP Q06337
E	1152	LYS	-	expression tag	UNP Q06337
E	1153	LEU	-	expression tag	UNP Q06337
E	1154	ASN	-	expression tag	UNP Q06337
E	1155	ASP	-	expression tag	UNP Q06337
E	1156	ALA	-	expression tag	UNP Q06337
E	1157	GLN	-	expression tag	UNP Q06337
E	1158	ALA	-	expression tag	UNP Q06337
E	1159	PRO	-	expression tag	UNP Q06337
E	1160	LYS	-	expression tag	UNP Q06337
E	1161	VAL	-	expression tag	UNP Q06337
E	1162	ASP	-	expression tag	UNP Q06337
E	1163	ALA	-	expression tag	UNP Q06337
E	1164	ASN	-	expression tag	UNP Q06337
E	1165	SER	-	expression tag	UNP Q06337
E	1166	ALA	-	expression tag	UNP Q06337
E	1167	ALA	-	expression tag	UNP Q06337
E	1168	LEU	-	expression tag	UNP Q06337

- Molecule 13 is a protein called Actin-related protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	414	Total	C	N	O	S	0	0
			3278	2088	541	638	11		

- Molecule 14 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	357	Total	C	N	O	S	0	0
			2788	1772	468	531	17		

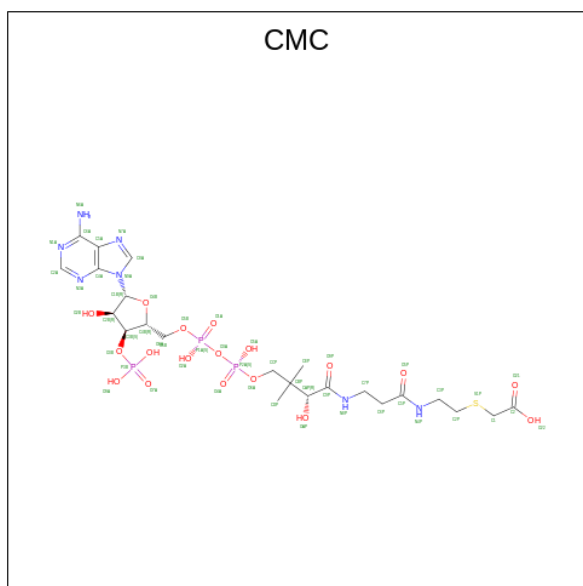
- Molecule 15 is a protein called SWR1-complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	237	Total	C	N	O	S	0	0
			1989	1275	337	370	7		

- Molecule 16 is a protein called Transcription-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	3513	Total	C	N	O	S	0	0
			28729	18596	4776	5237	120		

- Molecule 17 is CARBOXYMETHYL COENZYME *A (three-letter code: CMC) (formula: $C_{23}H_{38}N_7O_{18}P_3S$) (labeled as "Ligand of Interest" by depositor).

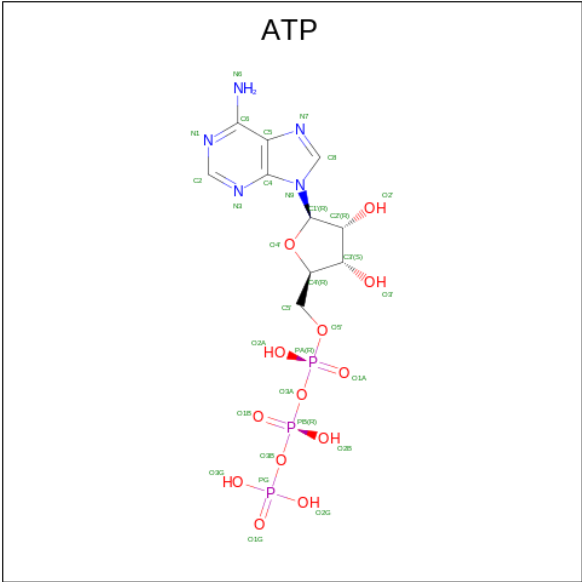


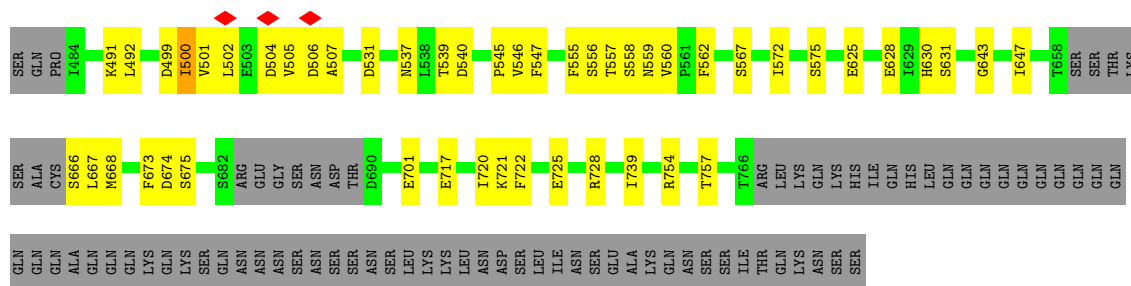
Mol	Chain	Residues	Atoms						AltConf
17	B	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	F	1	Total	Mg	0
			1	1	
18	G	1	Total	Mg	0
			1	1	

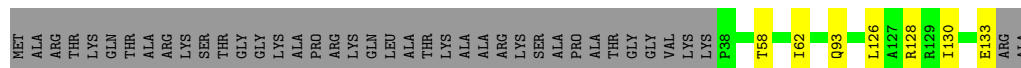
- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).





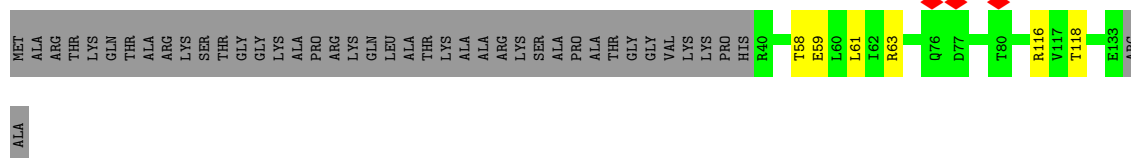
• Molecule 4: Histone H3

Chain O: 65% 5% 29%



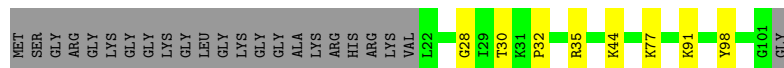
• Molecule 4: Histone H3

Chain A: 65% 0% 31%



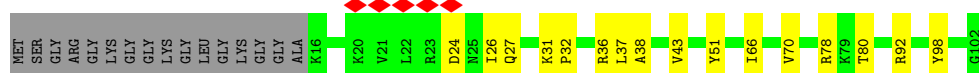
• Molecule 5: Histone H4

Chain Q: 70% 8% 22%



• Molecule 5: Histone H4

Chain B: 5% 69% 16% 16%



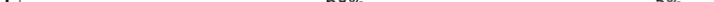
• Molecule 6: Histone H2A

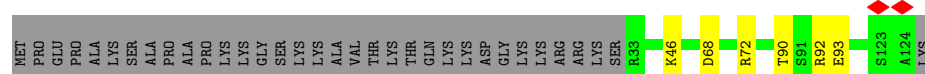
Chain S: 77% 5% 18%



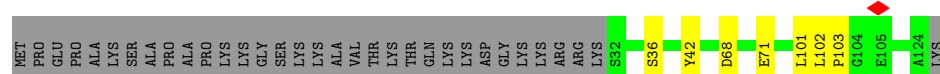
• Molecule 6: Histone H2A

Met	Ser	Gly	Arg	Gly	Lys	Gln	Gly	Lys	Thr	Arg	A12	R29	R71	I79	P80	R81	H82	D90	E91	E92	L93	L115	L116	P117	Lys	Lys	Thr	Glu	Ser	Ser	Lys	Ala	Lys	Lys	Ser	Ser
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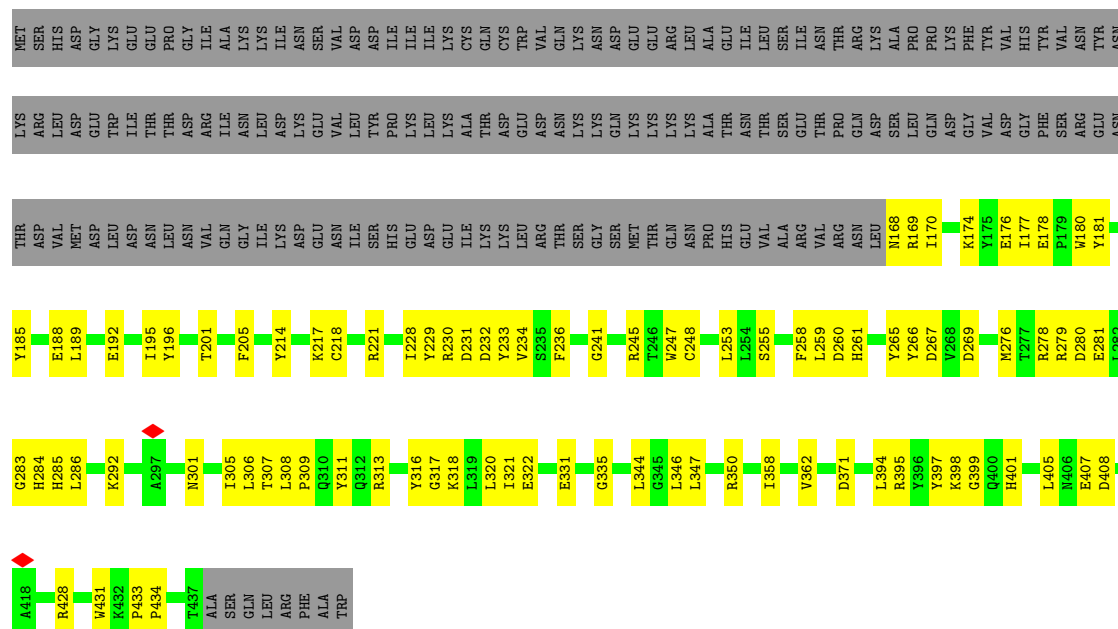
Chain U:  68% 5% 27%

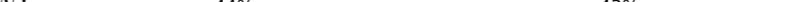


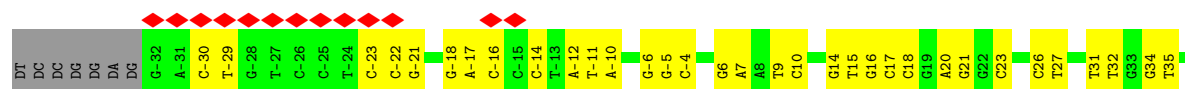
Chain D:  68% 6% 26%

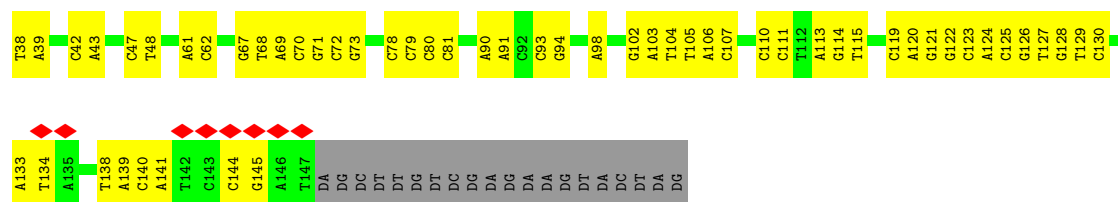


Chain P: 41% 20% 39%

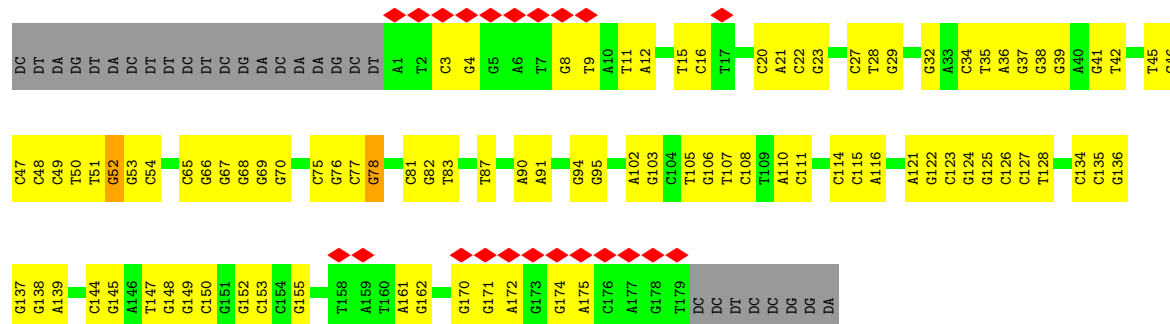


Chain W: 

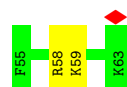
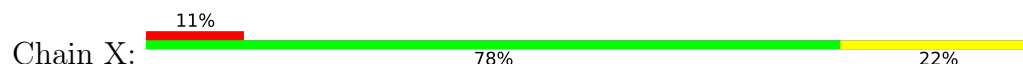




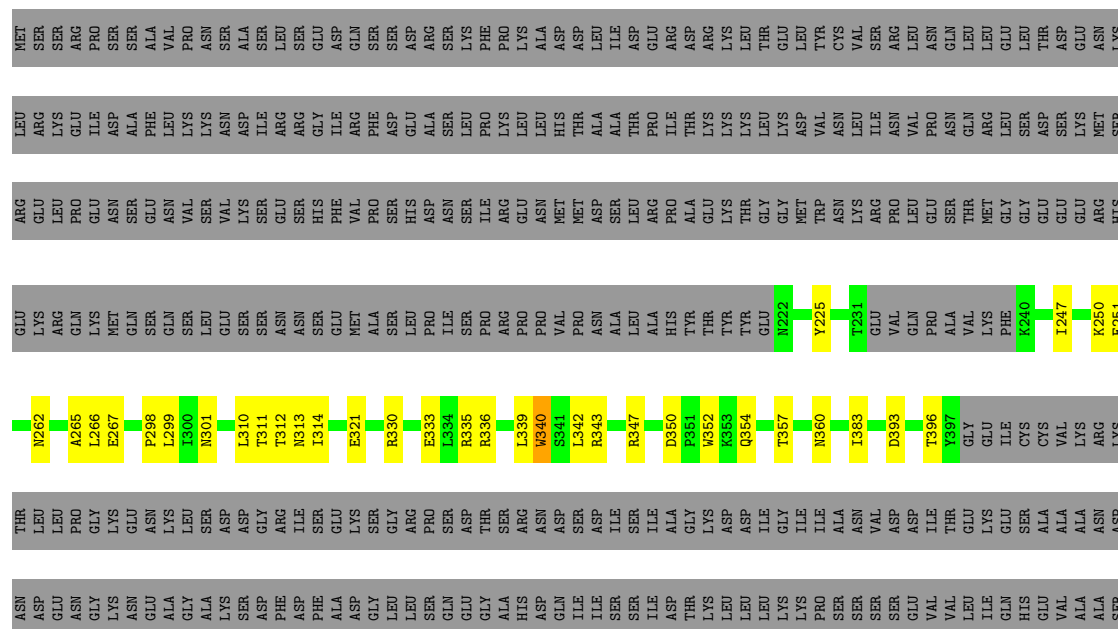
• Molecule 10: DNA (207-mer)

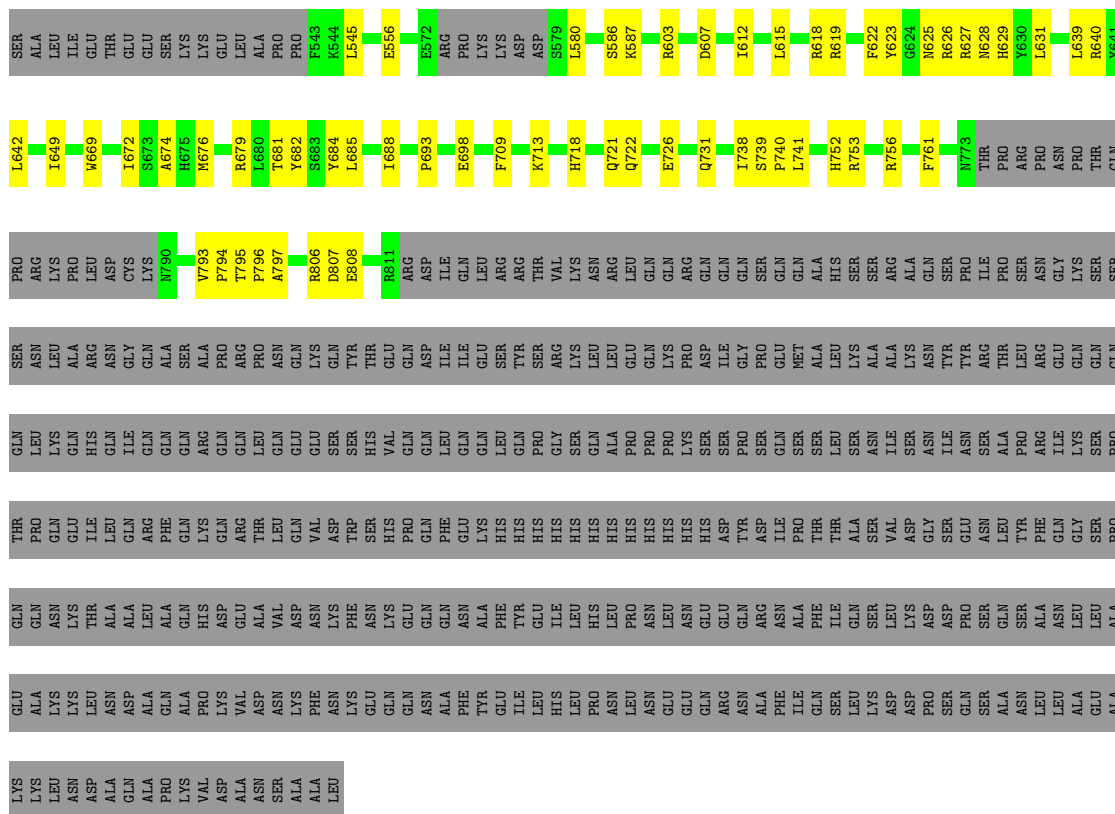


• Molecule 11: Epl1 arginine anchor

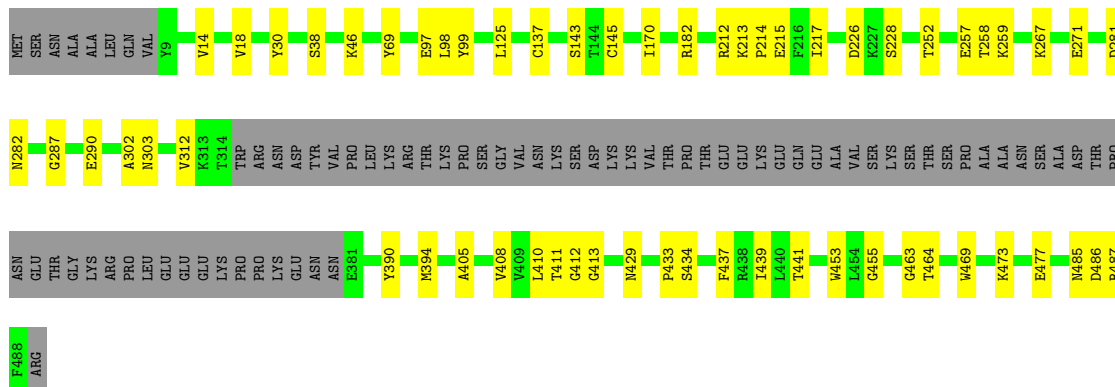


• Molecule 12: Chromatin modification-related protein EAF1

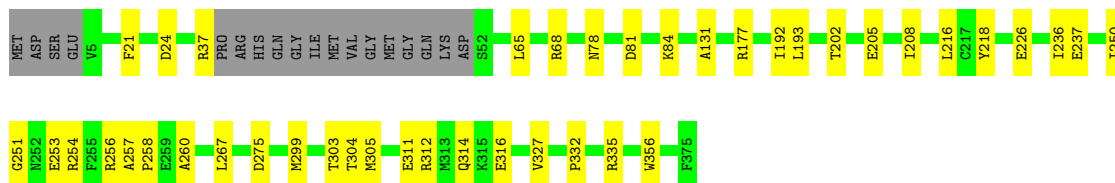
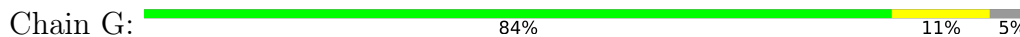


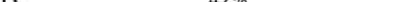


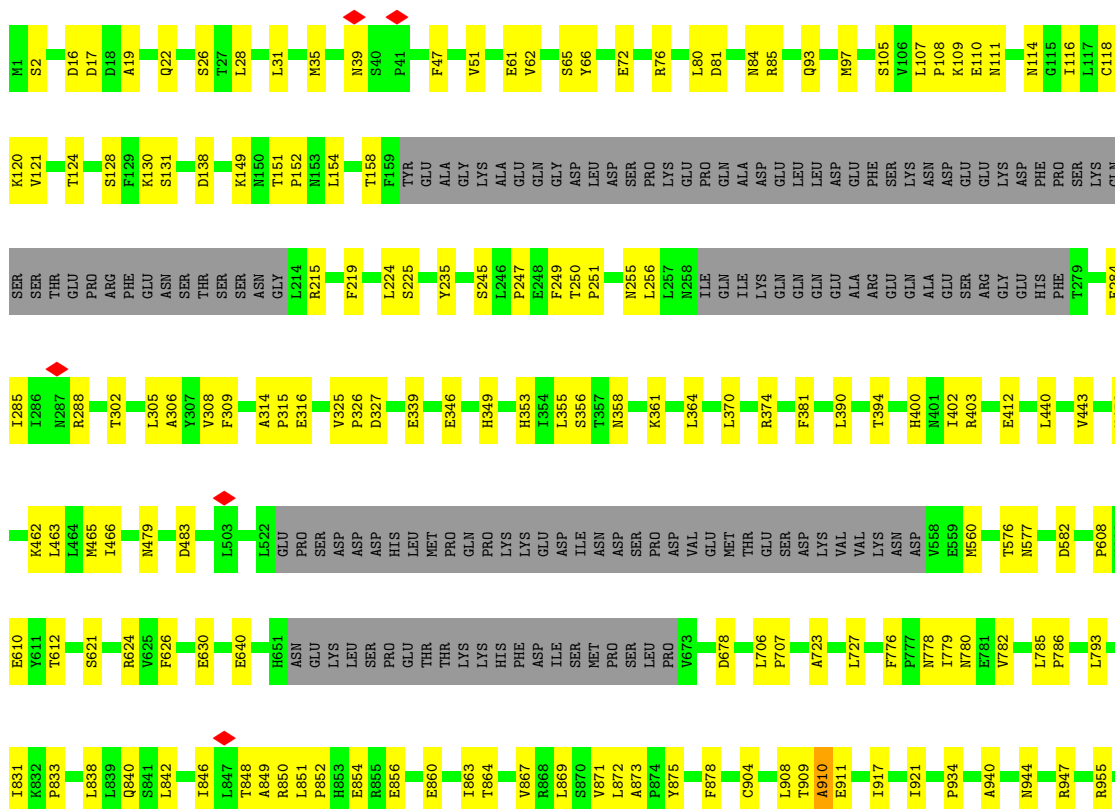
- Molecule 13: Actin-related protein 4



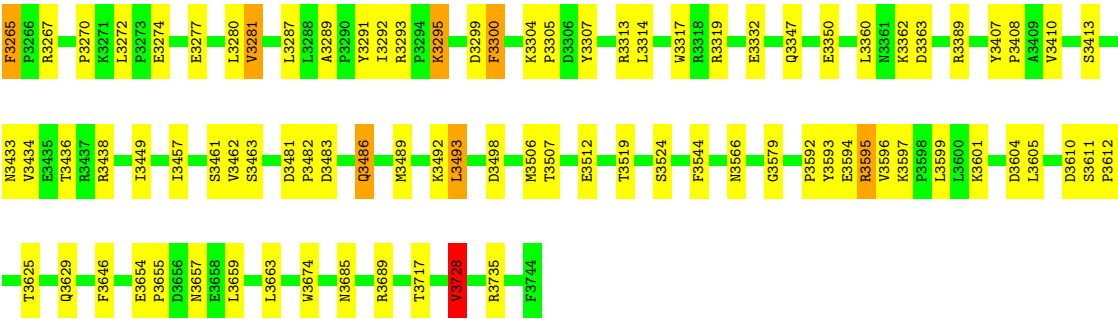
- Molecule 14: Actin



Chain K:  42% 8% 50%



F3121	L2936	M2605	E2444	L2310	E2444	E2405	E2529	K2873	F3063	T3240	F3121	L1507	E1683	S1818	E1976	VAL	K2041	E1863	I1771	D1607	E1094	K1051	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
I3128	T2972	T2613	R2450	K2313	E2614	E2615	Q2531	F2407	Q2501	T3241	I3128	L1509	W1684	G1819	Q1981	GLU	K2042	E1885	A1772	V1607	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
W3131	F2982	S2616	R2456	Y2316	S2617	L2616	R2457	Y2316	Q2501	T3241	W3131	L1513	K1686	E1824	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
Y3132	E2998	L2618	D2457	L2320	E2617	L2618	D2457	L2320	Q2501	T3241	Y3132	L1532	K1687	E1825	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
F3136	T3001	P2619	E2461	S2328	E2618	L2619	D2461	S2328	Q2501	T3241	F3136	L1532	K1688	E1826	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
L3140	Q3018	P2620	E2462	S2329	E2619	L2620	D2462	S2329	Q2501	T3241	L3140	L1532	K1689	E1827	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
M3151	A3020	H2821	E2463	L2339	E2620	L2621	D2463	L2339	Q2501	T3241	M3151	L1532	K1690	E1828	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
V3152	F3022	H2822	E2464	L2340	E2621	L2622	D2464	L2340	Q2501	T3241	V3152	L1532	K1691	E1829	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
R3153	T3024	H2823	E2465	L2341	E2622	L2623	D2465	L2341	Q2501	T3241	R3153	L1532	K1692	E1830	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
R3158	T3024	H2824	E2466	L2342	E2623	L2624	D2466	L2342	Q2501	T3241	R3158	L1532	K1693	E1831	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
Q3182	K3028	H2825	E2467	L2343	E2624	L2625	D2467	L2343	Q2501	T3241	Q3182	L1532	K1694	E1832	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
ARG	F3029	H2826	E2468	L2344	E2625	L2626	D2468	L2344	Q2501	T3241	ARG	L1532	K1695	E1833	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
GLN	T3030	H2827	E2469	L2345	E2626	L2627	D2469	L2345	Q2501	T3241	GLN	L1532	K1696	E1834	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
THR	L3030	H2828	E2470	L2346	E2627	L2628	D2470	L2346	Q2501	T3241	THR	L1532	K1697	E1835	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
MET	A3035	H2829	E2471	L2347	E2628	L2629	D2471	L2347	Q2501	T3241	MET	L1532	K1698	E1836	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
ALA	Y3036	H2830	E2472	L2348	E2629	L2630	D2472	L2348	Q2501	T3241	ALA	L1532	K1699	E1837	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
VAL	E3037	H2831	E2473	L2349	E2630	L2631	D2473	L2349	Q2501	T3241	VAL	L1532	K1700	E1838	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
MET	E3038	H2832	E2474	L2350	E2631	L2632	D2474	L2350	Q2501	T3241	MET	L1532	K1701	E1839	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
GLY	A3039	H2833	E2475	L2351	E2632	L2633	D2475	L2351	Q2501	T3241	GLY	L1532	K1702	E1840	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
LYS	N3040	H2834	E2476	L2352	E2633	L2634	D2476	L2352	Q2501	T3241	LYS	L1532	K1703	E1841	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
PRO	T3045	H2835	E2477	L2353	E2634	L2635	D2477	L2353	Q2501	T3241	PRO	L1532	K1704	E1842	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
ASP	A3046	H2836	E2478	L2354	E2635	L2636	D2478	L2354	Q2501	T3241	ASP	L1532	K1705	E1843	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
THR	Y3047	H2837	E2479	L2355	E2636	L2637	D2479	L2355	Q2501	T3241	THR	L1532	K1706	E1844	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
ASN	Q3048	H2838	E2480	L2356	E2637	L2638	D2480	L2356	Q2501	T3241	ASN	L1532	K1707	E1845	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
ASP	A3049	H2839	E2481	L2357	E2638	L2639	D2481	L2357	Q2501	T3241	ASP	L1532	K1708	E1846	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
ASN	D3050	H2840	E2482	L2358	E2639	L2640	D2482	L2358	Q2501	T3241	ASN	L1532	K1709	E1847	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
GLY	F3063	H2841	E2483	L2359	E2640	L2641	D2483	L2359	Q2501	T3241	GLY	L1532	K1710	E1848	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
ARG	Q3067	H2842	E2484	L2360	E2641	L2642	D2484	L2360	Q2501	T3241	ARG	L1532	K1711	E1849	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
R3067	L3068	H2843	E2485	L2361	E2642	L2643	D2485	L2361	Q2501	T3241	R3067	L1532	K1712	E1850	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
S3069	E3070	H2844	E2486	L2362	E2643	L2644	D2486	L2362	Q2501	T3241	S3069	L1532	K1713	E1851	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
E3210	N3073	H2845	E2487	L2363	E2644	L2645	D2487	L2363	Q2501	T3241	E3210	L1532	K1714	E1852	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
T3240	I3074	H2846	E2488	L2364	E2645	L2646	D2488	L2364	Q2501	T3241	T3240	L1532	K1715	E1853	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
T3241	S3075	H2847	E2489	L2365	E2646	L2647	D2489	L2365	Q2501	T3241	T3241	L1532	K1716	E1854	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
D3244	F3076	H2848	E2490	L2366	E2647	L2648	D2490	L2366	Q2501	T3241	D3244	L1532	K1717	E1855	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
R3247	A3078	H2849	E2491	L2367	E2648	L2649	D2491	L2367	Q2501	T3241	R3247	L1532	K1718	E1856	F1988	THR	E1897	K1888	F1776	N1626	E1093	K1052	V1047	K1044	A1033	S1032	S1335	K1330	Q1331	E1532	D1536	S1329	H1014	Y1012	I1007	Y1007	Y993
L3248	S3079	H2850	E2492	L2368	E2649	L2650	D2492	L2368	Q2501	T3241	L324																										



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	474949	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.268	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.032	Depositor
Map size (\AA)	407.02, 407.02, 407.02	wwPDB
Map dimensions	94, 94, 94	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	4.33, 4.33, 4.33	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CMC, ATP, MG

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	Y	0.25	0/401	0.36	0/535
2	V	0.25	0/934	0.37	0/1251
3	H	0.71	0/2298	0.63	0/3093
3	T	0.25	0/2341	0.42	0/3153
4	A	0.31	0/784	0.40	0/1052
4	O	0.31	0/803	0.39	0/1078
5	B	0.32	0/711	0.45	0/948
5	Q	0.33	0/648	0.45	0/868
6	N	0.30	0/824	0.42	0/1113
6	S	0.30	0/824	0.42	0/1113
7	D	0.32	0/736	0.41	0/991
7	U	0.31	0/730	0.41	0/983
8	P	0.27	0/2347	0.44	0/3171
9	W	0.69	0/4107	0.98	0/6330
10	I	0.69	0/4150	0.96	2/6410 (0.0%)
11	X	0.24	0/83	0.51	0/107
12	E	0.67	0/3527	0.62	0/4769
13	F	0.69	0/3350	0.57	0/4544
14	G	0.57	0/2849	0.54	0/3859
15	K	0.70	0/2036	0.57	0/2739
16	L	0.58	3/29358 (0.0%)	0.58	2/39779 (0.0%)
All	All	0.58	3/63841 (0.0%)	0.63	4/87886 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
16	L	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	2755	PHE	CB-CG	-5.67	1.41	1.51
16	L	3728	VAL	CB-CG2	-5.26	1.41	1.52
16	L	3512	GLU	CB-CG	-5.12	1.42	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	2626	LEU	CB-CG-CD2	-6.70	99.61	111.00
10	I	78	DG	O4'-C4'-C3'	-6.18	102.03	104.50
16	L	3263	LEU	CA-CB-CG	5.95	129.00	115.30
10	I	52	DG	O4'-C1'-N9	5.29	111.70	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	L	2621	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	396	0	372	10	0
2	V	923	0	955	24	0
3	H	2250	0	2192	55	0
3	T	2294	0	2236	75	0
4	A	774	0	813	5	0
4	O	791	0	828	4	0
5	B	703	0	753	13	0
5	Q	641	0	684	6	0
6	N	814	0	869	8	0
6	S	814	0	869	4	0
7	D	725	0	745	7	0
7	U	719	0	740	5	0
8	P	2286	0	2268	71	0
9	W	3666	0	2018	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	I	3695	0	2007	67	0
11	X	82	0	92	2	0
12	E	3448	0	3448	95	0
13	F	3278	0	3238	33	0
14	G	2788	0	2760	28	0
15	K	1989	0	1961	39	0
16	L	28729	0	29144	490	0
17	B	51	0	33	3	0
18	F	1	0	0	0	0
18	G	1	0	0	0	0
19	F	31	0	12	1	0
19	G	31	0	12	1	0
All	All	61920	0	59049	999	0

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

All (999) 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)
12:E:640:ARG:NH2	12:E:726:GLU:OE1	1.98	0.96
16:L:944:ASN:OD1	16:L:947:ARG:NH2	2.01	0.93
12:E:312:THR:OG1	16:L:3728:VAL:O	1.88	0.89
16:L:3244:ASP:OD1	16:L:3247:ARG:NH1	2.13	0.82
15:K:262:LYS:NZ	3:H:545:PRO:O	2.14	0.80
3:H:500:ILE:HD12	3:H:501:VAL:H	1.46	0.80
3:T:214:ILE:HD13	3:T:280:ARG:HG3	1.62	0.79
16:L:1847:ALA:O	16:L:1849:LEU:N	2.15	0.79
16:L:1328:HIS:O	16:L:1331:GLN:NE2	2.16	0.79
3:H:506:ASP:OD1	3:H:507:ALA:N	2.16	0.79
8:P:229:TYR:HB3	8:P:236:PHE:HB2	1.66	0.77
16:L:2341:ASP:O	16:L:2385:ARG:NH1	2.18	0.77
16:L:3109:SER:O	16:L:3689:ARG:NH1	2.18	0.76
16:L:370:LEU:O	16:L:374:ARG:NH2	2.18	0.76
16:L:400:HIS:O	16:L:403:ARG:NE	2.18	0.75
12:E:684:TYR:HB3	16:L:2755:PHE:CE2	2.21	0.75
16:L:85:ARG:NH2	16:L:1976:GLU:O	2.21	0.73
16:L:80:LEU:O	16:L:84:ASN:ND2	2.21	0.73
16:L:1601:ASN:ND2	16:L:1632:GLU:O	2.21	0.72
12:E:343:ARG:NH2	3:H:531:ASP:OD2	2.21	0.72
16:L:1913:ILE:O	16:L:1956:ARG:NH1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:1426:GLU:OE1	16:L:1427:GLU:N	2.24	0.71
8:P:259:LEU:HG	8:P:261:HIS:H	1.55	0.71
9:W:47:DC:H2''	9:W:48:DT:H71	1.73	0.70
3:H:504:ASP:HB3	3:H:507:ALA:HB3	1.74	0.69
16:L:3109:SER:OG	16:L:3689:ARG:NH1	2.24	0.69
15:K:313:ARG:O	3:H:500:ILE:O	2.11	0.69
16:L:16:ASP:OD1	16:L:17:ASP:N	2.25	0.69
17:B:501:CMC:H2B	8:P:313:ARG:HG2	1.74	0.68
16:L:3629:GLN:OE1	16:L:3728:VAL:HG21	1.92	0.68
13:F:99:TYR:OH	14:G:177:ARG:NH1	2.27	0.68
16:L:1849:LEU:HB3	16:L:1853:VAL:HG13	1.75	0.68
12:E:350:ASP:OD2	15:K:206:TYR:OH	2.10	0.67
10:I:45:DT:H2''	10:I:46:DC:H5'	1.78	0.66
10:I:136:DG:H2'	10:I:137:DG:C8	2.31	0.66
3:H:501:VAL:HG12	3:H:502:LEU:N	2.10	0.66
16:L:1834:LEU:O	16:L:1838:HIS:ND1	2.28	0.66
3:T:203:ARG:NH1	3:T:219:GLU:O	2.29	0.66
10:I:123:DC:H2''	10:I:124:DG:C8	2.32	0.65
12:E:556:GLU:N	12:E:556:GLU:OE1	2.29	0.65
8:P:292:LYS:NZ	8:P:331:GLU:OE2	2.30	0.65
16:L:154:LEU:O	16:L:158:THR:OG1	2.14	0.65
16:L:1750:PHE:O	16:L:1799:ARG:NH1	2.30	0.64
4:A:63:ARG:HD2	10:I:91:DA:H4'	1.79	0.64
12:E:262:ASN:ND2	3:H:628:GLU:OE2	2.28	0.64
3:T:128:MET:O	8:P:176:GLU:N	2.25	0.64
9:W:98:DA:H5'	9:W:98:DA:C8	2.33	0.64
12:E:674:ALA:CB	16:L:2626:LEU:HD21	2.27	0.64
14:G:299:MET:HB3	14:G:304:THR:HG21	1.80	0.64
3:T:126:ALA:HB3	8:P:309:PRO:HB2	1.79	0.64
16:L:3274:GLU:N	16:L:3274:GLU:OE2	2.30	0.64
9:W:72:DC:H2''	9:W:73:DG:C8	2.33	0.64
3:T:316:GLU:HG3	8:P:267:ASP:N	2.13	0.64
1:Y:15:LEU:HD11	3:T:372:ARG:HG3	1.79	0.63
16:L:3629:GLN:OE1	16:L:3728:VAL:CG2	2.47	0.63
13:F:30:TYR:OH	13:F:98:LEU:O	2.17	0.63
6:S:20:ARG:NH2	10:I:32:DG:OP1	2.27	0.63
9:W:80:DC:H2''	9:W:81:DC:C5	2.34	0.63
16:L:2620:PRO:O	16:L:2621:HIS:CG	2.52	0.63
9:W:90:DA:H1'	9:W:91:DA:C8	2.34	0.63
16:L:610:GLU:OE2	16:L:1582:ARG:NH2	2.32	0.62
16:L:2415:ARG:CZ	16:L:2415:ARG:HA	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:11:LEU:HD21	3:T:374:LYS:HE2	1.82	0.62
8:P:196:TYR:HB2	8:P:205:PHE:HB2	1.80	0.62
9:W:78:DC:H2''	9:W:79:DC:C5	2.35	0.62
16:L:2620:PRO:O	16:L:2621:HIS:ND1	2.32	0.62
16:L:3075:ILE:HG22	16:L:3077:PHE:H	1.64	0.62
16:L:3481:ASP:OD1	16:L:3482:PRO:HD2	2.00	0.61
2:V:65:GLU:OE1	3:T:380:ARG:NH1	2.28	0.61
3:H:558:SER:HB3	16:L:3519:THR:HG22	1.81	0.61
12:E:225:TYR:HB2	16:L:3295:LYS:NZ	2.16	0.61
16:L:17:ASP:OD1	16:L:26:SER:OG	2.18	0.61
16:L:867:VAL:HG21	16:L:872:LEU:HA	1.82	0.61
16:L:3304:LYS:N	16:L:3305:PRO:HD2	2.14	0.61
12:E:684:TYR:HB3	16:L:2755:PHE:CZ	2.36	0.61
8:P:185:TYR:CZ	8:P:253:LEU:HB3	2.36	0.60
9:W:-12:DA:H2'	9:W:-11:DT:H71	1.83	0.60
12:E:360:ASN:OD1	15:K:182:ARG:NH2	2.33	0.60
14:G:237:GLU:HA	14:G:251:GLY:HA2	1.81	0.60
16:L:3260:TYR:O	16:L:3263:LEU:HD23	2.02	0.60
16:L:840:GLN:NE2	16:L:878:PHE:O	2.35	0.60
16:L:2748:GLU:O	16:L:2752:HIS:HB2	2.00	0.60
4:A:61:LEU:HD12	5:B:37:LEU:HD23	1.84	0.60
15:K:113:LYS:O	15:K:116:GLN:NE2	2.35	0.60
16:L:1626:ASN:OD1	16:L:1630:ARG:NH2	2.35	0.59
3:T:313:ARG:HH21	3:T:315:ARG:HG3	1.66	0.59
14:G:311:GLU:OE2	14:G:311:GLU:N	2.31	0.59
9:W:126:DG:H2''	9:W:127:DT:O5'	2.01	0.59
3:T:305:GLU:HG3	3:T:310:VAL:HG11	1.84	0.59
15:K:120:ILE:HD12	15:K:177:LYS:HG2	1.84	0.59
15:K:288:ASP:OD1	15:K:289:GLN:N	2.34	0.59
8:P:258:PHE:HB2	8:P:306:LEU:HD11	1.84	0.59
12:E:674:ALA:HB3	16:L:2626:LEU:HD21	1.84	0.59
16:L:1386:ASP:OD2	16:L:1412:ARG:NH1	2.36	0.59
10:I:110:DA:H1'	10:I:111:DC:H5'	1.85	0.58
16:L:3265:PHE:HA	16:L:3267:ARG:HG3	1.85	0.58
9:W:138:DT:H2''	9:W:139:DA:C8	2.38	0.58
16:L:2413:THR:HA	16:L:2416:MET:SD	2.43	0.58
16:L:3299:ASP:OD2	16:L:3313:ARG:HD3	2.02	0.58
16:L:3153:ARG:NH1	16:L:3210:GLU:OE2	2.36	0.58
1:Y:1:MET:HG3	1:Y:3:ASP:H	1.68	0.58
2:V:92:THR:HG22	3:T:251:THR:HB	1.86	0.58
16:L:1098:ASP:OD1	16:L:1098:ASP:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:68:DT:H2''	9:W:69:DA:C8	2.38	0.58
16:L:2807:ARG:NH2	16:L:2863:HIS:O	2.37	0.58
16:L:3332:GLU:OE2	16:L:3389:ARG:NE	2.36	0.58
16:L:2625:TYR:CZ	16:L:2664:GLU:OE1	2.57	0.58
16:L:576:THR:O	16:L:576:THR:HG22	2.04	0.57
8:P:228:ILE:HB	8:P:431:TRP:HB2	1.85	0.57
9:W:129:DT:H2''	9:W:130:DC:C5	2.39	0.57
14:G:218:TYR:OH	14:G:226:GLU:OE2	2.20	0.57
10:I:105:DT:H2''	10:I:106:DG:C8	2.38	0.57
16:L:778:ASN:OD1	16:L:779:ILE:N	2.37	0.57
9:W:34:DG:H2'	9:W:35:DT:C6	2.40	0.57
3:T:227:SER:OG	3:T:229:MET:SD	2.62	0.57
5:B:92:ARG:HH21	7:D:101:LEU:HD23	1.68	0.57
16:L:128:SER:O	16:L:131:SER:OG	2.21	0.57
16:L:2643:ILE:HB	16:L:2658:ASN:ND2	2.19	0.57
9:W:126:DG:H2'	9:W:127:DT:C6	2.40	0.57
16:L:358:ASN:O	16:L:361:LYS:NZ	2.35	0.57
9:W:124:DA:H1'	9:W:125:DC:H5'	1.86	0.56
14:G:192:ILE:HD11	14:G:256:ARG:HE	1.70	0.56
16:L:130:LYS:NZ	16:L:224:LEU:O	2.33	0.56
3:T:236:ASN:OD1	3:T:245:HIS:NE2	2.33	0.56
3:H:556:SER:O	3:H:558:SER:N	2.37	0.56
3:H:722:PHE:CG	3:H:722:PHE:O	2.58	0.56
16:L:1685:LEU:HB3	16:L:1688:LYS:HB3	1.87	0.56
16:L:2373:ALA:HB1	16:L:2415:ARG:HB3	1.87	0.56
16:L:3483:ASP:OD1	16:L:3483:ASP:N	2.34	0.56
16:L:3657:ASN:ND2	16:L:3657:ASN:O	2.39	0.56
16:L:3610:ASP:OD1	16:L:3610:ASP:N	2.39	0.56
12:E:299:LEU:HD13	15:K:278:LEU:HD12	1.87	0.56
16:L:1509:LEU:O	16:L:1513:TYR:OH	2.19	0.56
16:L:2206:LEU:HA	16:L:2209:VAL:HG12	1.87	0.56
16:L:2755:PHE:CE2	16:L:2757:ASP:HB2	2.41	0.56
8:P:168:ASN:ND2	8:P:192:GLU:O	2.37	0.56
16:L:2369:VAL:CG2	16:L:2412:ILE:HD11	2.36	0.56
1:Y:15:LEU:HD13	3:T:375:ILE:HD12	1.87	0.56
12:E:795:THR:O	12:E:797:ALA:N	2.39	0.56
3:H:717:GLU:N	3:H:717:GLU:OE1	2.38	0.56
12:E:330:ARG:NH1	12:E:333:GLU:OE2	2.35	0.56
16:L:3611:SER:HB3	16:L:3674:TRP:HE1	1.70	0.56
12:E:339:LEU:N	12:E:339:LEU:HD23	2.21	0.55
13:F:281:ASP:OD1	13:F:282:ASN:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:1052:LEU:HB2	16:L:1055:ILE:HD11	1.88	0.55
3:H:501:VAL:CG1	3:H:502:LEU:N	2.69	0.55
16:L:235:TYR:OH	16:L:316:GLU:OE2	2.22	0.55
16:L:2484:LYS:HE3	16:L:2535:ARG:HD2	1.88	0.55
16:L:2593:THR:HA	16:L:2596:ILE:HG13	1.87	0.55
16:L:3593:TYR:HB2	16:L:3596:VAL:HG12	1.87	0.55
16:L:2422:VAL:HA	16:L:2463:ILE:HD11	1.88	0.55
16:L:2774:ASP:N	16:L:2774:ASP:OD1	2.35	0.55
12:E:335:ARG:NH2	3:H:539:THR:HG21	2.22	0.55
16:L:65:SER:OG	16:L:72:GLU:OE2	2.23	0.55
16:L:2373:ALA:HB1	16:L:2415:ARG:CB	2.37	0.55
10:I:149:DG:H2"	10:I:150:DC:C5	2.42	0.55
12:E:607:ASP:O	16:L:2574:ASN:OD1	2.25	0.55
12:E:753:ARG:HA	12:E:756:ARG:HB2	1.89	0.55
16:L:1774:SER:OG	16:L:1777:GLU:OE2	2.24	0.55
16:L:2768:ASP:OD1	16:L:2769:TRP:N	2.40	0.55
9:W:-30:DC:H2"	9:W:-29:DT:H71	1.90	0.54
12:E:311:THR:O	12:E:313:ASN:N	2.40	0.54
12:E:649:ILE:HG12	12:E:688:ILE:HB	1.89	0.54
16:L:3289:ALA:HB2	16:L:3293:ARG:NH1	2.22	0.54
12:E:807:ASP:OD1	12:E:808:GLU:N	2.40	0.54
13:F:302:ALA:O	13:F:303:ASN:OD1	2.25	0.54
14:G:304:THR:O	14:G:335:ARG:NH1	2.40	0.54
16:L:2294:GLN:HG2	16:L:2295:PRO:HD3	1.89	0.54
3:T:328:ILE:HG23	3:T:329:LEU:HD22	1.89	0.54
16:L:107:LEU:HB2	16:L:108:PRO:HD3	1.89	0.54
16:L:2089:SER:OG	16:L:2090:LEU:N	2.41	0.54
16:L:2854:GLU:OE1	16:L:2884:TRP:NE1	2.35	0.54
16:L:3021:GLU:HA	16:L:3024:THR:HG22	1.89	0.54
3:T:141:PHE:N	8:P:281:GLU:O	2.22	0.54
16:L:2755:PHE:CD1	16:L:2756:THR:N	2.76	0.54
10:I:65:DC:H2"	10:I:66:DG:C8	2.42	0.54
8:P:177:ILE:HD12	8:P:258:PHE:HZ	1.73	0.54
7:U:68:ASP:OD2	5:B:98:TYR:OH	2.25	0.54
12:E:312:THR:OG1	16:L:3728:VAL:HG22	2.08	0.54
13:F:212:ARG:NH2	13:F:271:GLU:OE1	2.35	0.54
13:F:411:THR:HG22	13:F:412:GLY:H	1.73	0.54
16:L:776:PHE:HB3	16:L:779:ILE:HB	1.90	0.54
3:T:132:GLU:HG2	3:T:135:LYS:HD2	1.90	0.53
3:T:316:GLU:HB2	8:P:267:ASP:HB3	1.91	0.53
9:W:17:DC:H2"	9:W:18:DC:C5	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:3:DC:H2''	10:I:4:DG:C8	2.43	0.53
1:Y:21:ASP:O	1:Y:25:GLN:HG2	2.08	0.53
10:I:27:DC:H2''	10:I:28:DT:C5	2.43	0.53
12:E:794:PRO:O	12:E:795:THR:OG1	2.26	0.53
13:F:469:TRP:O	15:K:86:ASN:ND2	2.40	0.53
3:H:500:ILE:O	3:H:501:VAL:CG2	2.56	0.53
3:H:500:ILE:CD1	3:H:501:VAL:H	2.20	0.53
16:L:85:ARG:NH2	16:L:1975:VAL:O	2.38	0.53
3:T:313:ARG:HH12	8:P:265:TYR:HA	1.73	0.53
12:E:615:LEU:HG	16:L:2456:ARG:CZ	2.38	0.53
15:K:314:LYS:O	15:K:315:ARG:CB	2.56	0.53
16:L:872:LEU:HD12	16:L:873:ALA:N	2.23	0.53
16:L:2613:ILE:HG22	16:L:2615:SER:H	1.74	0.53
14:G:131:ALA:HB1	14:G:356:TRP:HB3	1.89	0.53
16:L:2412:ILE:HB	16:L:2415:ARG:HB2	1.89	0.53
16:L:2493:CYS:SG	16:L:2494:LEU:HD23	2.49	0.53
16:L:3407:TYR:HB3	16:L:3408:PRO:HD3	1.91	0.53
8:P:292:LYS:HE3	8:P:301:ASN:HA	1.91	0.53
3:H:557:THR:HG22	3:H:625:GLU:HG3	1.90	0.53
16:L:305:LEU:HA	16:L:308:VAL:HG22	1.89	0.53
16:L:1007:TYR:HA	16:L:1014:ARG:HH22	1.74	0.53
9:W:70:DC:H2''	9:W:71:DG:C8	2.44	0.53
16:L:2619:PRO:HB2	16:L:2624:LYS:HE3	1.91	0.53
3:T:133:TYR:CG	8:P:174:LYS:HB3	2.43	0.53
12:E:336:ARG:NH1	12:E:336:ARG:HB3	2.23	0.53
16:L:621:SER:O	16:L:624:ARG:NH2	2.42	0.53
8:P:188:GLU:O	8:P:192:GLU:HG2	2.07	0.53
10:I:36:DA:H2''	10:I:37:DG:C8	2.44	0.53
3:H:537:ASN:OD1	3:H:539:THR:HG22	2.09	0.53
16:L:479:ASN:ND2	16:L:640:GLU:OE1	2.42	0.53
16:L:2284:LYS:HA	16:L:2287:LYS:HG2	1.91	0.53
13:F:433:PRO:O	13:F:434:SER:OG	2.11	0.53
16:L:66:TYR:CD2	16:L:114:ASN:HA	2.44	0.53
16:L:1638:GLU:O	16:L:1642:LYS:NZ	2.40	0.53
16:L:2405:GLU:OE1	16:L:2411:GLU:HG2	2.09	0.53
16:L:2864:THR:O	16:L:2873:LYS:NZ	2.40	0.53
12:E:354:GLN:NE2	15:K:180:ASP:O	2.42	0.52
15:K:313:ARG:HB2	3:H:501:VAL:HG21	1.91	0.52
9:W:105:DT:H2''	9:W:106:DA:O5'	2.08	0.52
16:L:577:ASN:ND2	16:L:582:ASP:OD2	2.42	0.52
16:L:2444:GLU:O	16:L:2450:ARG:NE	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:244:SER:O	3:T:244:SER:OG	2.28	0.52
3:T:310:VAL:HG12	3:T:313:ARG:HD3	1.91	0.52
15:K:313:ARG:HB2	3:H:501:VAL:CG2	2.39	0.52
16:L:1775:ASN:OD1	16:L:1776:LYS:N	2.42	0.52
3:T:295:LEU:HD23	3:T:296:LYS:O	2.10	0.52
16:L:863:ILE:HG13	16:L:864:THR:HG23	1.92	0.52
2:V:44:GLN:NE2	2:V:48:GLN:OE1	2.42	0.52
8:P:245:ARG:NH1	8:P:269:ASP:OD2	2.43	0.52
15:K:167:GLU:N	15:K:167:GLU:OE1	2.38	0.52
16:L:381:PHE:HB2	16:L:1857:HIS:HA	1.91	0.52
9:W:123:DC:H2''	9:W:124:DA:C8	2.44	0.52
16:L:1562:LEU:O	16:L:1602:ARG:NH1	2.41	0.52
3:T:197:GLU:OE2	3:T:283:LYS:NZ	2.33	0.52
3:T:376:LYS:HG2	3:T:391:LEU:HD13	1.91	0.52
10:I:66:DG:H2'	10:I:67:DG:C8	2.44	0.52
16:L:245:SER:OG	16:L:247:PRO:O	2.23	0.52
16:L:1141:ASP:OD1	16:L:1141:ASP:N	2.35	0.52
16:L:2627:ALA:O	16:L:2628:ILE:HD13	2.10	0.52
16:L:2720:PRO:O	16:L:2721:TYR:CG	2.62	0.52
16:L:846:ILE:HG21	16:L:854:GLU:OE1	2.10	0.52
16:L:2772:ASP:OD1	16:L:2772:ASP:N	2.41	0.52
16:L:3277:GLU:O	16:L:3281:VAL:HG12	2.10	0.52
9:W:110:DC:H2''	9:W:111:DC:C5	2.45	0.52
12:E:631:LEU:HD13	12:E:713:LYS:HG2	1.92	0.52
2:V:98:ALA:HB3	3:T:238:LEU:HD11	1.92	0.51
3:T:167:ARG:HD3	3:T:282:ARG:CZ	2.40	0.51
10:I:81:DC:H2''	10:I:82:DG:C8	2.44	0.51
3:H:547:PHE:CD1	3:H:572:ILE:HD12	2.45	0.51
16:L:1062:ASP:OD1	16:L:1062:ASP:N	2.43	0.51
16:L:2104:VAL:HG21	16:L:2121:ILE:HD11	1.92	0.51
16:L:2177:LYS:HG3	16:L:2179:TRP:HB2	1.92	0.51
6:N:92:GLU:OE1	11:X:58:ARG:NH1	2.41	0.51
3:T:177:ASN:HD21	3:T:183:ILE:HG23	1.76	0.51
10:I:107:DT:H2'	10:I:108:DC:C6	2.45	0.51
12:E:625:ASN:O	12:E:627:ARG:NE	2.42	0.51
3:H:505:VAL:HG22	16:L:2720:PRO:HB2	1.92	0.51
16:L:3462:VAL:O	16:L:3463:SER:OG	2.20	0.51
8:P:232:ASP:OD1	8:P:232:ASP:N	2.44	0.51
16:L:1825:LEU:HD12	16:L:1828:ASP:HA	1.93	0.51
2:V:88:VAL:O	2:V:92:THR:HG23	2.11	0.51
2:V:112:GLU:OE2	3:T:335:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:321:ARG:NH1	10:I:87:DT:O3'	2.35	0.51
10:I:49:DC:H2''	10:I:50:DT:H72	1.92	0.51
16:L:2:SER:OG	16:L:39:ASN:O	2.15	0.51
16:L:47:PHE:O	16:L:51:VAL:HG13	2.11	0.51
12:E:298:PRO:HG2	12:E:301:ASN:ND2	2.26	0.51
16:L:3646:PHE:HB2	16:L:3717:THR:HG22	1.93	0.51
16:L:3685:ASN:N	16:L:3685:ASN:OD1	2.44	0.51
14:G:260:ALA:HB1	14:G:267:LEU:HD11	1.92	0.51
2:V:3:PRO:HG2	3:T:326:ILE:O	2.11	0.51
12:E:347:ARG:NH2	12:E:580:LEU:O	2.43	0.51
16:L:3202:ARG:HG2	16:L:3204:PRO:HD2	1.93	0.51
9:W:34:DG:H2''	9:W:35:DT:O5'	2.11	0.51
10:I:37:DG:H2''	10:I:38:DG:C8	2.45	0.51
16:L:219:PHE:HA	16:L:308:VAL:HG11	1.92	0.51
9:W:-11:DT:H2''	9:W:-10:DA:C8	2.46	0.50
12:E:607:ASP:OD1	12:E:607:ASP:N	2.40	0.50
3:H:505:VAL:HG22	16:L:2720:PRO:CB	2.41	0.50
3:H:630:HIS:O	3:H:631:SER:OG	2.29	0.50
16:L:284:GLU:HG2	16:L:285:ILE:H	1.76	0.50
16:L:934:PRO:HD3	16:L:2829:VAL:HG21	1.92	0.50
16:L:1327:ASP:O	16:L:1330:LYS:NZ	2.42	0.50
8:P:280:ASP:N	8:P:283:GLY:O	2.43	0.50
9:W:98:DA:H5'	9:W:98:DA:H8	1.75	0.50
13:F:213:LYS:HB3	13:F:214:PRO:HD3	1.93	0.50
3:H:546:VAL:O	3:H:575:SER:HA	2.11	0.50
16:L:2272:VAL:N	16:L:2273:PRO:CD	2.74	0.50
16:L:2373:ALA:CB	16:L:2415:ARG:HG3	2.41	0.50
16:L:2773:ARG:NH2	16:L:2805:GLU:OE2	2.43	0.50
16:L:3050:ASP:OD1	16:L:3050:ASP:N	2.42	0.50
16:L:3433:ASN:HB3	16:L:3436:THR:OG1	2.11	0.50
2:V:44:GLN:O	2:V:48:GLN:HG3	2.11	0.50
8:P:407:GLU:HG2	8:P:408:ASP:N	2.27	0.50
9:W:121:DG:H2''	9:W:122:DG:C8	2.46	0.50
9:W:90:DA:H1'	9:W:91:DA:N7	2.26	0.50
16:L:118:CYS:HA	16:L:121:VAL:HG22	1.93	0.50
16:L:1741:ASN:OD1	16:L:1742:PRO:HD3	2.11	0.50
16:L:2616:LEU:O	16:L:2618:LEU:N	2.45	0.50
12:E:642:LEU:HD23	12:E:642:LEU:H	1.76	0.50
16:L:2204:GLU:OE1	16:L:2204:GLU:N	2.43	0.50
2:V:50:HIS:CD2	3:T:393:ASN:H	2.30	0.50
3:T:332:GLN:HG3	3:T:333:ARG:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:138:DG:H2''	10:I:139:DA:C8	2.47	0.50
16:L:1444:PHE:HB3	16:L:1463:LEU:HD21	1.93	0.50
16:L:1844:ASN:HA	16:L:1848:ILE:HG13	1.94	0.50
16:L:2621:HIS:HA	16:L:2624:LYS:HG2	1.93	0.50
9:W:72:DC:H2''	9:W:73:DG:H8	1.74	0.50
10:I:106:DG:H2''	10:I:107:DT:H5''	1.93	0.50
10:I:144:DC:H2''	10:I:145:DG:C8	2.46	0.50
16:L:1298:ASN:OD1	16:L:1303:VAL:HG11	2.11	0.50
3:T:328:ILE:O	3:T:332:GLN:HG2	2.12	0.49
12:E:225:TYR:HB2	16:L:3295:LYS:CE	2.42	0.49
12:E:628:ASN:HA	12:E:631:LEU:HD12	1.94	0.49
16:L:76:ARG:HH12	16:L:116:ILE:HG13	1.76	0.49
16:L:1028:MET:O	16:L:2493:CYS:SG	2.68	0.49
16:L:1988:PHE:O	16:L:1992:HIS:ND1	2.45	0.49
16:L:2181:MET:HA	16:L:2184:LEU:HG	1.93	0.49
8:P:346:LEU:O	8:P:350:ARG:HG2	2.12	0.49
15:K:285:PRO:CB	16:L:2719:LEU:HD21	2.42	0.49
16:L:1704:LYS:O	16:L:1708:GLU:HG2	2.12	0.49
13:F:485:ASN:OD1	13:F:486:ASP:N	2.43	0.49
3:H:539:THR:HG23	3:H:540:ASP:N	2.26	0.49
16:L:402:ILE:HG13	16:L:403:ARG:H	1.77	0.49
16:L:2768:ASP:O	16:L:2770:ASN:ND2	2.45	0.49
5:Q:77:LYS:HE2	7:U:92:ARG:CZ	2.42	0.49
12:E:311:THR:HA	16:L:3629:GLN:OE1	2.12	0.49
9:W:-23:DC:H2''	9:W:-22:DC:C5	2.47	0.49
12:E:679:ARG:O	16:L:2664:GLU:HG2	2.13	0.49
16:L:3524:SER:O	16:L:3524:SER:OG	2.24	0.49
12:E:603:ARG:HE	3:H:631:SER:HB3	1.78	0.49
16:L:2275:LEU:HA	16:L:2278:LEU:HD13	1.94	0.49
8:P:170:ILE:HG12	8:P:195:ILE:HB	1.94	0.49
9:W:68:DT:H2''	9:W:69:DA:N7	2.27	0.49
16:L:910:ALA:HB2	16:L:955:ARG:NH1	2.28	0.49
16:L:1830:LYS:O	16:L:1830:LYS:HG3	2.12	0.49
16:L:2499:ILE:HD12	16:L:2502:GLU:HB2	1.94	0.49
16:L:3023:PHE:HB3	16:L:3046:ALA:HB2	1.93	0.49
10:I:15:DT:H4'	10:I:16:DC:OP1	2.12	0.49
11:X:58:ARG:O	11:X:59:LYS:HG2	2.13	0.49
16:L:908:LEU:O	16:L:909:THR:HG22	2.12	0.49
16:L:3121:PHE:CD2	16:L:3151:MET:HB2	2.48	0.49
9:W:-6:DG:H2''	9:W:-5:DG:C8	2.48	0.49
16:L:2540:ASP:OD1	16:L:2541:PHE:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:2755:PHE:CD2	16:L:2757:ASP:HB2	2.48	0.49
16:L:3128:ILE:HD11	16:L:3158:ARG:HD2	1.94	0.49
2:V:96:LEU:HD21	3:T:253:PHE:HE2	1.78	0.49
3:T:315:ARG:NH2	8:P:266:TYR:OH	2.46	0.49
12:E:625:ASN:O	12:E:627:ARG:NH2	2.41	0.49
13:F:252:THR:HB	13:F:257:GLU:OE2	2.13	0.49
16:L:793:LEU:HG	16:L:831:ILE:HD11	1.93	0.49
2:V:11:ILE:HA	2:V:14:VAL:HG12	1.95	0.48
16:L:2653:LYS:HA	16:L:2656:GLU:HG3	1.96	0.48
3:T:379:LYS:O	3:T:383:ASN:N	2.45	0.48
15:K:120:ILE:HG23	15:K:177:LYS:HG2	1.94	0.48
12:E:265:ALA:O	12:E:266:LEU:HG	2.13	0.48
12:E:622:PHE:O	12:E:623:TYR:HB3	2.13	0.48
16:L:2762:CYS:HA	16:L:2769:TRP:CZ3	2.48	0.48
9:W:114:DG:H2''	9:W:115:DT:H5'	1.96	0.48
12:E:625:ASN:OD1	16:L:2414:VAL:HG22	2.13	0.48
12:E:684:TYR:CD1	16:L:2755:PHE:CZ	3.02	0.48
16:L:678:ASP:OD1	16:L:678:ASP:N	2.45	0.48
16:L:867:VAL:HG22	16:L:869:LEU:N	2.27	0.48
16:L:1048:ASN:HA	16:L:1051:LYS:HE2	1.94	0.48
16:L:3045:THR:HA	16:L:3048:GLN:HG3	1.95	0.48
12:E:796:PRO:HD2	16:L:3080:ASN:OD1	2.13	0.48
3:H:674:ASP:OD1	3:H:675:SER:N	2.46	0.48
16:L:1848:ILE:O	16:L:1849:LEU:HB2	2.14	0.48
16:L:3140:LEU:HD22	16:L:3152:VAL:HG23	1.94	0.48
14:G:205:GLU:O	14:G:208:ILE:N	2.45	0.48
16:L:2917:LEU:HB3	16:L:2918:PRO:HD3	1.96	0.48
3:T:125:ASP:O	8:P:178:GLU:HB3	2.13	0.48
12:E:335:ARG:HD3	12:E:343:ARG:HD2	1.96	0.48
12:E:731:GLN:OE1	12:E:739:SER:N	2.36	0.48
16:L:3063:PHE:CZ	16:L:3067:ARG:HD2	2.48	0.48
14:G:78:ASN:ND2	14:G:81:ASP:OD2	2.47	0.48
16:L:2272:VAL:CG1	16:L:2273:PRO:HD3	2.44	0.48
16:L:2616:LEU:O	16:L:2616:LEU:HD12	2.14	0.48
3:T:124:PRO:HB2	8:P:180:TRP:CD1	2.48	0.48
3:T:332:GLN:HG3	3:T:333:ARG:N	2.28	0.48
10:I:127:DC:H2'	10:I:128:DT:C6	2.48	0.48
16:L:3087:GLN:O	16:L:3091:LEU:HD23	2.14	0.48
16:L:3131:TRP:CH2	16:L:3362:LYS:O	2.66	0.48
3:T:238:LEU:O	3:T:242:ILE:HG13	2.14	0.48
3:T:351:VAL:O	3:T:355:GLU:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:71:ARG:HH22	8:P:399:GLY:HA3	1.79	0.48
16:L:440:LEU:O	16:L:443:VAL:HG12	2.14	0.48
16:L:779:ILE:HG22	16:L:780:ASN:H	1.79	0.48
16:L:2249:GLU:HG2	16:L:2251:SER:H	1.79	0.48
16:L:3260:TYR:O	16:L:3263:LEU:CD2	2.62	0.48
16:L:3291:TYR:CE1	16:L:3292:ILE:HG12	2.48	0.48
3:T:239:ASN:HD21	3:T:248:HIS:HA	1.79	0.47
16:L:2411:GLU:OE2	16:L:2416:MET:SD	2.72	0.47
16:L:2626:LEU:C	16:L:2628:ILE:H	2.17	0.47
8:P:358:ILE:O	8:P:362:VAL:HG23	2.14	0.47
14:G:237:GLU:OE2	14:G:250:ILE:N	2.47	0.47
15:K:44:ARG:NH2	3:H:701:GLU:OE1	2.42	0.47
16:L:2786:VAL:HG23	16:L:2786:VAL:O	2.14	0.47
3:T:281:GLU:O	3:T:285:GLU:HG3	2.14	0.47
5:B:31:LYS:HG3	5:B:51:TYR:CE2	2.49	0.47
10:I:115:DC:H2"	10:I:116:DA:C8	2.50	0.47
15:K:303:LEU:O	15:K:307:LEU:HD23	2.14	0.47
16:L:346:GLU:HA	16:L:349:HIS:HB2	1.96	0.47
16:L:1368:LEU:HG	16:L:1368:LEU:O	2.14	0.47
12:E:335:ARG:CZ	3:H:539:THR:HG21	2.44	0.47
16:L:1898:ASP:OD1	16:L:1899:THR:N	2.47	0.47
16:L:3132:TYR:OH	16:L:3363:ASP:OD1	2.23	0.47
9:W:-18:DG:H2"	9:W:-17:DA:C8	2.49	0.47
9:W:6:DG:H2"	9:W:7:DA:H8	1.79	0.47
16:L:61:GLU:O	16:L:62:VAL:HG12	2.15	0.47
16:L:84:ASN:OD1	16:L:120:LYS:HB3	2.15	0.47
16:L:1366:THR:HG22	16:L:1367:PHE:CG	2.50	0.47
16:L:1397:GLN:NE2	16:L:1400:THR:O	2.37	0.47
16:L:1989:LEU:O	16:L:1993:PRO:HD2	2.15	0.47
16:L:2166:ASP:HA	16:L:2169:TYR:CE2	2.50	0.47
16:L:2411:GLU:OE1	16:L:2416:MET:SD	2.73	0.47
16:L:2540:ASP:OD1	16:L:2540:ASP:N	2.46	0.47
12:E:619:ARG:HG2	16:L:2457:ASP:OD2	2.15	0.47
3:H:555:PHE:HD1	3:H:556:SER:O	1.98	0.47
16:L:626:PHE:HB3	16:L:630:GLU:HB2	1.96	0.47
16:L:2421:LEU:HB3	16:L:2463:ILE:HG12	1.97	0.47
16:L:3287:LEU:HD13	16:L:3292:ILE:HG22	1.96	0.47
16:L:3654:GLU:N	16:L:3655:PRO:HD3	2.30	0.47
2:V:42:TYR:HB3	2:V:75:SER:OG	2.15	0.47
6:S:90:ASP:HB3	6:S:93:LEU:HB2	1.97	0.47
6:N:90:ASP:HB3	6:N:93:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:110:DA:H2''	10:I:111:DC:OP2	2.15	0.47
10:I:170:DG:H2'	10:I:171:DG:C8	2.49	0.47
12:E:299:LEU:HD12	12:E:321:GLU:HG3	1.96	0.47
14:G:216:LEU:O	14:G:254:ARG:HD3	2.14	0.47
16:L:130:LYS:NZ	16:L:225:SER:OG	2.47	0.47
16:L:255:ASN:OD1	16:L:256:LEU:HD12	2.14	0.47
16:L:785:LEU:N	16:L:786:PRO:HD2	2.30	0.47
16:L:1012:HIS:CD2	16:L:2429:ILE:HD13	2.49	0.47
16:L:1756:ILE:HG13	16:L:1757:LYS:HG2	1.95	0.47
16:L:2402:PHE:CZ	16:L:2416:MET:HB2	2.50	0.47
3:T:166:GLU:HA	3:T:169:GLU:HG2	1.96	0.47
5:B:38:ALA:HB1	5:B:43:VAL:HB	1.96	0.47
13:F:215:GLU:O	13:F:217:ILE:HG13	2.15	0.47
16:L:1615:MET:HB2	16:L:1650:PHE:CE2	2.49	0.47
16:L:1796:LEU:HG	16:L:1798:ALA:H	1.80	0.47
16:L:3625:THR:O	16:L:3629:GLN:HB2	2.15	0.47
9:W:26:DC:H2''	9:W:27:DT:C6	2.50	0.47
12:E:622:PHE:CD1	16:L:2417:GLU:HB2	2.50	0.47
12:E:793:VAL:HG13	16:L:3040:ASN:ND2	2.30	0.47
16:L:2316:TYR:O	16:L:2320:LEU:CB	2.63	0.47
16:L:3350:GLU:N	16:L:3350:GLU:OE1	2.48	0.47
2:V:94:LEU:HA	2:V:97:ILE:HG22	1.96	0.47
8:P:170:ILE:HG23	8:P:195:ILE:HG22	1.97	0.47
12:E:628:ASN:OD1	12:E:631:LEU:HB2	2.14	0.47
12:E:718:HIS:O	12:E:722:GLN:HG2	2.15	0.47
13:F:226:ASP:OD2	13:F:228:SER:OG	2.22	0.47
16:L:2418:GLN:HB3	16:L:2419:PRO:HD2	1.97	0.47
16:L:2418:GLN:OE1	16:L:2462:PHE:CD1	2.67	0.47
16:L:2651:ASN:HB3	16:L:2653:LYS:HG2	1.97	0.47
3:T:197:GLU:HG3	3:T:201:HIS:CE1	2.50	0.46
10:I:152:DG:H2''	10:I:153:DC:C5	2.49	0.46
16:L:412:GLU:HG2	16:L:463:LEU:HD21	1.97	0.46
16:L:2619:PRO:HG2	16:L:2624:LYS:NZ	2.30	0.46
16:L:2721:TYR:HB2	16:L:2726:TYR:HB2	1.96	0.46
8:P:231:ASP:OD1	8:P:234:VAL:N	2.35	0.46
15:K:124:THR:OG1	15:K:127:GLU:OE1	2.14	0.46
16:L:355:LEU:HD21	16:L:364:LEU:HD23	1.98	0.46
16:L:1171:ILE:HD11	16:L:1193:LEU:CD2	2.45	0.46
16:L:1683:GLU:HB2	16:L:1687:LYS:H	1.80	0.46
3:T:201:HIS:NE2	3:T:290:GLU:OE2	2.48	0.46
3:T:277:ASP:O	3:T:281:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:8:DG:H2''	10:I:9:DT:H5'	1.97	0.46
16:L:2685:TYR:CD1	16:L:2685:TYR:N	2.83	0.46
4:O:62:ILE:HB	4:O:93:GLN:HE21	1.81	0.46
5:B:92:ARG:NH2	7:D:101:LEU:HD23	2.30	0.46
9:W:47:DC:H2''	9:W:48:DT:C7	2.44	0.46
16:L:1137:ASN:N	16:L:1137:ASN:OD1	2.47	0.46
16:L:1533:GLU:O	16:L:1537:THR:HG23	2.15	0.46
16:L:1849:LEU:O	16:L:1853:VAL:HG22	2.16	0.46
8:P:276:MET:O	8:P:286:LEU:HD12	2.15	0.46
9:W:15:DT:H4'	9:W:16:DG:OP1	2.15	0.46
15:K:324:ASN:N	15:K:324:ASN:OD1	2.48	0.46
16:L:1377:LEU:HA	16:L:1380:GLU:HG2	1.96	0.46
16:L:1787:THR:O	16:L:1791:LEU:HG	2.15	0.46
16:L:2169:TYR:HA	16:L:2172:PHE:HB3	1.96	0.46
9:W:-17:DA:H2''	9:W:-16:DC:C2	2.50	0.46
9:W:113:DA:H2''	9:W:114:DG:H8	1.81	0.46
12:E:684:TYR:CD1	16:L:2755:PHE:CE2	3.03	0.46
15:K:291:ILE:HG12	16:L:2713:LYS:HD3	1.97	0.46
16:L:1327:ASP:N	16:L:1327:ASP:OD1	2.48	0.46
3:T:188:GLU:OE1	3:T:262:ARG:NH2	2.48	0.46
3:T:265:ILE:O	3:T:269:GLU:HG2	2.15	0.46
12:E:669:TRP:O	12:E:693:PRO:HB3	2.16	0.46
16:L:462:LYS:O	16:L:466:ILE:HG13	2.15	0.46
16:L:1603:PHE:O	16:L:1605:ASN:N	2.48	0.46
16:L:2350:ARG:HA	16:L:2353:VAL:HG22	1.97	0.46
12:E:685:LEU:O	16:L:2755:PHE:CD1	2.68	0.46
13:F:125:LEU:HD23	13:F:137:CYS:SG	2.56	0.46
16:L:1962:THR:N	16:L:1963:PRO:HD2	2.31	0.46
3:T:191:ILE:HG22	3:T:264:LEU:HD13	1.97	0.46
3:T:239:ASN:ND2	3:T:248:HIS:HA	2.31	0.46
9:W:14:DG:H2''	9:W:15:DT:H5'	1.97	0.46
9:W:104:DT:C6	9:W:105:DT:H72	2.51	0.46
10:I:127:DC:H2'	10:I:128:DT:C5	2.51	0.46
12:E:312:THR:O	12:E:312:THR:CG2	2.63	0.46
3:H:643:GLY:N	3:H:647:ILE:O	2.44	0.46
16:L:465:MET:HE2	16:L:630:GLU:HB3	1.98	0.46
16:L:2411:GLU:CD	16:L:2416:MET:SD	2.94	0.46
16:L:2474:GLN:HG2	16:L:2546:ILE:HD12	1.98	0.46
16:L:3024:THR:O	16:L:3028:MET:HG3	2.16	0.46
3:T:172:LEU:HD12	3:T:176:VAL:HB	1.96	0.46
9:W:107:DC:H5'	9:W:107:DC:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:383:ILE:HG12	12:E:545:LEU:HD13	1.97	0.46
13:F:46:LYS:O	13:F:69:TYR:O	2.34	0.46
14:G:257:ALA:HB3	14:G:258:PRO:HD3	1.98	0.46
16:L:1950:THR:N	16:L:1951:PRO:HD2	2.31	0.46
16:L:2521:ASN:HA	16:L:2524:LYS:HG2	1.98	0.46
16:L:2726:TYR:HA	16:L:2729:TRP:CE3	2.51	0.46
10:I:75:DC:H2"	10:I:76:DG:C8	2.50	0.45
13:F:408:VAL:O	13:F:439:ILE:O	2.34	0.45
15:K:51:GLY:O	15:K:52:GLU:HG2	2.17	0.45
16:L:306:ALA:HA	16:L:309:PHE:CD1	2.51	0.45
16:L:326:PRO:HB3	16:L:364:LEU:HD13	1.97	0.45
16:L:1954:HIS:O	16:L:1958:ASN:HB2	2.15	0.45
16:L:3594:GLU:H	16:L:3595:ARG:NH1	2.14	0.45
15:K:313:ARG:O	3:H:501:VAL:HG22	2.16	0.45
16:L:1532:VAL:O	16:L:1536:ASP:N	2.49	0.45
6:N:71:ARG:NH2	8:P:399:GLY:HA3	2.32	0.45
16:L:249:PHE:CD1	16:L:288:ARG:HD2	2.51	0.45
16:L:1033:ALA:O	16:L:2531:GLN:NE2	2.50	0.45
16:L:1277:GLU:HB3	16:L:1280:LEU:HB2	1.99	0.45
2:V:62:HIS:HB3	2:V:65:GLU:HB2	1.98	0.45
10:I:81:DC:H2"	10:I:82:DG:H8	1.80	0.45
16:L:1063:LEU:HD22	16:L:3319:ARG:HD3	1.97	0.45
16:L:1827:GLU:HG2	16:L:1829:LYS:HG2	1.98	0.45
16:L:2310:LEU:HA	16:L:2313:LYS:HD2	1.99	0.45
16:L:3449:ILE:HG23	16:L:3457:ILE:HG13	1.97	0.45
12:E:225:TYR:HB2	16:L:3295:LYS:HE2	1.98	0.45
12:E:639:LEU:HG	12:E:640:ARG:H	1.80	0.45
16:L:2038:TRP:O	16:L:2042:THR:HG23	2.16	0.45
16:L:2785:ASP:OD1	16:L:2785:ASP:N	2.45	0.45
16:L:3068:LEU:CD1	16:L:3078:ALA:HB2	2.46	0.45
10:I:121:DA:H2"	10:I:122:DG:C8	2.52	0.45
13:F:463:GLY:O	13:F:464:THR:OG1	2.23	0.45
16:L:306:ALA:HA	16:L:309:PHE:CE1	2.52	0.45
16:L:863:ILE:O	16:L:864:THR:OG1	2.29	0.45
1:Y:19:LEU:HD23	3:T:368:ILE:HD13	1.98	0.45
5:Q:32:PRO:HA	5:Q:35:ARG:HG2	1.98	0.45
6:N:29:ARG:NH1	7:D:36:SER:O	2.50	0.45
8:P:278:ARG:HG3	8:P:285:HIS:HB2	1.97	0.45
10:I:77:DC:H2"	10:I:78:DG:C8	2.52	0.45
16:L:339:GLU:HB2	16:L:1897:GLU:HB2	1.99	0.45
16:L:612:THR:HB	16:L:1532:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:782:VAL:HG23	16:L:785:LEU:HD21	1.98	0.45
16:L:850:ARG:C	16:L:852:PRO:HD3	2.37	0.45
16:L:1474:PRO:HB2	16:L:1478:LEU:HD11	1.99	0.45
16:L:2721:TYR:O	16:L:2723:GLN:N	2.49	0.45
16:L:2982:PHE:CE1	16:L:3018:GLN:HB2	2.52	0.45
5:Q:98:TYR:OH	7:D:68:ASP:OD2	2.27	0.45
12:E:343:ARG:HB3	3:H:537:ASN:HA	1.99	0.45
16:L:1779:GLN:OE1	16:L:1824:TYR:OH	2.29	0.45
16:L:2272:VAL:HG12	16:L:2273:PRO:HD3	1.99	0.45
2:V:109:ALA:O	2:V:113:GLU:HG3	2.17	0.45
6:S:79:ILE:HG12	6:S:82:HIS:CE1	2.52	0.45
9:W:-22:DC:H2"	9:W:-21:DG:C8	2.51	0.45
15:K:310:ASP:O	15:K:312:THR:N	2.48	0.45
16:L:846:ILE:HB	16:L:849:ALA:HB2	1.99	0.45
16:L:848:THR:OG1	16:L:1156:TYR:HB3	2.16	0.45
16:L:2301:LEU:HD23	16:L:2301:LEU:O	2.17	0.45
16:L:3595:ARG:O	16:L:3601:LYS:NZ	2.38	0.45
3:T:141:PHE:HB2	8:P:221:ARG:HD3	1.97	0.44
5:B:24:ASP:HB2	5:B:26:ILE:HG22	1.99	0.44
5:B:32:PRO:O	5:B:36:ARG:HG3	2.17	0.44
6:N:79:ILE:HG12	6:N:82:HIS:CE1	2.52	0.44
14:G:314:GLN:NE2	14:G:327:VAL:O	2.50	0.44
16:L:838:LEU:O	16:L:842:LEU:HB2	2.17	0.44
16:L:1278:GLU:HG2	16:L:1320:ILE:HG12	1.99	0.44
16:L:1504:SER:HB2	16:L:1558:ILE:HG22	1.99	0.44
12:E:266:LEU:O	12:E:267:GLU:HB3	2.18	0.44
12:E:684:TYR:CB	16:L:2755:PHE:CE2	2.96	0.44
12:E:731:GLN:OE1	12:E:738:ILE:N	2.50	0.44
13:F:429:ASN:OD1	3:H:728:ARG:NH2	2.50	0.44
16:L:81:ASP:HA	16:L:84:ASN:HD22	1.82	0.44
16:L:109:LYS:HD2	16:L:114:ASN:HD21	1.82	0.44
16:L:1031:SER:OG	16:L:2493:CYS:SG	2.76	0.44
16:L:2461:GLU:HB3	16:L:2591:TYR:CD2	2.53	0.44
16:L:2499:ILE:HG23	16:L:2500:LEU:HD22	2.00	0.44
16:L:2972:THR:O	16:L:2973:LEU:HD22	2.17	0.44
12:E:314:ILE:HG23	15:K:278:LEU:HD22	1.99	0.44
12:E:339:LEU:O	12:E:340:TRP:CB	2.65	0.44
13:F:145:CYS:O	13:F:455:GLY:HA3	2.18	0.44
16:L:19:ALA:HB3	16:L:22:GLN:HE22	1.82	0.44
16:L:904:CYS:O	16:L:908:LEU:HD12	2.18	0.44
16:L:1340:LYS:HD3	16:L:1345:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:2248:GLN:NE2	16:L:2249:GLU:OE2	2.50	0.44
9:W:127:DT:H2''	9:W:128:DG:C8	2.52	0.44
14:G:37:ARG:HH12	14:G:84:LYS:HD2	1.83	0.44
14:G:304:THR:HG22	14:G:335:ARG:HH11	1.83	0.44
16:L:2483:GLU:HG2	16:L:2485:GLU:H	1.82	0.44
2:V:74:GLU:HG2	2:V:78:LYS:HE3	1.98	0.44
3:T:166:GLU:O	3:T:170:THR:HG23	2.18	0.44
8:P:233:TYR:HE2	8:P:316:TYR:HE1	1.66	0.44
8:P:233:TYR:CD2	8:P:234:VAL:HG13	2.52	0.44
10:I:65:DC:H2''	10:I:66:DG:H8	1.82	0.44
16:L:2557:HIS:ND1	16:L:2605:MET:HG2	2.32	0.44
16:L:3566:ASN:OD1	16:L:3566:ASN:N	2.50	0.44
9:W:-23:DC:H2''	9:W:-22:DC:H5	1.81	0.44
9:W:107:DC:H5'	9:W:107:DC:H6	1.82	0.44
10:I:41:DG:H2'	10:I:42:DT:H71	1.99	0.44
12:E:266:LEU:HD21	12:E:607:ASP:OD1	2.18	0.44
13:F:14:VAL:HG21	15:K:91:LEU:HD13	1.99	0.44
14:G:193:LEU:HA	14:G:253:GLU:OE2	2.17	0.44
16:L:302:THR:O	16:L:305:LEU:HG	2.17	0.44
16:L:869:LEU:HD23	16:L:871:VAL:O	2.17	0.44
16:L:3035:ALA:HB1	16:L:3038:GLU:OE2	2.18	0.44
16:L:2621:HIS:HA	16:L:2624:LYS:CG	2.47	0.44
16:L:3261:ASN:ND2	16:L:3486:GLN:OE1	2.43	0.44
2:V:76:LEU:HD12	2:V:76:LEU:HA	1.86	0.44
3:T:176:VAL:HG22	3:T:274:LYS:HE3	2.00	0.44
9:W:61:DA:H2''	9:W:62:DC:H5'	2.00	0.44
14:G:202:THR:HG23	14:G:205:GLU:HG3	1.99	0.44
3:H:666:SER:OG	3:H:667:LEU:N	2.50	0.44
16:L:2011:MET:HB2	16:L:2028:ALA:HB1	2.00	0.44
16:L:2037:TYR:O	16:L:2041:LYS:HB2	2.18	0.44
16:L:2421:LEU:HD12	16:L:2462:PHE:HD2	1.83	0.44
16:L:3592:PRO:O	16:L:3611:SER:HA	2.17	0.44
2:V:50:HIS:O	2:V:54:ARG:HG3	2.17	0.44
7:D:42:TYR:OH	9:W:21:DG:O5'	2.32	0.44
16:L:453:ASN:OD1	16:L:453:ASN:N	2.51	0.44
16:L:1563:PRO:O	16:L:1565:GLN:N	2.48	0.44
16:L:2285:LEU:O	16:L:2288:ASP:OD2	2.35	0.44
16:L:2344:MET:HB3	16:L:2348:PHE:CZ	2.53	0.44
16:L:2345:ASP:OD2	16:L:2346:GLN:N	2.51	0.44
8:P:255:SER:HA	8:P:306:LEU:HD13	1.98	0.43
12:E:225:TYR:HB2	16:L:3295:LYS:HZ3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:267:LYS:HA	13:F:282:ASN:HD21	1.83	0.43
3:H:722:PHE:O	3:H:722:PHE:CD2	2.71	0.43
16:L:856:GLU:OE1	16:L:856:GLU:N	2.48	0.43
16:L:2249:GLU:OE1	16:L:2252:SER:N	2.51	0.43
16:L:3067:ARG:O	16:L:3070:GLU:HG2	2.18	0.43
16:L:3291:TYR:CD1	16:L:3292:ILE:HG12	2.53	0.43
16:L:3489:MET:O	16:L:3493:LEU:HB2	2.18	0.43
9:W:67:DG:H2''	9:W:68:DT:C5	2.53	0.43
13:F:287:GLY:HA2	13:F:290:GLU:HB3	2.00	0.43
13:F:405:ALA:O	13:F:437:PHE:HA	2.19	0.43
3:H:500:ILE:O	3:H:501:VAL:HG23	2.18	0.43
16:L:61:GLU:O	16:L:62:VAL:CG1	2.66	0.43
16:L:314:ALA:HB3	16:L:315:PRO:HD3	2.00	0.43
16:L:560:MET:SD	16:L:1767:PHE:HB2	2.58	0.43
16:L:2631:ASN:O	16:L:2632:ALA:C	2.56	0.43
16:L:3304:LYS:N	16:L:3305:PRO:CD	2.79	0.43
10:I:90:DA:H2''	10:I:91:DA:N7	2.32	0.43
12:E:247:ILE:HG21	3:H:673:PHE:HZ	1.84	0.43
16:L:1742:PRO:HA	16:L:1745:LEU:HB2	2.00	0.43
16:L:1841:ILE:O	16:L:1844:ASN:CG	2.56	0.43
16:L:2274:LEU:HG	16:L:2277:PRO:HG3	2.00	0.43
17:B:501:CMC:H133	8:P:344:LEU:HG	2.00	0.43
9:W:93:DC:H2''	9:W:94:DG:C8	2.53	0.43
9:W:119:DC:H2''	9:W:120:DA:N7	2.32	0.43
12:E:761:PHE:CZ	16:L:2715:ARG:HG3	2.53	0.43
13:F:182:ARG:NE	13:F:312:VAL:HG11	2.33	0.43
14:G:275:ASP:OD1	14:G:275:ASP:N	2.46	0.43
15:K:285:PRO:HG3	16:L:2719:LEU:CD2	2.48	0.43
3:H:499:ASP:O	3:H:500:ILE:C	2.56	0.43
3:H:500:ILE:HD12	3:H:501:VAL:N	2.25	0.43
16:L:483:ASP:OD1	16:L:483:ASP:N	2.50	0.43
16:L:1144:LEU:HD23	16:L:1144:LEU:H	1.83	0.43
16:L:1782:PHE:O	16:L:1785:ASP:OD2	2.36	0.43
16:L:2413:THR:O	16:L:2416:MET:HG2	2.19	0.43
16:L:2434:ARG:O	16:L:2437:THR:HG22	2.19	0.43
16:L:3088:ALA:O	16:L:3092:TYR:HB2	2.18	0.43
16:L:3360:LEU:HD12	16:L:3360:LEU:O	2.18	0.43
1:Y:23:ARG:HA	3:T:396:ARG:HH21	1.82	0.43
5:B:66:ILE:O	5:B:70:VAL:HG23	2.18	0.43
7:D:102:LEU:HA	7:D:103:PRO:HD3	1.89	0.43
9:W:133:DA:H2'	9:W:134:DT:H71	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:681:THR:HG22	12:E:682:TYR:N	2.34	0.43
13:F:38:SER:HB3	13:F:97:GLU:HB3	2.00	0.43
13:F:410:LEU:HB3	13:F:441:THR:HG22	2.01	0.43
15:K:198:LEU:HG	15:K:198:LEU:O	2.17	0.43
16:L:1369:THR:HB	16:L:1370:PHE:CE2	2.53	0.43
16:L:1618:ARG:NH1	16:L:1668:ASN:OD1	2.39	0.43
16:L:3263:LEU:HD11	16:L:3270:PRO:HB3	2.01	0.43
3:T:128:MET:HB2	8:P:176:GLU:HB3	1.98	0.43
10:I:20:DC:H2''	10:I:21:DA:C8	2.53	0.43
10:I:137:DG:C6	10:I:138:DG:C6	3.06	0.43
12:E:612:ILE:HG22	12:E:612:ILE:O	2.19	0.43
12:E:684:TYR:HD1	16:L:2755:PHE:HZ	1.66	0.43
13:F:18:VAL:HG22	13:F:453:TRP:NE1	2.34	0.43
3:H:739:ILE:HD11	16:L:3492:LYS:HD2	2.01	0.43
16:L:111:ASN:O	16:L:114:ASN:HB2	2.18	0.43
16:L:325:VAL:N	16:L:326:PRO:CD	2.82	0.43
16:L:851:LEU:N	16:L:852:PRO:HD3	2.33	0.43
16:L:1644:LEU:HD21	16:L:1676:MET:HG3	2.00	0.43
16:L:1651:TYR:O	16:L:1655:ILE:HG13	2.18	0.43
10:I:171:DG:H2''	10:I:172:DA:C8	2.54	0.43
13:F:258:THR:HG23	13:F:259:LYS:HD3	2.00	0.43
16:L:1136:PRO:HD3	16:L:2503:TYR:CZ	2.53	0.43
16:L:2418:GLN:OE1	16:L:2462:PHE:CG	2.72	0.43
16:L:2631:ASN:O	16:L:2633:TRP:N	2.51	0.43
16:L:2806:SER:O	16:L:2806:SER:OG	2.32	0.43
16:L:2879:ARG:HA	16:L:2879:ARG:HD2	1.89	0.43
16:L:3507:THR:CG2	16:L:3735:ARG:HD3	2.49	0.43
16:L:3599:LEU:HB3	16:L:3604:ASP:OD2	2.18	0.43
4:O:128:ARG:NE	4:O:133:GLU:OE1	2.49	0.43
8:P:344:LEU:O	8:P:347:LEU:HG	2.18	0.43
10:I:51:DT:C2	10:I:52:DG:C8	3.07	0.43
10:I:69:DG:H1'	10:I:70:DG:C8	2.53	0.43
14:G:303:THR:HG22	14:G:303:THR:O	2.19	0.43
16:L:1376:ARG:O	16:L:1379:GLN:HG3	2.17	0.43
16:L:2418:GLN:OE1	16:L:2418:GLN:HA	2.18	0.43
16:L:3249:ILE:HD13	16:L:3317:TRP:HB3	2.01	0.43
3:T:126:ALA:HB1	8:P:177:ILE:HG22	2.00	0.43
8:P:405:LEU:HD12	8:P:405:LEU:O	2.18	0.43
10:I:50:DT:H2'	10:I:51:DT:H71	2.01	0.43
16:L:850:ARG:HB3	16:L:852:PRO:HD3	1.99	0.43
16:L:1849:LEU:HB3	16:L:1853:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:46:LYS:HA	7:U:46:LYS:HD3	1.81	0.43
8:P:169:ARG:HD2	8:P:176:GLU:OE2	2.19	0.43
9:W:20:DA:H2''	9:W:21:DG:C8	2.54	0.43
9:W:31:DT:C6	9:W:32:DT:H72	2.53	0.43
9:W:38:DT:H2''	9:W:39:DA:N7	2.34	0.43
12:E:250:LYS:HG3	12:E:251:GLU:H	1.83	0.43
12:E:310:LEU:O	12:E:314:ILE:HG12	2.18	0.43
16:L:833:PRO:HG3	16:L:875:TYR:CZ	2.54	0.43
16:L:1730:LEU:O	16:L:1734:GLU:HG2	2.18	0.43
16:L:2721:TYR:HE1	16:L:2723:GLN:OE1	2.01	0.43
16:L:3019:LYS:HG3	16:L:3049:ILE:CD1	2.48	0.43
16:L:3036:TYR:CE1	16:L:3067:ARG:HG2	2.54	0.43
3:T:162:TYR:O	8:P:217:LYS:NZ	2.51	0.42
8:P:308:LEU:N	8:P:308:LEU:HD23	2.34	0.42
8:P:395:ARG:HA	8:P:395:ARG:HH11	1.84	0.42
10:I:53:DG:H2'	10:I:54:DC:C6	2.54	0.42
12:E:761:PHE:HZ	16:L:2715:ARG:HG3	1.84	0.42
16:L:138:ASP:OD1	16:L:138:ASP:N	2.45	0.42
16:L:1234:GLN:OE1	16:L:1271:THR:HB	2.18	0.42
16:L:2279:MET:SD	16:L:2328:SER:HB2	2.59	0.42
16:L:2483:GLU:HG3	16:L:2485:GLU:OE1	2.19	0.42
16:L:2628:ILE:HG13	16:L:2665:LEU:HD21	2.00	0.42
16:L:3036:TYR:O	16:L:3063:PHE:HZ	2.02	0.42
4:O:126:LEU:O	4:O:130:ILE:HG12	2.19	0.42
8:P:311:TYR:HB3	8:P:316:TYR:CD2	2.54	0.42
10:I:124:DG:H2''	10:I:125:DG:H8	1.84	0.42
12:E:586:SER:O	12:E:587:LYS:HB2	2.19	0.42
12:E:649:ILE:O	12:E:741:LEU:O	2.38	0.42
13:F:413:GLY:HA3	19:F:1002:ATP:C5'	2.48	0.42
15:K:118:LEU:O	15:K:120:ILE:HG12	2.19	0.42
15:K:197:THR:O	15:K:198:LEU:HB3	2.19	0.42
3:H:557:THR:CG2	3:H:625:GLU:HG3	2.48	0.42
16:L:390:LEU:O	16:L:394:THR:HG23	2.19	0.42
16:L:1490:SER:O	16:L:1492:HIS:N	2.52	0.42
16:L:1789:PHE:CD2	16:L:1794:LYS:HD3	2.54	0.42
16:L:1804:LYS:HG3	16:L:1863:GLU:HB2	2.01	0.42
2:V:50:HIS:CE1	3:T:392:ILE:HA	2.54	0.42
5:B:24:ASP:OD2	5:B:27:GLN:NE2	2.45	0.42
8:P:181:TYR:CD1	8:P:260:ASP:HB2	2.54	0.42
8:P:371:ASP:OD1	8:P:371:ASP:N	2.51	0.42
8:P:431:TRP:CZ2	8:P:434:PRO:HD3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:93:DC:H2''	9:W:94:DG:H8	1.85	0.42
12:E:640:ARG:N	12:E:640:ARG:HD2	2.33	0.42
12:E:709:PHE:CE2	12:E:721:GLN:HG3	2.53	0.42
13:F:143:SER:HB3	13:F:170:ILE:HD11	2.00	0.42
3:H:720:ILE:HG21	3:H:725:GLU:OE2	2.20	0.42
16:L:2036:LEU:HD13	16:L:2123:ILE:HG13	2.00	0.42
16:L:2121:ILE:HD12	16:L:2169:TYR:CE2	2.54	0.42
16:L:2405:GLU:HG3	16:L:2408:ASN:HB3	2.02	0.42
16:L:2411:GLU:O	16:L:2412:ILE:HD13	2.19	0.42
1:Y:27:ASP:OD1	3:T:396:ARG:NH1	2.52	0.42
2:V:38:GLU:HG3	2:V:75:SER:OG	2.19	0.42
3:T:147:TYR:CE1	8:P:230:ARG:HB3	2.54	0.42
3:T:238:LEU:HD23	3:T:238:LEU:HA	1.85	0.42
5:B:24:ASP:OD1	5:B:24:ASP:N	2.46	0.42
9:W:128:DG:H2''	9:W:129:DT:C6	2.54	0.42
9:W:144:DC:H2''	9:W:145:DG:C8	2.54	0.42
15:K:173:PHE:O	15:K:177:LYS:HG3	2.20	0.42
3:H:500:ILE:HG21	16:L:2715:ARG:HH22	1.84	0.42
3:H:558:SER:CB	16:L:3519:THR:HG22	2.48	0.42
16:L:608:PRO:O	16:L:612:THR:N	2.49	0.42
16:L:1939:ARG:NH2	16:L:1981:GLN:OE1	2.53	0.42
16:L:2120:ALA:HA	16:L:2123:ILE:HG22	2.00	0.42
16:L:2568:TYR:CZ	16:L:2616:LEU:HD23	2.55	0.42
8:P:305:ILE:HD11	8:P:320:LEU:HB3	2.00	0.42
10:I:68:DG:H1'	10:I:69:DG:H5'	2.02	0.42
3:H:560:VAL:O	3:H:567:SER:HB2	2.19	0.42
16:L:2409:ASN:OD1	16:L:2411:GLU:O	2.37	0.42
16:L:2627:ALA:O	16:L:2632:ALA:HB3	2.20	0.42
16:L:3249:ILE:HD11	16:L:3317:TRP:CE3	2.55	0.42
7:U:90:THR:OG1	7:U:93:GLU:OE1	2.31	0.42
17:B:501:CMC:H121	8:P:307:THR:HB	2.01	0.42
9:W:6:DG:H1'	9:W:7:DA:H5'	2.02	0.42
13:F:486:ASP:O	13:F:487:ARG:HG2	2.19	0.42
15:K:303:LEU:O	15:K:307:LEU:CD2	2.67	0.42
3:H:500:ILE:C	3:H:501:VAL:HG23	2.40	0.42
16:L:250:THR:OG1	16:L:251:PRO:HD3	2.20	0.42
16:L:723:ALA:O	16:L:727:LEU:HG	2.20	0.42
16:L:1044:LYS:HA	16:L:1047:VAL:HG12	2.02	0.42
16:L:1105:ASN:OD1	16:L:2529:SER:OG	2.38	0.42
16:L:1829:LYS:HD3	16:L:1829:LYS:HA	1.94	0.42
16:L:3434:VAL:O	16:L:3438:ARG:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:130:TRP:CZ2	3:T:132:GLU:HB2	2.54	0.42
8:P:230:ARG:O	8:P:428:ARG:HD3	2.19	0.42
9:W:-5:DG:H1'	9:W:-4:DC:H5'	2.00	0.42
10:I:11:DT:H2''	10:I:12:DA:H8	1.85	0.42
15:K:247:SER:O	15:K:251:ILE:HG12	2.19	0.42
15:K:310:ASP:OD1	15:K:312:THR:CG2	2.68	0.42
3:H:559:ASN:HB3	3:H:562:PHE:HD2	1.85	0.42
16:L:940:ALA:O	16:L:944:ASN:ND2	2.52	0.42
16:L:2243:ILE:HG13	16:L:2252:SER:O	2.20	0.42
16:L:2626:LEU:C	16:L:2628:ILE:N	2.73	0.42
16:L:2774:ASP:HA	16:L:2777:GLU:OE1	2.19	0.42
16:L:3248:LEU:O	16:L:3251:VAL:HG12	2.19	0.42
16:L:3507:THR:HG22	16:L:3735:ARG:HD3	2.01	0.42
3:T:167:ARG:NH1	3:T:285:GLU:OE1	2.42	0.42
14:G:37:ARG:N	14:G:65:LEU:HD11	2.35	0.42
3:H:491:LYS:O	3:H:492:LEU:HD12	2.19	0.42
16:L:706:LEU:N	16:L:707:PRO:HD2	2.35	0.42
16:L:1389:ASP:OD1	16:L:1389:ASP:N	2.49	0.42
16:L:1818:SER:OG	16:L:1819:GLY:N	2.52	0.42
16:L:2029:ILE:HG13	16:L:2116:LEU:HD12	2.00	0.42
16:L:2276:THR:N	16:L:2277:PRO:HD2	2.35	0.42
16:L:2373:ALA:HB1	16:L:2415:ARG:CG	2.50	0.42
16:L:2491:ILE:O	16:L:2492:TYR:CG	2.73	0.42
16:L:2794:PHE:CE1	16:L:2904:TRP:HZ2	2.38	0.42
16:L:3300:PHE:CD2	16:L:3300:PHE:C	2.92	0.42
2:V:92:THR:O	2:V:96:LEU:HG	2.20	0.42
5:Q:44:LYS:HD2	6:N:115:LEU:HB3	2.02	0.42
5:B:78:ARG:NH1	5:B:80:THR:O	2.53	0.42
8:P:201:THR:HA	8:P:247:TRP:CD1	2.55	0.42
8:P:228:ILE:HG21	8:P:431:TRP:HD1	1.83	0.42
8:P:394:LEU:HD12	8:P:394:LEU:HA	1.84	0.42
8:P:395:ARG:O	8:P:401:HIS:HA	2.20	0.42
9:W:-6:DG:C2	10:I:155:DG:N1	2.88	0.42
12:E:225:TYR:CB	16:L:3295:LYS:NZ	2.82	0.42
12:E:618:ARG:O	12:E:618:ARG:HG3	2.20	0.42
16:L:860:GLU:O	16:L:864:THR:OG1	2.37	0.42
16:L:2783:VAL:HG13	16:L:2791:ARG:HD2	2.02	0.42
16:L:3280:LEU:HD12	16:L:3281:VAL:N	2.35	0.42
16:L:3313:ARG:NH2	16:L:3314:LEU:HD23	2.34	0.42
16:L:3461:SER:OG	16:L:3462:VAL:O	2.28	0.42
12:E:672:ILE:O	12:E:676:MET:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:305:MET:HB2	19:G:502:ATP:C6	2.55	0.42
3:H:720:ILE:O	3:H:721:LYS:HG2	2.20	0.42
16:L:151:THR:OG1	16:L:152:PRO:HD3	2.20	0.42
16:L:2316:TYR:O	16:L:2320:LEU:HB2	2.19	0.42
16:L:2616:LEU:HD12	16:L:2616:LEU:C	2.40	0.42
16:L:2621:HIS:CD2	16:L:2621:HIS:C	2.93	0.42
16:L:3240:THR:OG1	16:L:3241:THR:N	2.52	0.42
16:L:3410:VAL:O	16:L:3413:SER:OG	2.33	0.42
16:L:3611:SER:HB2	16:L:3612:PRO:HD3	2.02	0.42
1:Y:26:GLU:HG3	3:T:361:TRP:CD1	2.55	0.41
2:V:2:ASP:HB3	2:V:5:LEU:HB3	2.01	0.41
10:I:47:DC:H1'	10:I:48:DC:C5	2.55	0.41
12:E:311:THR:HG1	12:E:314:ILE:HG12	1.84	0.41
12:E:311:THR:OG1	12:E:314:ILE:HG12	2.18	0.41
14:G:332:PRO:O	14:G:335:ARG:HG3	2.20	0.41
15:K:214:LYS:HG3	15:K:223:LEU:HD11	2.02	0.41
16:L:917:ILE:HD12	16:L:921:ILE:HD13	2.01	0.41
16:L:1547:MET:HB3	16:L:1548:PRO:HD3	2.02	0.41
9:W:42:DC:H2''	9:W:43:DA:C8	2.54	0.41
12:E:393:ASP:HA	12:E:396:THR:HG22	2.02	0.41
12:E:625:ASN:ND2	16:L:2414:VAL:HG22	2.34	0.41
16:L:3109:SER:C	16:L:3689:ARG:HH11	2.24	0.41
5:Q:91:LYS:NZ	7:D:71:GLU:OE1	2.52	0.41
8:P:214:TYR:O	8:P:218:CYS:N	2.53	0.41
9:W:-14:DC:H6	9:W:-14:DC:H2'	1.70	0.41
9:W:23:DC:H5'	9:W:23:DC:H6	1.85	0.41
9:W:79:DC:H4'	9:W:80:DC:OP1	2.20	0.41
9:W:125:DC:C2	9:W:126:DG:C5	3.09	0.41
16:L:466:ILE:HA	16:L:1716:LEU:HD21	2.01	0.41
16:L:2416:MET:CG	16:L:2417:GLU:N	2.83	0.41
1:Y:8:TYR:HE1	3:T:375:ILE:HG23	1.84	0.41
3:T:167:ARG:HG2	3:T:278:TYR:OH	2.20	0.41
9:W:123:DC:C2'	9:W:124:DA:C8	3.03	0.41
10:I:47:DC:H4'	10:I:48:DC:H5'	2.01	0.41
10:I:82:DG:H2'	10:I:83:DT:H71	2.02	0.41
10:I:126:DC:H2''	10:I:127:DC:O5'	2.20	0.41
10:I:127:DC:H2''	10:I:128:DT:O5'	2.21	0.41
12:E:752:HIS:O	12:E:752:HIS:ND1	2.53	0.41
3:H:668:MET:H	3:H:668:MET:HG2	1.71	0.41
16:L:909:THR:O	16:L:911:GLU:N	2.53	0.41
16:L:1335:SER:N	16:L:1336:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:3659:LEU:O	16:L:3663:LEU:HB2	2.21	0.41
8:P:431:TRP:CZ2	8:P:433:PRO:HA	2.55	0.41
9:W:140:DC:H2''	9:W:141:DA:C8	2.56	0.41
10:I:53:DG:H2''	10:I:54:DC:H5'	2.02	0.41
12:E:626:ARG:CZ	12:E:629:HIS:ND1	2.83	0.41
16:L:224:LEU:O	16:L:225:SER:OG	2.29	0.41
16:L:2313:LYS:HA	16:L:2316:TYR:CD2	2.56	0.41
16:L:3604:ASP:OD1	16:L:3604:ASP:N	2.53	0.41
2:V:23:TYR:O	2:V:26:GLU:HG2	2.21	0.41
8:P:397:TYR:CE2	8:P:398:LYS:HE3	2.56	0.41
10:I:94:DG:C4	10:I:95:DG:C8	3.09	0.41
15:K:120:ILE:HG22	15:K:120:ILE:O	2.19	0.41
16:L:31:LEU:HD12	16:L:35:MET:O	2.21	0.41
16:L:846:ILE:HB	16:L:849:ALA:CB	2.51	0.41
16:L:2394:PHE:O	16:L:2397:ILE:HG12	2.19	0.41
3:T:313:ARG:NH2	8:P:265:TYR:O	2.54	0.41
8:P:279:ARG:HA	8:P:284:HIS:HA	2.02	0.41
9:W:102:DG:C6	9:W:103:DA:C6	3.08	0.41
12:E:352:TRP:NE1	15:K:119:SER:OG	2.50	0.41
12:E:357:THR:OG1	12:E:360:ASN:OD1	2.38	0.41
16:L:105:SER:O	16:L:109:LYS:HE2	2.20	0.41
16:L:149:LYS:O	16:L:152:PRO:HD2	2.21	0.41
16:L:284:GLU:O	16:L:285:ILE:HD13	2.21	0.41
16:L:1093:LYS:O	16:L:1094:GLU:CG	2.69	0.41
16:L:2198:ASP:OD2	16:L:2203:GLN:HA	2.21	0.41
16:L:2339:LEU:HD23	16:L:2344:MET:HE3	2.02	0.41
16:L:2488:LEU:HD12	16:L:2491:ILE:HD13	2.03	0.41
16:L:2504:LEU:O	16:L:2504:LEU:HG	2.21	0.41
3:T:147:TYR:OH	8:P:428:ARG:O	2.22	0.41
5:Q:28:GLY:O	5:Q:30:THR:HG23	2.21	0.41
8:P:189:LEU:O	8:P:195:ILE:HD11	2.21	0.41
8:P:301:ASN:HB3	8:P:335:GLY:HA3	2.03	0.41
10:I:49:DC:H2''	10:I:50:DT:C7	2.49	0.41
10:I:134:DC:H2''	10:I:135:DC:C6	2.56	0.41
12:E:612:ILE:HG23	12:E:615:LEU:HD13	2.03	0.41
12:E:698:GLU:HG3	12:E:740:PRO:HG3	2.01	0.41
3:H:501:VAL:HG12	3:H:502:LEU:C	2.40	0.41
3:H:505:VAL:CG2	16:L:2720:PRO:HB2	2.50	0.41
16:L:28:LEU:H	16:L:28:LEU:HD23	1.86	0.41
16:L:1503:LEU:O	16:L:1507:LEU:HB2	2.20	0.41
16:L:1708:GLU:OE1	16:L:1708:GLU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:1957:MET:HG2	16:L:1966:TRP:CD1	2.56	0.41
16:L:2744:ASP:OD1	16:L:2745:VAL:N	2.54	0.41
16:L:3629:GLN:HE21	16:L:3629:GLN:HB3	1.68	0.41
3:T:188:GLU:HG2	3:T:267:LEU:HD11	2.02	0.41
4:A:116:ARG:NH1	4:A:118:THR:O	2.54	0.41
8:P:318:LYS:O	8:P:322:GLU:HG3	2.20	0.41
10:I:22:DC:H2''	10:I:23:DG:H8	1.86	0.41
10:I:28:DT:H1'	10:I:29:DG:C8	2.55	0.41
10:I:102:DA:C6	10:I:103:DG:C6	3.09	0.41
10:I:114:DC:H2''	10:I:115:DC:C6	2.55	0.41
10:I:161:DA:H2''	10:I:162:DG:N7	2.35	0.41
10:I:174:DG:H2''	10:I:175:DA:C8	2.56	0.41
14:G:21:PHE:HB2	14:G:24:ASP:OD1	2.21	0.41
14:G:236:ILE:HG22	14:G:236:ILE:O	2.20	0.41
15:K:314:LYS:O	15:K:315:ARG:HB3	2.21	0.41
16:L:110:GLU:O	16:L:215:ARG:NH2	2.40	0.41
16:L:327:ASP:OD2	16:L:327:ASP:N	2.49	0.41
16:L:848:THR:HB	16:L:1156:TYR:CD1	2.56	0.41
16:L:1365:ASN:O	16:L:1365:ASN:ND2	2.50	0.41
16:L:1771:ILE:O	16:L:1779:GLN:NE2	2.53	0.41
16:L:1784:ASN:HD21	16:L:1832:LYS:HB3	1.86	0.41
16:L:1847:ALA:C	16:L:1849:LEU:H	2.21	0.41
16:L:1885:ASP:O	16:L:1888:LYS:HG2	2.21	0.41
16:L:2349:LEU:O	16:L:2353:VAL:HG13	2.20	0.41
16:L:3136:PHE:O	16:L:3140:LEU:HG	2.21	0.41
3:T:337:LEU:O	3:T:341:LEU:HG	2.20	0.41
10:I:82:DG:C2'	10:I:83:DT:H71	2.50	0.41
16:L:1628:VAL:HG12	16:L:1679:THR:HG21	2.02	0.41
16:L:2031:LEU:O	16:L:2035:ILE:HG13	2.21	0.41
2:V:39:LYS:HA	2:V:42:TYR:CD1	2.56	0.40
9:W:-18:DG:H2''	9:W:-17:DA:N7	2.36	0.40
9:W:9:DT:H2''	9:W:10:DC:H6	1.86	0.40
9:W:17:DC:H2''	9:W:18:DC:C6	2.55	0.40
12:E:806:ARG:HB3	12:E:806:ARG:CZ	2.50	0.40
16:L:109:LYS:HB2	16:L:114:ASN:ND2	2.37	0.40
16:L:993:VAL:HG12	16:L:993:VAL:O	2.21	0.40
16:L:3063:PHE:CE2	16:L:3067:ARG:HD2	2.56	0.40
16:L:3073:ASN:ND2	16:L:3689:ARG:HG2	2.37	0.40
4:O:58:THR:HG21	6:N:81:ARG:HD3	2.03	0.40
5:B:31:LYS:HG3	5:B:51:TYR:CZ	2.56	0.40
8:P:241:GLY:HA2	8:P:248:CYS:SG	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:38:DG:H1'	10:I:39:DG:N7	2.36	0.40
13:F:473:LYS:O	13:F:477:GLU:HG2	2.21	0.40
16:L:120:LYS:O	16:L:124:THR:HG23	2.22	0.40
16:L:353:HIS:O	16:L:356:SER:OG	2.39	0.40
16:L:1831:PRO:HB2	16:L:1834:LEU:HB2	2.04	0.40
16:L:2236:ILE:HD11	16:L:2259:LEU:HG	2.03	0.40
16:L:2998:GLU:HG2	16:L:3001:THR:OG1	2.20	0.40
16:L:3030:LEU:O	16:L:3035:ALA:HB3	2.21	0.40
6:S:106:GLY:HA3	4:A:58:THR:HG22	2.03	0.40
9:W:69:DA:H2''	9:W:70:DC:C5	2.56	0.40
10:I:34:DC:H2'	10:I:35:DT:H72	2.04	0.40
12:E:340:TRP:NE1	12:E:342:LEU:HB2	2.36	0.40
13:F:390:TYR:O	13:F:394:MET:HG2	2.21	0.40
16:L:1604:HIS:HA	16:L:1607:VAL:HG12	2.03	0.40
16:L:2573:LYS:O	16:L:2574:ASN:HB2	2.20	0.40
16:L:2622:LEU:O	16:L:2626:LEU:HD23	2.21	0.40
16:L:3544:PHE:CE1	16:L:3579:GLY:HA2	2.56	0.40
7:U:68:ASP:O	7:U:72:ARG:HG3	2.20	0.40
4:A:59:GLU:OE2	4:A:59:GLU:N	2.54	0.40
10:I:147:DT:H1'	10:I:148:DG:C8	2.57	0.40
15:K:51:GLY:C	15:K:52:GLU:HG2	2.41	0.40
3:H:754:ARG:O	3:H:757:THR:HG22	2.22	0.40
16:L:1133:LEU:H	16:L:1133:LEU:HD23	1.86	0.40
16:L:2785:ASP:O	16:L:2786:VAL:CG2	2.69	0.40
16:L:3597:LYS:NZ	16:L:3605:LEU:HD11	2.37	0.40
3:T:187:ASP:O	3:T:191:ILE:HG12	2.22	0.40
8:P:317:GLY:O	8:P:321:ILE:HG13	2.22	0.40
10:I:148:DG:H2''	10:I:149:DG:C8	2.56	0.40
14:G:37:ARG:HG2	14:G:68:ARG:HH21	1.87	0.40
14:G:312:ARG:O	14:G:316:GLU:HG2	2.21	0.40
16:L:80:LEU:HD11	16:L:120:LYS:HB2	2.01	0.40
16:L:93:GLN:O	16:L:97:MET:HG2	2.21	0.40
16:L:1029:THR:HG22	16:L:1029:THR:O	2.22	0.40
16:L:1847:ALA:CB	16:L:1851:TYR:HE2	2.34	0.40
16:L:2620:PRO:HB2	16:L:2623:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	44/113 (39%)	44 (100%)	0	0	100	100
2	V	111/282 (39%)	111 (100%)	0	0	100	100
3	H	263/832 (32%)	233 (89%)	29 (11%)	1 (0%)	30	68
3	T	272/832 (33%)	262 (96%)	10 (4%)	0	100	100
4	A	92/136 (68%)	91 (99%)	1 (1%)	0	100	100
4	O	94/136 (69%)	94 (100%)	0	0	100	100
5	B	85/103 (82%)	82 (96%)	3 (4%)	0	100	100
5	Q	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
6	N	104/130 (80%)	104 (100%)	0	0	100	100
6	S	104/130 (80%)	104 (100%)	0	0	100	100
7	D	91/126 (72%)	91 (100%)	0	0	100	100
7	U	90/126 (71%)	90 (100%)	0	0	100	100
8	P	268/445 (60%)	263 (98%)	5 (2%)	0	100	100
11	X	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
12	E	405/1168 (35%)	363 (90%)	41 (10%)	1 (0%)	44	78
13	F	410/489 (84%)	384 (94%)	26 (6%)	0	100	100
14	G	353/375 (94%)	343 (97%)	10 (3%)	0	100	100
15	K	229/476 (48%)	211 (92%)	17 (7%)	1 (0%)	30	68
16	L	3489/3744 (93%)	3203 (92%)	284 (8%)	2 (0%)	48	83
All	All	6589/9755 (68%)	6155 (93%)	429 (6%)	5 (0%)	50	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	K	315	ARG
3	H	500	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	L	1848	ILE
12	E	340	TRP
16	L	910	ALA

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	Y	44/100 (44%)	44 (100%)	0	100	100
2	V	106/258 (41%)	106 (100%)	0	100	100
3	H	256/769 (33%)	256 (100%)	0	100	100
3	T	259/769 (34%)	259 (100%)	0	100	100
4	A	82/111 (74%)	82 (100%)	0	100	100
4	O	84/111 (76%)	84 (100%)	0	100	100
5	B	72/79 (91%)	72 (100%)	0	100	100
5	Q	66/79 (84%)	66 (100%)	0	100	100
6	N	83/102 (81%)	83 (100%)	0	100	100
6	S	83/102 (81%)	83 (100%)	0	100	100
7	D	79/106 (74%)	79 (100%)	0	100	100
7	U	78/106 (74%)	78 (100%)	0	100	100
8	P	253/414 (61%)	253 (100%)	0	100	100
11	X	9/9 (100%)	9 (100%)	0	100	100
12	E	379/1054 (36%)	379 (100%)	0	100	100
13	F	367/434 (85%)	367 (100%)	0	100	100
14	G	305/320 (95%)	305 (100%)	0	100	100
15	K	221/441 (50%)	221 (100%)	0	100	100
16	L	3238/3452 (94%)	3218 (99%)	20 (1%)	84	88
All	All	6064/8816 (69%)	6044 (100%)	20 (0%)	90	92

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	L	1365	ASN
16	L	1804	LYS
16	L	1853	VAL
16	L	2181	MET
16	L	2521	ASN
16	L	2679	TRP
16	L	3263	LEU
16	L	3265	PHE
16	L	3272	LEU
16	L	3281	VAL
16	L	3295	LYS
16	L	3300	PHE
16	L	3307	TYR
16	L	3347	GLN
16	L	3486	GLN
16	L	3493	LEU
16	L	3498	ASP
16	L	3506	MET
16	L	3595	ARG
16	L	3728	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
12	E	222	ASN
16	L	1605	ASN
16	L	2907	HIS
16	L	2913	ASN
16	L	2941	HIS
16	L	2992	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	ATP	G	502	18	26,33,33	0.69	0	31,52,52	0.82	1 (3%)
17	CMC	B	501	5	45,53,54	0.58	0	55,78,80	0.77	1 (1%)
19	ATP	F	1002	18	26,33,33	0.74	0	31,52,52	0.76	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	ATP	G	502	18	-	0/18/38/38	0/3/3/3
17	CMC	B	501	5	-	6/46/67/68	0/3/3/3
19	ATP	F	1002	18	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	501	CMC	C5A-C6A-N6A	2.35	123.93	120.35
19	G	502	ATP	C5-C6-N6	2.27	123.80	120.35
19	F	1002	ATP	C5-C6-N6	2.26	123.79	120.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

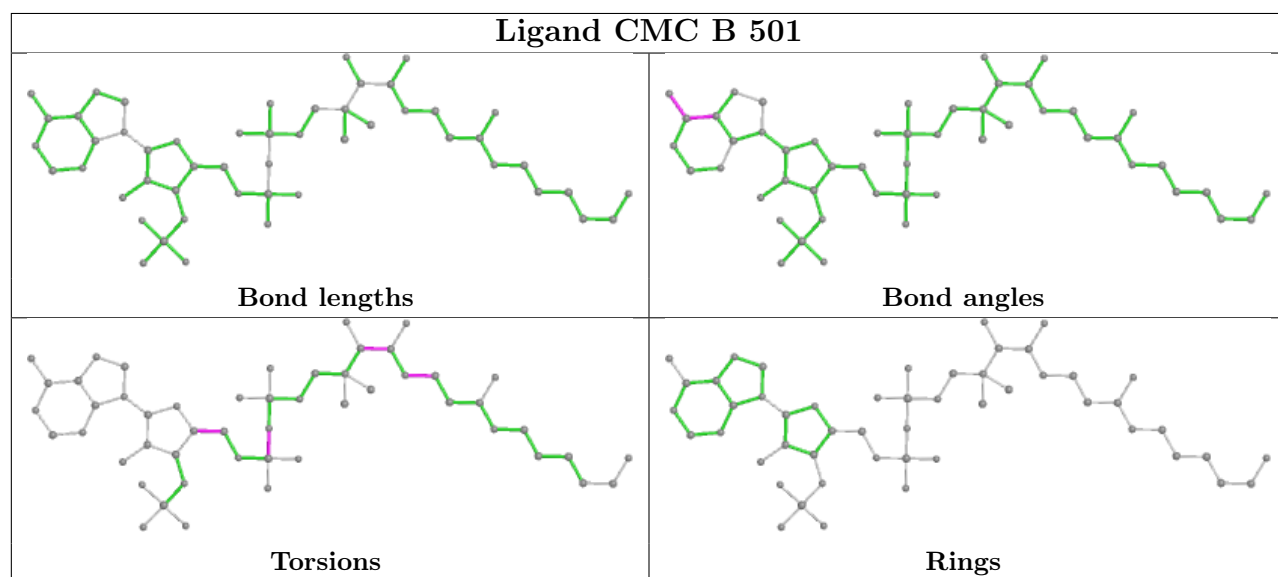
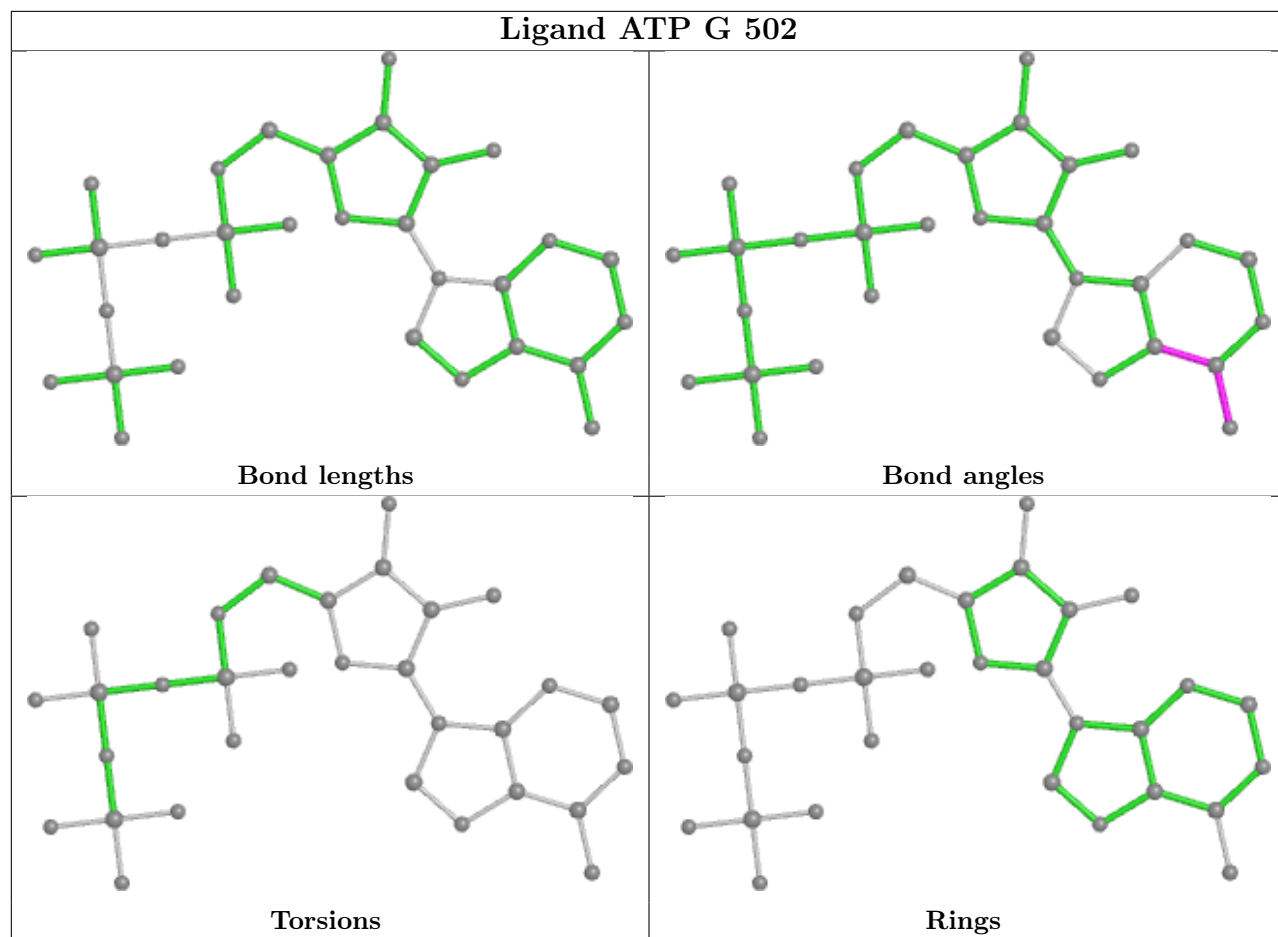
Mol	Chain	Res	Type	Atoms
17	B	501	CMC	O4B-C4B-C5B-O5B
17	B	501	CMC	C3B-C4B-C5B-O5B
17	B	501	CMC	P2A-O3A-P1A-O1A
17	B	501	CMC	C6P-C7P-N8P-C9P
19	F	1002	ATP	C5'-O5'-PA-O3A
19	F	1002	ATP	PG-O3B-PB-O2B
19	F	1002	ATP	C5'-O5'-PA-O2A
17	B	501	CMC	O9P-C9P-CAP-OAP
19	F	1002	ATP	O4'-C4'-C5'-O5'
17	B	501	CMC	P2A-O3A-P1A-O2A

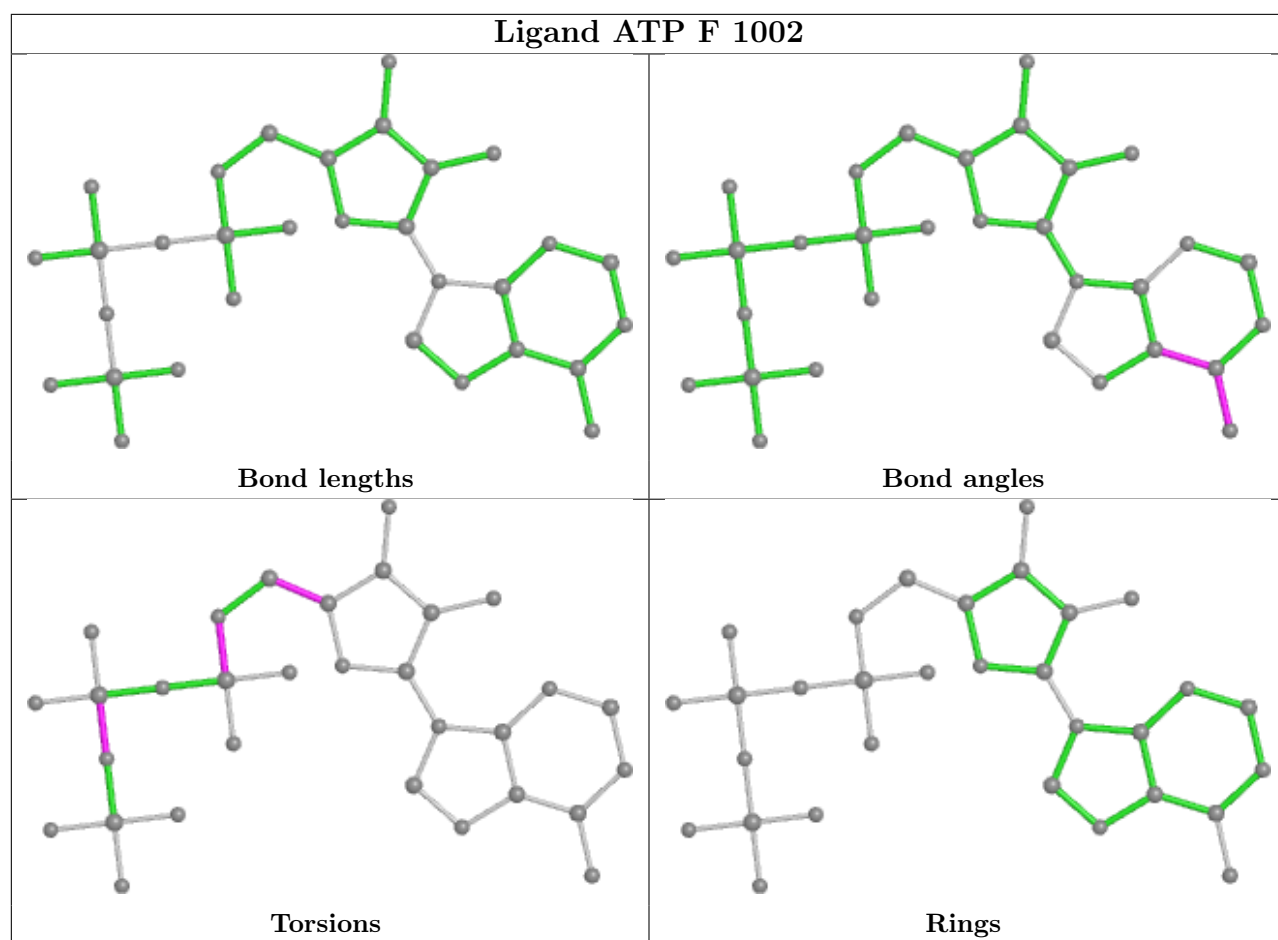
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	G	502	ATP	1	0
17	B	501	CMC	3	0
19	F	1002	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

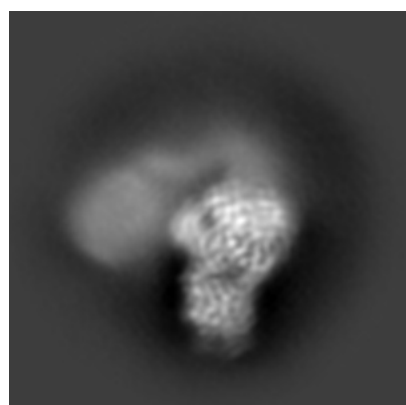
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32150. These allow visual inspection of the internal detail of the map and identification of artifacts.

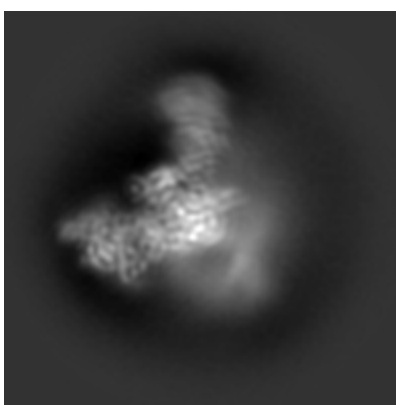
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

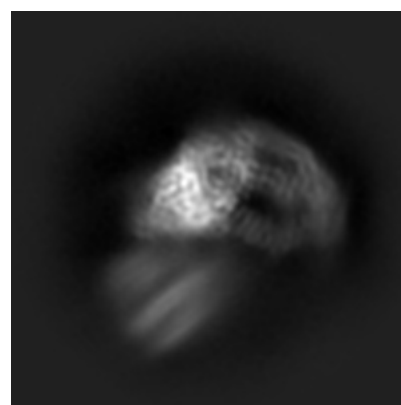
6.1.1 Primary map



X



Y

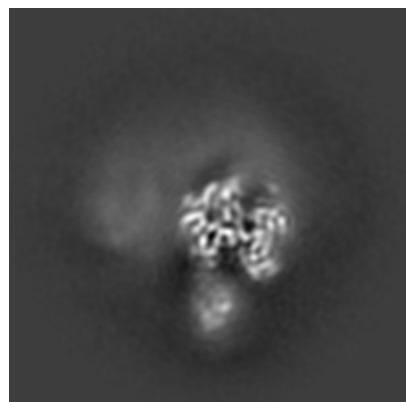


Z

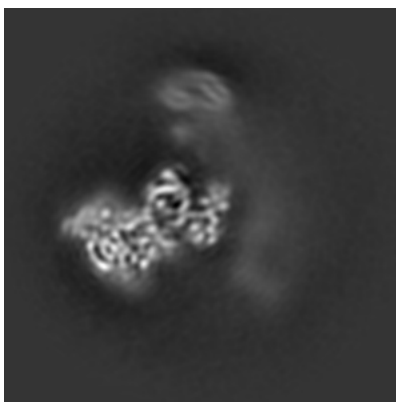
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

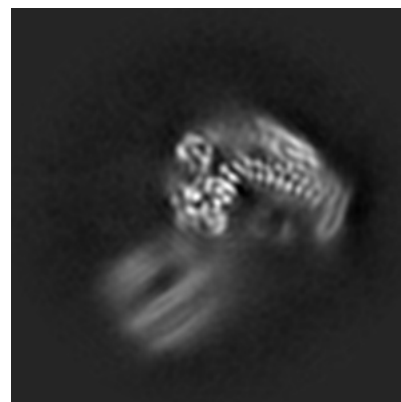
6.2.1 Primary map



X Index: 47



Y Index: 47

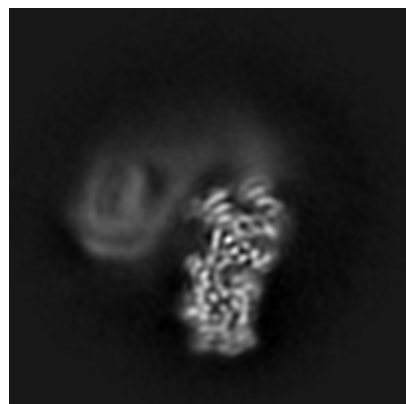


Z Index: 47

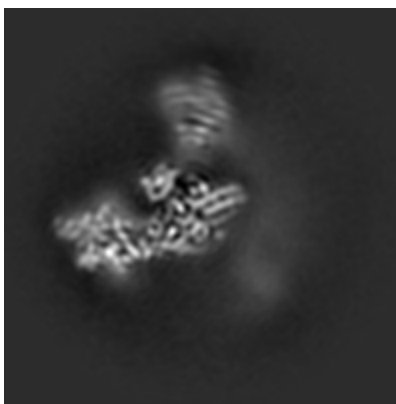
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

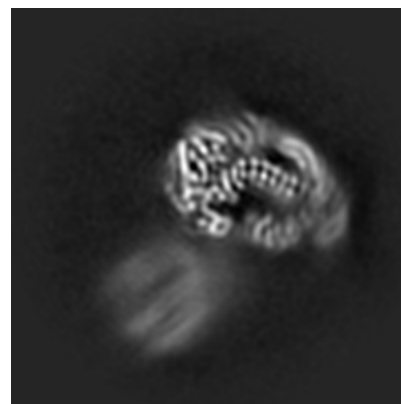
6.3.1 Primary map



X Index: 41



Y Index: 51

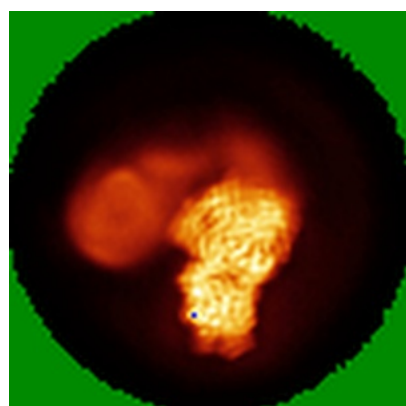


Z Index: 44

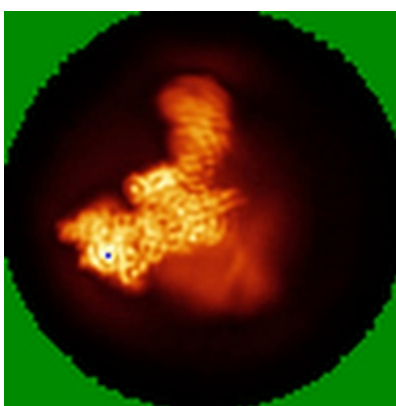
The images above show the largest variance slices of the map in three orthogonal directions.

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

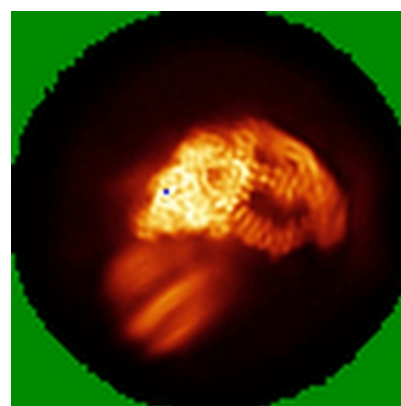
6.4.1 Primary map



X



Y

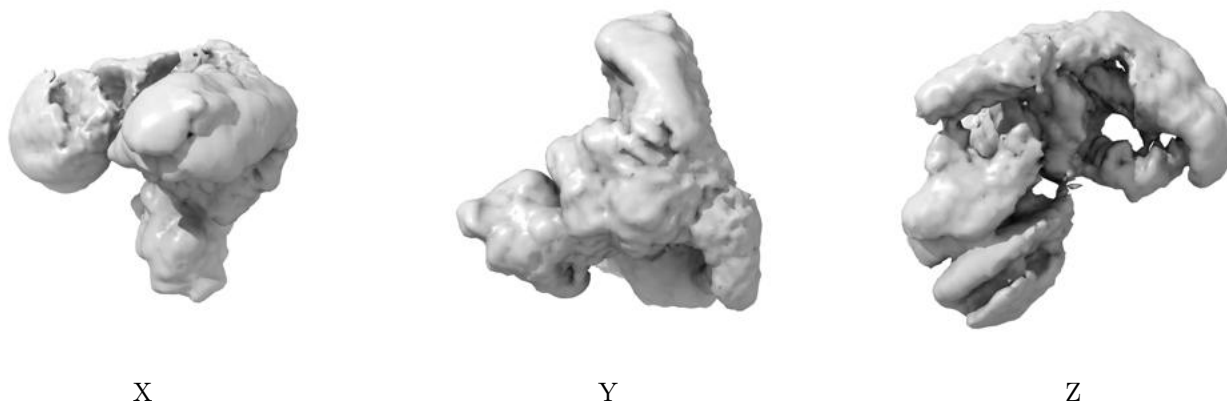


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

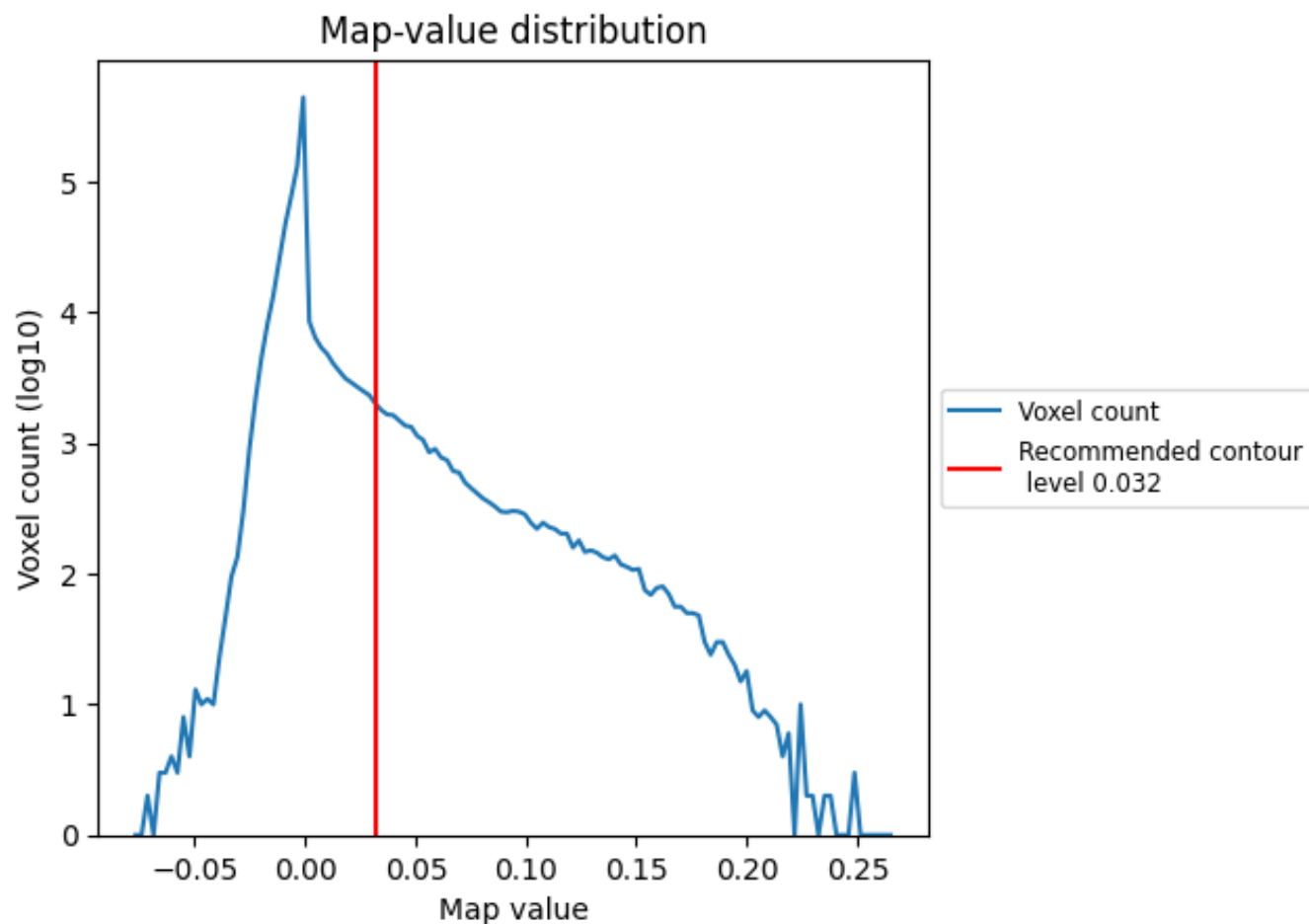
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

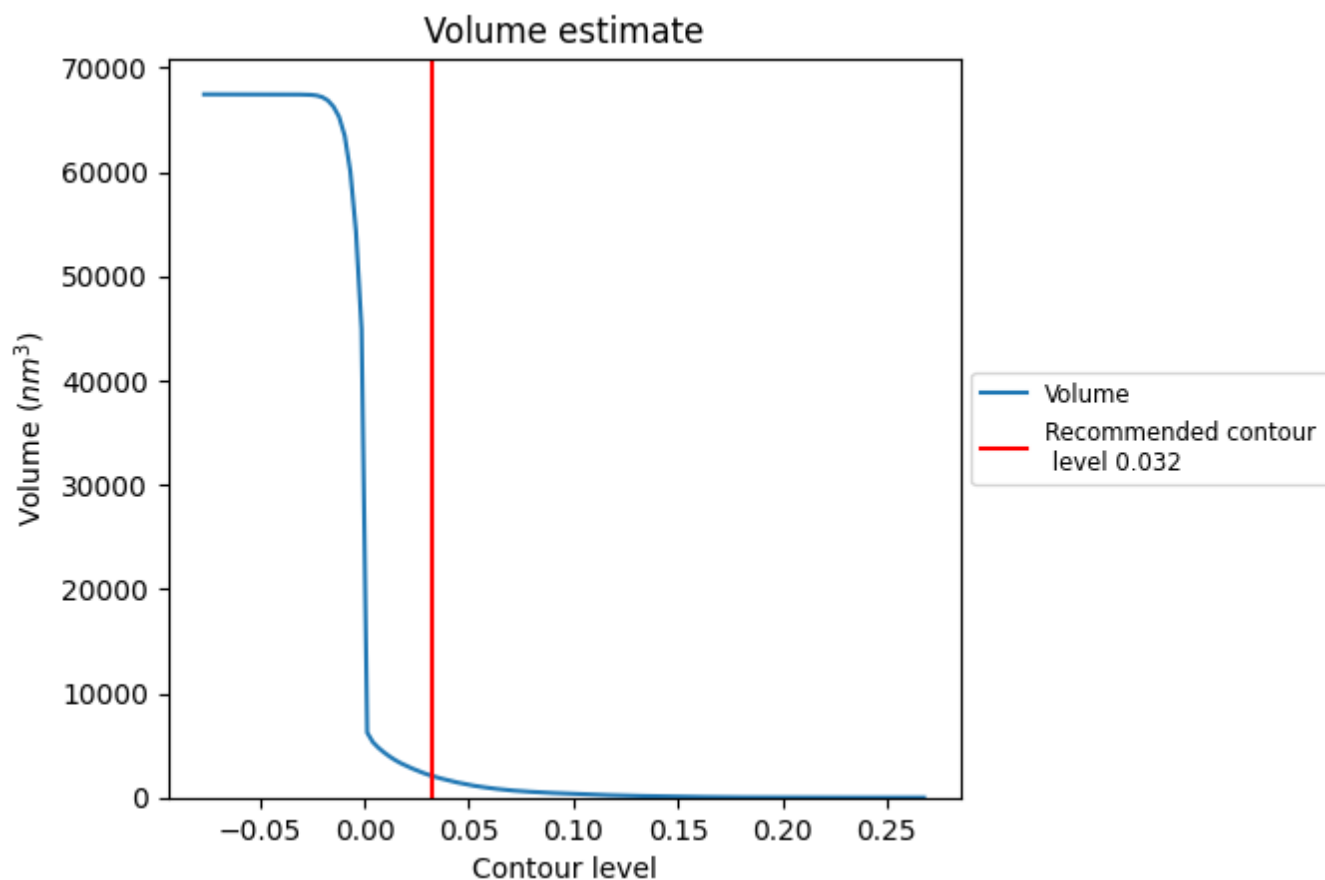
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

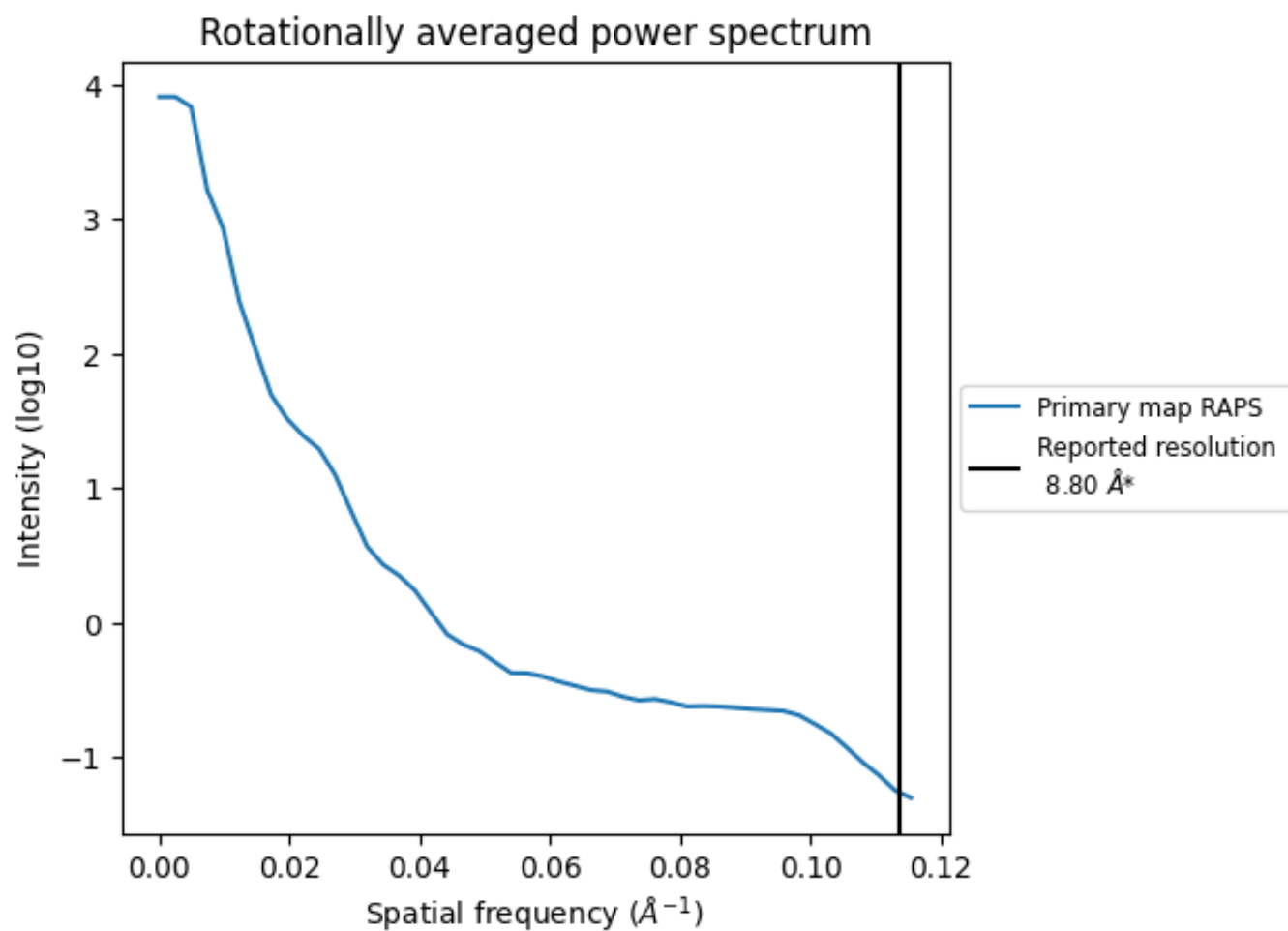
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2095 nm³; this corresponds to an approximate mass of 1893 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 0.114 Å⁻¹

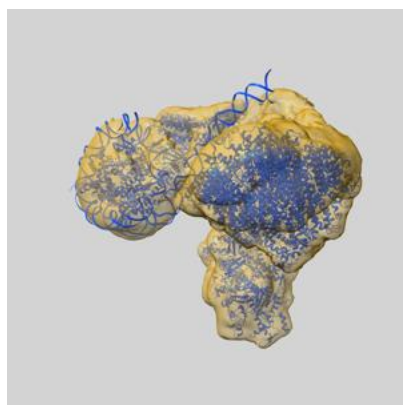
8 Fourier-Shell correlation

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

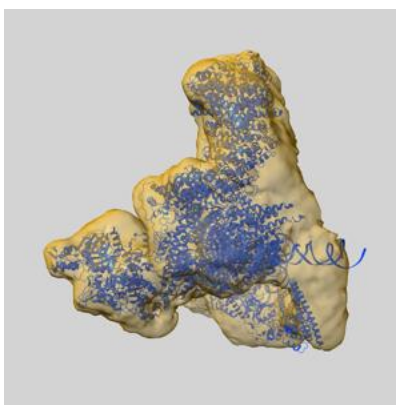
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32150 and PDB model 7VVZ. Per-residue inclusion information can be found in section 3 on page 13.

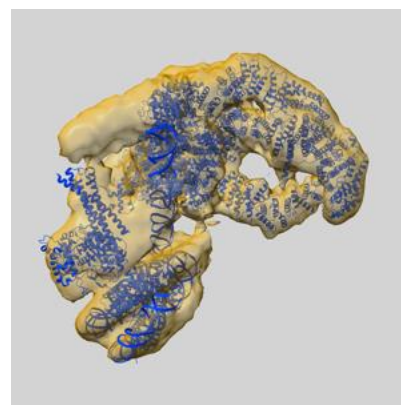
9.1 Map-model overlay [i](#)



X



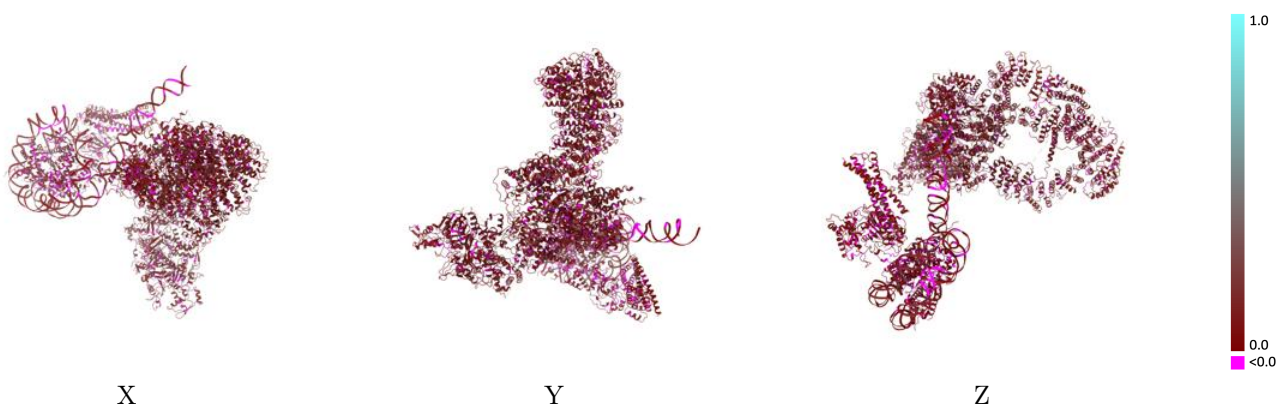
Y



Z

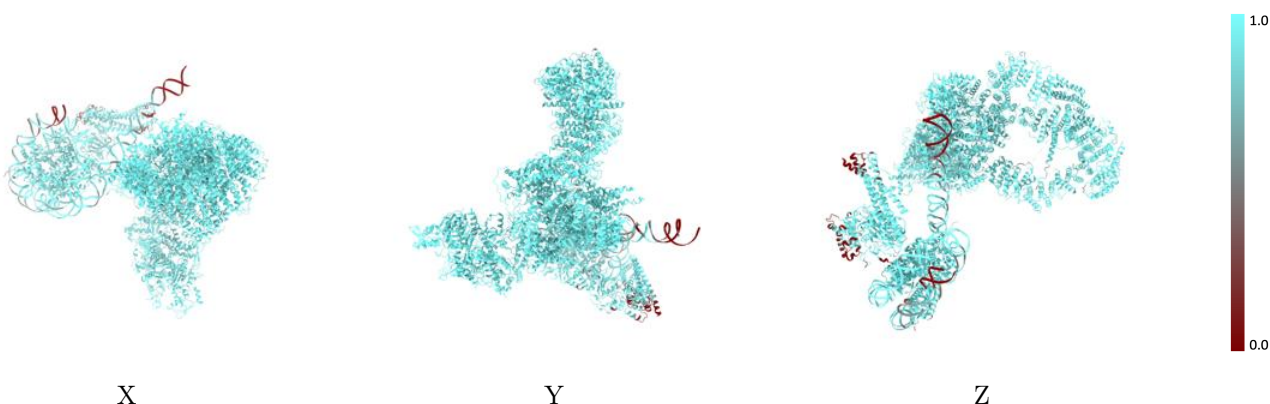
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



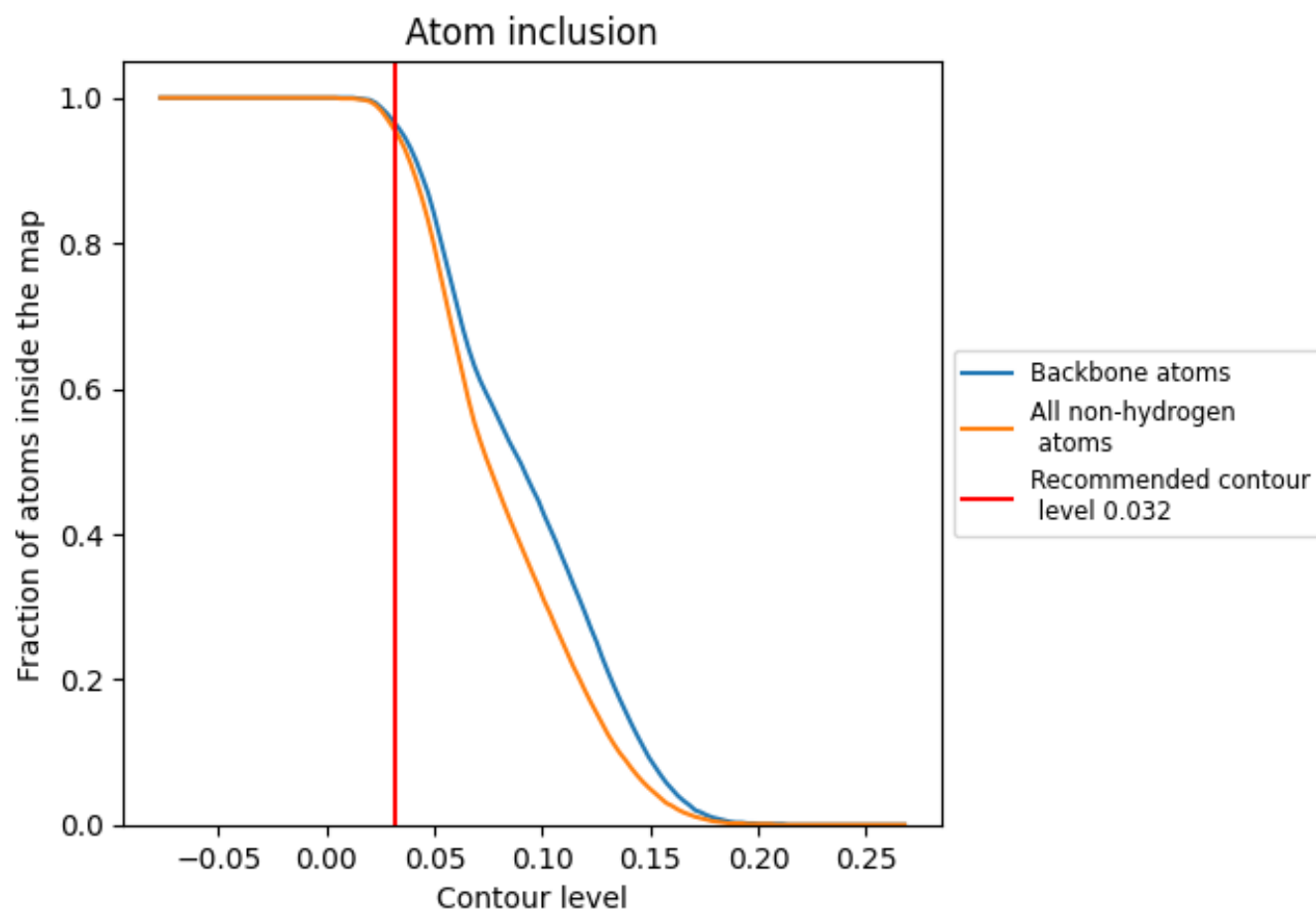
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.032).













































9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9540	 0.1080
A	 0.9540	 0.0710
B	 0.9380	 0.0550
D	 0.9830	 0.0560
E	 0.9990	 0.1360
F	 1.0000	 0.1220
G	 0.9980	 0.1180
H	 0.9840	 0.1200
I	 0.8130	 0.0880
K	 0.9910	 0.1310
L	 0.9830	 0.1260
N	 0.9910	 0.0370
O	 1.0000	 0.0500
P	 0.9850	 0.0680
Q	 1.0000	 0.0320
S	 0.9730	 0.0490
T	 0.7880	 0.0650
U	 0.9830	 0.0670
V	 0.8430	 0.0470
W	 0.8130	 0.0750
X	 0.8850	 0.0650
Y	 0.7530	 0.0780

