



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 12:15 PM UTC

PDB ID : 9G2C / pdb_00009g2c
EMDB ID : EMD-50972
Title : Yeast RNA polymerase I elongation complex stalled by an apurinic site, open state
Authors : Santos-Aledo, A.; Plaza-Pegueroles, A.; Ruiz, F.M.; Fernandez-Tornero, C.
Deposited on : 2024-07-10
Resolution : 3.50 Å(reported)
Based on initial model : 6hko

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

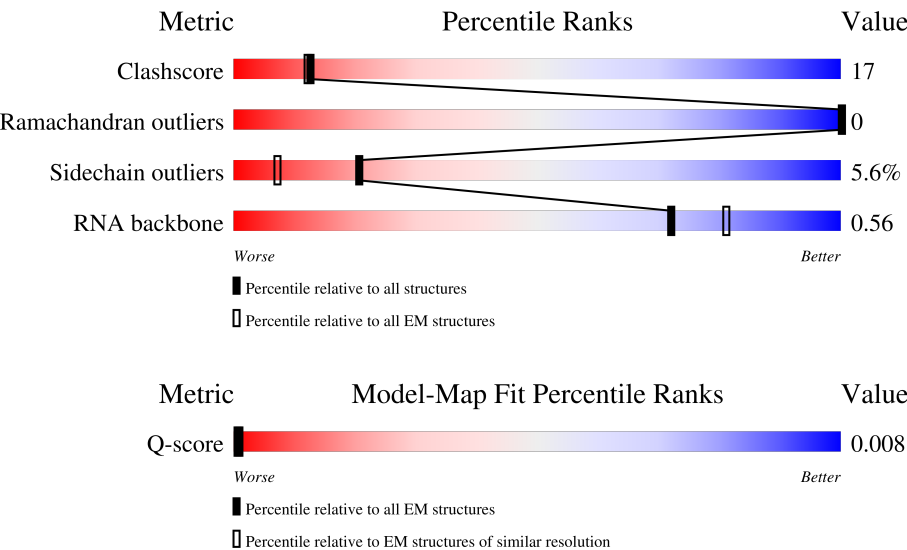
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	1664	60% 46% 23% • 30%
2	B	1203	82% 55% 36% • 6%
3	C	335	82% 59% 29% • 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	215	
5	F	155	
6	G	326	
7	H	146	
8	I	125	
9	J	70	
10	K	142	
11	L	70	
12	M	415	
13	N	233	
14	R	12	
15	S	38	
16	T	38	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 29270 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 DNA-directed RNA polymerase I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1172	Total	C	N	O	S	0	0
			9243	5827	1599	1768	49		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1127	Total	C	N	O	S	0	0
			8963	5676	1577	1660	50		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	304	Total	C	N	O	S	0	0
			2415	1535	414	458	8		

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	181	Total	C	N	O	S	0	0
			1488	943	263	274	8		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	103	Total	C	N	O	S	0	0
			839	530	148	158	3		

- Molecule 6 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	60	Total	C	N	O	S	0	0
			472	305	75	89	3		

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 8 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	57	Total	C	N	O	S	0	0
			423	267	70	82	4		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	68	Total	C	N	O	S	0	0
			561	357	100	99	5		

- Molecule 10 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	97	Total	C	N	O	S	0	0
			758	476	123	155	4		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	71	Total	C	N	O	0	0
			571	359	99	113		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	86	Total	C	N	O	S	0	0
			679	437	116	124	2		

- Molecule 14 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	9	Total	C	N	O	P	0	0
			197	88	40	60	9		

- Molecule 15 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	27	Total	C	N	O	P	0	0
			546	262	89	168	27		

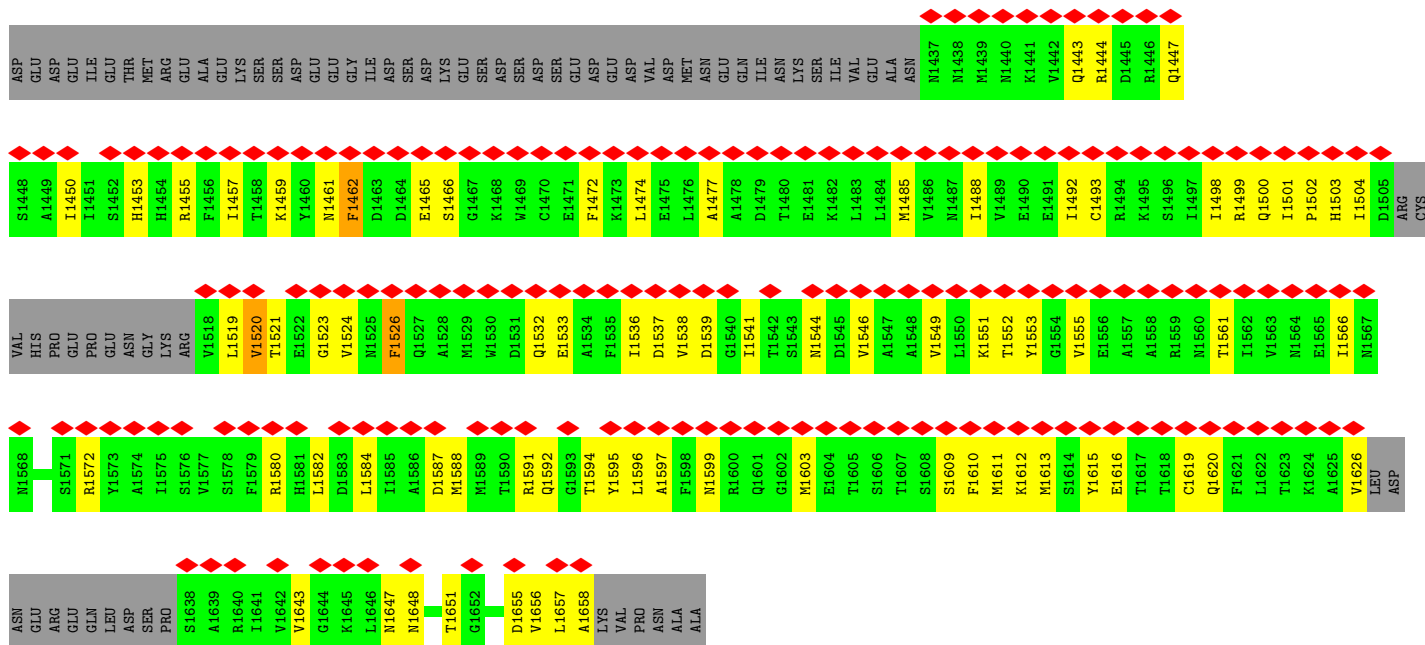
- Molecule 16 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	35	Total	C	N	O	P	0	0
			707	337	127	208	35		

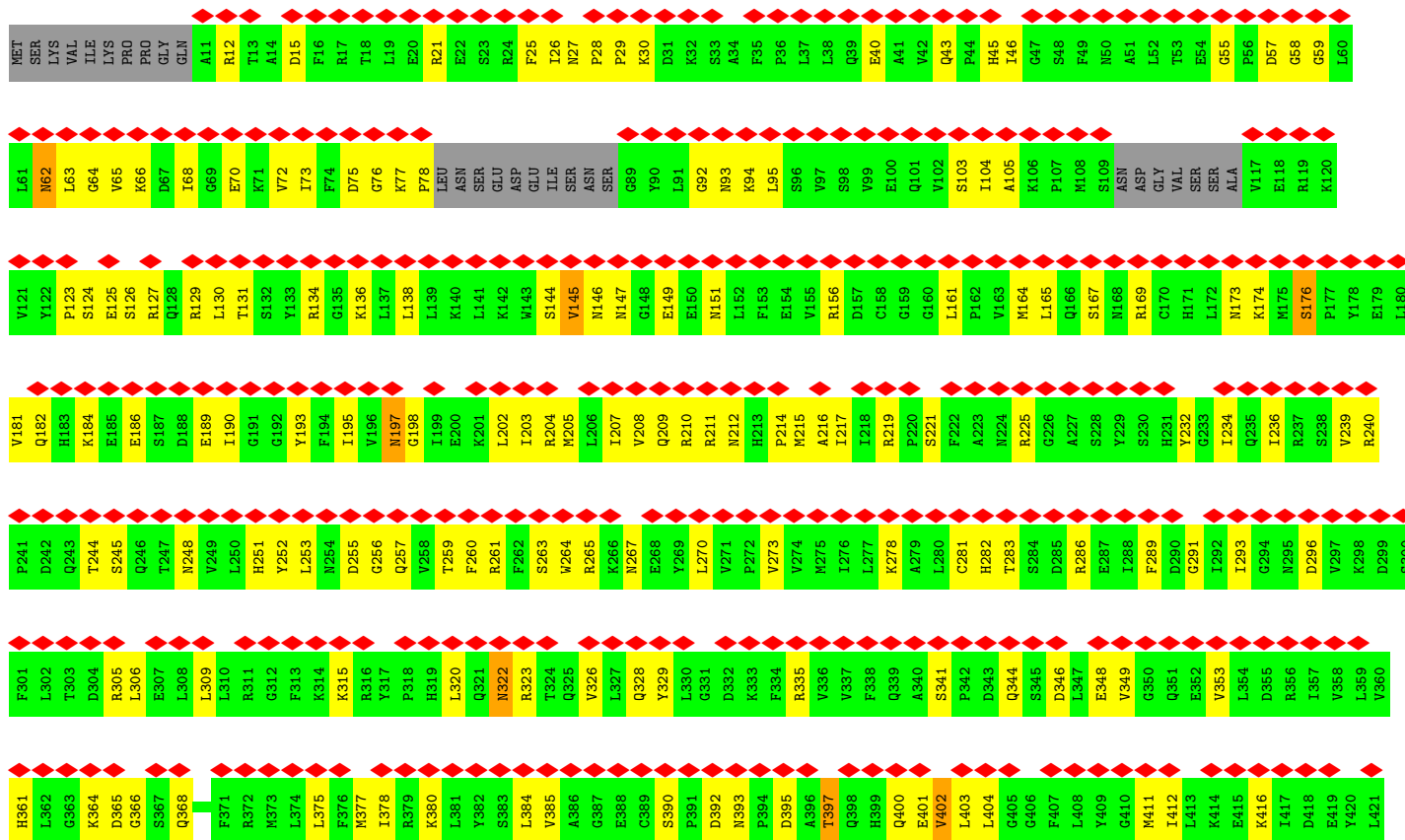
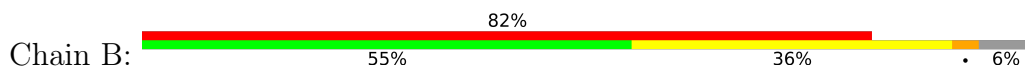
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	B	1	Total	Zn	0
			1	1	
17	I	1	Total	Zn	0
			1	1	
17	J	1	Total	Zn	0
			1	1	
17	L	1	Total	Zn	0
			1	1	

A1328	D1268	L1148	H1088	L1027	T965	I903	R843	D782	P722	G663	M601
I1329	K1269	D1149	L1089	E1028	L966	T904	T844	K783	Y723	S664	G602
V1330	I1270	K1150	D1090	G1029	P967	S905	D845		P724	P665	H603
F1331	I1271	N1151	V1091	V1030	S968	Q906	I846	Y786	W726	V666	K604
E1332	T1272	S1152	E1092	H1031	F969	V908	L847	G787	G728	R667	V605
T1333	T1273	K1153	S1093	S1032	K970	S909	K848	S789	K729	T727	R606
K1334			A1094	V1034	P971	K910	T849	K790	I731	I670	L608
E1274		LEU	E1094	D1035	Y972	C911	S850	I791	G730	Q671	P609
T1275		PHE	S1095	M1036	E973	N1036	V851	G792	I730	D672	N610
T1276		LYS	K1096	S1037	T974	V912	D852	I793	T733	H673	E611
G1277		SER	Y1097	I1038	D975	P913	T853	V794	T734	I674	K612
		ASP	S1098	R1039	A976	G915	G854	H795	I735	S675	T613
		G1160	K1099	D1040	M977	T916	R855	L797	L736	A676	L614
		V1161	T1101	A1041	A978	N917	E857	H798	L737	G677	R615
		M1162	L1102	D1042	G979	K918	A858	E799	N738	V678	L616
		E1163	K1103	G1043	T981	K919	A859	V800	V739	W679	H617
		K1164	Y1104	T1044	G980	F920	E860	Y801	T740	L680	V618
		L1165	R1105	V1045	K983	P921	V861	G802	P741	T681	A619
		F1166	K1106	Q1047	R985	C922	T862	P803	F742	S682	N620
		A1167	K1107	F1048	F986	S924	N863	V805	D743	K683	T621
		L1169	H1108	M1049	Y987	N925	L864	A806	M744	D684	G622
		M1170	S1109	Y1050	S988	Q926	D665	A807	P745	S685	A623
		Q1171	K1110	G1051	G989	A927	K866	K808	G746	S686	Y624
		L1172	E1111	D1052	T990	M928	D667	V809	I747	F686	N625
		K1173	P1112	D1053	K991		T868	L810	N748	T688	A626
		Y1174	H1113	A1054	P992	S931	P669	L810	L749	R689	ASP
		M1175	Y1114	I1055	Q993	G932	A870	S811	I750	E590	PHE
		S1177	K1115	D1056	E994	A933	D871	V812	S751	Q691	GLY
		L1178	Q1116	D1057	Y995	K934	D872	L813	K752	Y692	ASP
		T1179	S1117	T1058	Y996	G935	P873	G814	N753	G693	E632
		N1180	V1118	K1059	F997	N937	E874	R815	K754	Q694	M633
		N1180	K1119	E1060	H998	N937	L875	L816	I755	Y695	N634
		P1181	Y1120	S1061	A1001	V938	L876	F817	K756	I696	M635
		G1182	D1121	H1062	G1002	N939	T877	N819	N757	Y697	H636
		E1183	P1122	M1063	E1003		K877	T820	F758	G698	F637
		A1184	V1123	T1064	L1004	Q942	R878	I821	Y759	C699	F638
		V1185	L1124	Q1065		I943	L879	T822	W760	I700	Q639
		G1186	A1125			M944	Q880	A823	G761	R701	N640
		T1187	K1126	F1068	T1007	C945	E881	T824	K762	E641	
		I1188	C1069	C1069	D1008	L946	E881	F826	G763	E703	N642
		L1188	A1189	L1070	T1009	L947	E882	A825	S764	D704	A643
		S1190	N1128	D1071	A1010	Q948	L883	R884	L765	G705	R644
		E1249	P1129	N1072	V1011	Q949	R884	T827	E766	H706	A645
		Q1250	A1130	Y1072	K1012	Q950	D885	C828	N767	T707	E646
		A1251	K1131	Y1073	T1013	A951	N886	G829	E768	T708	A647
		D1252	Y1132	Y1074	S1014	L952	N887	M830	V769	R709	L648
		T1253	L1133	A1075	R1015	E953	K888	D831	L770	S710	N649
		F1254	G1134	L1076	S1016	G954	V889	L833	K771	K711	L650
		C1255	S1135	L1077	G1017	R955	S889	R834	I770	I712	A651
		S1197	V1136	K1078	Y1018	R956	G890	L835	G773	V713	N652
		T1198	S1137	K1079	L1019	V957	L892	T836	D774	T714	T653
		Q1199	E1138	Y1080	Q1020	P958	D893	A837	A775	L715	D654
		M1200	N1139	T1201	R1021	V959	A894	E838	L776	P716	S655
		T1202	F1140	M1081	C1022	N960	V895	G839	L777	T717	Q656
		L1203	Q1141	P1082	L1023	V961	T896	N840	L778	I718	Y657
		N1203	D1142	S1083	T1024	S962	S897	K841	G779	I719	L658
		T1204	K1143	A1084	L1024	G963	S898	W842	I780	F720	T659
		PHE	L1144	L1085	K1025	K964	V900		L781		P660
		HIS	E1145	I1086	Q1026		A902				
		PHE	S1146	E1087							
			F1147								

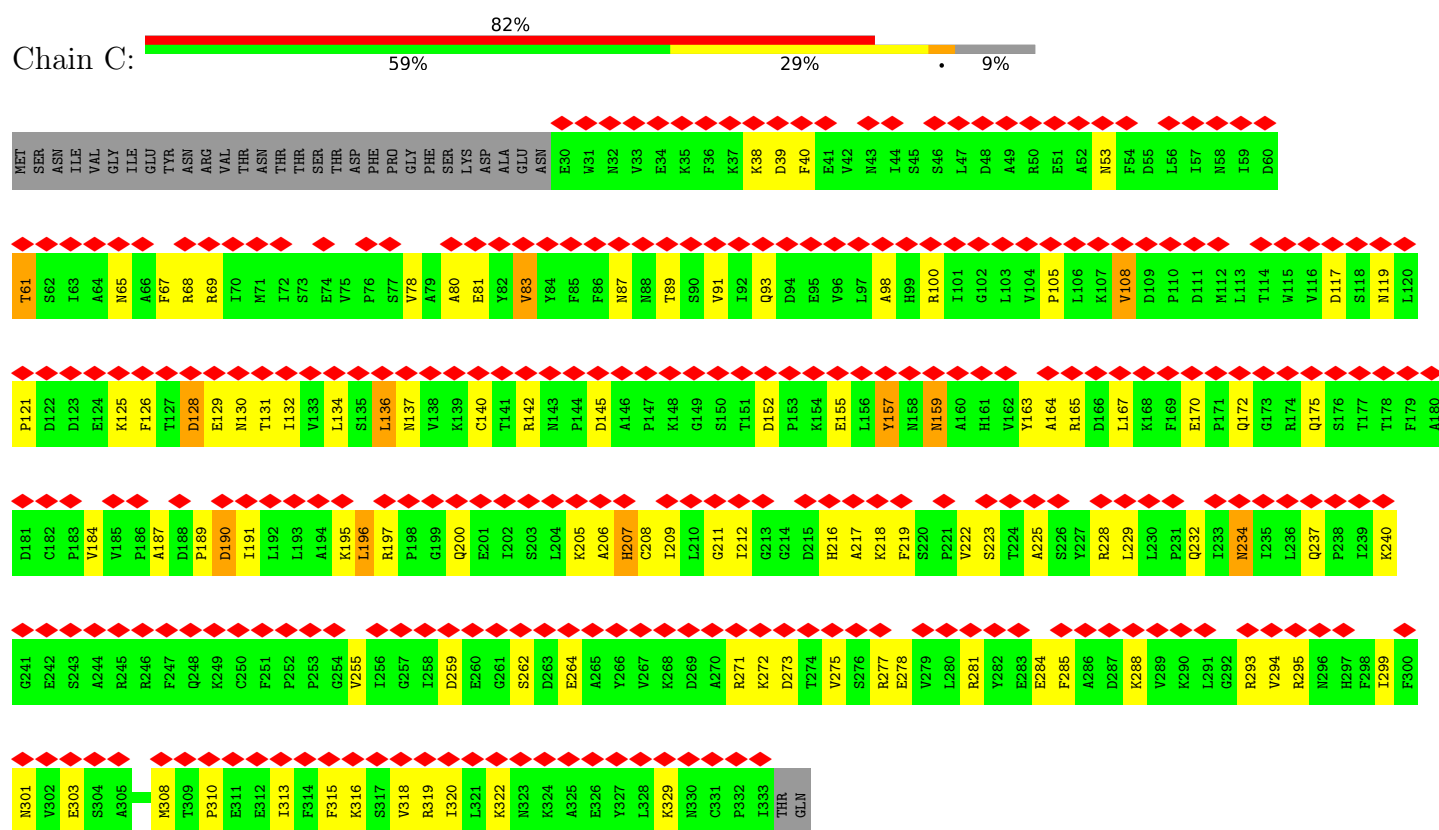


• Molecule 2: DNA-directed RNA polymerase I subunit RPA135

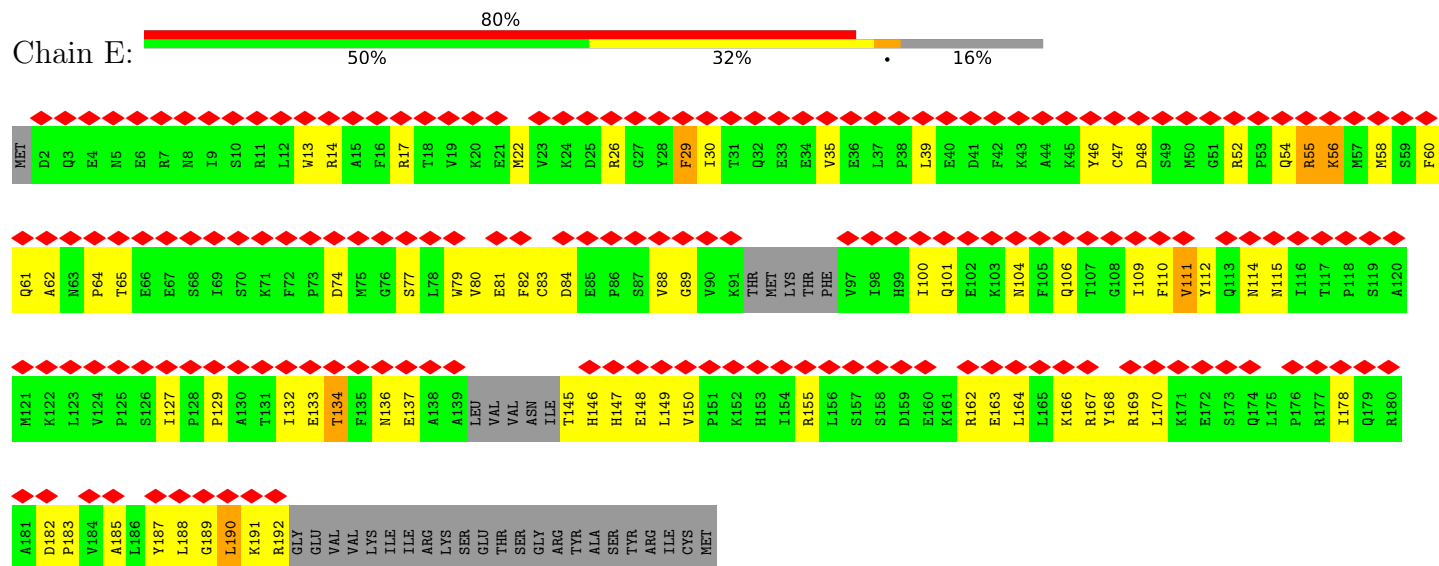


ILE	PHE	ILE	ASP	D1155	S1156	Q1157	I1158	TRP	GLU	ASP	GLY	PHE	V1168	G1169	G1170	N1171	E1172	T1173	T1174	T1175	V1176	A1177	I1178	P1179	F1180	V1181	L1182	K1183	Y1184	L1185	D1186	S1187	E1188	L1189	S1190	A1191	M1192	G1193	I1194	R1195	L1196	R1197	Y1198	M1199	V1200	E1201	P1202	K1203														
R1091	L1092	L1093	N1094	SER	ASP	ASP	THR	THR	GLN	ALA	SER	V1103	C1104	R1105	S981	E1106	C1107	G1108	S1109	ILE	LEU	THR	T1113	Q1114	Q1115	S1116	V1117	R1119	I1120	G1121	S1122	I1123	S1124	T1125	V1126	C1127	C1128	R1129	R1130	R1131	SER	MET	ARG	PHE	GLU	ASP	ALA	LYS	LYS	LEU	LEU	THR	LYS	SER	GLU	ASP	GLY	GLU	LYS			
V1031	Y1032	Y1033	Q1034	R1035	L1036	R1037	H1038	M1039	VAL	ASN	ASN	K1043	F1044	Q1045	S981	P982	R983	R984	I985	E986	D989	D990	A993	D994	Y995	P996	G997	E998	Q999	L1000	K1001	K1002	A1003	G1004	Y1005	N1006	G1009	M1010	E1011	P1012	ARG	M1013	Y1014	S1015	G1016	R1076	D1077	LVS	A1078	L1079	LVS	L1080	H1081	E1082	G1083	T1084	S1085	F1086	L1087	L1088	Q1089	D1090
R906	I907	R908	R909	T910	P911	Q912	I913	G914	D915	R916	F917	S918	S919	R920	H921	G922	Q923	R924	G925	Y926	C927	S928	R929	D994	K930	W931	P932	T933	I934	N936	P937	F938	S939	E940	T941	G942	I943	Q944	P945	D946	I947	Y948	I949	N950	P951	H952	A953	R954	P955	S956	H958	G961	N962	E965	S966	L967						
A968	G969	K970	A971	G972	A973	L974	H975	G976	I977	A978	Q979	D980	S981	T982	P983	R984	I985	E986	D989	D990	A993	D994	Y995	P996	G997	E998	Q999	L1000	K1001	K1002	A1003	G1004	Y1005	N1006	G1009	M1010	E1011	P1012	ARG	M1013	Y1014	S1015	G1016	R1076	D1077	LVS	A1078	L1079	LVS	L1080	H1081	E1082	G1083	T1084	S1085	F1086	L1087	L1088	Q1089	D1090		
P846	Y847	I848	G849	T850	Y851	H852	E853	E854	G855	D856	P857	I858	C859	A860	Y861	F862	D863	T864	T865	L866	N867	K868	T869	K870	L871	K872	T873	Y874	H875	S876	S877	E878	P879	A880	Y881	T882	E883	E884	N886	L887	I888	G889	D890	E891	S892	N893	K894	F895	Q896	E897	L898	Q899	T900	Y901	S902	T903	K904	Y905				
A786	M787	I788	I789	N790	S791	H792	A793	D794	E795	R796	F797	F798	G799	Y800	G801	T802	M803	Y804	K805	T806	E807	K808	Y809	D810	L811	A812	L813	R814	R815	N816	R817	G818	D819	P820	I821	T822	Q823	H824	F825	G826	F827	G828	N829	D830	E831	W832	P833	K834	E835	W836	L837	E838	K839	L840	D841	E842	D843	G844	L845			
T725	M726	G727	T728	E729	G730	V731	A732	L733	C734	H735	R736	D738	N739	K740	L741	Y742	R743	L744	Q745	T746	G747	Q748	T749	P750	I751	V752	K753	A754	N755	L756	Y757	D758	D759	M762	D763	T764	F765	P766	N767	G768	F769	N770	A771	V772	V773	A774	V775	I776	S777	Y778	T779	Y781	D782	M783	D784	D785						
I603	I604	A605	D606	T607	L608	R609	Y610	W611	K612	V613	G615	K616	T617	P618	G619	L620	P621	I622	D623	L624	E625	G626	Y628	V629	P630	P631	S632	T633	R634	G635	Q636	Y637	P638	G639	L640	Y641	L642	F643	G644	G645	H646	S647	R648	M649	L650	P651	P652	G653	R654	Y655	L656	P657	L658	D659	K660	E661	D662					
N543	H544	F545	H547	K548	C549	I551	S552	T553	Q554	Q555	S556	D557	V558	S559	R560	I561	S562	S563	I564	L565	Y566	S567	L568	G569	V570	A571	P572	A573	S574	H575	T576	F577	A578	A579	G580	P581	S582	L583	C584	C585	V586	Q587	I588	D589	G590	K591	I592	I593	Q594	W595	V596	S597	H598	E599	Q600	G601	K602					
S482	G483	Y484	T485	V486	V487	A488	E489	K490	I491	M492	Y493	R495	F496	I497	S498	H499	F500	R501	M502	V503	H504	R505	G506	S507	F508	F509	A510	Q511	L512	K513	T514	T515	T516	V517	R518	K519	L520	L521	P522	E523	S524	W525	G526	F527	L528	C529	H532	T533	P534	D535	G536	S537	P538	C539	G540	L541	L542					
Q422	N423	I424	I425	A426	Q427	V428	R429	M430	D431	I432	N433	R434	G435	M436	A437	I438	N439	F440	K441	D442	K443	R444	Y445	S446	R448	V449	L450	M451	R452	V453	N454	E455	N456	I457	G458	S459	K460	M461	Q462	Y463	F464	L465	S466	T467	G468	N469	L470	V471	S472	Q473	G475	L476	D477	L478	Q479	Q480	V481					

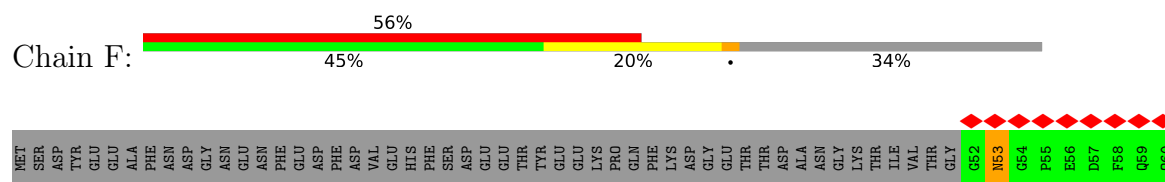
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



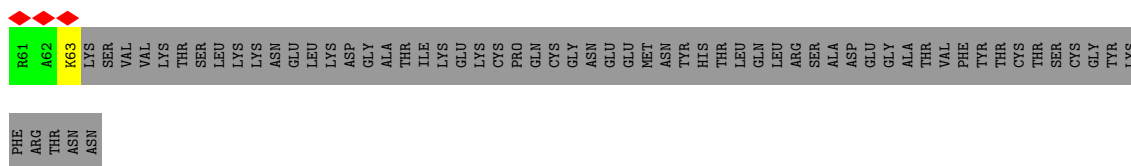
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



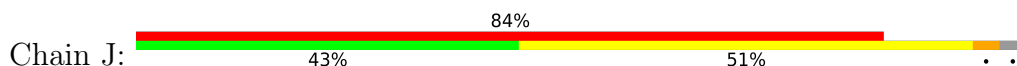
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



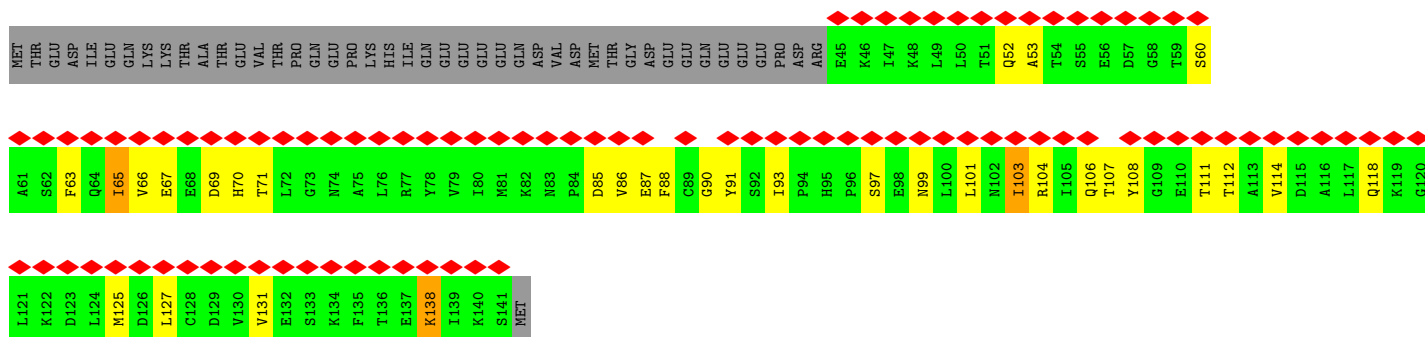




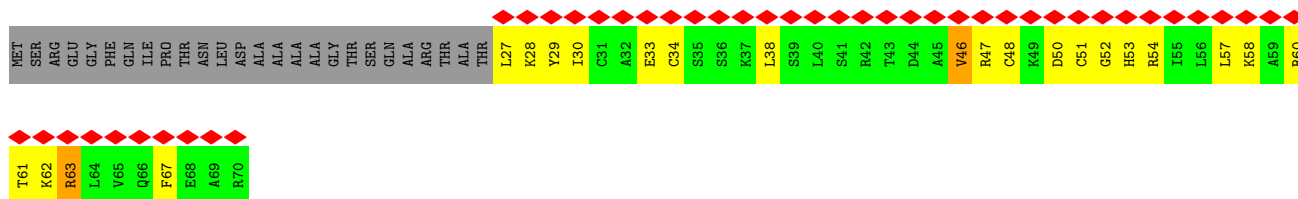
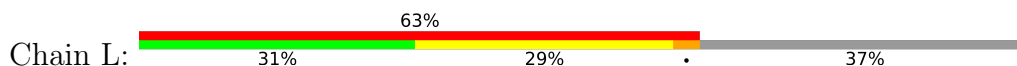
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC5



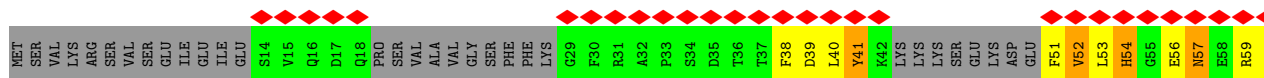
- Molecule 10: DNA-directed RNA polymerases I and III subunit RPAC2



- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 12: DNA-directed RNA polymerase I subunit RPA49



C1	T2	A3	C4	C5	G6	A7	T8	A9	A10	G11	C12	A13	G14	A15	T16	N17	C18	T19	C20	T21	C22	G23	A24	T25	T26	G27	C28	G29	T30	A31	T32	G33	A34	A35	DA	DT	DC
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	----



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117941	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.138	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	301.536, 301.536, 301.536	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.047, 1.047, 1.047	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.16	0/9393	0.31	0/12678
2	B	0.19	0/9158	0.30	0/12370
3	C	0.18	0/2467	0.27	0/3344
4	E	0.15	0/1519	0.34	0/2044
5	F	0.15	0/854	0.31	0/1151
6	G	0.14	0/483	0.35	0/656
7	H	0.16	0/1070	0.24	0/1449
8	I	0.14	0/428	0.35	0/578
9	J	0.22	0/570	0.30	0/765
10	K	0.17	0/768	0.25	0/1037
11	L	0.16	0/354	0.31	0/468
12	M	0.11	0/578	0.29	0/768
13	N	0.13	0/691	0.32	0/928
14	R	0.10	0/221	0.21	0/343
15	S	0.17	0/607	0.37	0/931
16	T	0.18	0/779	0.36	0/1197
All	All	0.17	0/29940	0.30	0/40707

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9243	0	9314	312	0
2	B	8963	0	8881	354	0
3	C	2415	0	2403	88	0
4	E	1488	0	1490	64	0
5	F	839	0	852	27	0
6	G	472	0	474	23	0
7	H	1052	0	1021	29	0
8	I	423	0	425	20	0
9	J	561	0	573	46	0
10	K	758	0	756	28	0
11	L	352	0	374	22	0
12	M	571	0	557	23	0
13	N	679	0	699	19	0
14	R	197	0	99	7	0
15	S	546	0	309	11	0
16	T	707	0	392	12	0
17	B	1	0	0	0	0
17	I	1	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
All	All	29270	0	28619	957	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 17.

All (957) 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)
9:J:43:ARG:HD2	9:J:45:CYS:SG	1.92	1.09
2:B:1104:CYS:SG	2:B:1107:CYS:HB2	2.07	0.93
8:I:30:CYS:SG	8:I:33:CYS:HB2	2.17	0.85
1:A:1325:LEU:HD13	1:A:1492:ILE:HG23	1.56	0.85
9:J:57:ILE:O	9:J:61:LEU:HB2	1.81	0.81
1:A:1450:ILE:HD13	1:A:1459:LYS:HD3	1.62	0.79
12:M:70:SER:HB2	12:M:73:SER:HB3	1.64	0.78
1:A:1225:ILE:HG23	1:A:1226:VAL:HG13	1.66	0.78
1:A:1533:GLU:HA	1:A:1538:VAL:HB	1.66	0.78
4:E:48:ASP:HA	4:E:56:LYS:HB2	1.64	0.77
1:A:734:THR:O	1:A:738:ASN:ND2	2.19	0.76
2:B:184:LYS:HE3	9:J:69:ARG:HH21	1.51	0.74
9:J:69:ARG:HH22	11:L:33:GLU:HA	1.50	0.74
6:G:48:SER:HB2	6:G:68:PRO:HB3	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ILE:HG23	1:A:577:VAL:HG22	1.71	0.72
2:B:909:ARG:NH1	2:B:1039:MET:SD	2.62	0.72
2:B:252:TYR:OH	2:B:305:ARG:NH1	2.22	0.72
16:T:7:DA:H3'	16:T:8:DT:H71	1.71	0.71
2:B:840:LEU:HD21	2:B:860:ALA:HB2	1.71	0.71
1:A:956:ARG:HH21	1:A:979:GLY:HA3	1.56	0.71
2:B:103:SER:HB3	2:B:138:LEU:HB2	1.72	0.71
3:C:100:ARG:NH2	9:J:3:VAL:O	2.24	0.71
7:H:91:ASP:OD1	7:H:91:ASP:N	2.24	0.70
15:S:5:DT:H3	16:T:34:DA:H61	1.40	0.70
1:A:647:ALA:HA	1:A:651:ALA:HB3	1.73	0.70
1:A:855:ARG:NH2	1:A:866:LYS:O	2.24	0.70
4:E:54:GLN:HG2	4:E:56:LYS:H	1.55	0.70
5:F:135:ARG:HD2	5:F:143:PHE:HB3	1.73	0.70
13:N:38:PHE:HB3	13:N:111:VAL:HG13	1.72	0.70
2:B:547:HIS:O	2:B:651:ARG:NH2	2.26	0.69
12:M:82:ASN:HB2	12:M:87:SER:HB3	1.75	0.69
2:B:186:GLU:HB3	2:B:189:GLU:HB2	1.75	0.69
2:B:335:ARG:NH2	2:B:346:ASP:OD1	2.26	0.69
3:C:293:ARG:O	3:C:295:ARG:NH1	2.26	0.69
1:A:430:ILE:HA	1:A:433:ASP:HB3	1.74	0.68
2:B:77:LYS:NZ	2:B:78:PRO:O	2.26	0.68
2:B:822:THR:HB	2:B:864:ASP:HB3	1.75	0.68
5:F:62:GLU:OE1	6:G:119:HIS:NE2	2.26	0.68
2:B:390:SER:OG	2:B:634:ARG:O	2.12	0.68
2:B:1047:ARG:NH1	2:B:1066:HIS:O	2.26	0.68
2:B:212:ASN:ND2	2:B:589:ASP:OD1	2.26	0.68
1:A:812:VAL:HG23	1:A:815:ARG:HH21	1.58	0.68
9:J:10:CYS:SG	9:J:43:ARG:NH2	2.65	0.68
2:B:214:PRO:O	2:B:380:LYS:NZ	2.26	0.68
11:L:60:ARG:HH12	11:L:63:ARG:HB3	1.59	0.68
2:B:75:ASP:HB3	2:B:93:ASN:H	1.59	0.68
1:A:1307:ASP:OD1	1:A:1499:ARG:NH2	2.26	0.67
6:G:53:TYR:OH	6:G:62:MET:SD	2.48	0.67
9:J:10:CYS:SG	9:J:11:GLY:N	2.68	0.67
9:J:68:LYS:NZ	11:L:34:CYS:O	2.27	0.67
2:B:564:ILE:O	2:B:567:SER:OG	2.12	0.67
1:A:1544:ASN:HD21	1:A:1561:THR:HG22	1.59	0.67
2:B:556:SER:HB2	2:B:621:PRO:HG2	1.77	0.67
2:B:609:ARG:NH2	2:B:668:GLU:OE2	2.27	0.67
1:A:1546:VAL:O	1:A:1551:LYS:NZ	2.27	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:LEU:HB2	1:A:636:HIS:HB2	1.76	0.66
2:B:1070:ARG:NH1	16:T:19:DT:OP1	2.28	0.66
1:A:637:PHE:O	1:A:639:GLN:NE2	2.27	0.66
2:B:819:ASP:OD1	2:B:819:ASP:N	2.28	0.66
2:B:526:GLY:HA2	2:B:696:ILE:HG22	1.78	0.66
3:C:164:ALA:HB2	3:C:191:ILE:HG12	1.78	0.66
12:M:51:PHE:HD2	12:M:52:VAL:HG12	1.60	0.66
1:A:404:SER:O	1:A:408:LYS:NZ	2.28	0.65
1:A:1003:ARG:HD2	2:B:520:LEU:HB2	1.77	0.65
2:B:259:THR:HB	2:B:270:LEU:HD21	1.78	0.65
2:B:181:VAL:HG11	9:J:62:ARG:HE	1.62	0.65
3:C:222:VAL:HG11	3:C:225:ALA:HB2	1.76	0.65
1:A:588:LEU:HD21	2:B:1087:LEU:HD11	1.79	0.65
1:A:1651:THR:O	5:F:92:ARG:NH1	2.29	0.65
1:A:880:GLN:OE1	1:A:972:TYR:OH	2.13	0.65
1:A:782:ASP:OD1	1:A:783:LYS:N	2.27	0.65
2:B:974:LEU:O	9:J:47:ARG:NH2	2.30	0.65
8:I:34:LYS:HG3	12:M:59:ARG:HH11	1.62	0.64
2:B:211:ARG:HE	2:B:239:VAL:HG21	1.63	0.64
9:J:57:ILE:O	9:J:61:LEU:CB	2.45	0.64
2:B:126:SER:HA	2:B:129:ARG:HB2	1.80	0.64
6:G:53:TYR:HB3	6:G:105:ILE:HG13	1.80	0.64
12:M:81:PHE:HA	12:M:88:ILE:HA	1.78	0.64
3:C:206:ALA:O	3:C:207:HIS:ND1	2.28	0.64
3:C:128:ASP:O	3:C:175:GLN:NE2	2.31	0.64
2:B:127:ARG:NH2	2:B:193:TYR:OH	2.30	0.64
2:B:1010:ASN:HB3	2:B:1025:ASP:HB2	1.78	0.64
2:B:1115:GLN:HB2	2:B:1126:VAL:HG12	1.80	0.64
1:A:1050:TYR:HD2	1:A:1179:ILE:HD13	1.63	0.63
4:E:127:ILE:HG22	4:E:129:PRO:HD2	1.80	0.63
1:A:1028:GLU:HA	1:A:1187:ILE:HD11	1.80	0.63
9:J:69:ARG:NH1	11:L:33:GLU:O	2.31	0.63
2:B:320:LEU:HB3	2:B:326:VAL:HG12	1.81	0.63
2:B:933:THR:OG1	2:B:944:GLN:OE1	2.16	0.63
3:C:222:VAL:HG22	3:C:313:ILE:HD12	1.80	0.63
1:A:703:GLU:O	10:K:52:GLN:NE2	2.32	0.62
4:E:64:PRO:HG3	4:E:77:SER:HA	1.81	0.62
14:R:4:A:H2'	14:R:5:A:C8	2.34	0.62
1:A:559:ASN:OD1	1:A:559:ASN:N	2.31	0.62
1:A:1315:ASN:OD1	1:A:1319:ASN:ND2	2.32	0.62
2:B:694:THR:OG1	2:B:702:ASN:OD1	2.16	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:THR:OG1	3:C:200:GLN:NE2	2.30	0.62
2:B:282:HIS:HE1	12:M:106:LYS:HD2	1.63	0.62
2:B:1158:ILE:HA	2:B:1168:VAL:HG23	1.81	0.62
2:B:821:ILE:HD11	2:B:899:GLN:HG2	1.81	0.62
2:B:216:ALA:HB1	2:B:384:LEU:HD22	1.81	0.62
1:A:1251:ALA:HA	1:A:1536:ILE:HD13	1.82	0.62
9:J:43:ARG:CD	9:J:45:CYS:SG	2.79	0.62
2:B:1006:ASN:OD1	2:B:1010:ASN:N	2.32	0.62
1:A:1129:PRO:HA	1:A:1135:SER:HB2	1.82	0.62
1:A:1246:VAL:HG11	1:A:1536:ILE:HA	1.81	0.62
2:B:94:LYS:NZ	2:B:147:ASN:OD1	2.27	0.62
2:B:293:ILE:HG23	2:B:296:ASP:HB2	1.82	0.62
2:B:588:ILE:HG12	2:B:642:LEU:HD12	1.82	0.62
1:A:833:LEU:HA	1:A:944:MET:HE2	1.80	0.61
2:B:698:SER:O	2:B:702:ASN:ND2	2.33	0.61
7:H:8:ASP:OD1	7:H:9:ILE:N	2.31	0.61
10:K:88:PHE:HB3	10:K:106:GLN:HB2	1.82	0.61
1:A:1258:ILE:HD11	1:A:1501:ILE:HD13	1.82	0.61
2:B:58:GLY:HA3	2:B:62:ASN:HB3	1.83	0.61
3:C:228:ARG:NH2	3:C:271:ARG:O	2.31	0.61
2:B:1064:LYS:NZ	16:T:22:DC:OP2	2.29	0.61
1:A:546:LEU:HA	1:A:549:MET:HG3	1.83	0.61
1:A:1553:TYR:OH	4:E:147:HIS:ND1	2.33	0.61
2:B:207:ILE:HD11	2:B:400:GLN:HB3	1.82	0.61
2:B:834:LYS:HZ2	2:B:835:GLU:H	1.48	0.61
4:E:52:ARG:NH2	4:E:54:GLN:OE1	2.31	0.61
2:B:21:ARG:HH21	9:J:54:VAL:HA	1.66	0.61
11:L:34:CYS:SG	11:L:50:ASP:CG	2.75	0.61
2:B:1105:ARG:HB3	2:B:1172:GLU:HB3	1.83	0.61
3:C:126:PHE:HA	3:C:130:ASN:HD21	1.64	0.61
2:B:1107:CYS:HB3	2:B:1130:ARG:HH11	1.65	0.61
1:A:718:THR:OG1	1:A:730:GLN:OE1	2.18	0.61
2:B:46:ILE:HD13	2:B:164:MET:HE3	1.82	0.61
4:E:88:VAL:O	4:E:115:ASN:ND2	2.34	0.61
1:A:1018:TYR:HA	1:A:1021:ARG:HG2	1.83	0.60
2:B:492:ASN:ND2	2:B:725:THR:O	2.25	0.60
2:B:512:LEU:HD13	15:S:23:DC:H2"	1.83	0.60
2:B:785:ASP:OD1	2:B:957:ARG:NH1	2.34	0.60
1:A:811:SER:OG	1:A:815:ARG:NH1	2.35	0.60
1:A:991:LYS:N	1:A:994:GLU:OE1	2.32	0.60
2:B:795:GLU:OE1	3:C:217:ALA:N	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1239:THR:HA	1:A:1520:VAL:HG22	1.83	0.60
2:B:264:TRP:CD1	2:B:265:ARG:HG2	2.35	0.60
2:B:623:ASP:O	2:B:648:ARG:NH2	2.24	0.60
1:A:498:PRO:HB3	1:A:612:LYS:HA	1.83	0.60
6:G:89:ILE:HG21	6:G:103:LYS:HB3	1.83	0.60
13:N:33:LYS:HG2	13:N:119:LEU:HD22	1.84	0.60
1:A:1127:TYR:HB3	1:A:1132:TYR:HD2	1.66	0.60
1:A:1657:LEU:HD11	6:G:104:LEU:HD23	1.83	0.60
2:B:744:LEU:HA	2:B:801:GLY:HA2	1.83	0.60
2:B:77:LYS:HB3	2:B:92:GLY:HA2	1.83	0.60
10:K:86:VAL:HA	10:K:107:THR:HA	1.84	0.60
1:A:689:ARG:NH2	10:K:87:GLU:O	2.35	0.60
1:A:652:ASN:ND2	1:A:654:ASP:OD1	2.34	0.60
3:C:69:ARG:NH2	10:K:69:ASP:OD2	2.35	0.60
2:B:209:GLN:NE2	2:B:215:MET:SD	2.63	0.59
1:A:672:ASP:HB2	2:B:783:MET:HE2	1.83	0.59
2:B:21:ARG:NH2	9:J:54:VAL:HA	2.16	0.59
2:B:1047:ARG:HH12	2:B:1051:PRO:HG2	1.67	0.59
2:B:547:HIS:CE1	2:B:695:ASN:HA	2.37	0.59
2:B:662:ASP:OD1	2:B:663:ILE:N	2.35	0.59
1:A:729:LYS:NZ	1:A:766:GLU:OE2	2.29	0.59
2:B:12:ARG:NH1	9:J:32:GLU:OE1	2.30	0.59
4:E:145:THR:OG1	4:E:146:HIS:N	2.34	0.59
9:J:9:SER:HB2	9:J:45:CYS:HB2	1.83	0.59
1:A:396:ILE:O	1:A:400:ASN:ND2	2.36	0.59
2:B:456:ASN:HB3	2:B:459:SER:HB3	1.84	0.59
2:B:568:LEU:HA	13:N:140:SER:HA	1.85	0.59
7:H:81:PRO:O	7:H:83:GLN:NE2	2.35	0.59
1:A:855:ARG:HH22	1:A:867:ASP:HA	1.66	0.59
1:A:1299:ASN:HB2	1:A:1466:SER:HA	1.85	0.59
2:B:25:PHE:HB3	9:J:58:GLU:HB2	1.83	0.59
3:C:78:VAL:HG21	3:C:108:VAL:HG23	1.85	0.59
1:A:641:GLU:N	1:A:641:GLU:OE1	2.36	0.59
1:A:1018:TYR:HD2	1:A:1223:ARG:HH12	1.48	0.59
1:A:995:TYR:OH	2:B:715:ASN:ND2	2.35	0.59
2:B:651:ARG:HH11	2:B:652:PRO:HD2	1.68	0.59
2:B:1012:PRO:HG2	3:C:275:VAL:HB	1.85	0.59
3:C:105:PRO:HB2	3:C:187:ALA:HB3	1.83	0.58
4:E:46:TYR:HB3	4:E:55:ARG:HB3	1.85	0.58
1:A:617:HIS:HD2	1:A:619:ALA:H	1.50	0.58
1:A:1181:PRO:HD2	5:F:86:THR:HG21	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:167:ARG:O	4:E:169:ARG:NH2	2.37	0.58
1:A:874:GLU:O	1:A:878:ARG:HG2	2.03	0.58
1:A:1275:THR:HB	1:A:1289:SER:HB2	1.85	0.58
2:B:890:ASP:O	11:L:54:ARG:NE	2.36	0.58
3:C:216:HIS:HD2	3:C:218:LYS:H	1.51	0.58
1:A:131:ASP:O	4:E:192:ARG:NH1	2.36	0.58
2:B:518:ARG:NH1	2:B:539:CYS:O	2.36	0.58
11:L:48:CYS:O	11:L:52:GLY:N	2.37	0.58
1:A:515:ASN:HB3	5:F:115:THR:HB	1.86	0.58
10:K:66:VAL:HG12	10:K:67:GLU:HG2	1.85	0.58
2:B:656:LEU:HB3	13:N:148:ILE:HG21	1.85	0.58
4:E:100:ILE:HG22	4:E:127:ILE:HD11	1.85	0.58
7:H:63:LEU:HB3	7:H:88:SER:HB2	1.85	0.58
2:B:954:PHE:HE2	2:B:962:MET:HB3	1.69	0.58
6:G:55:GLU:HA	6:G:102:GLU:HA	1.86	0.58
4:E:61:GLN:HE21	4:E:62:ALA:H	1.51	0.58
2:B:651:ARG:HD2	2:B:652:PRO:HD2	1.84	0.57
4:E:106:GLN:HA	4:E:129:PRO:HB2	1.85	0.57
2:B:557:ASP:OD2	2:B:560:ARG:NH2	2.36	0.57
4:E:101:GLN:HB3	4:E:127:ILE:HD13	1.85	0.57
1:A:1243:TRP:HB2	1:A:1537:ASP:H	1.70	0.57
2:B:401:GLU:OE1	2:B:402:VAL:N	2.37	0.57
2:B:651:ARG:NH2	2:B:695:ASN:O	2.37	0.57
2:B:886:ASN:ND2	2:B:902:SER:O	2.38	0.57
9:J:14:VAL:HA	9:J:17:LYS:HD2	1.85	0.57
1:A:410:LYS:NZ	1:A:410:LYS:O	2.37	0.57
1:A:831:ASP:N	1:A:831:ASP:OD1	2.37	0.57
1:A:1299:ASN:ND2	1:A:1465:GLU:O	2.37	0.57
2:B:470:LEU:HD21	2:B:476:LEU:HD23	1.85	0.57
14:R:4:A:H2'	14:R:5:A:H8	1.68	0.57
1:A:1124:LEU:HD12	1:A:1129:PRO:HB3	1.86	0.57
3:C:211:GLY:HA3	3:C:219:PHE:CG	2.40	0.57
13:N:114:GLU:HG2	13:N:118:SER:HB3	1.85	0.57
1:A:551:VAL:HG22	1:A:554:ARG:HH21	1.69	0.57
9:J:3:VAL:HG11	9:J:18:TRP:HB2	1.87	0.57
1:A:597:LYS:HE2	1:A:660:PRO:HG3	1.87	0.57
12:M:80:LEU:HB2	12:M:89:GLN:HB2	1.86	0.57
3:C:195:LYS:NZ	9:J:58:GLU:OE2	2.29	0.56
1:A:1498:ILE:HG22	1:A:1499:ARG:HG2	1.86	0.56
2:B:273:VAL:HG11	2:B:378:ILE:HD11	1.85	0.56
1:A:589:MET:HB3	1:A:633:MET:HE2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1124:LEU:HD21	1:A:1137:SER:HA	1.86	0.56
1:A:1325:LEU:HB3	1:A:1492:ILE:HG12	1.86	0.56
2:B:1196:LEU:HD22	2:B:1197:ARG:H	1.70	0.56
3:C:275:VAL:HG21	3:C:293:ARG:HH22	1.70	0.56
3:C:278:GLU:OE2	3:C:281:ARG:NH1	2.38	0.56
8:I:33:CYS:O	8:I:34:LYS:HG2	2.05	0.56
16:T:5:DC:H2''	16:T:6:DG:C8	2.40	0.56
2:B:219:ARG:NE	15:S:23:DC:H42	2.04	0.56
2:B:392:ASP:OD2	2:B:636:GLN:NE2	2.26	0.56
2:B:395:ASP:HA	2:B:505:ARG:HH21	1.71	0.56
6:G:100:THR:HG22	6:G:102:GLU:H	1.69	0.56
1:A:460:LEU:N	1:A:466:LEU:H	2.02	0.56
1:A:1217:LEU:HD22	1:A:1572:ARG:HD2	1.87	0.56
2:B:124:SER:HA	2:B:127:ARG:HD2	1.87	0.56
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.86	0.56
7:H:98:TYR:OH	7:H:139:ASN:ND2	2.34	0.56
2:B:651:ARG:HH22	2:B:695:ASN:HB2	1.69	0.56
1:A:797:LEU:HD21	1:A:805:VAL:HG12	1.88	0.56
2:B:899:GLN:OE1	2:B:899:GLN:N	2.39	0.56
2:B:676:VAL:HG13	2:B:677:THR:HG23	1.88	0.55
2:B:834:LYS:HZ2	2:B:835:GLU:N	2.04	0.55
1:A:880:GLN:NE2	2:B:633:THR:O	2.38	0.55
1:A:968:SER:HA	2:B:674:ILE:O	2.06	0.55
1:A:1609:SER:HA	1:A:1612:LYS:HD3	1.88	0.55
1:A:1459:LYS:HA	1:A:1472:PHE:HA	1.89	0.55
2:B:341:SER:N	2:B:344:GLN:OE1	2.39	0.55
2:B:1052:VAL:HA	2:B:1059:PRO:HA	1.88	0.55
4:E:52:ARG:O	4:E:55:ARG:NE	2.38	0.55
1:A:1329:ILE:O	1:A:1332:GLU:HG3	2.06	0.55
2:B:442:ASP:OD2	2:B:445:TYR:N	2.38	0.55
2:B:792:SER:O	2:B:796:ARG:HG2	2.06	0.55
2:B:1075:GLU:OE1	2:B:1075:GLU:N	2.38	0.55
3:C:259:ASP:OD2	3:C:262:SER:N	2.38	0.55
1:A:1003:ARG:NH2	2:B:533:THR:OG1	2.39	0.55
1:A:834:ARG:NH1	1:A:987:TYR:OH	2.39	0.55
2:B:203:ILE:HD13	2:B:485:THR:HG22	1.87	0.55
2:B:962:MET:HE1	2:B:1033:TYR:HE1	1.71	0.55
2:B:1126:VAL:HG11	2:B:1173:THR:HB	1.89	0.55
3:C:172:GLN:N	3:C:175:GLN:OE1	2.37	0.55
5:F:79:ARG:NH1	5:F:145:ASP:O	2.29	0.55
10:K:65:ILE:HD12	10:K:101:LEU:HD23	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1251:ALA:HA	1:A:1536:ILE:HG21	1.88	0.55
2:B:676:VAL:N	2:B:680:GLU:OE2	2.35	0.55
15:S:34:DG:H2"	15:S:35:DG:C8	2.41	0.55
4:E:188:LEU:HD11	4:E:190:LEU:HD12	1.89	0.55
1:A:1233:ILE:HG23	1:A:1236:PRO:HD2	1.89	0.55
1:A:1592:GLN:HE22	1:A:1594:THR:C	2.14	0.55
3:C:271:ARG:HH11	3:C:299:ILE:HD12	1.72	0.55
1:A:550:SER:HB3	1:A:553:GLN:HG3	1.89	0.55
2:B:164:MET:O	2:B:167:SER:OG	2.19	0.55
1:A:399:LEU:HB3	1:A:423:LEU:HD13	1.89	0.54
1:A:1587:ASP:HA	1:A:1591:ARG:HB2	1.89	0.54
2:B:145:VAL:HG21	2:B:441:LYS:HG2	1.88	0.54
10:K:67:GLU:OE1	10:K:99:ASN:ND2	2.39	0.54
1:A:1034:TYR:CZ	5:F:136:ARG:HB3	2.42	0.54
2:B:104:ILE:HG12	2:B:169:ARG:NE	2.22	0.54
2:B:217:ILE:HG22	2:B:219:ARG:H	1.72	0.54
2:B:568:LEU:HD13	2:B:604:ILE:HD12	1.89	0.54
2:B:839:LYS:HD2	2:B:856:ASP:HB3	1.87	0.54
1:A:399:LEU:HD22	1:A:423:LEU:HB2	1.87	0.54
2:B:404:LEU:HD11	2:B:551:ILE:HG21	1.89	0.54
10:K:91:TYR:HB2	10:K:101:LEU:HD11	1.89	0.54
1:A:1603:MET:HG3	1:A:1615:TYR:HD2	1.72	0.54
4:E:47:CYS:O	4:E:56:LYS:NZ	2.37	0.54
8:I:34:LYS:HG3	12:M:59:ARG:HD2	1.89	0.54
3:C:329:LYS:NZ	10:K:118:GLN:OE1	2.40	0.54
4:E:136:ASN:OD1	4:E:137:GLU:N	2.41	0.54
1:A:466:LEU:HD23	2:B:1185:LEU:HD23	1.90	0.54
1:A:1097:TYR:OH	1:A:1121:ASP:OD1	2.19	0.54
1:A:1127:TYR:HB3	1:A:1132:TYR:CD2	2.41	0.54
1:A:1655:ASP:OD1	1:A:1656:VAL:N	2.40	0.54
11:L:60:ARG:NH1	11:L:61:THR:O	2.41	0.54
1:A:963:GLY:HA3	1:A:972:TYR:CE1	2.43	0.54
2:B:912:GLN:N	2:B:915:ASP:OD2	2.41	0.54
2:B:968:ALA:HB1	2:B:979:GLN:HG2	1.90	0.54
4:E:109:ILE:HA	4:E:132:ILE:HD13	1.89	0.54
1:A:1240:LEU:HB3	1:A:1541:ILE:HG12	1.90	0.54
8:I:25:GLY:HA2	8:I:39:LYS:HB2	1.90	0.54
1:A:1603:MET:HE1	1:A:1611:MET:HE2	1.89	0.54
2:B:785:ASP:OD2	2:B:957:ARG:NH2	2.41	0.54
2:B:245:SER:OG	2:B:476:LEU:O	2.26	0.54
3:C:53:ASN:HD22	3:C:301:ASN:HD22	1.55	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:THR:O	1:A:433:ASP:N	2.40	0.53
3:C:223:SER:OG	3:C:303:GLU:OE1	2.25	0.53
3:C:255:VAL:HG22	3:C:272:LYS:HB3	1.88	0.53
7:H:40:LEU:HD13	7:H:123:MET:HB2	1.90	0.53
12:M:112:LYS:HG2	12:M:113:ILE:HG13	1.89	0.53
1:A:754:LYS:O	1:A:756:LYS:NZ	2.41	0.53
1:A:483:VAL:HA	1:A:632:GLU:HA	1.90	0.53
2:B:892:SER:HB2	2:B:894:LYS:HG2	1.89	0.53
2:B:281:CYS:SG	2:B:283:THR:OG1	2.64	0.53
3:C:132:ILE:HD12	3:C:184:VAL:HG11	1.90	0.53
1:A:510:PRO:HA	1:A:576:LYS:HA	1.90	0.53
1:A:1260:LYS:HE2	1:A:1500:GLN:HG3	1.91	0.53
2:B:251:HIS:CE1	2:B:261:ARG:HE	2.26	0.53
3:C:284:GLU:O	3:C:288:LYS:NZ	2.38	0.53
8:I:21:ASN:O	8:I:21:ASN:ND2	2.41	0.53
1:A:1314:GLN:NE2	1:A:1318:SER:OG	2.40	0.53
2:B:443:LYS:HA	2:B:446:MET:HE2	1.91	0.53
2:B:743:ARG:NH1	2:B:804:TYR:OH	2.41	0.53
3:C:69:ARG:NE	10:K:71:THR:OG1	2.42	0.53
1:A:479:ALA:HB1	2:B:1069:ILE:HD11	1.90	0.53
2:B:608:LEU:HD22	2:B:626:ILE:HD12	1.91	0.53
7:H:133:ASN:OD1	7:H:133:ASN:N	2.41	0.53
1:A:1036:ASN:ND2	1:A:1049:MET:HA	2.24	0.53
1:A:1526:PHE:HE2	1:A:1549:VAL:HG22	1.74	0.53
2:B:57:ASP:OD1	2:B:57:ASP:N	2.42	0.53
2:B:129:ARG:HG2	2:B:888:ILE:HG23	1.90	0.53
2:B:708:ASP:OD1	2:B:708:ASP:N	2.32	0.53
1:A:461:GLU:H	1:A:465:GLY:HA3	1.75	0.52
2:B:105:ALA:HB3	2:B:136:LYS:HB3	1.90	0.52
7:H:92:ASP:N	7:H:92:ASP:OD1	2.41	0.52
1:A:1276:THR:OG1	8:I:45:LEU:N	2.42	0.52
1:A:1325:LEU:HD22	1:A:1492:ILE:HG12	1.91	0.52
2:B:240:ARG:HD2	2:B:244:THR:HB	1.92	0.52
2:B:815:ARG:HH11	2:B:820:PRO:HA	1.74	0.52
2:B:890:ASP:OD1	2:B:890:ASP:N	2.41	0.52
2:B:968:ALA:HB2	2:B:996:PHE:CE2	2.44	0.52
12:M:81:PHE:HB3	12:M:88:ILE:HG23	1.91	0.52
2:B:989:ASP:N	2:B:989:ASP:OD1	2.41	0.52
3:C:315:PHE:HB3	3:C:319:ARG:HH21	1.73	0.52
2:B:144:SER:OG	2:B:151:ASN:ND2	2.42	0.52
2:B:232:TYR:CE2	2:B:385:VAL:HA	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:983:PRO:HB2	2:B:984:TRP:CE3	2.45	0.52
4:E:29:PHE:H	4:E:65:THR:HB	1.74	0.52
1:A:772:LYS:NZ	7:H:101:ALA:O	2.42	0.52
1:A:1012:LYS:NZ	1:A:1202:LEU:O	2.43	0.52
1:A:755:ILE:HD12	1:A:780:ILE:HD11	1.90	0.52
2:B:123:PRO:C	2:B:125:GLU:H	2.17	0.52
3:C:152:ASP:OD1	3:C:152:ASP:N	2.42	0.52
6:G:88:LYS:CB	6:G:119:HIS:H	2.23	0.52
2:B:251:HIS:HE1	2:B:261:ARG:HE	1.57	0.52
2:B:915:ASP:OD1	2:B:915:ASP:N	2.39	0.52
1:A:496:GLY:N	1:A:615:ARG:O	2.41	0.52
1:A:855:ARG:NH2	1:A:856:GLU:OE2	2.43	0.52
1:A:1010:ALA:O	1:A:1013:THR:OG1	2.28	0.52
3:C:237:GLN:HG3	3:C:288:LYS:HG2	1.91	0.52
1:A:597:LYS:N	1:A:1191:GLN:OE1	2.42	0.51
1:A:863:ASN:HD21	8:I:63:LYS:HE3	1.74	0.51
1:A:942:GLN:NE2	2:B:958:MET:SD	2.83	0.51
1:A:1185:VAL:HB	1:A:1584:LEU:HD11	1.92	0.51
2:B:741:LEU:HD12	2:B:804:TYR:HD2	1.75	0.51
2:B:209:GLN:OE1	2:B:210:ARG:N	2.43	0.51
2:B:727:GLY:HA2	2:B:767:ASN:CG	2.35	0.51
2:B:833:PRO:HD2	2:B:836:TRP:CH2	2.45	0.51
9:J:41:LEU:HD11	9:J:50:ILE:HD12	1.93	0.51
12:M:54:HIS:NE2	12:M:56:GLU:OE2	2.43	0.51
1:A:1034:TYR:HA	1:A:1181:PRO:HB3	1.92	0.51
1:A:1658:ALA:HB1	6:G:54:LEU:HD23	1.93	0.51
2:B:465:LEU:HA	2:B:485:THR:HG21	1.92	0.51
2:B:790:ASN:OD1	2:B:793:ALA:N	2.32	0.51
12:M:54:HIS:CE1	12:M:56:GLU:HG2	2.45	0.51
1:A:683:LYS:NZ	7:H:41:ASP:OD2	2.42	0.51
1:A:1444:ARG:NH1	1:A:1444:ARG:O	2.42	0.51
5:F:120:ILE:O	5:F:124:GLU:HG2	2.10	0.51
9:J:7:CYS:HB3	9:J:11:GLY:H	1.76	0.51
11:L:33:GLU:HB2	11:L:53:HIS:CD2	2.46	0.51
1:A:139:ILE:HB	1:A:185:ARG:HA	1.92	0.51
1:A:1552:THR:HA	4:E:183:PRO:HG2	1.93	0.51
1:A:1647:ASN:OD1	1:A:1648:ASN:N	2.37	0.51
2:B:861:TYR:CZ	2:B:870:LYS:HB2	2.45	0.51
2:B:1025:ASP:OD2	3:C:277:ARG:NH1	2.44	0.51
3:C:155:GLU:N	3:C:155:GLU:OE1	2.43	0.51
1:A:317:SER:OG	1:A:431:GLN:NE2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:ASP:OD1	1:A:888:LYS:HB2	2.11	0.51
2:B:232:TYR:HD2	2:B:385:VAL:HG22	1.76	0.51
9:J:8:PHE:H	9:J:49:MET:HE3	1.75	0.51
1:A:1459:LYS:HE2	1:A:1461:ASN:HD21	1.76	0.51
1:A:1566:ILE:HG23	1:A:1582:LEU:HD13	1.93	0.51
2:B:654:ARG:NH2	2:B:659:ASP:O	2.44	0.51
2:B:1113:THR:OG1	2:B:1114:GLN:N	2.43	0.51
1:A:646:GLU:OE1	2:B:1087:LEU:N	2.37	0.50
1:A:882:ILE:O	1:A:889:SER:OG	2.25	0.50
2:B:803:MET:HB2	2:B:907:ILE:HB	1.92	0.50
4:E:110:PHE:O	4:E:134:THR:OG1	2.19	0.50
1:A:799:GLU:HG2	1:A:1068:PHE:HE2	1.76	0.50
2:B:565:LEU:HD13	2:B:593:ILE:HD11	1.94	0.50
3:C:164:ALA:HB3	3:C:189:PRO:HA	1.93	0.50
6:G:108:THR:N	6:G:113:PHE:O	2.43	0.50
1:A:507:TYR:HB2	1:A:637:PHE:CZ	2.46	0.50
1:A:921:PRO:HG3	7:H:19:ARG:HB3	1.92	0.50
5:F:112:GLU:HG3	5:F:114:GLU:HG2	1.93	0.50
1:A:704:ASP:HB2	1:A:706:HIS:CE1	2.47	0.50
1:A:1076:LEU:HA	1:A:1079:LYS:HG2	1.94	0.50
2:B:841:ASP:HB3	2:B:847:TYR:CE2	2.46	0.50
1:A:946:LEU:HD11	1:A:983:LYS:HA	1.92	0.50
1:A:947:LEU:HD22	1:A:982:VAL:HG11	1.93	0.50
1:A:1457:ILE:HD12	1:A:1472:PHE:HB2	1.92	0.50
2:B:641:TYR:HB3	2:B:643:PHE:HE2	1.77	0.50
2:B:600:GLN:O	2:B:604:ILE:HG12	2.12	0.50
1:A:956:ARG:NH2	1:A:979:GLY:HA3	2.26	0.50
1:A:1197:SER:HA	1:A:1200:MET:HB2	1.94	0.50
6:G:93:ASP:CG	6:G:94:PRO:HD2	2.37	0.50
1:A:135:LYS:HD2	4:E:192:ARG:HH21	1.77	0.50
1:A:949:GLN:OE1	1:A:950:GLN:N	2.45	0.50
2:B:248:ASN:HD22	2:B:260:PHE:HZ	1.60	0.50
2:B:397:THR:HA	2:B:400:GLN:HB2	1.94	0.50
2:B:547:HIS:HE1	2:B:695:ASN:HA	1.74	0.50
2:B:722:GLY:O	2:B:725:THR:OG1	2.24	0.50
3:C:216:HIS:CD2	3:C:218:LYS:H	2.29	0.50
7:H:80:ARG:HG3	10:K:108:TYR:CZ	2.47	0.50
11:L:27:LEU:N	11:L:38:LEU:O	2.44	0.50
1:A:948:GLY:O	1:A:982:VAL:N	2.44	0.49
2:B:291:GLY:HA3	2:B:375:LEU:HD23	1.94	0.49
2:B:614:GLU:O	2:B:616:LYS:NZ	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:GLY:HA3	1:A:554:ARG:NH1	2.26	0.49
1:A:1039:ARG:NH1	5:F:139:PRO:HG2	2.27	0.49
2:B:129:ARG:HH21	11:L:54:ARG:HB2	1.77	0.49
2:B:494:TYR:HB3	2:B:700:LEU:HD21	1.94	0.49
1:A:1270:VAL:H	8:I:51:THR:HG1	1.60	0.49
2:B:146:ASN:ND2	2:B:149:GLU:OE1	2.43	0.49
5:F:119:ARG:NH1	5:F:122:MET:SD	2.85	0.49
8:I:34:LYS:HE3	12:M:59:ARG:HB3	1.94	0.49
11:L:46:VAL:HG13	11:L:54:ARG:HA	1.93	0.49
14:R:7:C:H2'	14:R:8:G:H8	1.77	0.49
1:A:514:TYR:OH	5:F:117:PRO:HG3	2.13	0.49
2:B:208:VAL:O	2:B:401:GLU:N	2.45	0.49
2:B:320:LEU:HD21	2:B:329:TYR:CG	2.48	0.49
1:A:1261:VAL:HG12	1:A:1498:ILE:HD12	1.93	0.49
1:A:1532:GLN:OE1	4:E:14:ARG:NH1	2.45	0.49
5:F:133:VAL:HG11	6:G:104:LEU:HD21	1.94	0.49
4:E:164:LEU:HA	4:E:167:ARG:HG2	1.95	0.49
1:A:314:TYR:HD2	1:A:316:LEU:HD23	1.77	0.49
1:A:715:LEU:HB3	1:A:730:GLN:HE21	1.78	0.49
2:B:204:ARG:HD2	2:B:486:VAL:HB	1.95	0.49
2:B:883:GLU:HB2	2:B:906:ARG:HB2	1.94	0.49
3:C:196:LEU:HG	3:C:200:GLN:HG3	1.95	0.49
1:A:671:GLN:HB2	2:B:952:HIS:CD2	2.48	0.49
15:S:32:DT:H1'	15:S:33:DC:H5'	1.95	0.49
2:B:40:GLU:HA	2:B:43:GLN:HB2	1.94	0.49
2:B:528:LEU:HD13	2:B:543:ASN:HD22	1.76	0.49
2:B:569:GLY:H	13:N:140:SER:HB3	1.77	0.49
2:B:641:TYR:HB3	2:B:643:PHE:CE2	2.47	0.49
2:B:750:PRO:HD2	2:B:753:LYS:HE3	1.94	0.49
2:B:786:ALA:HB1	2:B:928:SER:HB2	1.95	0.49
4:E:48:ASP:HB3	4:E:52:ARG:H	1.78	0.49
10:K:112:THR:HG22	10:K:114:VAL:H	1.77	0.49
12:M:57:ASN:HD21	12:M:60:LEU:C	2.21	0.49
1:A:507:TYR:HB2	1:A:637:PHE:HZ	1.76	0.48
1:A:867:ASP:OD1	1:A:867:ASP:N	2.46	0.48
1:A:1501:ILE:HD11	1:A:1504:ILE:HG13	1.94	0.48
2:B:543:ASN:OD1	2:B:543:ASN:N	2.46	0.48
2:B:875:HIS:O	2:B:875:HIS:ND1	2.43	0.48
11:L:48:CYS:SG	11:L:51:CYS:N	2.85	0.48
16:T:25:DT:H2'	16:T:26:DT:C6	2.48	0.48
1:A:396:ILE:HG13	1:A:427:PHE:HB3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1502:PRO:HB2	1:A:1503:HIS:HD2	1.78	0.48
2:B:281:CYS:HG	2:B:283:THR:HG1	1.59	0.48
4:E:155:ARG:HH22	4:E:187:TYR:HD2	1.62	0.48
4:E:168:TYR:HB3	4:E:170:LEU:HG	1.94	0.48
15:S:36:DT:H2''	15:S:37:DA:C8	2.48	0.48
2:B:181:VAL:HG13	9:J:63:TYR:HE1	1.78	0.48
3:C:240:LYS:NZ	3:C:264:GLU:HB2	2.29	0.48
1:A:1126:LYS:HB3	1:A:1127:TYR:CD2	2.48	0.48
1:A:1288:ARG:HB2	1:A:1477:ALA:O	2.14	0.48
2:B:125:GLU:O	2:B:126:SER:OG	2.25	0.48
4:E:26:ARG:HD3	4:E:188:LEU:HB2	1.95	0.48
1:A:264:ASN:ND2	1:A:265:ARG:HG3	2.28	0.48
1:A:1039:ARG:CZ	5:F:139:PRO:HG2	2.44	0.48
4:E:79:TRP:HB2	4:E:104:ASN:HD21	1.77	0.48
9:J:44:TYR:HA	9:J:47:ARG:HB2	1.95	0.48
11:L:33:GLU:HB2	11:L:53:HIS:HD2	1.79	0.48
14:R:6:U:H2'	14:R:7:C:H6	1.78	0.48
1:A:928:MET:SD	2:B:952:HIS:ND1	2.77	0.48
2:B:839:LYS:HE2	2:B:852:VAL:HA	1.94	0.48
4:E:132:ILE:HD11	4:E:134:THR:HG23	1.96	0.48
4:E:182:ASP:HB2	4:E:185:ALA:HB3	1.94	0.48
14:R:6:U:H2'	14:R:7:C:C6	2.48	0.48
1:A:556:ALA:H	1:A:559:ASN:ND2	2.12	0.48
1:A:657:TYR:CE2	1:A:665:PRO:HB3	2.49	0.48
3:C:145:ASP:OD1	3:C:145:ASP:N	2.40	0.48
2:B:564:ILE:HG21	2:B:620:LEU:HD11	1.94	0.48
2:B:731:VAL:HG23	9:J:63:TYR:HE2	1.79	0.48
2:B:1025:ASP:OD1	2:B:1025:ASP:N	2.42	0.48
3:C:67:PHE:CE1	3:C:318:VAL:HG12	2.49	0.48
8:I:12:ASP:CG	8:I:33:CYS:SG	2.94	0.48
10:K:63:PHE:HZ	10:K:114:VAL:HG22	1.79	0.48
15:S:31:DA:H2'	15:S:32:DT:H72	1.96	0.48
3:C:195:LYS:HD2	9:J:57:ILE:HD12	1.96	0.48
1:A:579:ARG:HH22	1:A:585:ASP:CG	2.22	0.48
1:A:1130:ALA:HB2	1:A:1178:LEU:HD12	1.95	0.48
1:A:1526:PHE:CE2	1:A:1549:VAL:HG22	2.48	0.48
2:B:393:ASN:ND2	2:B:395:ASP:OD1	2.36	0.48
4:E:89:GLY:HA2	4:E:115:ASN:HB2	1.96	0.47
3:C:190:ASP:N	3:C:190:ASP:OD1	2.46	0.47
9:J:10:CYS:SG	9:J:12:LYS:N	2.85	0.47
1:A:749:LEU:HD23	1:A:750:ILE:N	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:VAL:HG22	1:A:1038:ILE:HD12	1.97	0.47
1:A:1040:ASP:OD1	1:A:1040:ASP:N	2.46	0.47
2:B:131:THR:O	2:B:198:GLY:N	2.46	0.47
4:E:47:CYS:HA	4:E:55:ARG:HH12	1.79	0.47
5:F:61:HIS:HA	5:F:64:ILE:HB	1.95	0.47
9:J:64:ASN:OD1	9:J:67:GLU:N	2.47	0.47
2:B:255:ASP:OD1	2:B:256:GLY:N	2.48	0.47
2:B:444:ARG:O	2:B:448:ARG:HG3	2.13	0.47
3:C:308:MET:HE2	3:C:316:LYS:HZ1	1.77	0.47
1:A:436:ALA:HA	1:A:439:ASP:O	2.13	0.47
1:A:1032:VAL:HG21	1:A:1179:ILE:HD12	1.95	0.47
4:E:55:ARG:HG3	4:E:58:MET:HE2	1.96	0.47
4:E:61:GLN:HE21	4:E:62:ALA:N	2.12	0.47
1:A:1619:CYS:SG	1:A:1620:GLN:N	2.88	0.47
2:B:251:HIS:HE1	2:B:261:ARG:HH21	1.63	0.47
2:B:252:TYR:HH	2:B:305:ARG:NH1	2.13	0.47
2:B:852:VAL:HG13	2:B:856:ASP:HB2	1.96	0.47
1:A:482:SER:OG	1:A:483:VAL:N	2.48	0.47
1:A:643:ALA:HB1	2:B:1087:LEU:HD12	1.96	0.47
1:A:715:LEU:HD13	1:A:734:THR:HB	1.95	0.47
1:A:1033:SER:OG	1:A:1037:SER:O	2.32	0.47
1:A:1176:ARG:NH2	5:F:154:ASP:O	2.48	0.47
1:A:1539:ASP:OD1	4:E:147:HIS:NE2	2.35	0.47
2:B:512:LEU:HG	2:B:514:THR:H	1.80	0.47
3:C:234:ASN:OD1	3:C:234:ASN:N	2.48	0.47
4:E:155:ARG:HE	4:E:188:LEU:HB3	1.79	0.47
16:T:19:DT:H2'	16:T:20:DC:C6	2.50	0.47
1:A:703:GLU:HA	10:K:53:ALA:HB2	1.97	0.47
1:A:980:GLY:HA2	1:A:997:PHE:CD2	2.49	0.47
2:B:679:GLN:OE1	13:N:157:ARG:N	2.48	0.47
1:A:653:THR:OG1	1:A:667:ARG:NH1	2.47	0.47
1:A:1062:HIS:CD2	1:A:1065:GLN:HG3	2.49	0.47
1:A:1228:THR:OG1	15:S:27:DG:OP1	2.33	0.47
1:A:1533:GLU:HG2	1:A:1539:ASP:HA	1.97	0.47
2:B:263:SER:OG	2:B:267:ASN:O	2.26	0.47
11:L:30:ILE:N	11:L:57:LEU:O	2.48	0.47
1:A:556:ALA:H	1:A:559:ASN:HD21	1.62	0.47
2:B:1196:LEU:HB3	2:B:1198:TYR:CE1	2.50	0.47
6:G:58:LEU:HG	6:G:59:GLN:H	1.79	0.47
10:K:85:ASP:OD2	10:K:111:THR:OG1	2.20	0.47
1:A:537:GLN:HB3	1:A:576:LYS:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:ASN:N	1:A:620:ASN:OD1	2.47	0.46
1:A:880:GLN:HE22	1:A:884:ARG:HH21	1.63	0.46
5:F:136:ARG:HD3	5:F:146:TRP:CD1	2.50	0.46
1:A:1307:ASP:OD1	1:A:1307:ASP:N	2.48	0.46
3:C:53:ASN:ND2	3:C:301:ASN:HD22	2.12	0.46
3:C:229:LEU:HB2	3:C:293:ARG:HD3	1.96	0.46
1:A:842:TRP:CD2	1:A:910:LYS:HE3	2.50	0.46
1:A:1050:TYR:CD2	1:A:1179:ILE:HD13	2.47	0.46
2:B:197:ASN:OD1	2:B:197:ASN:N	2.47	0.46
2:B:742:TYR:CD1	2:B:803:MET:HG2	2.50	0.46
8:I:13:CYS:SG	8:I:33:CYS:HA	2.55	0.46
13:N:159:ASP:OD1	13:N:159:ASP:N	2.48	0.46
1:A:1194:GLY:O	1:A:1197:SER:OG	2.20	0.46
2:B:125:GLU:C	2:B:127:ARG:H	2.23	0.46
1:A:1050:TYR:HB3	1:A:1054:ALA:HA	1.97	0.46
5:F:137:TYR:HB3	5:F:143:PHE:CD1	2.51	0.46
8:I:28:VAL:O	8:I:30:CYS:N	2.45	0.46
9:J:13:VAL:O	9:J:17:LYS:NZ	2.41	0.46
10:K:138:LYS:HA	10:K:138:LYS:HD2	1.83	0.46
12:M:39:ASP:OD2	12:M:54:HIS:ND1	2.49	0.46
1:A:511:VAL:HG11	1:A:561:LEU:HD13	1.98	0.46
1:A:1588:MET:O	1:A:1596:LEU:N	2.46	0.46
2:B:322:ASN:HD21	12:M:108:LEU:HD23	1.80	0.46
4:E:112:TYR:HD2	4:E:114:ASN:H	1.62	0.46
7:H:23:VAL:HA	7:H:43:ASN:HA	1.97	0.46
8:I:39:LYS:HG2	8:I:40:SER:H	1.81	0.46
9:J:8:PHE:HB2	9:J:48:ARG:HH22	1.81	0.46
13:N:141:GLU:OE1	13:N:141:GLU:N	2.49	0.46
1:A:425:ASN:HA	1:A:428:VAL:HB	1.98	0.46
1:A:1153:LYS:HB3	1:A:1161:VAL:HB	1.98	0.46
1:A:1555:VAL:HG21	4:E:182:ASP:HB3	1.98	0.46
2:B:225:ARG:HH12	2:B:261:ARG:CZ	2.29	0.46
2:B:969:GLY:HA3	2:B:1030:VAL:HG22	1.96	0.46
4:E:147:HIS:H	4:E:150:VAL:HB	1.80	0.46
15:S:23:DC:H5"	15:S:23:DC:H6	1.81	0.46
1:A:671:GLN:HG3	2:B:783:MET:HB3	1.98	0.46
2:B:75:ASP:OD1	2:B:76:GLY:N	2.48	0.46
2:B:864:ASP:O	2:B:867:ASN:ND2	2.49	0.46
9:J:14:VAL:HB	9:J:50:ILE:HD11	1.98	0.46
1:A:1124:LEU:HD22	1:A:1124:LEU:H	1.81	0.46
1:A:1326:GLU:OE1	1:A:1329:ILE:HD12	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1443:GLN:O	1:A:1447:GLN:HG3	2.16	0.46
1:A:1626:VAL:HG11	2:B:1194:ILE:HG23	1.98	0.46
3:C:129:GLU:OE1	3:C:129:GLU:N	2.47	0.46
1:A:475:ARG:NH1	16:T:20:DC:OP1	2.43	0.46
2:B:568:LEU:HD23	13:N:141:GLU:H	1.81	0.46
11:L:47:ARG:HD3	11:L:52:GLY:HA2	1.96	0.46
1:A:701:ARG:NH1	10:K:93:ILE:O	2.50	0.45
2:B:733:LEU:HD12	2:B:743:ARG:HD2	1.98	0.45
4:E:189:GLY:O	4:E:191:LYS:NZ	2.32	0.45
15:S:29:DT:H2'	15:S:30:DT:O4'	2.16	0.45
1:A:508:PRO:HB2	1:A:576:LYS:HE2	1.97	0.45
2:B:103:SER:O	2:B:169:ARG:NH2	2.49	0.45
2:B:560:ARG:O	2:B:563:SER:OG	2.25	0.45
2:B:842:GLU:OE1	11:L:58:LYS:NZ	2.45	0.45
4:E:188:LEU:HD21	4:E:190:LEU:HB2	1.99	0.45
16:T:19:DT:H2'	16:T:20:DC:H6	1.80	0.45
1:A:613:THR:HG23	1:A:615:ARG:HD3	1.99	0.45
1:A:720:PHE:HE2	7:H:98:TYR:HB2	1.81	0.45
2:B:289:PHE:HA	2:B:306:LEU:HD21	1.98	0.45
2:B:651:ARG:HD2	2:B:651:ARG:HA	1.85	0.45
1:A:1290:TYR:HB2	1:A:1474:LEU:HB2	1.98	0.45
4:E:29:PHE:HB3	4:E:65:THR:HG21	1.97	0.45
12:M:38:PHE:CE2	12:M:40:LEU:HB2	2.52	0.45
2:B:286:ARG:HD3	8:I:9:PHE:CD1	2.51	0.45
2:B:1116:SER:N	2:B:1125:THR:O	2.42	0.45
12:M:38:PHE:HD1	12:M:53:LEU:HD13	1.81	0.45
1:A:1036:ASN:HD22	1:A:1049:MET:HA	1.82	0.45
1:A:1314:GLN:HB2	1:A:1462:PHE:CE1	2.52	0.45
2:B:349:VAL:O	2:B:353:VAL:HG13	2.17	0.45
3:C:322:LYS:HE3	10:K:125:MET:HE1	1.99	0.45
5:F:137:TYR:HA	5:F:143:PHE:HA	1.99	0.45
13:N:35:LEU:HD21	13:N:118:SER:O	2.16	0.45
13:N:35:LEU:HD22	13:N:117:GLU:HA	1.99	0.45
1:A:1322:ILE:O	1:A:1326:GLU:HG2	2.17	0.45
2:B:134:ARG:NH2	2:B:462:GLN:HE22	2.15	0.45
2:B:469:ASN:OD1	2:B:469:ASN:N	2.49	0.45
2:B:751:ILE:HG12	9:J:52:THR:HG21	1.97	0.45
3:C:134:LEU:HD23	3:C:167:LEU:HB3	1.98	0.45
7:H:139:ASN:N	7:H:139:ASN:OD1	2.48	0.45
1:A:998:HIS:HE2	2:B:712:SER:H	1.65	0.45
1:A:1018:TYR:HD1	1:A:1021:ARG:HD3	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1031:HIS:ND1	1:A:1039:ARG:O	2.46	0.45
2:B:15:ASP:OD1	2:B:15:ASP:N	2.48	0.45
2:B:253:LEU:HD12	2:B:257:GLN:HE21	1.82	0.45
2:B:789:ILE:HD11	2:B:930:LYS:HG2	1.98	0.45
3:C:87:ASN:HB2	11:L:62:LYS:HD3	1.98	0.45
7:H:35:GLN:N	7:H:35:GLN:OE1	2.49	0.45
1:A:568:VAL:HG12	1:A:571:HIS:CE1	2.51	0.45
1:A:1310:LYS:HD2	1:A:1465:GLU:HA	1.99	0.45
2:B:1093:LEU:HG	2:B:1094:ASN:H	1.81	0.45
3:C:69:ARG:NH1	10:K:70:HIS:HB2	2.32	0.45
3:C:255:VAL:HG11	3:C:273:ASP:HB2	1.99	0.45
1:A:652:ASN:OD1	1:A:652:ASN:N	2.50	0.45
1:A:1329:ILE:HG22	1:A:1455:ARG:HH12	1.82	0.45
2:B:125:GLU:OE2	2:B:129:ARG:NH1	2.50	0.45
2:B:525:TRP:NE1	2:B:690:GLU:OE2	2.45	0.45
1:A:1546:VAL:HG21	1:A:1595:TYR:CE1	2.53	0.44
1:A:1546:VAL:HG11	1:A:1595:TYR:OH	2.16	0.44
3:C:100:ARG:HH22	9:J:3:VAL:N	2.15	0.44
2:B:566:TYR:HB3	12:M:73:SER:HB2	1.98	0.44
1:A:1050:TYR:CE1	1:A:1580:ARG:HB3	2.52	0.44
2:B:974:LEU:HD21	9:J:44:TYR:HD2	1.83	0.44
1:A:551:VAL:HG22	1:A:554:ARG:NH2	2.32	0.44
1:A:610:ASN:ND2	10:K:97:SER:OG	2.50	0.44
2:B:368:GLN:O	2:B:368:GLN:NE2	2.51	0.44
2:B:742:TYR:CE2	2:B:1037:ARG:HD2	2.52	0.44
3:C:117:ASP:OD2	3:C:119:ASN:ND2	2.49	0.44
5:F:72:LYS:O	5:F:142:SER:HA	2.18	0.44
10:K:60:SER:OG	10:K:106:GLN:HG2	2.18	0.44
1:A:597:LYS:HB2	2:B:1082:HIS:CE1	2.52	0.44
1:A:819:ASN:O	1:A:822:THR:OG1	2.34	0.44
2:B:705:PRO:HG3	2:B:920:ARG:CZ	2.48	0.44
2:B:884:GLU:HB3	2:B:904:LYS:HE2	1.99	0.44
2:B:938:PHE:CE1	2:B:1014:TYR:HB2	2.52	0.44
3:C:137:ASN:O	3:C:137:ASN:ND2	2.50	0.44
4:E:22:MET:HG2	4:E:187:TYR:CZ	2.53	0.44
1:A:618:TYR:CD1	1:A:670:ILE:HD11	2.53	0.44
2:B:548:LYS:O	2:B:651:ARG:NH1	2.51	0.44
2:B:591:LYS:O	2:B:593:ILE:HG23	2.18	0.44
3:C:170:GLU:OE1	3:C:172:GLN:NE2	2.51	0.44
6:G:56:ASN:ND2	6:G:101:SER:O	2.51	0.44
7:H:128:ASN:N	7:H:128:ASN:OD1	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:10:DA:H2"	16:T:11:DG:N7	2.33	0.44
1:A:827:THR:OG1	2:B:775:VAL:O	2.24	0.44
1:A:1085:LEU:O	1:A:1089:LEU:HD11	2.17	0.44
1:A:1236:PRO:HB2	1:A:1524:VAL:HG22	1.99	0.44
1:A:1321:PHE:HA	1:A:1325:LEU:HD12	1.99	0.44
1:A:1596:LEU:HG	1:A:1597:ALA:H	1.83	0.44
2:B:64:GLY:O	2:B:68:ILE:HG13	2.18	0.44
2:B:70:GLU:O	2:B:72:VAL:HG23	2.18	0.44
2:B:129:ARG:NH1	2:B:891:GLU:OE2	2.51	0.44
2:B:697:LEU:HB3	2:B:702:ASN:ND2	2.33	0.44
2:B:770:ASN:O	9:J:48:ARG:NH1	2.51	0.44
3:C:191:ILE:HA	9:J:16:ASP:HA	1.99	0.44
9:J:8:PHE:HB2	9:J:48:ARG:NH2	2.33	0.44
1:A:720:PHE:CE2	7:H:98:TYR:HB2	2.52	0.44
1:A:1274:GLU:O	8:I:46:LYS:HA	2.18	0.44
1:A:1485:MET:HA	1:A:1488:ILE:HD11	2.00	0.44
1:A:1546:VAL:HG21	1:A:1595:TYR:CZ	2.53	0.44
2:B:377:MET:HE2	2:B:377:MET:HB3	1.89	0.44
2:B:672:MET:HE3	2:B:688:HIS:CE1	2.52	0.44
2:B:730:GLY:HA2	2:B:765:PHE:CE2	2.53	0.44
2:B:834:LYS:HG3	2:B:835:GLU:H	1.83	0.44
3:C:83:VAL:HG11	3:C:98:ALA:HB1	2.00	0.44
4:E:61:GLN:HE22	4:E:79:TRP:CD1	2.36	0.44
13:N:31:LYS:HB3	13:N:119:LEU:HD11	2.00	0.44
1:A:1566:ILE:HD13	1:A:1582:LEU:HD22	2.00	0.43
2:B:731:VAL:HG12	9:J:60:PHE:HD1	1.83	0.43
2:B:773:VAL:N	2:B:1029:GLY:O	2.51	0.43
2:B:782:ASP:HA	2:B:786:ALA:HB3	2.00	0.43
2:B:826:GLY:O	2:B:862:PHE:N	2.51	0.43
2:B:827:PHE:HB2	2:B:869:THR:HG21	2.00	0.43
3:C:142:ARG:HA	3:C:157:TYR:HB3	2.00	0.43
1:A:502:ALA:HB1	1:A:530:TRP:CD1	2.53	0.43
1:A:1610:PHE:HA	1:A:1613:MET:HE2	2.00	0.43
2:B:645:GLY:HA3	2:B:648:ARG:HE	1.83	0.43
2:B:861:TYR:CE2	2:B:870:LYS:HB2	2.54	0.43
7:H:25:ARG:HA	7:H:41:ASP:OD1	2.18	0.43
2:B:181:VAL:HG13	9:J:63:TYR:CE1	2.53	0.43
3:C:125:LYS:HB2	3:C:125:LYS:HE3	1.79	0.43
3:C:190:ASP:HB2	9:J:16:ASP:HB2	1.99	0.43
3:C:197:ARG:HA	3:C:197:ARG:HD3	1.79	0.43
4:E:147:HIS:CD2	4:E:148:GLU:HG3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:56:ASN:HA	6:G:61:VAL:HG11	2.00	0.43
12:M:41:TYR:CD1	13:N:27:ASP:HB2	2.53	0.43
14:R:5:A:H2'	14:R:6:U:C6	2.53	0.43
1:A:399:LEU:HD13	1:A:423:LEU:HA	2.00	0.43
2:B:403:LEU:HD23	2:B:403:LEU:H	1.82	0.43
2:B:571:ALA:O	2:B:594:GLY:HA2	2.18	0.43
2:B:613:VAL:HG23	2:B:658:LEU:HD12	2.00	0.43
2:B:853:GLU:HG3	2:B:854:GLU:H	1.82	0.43
2:B:950:ASN:HD22	2:B:952:HIS:HB2	1.82	0.43
7:H:100:THR:HG22	7:H:139:ASN:HA	1.99	0.43
1:A:668:GLY:HA3	1:A:787:GLY:O	2.18	0.43
1:A:924:SER:O	1:A:928:MET:HG2	2.18	0.43
1:A:1217:LEU:HD13	1:A:1572:ARG:NE	2.33	0.43
1:A:1228:THR:HA	1:A:1599:ASN:ND2	2.33	0.43
2:B:57:ASP:O	2:B:62:ASN:ND2	2.51	0.43
2:B:281:CYS:SG	2:B:282:HIS:N	2.91	0.43
2:B:714:ARG:HD3	2:B:714:ARG:HA	1.71	0.43
2:B:1006:ASN:OD1	2:B:1009:GLY:N	2.51	0.43
3:C:80:ALA:HA	3:C:208:CYS:HA	1.99	0.43
6:G:65:HIS:C	6:G:68:PRO:HD2	2.44	0.43
11:L:60:ARG:NH1	11:L:63:ARG:HB3	2.30	0.43
1:A:975:ASP:OD2	1:A:977:MET:HB3	2.19	0.43
1:A:1087:GLU:OE1	1:A:1087:GLU:N	2.50	0.43
1:A:1221:ARG:NH1	1:A:1224:GLU:OE1	2.52	0.43
2:B:504:HIS:CE1	2:B:506:GLY:H	2.36	0.43
4:E:46:TYR:O	4:E:55:ARG:NH1	2.52	0.43
1:A:730:GLN:O	1:A:734:THR:HG22	2.18	0.43
2:B:724:GLN:HE22	2:B:1037:ARG:NH2	2.16	0.43
4:E:60:PHE:O	4:E:82:PHE:N	2.52	0.43
5:F:135:ARG:HH12	6:G:92:ALA:HB3	1.83	0.43
9:J:48:ARG:HE	9:J:48:ARG:HB2	1.49	0.43
12:M:38:PHE:CZ	12:M:40:LEU:HB2	2.54	0.43
16:T:9:DA:H2''	16:T:10:DA:C8	2.53	0.43
1:A:699:CYS:SG	1:A:816:LEU:HB2	2.58	0.43
1:A:711:LYS:HA	10:K:104:ARG:HH21	1.83	0.43
1:A:1148:LEU:HD21	1:A:1166:PHE:CD2	2.54	0.43
2:B:182:GLN:O	9:J:69:ARG:HD3	2.18	0.43
2:B:648:ARG:NH1	2:B:650:LEU:HD21	2.33	0.43
2:B:816:ASN:HB2	2:B:819:ASP:OD1	2.19	0.43
2:B:824:HIS:O	2:B:862:PHE:N	2.51	0.43
2:B:840:LEU:HB2	2:B:857:PRO:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:83:CYS:HB3	4:E:111:VAL:HG13	2.00	0.43
5:F:53:ASN:OD1	5:F:53:ASN:N	2.52	0.43
1:A:596:HIS:CE1	1:A:598:ALA:HB3	2.53	0.43
1:A:617:HIS:CD2	1:A:619:ALA:H	2.34	0.43
1:A:993:GLN:OE1	1:A:993:GLN:N	2.37	0.43
2:B:771:ALA:HB2	2:B:798:PHE:HZ	1.83	0.43
5:F:130:ILE:HB	5:F:132:LEU:HD22	2.01	0.43
8:I:38:PRO:HG2	8:I:41:GLN:HE21	1.83	0.43
1:A:672:ASP:CG	2:B:783:MET:HG2	2.44	0.42
1:A:1022:CYS:SG	1:A:1227:MET:HE1	2.59	0.42
2:B:654:ARG:HB2	2:B:691:PHE:CD2	2.54	0.42
2:B:842:GLU:HB2	2:B:845:LEU:O	2.18	0.42
1:A:699:CYS:SG	1:A:812:VAL:HG13	2.59	0.42
1:A:745:PRO:HG2	1:A:1074:TYR:HB2	2.01	0.42
2:B:55:GLY:HA3	2:B:59:GLY:HA2	2.01	0.42
2:B:126:SER:HB2	2:B:131:THR:C	2.44	0.42
2:B:361:HIS:CE1	2:B:590:GLY:HA3	2.54	0.42
9:J:2:ILE:HD11	9:J:56:LEU:H	1.84	0.42
10:K:70:HIS:CD2	10:K:70:HIS:H	2.37	0.42
1:A:1162:ASN:OD1	1:A:1162:ASN:N	2.51	0.42
2:B:412:ILE:HG12	2:B:461:MET:HE1	2.01	0.42
2:B:676:VAL:O	2:B:693:PRO:HG3	2.19	0.42
2:B:799:GLY:O	2:B:911:PRO:HD3	2.19	0.42
2:B:936:MET:HE3	2:B:937:PRO:HD2	2.02	0.42
2:B:364:LYS:C	2:B:366:GLY:H	2.28	0.42
3:C:129:GLU:H	3:C:129:GLU:CD	2.25	0.42
3:C:271:ARG:NE	13:N:175:TYR:OH	2.51	0.42
5:F:93:ILE:HG23	5:F:132:LEU:HD11	2.02	0.42
10:K:90:GLY:O	10:K:103:ILE:HD13	2.19	0.42
11:L:28:LYS:HG3	11:L:29:TYR:CG	2.55	0.42
1:A:688:THR:OG1	1:A:689:ARG:N	2.52	0.42
1:A:1657:LEU:HB2	6:G:106:LYS:HA	2.01	0.42
2:B:412:ILE:O	2:B:416:LYS:HG2	2.20	0.42
2:B:751:ILE:HD12	2:B:1030:VAL:HG21	2.01	0.42
2:B:853:GLU:N	2:B:856:ASP:OD2	2.37	0.42
2:B:896:GLN:N	2:B:896:GLN:OE1	2.53	0.42
13:N:114:GLU:C	13:N:116:LYS:H	2.28	0.42
1:A:516:ILE:O	1:A:520:ARG:N	2.49	0.42
1:A:556:ALA:N	1:A:559:ASN:OD1	2.52	0.42
1:A:1459:LYS:HG3	1:A:1472:PHE:HB3	2.00	0.42
2:B:758:ASP:OD1	2:B:758:ASP:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:PHE:CE2	10:K:131:VAL:HG12	2.54	0.42
4:E:162:ARG:O	4:E:166:LYS:HG2	2.20	0.42
6:G:108:THR:OG1	6:G:111:THR:O	2.25	0.42
1:A:719:ILE:O	1:A:724:PRO:HA	2.20	0.42
1:A:1338:ARG:HH11	1:A:1338:ARG:HA	1.85	0.42
2:B:124:SER:HA	2:B:127:ARG:HB2	2.01	0.42
2:B:130:LEU:HD12	2:B:198:GLY:HA3	2.01	0.42
2:B:323:ARG:O	2:B:326:VAL:HG22	2.19	0.42
2:B:697:LEU:HB3	2:B:702:ASN:HD21	1.83	0.42
7:H:26:ILE:HD11	7:H:42:ILE:HG12	2.02	0.42
13:N:31:LYS:HD2	13:N:119:LEU:HD21	2.01	0.42
1:A:575:LYS:HE2	1:A:575:LYS:HB2	1.89	0.42
2:B:1197:ARG:H	2:B:1197:ARG:HG2	1.62	0.42
3:C:65:ASN:OD1	3:C:68:ARG:NH2	2.48	0.42
6:G:56:ASN:N	6:G:57:PRO:HD3	2.34	0.42
13:N:162:LYS:HD3	13:N:162:LYS:HA	1.92	0.42
1:A:485:SER:OG	1:A:615:ARG:NE	2.53	0.42
1:A:1150:LYS:HA	1:A:1150:LYS:HD3	1.86	0.42
2:B:65:VAL:HA	2:B:68:ILE:HG13	2.01	0.42
2:B:161:LEU:HD23	2:B:161:LEU:HA	1.85	0.42
2:B:244:THR:HG23	2:B:411:MET:HE1	2.02	0.42
2:B:810:ASP:OD1	2:B:812:ALA:N	2.51	0.42
3:C:232:GLN:HB2	3:C:294:VAL:HG13	2.02	0.42
8:I:31:SER:C	8:I:33:CYS:H	2.28	0.42
15:S:30:DT:C2	15:S:31:DA:C8	3.08	0.42
1:A:527:PRO:HA	1:A:580:HIS:CE1	2.54	0.42
1:A:587:VAL:HG12	1:A:637:PHE:HD1	1.85	0.42
1:A:886:ASN:O	1:A:955:ARG:NH2	2.44	0.42
1:A:1222:LEU:O	1:A:1226:VAL:HG22	2.20	0.42
1:A:1225:ILE:O	1:A:1588:MET:HE1	2.20	0.42
2:B:26:ILE:HG22	2:B:27:ASN:ND2	2.35	0.42
6:G:110:ASP:OD1	6:G:111:THR:N	2.49	0.42
7:H:88:SER:OG	7:H:91:ASP:OD1	2.25	0.42
1:A:611:GLU:HB3	2:B:913:ILE:HD11	2.02	0.41
1:A:624:TYR:CE1	1:A:633:MET:HE1	2.55	0.41
2:B:909:ARG:HD3	2:B:909:ARG:HA	1.87	0.41
3:C:310:PRO:HA	3:C:313:ILE:HG12	2.02	0.41
1:A:496:GLY:HA3	1:A:615:ARG:HB2	2.02	0.41
1:A:1215:VAL:HG13	1:A:1217:LEU:HD21	2.02	0.41
2:B:28:PRO:HA	2:B:29:PRO:HD3	1.98	0.41
2:B:30:LYS:HA	2:B:176:SER:OG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:ARG:HD2	2:B:156:ARG:HA	1.85	0.41
2:B:165:LEU:HD11	2:B:195:ILE:HD11	2.01	0.41
2:B:221:SER:O	2:B:225:ARG:HG2	2.20	0.41
2:B:524:SER:O	2:B:524:SER:OG	2.37	0.41
2:B:585:CYS:HB2	2:B:595:TRP:CZ3	2.54	0.41
2:B:623:ASP:OD1	2:B:623:ASP:N	2.46	0.41
2:B:851:TYR:CE1	2:B:879:PRO:HB2	2.56	0.41
3:C:159:ASN:OD1	3:C:159:ASN:N	2.53	0.41
1:A:586:VAL:HG11	1:A:648:LEU:HG	2.01	0.41
1:A:610:ASN:CG	1:A:611:GLU:H	2.29	0.41
1:A:727:THR:O	1:A:731:ILE:HG13	2.21	0.41
1:A:942:GLN:HA	1:A:946:LEU:O	2.20	0.41
1:A:1264:SER:HB3	1:A:1493:CYS:HB3	2.01	0.41
2:B:480:GLN:CD	2:B:507:SER:H	2.28	0.41
2:B:832:TRP:HD1	2:B:836:TRP:CE3	2.38	0.41
3:C:320:ILE:HD13	3:C:320:ILE:HA	1.94	0.41
4:E:62:ALA:HB3	4:E:80:VAL:HB	2.01	0.41
14:R:7:C:H2'	14:R:8:G:C8	2.53	0.41
1:A:1236:PRO:HD2	1:A:1524:VAL:HG21	2.03	0.41
1:A:1311:GLU:OE1	1:A:1311:GLU:N	2.46	0.41
2:B:730:GLY:HA2	2:B:765:PHE:HE2	1.85	0.41
2:B:954:PHE:N	2:B:955:PRO:HD2	2.35	0.41
2:B:970:LYS:HG2	2:B:1000:LEU:HD21	2.01	0.41
3:C:216:HIS:HB3	3:C:218:LYS:HG2	2.01	0.41
6:G:98:GLU:N	6:G:98:GLU:OE1	2.53	0.41
1:A:1504:ILE:HA	1:A:1523:GLY:HA3	2.02	0.41
3:C:136:LEU:HD22	3:C:136:LEU:HA	1.83	0.41
4:E:13:TRP:CD2	4:E:39:LEU:HD13	2.55	0.41
5:F:130:ILE:HG13	5:F:148:VAL:HG21	2.02	0.41
16:T:32:DT:H6	16:T:32:DT:H2'	1.72	0.41
2:B:45:HIS:NE2	2:B:205:MET:HE3	2.35	0.41
2:B:104:ILE:HG12	2:B:169:ARG:HE	1.86	0.41
2:B:777:SER:HB2	2:B:951:PRO:HD2	2.02	0.41
2:B:815:ARG:HG3	2:B:821:ILE:HG23	2.02	0.41
2:B:1020:GLU:HG2	3:C:61:THR:HG21	2.03	0.41
3:C:140:CYS:HB2	3:C:196:LEU:HD23	2.01	0.41
4:E:127:ILE:H	4:E:127:ILE:HG13	1.66	0.41
7:H:28:ALA:HB3	7:H:38:LEU:HB3	2.02	0.41
12:M:82:ASN:N	12:M:87:SER:O	2.53	0.41
2:B:232:TYR:CD2	2:B:385:VAL:HG22	2.55	0.41
2:B:795:GLU:HB3	3:C:216:HIS:NE2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:825:PHE:CE2	2:B:899:GLN:HA	2.56	0.41
4:E:47:CYS:HA	4:E:55:ARG:NH1	2.36	0.41
1:A:1223:ARG:O	1:A:1227:MET:HB2	2.19	0.41
2:B:328:GLN:OE1	12:M:110:GLY:N	2.36	0.41
2:B:440:PHE:HD1	2:B:445:TYR:HE2	1.68	0.41
2:B:795:GLU:HB3	3:C:216:HIS:CD2	2.56	0.41
1:A:403:LEU:HD12	1:A:423:LEU:HD22	2.01	0.41
1:A:640:ASN:OD1	1:A:640:ASN:N	2.54	0.41
1:A:1243:TRP:HB2	1:A:1537:ASP:N	2.35	0.41
1:A:1330:VAL:HG23	1:A:1455:ARG:CZ	2.51	0.41
1:A:1591:ARG:HH21	1:A:1596:LEU:HD23	1.86	0.41
1:A:1655:ASP:HB3	5:F:135:ARG:HB3	2.02	0.41
2:B:73:ILE:HD11	2:B:429:ARG:HE	1.86	0.41
2:B:95:LEU:HD21	2:B:440:PHE:CD1	2.56	0.41
2:B:239:VAL:HA	2:B:244:THR:O	2.20	0.41
2:B:245:SER:OG	2:B:477:ASP:HB2	2.21	0.41
2:B:1128:CYS:SG	2:B:1131:CYS:N	2.85	0.41
4:E:13:TRP:O	4:E:17:ARG:HG3	2.20	0.41
4:E:74:ASP:OD1	4:E:74:ASP:N	2.52	0.41
4:E:155:ARG:HH21	4:E:188:LEU:HB3	1.86	0.41
4:E:155:ARG:CZ	4:E:187:TYR:HB3	2.51	0.41
7:H:5:LEU:HD11	7:H:61:SER:HB2	2.02	0.41
7:H:93:TYR:CD2	7:H:145:ARG:HB2	2.55	0.41
11:L:46:VAL:HG11	11:L:54:ARG:CZ	2.50	0.41
1:A:396:ILE:HD11	1:A:426:ALA:HB3	2.03	0.41
1:A:494:GLU:HG2	1:A:604:LYS:HB2	2.02	0.41
1:A:725:LEU:HD23	1:A:725:LEU:HA	1.90	0.41
1:A:756:LYS:HA	1:A:756:LYS:HD3	1.88	0.41
1:A:772:LYS:NZ	7:H:102:TYR:HA	2.36	0.41
1:A:1258:ILE:HD12	1:A:1258:ILE:HA	1.87	0.41
1:A:1546:VAL:HG11	1:A:1595:TYR:CZ	2.56	0.41
2:B:743:ARG:HH22	3:C:93:GLN:HE22	1.69	0.41
2:B:750:PRO:HG3	2:B:1032:TYR:CE2	2.55	0.41
2:B:1017:ALA:HB1	10:K:70:HIS:ND1	2.36	0.41
3:C:38:LYS:HE3	3:C:38:LYS:HB2	1.79	0.41
7:H:117:SER:HA	7:H:122:LEU:HA	2.03	0.41
8:I:60:LEU:HD23	8:I:60:LEU:HA	1.93	0.41
11:L:48:CYS:SG	11:L:50:ASP:CG	3.00	0.41
1:A:475:ARG:HB2	2:B:1059:PRO:HD2	2.03	0.40
1:A:810:LEU:HA	1:A:810:LEU:HD23	1.86	0.40
2:B:207:ILE:HA	2:B:402:VAL:HA	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:796:ARG:HE	3:C:217:ALA:HB1	1.85	0.40
3:C:121:PRO:O	3:C:125:LYS:N	2.54	0.40
3:C:272:LYS:HD2	13:N:175:TYR:CE2	2.55	0.40
3:C:285:PHE:HD1	3:C:288:LYS:HD2	1.86	0.40
2:B:173:ASN:ND2	2:B:174:LYS:HG3	2.36	0.40
2:B:328:GLN:HA	2:B:346:ASP:HB3	2.03	0.40
3:C:126:PHE:HB3	3:C:131:THR:HG21	2.04	0.40
3:C:163:TYR:HD2	3:C:165:ARG:NH1	2.19	0.40
1:A:257:ASN:HB2	1:A:260:GLN:HB2	2.04	0.40
1:A:316:LEU:O	1:A:320:VAL:HG23	2.21	0.40
1:A:523:VAL:HA	1:A:533:ALA:HB3	2.03	0.40
1:A:1007:ILE:HG21	2:B:515:THR:HG23	2.02	0.40
1:A:1450:ILE:HG22	1:A:1457:ILE:HD11	2.03	0.40
2:B:344:GLN:HG2	2:B:348:GLU:CD	2.46	0.40
2:B:509:PHE:HD2	2:B:517:VAL:HG21	1.86	0.40
2:B:815:ARG:NH1	2:B:820:PRO:HA	2.36	0.40
2:B:1123:ILE:H	2:B:1123:ILE:HG13	1.57	0.40
2:B:1129:ARG:HG3	2:B:1130:ARG:N	2.35	0.40
4:E:132:ILE:HD12	4:E:133:GLU:H	1.87	0.40
7:H:128:ASN:H	7:H:132:LEU:HD13	1.87	0.40
2:B:315:LYS:HE2	2:B:315:LYS:HB2	1.99	0.40
2:B:974:LEU:HD23	2:B:974:LEU:HA	1.87	0.40
2:B:1105:ARG:HH21	2:B:1174:THR:HB	1.86	0.40
3:C:205:LYS:HE2	3:C:205:LYS:HB2	1.85	0.40
4:E:26:ARG:HA	4:E:26:ARG:HD2	1.81	0.40
4:E:81:GLU:OE1	4:E:81:GLU:N	2.54	0.40
7:H:111:LEU:HD23	7:H:111:LEU:HA	1.92	0.40
9:J:42:LYS:HE2	9:J:42:LYS:HB2	1.91	0.40
1:A:532:GLY:H	1:A:580:HIS:HB2	1.86	0.40
1:A:846:ILE:O	1:A:849:THR:OG1	2.32	0.40
1:A:1248:ASP:OD1	1:A:1248:ASP:N	2.43	0.40
1:A:1450:ILE:HA	1:A:1453:HIS:CD2	2.57	0.40
2:B:66:LYS:C	2:B:66:LYS:HZ2	2.29	0.40
2:B:234:ILE:HD12	2:B:380:LYS:HE2	2.04	0.40
2:B:282:HIS:HB2	2:B:323:ARG:HD2	2.03	0.40
2:B:461:MET:HA	2:B:461:MET:HE2	2.03	0.40
3:C:128:ASP:OD1	3:C:128:ASP:N	2.53	0.40
4:E:22:MET:HE2	4:E:22:MET:HB3	1.86	0.40
5:F:108:PHE:HE2	5:F:131:PRO:HD3	1.86	0.40
8:I:6:SER:HA	8:I:45:LEU:HD21	2.03	0.40
10:K:91:TYR:H	10:K:91:TYR:HD1	1.70	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	A	1146/1664 (69%)	1044 (91%)	102 (9%)	0	100	100
2	B	1109/1203 (92%)	1013 (91%)	96 (9%)	0	100	100
3	C	302/335 (90%)	291 (96%)	11 (4%)	0	100	100
4	E	175/215 (81%)	146 (83%)	29 (17%)	0	100	100
5	F	101/155 (65%)	91 (90%)	10 (10%)	0	100	100
6	G	56/326 (17%)	43 (77%)	13 (23%)	0	100	100
7	H	127/146 (87%)	120 (94%)	7 (6%)	0	100	100
8	I	53/125 (42%)	34 (64%)	19 (36%)	0	100	100
9	J	66/70 (94%)	58 (88%)	8 (12%)	0	100	100
10	K	95/142 (67%)	92 (97%)	3 (3%)	0	100	100
11	L	42/70 (60%)	36 (86%)	6 (14%)	0	100	100
12	M	61/415 (15%)	50 (82%)	11 (18%)	0	100	100
13	N	76/233 (33%)	59 (78%)	17 (22%)	0	100	100
All	All	3409/5099 (67%)	3077 (90%)	332 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1033/1465 (70%)	991 (96%)	42 (4%)	27	53
2	B	985/1053 (94%)	927 (94%)	58 (6%)	18	44
3	C	268/296 (90%)	252 (94%)	16 (6%)	17	44
4	E	166/197 (84%)	154 (93%)	12 (7%)	13	38
5	F	91/137 (66%)	86 (94%)	5 (6%)	19	46
6	G	55/291 (19%)	48 (87%)	7 (13%)	4	21
7	H	115/128 (90%)	110 (96%)	5 (4%)	26	51
8	I	50/110 (46%)	42 (84%)	8 (16%)	2	14
9	J	63/65 (97%)	59 (94%)	4 (6%)	16	42
10	K	87/130 (67%)	83 (95%)	4 (5%)	24	50
11	L	39/57 (68%)	36 (92%)	3 (8%)	12	37
12	M	65/371 (18%)	61 (94%)	4 (6%)	16	43
13	N	79/220 (36%)	73 (92%)	6 (8%)	12	37
All	All	3096/4520 (68%)	2922 (94%)	174 (6%)	21	46

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	409	ASP
1	A	410	LYS
1	A	419	ILE
1	A	428	VAL
1	A	433	ASP
1	A	435	ASN
1	A	485	SER
1	A	500	VAL
1	A	559	ASN
1	A	571	HIS
1	A	581	ILE
1	A	620	ASN
1	A	670	ILE
1	A	671	GLN
1	A	769	VAL
1	A	812	VAL
1	A	990	ILE
1	A	1013	THR
1	A	1025	LYS
1	A	1026	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1030	VAL
1	A	1031	HIS
1	A	1038	ILE
1	A	1040	ASP
1	A	1072	ASN
1	A	1089	LEU
1	A	1091	VAL
1	A	1199	GLN
1	A	1222	LEU
1	A	1235	THR
1	A	1240	LEU
1	A	1246	VAL
1	A	1324	LEU
1	A	1330	VAL
1	A	1334	LYS
1	A	1462	PHE
1	A	1519	LEU
1	A	1520	VAL
1	A	1521	THR
1	A	1526	PHE
1	A	1616	GLU
1	A	1643	VAL
2	B	62	ASN
2	B	63	LEU
2	B	145	VAL
2	B	176	SER
2	B	190	ILE
2	B	197	ASN
2	B	202	LEU
2	B	236	ILE
2	B	278	LYS
2	B	309	LEU
2	B	322	ASN
2	B	365	ASP
2	B	397	THR
2	B	402	VAL
2	B	469	ASN
2	B	503	VAL
2	B	543	ASN
2	B	547	HIS
2	B	565	LEU
2	B	626	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	685	VAL
2	B	689	VAL
2	B	690	GLU
2	B	696	ILE
2	B	699	ILE
2	B	723	LYS
2	B	725	THR
2	B	752	VAL
2	B	769	PHE
2	B	788	ILE
2	B	794	ASP
2	B	808	LYS
2	B	810	ASP
2	B	819	ASP
2	B	834	LYS
2	B	842	GLU
2	B	845	LEU
2	B	885	VAL
2	B	886	ASN
2	B	890	ASP
2	B	898	LEU
2	B	900	THR
2	B	907	ILE
2	B	915	ASP
2	B	979	GLN
2	B	989	ASP
2	B	994	ASP
2	B	1025	ASP
2	B	1030	VAL
2	B	1033	TYR
2	B	1052	VAL
2	B	1115	GLN
2	B	1123	ILE
2	B	1171	ASN
2	B	1178	ILE
2	B	1185	LEU
2	B	1186	ASP
2	B	1196	LEU
3	C	39	ASP
3	C	61	THR
3	C	81	GLU
3	C	83	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	91	VAL
3	C	108	VAL
3	C	128	ASP
3	C	136	LEU
3	C	157	TYR
3	C	159	ASN
3	C	190	ASP
3	C	196	LEU
3	C	207	HIS
3	C	209	ILE
3	C	212	ILE
3	C	234	ASN
4	E	29	PHE
4	E	30	ILE
4	E	35	VAL
4	E	55	ARG
4	E	56	LYS
4	E	84	ASP
4	E	111	VAL
4	E	134	THR
4	E	149	LEU
4	E	163	GLU
4	E	178	ILE
4	E	190	LEU
5	F	53	ASN
5	F	63	GLN
5	F	108	PHE
5	F	123	LYS
5	F	130	ILE
6	G	53	TYR
6	G	54	LEU
6	G	93	ASP
6	G	95	LEU
6	G	106	LYS
6	G	108	THR
6	G	120	VAL
7	H	91	ASP
7	H	92	ASP
7	H	112	ILE
7	H	133	ASN
7	H	139	ASN
8	I	12	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	I	24	LEU
8	I	28	VAL
8	I	42	PHE
8	I	47	VAL
8	I	48	VAL
8	I	49	THR
8	I	51	THR
9	J	5	VAL
9	J	10	CYS
9	J	25	LEU
9	J	57	ILE
10	K	65	ILE
10	K	103	ILE
10	K	127	LEU
10	K	138	LYS
11	L	46	VAL
11	L	63	ARG
11	L	67	PHE
12	M	41	TYR
12	M	52	VAL
12	M	54	HIS
12	M	57	ASN
13	N	30	LYS
13	N	58	PHE
13	N	109	LEU
13	N	121	ILE
13	N	155	VAL
13	N	159	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	ASN
1	A	322	ASN
1	A	400	ASN
1	A	407	GLN
1	A	431	GLN
1	A	432	ASN
1	A	435	ASN
1	A	470	HIS
1	A	493	ASN
1	A	553	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	580	HIS
1	A	610	ASN
1	A	617	HIS
1	A	671	GLN
1	A	738	ASN
1	A	863	ASN
1	A	906	GLN
1	A	1036	ASN
1	A	1108	HIS
1	A	1141	GLN
1	A	1299	ASN
1	A	1314	GLN
1	A	1336	GLN
1	A	1447	GLN
1	A	1461	ASN
1	A	1503	HIS
1	A	1544	ASN
2	B	151	ASN
2	B	248	ASN
2	B	251	HIS
2	B	257	GLN
2	B	282	HIS
2	B	361	HIS
2	B	368	GLN
2	B	422	GLN
2	B	433	ASN
2	B	462	GLN
2	B	473	GLN
2	B	532	HIS
2	B	547	HIS
2	B	554	GLN
2	B	555	GLN
2	B	600	GLN
2	B	673	ASN
2	B	711	GLN
2	B	715	ASN
2	B	724	GLN
2	B	867	ASN
2	B	886	ASN
2	B	950	ASN
2	B	1008	HIS
2	B	1089	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	200	GLN
3	C	216	HIS
3	C	297	HIS
3	C	301	ASN
4	E	32	GLN
4	E	101	GLN
4	E	104	ASN
5	F	63	GLN
6	G	56	ASN
6	G	65	HIS
8	I	32	GLN
8	I	41	GLN
10	K	52	GLN
11	L	66	GLN
12	M	89	GLN
13	N	41	ASN
13	N	103	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	R	8/12 (66%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	R	5	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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
16	3DR	T	17	16	8,11,12	1.49	1 (12%)	7,14,17	1.58	1 (14%)

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
16	3DR	T	17	16	-	0/3/15/16	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	17	3DR	C2'-C1'	2.58	1.58	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	17	3DR	O4'-C4'-C3'	3.69	109.15	103.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

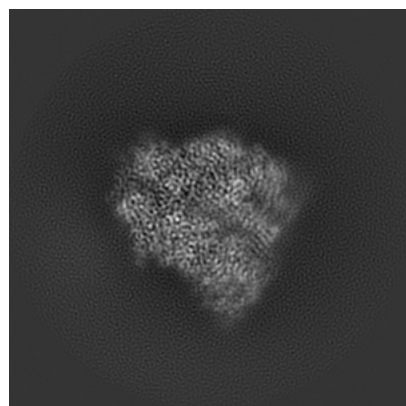
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50972. These allow visual inspection of the internal detail of the map and identification of artifacts.

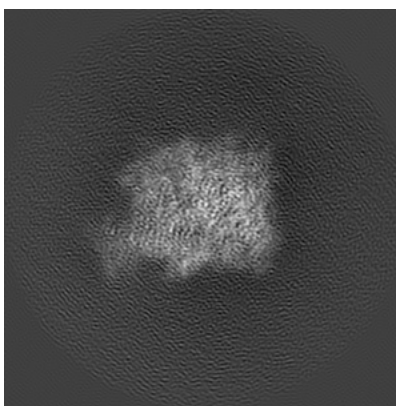
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

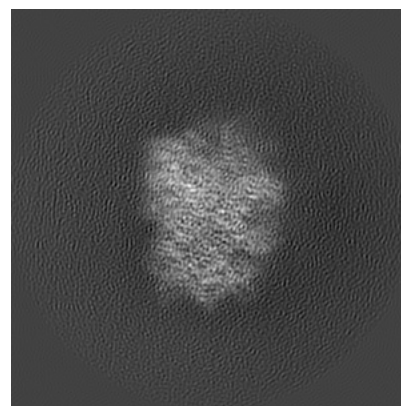
6.1.1 Primary map



X

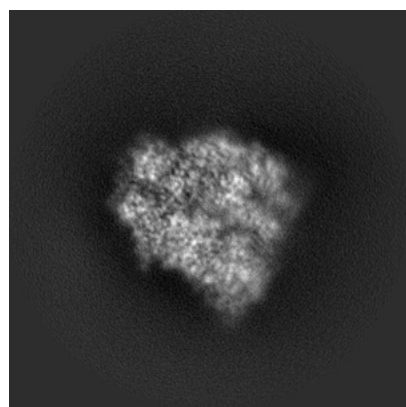


Y

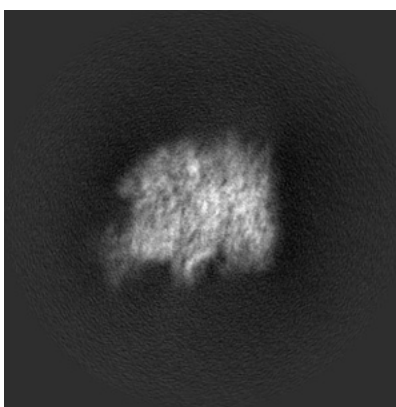


Z

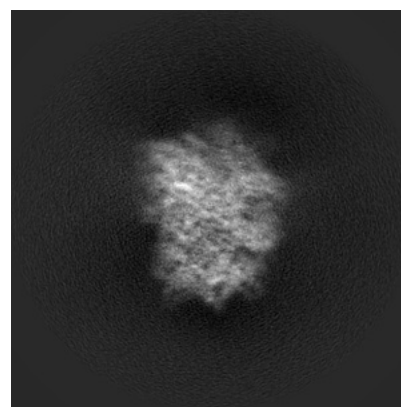
6.1.2 Raw map



X



Y

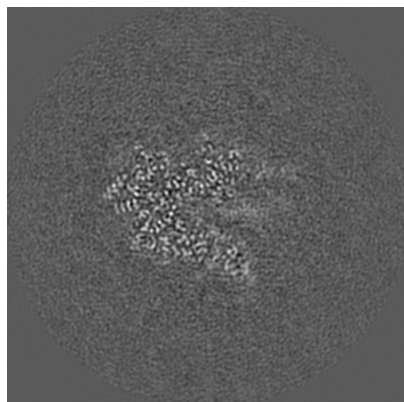


Z

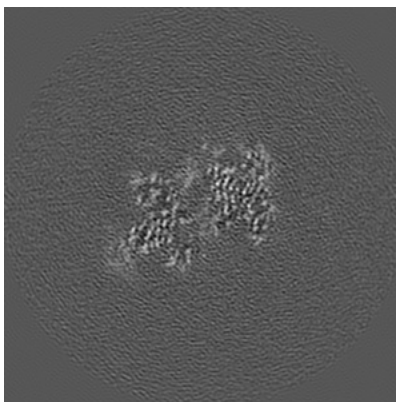
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

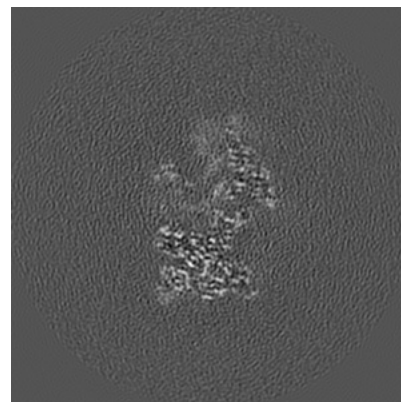
6.2.1 Primary map



X Index: 144

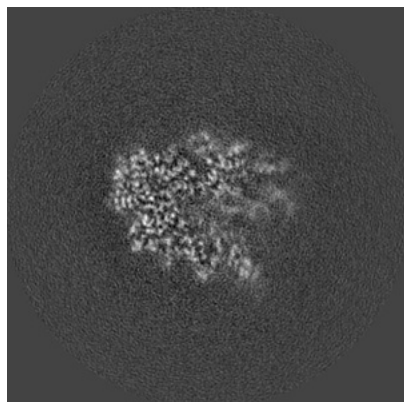


Y Index: 144

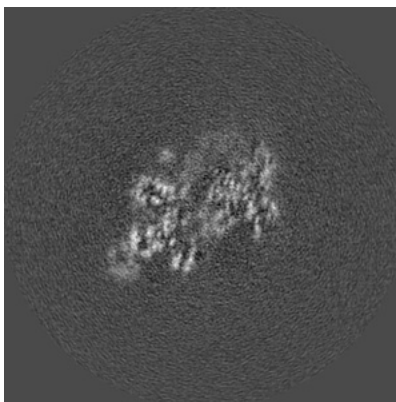


Z Index: 144

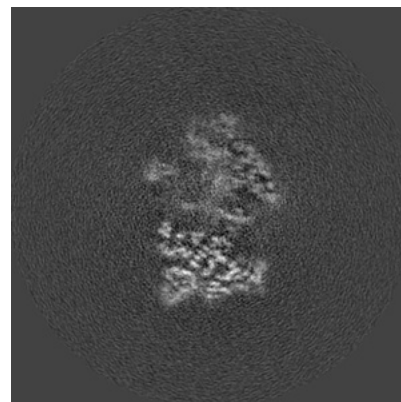
6.2.2 Raw map



X Index: 144



Y Index: 144

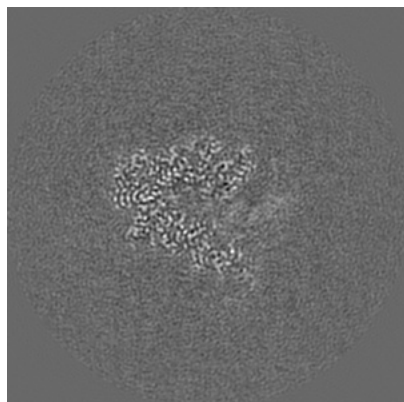


Z Index: 144

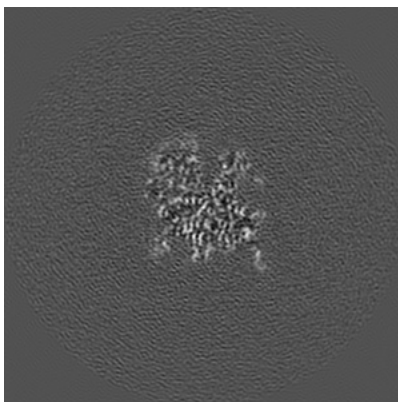
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

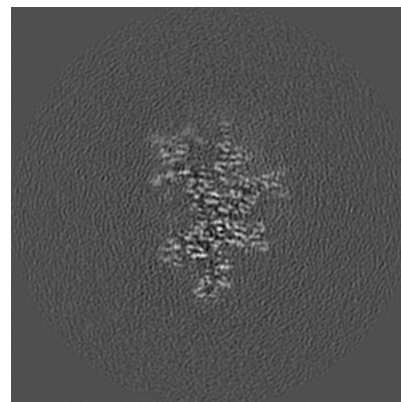
6.3.1 Primary map



X Index: 139

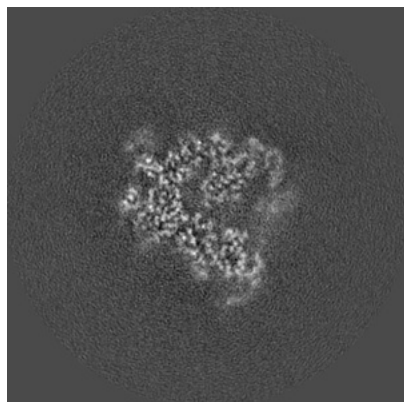


Y Index: 120

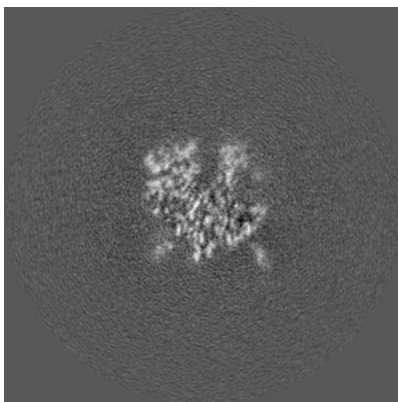


Z Index: 162

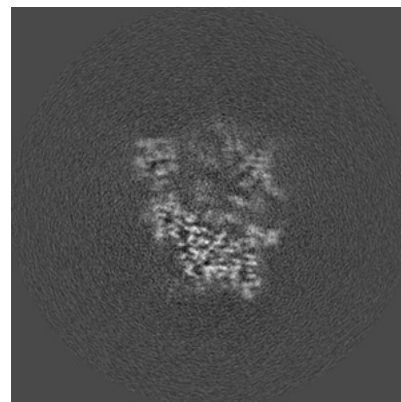
6.3.2 Raw map



X Index: 131



Y Index: 119

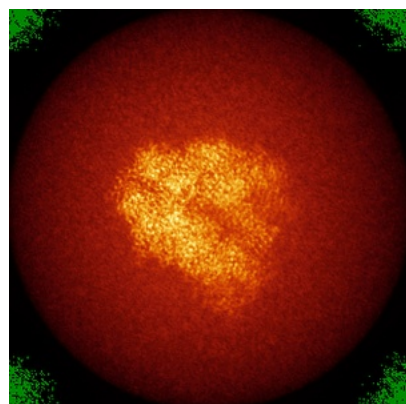


Z Index: 135

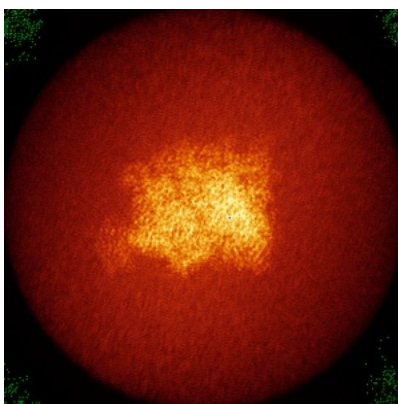
The images above show the largest variance slices of the map in three orthogonal directions.

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

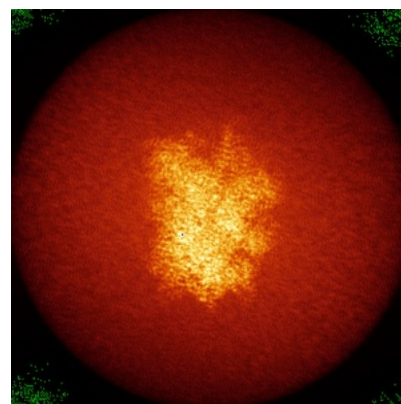
6.4.1 Primary map



X

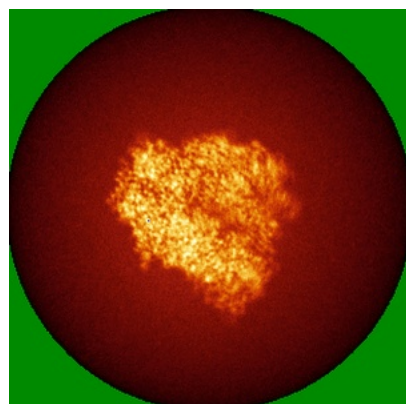


Y

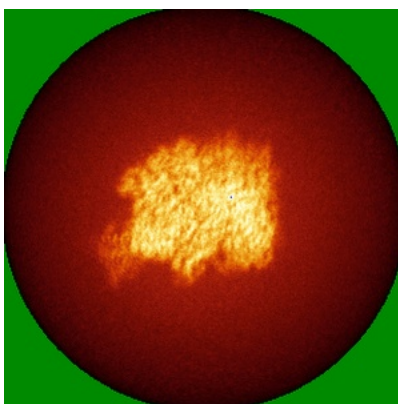


Z

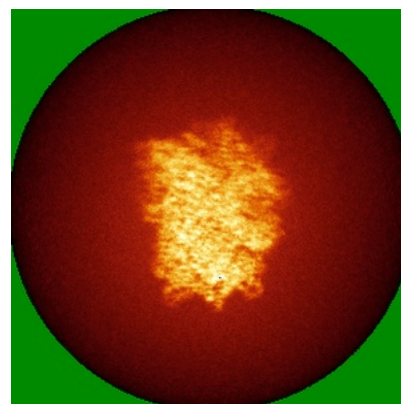
6.4.2 Raw map



X



Y

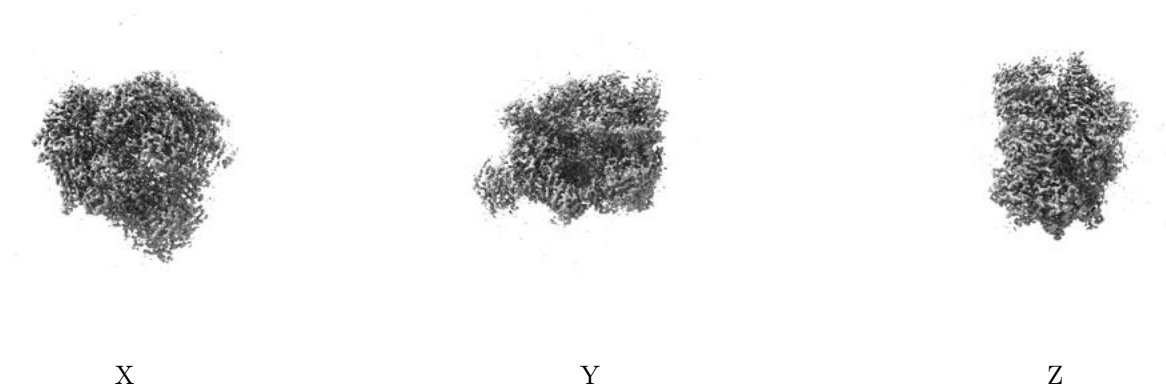


Z

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

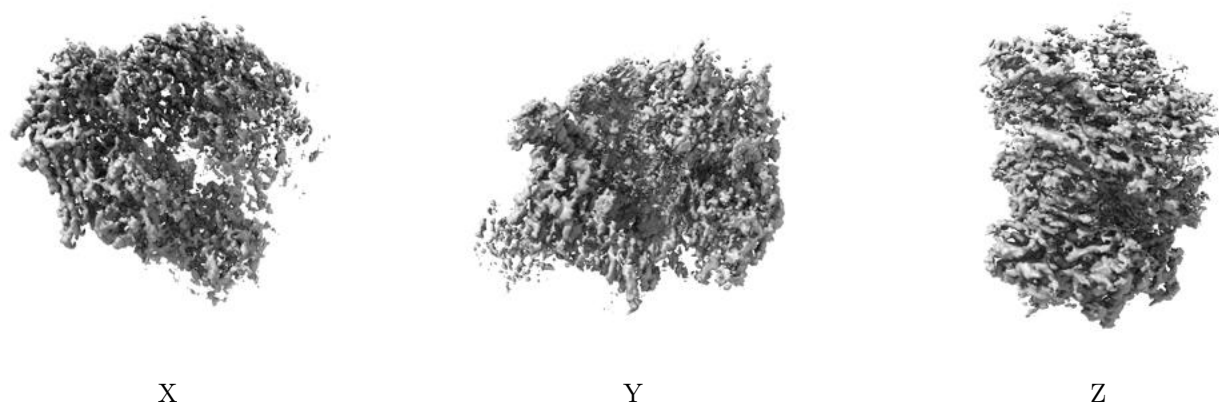
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

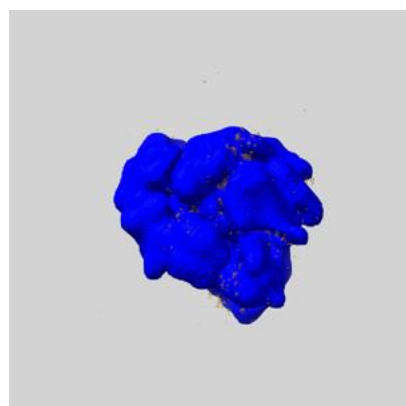
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

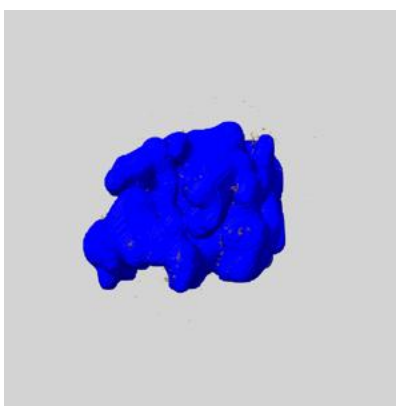
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

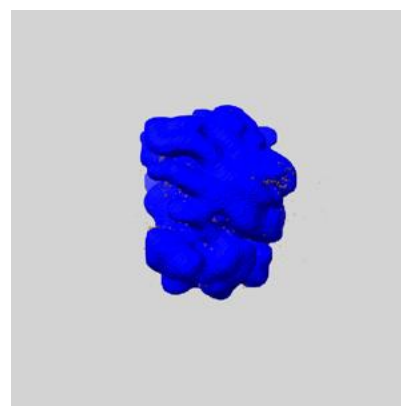
6.6.1 emd_50972_msk_1.map [i](#)



X



Y

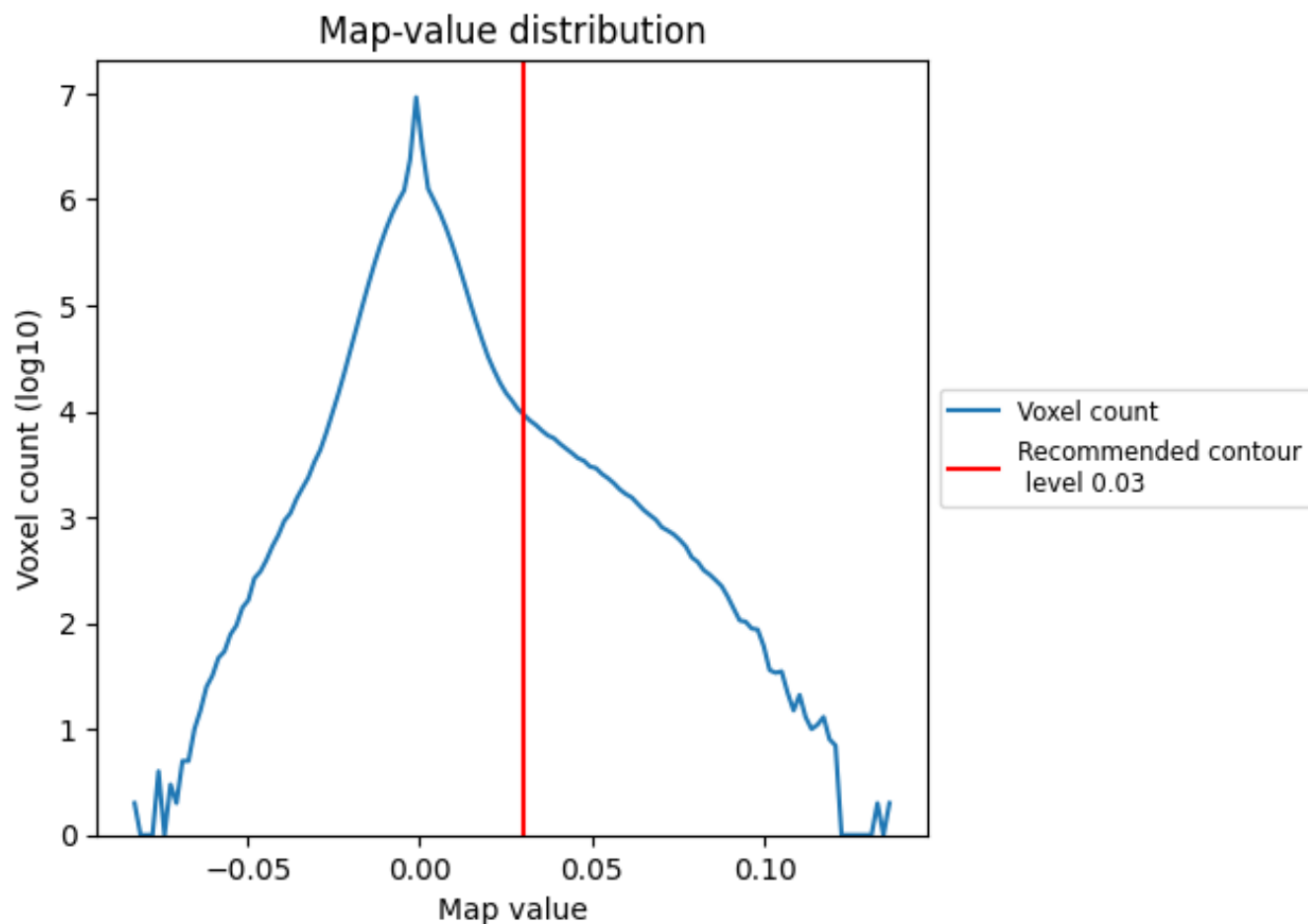


Z

7 Map analysis [i](#)

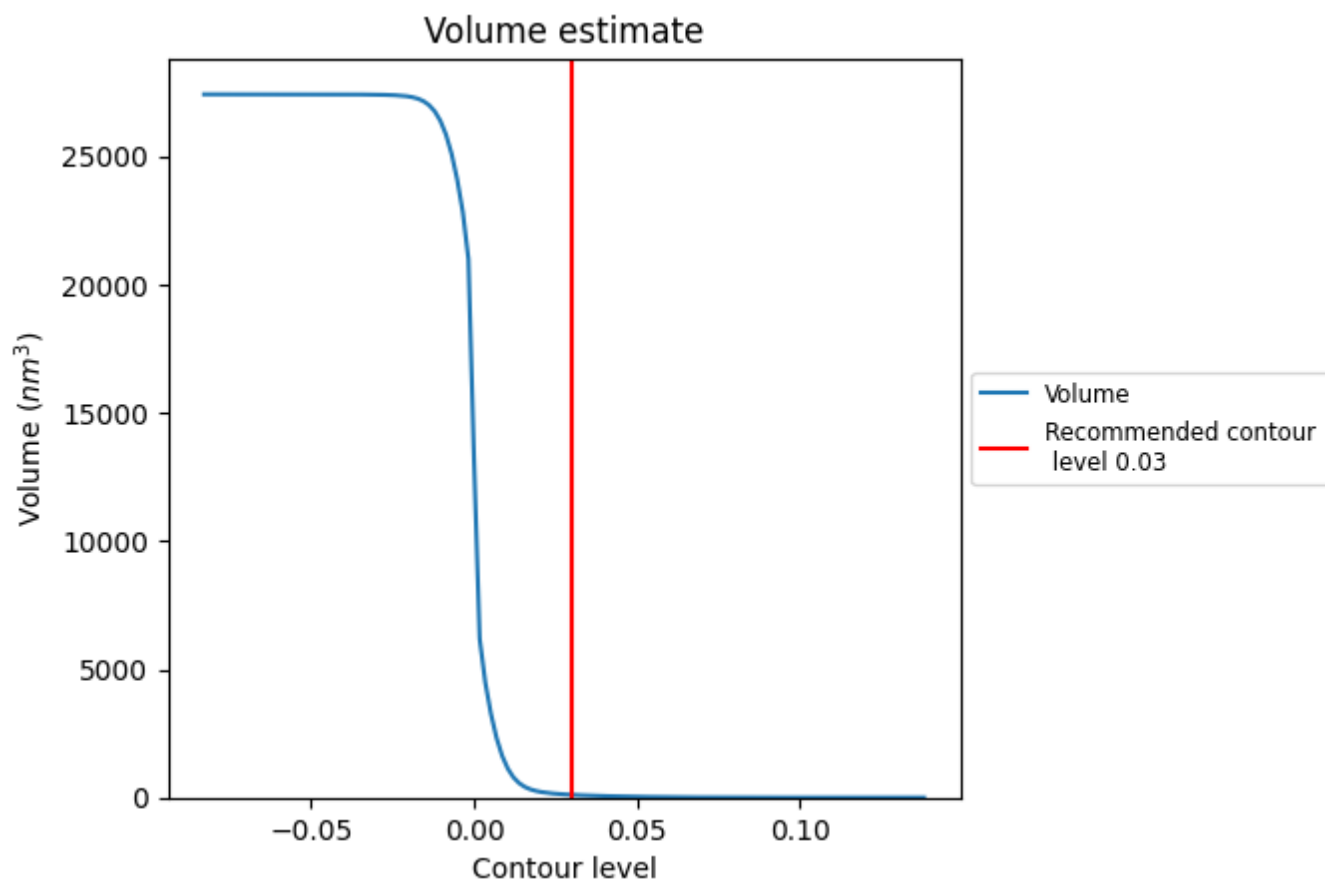
This section contains the results of statistical analysis of the map.

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.

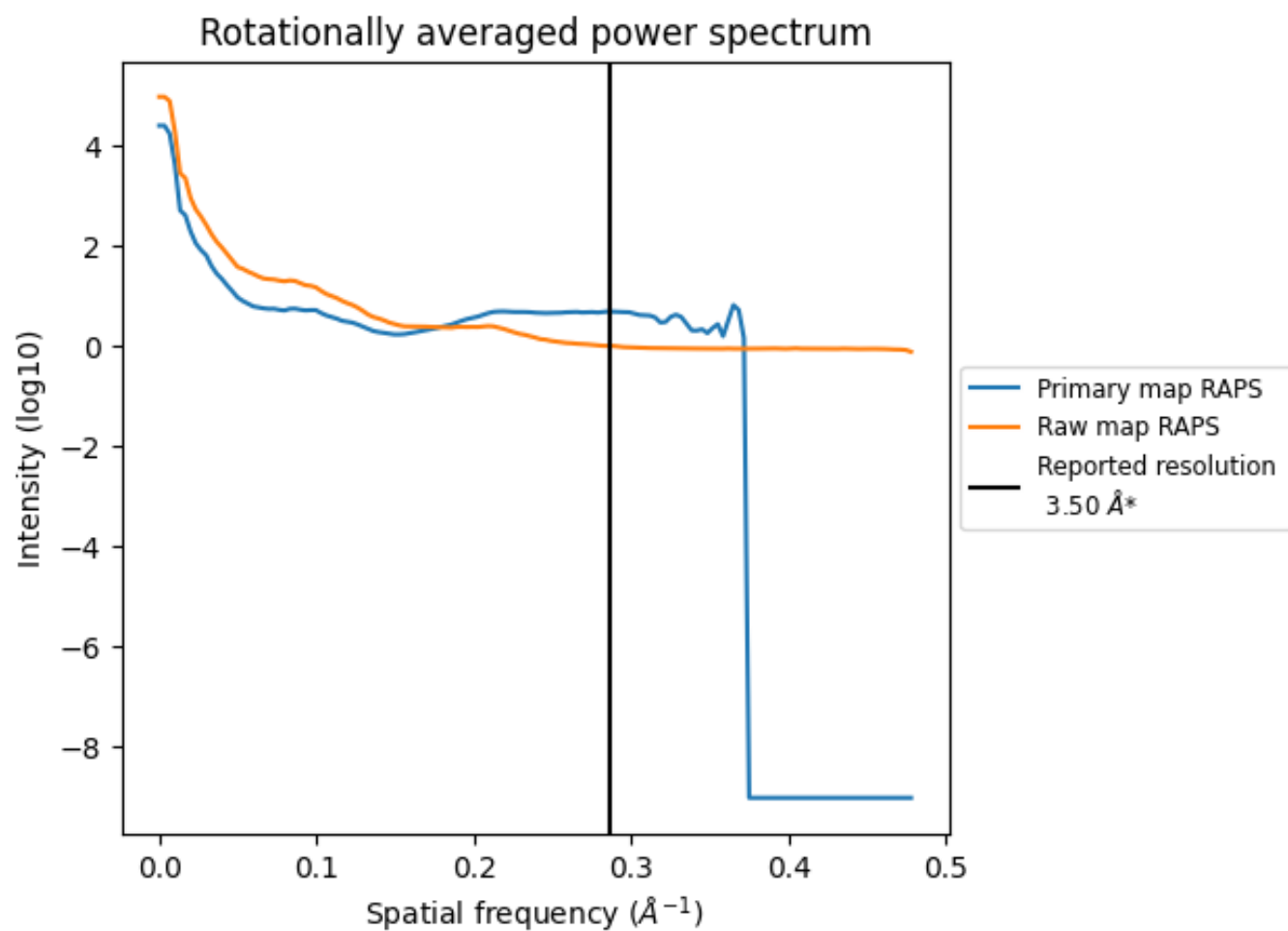
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 107 nm³; this corresponds to an approximate mass of 97 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 ⓘ

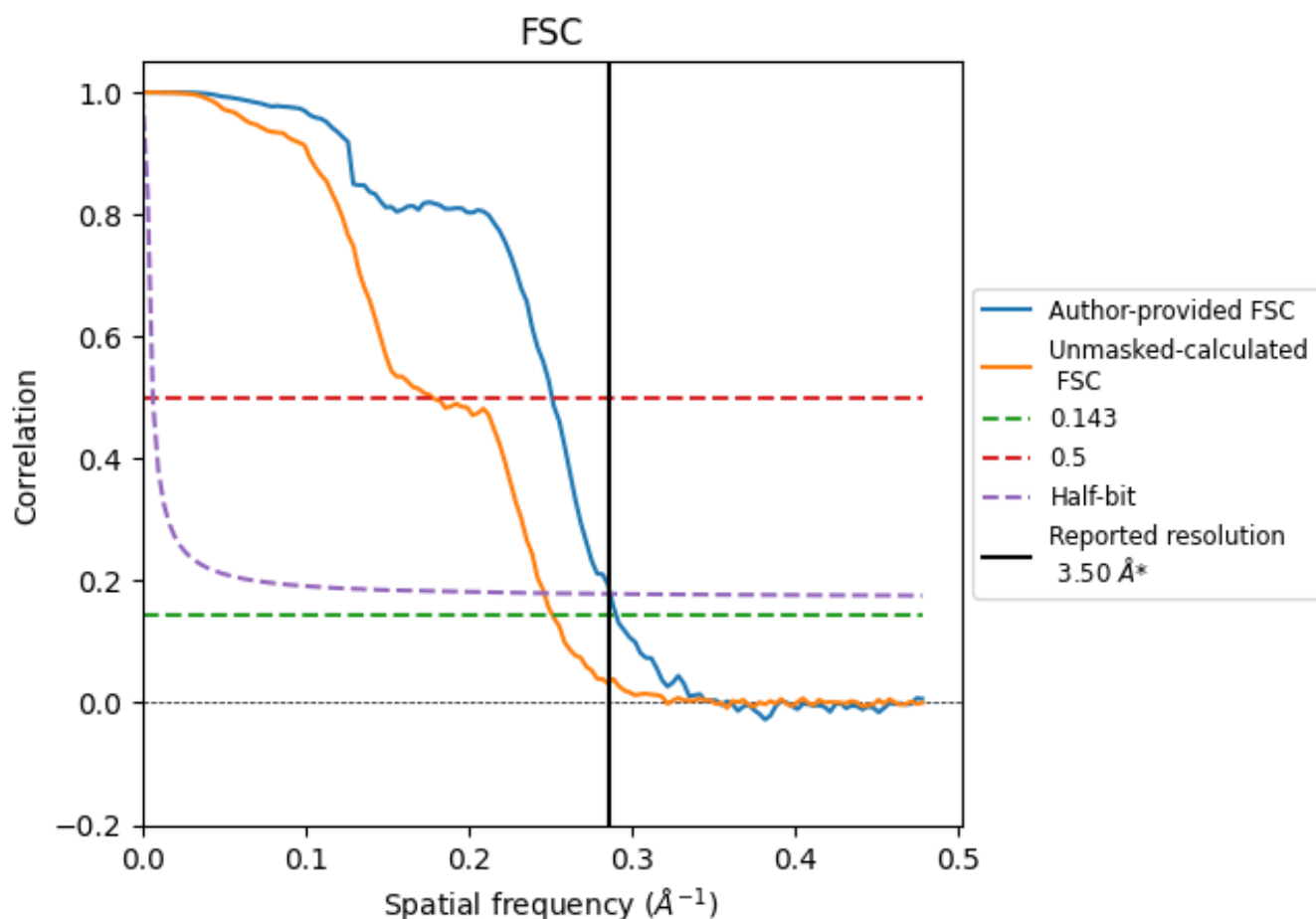


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

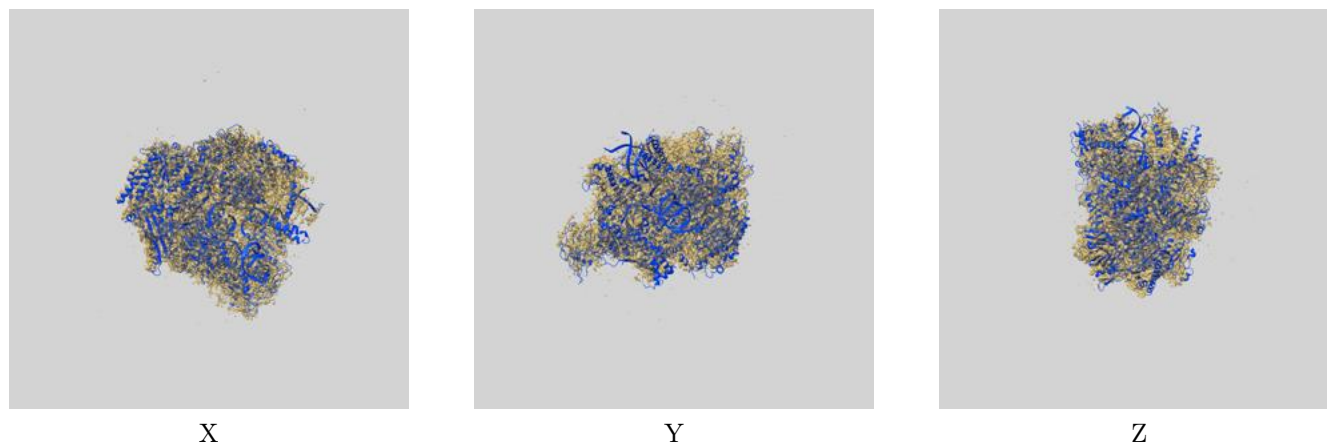
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.44	3.98	3.49
Unmasked-calculated*	3.98	5.62	4.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

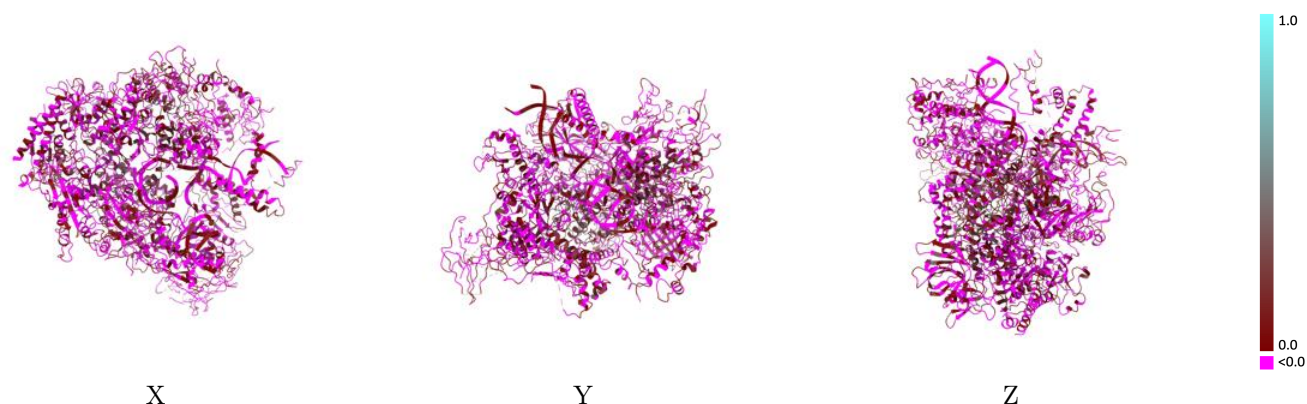
This section contains information regarding the fit between EMDB map EMD-50972 and PDB model 9G2C. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



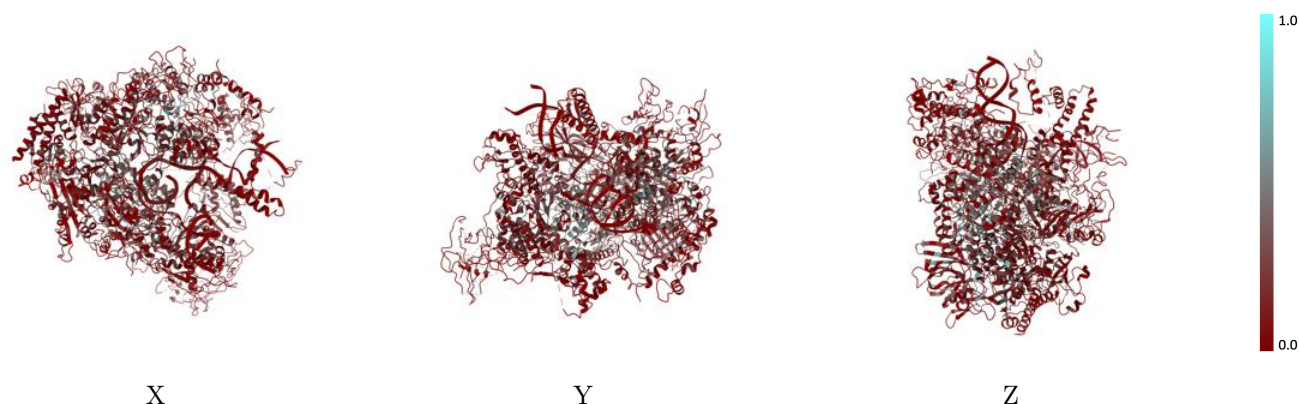
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



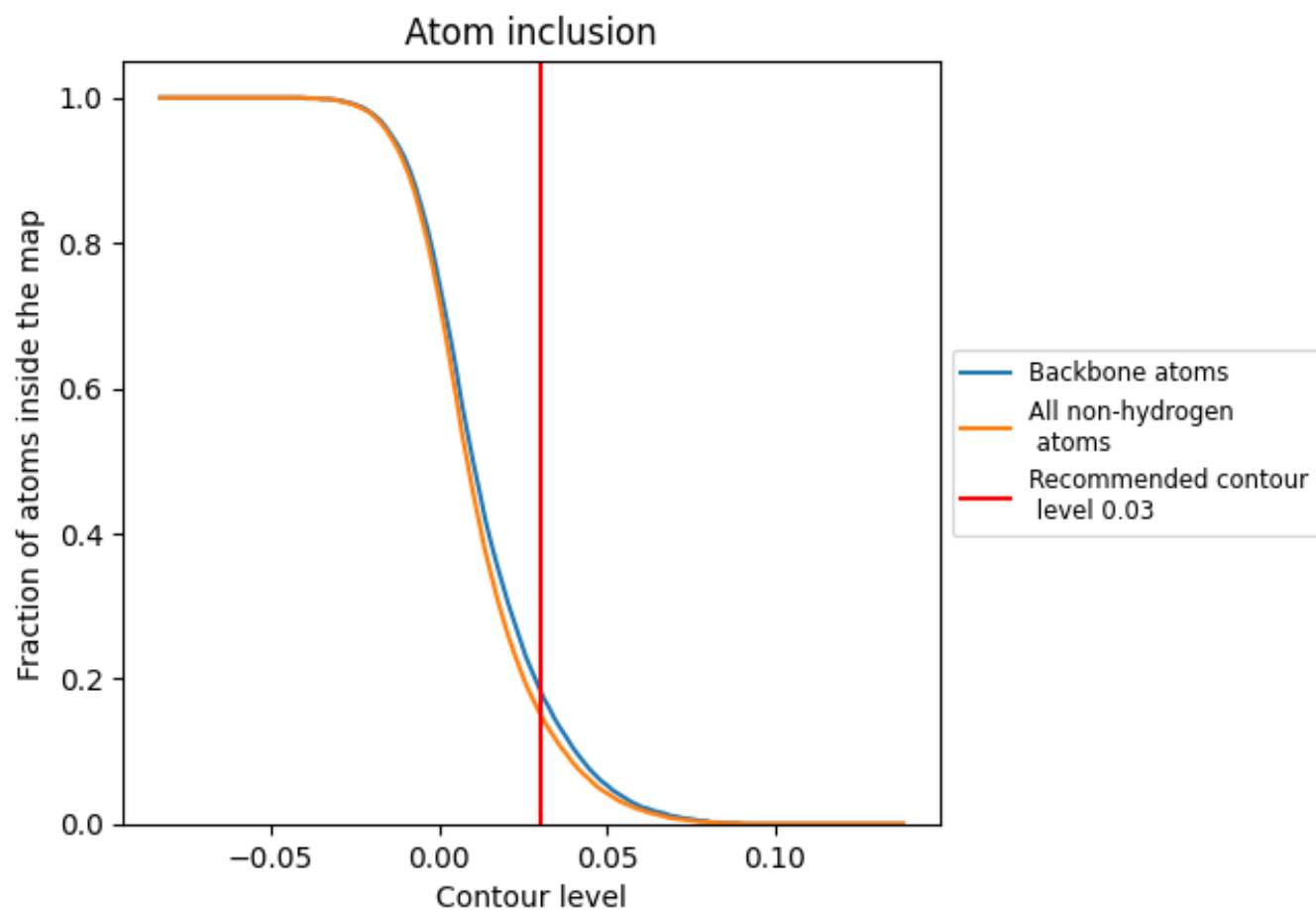
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 19% of all backbone atoms, 15% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.1530	 0.0080
A	 0.1840	 0.0300
B	 0.1700	 -0.0090
C	 0.1460	 0.0110
E	 0.0930	 -0.0340
F	 0.2100	 0.0900
G	 0.1130	 0.0330
H	 0.1530	 0.0080
I	 0.0740	 0.0280
J	 0.1530	 -0.0810
K	 0.0870	 -0.0290
L	 0.0760	 0.0240
M	 0.0530	 -0.0300
N	 0.0830	 0.0190
R	 0.1320	 -0.0100
S	 0.0130	 0.0120
T	 0.0450	 0.0090

