



Full wwPDB EM Validation Report ⓘ

Nov 9, 2022 – 10:27 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:

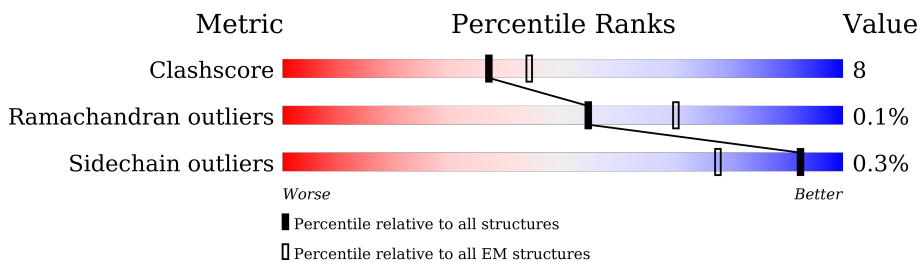
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	 75% 7% 18%
6	S	130	 77% 5% 18%
7	D	126	 68% 6% 26%
7	U	126	 68% 5% 27%
8	P	445	 41% 20% 39%
9	W	207	 10% 44% 43% 13%
10	I	207	 11% 42% 44% 14%
11	X	9	 11% 78% 22%
12	E	1168	 28% 8% 64%
13	F	489	 73% 12% 15%
14	G	375	 84% 11% 5%
15	K	476	 42% 8% 50%
16	L	3744	 76% 18% 6%

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
			Total	C	N	O	S		
1	Y	46	396	245	64	86	1	0	0

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

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

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

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

- Molecule 4 is a protein called Histone H3.

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

- Molecule 5 is a protein called Histone H4.

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

- 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
			Total	C	N	O	S		
12	E	415	3448	2193	619	622	14	0	0

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
			Total	C	N	O	S		
13	F	414	3278	2088	541	638	11	0	0

- Molecule 14 is a protein called Actin.

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

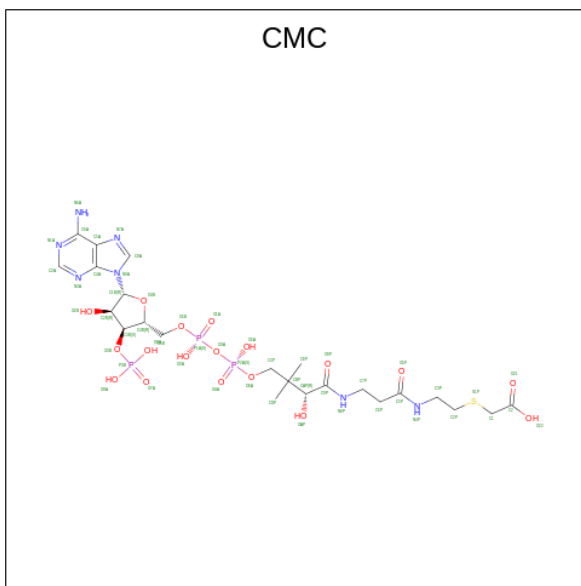
- Molecule 15 is a protein called SWR1-complex protein 4.

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

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

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

- 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).

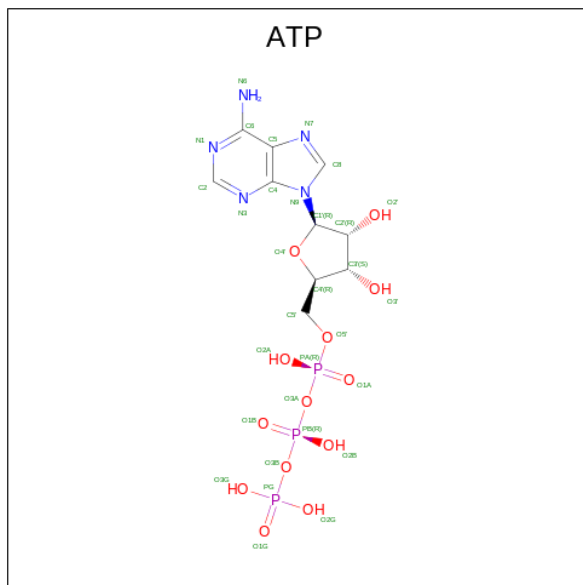


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
17	B	1	51	23	7	17	3	1	0

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

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

- 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).

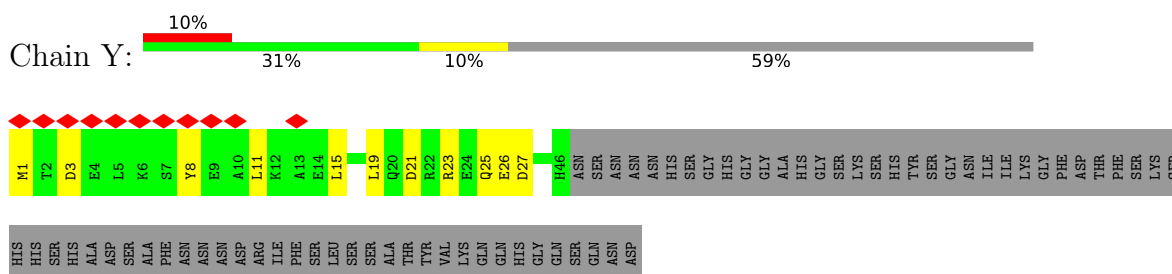


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
19	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
19	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

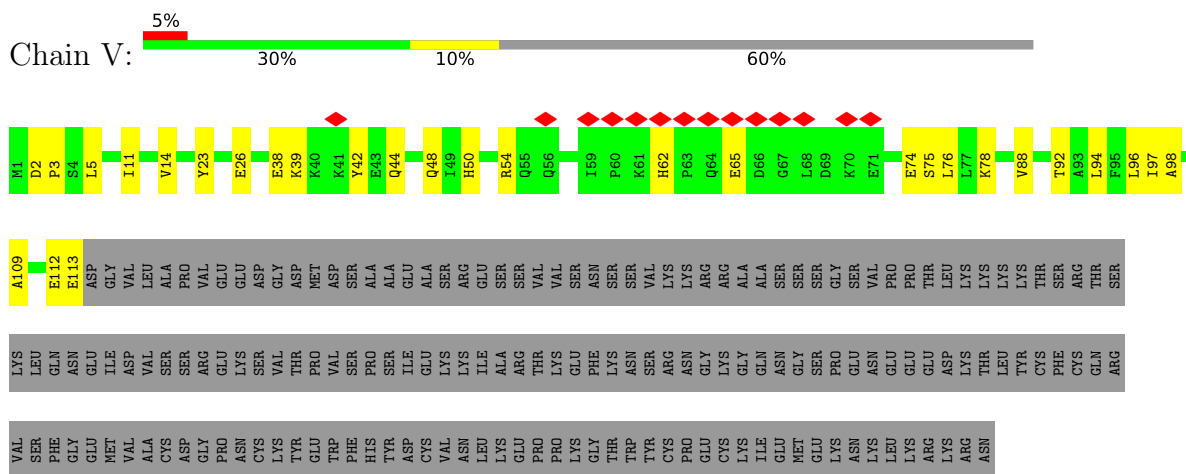
3 Residue-property plots

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

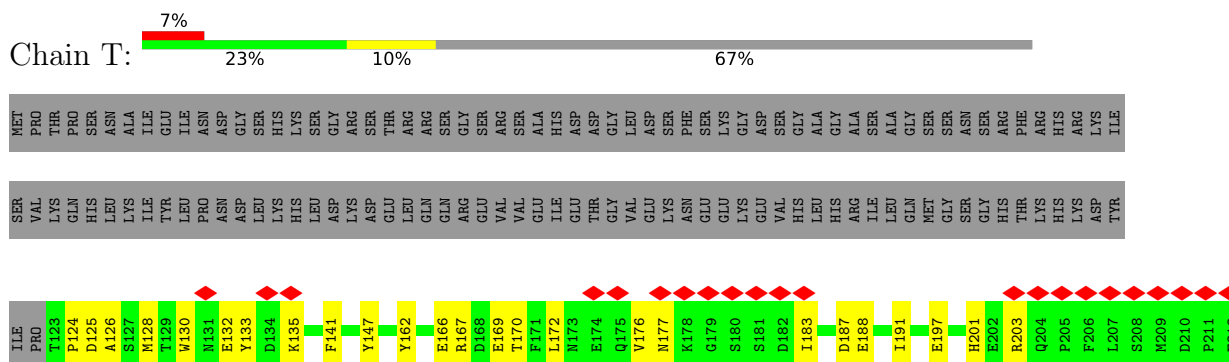
- Molecule 1: Chromatin modification-related protein EAF6

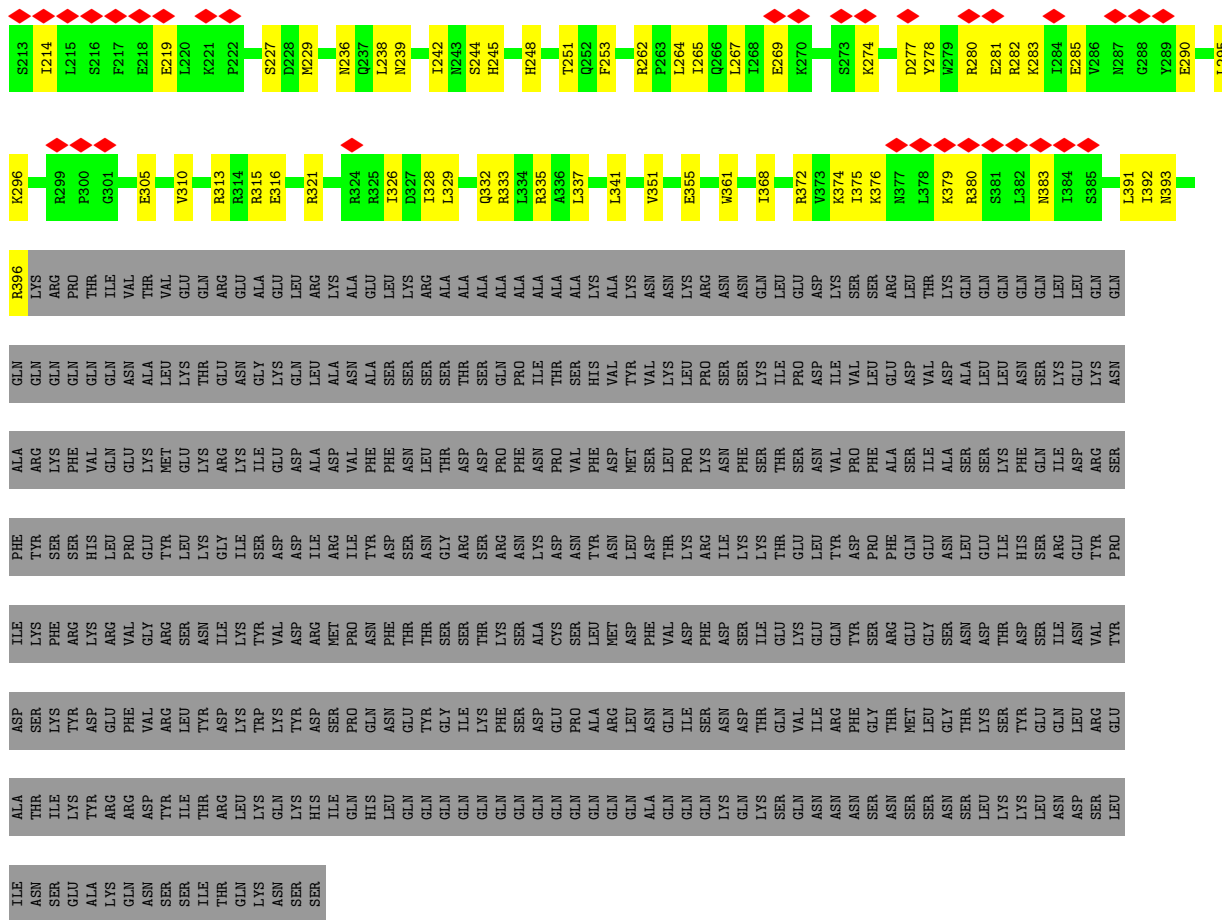


- Molecule 2: Chromatin modification-related protein YNG2

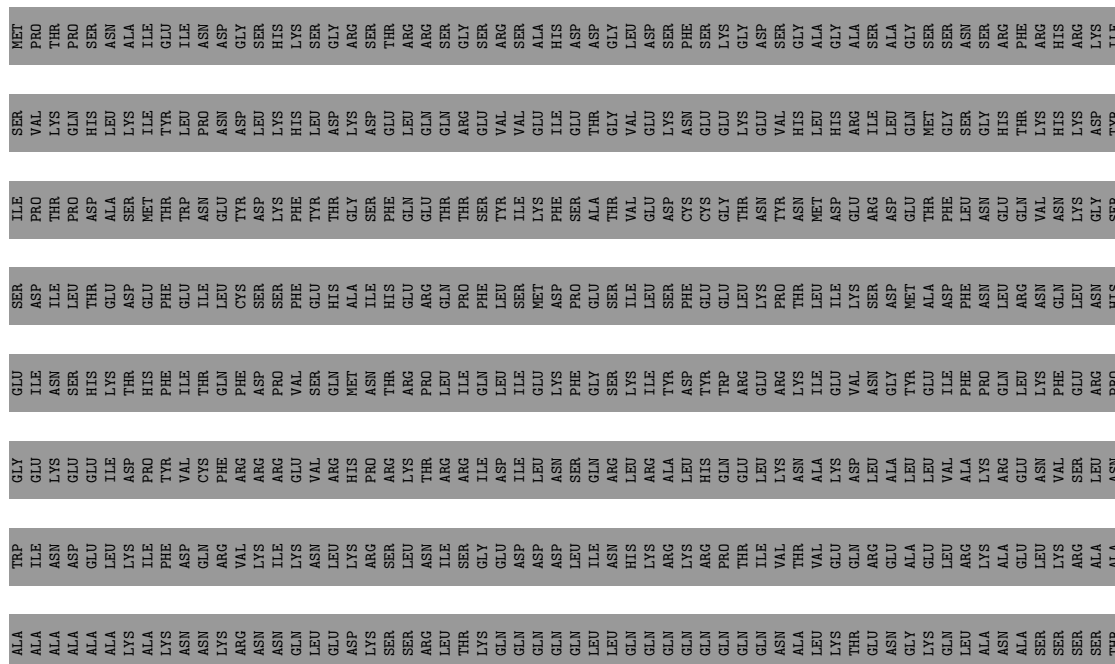


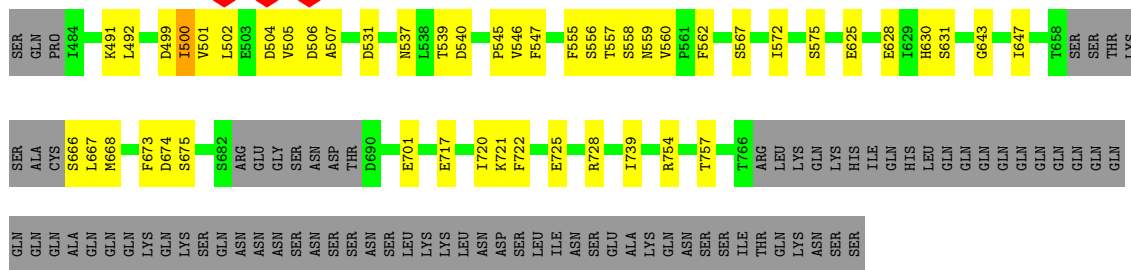
- Molecule 3: Enhancer of polycomb-like protein 1



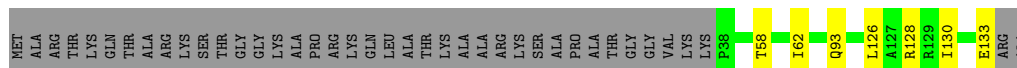


● Molecule 3: Enhancer of polycomb-like protein 1

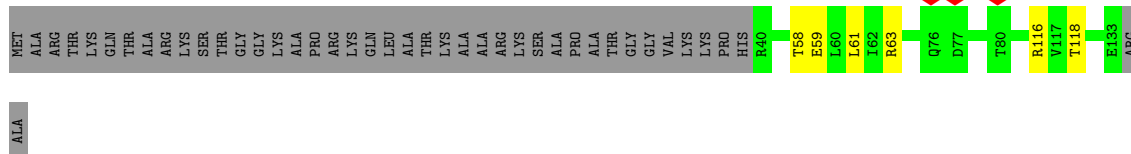




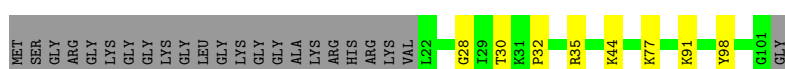
• Molecule 4: Histone H3



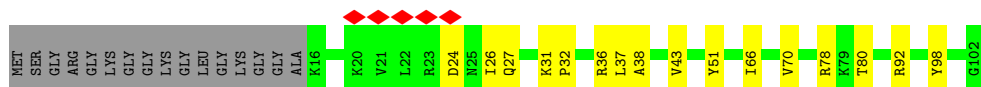
• Molecule 4: Histone H3



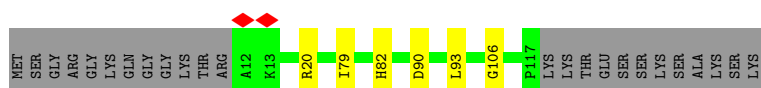
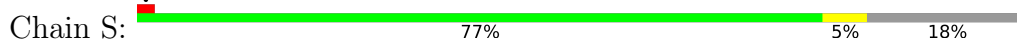
• Molecule 5: Histone H4



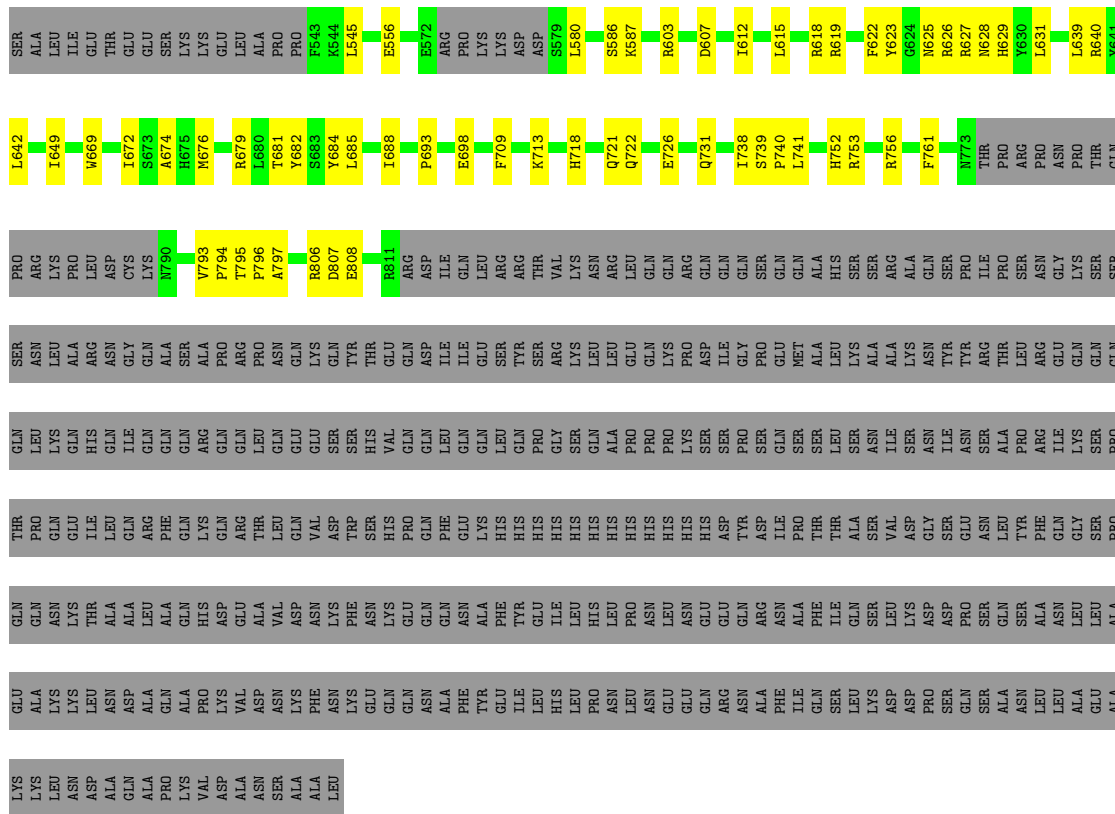
• Molecule 5: Histone H4



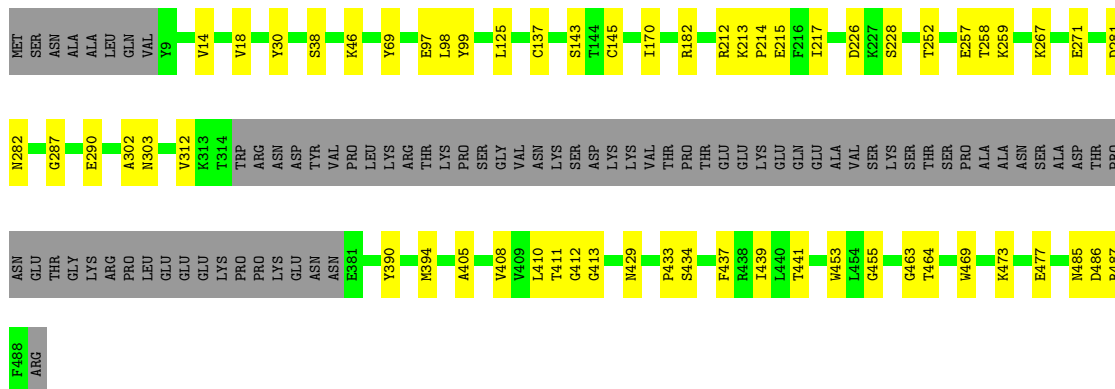
• Molecule 6: Histone H2A



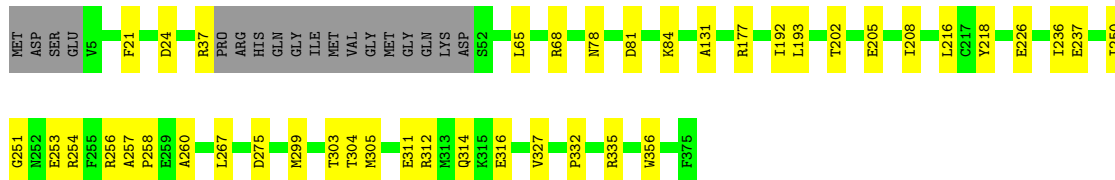
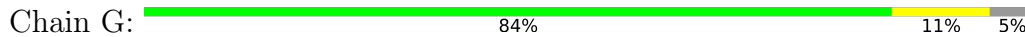
• Molecule 6: Histone H2A



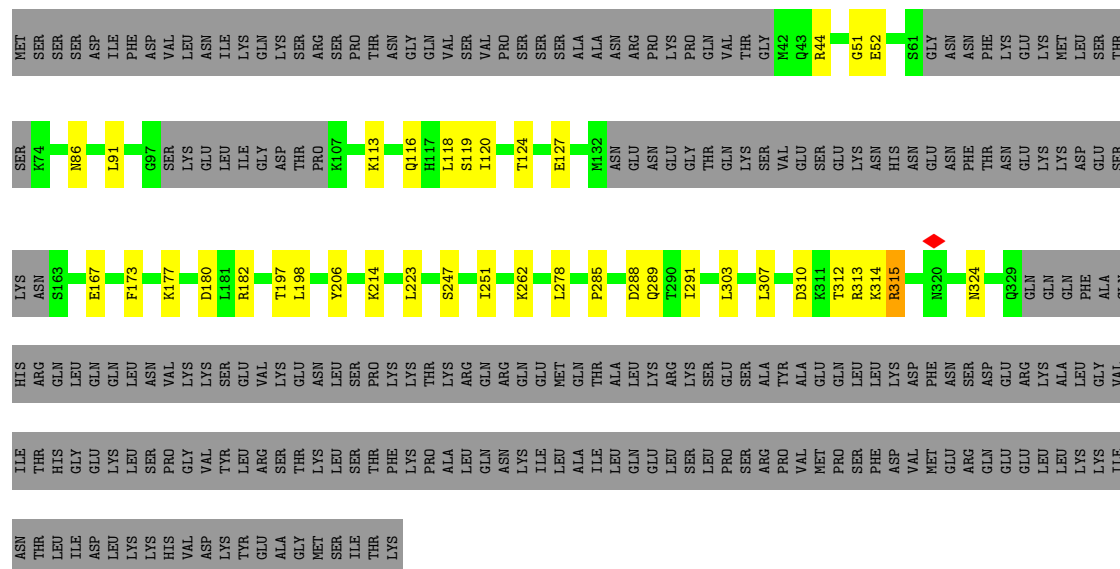
• Molecule 13: Actin-related protein 4



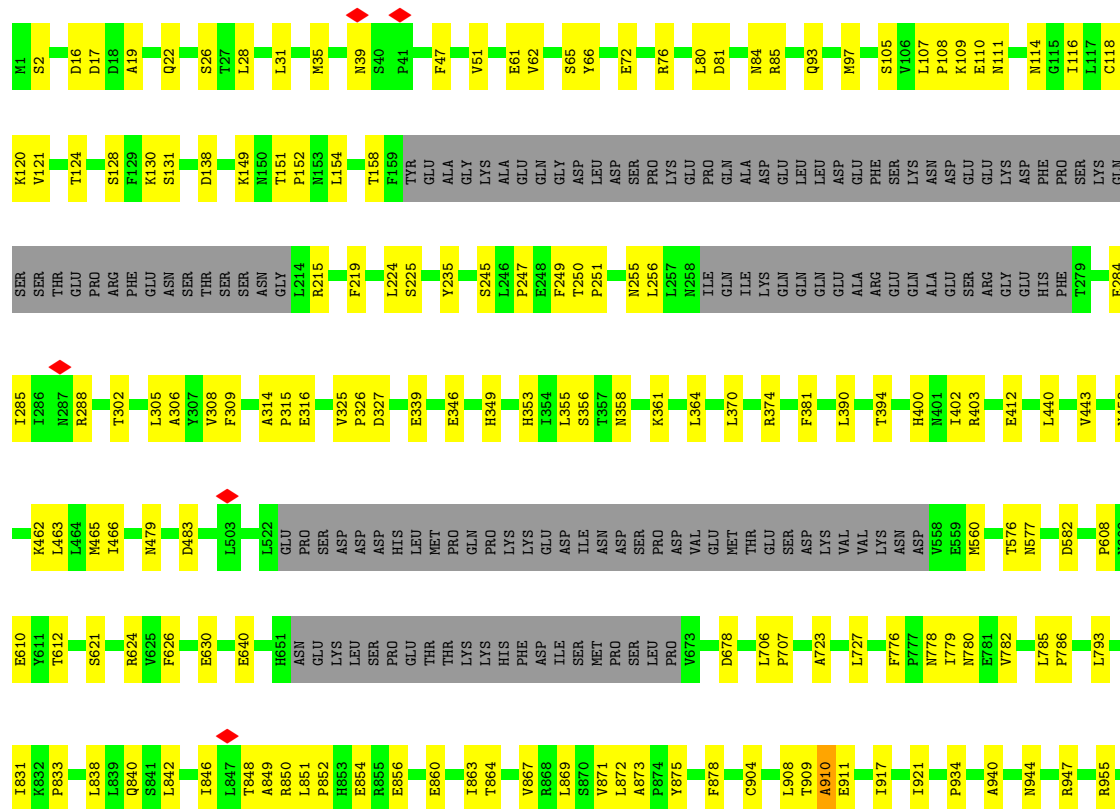
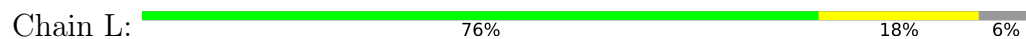
• Molecule 14: Actin



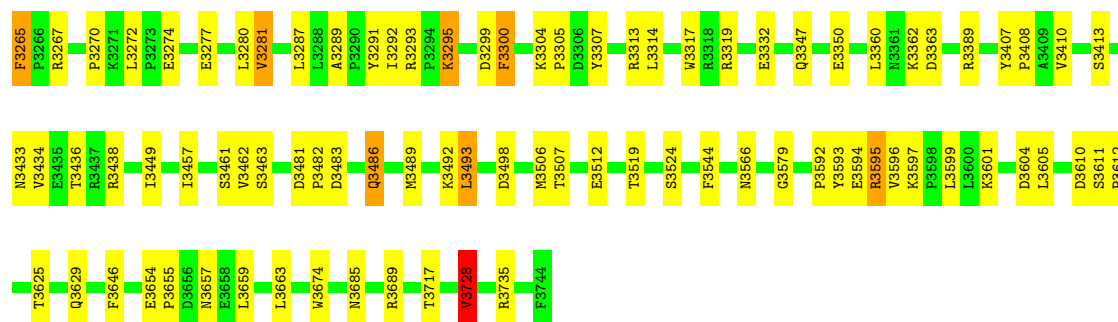
• Molecule 15: SWR1-complex protein 4



• Molecule 16: Transcription-associated protein 1



F3121	I3128	W3131	Y3132	F3136	L3140	M3151	V3152	R3153	R3158	Q3182	ARG	GLN	THR	MET	ALA	VAL	MET	GLY	ASP	LYS	PRO	THR	ASP	THR	ASN	ASP	ARG	ASN	ASN	GLY	ARG	F3067	L3068	P3204	E3210	T3240	T3241	D3244	R3247	L3248	N3249	V3251	Y3260	N3261	R3262	P3264													
L2936	T2972	L2973	F2982	E2998	T3001	Q3018	K3019	V3152	R3153	L3140	M3151	V3152	R3153	R3158	Q3182	ARG	GLN	THR	MET	ALA	VAL	MET	GLY	ASP	LYS	PRO	THR	ASP	THR	ASN	ASP	ARG	F3067	L3068	P3204	E3210	T3240	T3241	D3244	R3247	L3248	N3249	V3251	Y3260	N3261	R3262	P3264												
F2785	T2786	D2787	C2788	D2788	W2789	N2770	S2771	R2772	R2773	D2774	E2777	V2783	M2784	D2785	V2786	R2791	F2794	E2805	S2806	R2807	E2829	E2854	H2863	T2864	K2873	R2879	W2884	W2904	L2917	P2918	Q2924	GLN	SER	ASN	SER	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN													
M2605	I2613	E2614	S2615	L2616	E2617	L2618	P2619	P2620	H2621	V2623	K2624	Y2625	L2626	A2627	L2628	N2631	A2632	W2633	I2643	N2651	T2652	K2653	E2656	A2657	M2658	E2664	L2665	W2679	Y2685	K2713	A2714	R2715	L2719	P2720	Y2721	S2722	Q2723	Y2726	W2729	D2744	W2745	E2748	H2752																
E2444	R2450	R2456	D2457	E2461	I2463	Q2474	E2483	K2484	Q2346	L2347	F2348	L2349	R2350	V2353	V2369	A2373	R2385	E2502	C2493	L2494	I2499	L2500	Q2501	E2502	Y2503	L2504	M2521	K2524	S2529	M2530	Q2531	R2535	D2540	F2541	I2546	H2557	Y2568	K2573	N2574	H2591	T2593	I2596																	
L2310	K2313	Y2316	L2320	S2328	L2339	L2340	D2341	M2344	D2345	Q2346	L2347	F2348	L2349	R2350	V2353	V2369	A2373	R2385	E2502	C2493	L2494	I2499	L2500	Q2501	E2502	Y2503	L2504	M2521	K2524	S2529	M2530	Q2531	R2535	D2540	F2541	I2546	H2557	Y2568	K2573	N2574	H2591	T2593	I2596																
Y2169	F2172	K2177	E2178	W2179	I2180	M2181	L2184	D2198	H2199	H2200	Q2203	E2204	L2206	V2209	I2236	I2243	Q2248	E2249	T2250	S2251	S2252	L2259	V2272	P2273	L2274	L2275	T2276	P2277	L2278	M2279	K2284	L2285	C2286	K2287	D2288	Q2294	P2295	K2296	D2297	A2298	M2299	A2300	L2301																
VAL	GLU	ALA	ASP	THR	THR	ALA	ILE	ILE	VAL	ASP	ALA	ASN	ASN	SER	ASN	PRO	ILE	S2089	L2090	V2104	ASN	HIS	ARG	ALA	ILE	GLU	THR	E2115	L2116	A2120	I2121	N2122	I2123	P2130	HIS	TRP	THR	ASN	VAL	GLY	ASP	VAL	VAL	MET	SER	ASP	SER	SER	GLN	ASP	LEU	ILE	PHE	GLN	ASP	LEU	ASP	E2154	D2166
E1976	Q1981	F1988	L1989	H1992	P1993	M2011	F2016	MET	SER	ASN	ASN	ASN	PRO	ASN	ILE	S2089	L2090	V2104	ASN	HIS	ARG	ALA	ILE	GLU	THR	E2115	L2116	A2120	I2121	N2122	I2123	P2130	HIS	TRP	THR	ASN	VAL	GLY	ASP	VAL	VAL	MET	SER	ASP	SER	SER	GLN	ASP	LEU	ASP	E2154	D2166							
S1818	G1819	Y1824	L1825	V1826	E1827	D1828	K1829	P1830	P1831	ASP	K1832	W1833	L1834	H1838	I1841	N1844	A1847	I1848	L1849	A1850	Y1851	D1852	V1853	F1857	E1863	D1885	K1888	E1897	D1898	T1899	I1913	F1782	I1783	N1784	D1785	A1786	T1787	L1788	F1789	V1790	L1791	K1794	C1795	L1796	D1797	A1798	R1799	K1804	V1975										
L1507	E1508	L1509	Y1513	V1532	E1533	D1536	K1530	Q1531	S1535	P1536	K1547	P1548	I1558	L1562	P1563	P1564	Q1565	R1582	M1601	R1602	F1603	H1604	M1605	P1606	Y1607	M1615	R1618	N1626	V1628	V1629	P1631	E1632	E1638	K1642	L1643	L1644	F1650	Y1651	I1655	I1655	D1491	H1492	L1503	S1504															
Y1993	Y1007	H1012	Y1013	R1014	M1028	T1029	K1030	Q1031	S1031	S1032	A1033	K1044	V1047	M1048	K1051	L1052	T1055	D1062	L1063	K1093	E1094	D1098	N1105	L1133	P1136	N1137	D1141	L1144	Y1156	I1171	L1193	Q1234	T1271	E1277	D1278	L1279	L1280	N1288																					
V1303	I1320	D1327	H1328	S1329	M1028	T1029	K1030	Q1031	S1031	S1032	A1033	K1044	V1047	M1048	K1051	L1052	T1055	D1062	L1063	K1093	E1094	D1098	N1105	L1133	P1136	N1137	D1141	L1144	Y1156	I1171	L1193	Q1234	T1271	E1277	D1278	L1279	L1280	N1288																					



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: MG, CMC, ATP

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%)	34	72
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%)	47	81
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%)	34	72
16	L	3489/3744 (93%)	3203 (92%)	284 (8%)	2 (0%)	51	86
All	All	6589/9755 (68%)	6155 (93%)	429 (6%)	5 (0%)	54	86

All (5) Ramachandran outliers are listed below:

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

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

5.3.2 Protein sidechains [i](#)

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%)	86	92
All	All	6064/8816 (69%)	6044 (100%)	20 (0%)	92	95

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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
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%)
19	ATP	G	502	18	26,33,33	0.69	0	31,52,52	0.82	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
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
19	ATP	G	502	18	-	0/18/38/38	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($^{\circ}$)	Ideal($^{\circ}$)
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:

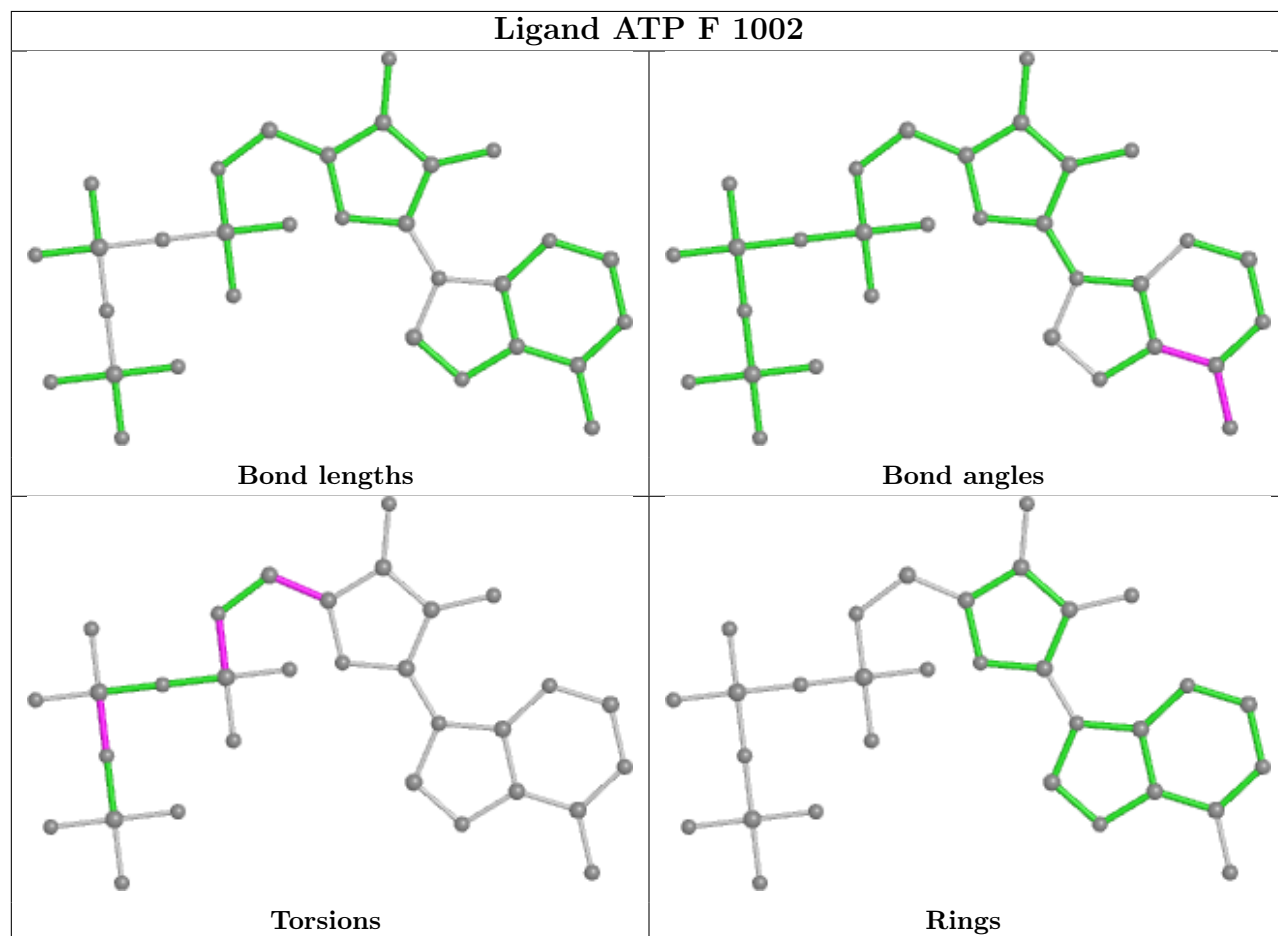
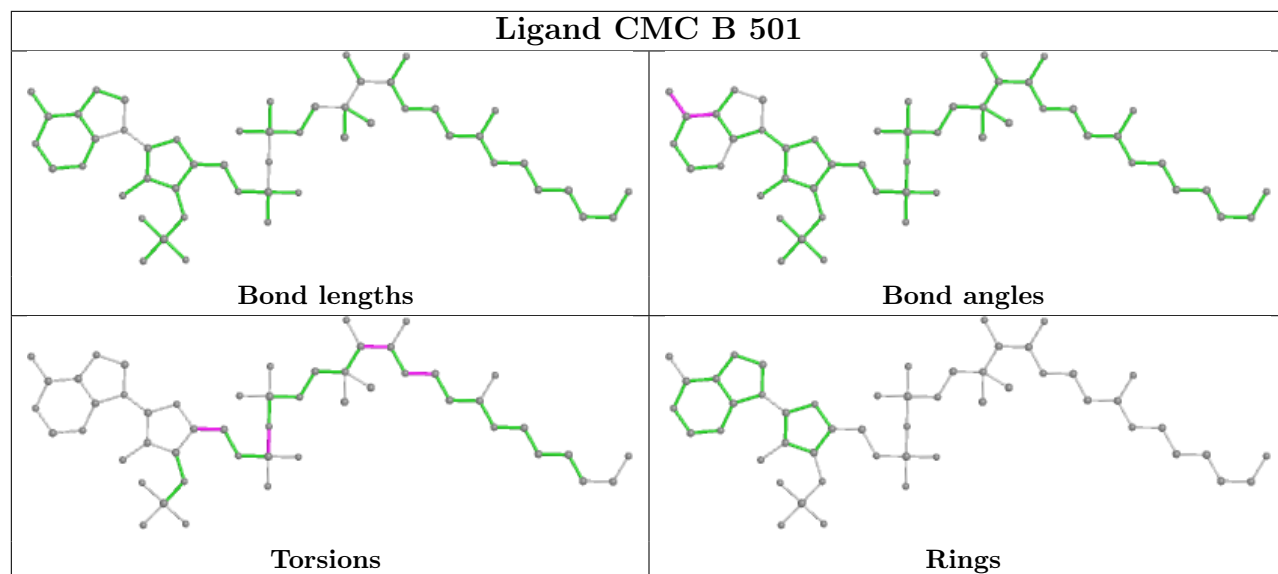
Mol	Chain	Res	Type	Atoms
17	B	501	CMC	O4B-C4B-C5B-O5B
17	B	501	CMC	C3B-C4B-C5B-O5B
17	B	501	CMC	P2A-O3A-P1A-O1A
17	B	501	CMC	C6P-C7P-N8P-C9P
19	F	1002	ATP	C5'-O5'-PA-O3A
19	F	1002	ATP	PG-O3B-PB-O2B
19	F	1002	ATP	C5'-O5'-PA-O2A
17	B	501	CMC	O9P-C9P-CAP-OAP
19	F	1002	ATP	O4'-C4'-C5'-O5'
17	B	501	CMC	P2A-O3A-P1A-O2A

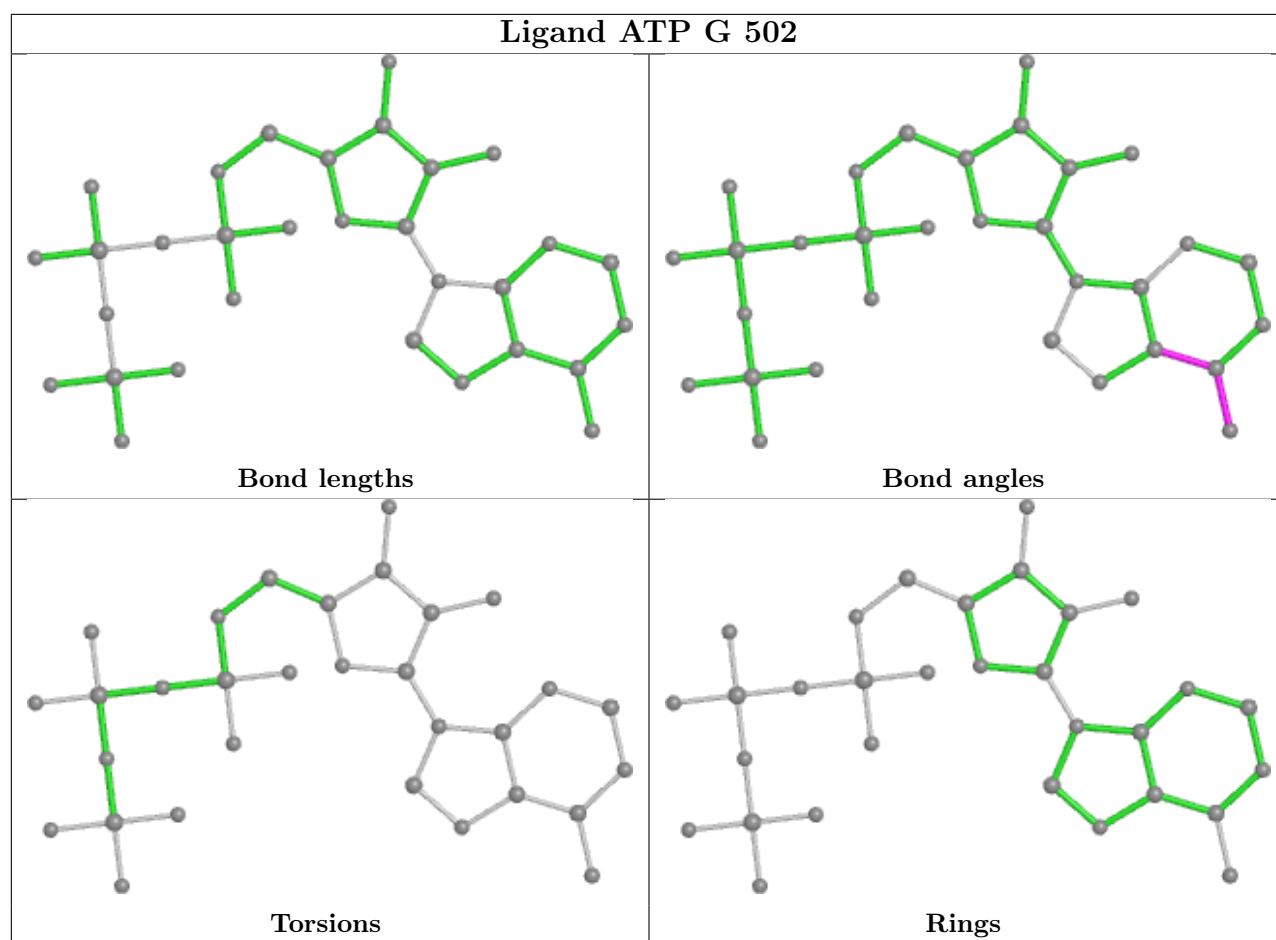
There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

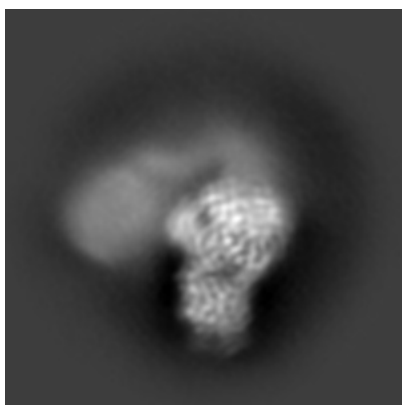
6 Map visualisation [i](#)

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.

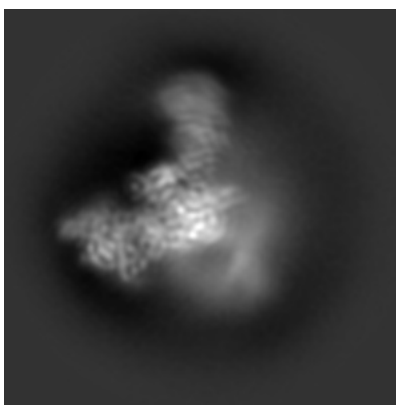
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

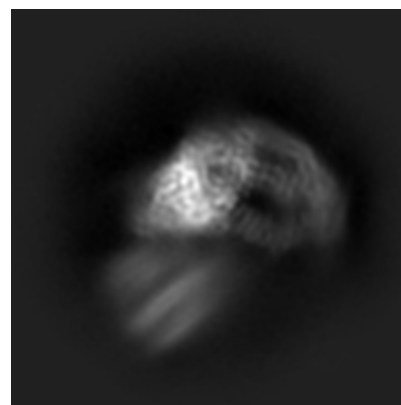
6.1.1 Primary map



X



Y

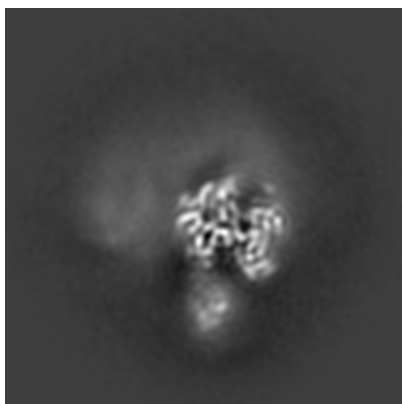


Z

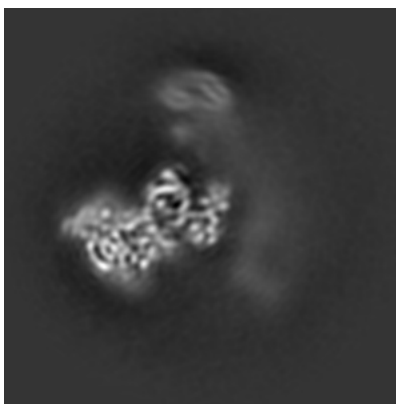
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

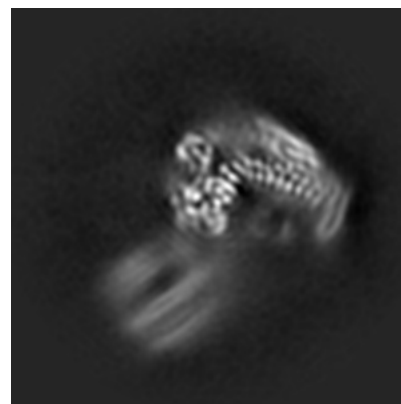
6.2.1 Primary map



X Index: 47



Y Index: 47

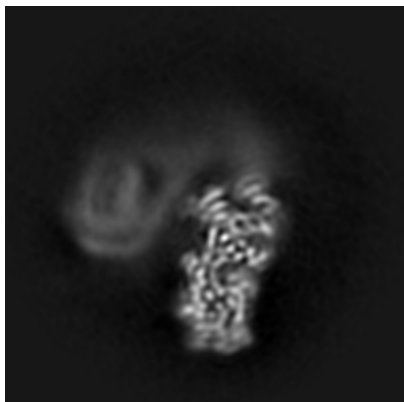


Z Index: 47

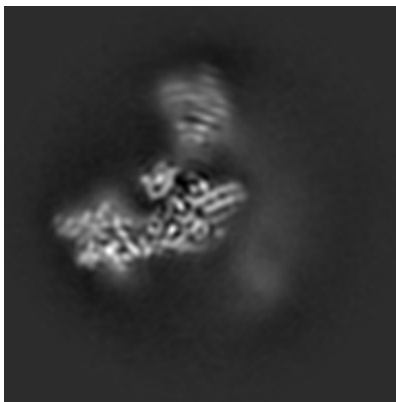
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

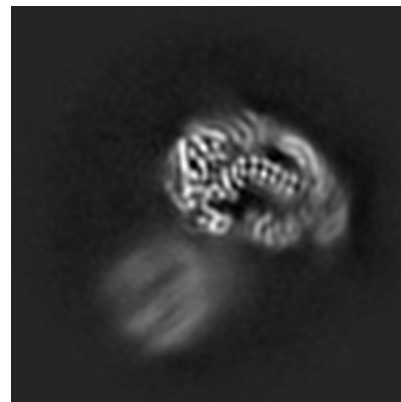
6.3.1 Primary map



X Index: 41



Y Index: 51

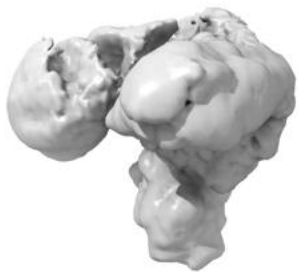


Z Index: 44

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

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

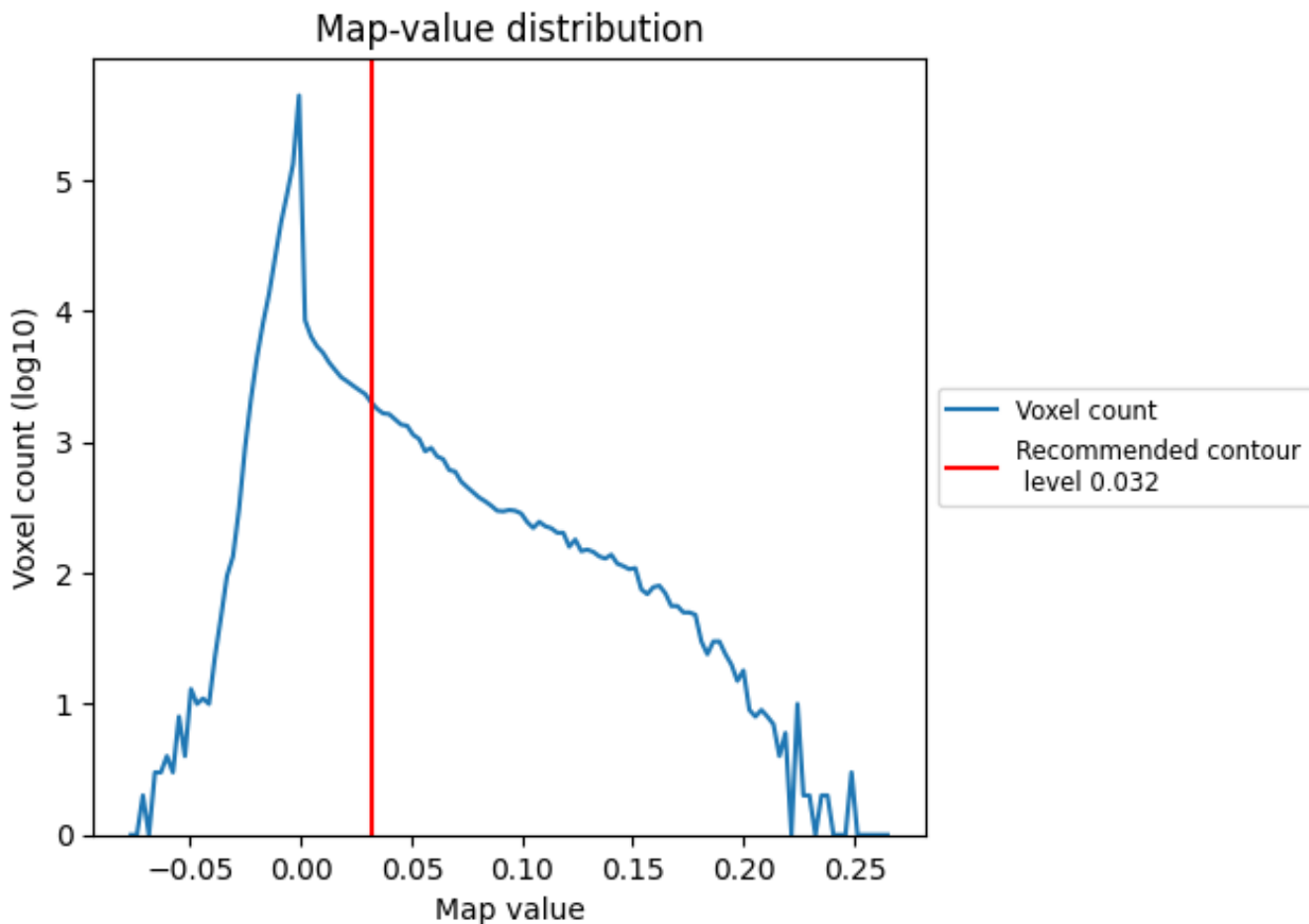
6.5 Mask visualisation

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

7 Map analysis [i](#)

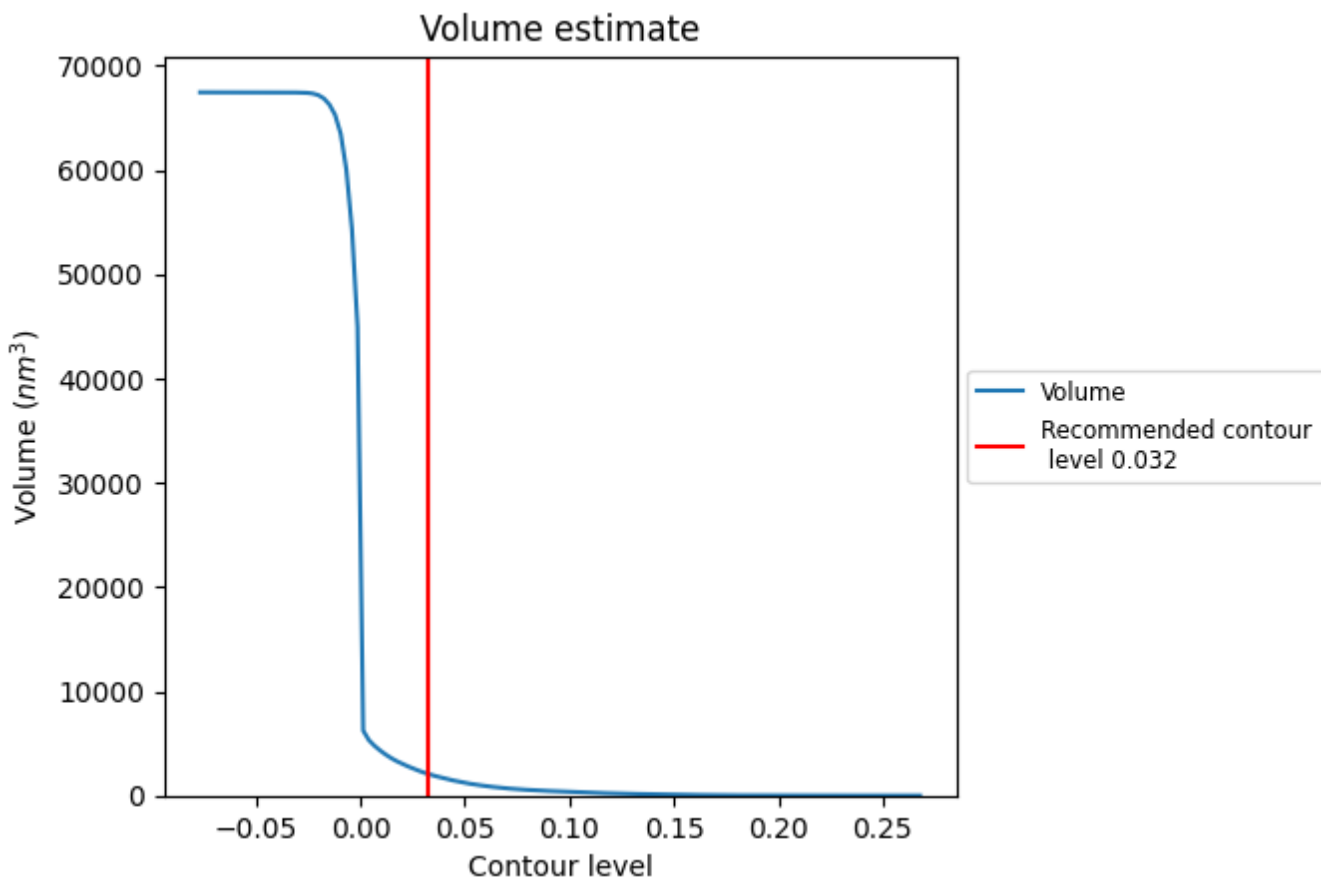
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

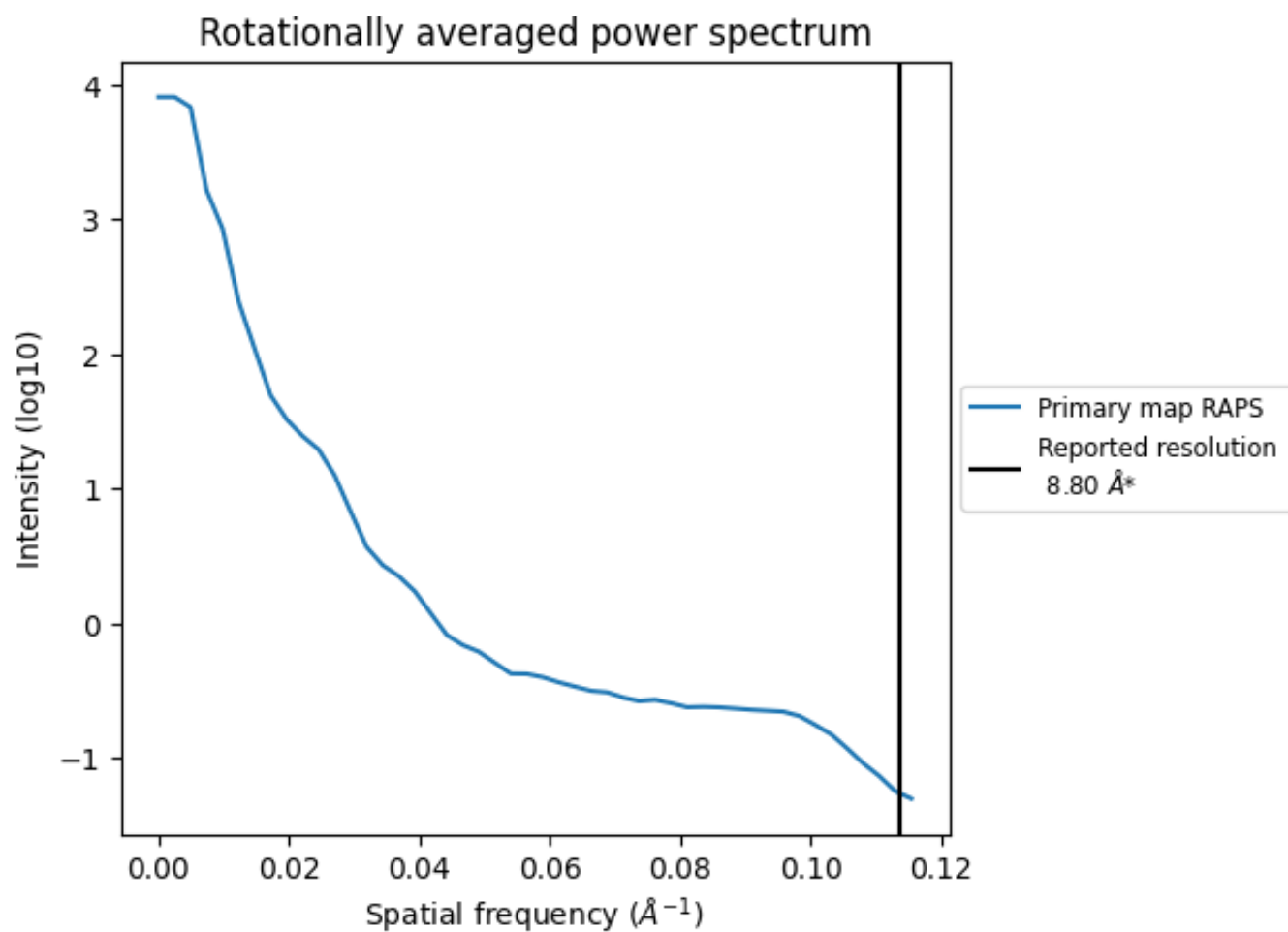
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.114 Å⁻¹

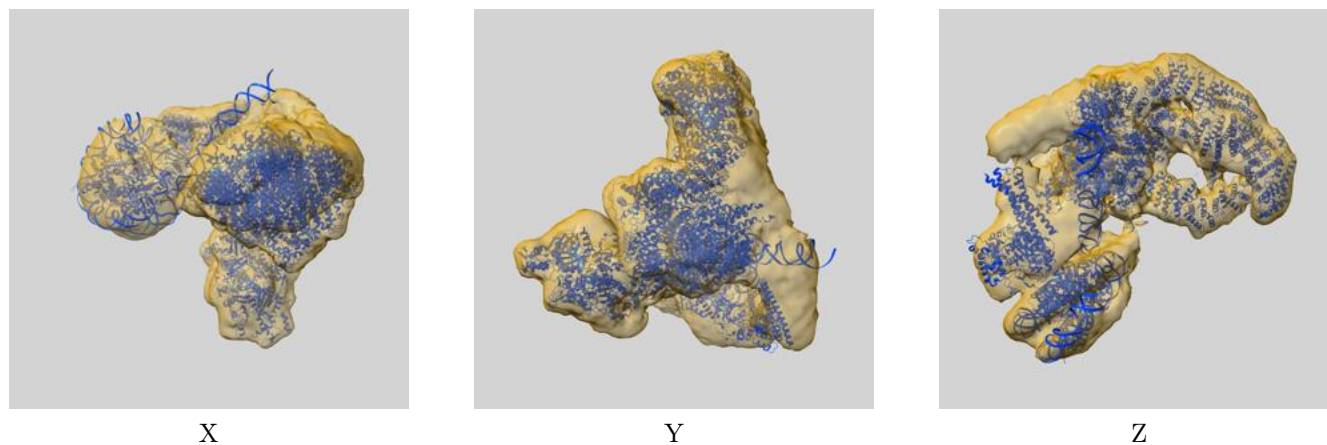
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

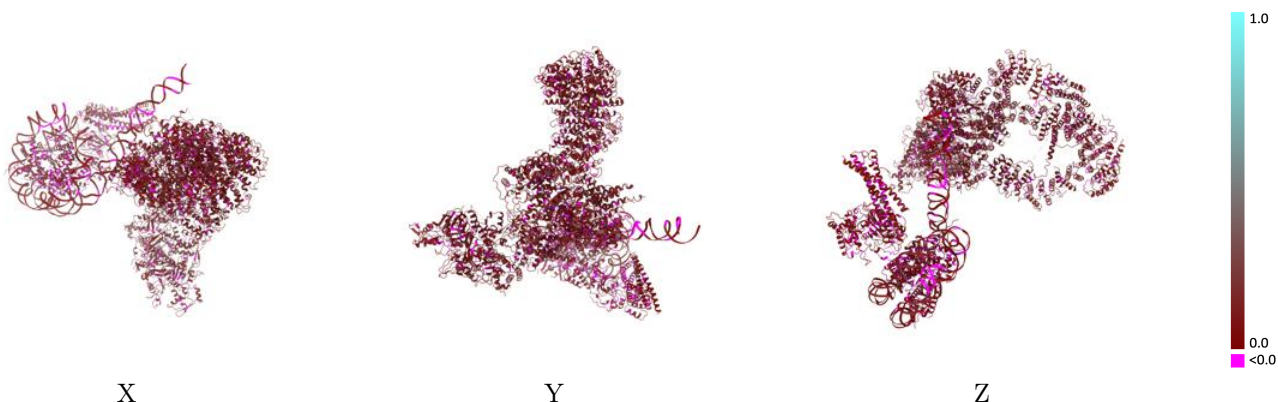
This section contains information regarding the fit between EMDB map EMD-32150 and PDB model 7VVZ. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



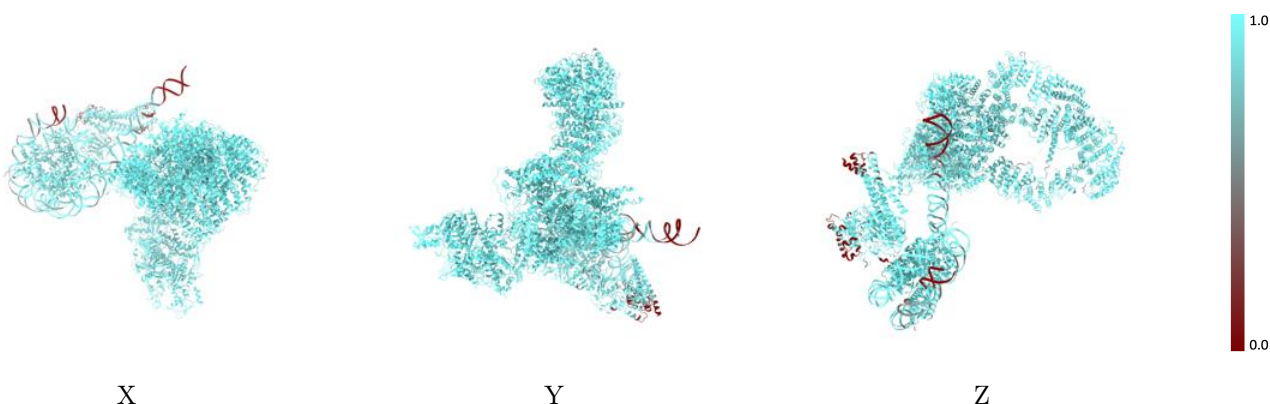
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



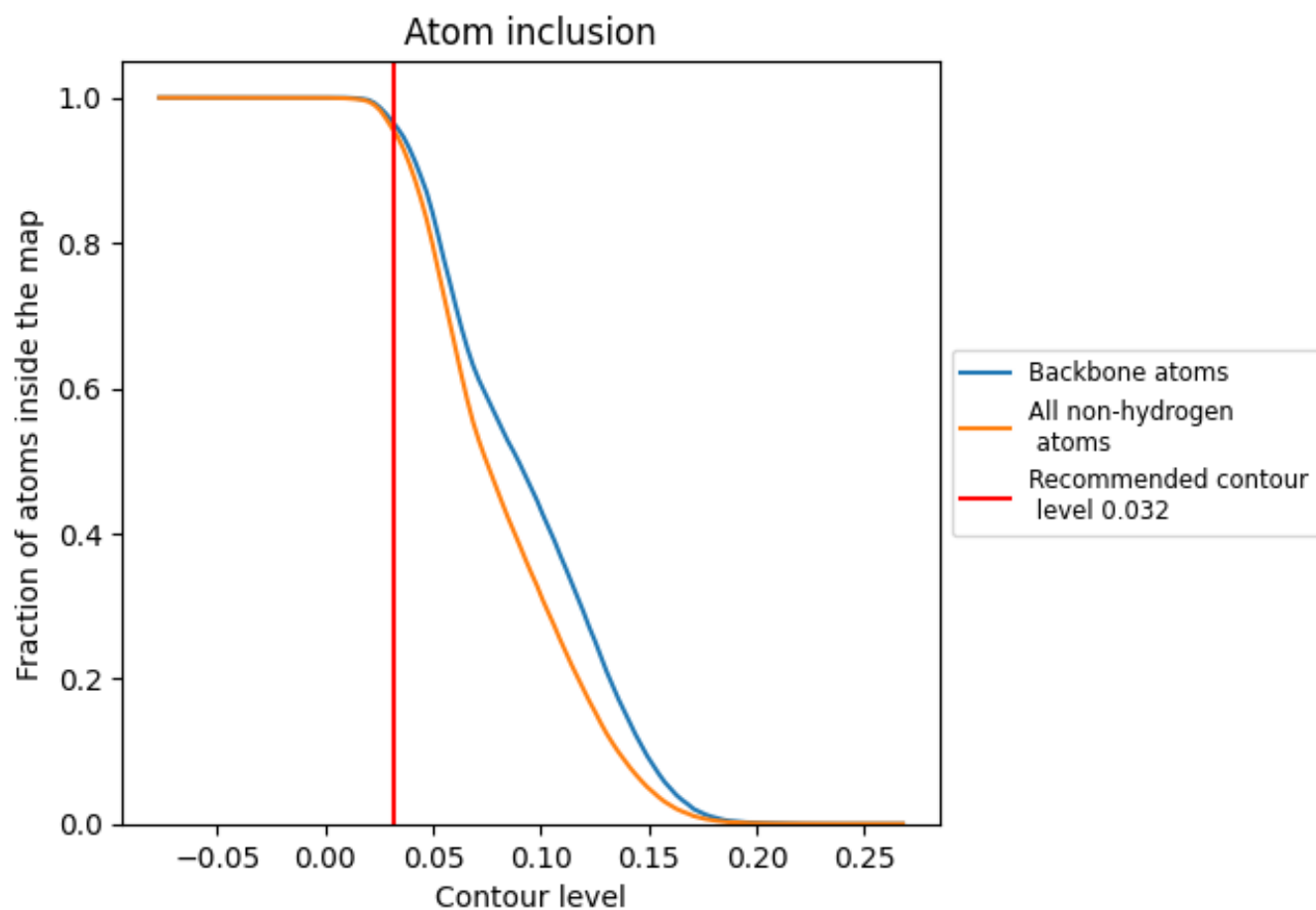
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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	 0.9537	 0.1080
A	 0.9544	 0.0710
B	 0.9378	 0.0550
D	 0.9831	 0.0560
E	 0.9985	 0.1360
F	 0.9997	 0.1220
G	 0.9978	 0.1180
H	 0.9841	 0.1200
I	 0.8133	 0.0880
K	 0.9913	 0.1310
L	 0.9827	 0.1260
N	 0.9911	 0.0370
O	 1.0000	 0.0500
P	 0.9852	 0.0680
Q	 1.0000	 0.0320
S	 0.9734	 0.0490
T	 0.7882	 0.0650
U	 0.9829	 0.0670
V	 0.8434	 0.0470
W	 0.8126	 0.0750
X	 0.8846	 0.0650
Y	 0.7532	 0.0780

