



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 01:34 AM UTC

PDB ID : 6FTX / pdb_00006ftx
EMDB ID : EMD-4318
Title : Structure of the chromatin remodelling enzyme Chd1 bound to a ubiquitiny-
lated nucleosome
Authors : Sundaramoorthy, R.; Owen-hughes, T.; Norman, D.G.; Hughes, A.
Deposited on : 2018-02-25
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

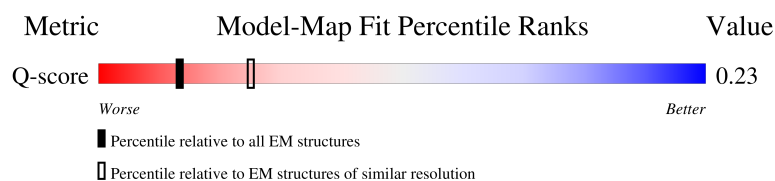
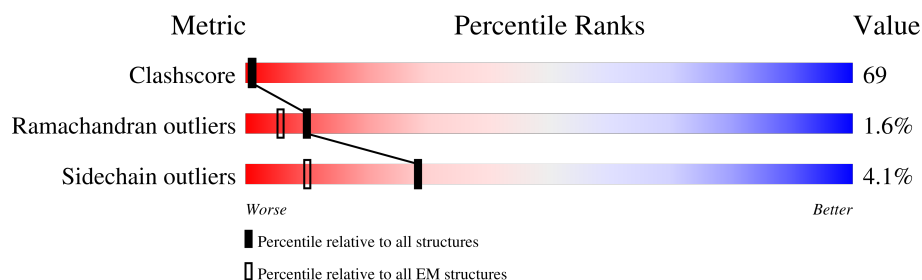
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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.



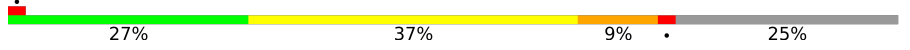
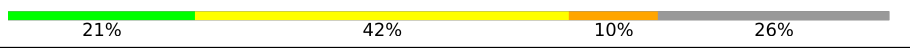
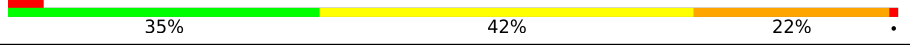
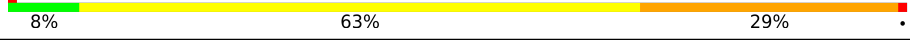
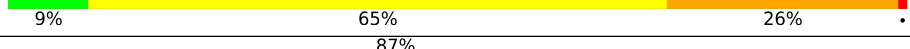
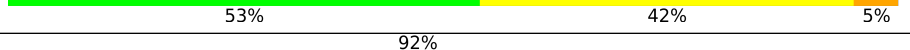
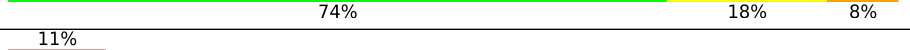
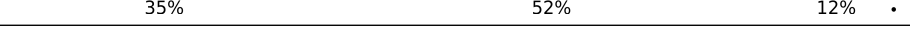
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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	97	27% 54% 16% .
2	B	103	15% 48% 16% . 19%
2	F	103	8% 26% 46% 15% . 11%
3	C	130	23% 33% 20% . 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	130	
4	D	126	
4	H	126	
5	E	110	
6	I	159	
7	J	160	
8	N	76	
8	O	76	
9	W	878	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	ADP	W	1302	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21049 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	97	Total	C	N	O	S	0	0
			802	506	155	138	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
2	F	92	Total	C	N	O	S	0	0
			686	430	134	121	1		

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	103	Total	C	N	O	0	0
			795	501	155	139		
3	G	105	Total	C	N	O	0	0
			809	510	158	141		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	conflict	UNP P06897
G	99	ARG	GLY	conflict	UNP P06897

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	95	Total	C	N	O	S	0	0
			745	469	134	140	2		
4	H	93	Total	C	N	O	S	0	0
			726	457	130	137	2		

- Molecule 5 is a protein called Histone H3.3C.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	110	Total	C	N	O	S	0	0
			866	543	168	152	3		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	26	ALA	-	expression tag	UNP P02302
E	27	ALA	-	expression tag	UNP P02302
E	28	ALA	-	expression tag	UNP P02302
E	30	ALA	PRO	conflict	UNP P02302
E	32	ALA	THR	conflict	UNP P02302
E	33	ALA	GLY	conflict	UNP P02302
E	34	ALA	GLY	conflict	UNP P02302
E	35	ALA	VAL	conflict	UNP P02302
E	36	ALA	LYS	conflict	UNP P02302
E	37	ALA	LYS	conflict	UNP P02302
E	38	ALA	PRO	conflict	UNP P02302
E	86	SER	ARG	conflict	UNP P02302

- Molecule 6 is a DNA chain called DNA (159-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	159	Total	C	N	O	P	0	0
			3238	1537	590	952	159		

- Molecule 7 is a DNA chain called DNA (160-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	160	Total	C	N	O	P	0	0
			3298	1562	616	961	159		

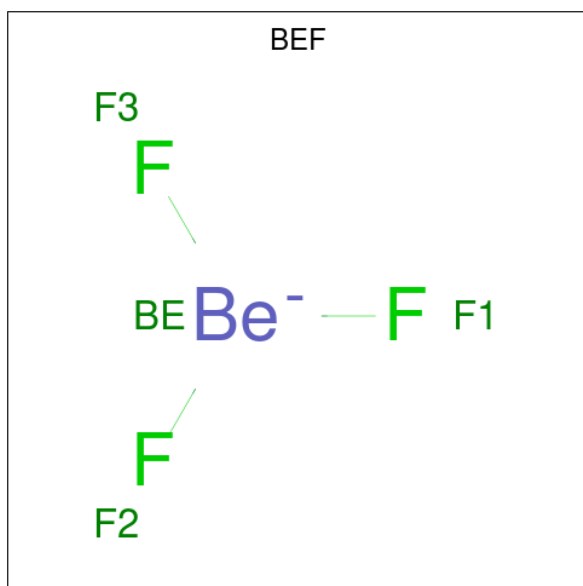
- Molecule 8 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	76	Total	C	N	O	S	0	0
			601	378	105	117	1		
8	O	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

- Molecule 9 is a protein called Chromatin-remodeling ATPase.

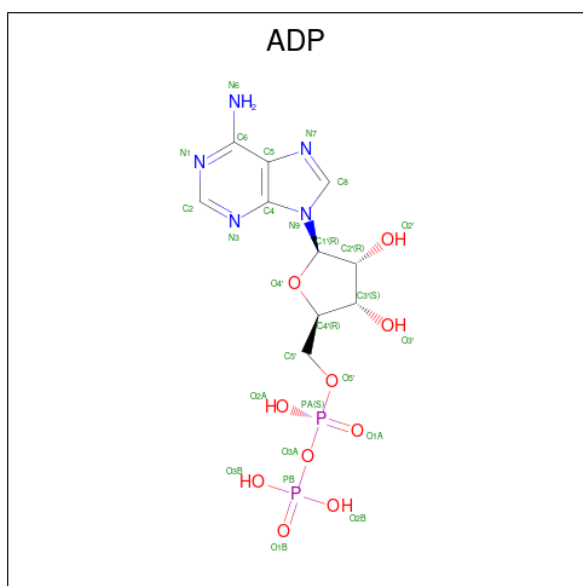
Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	878	Total	C	N	O	S	2	0
			7189	4568	1260	1334	27		

- Molecule 10 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			AltConf
10	W	1	Total	Be	F	0
			4	1	3	

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).

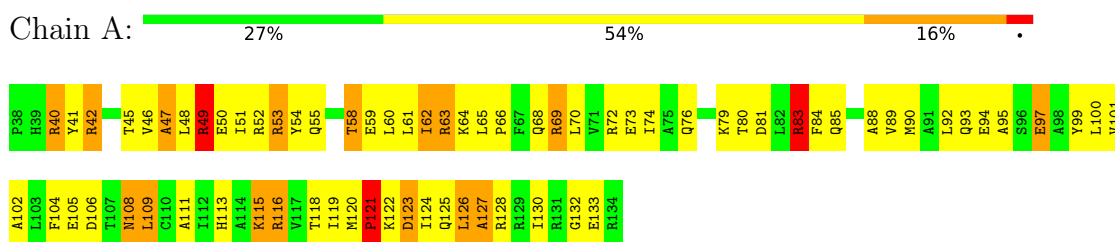


Mol	Chain	Residues	Atoms					AltConf
11	W	1	Total	C	N	O	P	0
			27	10	5	10	2	

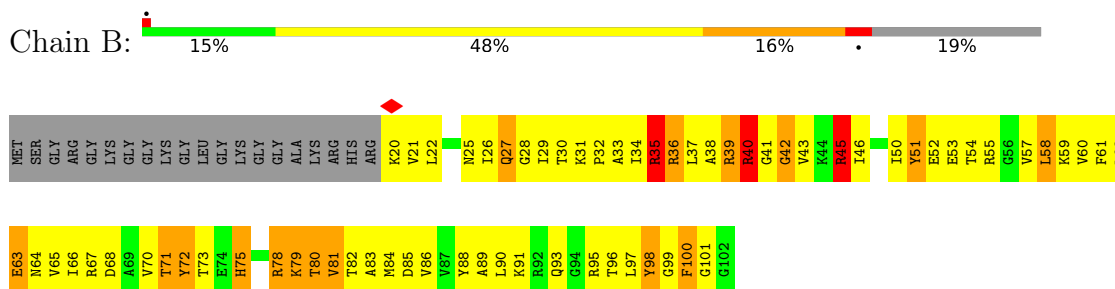
3 Residue-property plots

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.

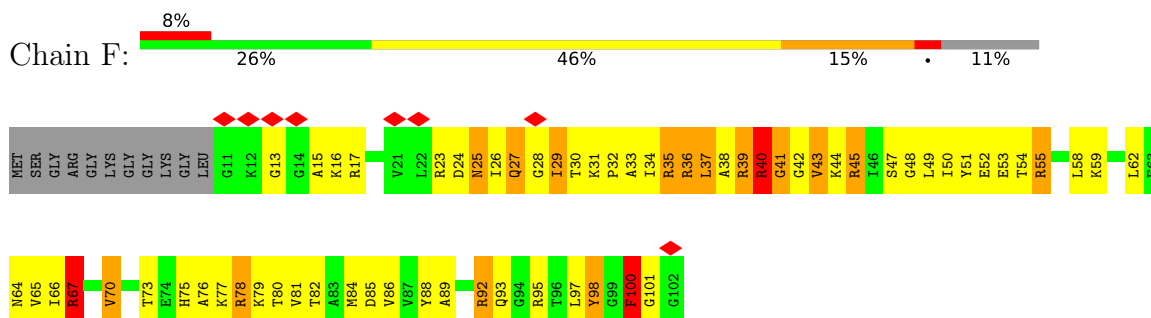
• Molecule 1: Histone H3



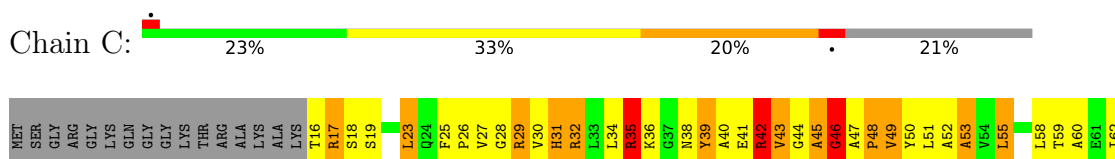
• Molecule 2: Histone H4

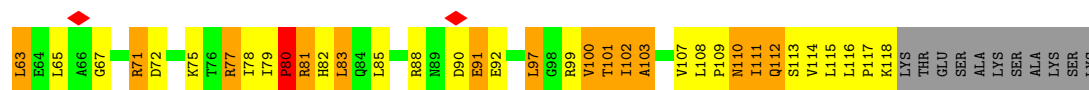


• Molecule 2: Histone H4

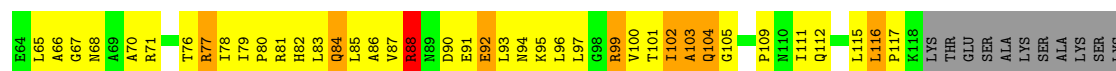
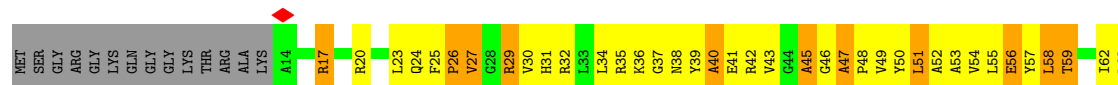
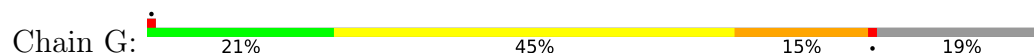


• Molecule 3: Histone H2A type 1

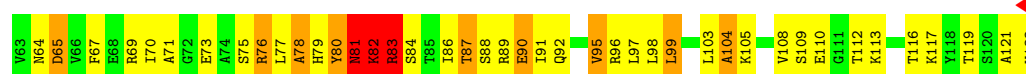
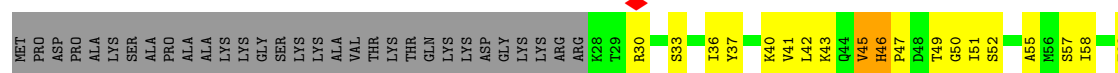
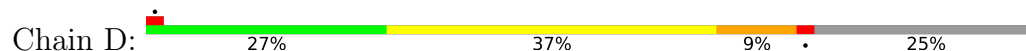




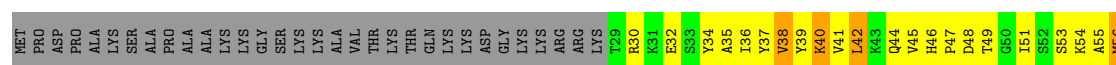
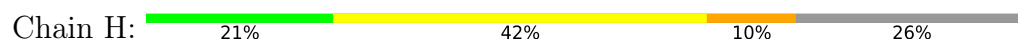
• Molecule 3: Histone H2A type 1



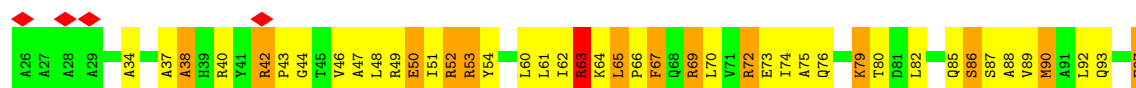
• Molecule 4: Histone H2B



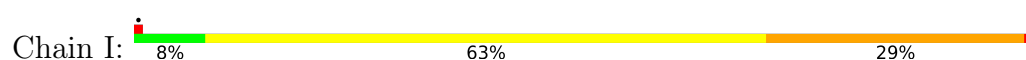
• Molecule 4: Histone H2B



• Molecule 5: Histone H3.3C



• Molecule 6: DNA (159-MER)



E1177	E1178	D1179	E1180	K1181	L1182	L1183	G1184	G1185	G1186	F1187	K1188	F1189	G1190	Y1191	G1192	S1193	W1194	I1197	R1198	D1199	D1200	F1201	F1202	G1203	I1205	T1206	K1207	K1208	I1209	K1245	V1246	P1247	G1248	A1249	I1250	L1251	L1252	G1253	R1254	R1255	Y1256	D1257	Y1258	L1259	L1260	S1261	F1262	L1263	R1264	G1265	G1266	G1267	G1268	W1170	S1171	W1174	T1175	K1176	L1107	S1108	L1109	K1110	K1111	L1112	E1113	K1114	K1115	A1116	V1117	L1118	F1119	N1120	F1121	V1124	L1127	N1128	A1129	L1132	L1133	E1137	D1138	L1139	K1140	K1143	N1144	L1145	L1146	N1147	S1148	N1149	Y1150	K1151	D1152	D1153	P1154	L1155	K1156	F1157	S1158	L1159	G1160	N1161	N1162	T1163	P1164	K1165	W1170	S1171	W1174	T1175	K1176	T1039	L1040	P1041	V1042	K1043	S1044	F1045	E1046	K1047	Y1048	G1049	E1050	T1051	Y1052	D1053	E1054	M1055	M1056	A1059	E1066	E1067	R1070	I1073	L1074	E1075	K1076	L1077	E1078	K1079	H1080	A1081	T1082	A1083	Y1084	R1085	A1086	K1087	L1088	K1089	S1090	G1091	E1092	T1093	K1094	A1095	E1096	N1097	Q1098	P1099	K1100	D1101	PH103	L1104	T1105	R1106	A805	H806	R807	I808	G809	Q810	K811	N812	H813	V814	M815	V816	Y817	R818	R819	L820	V821	S822	K823	T824	V825	E826	E827	E828	V829	A833	R834	K835	K836	M837	R838	D1005	M1006	D1007	E1013	V1014	L1017	Y1018	L1022	K1023	F1024	G1025	N1026	L1027	K1028	E1029	I1030	L1031	D1032	E1033	L1034	I1035	A1036	D1037	G1038	A858	S859	N860	Y863	L864	F865	D866	N867	E868	E869	V872	L873	Q874	G875	T881	M881	T882	R888	G889	L890	I891	M892	S893	S894	G895	K896	M897	V898	L899	L703	L704	T705	R706	L707	K708	H712	R713	V714	L715	I716	F717	S718	Q719	V721	R722	M723	L724	D725	I726	D729	Y730	L731	S732	I733	F738	Q739	R740	L741	D742	G743	T744	P746	Q749	R750	R751	I752	S753	T754	D755	H756	D764	F765	V766	F767	M768	L769	S770	T771	R772	A773	G774	G775	L776	G777	I778	N779	L780	M781	D784	T785	V786	F787	I788	F789	D790	S791	D792	N793	N794	P795	Q796	A797	D798	L799	Q800	A801	M802	A803	R804	R524	L525	Y526	E527	S528	F532	K533	V534	A535	N536	R537	M538	L539	T540	G542	T543	P544	L545	Q546	N547	K550	E551	L552	A553	A554	L555	V556	L559	M560	P561	G562	R563	F564	N574	Q575	D576	E577	E578	Q579	E580	E581	Y582	I583	H584	D585	L586	H587	R588	R589	I590	Q591	P592	F593	I594	L595	R596	R597	L598	K599	R600	D601	V602	L606	S608	K609	T610	E611	R612	G613	L614	R615	V616	E617	L618	S619	D620	V621	Q622	T623	E624	Y625	G626	K627	M628	L629	R630	T631	K632	M633	Y634	S635	A636	L637	T638	A639	G640	A641	K642	G643	G644	H645	S647	L648	L649	M650	T651	M652	N653	E654	L655	K656	K657	S461	S462	R463	D464	T465	I466	R467	E468	Y469	E470	F471	Y472	T473	M474	R476	A477	K478	G479	K480	K481	T482	M483	K484	F485	M486	L487	L488	L489	T490	P491	H492	E493	Y494	I495	R499	L502	G503	S504	I505	K506	V507	Q508	F509	M510	A511	V512	D513	E514	A515	H516	R517	L518	K519	N520	A521	P522	S523	S431	P432	Q433	R434	G435	L436	M437	P438	A439	K440	L441	D442	T443	A448	P449	D450	L451	N452	C455	Y456	M457	G458	N459	D395	K393	V328	I327	D326	Y325	F389	N385	I384	V386	M387	A388	N323	G322	E322	A319	E318	D317	N316	Y316	L314	R313	D312	W311	V309	L308	Y307	G306	I371	F370	P369	P368	Q367	V366	E362	F361	R360	N295	A296	S297	G297	L298	P427	H428	I429	M430	V431	P432	V433	L434	S435	T436	M437	P438	A439	K440	L441	D442	T443	A448	P449	D450	L451	N452	C455	Y456	M457	G458	N459	D395	K393	V328	I327	D326	Y325	F389	N385	I384	V386	M387	A388	N323	G322	E322	A319	E318	D317	N316	Y316	L314	R313	D312	W311	V309	L308	Y307	G306	I371	F370	P369	P368	Q367	V366	E362	F361	R360	N295	A296	S297	G297	L298	P427	H428	I429	M430	V431	P432	V433	L434	S435	T436	M437	P438	A439	K440	L441	D442	T443	A448	P449	D450	L451	N452	C455	Y456	M457	G458	N459	D395	K393	V328	I327	D326	Y325	F389	N385	I384	V386	M387	A388	N323	G322	E322	A319	E318	D317	N316	Y316	L314	R313	D312	W311	V309	L308	Y307	G306	I371	F370	P369	P368	Q367	V366	E362	F361	R360	N295	A296	S297	G297	L298	P427	H428	I429	M430	V431	P432	V433	L434	S435	T436	M437	P438	A439	K440	L441	D442	T443	A448	P449	D450	L451	N452	C455	Y456	M457	G458	N459	D395	K393	V328	I327	D326	Y325	F389	N385	I384	V386	M387	A388	N323	G322	E322	A319	E318	D317	N316	Y316	L314	R313	D312	W311	V309	L308	Y307	G306	I371	F370	P369	P368	Q367	V366	E362	F361	R360	N295	A296	S297	G297	L298	P427	H428	I429	M430	V431	P432	V433	L434	S435	T436	M437	P438	A439	K440	L441	D442	T443	A448	P449	D450	L451	N452	C455	Y456	M457	G458	N459	D395	K393	V328	I327	D326	Y325	F389	N385	I384	V386	M387	A388	N323	G322	E322	A319	E318	D317	N316	Y316	L314	R313	D312	W311	V309	L308	Y307	G306	I371	F370	P369	P368	Q367	V366	E362	F361	R360	N295	A296	S297	G297	L298	P427	H428	I429	M430	V431	P432	V433	L434	S435	T436	M437	P438	A439	K440	L441	D442	T443	A448	P449	D450	L451	N452	C455	Y456	M457	G458	N459	D395	K393	V328	I327	D326	Y325	F389	N385	I384	V386	M387	A388	N323	G322	E322	A319	E318	D317	N316	Y316	L314	R313	D312	W311	V309	L308	Y307	G306	I371	F370	P369	P368	Q367	V366	E362	F361	R360	N295	A296	S297	G297	L298	P427	H428	I429	M430	V431	P432	V433	L434	S435	T436	M437	P438	A439	K440	L441	D442	T443	A448	P449	D450	L451	N452	C455	Y456	M457	G458	N459	D395	K393	V328	I327	D326	Y325	F389	N385	I384	V386	M387	A388	N323	G322	E322	A319	E318	D317	N316	Y316	L314	R313	D312	W311	V309	L308	Y307	G306	I371	F370	P369	P368	Q367	V366	E362	F361	R360	N295	A296	S297	G297	L298	P427	H428	I429	M430	V431	P432	V433	L434	S435	T436	M437	P438	A439	K440	L441	D442	T443	A448	P449	D450	L451	N452	C455	Y456	M457	G458	N459	D395	K393	V328	I327	D326	Y325	F389	N385	I384	V386	M387	A388	N323	G322	E322	A319	E318	D317	N316	Y316	L314	R313	D312	W311	V309	L308	Y307	G306	I371	F370	P369	P368	Q367	V366	E362	F361	R360	N295	A296	S297	G297	L298	P427	H428	I429	M430	V431	P432	V433	L434	S435	T436	M437	P438	A439	K440	L441	D442	T443	A448	P449	D450	L451	N452	C455	Y456	M457	G458	N459	D395	K393	V328	I327	D326	Y325	F389	N385	I384	V386	M387	A388	N323	G322	E322	A319	E318	D317	N316	Y316	L314	R313	D312	W311	V309	L308	Y307	G306	I371	F370	P369	P368	Q367	V366	E362	F361	R360	N295	A296	S297	G297	L298	P427	H428	I429	M430	V431	P432	V433	L434	S435	T436	M437	P438	A439	K440	L441	D442	T443	A448	P449	D450	L451	N452	C455	Y456	M457	G458	N459	D395	K393	V328	I327	D326	Y325	F389	N385	I384	V386	M387	A388	N323	G322	E322	A319	E318	D317	N316	Y316	L314	R313	D312	W311	V309	L308	Y307	G306	I371	F370	P369	P368	Q367	V366	E362	F361	R360	N295	A296	S297	G297	L298	P427	H428	I429	M430	V431	P432	V433	L434	S435	T436	M437	P438	A439	K440	L441	D442	T443	A448	P449	D450	L451	N452	C455	Y456	M457	G458	N459	D395	K393	V328	I327	D326	Y325	F389	N385	I384	V386	M387	A388	N323	G322	E322	A319	E318	D317	N316	Y316	L314	R313	D312	W311	V309	L308	Y307	G306	I371	F370	P369	P368	Q367	V366	E362	F361	R360	N295	A296	S297	G297	L298	P427	H428	I429	M430	V431	P432	V433	L434	S435	T436	M437	P438	A439	K440	L441	D442	T443	A448	P449	D450	L451	N452	C455	Y456	M457	G458	N459	D395	K393	V328	I327	D326	Y325	F389	N385	I384	V386	M387	A388	N323	G322	E322	A319	E318	D317	N316	Y316	L314	R313	D312	W311	V309	L308	Y307	G306	I371	F370	P369	P368	Q367	V366	E362	F361	R360	N295	A296	S297	G297	L298	P427	H428	I429	M430	V431	P432	V433	L434	S435	T436	M437	P438	A439	K440	L441	D442	T443	A448	P449	D450	L451	N452	C455	Y456	M457	G458	N459	D395	K393	V328	I327	D326	Y325	F389	N385	I384	V386	M387	A388	N323	G322	E322	A319	E318	D317	N316	Y316	L314	R313	D312	W311	V309	L308	Y307	G306	I371	F370	P369	P368	Q367	V366	E362	F361	R360	N295	A296	S297	G297	L298	P427	H428	I429	M430	V431	P432	V433	L434	S435	T436	M437	P438	A439	K440	L441	D442	T443	A448	P449	D450	L451	N452	C455	Y456	M457	G458	N459	D395	K393	V328	I327	D326	Y325	F389	N385	I384	V386	M387	A388	N323	G322	E322	A319	E318	D317	N316	Y316	L314	R313	D312	W311	V309	L308	Y307	G306	I371	F370	P369	P368	Q367	V366	E362	F361	R360	N295	A296	S297	G297	L298	P427	H428	I429	M430	V431	P432	V433	L434	S435	T436	M437	P438	A439	K440	L441	D442	T443	A448	P449	D450	L451	N452	C455	Y456	M457	G458	N459	D395	K393	V328
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	135000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, BEF

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	1.62	14/814 (1.7%)	1.76	11/1092 (1.0%)
2	B	1.58	9/669 (1.3%)	2.01	18/894 (2.0%)
2	F	1.67	13/693 (1.9%)	1.96	21/929 (2.3%)
3	C	1.83	22/805 (2.7%)	2.00	32/1088 (2.9%)
3	G	1.73	18/819 (2.2%)	1.90	22/1106 (2.0%)
4	D	1.62	18/756 (2.4%)	1.79	10/1015 (1.0%)
4	H	1.51	9/737 (1.2%)	1.83	19/993 (1.9%)
5	E	1.46	10/877 (1.1%)	1.78	18/1179 (1.5%)
6	I	0.80	7/3628 (0.2%)	1.31	56/5591 (1.0%)
7	J	0.80	7/3703 (0.2%)	1.27	42/5720 (0.7%)
8	N	1.27	1/607 (0.2%)	1.44	2/816 (0.2%)
8	O	1.34	4/607 (0.7%)	1.45	5/816 (0.6%)
9	W	1.43	96/7334 (1.3%)	1.54	66/9875 (0.7%)
All	All	1.32	228/22049 (1.0%)	1.55	322/31114 (1.0%)

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
1	A	0	7
2	B	0	5
2	F	0	7
3	C	0	7
3	G	0	4
4	D	0	3
4	H	0	4
5	E	0	6
6	I	0	1
7	J	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
8	N	0	1
8	O	0	4
9	W	0	17
All	All	0	68

All (228) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	102	ILE	C-O	12.04	1.36	1.24
4	D	87	THR	C-O	-11.80	1.10	1.23
3	C	92	GLU	C-O	11.53	1.35	1.23
1	A	121	PRO	C-O	-10.42	1.10	1.24
3	G	51	LEU	C-O	-9.98	1.12	1.24
3	G	112	GLN	C-O	-9.85	1.11	1.23
3	C	111	ILE	C-O	-9.40	1.13	1.24
1	A	111	ALA	C-O	-9.37	1.13	1.24
9	W	216	LYS	C-O	9.37	1.35	1.24
3	C	109	PRO	C-O	-9.36	1.13	1.23
3	C	55	LEU	C-O	-9.33	1.13	1.24
9	W	784	ASP	N-CA	9.32	1.57	1.46
9	W	767	PHE	C-O	-9.18	1.13	1.23
4	D	57	SER	C-O	9.11	1.34	1.24
2	F	85	ASP	N-CA	-9.06	1.35	1.46
1	A	127	ALA	C-O	-8.89	1.13	1.24
5	E	98	ALA	N-CA	-8.89	1.35	1.46
9	W	430	ILE	C-O	-8.87	1.14	1.24
9	W	550	LYS	N-CA	8.83	1.56	1.46
9	W	729	ASP	CG-OD2	8.83	1.42	1.25
9	W	797	ALA	N-CA	8.74	1.57	1.46
2	F	13	GLY	N-CA	8.70	1.57	1.45
2	B	35	ARG	C-O	8.66	1.34	1.24
6	I	27	DG	O3'-P	-8.62	1.48	1.61
9	W	730	TYR	N-CA	8.55	1.56	1.46
2	F	37	LEU	C-O	-8.34	1.13	1.24
7	J	-24	DT	P-OP2	8.31	1.65	1.48
1	A	106	ASP	C-O	8.23	1.33	1.24
3	G	40	ALA	C-O	-8.17	1.15	1.23
9	W	431	VAL	C-O	-8.09	1.15	1.24
1	A	118	THR	C-O	8.08	1.33	1.24
3	G	84	GLN	C-O	8.03	1.33	1.24
3	G	42	ARG	N-CA	7.92	1.55	1.46
4	D	95	VAL	C-O	7.79	1.33	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	36	ARG	C-O	7.75	1.33	1.24
1	A	127	ALA	N-CA	-7.67	1.36	1.46
4	D	64	ASN	C-O	-7.60	1.15	1.24
9	W	625	TYR	N-CA	-7.60	1.37	1.46
4	D	83	ARG	C-O	-7.59	1.13	1.23
9	W	338	PHE	N-CA	7.58	1.55	1.46
2	B	101	GLY	C-O	-7.57	1.14	1.23
9	W	342	GLU	C-O	-7.50	1.15	1.24
9	W	533	LYS	C-O	-7.50	1.14	1.24
4	D	65	ASP	CG-OD2	-7.49	1.11	1.25
4	H	53	SER	C-O	-7.49	1.15	1.24
7	J	-47	DC	O3'-P	7.49	1.72	1.61
5	E	102	ALA	N-CA	-7.47	1.37	1.46
9	W	494	TYR	N-CA	-7.46	1.36	1.46
2	B	45	ARG	N-CA	7.46	1.56	1.46
9	W	499	ARG	C-O	-7.40	1.15	1.24
9	W	436	THR	N-CA	7.39	1.55	1.46
2	F	41	GLY	C-O	-7.37	1.15	1.24
9	W	820	VAL	C-O	-7.32	1.16	1.23
9	W	770	SER	N-CA	7.29	1.54	1.45
9	W	401	ASP	N-CA	7.28	1.55	1.45
3	C	110	ASN	N-CA	-7.25	1.36	1.46
3	C	36	LYS	C-O	-7.21	1.14	1.24
4	D	76	ARG	C-O	-7.21	1.15	1.24
9	W	716	ILE	C-O	-7.21	1.16	1.24
6	I	-60	DG	P-OP2	7.20	1.62	1.48
2	B	78	ARG	C-O	7.18	1.32	1.23
6	I	-2	DC	C4'-O4'	7.16	1.59	1.45
2	F	43	VAL	C-O	-7.14	1.15	1.24
9	W	599	LYS	C-O	-7.10	1.16	1.24
9	W	488	LEU	C-O	-7.08	1.15	1.23
3	C	29	ARG	CD-NE	7.06	1.56	1.46
4	D	95	VAL	N-CA	-7.00	1.38	1.46
3	C	35	ARG	C-O	-6.99	1.14	1.24
3	C	53	ALA	C-O	6.96	1.32	1.24
3	G	66	ALA	N-CA	-6.95	1.37	1.46
9	W	489	LEU	C-O	-6.94	1.16	1.24
9	W	792	ASP	N-CA	6.94	1.55	1.46
3	C	23	LEU	C-O	-6.91	1.14	1.23
8	O	58	ASP	N-CA	6.86	1.54	1.46
3	G	41	GLU	C-O	-6.80	1.16	1.24
1	A	47	ALA	C-O	-6.80	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	40	ARG	NE-CZ	6.77	1.40	1.33
2	B	40	ARG	C-O	-6.77	1.16	1.24
9	W	361	PHE	N-CA	6.77	1.53	1.45
9	W	767	PHE	N-CA	-6.74	1.37	1.46
9	W	632	LYS	N-CA	6.71	1.54	1.46
9	W	753	SER	C-O	6.71	1.32	1.24
9	W	652	MET	N-CA	6.69	1.54	1.45
3	G	88	ARG	N-CA	6.64	1.54	1.46
8	O	8	LEU	N-CA	6.64	1.54	1.46
4	D	78	ALA	C-O	-6.60	1.16	1.24
4	D	45	VAL	C-O	-6.58	1.16	1.24
9	W	327	ILE	C-O	-6.58	1.16	1.24
9	W	357	GLN	C-O	6.55	1.31	1.23
3	G	116	LEU	N-CA	-6.49	1.36	1.45
3	G	105	GLY	C-O	6.46	1.31	1.23
4	D	73	GLU	CD-OE2	6.45	1.37	1.25
1	A	108	ASN	C-O	6.43	1.31	1.24
9	W	452	ASN	N-CA	6.43	1.54	1.45
3	G	23	LEU	C-O	-6.39	1.16	1.23
3	G	86	ALA	C-O	-6.37	1.16	1.24
3	C	58	LEU	C-O	6.37	1.31	1.24
9	W	490	THR	N-CA	-6.31	1.38	1.46
9	W	651	ILE	N-CA	6.29	1.54	1.46
9	W	1254[A]	ARG	C-O	6.29	1.31	1.24
9	W	1254[B]	ARG	C-O	6.29	1.31	1.24
4	H	114	ALA	N-CA	-6.27	1.38	1.46
9	W	669	GLU	N-CA	6.27	1.54	1.46
3	G	49	VAL	C-O	-6.25	1.17	1.24
9	W	433	PRO	C-O	6.25	1.30	1.23
9	W	424	GLN	C-O	-6.21	1.16	1.24
9	W	725	ASP	N-CA	6.16	1.53	1.46
9	W	756	HIS	C-O	-6.16	1.16	1.24
2	B	57	VAL	N-CA	-6.14	1.39	1.46
9	W	724	LEU	N-CA	-6.12	1.38	1.46
3	G	27	VAL	N-CA	-6.12	1.39	1.46
1	A	94	GLU	C-O	6.12	1.31	1.24
3	C	83	LEU	C-O	-6.10	1.17	1.24
9	W	669	GLU	CD-OE2	-6.09	1.13	1.25
4	D	46	HIS	CE1-NE2	6.07	1.38	1.32
9	W	790	ASP	C-O	-6.07	1.16	1.23
3	G	37	GLY	C-O	-6.06	1.20	1.24
9	W	494	TYR	C-O	-6.06	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	67	PHE	C-O	-6.04	1.17	1.24
9	W	594	ILE	N-CA	-5.99	1.38	1.46
9	W	817	TYR	N-CA	-5.96	1.38	1.46
5	E	97	GLU	N-CA	-5.95	1.39	1.46
6	I	19	DC	O3'-P	-5.95	1.52	1.61
1	A	126	LEU	C-O	-5.94	1.17	1.24
5	E	112	ILE	C-O	5.93	1.30	1.24
5	E	97	GLU	C-O	-5.92	1.17	1.24
9	W	731	LEU	C-O	5.86	1.31	1.24
9	W	826	GLU	CD-OE2	-5.86	1.14	1.25
4	H	70	ILE	C-O	-5.84	1.17	1.24
4	H	40	LYS	C-O	5.83	1.30	1.24
3	G	56	GLU	N-CA	-5.82	1.39	1.46
4	H	56	MET	CG-SD	-5.82	1.66	1.80
3	C	49	VAL	C-O	5.80	1.30	1.24
2	F	29	ILE	C-O	5.79	1.30	1.24
4	D	117	LYS	C-O	5.78	1.30	1.24
9	W	591	GLN	N-CA	5.78	1.53	1.46
2	F	25	ASN	N-CA	-5.75	1.38	1.46
9	W	493	GLU	CD-OE2	5.74	1.36	1.25
9	W	596	ARG	N-CA	5.74	1.53	1.46
9	W	464	ASP	C-O	5.72	1.30	1.24
9	W	394	GLY	N-CA	5.69	1.53	1.45
9	W	532	PHE	N-CA	5.68	1.53	1.46
1	A	123	ASP	N-CA	-5.68	1.39	1.46
4	D	82	LYS	N-CA	5.67	1.53	1.46
9	W	257	ARG	N-CA	5.66	1.53	1.46
9	W	729	ASP	C-O	-5.66	1.17	1.24
7	J	-39	DT	P-OP2	5.65	1.59	1.48
9	W	720	MET	N-CA	-5.65	1.39	1.46
1	A	49	ARG	NE-CZ	5.64	1.39	1.33
9	W	610	THR	N-CA	5.64	1.53	1.46
9	W	801	ALA	C-O	-5.63	1.17	1.24
9	W	730	TYR	C-O	-5.60	1.17	1.24
2	B	51	TYR	C-O	-5.60	1.17	1.24
2	F	70	VAL	N-CA	-5.59	1.39	1.46
9	W	398	ILE	C-O	-5.58	1.18	1.24
3	C	46	GLY	C-O	5.54	1.31	1.23
4	D	65	ASP	C-O	-5.54	1.17	1.24
9	W	562	GLY	N-CA	5.53	1.53	1.45
7	J	17	DA	P-OP2	5.52	1.59	1.48
9	W	743	GLY	C-O	-5.49	1.16	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	428	HIS	CE1-NE2	5.48	1.38	1.32
3	C	45	ALA	C-O	5.47	1.31	1.24
9	W	1249	ALA	C-O	-5.47	1.17	1.24
9	W	516	HIS	N-CA	-5.47	1.38	1.46
3	C	72	ASP	C-O	5.43	1.30	1.24
5	E	86	SER	C-O	5.42	1.30	1.24
9	W	339	GLN	C-O	5.42	1.30	1.24
3	C	31	HIS	CE1-NE2	5.42	1.38	1.32
6	I	22	DC	O3'-P	5.41	1.69	1.61
7	J	39	DA	P-OP2	5.38	1.59	1.48
9	W	411	THR	N-CA	5.38	1.52	1.46
4	H	116	THR	C-O	5.37	1.30	1.24
1	A	97	GLU	N-CA	-5.35	1.40	1.46
3	C	100	VAL	C-O	-5.33	1.18	1.24
5	E	37	ALA	N-CA	5.33	1.52	1.45
6	I	38	DT	P-OP2	5.32	1.59	1.48
3	G	103	ALA	C-O	-5.30	1.17	1.24
4	D	104	ALA	C-O	-5.29	1.18	1.24
9	W	384	ILE	N-CA	-5.29	1.40	1.46
5	E	104	PHE	N-CA	-5.29	1.40	1.46
9	W	719	GLN	C-O	-5.28	1.17	1.24
9	W	418	LEU	N-CA	-5.28	1.39	1.46
9	W	652	MET	C-O	-5.27	1.17	1.24
9	W	1053	ASP	C-O	5.26	1.30	1.24
9	W	554	ALA	N-CA	5.24	1.52	1.46
9	W	463	ARG	N-CA	-5.22	1.39	1.46
2	B	79	LYS	CA-C	-5.22	1.47	1.52
9	W	403	MET	N-CA	5.22	1.53	1.46
2	F	98	TYR	N-CA	-5.21	1.39	1.45
5	E	67	PHE	C-O	-5.20	1.18	1.24
9	W	337	HIS	N-CA	-5.20	1.40	1.46
9	W	312	ARG	N-CA	5.20	1.52	1.46
6	I	-46	DC	O3'-P	-5.20	1.53	1.61
9	W	729	ASP	N-CA	-5.20	1.40	1.46
2	F	78	ARG	C-O	5.20	1.30	1.24
9	W	419	ILE	N-CA	5.20	1.51	1.45
9	W	726	ILE	N-CA	-5.19	1.40	1.46
2	F	35	ARG	C-O	5.19	1.30	1.24
4	H	39	TYR	C-O	5.18	1.30	1.24
9	W	382	THR	C-O	5.18	1.30	1.24
9	W	787	VAL	C-O	-5.18	1.18	1.24
8	N	26	VAL	C-O	5.18	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	38	DG	O3'-P	-5.17	1.53	1.61
9	W	438	PRO	C-O	5.16	1.30	1.24
9	W	499	ARG	N-CA	5.16	1.52	1.46
3	C	112	GLN	C-O	-5.15	1.17	1.23
3	C	107	VAL	C-O	-5.15	1.16	1.23
4	H	105	LYS	C-O	-5.14	1.18	1.24
9	W	1248	GLY	C-O	-5.14	1.19	1.23
9	W	1266	GLY	N-CA	5.13	1.52	1.45
4	D	33	SER	C-O	-5.12	1.17	1.23
9	W	614	LEU	C-O	-5.12	1.18	1.23
9	W	777	GLY	C-O	-5.10	1.16	1.23
2	F	27	GLN	N-CA	5.09	1.52	1.46
9	W	1265	GLY	N-CA	5.08	1.52	1.45
8	O	57	SER	N-CA	5.08	1.52	1.46
1	A	53	ARG	C-O	5.07	1.30	1.24
9	W	314	LEU	N-CA	-5.06	1.39	1.46
3	G	27	VAL	C-O	-5.06	1.18	1.24
5	E	118	THR	C-O	5.04	1.29	1.24
9	W	658	ALA	CA-CB	-5.04	1.46	1.53
3	C	83	LEU	N-CA	-5.04	1.40	1.46
8	O	70	VAL	C-O	5.04	1.29	1.23
9	W	547	ASN	N-CA	5.04	1.52	1.46
9	W	593	PHE	C-O	-5.04	1.16	1.23
4	D	90	GLU	CD-OE2	-5.02	1.15	1.25
9	W	407	LYS	N-CA	-5.02	1.40	1.46
7	J	-16	DT	O3'-P	-5.00	1.53	1.61

All (322) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	39	TYR	N-CA-C	10.11	121.99	110.97
8	O	64	GLU	CB-CG-CD	9.58	128.88	112.60
2	B	40	ARG	NE-CZ-NH1	-9.04	112.46	121.50
3	G	17	ARG	CA-C-O	-8.82	111.56	120.82
7	J	-42	DG	P-O5'-C5'	-8.80	106.79	120.00
6	I	62	DT	C2'-C3'-O3'	-8.69	98.46	111.50
3	G	104	GLN	CA-C-O	-8.67	111.89	122.03
5	E	119	ILE	N-CA-CB	8.58	122.02	110.26
2	B	75	HIS	CA-CB-CG	-8.56	105.24	113.80
7	J	9	DT	C2'-C3'-O3'	-8.55	98.68	111.50
8	O	39	ASP	CA-CB-CG	8.52	121.12	112.60
3	G	109	PRO	N-CA-C	-8.39	98.12	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	-23	DC	C2'-C3'-O3'	8.35	124.03	111.50
6	I	7	DC	C2'-C3'-O3'	-8.31	99.04	111.50
5	E	127	ALA	O-C-N	8.18	130.83	122.08
4	D	81	ASN	CB-CA-C	8.17	124.91	110.37
7	J	-26	DC	C2'-C3'-O3'	-8.13	99.30	111.50
7	J	-13	DA	N9-C1'-C2'	8.06	125.59	113.50
2	B	27	GLN	CB-CG-CD	-8.06	98.90	112.60
6	I	16	DA	C2'-C3'-O3'	-8.00	99.50	111.50
6	I	22	DC	C4'-C3'-O3'	7.93	121.90	110.00
3	C	42	ARG	CB-CA-C	-7.90	100.64	113.37
6	I	11	DG	C4'-C3'-O3'	7.90	121.86	110.00
7	J	53	DC	C2'-C3'-O3'	-7.81	99.78	111.50
9	W	495	ILE	N-CA-CB	7.79	118.80	110.62
7	J	-53	DA	C2'-C3'-O3'	7.78	123.17	111.50
6	I	-29	DC	C2'-C3'-O3'	7.76	123.14	111.50
7	J	16	DA	C2'-C3'-O3'	-7.71	99.93	111.50
9	W	442	ASP	CA-CB-CG	7.68	120.28	112.60
7	J	-14	DA	C2'-C3'-O3'	7.68	123.01	111.50
6	I	54	DG	C2'-C3'-O3'	7.66	122.98	111.50
8	O	64	GLU	CB-CA-C	7.65	124.03	111.26
6	I	14	DT	C2'-C3'-O3'	7.64	122.96	111.50
6	I	-24	DG	C4'-C3'-O3'	7.57	121.35	110.00
3	G	47	ALA	CA-C-O	7.54	126.25	119.08
2	B	63	GLU	CB-CG-CD	7.52	125.38	112.60
3	G	37	GLY	CA-C-O	7.52	125.88	119.04
3	G	92	GLU	CB-CG-CD	7.47	125.29	112.60
2	B	98	TYR	CA-C-O	-7.39	112.19	120.32
3	C	62	ILE	N-CA-C	7.39	117.99	110.82
1	A	49	ARG	CB-CG-CD	7.32	128.13	111.30
3	G	17	ARG	O-C-N	7.28	129.57	122.07
6	I	-44	DA	C2'-C3'-O3'	-7.28	100.58	111.50
7	J	39	DA	O5'-P-OP2	7.28	129.84	108.00
5	E	90	MET	N-CA-C	-7.25	102.56	111.33
6	I	43	DT	C2'-C3'-O3'	7.21	122.32	111.50
7	J	21	DG	C2'-C3'-O3'	7.18	122.27	111.50
6	I	14	DT	C4'-C3'-O3'	-7.12	99.31	110.00
7	J	23	DG	C2'-C3'-O3'	7.07	122.11	111.50
4	D	80	TYR	CA-C-N	-7.06	110.41	122.56
4	D	80	TYR	C-N-CA	-7.06	110.41	122.56
6	I	-39	DT	N1-C1'-C2'	7.02	124.03	113.50
1	A	53	ARG	CA-C-O	7.01	128.20	120.63
7	J	-38	DA	C2'-C3'-O3'	6.98	121.97	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	-58	DC	C2'-C3'-O3'	6.95	121.92	111.50
2	B	100	PHE	CA-C-N	-6.92	114.89	121.46
2	B	100	PHE	C-N-CA	-6.92	114.89	121.46
4	H	39	TYR	CA-CB-CG	-6.91	101.45	113.90
3	G	29	ARG	CA-C-O	6.90	127.74	120.42
6	I	61	DA	C4'-C3'-O3'	6.89	120.33	110.00
4	D	46	HIS	CA-CB-CG	6.87	120.67	113.80
3	G	45	ALA	CA-C-N	-6.87	111.86	122.30
3	G	45	ALA	C-N-CA	-6.87	111.86	122.30
9	W	432	VAL	N-CA-CB	-6.85	105.85	111.67
7	J	-65	DT	C4'-C3'-O3'	6.84	120.26	110.00
2	B	53	GLU	CB-CG-CD	6.82	124.19	112.60
5	E	107	THR	N-CA-C	-6.81	102.94	111.11
2	B	42	GLY	CA-C-O	6.80	126.62	118.86
7	J	-64	DA	C2'-C3'-O3'	-6.79	101.32	111.50
2	F	40	ARG	CB-CG-CD	-6.78	95.70	111.30
6	I	-2	DC	C5'-C4'-O4'	-6.77	99.24	109.40
9	W	516	HIS	N-CA-C	-6.72	104.29	113.30
6	I	-47	DT	N1-C1'-C2'	6.63	123.44	113.50
9	W	608	SER	N-CA-C	6.62	119.11	110.43
1	A	115	LYS	CB-CA-C	-6.62	100.20	111.26
6	I	0	DC	O5'-P-OP2	-6.57	88.29	108.00
5	E	52	ARG	NE-CZ-NH1	-6.57	114.93	121.50
8	N	39	ASP	CA-CB-CG	6.54	119.14	112.60
6	I	-62	DC	C4'-C3'-O3'	6.54	119.81	110.00
6	I	-30	DG	C2'-C3'-O3'	6.54	121.31	111.50
2	F	36	ARG	N-CA-C	-6.52	103.44	111.33
2	F	100	PHE	CA-C-O	-6.51	113.33	120.36
2	F	100	PHE	O-C-N	6.51	131.04	123.30
6	I	64	DT	C4'-C3'-O3'	6.50	119.75	110.00
6	I	37	DC	C4'-C3'-O3'	6.49	119.74	110.00
3	C	18	SER	N-CA-C	-6.48	104.14	111.07
6	I	23	DA	C4'-C3'-O3'	6.45	119.67	110.00
6	I	-46	DC	C2'-C3'-O3'	-6.45	101.83	111.50
9	W	729	ASP	N-CA-CB	-6.44	100.63	110.16
6	I	-11	DG	C2'-C3'-O3'	-6.43	101.86	111.50
6	I	-68	DG	C4'-C3'-O3'	6.42	119.62	110.00
6	I	-19	DG	C2'-C3'-O3'	-6.41	101.88	111.50
7	J	44	DT	C4'-C3'-O3'	6.41	119.61	110.00
6	I	71	DA	C4'-C3'-O3'	-6.40	100.39	110.00
2	F	36	ARG	CA-C-O	6.40	127.54	120.63
6	I	-52	DG	C4'-C3'-O3'	6.39	119.58	110.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	-34	DG	C2'-C3'-O3'	-6.34	102.00	111.50
9	W	177	HIS	CA-C-N	6.32	127.02	121.58
9	W	177	HIS	C-N-CA	6.32	127.02	121.58
9	W	756	HIS	CA-CB-CG	6.32	120.12	113.80
2	F	52	GLU	CA-C-O	-6.31	114.15	120.90
9	W	271	ASP	CA-CB-CG	6.31	118.91	112.60
9	W	432	VAL	CA-C-N	6.31	126.26	119.76
9	W	432	VAL	C-N-CA	6.31	126.26	119.76
9	W	385	ASN	CA-CB-CG	6.30	118.90	112.60
7	J	-6	DG	N9-C1'-C2'	6.30	122.94	113.50
3	C	91	GLU	N-CA-C	6.29	118.13	111.28
6	I	63	DA	C4'-C3'-O3'	6.28	119.42	110.00
7	J	-66	DG	C4'-C3'-O3'	6.27	119.41	110.00
9	W	575	GLN	CA-C-N	6.25	128.98	120.54
9	W	575	GLN	C-N-CA	6.25	128.98	120.54
6	I	62	DT	C4'-C3'-O3'	6.24	119.37	110.00
4	H	40	LYS	N-CA-C	6.24	118.63	111.02
6	I	-7	DG	N9-C1'-C2'	6.22	122.84	113.50
3	C	42	ARG	N-CA-C	-6.22	99.22	109.80
9	W	695	GLY	CA-C-O	6.22	127.25	120.66
3	C	48	PRO	CA-C-O	6.22	129.56	119.86
6	I	-4	DC	C4'-C3'-O3'	6.20	119.30	110.00
4	H	65	ASP	CA-C-O	6.20	127.32	120.63
3	C	97	LEU	CA-C-N	6.20	126.69	119.94
3	C	97	LEU	C-N-CA	6.20	126.69	119.94
9	W	279	ASP	CA-CB-CG	6.19	118.79	112.60
9	W	730	TYR	CB-CA-C	-6.18	100.41	110.79
8	O	71	LEU	N-CA-C	-6.16	97.68	110.80
5	E	120	MET	CA-C-O	6.16	127.00	120.66
3	G	26	PRO	CB-CA-C	-6.15	106.70	111.87
9	W	420	PHE	N-CA-C	-6.14	104.43	112.41
3	G	109	PRO	CB-CA-C	6.14	118.89	111.46
2	B	36	ARG	CA-C-O	-6.12	114.06	120.55
9	W	292	ASP	CA-CB-CG	6.11	118.71	112.60
2	F	40	ARG	NE-CZ-NH2	6.10	124.69	119.20
2	F	52	GLU	CB-CG-CD	6.08	122.94	112.60
4	D	90	GLU	CB-CA-C	6.04	120.37	110.88
5	E	133	GLU	N-CA-C	-6.00	103.50	111.24
3	C	63	LEU	CA-C-O	5.99	127.31	120.90
9	W	1202	PHE	CA-CB-CG	5.99	119.79	113.80
7	J	-19	DG	C2'-C3'-O3'	-5.99	102.52	111.50
6	I	8	DC	C4'-C3'-O3'	5.97	118.96	110.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	-17	DT	C2'-C3'-O3'	5.97	120.45	111.50
6	I	-50	DC	C4'-C3'-O3'	5.96	118.95	110.00
9	W	390	LEU	N-CA-C	-5.96	105.66	113.17
6	I	-43	DT	C4'-C3'-O3'	5.96	118.94	110.00
9	W	612	ARG	CG-CD-NE	5.93	125.05	112.00
7	J	-47	DC	N1-C1'-C2'	5.92	122.38	113.50
6	I	-3	DG	O5'-P-OP1	-5.91	91.28	109.00
9	W	599	LYS	CA-C-O	-5.90	114.81	121.00
5	E	125	GLN	CA-C-O	-5.90	114.63	120.82
8	N	40	GLN	O-C-N	5.89	128.36	122.12
7	J	59	DC	C4'-C3'-O3'	5.88	118.82	110.00
2	F	70	VAL	N-CA-C	-5.87	104.63	110.62
9	W	433	PRO	N-CA-C	5.87	120.30	111.14
2	F	55	ARG	N-CA-C	-5.87	104.96	111.36
3	C	42	ARG	CA-C-O	-5.84	114.58	120.77
9	W	464	ASP	N-CA-C	5.84	117.72	111.36
9	W	806	HIS	CB-CA-C	-5.84	101.87	111.68
2	F	38	ALA	CA-C-O	5.83	126.61	120.42
6	I	-13	DA	C2'-C3'-O3'	5.82	120.23	111.50
6	I	44	DC	P-O5'-C5'	-5.81	111.28	120.00
2	B	85	ASP	CA-C-O	-5.81	114.39	120.55
2	B	58	LEU	N-CA-C	-5.79	104.33	111.33
9	W	418	LEU	N-CA-C	-5.79	105.98	113.16
9	W	1188	LYS	N-CA-C	5.78	118.80	111.69
6	I	7	DC	C4'-C3'-O3'	5.77	118.66	110.00
2	F	31	LYS	CB-CA-C	-5.76	102.04	112.76
4	H	76	ARG	NE-CZ-NH1	-5.75	115.75	121.50
9	W	770	SER	O-C-N	-5.74	116.18	122.84
3	G	46	GLY	O-C-N	-5.74	116.52	121.97
3	C	39	TYR	CB-CA-C	-5.74	102.12	110.96
7	J	49	DC	C4'-C3'-O3'	5.71	118.57	110.00
4	H	99	LEU	CA-C-N	5.71	125.73	119.90
4	H	99	LEU	C-N-CA	5.71	125.73	119.90
7	J	9	DT	N1-C1'-C2'	5.71	122.06	113.50
3	C	50	TYR	CB-CG-CD1	-5.71	112.24	120.80
4	H	81	ASN	N-CA-CB	5.70	119.22	110.79
7	J	19	DC	C4'-C3'-O3'	5.70	118.55	110.00
6	I	0	DC	P-O5'-C5'	5.70	128.54	120.00
7	J	13	DT	P-O5'-C5'	-5.69	111.47	120.00
4	H	105	LYS	CB-CA-C	5.68	120.51	110.85
3	C	102	ILE	CA-C-O	5.67	126.61	120.43
9	W	606	LEU	CA-C-N	5.66	125.61	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	W	606	LEU	C-N-CA	5.66	125.61	119.78
5	E	119	ILE	CA-CB-CG1	5.65	120.01	110.40
9	W	628	ASN	CA-CB-CG	-5.65	106.95	112.60
2	F	49	LEU	CA-C-O	5.64	126.75	120.82
5	E	119	ILE	N-CA-C	-5.64	101.54	109.21
9	W	1265	GLY	CA-C-N	5.62	126.19	120.00
9	W	1265	GLY	C-N-CA	5.62	126.19	120.00
9	W	1099	PRO	N-CA-C	5.62	120.15	111.21
3	C	59	THR	CA-C-O	5.61	126.49	120.55
9	W	792	ASP	CA-C-N	5.60	130.91	122.68
9	W	792	ASP	C-N-CA	5.60	130.91	122.68
2	F	55	ARG	CB-CG-CD	5.60	124.17	111.30
3	C	103	ALA	CA-C-O	-5.60	115.62	120.88
3	G	41	GLU	CA-C-O	-5.59	114.63	120.55
9	W	1137	GLU	N-CA-C	5.58	117.44	111.36
2	B	71	THR	OG1-CB-CG2	-5.58	98.15	109.30
7	J	22	DT	N1-C1'-C2'	5.57	121.86	113.50
1	A	102	ALA	N-CA-C	5.57	118.07	111.33
6	I	71	DA	C2'-C3'-O3'	5.57	119.85	111.50
6	I	8	DC	O5'-P-OP1	-5.56	92.31	109.00
2	B	40	ARG	NH1-CZ-NH2	5.55	126.52	119.30
9	W	337	HIS	CA-C-N	5.55	127.98	120.38
9	W	337	HIS	C-N-CA	5.55	127.98	120.38
9	W	771	THR	CA-CB-OG1	-5.55	101.28	109.60
1	A	109	LEU	CA-C-O	5.55	126.65	120.82
6	I	27	DG	C2'-C3'-O3'	-5.55	103.18	111.50
3	C	102	ILE	N-CA-C	5.54	116.25	108.17
7	J	27	DG	N9-C1'-C2'	5.54	121.80	113.50
3	G	26	PRO	N-CA-CB	5.53	106.02	102.92
3	G	45	ALA	CA-C-O	5.52	126.46	119.78
9	W	287	PRO	CB-CA-C	5.51	118.51	110.63
5	E	126	LEU	O-C-N	5.50	127.81	122.09
9	W	666	ASP	N-CA-CB	-5.50	101.67	110.19
7	J	-47	DC	C5'-C4'-O4'	-5.48	101.17	109.40
2	F	67	ARG	O-C-N	5.48	127.79	122.09
4	H	39	TYR	N-CA-C	5.48	116.93	111.07
1	A	62	ILE	CB-CA-C	-5.47	104.08	111.63
2	B	95	ARG	CB-CG-CD	5.47	123.88	111.30
7	J	-24	DT	C4'-C3'-O3'	5.47	118.20	110.00
7	J	-7	DG	N9-C1'-C2'	5.45	121.68	113.50
2	F	36	ARG	CG-CD-NE	-5.45	100.02	112.00
6	I	65	DA	C2'-C3'-O3'	5.44	119.66	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	97	GLU	N-CA-C	-5.44	105.25	111.07
4	D	99	LEU	CD1-CG-CD2	5.43	122.75	110.80
9	W	1031	LEU	CA-C-O	-5.43	115.09	120.90
9	W	595	LEU	CA-C-O	-5.42	113.58	120.20
6	I	4	DC	C2'-C3'-O3'	5.41	119.62	111.50
3	C	32	ARG	CB-CA-C	-5.41	101.66	110.85
9	W	432	VAL	CA-CB-CG1	5.41	119.59	110.40
9	W	587	HIS	CA-CB-CG	5.39	119.19	113.80
4	H	65	ASP	CA-CB-CG	5.38	117.98	112.60
7	J	14	DT	C2'-C3'-O3'	-5.38	103.43	111.50
2	F	35	ARG	N-CA-C	-5.38	105.42	111.28
4	H	76	ARG	NE-CZ-NH2	5.37	124.03	119.20
4	H	115	VAL	N-CA-C	-5.36	105.15	110.62
4	H	38	VAL	CA-C-O	5.36	126.53	120.95
9	W	771	THR	CA-C-O	-5.36	115.18	120.80
4	H	119	THR	CA-CB-OG1	-5.35	101.57	109.60
6	I	44	DC	C2'-C3'-O3'	5.35	119.53	111.50
6	I	-17	DT	N1-C1'-C2'	5.35	121.52	113.50
4	H	74	ALA	CA-C-O	5.34	126.43	120.82
3	C	102	ILE	CA-C-N	5.34	131.21	121.97
3	C	102	ILE	C-N-CA	5.34	131.21	121.97
6	I	-16	DT	O5'-P-OP2	-5.34	91.98	108.00
5	E	53	ARG	CA-C-O	5.33	126.07	120.42
7	J	-5	DG	C2'-C3'-O3'	-5.32	103.52	111.50
9	W	1059	ALA	N-CA-C	5.32	116.76	111.07
1	A	83	ARG	NE-CZ-NH1	-5.32	116.18	121.50
7	J	-42	DG	O5'-C5'-C4'	5.31	118.76	110.80
9	W	493	GLU	CB-CG-CD	-5.31	103.57	112.60
4	H	40	LYS	CB-CA-C	-5.30	102.49	110.92
3	C	101	THR	CA-C-N	-5.29	115.07	122.75
3	C	101	THR	C-N-CA	-5.29	115.07	122.75
5	E	79	LYS	CA-C-O	5.29	126.89	121.23
7	J	43	DA	C2'-C3'-O3'	5.29	119.43	111.50
4	H	109	SER	CA-C-O	-5.29	115.27	120.82
3	C	46	GLY	CA-C-N	5.28	126.33	119.78
3	C	46	GLY	C-N-CA	5.28	126.33	119.78
2	F	55	ARG	CG-CD-NE	-5.28	100.38	112.00
5	E	50	GLU	N-CA-C	-5.27	105.53	111.28
7	J	52	DC	C2'-C3'-O3'	-5.26	103.61	111.50
8	O	37	PRO	CB-CA-C	5.26	116.11	111.17
3	G	23	LEU	CA-C-O	5.26	127.01	121.33
7	J	72	DA	C4'-C3'-O3'	5.25	117.88	110.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	101	GLY	CA-C-O	-5.25	116.75	121.47
9	W	1206	THR	N-CA-C	5.25	117.00	111.28
2	B	93	GLN	OE1-CD-NE2	5.25	127.84	122.60
3	C	50	TYR	CB-CG-CD2	5.25	128.67	120.80
9	W	189	THR	N-CA-C	5.24	117.44	108.90
6	I	18	DC	N1-C1'-C2'	5.24	121.36	113.50
3	G	58	LEU	CA-C-O	5.24	126.10	120.55
7	J	50	DG	C4'-C3'-O3'	5.22	117.84	110.00
7	J	38	DG	O5'-P-OP2	5.21	123.64	108.00
9	W	492	TYR	CA-C-O	-5.21	114.90	120.42
9	W	596	ARG	N-CA-CB	5.20	118.76	110.65
7	J	-36	DG	N9-C1'-C2'	5.19	121.28	113.50
5	E	108	ASN	CB-CA-C	-5.18	102.51	110.81
6	I	21	DC	P-O5'-C5'	5.18	127.77	120.00
9	W	482	THR	CA-CB-OG1	-5.18	101.83	109.60
3	G	105	GLY	CA-C-O	5.17	126.38	121.05
9	W	273	GLU	O-C-N	5.16	127.59	122.12
9	W	1255	ARG	N-CA-C	5.16	116.59	111.07
3	C	62	ILE	CA-C-N	5.14	127.48	120.54
3	C	62	ILE	C-N-CA	5.14	127.48	120.54
9	W	724	LEU	CA-C-O	-5.14	114.97	120.42
4	D	50	GLY	CA-C-O	5.14	127.68	121.77
2	F	35	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	A	58	THR	CA-C-N	5.12	128.12	120.90
1	A	58	THR	C-N-CA	5.12	128.12	120.90
9	W	1040	LEU	N-CA-C	5.12	118.44	109.48
3	G	102	ILE	N-CA-C	5.12	115.27	108.11
9	W	367	GLN	CA-C-O	5.12	123.40	119.46
3	C	43	VAL	N-CA-CB	-5.11	103.07	111.45
3	C	72	ASP	CA-CB-CG	5.10	117.70	112.60
6	I	-58	DG	N9-C1'-C2'	5.10	121.15	113.50
9	W	1144	ASN	N-CA-C	5.10	116.53	111.07
1	A	53	ARG	N-CA-C	-5.10	105.16	111.33
7	J	45	DT	N1-C1'-C2'	5.09	121.14	113.50
1	A	49	ARG	NE-CZ-NH2	5.09	123.78	119.20
2	F	93	GLN	CA-C-O	5.09	125.31	119.35
4	D	64	ASN	N-CA-C	-5.08	105.82	111.36
4	H	42	LEU	CB-CA-C	-5.08	102.84	110.92
7	J	-68	DA	C2'-C3'-O3'	-5.08	103.88	111.50
3	G	59	THR	CA-C-O	5.06	126.32	120.90
5	E	126	LEU	CB-CA-C	-5.06	102.71	110.81
2	B	75	HIS	CA-C-O	5.06	125.92	120.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	58	LEU	CD1-CG-CD2	-5.06	99.67	110.80
4	D	50	GLY	O-C-N	-5.04	118.90	123.29
9	W	790	ASP	CA-C-O	-5.04	115.21	121.06
4	H	48	ASP	CA-C-O	-5.04	116.43	122.13
6	I	-27	DC	N1-C1'-C2'	5.04	121.06	113.50
6	I	-16	DT	P-O5'-C5'	5.04	127.55	120.00
3	C	113	SER	O-C-N	5.03	127.46	122.03
9	W	829	VAL	N-CA-C	-5.03	105.49	110.62
3	C	80	PRO	CA-C-N	5.03	127.01	120.28
3	C	80	PRO	C-N-CA	5.03	127.01	120.28
6	I	-27	DC	C4'-C3'-O3'	-5.02	102.46	110.00
4	D	113	LYS	N-CA-C	-5.02	105.72	111.14
5	E	105	GLU	CB-CG-CD	5.01	121.12	112.60
9	W	205	ASN	CA-CB-CG	5.01	117.61	112.60
9	W	432	VAL	O-C-N	-5.01	117.11	121.57
3	G	116	LEU	O-C-N	-5.01	116.02	121.53

There are no chirality outliers.

All (68) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ARG	Sidechain
1	A	40	ARG	Sidechain
1	A	42	ARG	Sidechain
1	A	49	ARG	Sidechain
1	A	63	ARG	Sidechain
1	A	69	ARG	Sidechain
1	A	83	ARG	Sidechain
2	B	35	ARG	Sidechain
2	B	39	ARG	Sidechain
2	B	40	ARG	Sidechain
2	B	45	ARG	Sidechain
2	B	72	TYR	Sidechain
3	C	101	THR	Peptide
3	C	29	ARG	Sidechain
3	C	35	ARG	Sidechain
3	C	42	ARG	Sidechain
3	C	71	ARG	Sidechain
3	C	77	ARG	Sidechain
3	C	81	ARG	Sidechain
4	D	30	ARG	Sidechain
4	D	81	ASN	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
4	D	83	ARG	Peptide
5	E	116	ARG	Sidechain
5	E	40	ARG	Sidechain
5	E	63	ARG	Sidechain
5	E	69	ARG	Sidechain
5	E	72	ARG	Sidechain
5	E	97	GLU	Mainchain
2	F	100	PHE	Peptide
2	F	39	ARG	Sidechain
2	F	40	ARG	Sidechain
2	F	45	ARG	Sidechain
2	F	67	ARG	Sidechain
2	F	92	ARG	Sidechain
2	F	95	ARG	Sidechain
3	G	71	ARG	Sidechain
3	G	77	ARG	Sidechain
3	G	88	ARG	Sidechain
3	G	99	ARG	Sidechain
4	H	34	TYR	Sidechain
4	H	76	ARG	Sidechain
4	H	89	ARG	Sidechain
4	H	96	ARG	Sidechain
6	I	-4	DC	Sidechain
7	J	-19	DG	Sidechain
7	J	46	DG	Sidechain
8	N	54	ARG	Sidechain
8	O	44	ILE	Peptide
8	O	54	ARG	Sidechain
8	O	72	ARG	Sidechain
8	O	74	ARG	Sidechain
9	W	1085	ARG	Sidechain
9	W	1112	ARG	Sidechain
9	W	1264	ARG	Sidechain
9	W	189	THR	Peptide
9	W	237	ARG	Sidechain
9	W	241	ARG	Sidechain
9	W	274	ARG	Sidechain
9	W	276	ARG	Sidechain
9	W	312	ARG	Sidechain
9	W	313	ARG	Sidechain
9	W	377	ARG	Sidechain
9	W	517	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
9	W	563	ARG	Sidechain
9	W	706	ARG	Sidechain
9	W	720	MET	Mainchain
9	W	722	ARG	Sidechain
9	W	797	ALA	Mainchain

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	A	802	0	841	152	0
2	B	662	0	709	148	0
2	F	686	0	693	148	0
3	C	795	0	846	161	0
3	G	809	0	864	164	0
4	D	745	0	773	115	0
4	H	726	0	747	120	0
5	E	866	0	903	147	0
6	I	3238	0	1783	523	0
7	J	3298	0	1798	555	0
8	N	601	0	629	64	0
8	O	601	0	629	18	0
9	W	7189	0	7208	930	0
10	W	4	0	0	0	0
11	W	27	0	12	12	0
All	All	21049	0	18435	2671	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 69.

All (2671) 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)
5:E:63:ARG:NH1	6:I:17:DA:C5'	1.73	1.51
5:E:63:ARG:NH1	6:I:17:DA:H5''	1.26	1.47
5:E:61:LEU:CD1	2:F:37:LEU:HA	1.50	1.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:345:LYS:HB3	9:W:1036:ALA:CB	1.48	1.40
8:O:54:ARG:HD2	8:O:59:TYR:CE2	1.59	1.38
9:W:481:LYS:HG3	9:W:483:MET:CE	1.55	1.34
5:E:61:LEU:HD13	2:F:37:LEU:CA	1.54	1.34
3:C:34:LEU:HD22	3:C:39:TYR:CE2	1.63	1.33
3:C:40:ALA:HB2	4:D:86:ILE:CD1	1.56	1.33
5:E:61:LEU:HD12	2:F:37:LEU:CD1	1.58	1.32
6:I:62:DT:H3	7:J:-62:DA:N6	1.28	1.30
3:G:91:GLU:O	3:G:95:LYS:HG3	1.29	1.29
8:N:40:GLN:HG2	8:N:72:ARG:NH2	1.48	1.29
9:W:481:LYS:CG	9:W:483:MET:HE3	1.63	1.28
3:C:34:LEU:CD2	3:C:39:TYR:HE2	1.46	1.28
9:W:518:LEU:HD12	9:W:518:LEU:O	1.30	1.27
2:F:17:ARG:CB	9:W:722:ARG:NH2	1.97	1.27
9:W:390:LEU:CD1	9:W:393:LYS:HD2	1.65	1.26
9:W:607:PRO:HB2	9:W:813:HIS:N	1.48	1.26
4:H:66:VAL:O	4:H:70:ILE:HD13	1.13	1.25
8:O:54:ARG:HD2	8:O:59:TYR:CZ	1.72	1.25
9:W:777:GLY:O	9:W:778:ILE:HG22	1.36	1.24
9:W:345:LYS:CB	9:W:1036:ALA:CB	2.17	1.23
5:E:61:LEU:CD1	2:F:37:LEU:HD12	1.66	1.23
9:W:414:PHE:CE2	9:W:538:MET:HE1	1.74	1.23
1:A:83:ARG:O	1:A:84:PHE:HD1	1.15	1.22
3:G:77:ARG:HB2	6:I:58:DG:OP1	1.37	1.22
9:W:607:PRO:CB	9:W:813:HIS:H	1.52	1.22
2:F:45:ARG:NH1	7:J:-4:DG:H4'	1.54	1.21
6:I:22:DC:OP1	9:W:519:LYS:HB3	1.35	1.21
9:W:414:PHE:CD2	9:W:538:MET:HE1	1.76	1.20
5:E:63:ARG:NH2	7:J:-13:DA:H5'	1.56	1.20
9:W:607:PRO:HG3	9:W:811:LYS:C	1.64	1.19
6:I:34:DT:H2''	6:I:35:DC:C6	1.76	1.19
9:W:345:LYS:CB	9:W:1036:ALA:HB3	1.72	1.18
1:A:84:PHE:CE1	2:B:81:VAL:HB	1.78	1.17
3:G:91:GLU:O	3:G:95:LYS:CG	1.90	1.17
4:H:66:VAL:O	4:H:70:ILE:CD1	1.92	1.17
3:C:97:LEU:HD11	4:D:62:PHE:CE2	1.80	1.16
7:J:-37:DG:H2''	7:J:-36:DG:N7	1.61	1.15
3:G:77:ARG:HD2	6:I:57:DA:H4'	1.25	1.14
9:W:390:LEU:HD12	9:W:393:LYS:HD2	1.21	1.14
9:W:518:LEU:CD1	9:W:555:LEU:HD12	1.78	1.14
1:A:120:MET:HB3	1:A:121:PRO:HD2	1.29	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:ARG:HD3	7:J:38:DG:H4'	1.18	1.13
9:W:345:LYS:HE2	9:W:1037:ASP:HB2	1.22	1.12
1:A:83:ARG:O	1:A:84:PHE:CD1	2.01	1.12
3:G:51:LEU:CD2	4:H:91:ILE:HG21	1.79	1.12
7:J:19:DC:H2''	7:J:20:DG:C8	1.85	1.11
7:J:34:DC:H2'	7:J:35:DT:H71	1.11	1.11
3:C:79:ILE:HG23	3:C:80:PRO:HD2	1.31	1.11
6:I:67:DA:N1	7:J:-67:DT:N3	1.99	1.11
9:W:345:LYS:HB3	9:W:1036:ALA:HB1	1.11	1.11
9:W:398:ILE:HG23	9:W:539:LEU:HD11	1.27	1.11
4:D:62:PHE:HA	2:F:98:TYR:CE1	1.86	1.10
9:W:295:ARG:HD2	9:W:1198:ARG:NH2	1.66	1.10
2:B:26:ILE:HD13	2:B:59:LYS:HD3	1.30	1.10
3:G:77:ARG:HD3	6:I:57:DA:O3'	1.49	1.10
6:I:-28:DT:H2''	6:I:-27:DC:C5	1.87	1.09
6:I:22:DC:O2	7:J:-21:DG:N1	1.85	1.09
7:J:-38:DA:C5	7:J:-37:DG:C6	2.41	1.09
9:W:1150:TYR:HD1	9:W:1156:LYS:HE2	1.04	1.09
6:I:-6:DT:H2''	6:I:-5:DA:C8	1.88	1.09
9:W:1150:TYR:CD1	9:W:1156:LYS:HE2	1.87	1.09
3:C:34:LEU:CD2	3:C:39:TYR:CE2	2.28	1.09
9:W:650:ASN:HA	9:W:654:GLU:HB3	1.27	1.08
3:C:40:ALA:CB	4:D:86:ILE:CD1	2.30	1.08
9:W:408:THR:HG23	9:W:440:TRP:CZ3	1.88	1.08
1:A:73:GLU:HG2	2:B:22:LEU:O	1.54	1.08
9:W:615:ARG:HB3	9:W:822:LYS:HD3	1.11	1.08
3:C:17:ARG:NE	6:I:-43:DT:OP1	1.87	1.07
6:I:5:DC:H2''	6:I:6:DC:C5	1.89	1.07
9:W:481:LYS:CD	9:W:483:MET:HE1	1.84	1.07
7:J:-69:DG:H2''	7:J:-68:DA:C8	1.90	1.07
9:W:523:SER:HB2	9:W:526:TYR:HB2	1.12	1.07
5:E:66:PRO:HB2	2:F:29:ILE:HG12	1.35	1.06
6:I:62:DT:O2	7:J:-62:DA:N1	1.87	1.06
9:W:1138:ASP:HB3	9:W:1260:LEU:HD23	1.37	1.06
7:J:-25:DC:C2'	7:J:-24:DT:H72	1.86	1.06
3:C:40:ALA:CB	4:D:86:ILE:HD12	1.87	1.05
8:N:43:LEU:HB2	8:N:50:LEU:HD12	1.35	1.05
7:J:42:DA:H2''	7:J:43:DA:O5'	1.52	1.05
3:C:112:GLN:HB2	3:C:115:LEU:HD12	1.37	1.04
1:A:73:GLU:CG	2:B:22:LEU:O	2.05	1.04
3:C:30:VAL:HG13	4:D:67:PHE:HE1	1.15	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:22:DC:O2	7:J:-21:DG:N2	1.88	1.04
9:W:419:ILE:HG21	9:W:451:LEU:HD11	1.35	1.04
6:I:22:DC:O2	7:J:-21:DG:C2	2.10	1.04
9:W:1055:MET:HE3	9:W:1121:PHE:CE2	1.92	1.04
5:E:63:ARG:HH12	6:I:17:DA:H5'	1.07	1.03
7:J:72:DA:C8	7:J:73:DT:H72	1.94	1.03
3:C:40:ALA:HB2	4:D:86:ILE:HD12	1.40	1.03
2:F:15:ALA:HA	9:W:729:ASP:HB3	1.03	1.03
9:W:645:HIS:CE1	9:W:649:LEU:HD11	1.94	1.03
5:E:60:LEU:HD13	5:E:93:GLN:CD	1.84	1.03
2:F:15:ALA:CA	9:W:729:ASP:HB3	1.89	1.03
7:J:-25:DC:H2'	7:J:-24:DT:H72	1.34	1.03
3:C:34:LEU:HD22	3:C:39:TYR:HE2	0.88	1.02
5:E:60:LEU:HD13	5:E:93:GLN:NE2	1.73	1.02
9:W:474:ASN:HB2	9:W:475:PRO:HD2	1.39	1.02
6:I:-12:DC:H2'	6:I:-11:DG:C8	1.94	1.02
6:I:34:DT:H2''	6:I:35:DC:C5	1.94	1.02
6:I:42:DC:H2''	6:I:43:DT:O5'	1.55	1.02
5:E:63:ARG:NH1	6:I:17:DA:H5'	1.55	1.02
9:W:518:LEU:CD1	9:W:555:LEU:CD1	2.37	1.02
9:W:599:LYS:O	9:W:601:ASP:N	1.91	1.02
9:W:643:GLY:HA2	9:W:646:PHE:CZ	1.93	1.02
6:I:-23:DC:N4	6:I:-22:DA:H62	1.55	1.01
7:J:24:DC:C2'	7:J:25:DT:H71	1.89	1.01
9:W:607:PRO:HG3	9:W:812:ASN:N	1.73	1.01
4:H:47:PRO:HD2	8:O:54:ARG:HH22	1.25	1.01
5:E:72:ARG:HH22	7:J:-23:DT:P	1.83	1.01
3:G:77:ARG:CD	6:I:57:DA:O3'	2.08	1.01
7:J:6:DA:H2''	7:J:7:DC:C5	1.95	1.01
9:W:523:SER:CB	9:W:526:TYR:HB2	1.91	1.01
6:I:-35:DA:N7	6:I:-34:DG:C6	2.29	1.00
8:N:45:PHE:HB3	8:N:59:TYR:CE2	1.95	1.00
2:F:15:ALA:HA	9:W:729:ASP:CB	1.91	1.00
3:G:67:GLY:HA2	3:G:78:ILE:HD11	1.43	1.00
7:J:-32:DT:H2''	7:J:-31:DA:C8	1.95	1.00
6:I:23:DA:C6	7:J:-22:DG:O6	2.15	1.00
6:I:55:DT:N3	7:J:-55:DA:N1	2.10	1.00
9:W:518:LEU:HD11	9:W:555:LEU:CD1	1.92	0.99
9:W:481:LYS:CG	9:W:483:MET:CE	2.28	0.99
7:J:32:DG:H2''	7:J:33:DT:C7	1.93	0.99
7:J:32:DG:C2'	7:J:33:DT:H72	1.92	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-4:DC:N4	7:J:4:DG:H1	1.61	0.99
1:A:100:LEU:HD23	2:B:37:LEU:HD13	1.44	0.98
4:H:47:PRO:HD2	8:O:54:ARG:NH2	1.79	0.98
7:J:-25:DC:C2'	7:J:-24:DT:C7	2.40	0.98
9:W:345:LYS:HE2	9:W:1037:ASP:CB	1.92	0.98
7:J:34:DC:H2'	7:J:35:DT:C7	1.92	0.98
6:I:-38:DC:C4	6:I:-37:DG:C6	2.51	0.98
7:J:33:DT:H2''	7:J:34:DC:H5	1.27	0.98
8:N:31:GLN:OE1	8:N:38:PRO:HD3	1.63	0.98
7:J:33:DT:H2''	7:J:34:DC:C5	1.98	0.98
9:W:770:SER:HB2	9:W:773:ALA:HB3	1.45	0.98
9:W:523:SER:HB2	9:W:526:TYR:CB	1.94	0.98
3:G:51:LEU:HD21	4:H:91:ILE:HG21	1.46	0.97
6:I:23:DA:C6	7:J:-22:DG:C6	2.51	0.97
4:H:62:PHE:O	4:H:66:VAL:HG23	1.62	0.97
5:E:65:LEU:H	5:E:66:PRO:HD2	1.29	0.97
6:I:-35:DA:C8	6:I:-34:DG:N7	2.32	0.97
7:J:24:DC:H2''	7:J:25:DT:C6	2.00	0.97
9:W:345:LYS:CE	9:W:1037:ASP:HB2	1.94	0.97
7:J:-17:DT:C5	7:J:-16:DT:C4	2.53	0.97
8:N:45:PHE:CB	8:N:59:TYR:HE2	1.77	0.97
2:B:98:TYR:HE1	4:H:62:PHE:HA	1.28	0.97
4:H:36:ILE:HD11	6:I:49:DC:OP2	1.63	0.97
1:A:100:LEU:CD2	2:B:37:LEU:HD13	1.94	0.97
7:J:-25:DC:H2''	7:J:-24:DT:C7	1.96	0.96
9:W:650:ASN:HA	9:W:654:GLU:CB	1.95	0.96
2:B:98:TYR:CE1	4:H:62:PHE:HA	1.99	0.96
6:I:67:DA:N6	7:J:-68:DA:C6	2.32	0.96
9:W:518:LEU:O	9:W:518:LEU:CD1	2.13	0.96
3:G:91:GLU:O	3:G:95:LYS:CD	2.14	0.96
9:W:656:LYS:HE2	9:W:826:GLU:HA	1.48	0.96
1:A:59:GLU:OE2	1:A:60:LEU:O	1.84	0.95
5:E:63:ARG:HH11	6:I:17:DA:H5''	1.14	0.95
9:W:770:SER:CB	9:W:773:ALA:HB3	1.96	0.95
9:W:609:LYS:HA	9:W:814:VAL:HB	1.47	0.95
3:C:63:LEU:HD12	4:D:41:VAL:HG12	1.47	0.95
3:G:97:LEU:O	3:G:100:VAL:HG22	1.67	0.95
4:H:36:ILE:HD11	6:I:49:DC:P	2.04	0.95
6:I:-4:DC:H42	7:J:4:DG:H1	1.00	0.95
6:I:23:DA:C6	6:I:24:DA:N6	2.35	0.95
6:I:-53:DG:N2	7:J:54:DT:C2	2.34	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:VAL:HG13	4:D:67:PHE:CE1	2.02	0.95
2:F:32:PRO:O	2:F:36:ARG:HG2	1.67	0.95
9:W:390:LEU:HD12	9:W:393:LYS:CD	1.97	0.95
9:W:611:GLU:HG2	9:W:816:VAL:HG12	1.47	0.95
6:I:-23:DC:N4	6:I:-22:DA:N6	2.15	0.94
9:W:379:PHE:HE1	9:W:597:ARG:HD2	1.31	0.94
9:W:433:PRO:HD3	9:W:513:ASP:HB3	1.49	0.94
8:N:31:GLN:OE1	8:N:38:PRO:CD	2.14	0.94
8:N:40:GLN:HG2	8:N:72:ARG:HH21	1.30	0.94
9:W:367:GLN:CD	9:W:371:ILE:HD11	1.91	0.94
9:W:390:LEU:HD13	9:W:393:LYS:HD2	1.49	0.94
7:J:6:DA:H2''	7:J:7:DC:C6	2.01	0.94
9:W:650:ASN:CA	9:W:654:GLU:HB3	1.97	0.94
5:E:65:LEU:HD22	6:I:17:DA:OP2	1.67	0.94
7:J:-21:DG:H2''	7:J:-20:DC:O5'	1.66	0.94
7:J:19:DC:C5	7:J:20:DG:O6	2.20	0.94
9:W:502:LEU:O	9:W:507:TRP:HZ3	1.50	0.94
9:W:607:PRO:HB2	9:W:813:HIS:H	0.77	0.94
7:J:4:DG:H2'	7:J:5:DT:C6	2.02	0.94
3:G:84:GLN:NE2	3:G:102:ILE:CG1	2.30	0.94
6:I:43:DT:N3	7:J:-43:DA:N1	2.15	0.94
3:G:51:LEU:HD23	4:H:91:ILE:HG21	1.47	0.94
8:O:54:ARG:CD	8:O:59:TYR:CE2	2.51	0.94
9:W:229:THR:HG22	9:W:230:TYR:H	1.33	0.94
9:W:607:PRO:HD2	9:W:810:GLN:O	1.68	0.94
9:W:607:PRO:CD	9:W:811:LYS:HA	1.98	0.94
3:C:65:LEU:CD2	3:C:90:ASP:OD2	2.16	0.93
3:C:79:ILE:HG12	4:D:52:SER:HB3	1.49	0.93
7:J:-55:DA:H2''	7:J:-54:DC:C5	2.02	0.93
2:B:84:MET:HE1	2:B:88:TYR:OH	1.67	0.93
8:N:43:LEU:CB	8:N:50:LEU:HD12	1.97	0.93
9:W:295:ARG:HD2	9:W:1198:ARG:HH22	1.22	0.93
3:C:40:ALA:HB2	4:D:86:ILE:HD11	1.48	0.93
9:W:607:PRO:HG3	9:W:811:LYS:CA	1.99	0.93
3:C:97:LEU:HD11	4:D:62:PHE:HE2	1.28	0.93
6:I:-38:DC:C4	6:I:-37:DG:O6	2.21	0.93
7:J:-37:DG:H2''	7:J:-36:DG:C8	2.03	0.93
9:W:347:LEU:HD22	9:W:483:MET:O	1.68	0.93
2:F:17:ARG:CB	9:W:722:ARG:HH21	1.72	0.93
9:W:470:GLU:HG2	9:W:485:PHE:CE2	2.04	0.93
9:W:794:ASN:OD1	9:W:795:PRO:HD2	1.68	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:42:ARG:H	5:E:43:PRO:CD	1.82	0.93
6:I:-35:DA:C5	6:I:-34:DG:C6	2.57	0.93
1:A:42:ARG:HB3	6:I:70:DG:OP1	1.68	0.92
2:B:25:ASN:OD1	2:B:26:ILE:N	2.03	0.92
4:H:55:ALA:HA	4:H:58:ILE:HD12	1.50	0.92
7:J:-8:DG:H2''	7:J:-7:DG:C8	2.03	0.92
3:C:32:ARG:HD2	6:I:-44:DA:OP1	1.68	0.92
9:W:481:LYS:CD	9:W:483:MET:CE	2.45	0.92
4:H:51:ILE:HD13	4:H:56:MET:HE3	1.48	0.92
9:W:813:HIS:O	9:W:814:VAL:HG23	1.68	0.92
9:W:414:PHE:CE2	9:W:538:MET:CE	2.52	0.92
7:J:24:DC:H2''	7:J:25:DT:C5	2.04	0.92
6:I:8:DC:N4	7:J:-8:DG:O6	2.03	0.92
9:W:1246:VAL:HG13	9:W:1247:PRO:HA	1.51	0.91
5:E:63:ARG:CZ	6:I:17:DA:H5''	2.00	0.91
3:G:91:GLU:HB3	3:G:95:LYS:HE3	1.52	0.91
1:A:65:LEU:HB3	1:A:66:PRO:HD3	1.50	0.91
1:A:116:ARG:NH1	1:A:120:MET:HG2	1.84	0.91
3:G:77:ARG:CB	6:I:58:DG:OP1	2.18	0.91
6:I:72:DT:H3	7:J:-72:DA:H61	0.98	0.91
9:W:1026:ASN:HA	9:W:1052:TYR:OH	1.69	0.91
7:J:24:DC:H2''	7:J:25:DT:H71	1.51	0.91
9:W:611:GLU:HG2	9:W:816:VAL:CG1	1.99	0.91
9:W:615:ARG:CB	9:W:822:LYS:HD3	2.00	0.91
6:I:-35:DA:N6	7:J:35:DT:O4	2.04	0.91
6:I:62:DT:C2	7:J:-62:DA:N1	2.39	0.91
6:I:19:DC:H42	7:J:-19:DG:H1	1.19	0.91
6:I:-30:DG:C8	6:I:-29:DC:C5	2.59	0.91
7:J:34:DC:C2'	7:J:35:DT:H71	2.00	0.91
1:A:41:TYR:HB3	1:A:45:THR:HG21	1.53	0.91
9:W:419:ILE:HG21	9:W:451:LEU:CD1	2.00	0.91
9:W:315:ASN:OD1	9:W:316:TYR:N	2.04	0.90
9:W:474:ASN:CB	9:W:475:PRO:CD	2.48	0.90
7:J:-38:DA:C5	7:J:-37:DG:O6	2.23	0.90
4:H:87:THR:HG22	4:H:90:GLU:HG2	1.51	0.90
8:O:54:ARG:CD	8:O:59:TYR:CZ	2.55	0.90
9:W:656:LYS:HE3	9:W:829:VAL:CG2	2.00	0.90
3:G:83:LEU:HD13	4:H:59:MET:SD	2.12	0.90
7:J:-64:DA:H2'	7:J:-63:DT:H72	1.51	0.90
9:W:654:GLU:OE2	9:W:664:LEU:HD23	1.71	0.90
5:E:63:ARG:NE	2:F:30:THR:HG21	1.87	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:LEU:CD2	2:B:62:LEU:HD11	2.01	0.90
9:W:398:ILE:HG12	9:W:539:LEU:HD21	1.52	0.90
9:W:629:ILE:HG21	9:W:650:ASN:ND2	1.87	0.90
5:E:61:LEU:HD12	2:F:37:LEU:HD12	0.91	0.89
1:A:83:ARG:C	1:A:84:PHE:CD1	2.51	0.89
3:C:32:ARG:CD	6:I:-44:DA:P	2.59	0.89
3:C:81:ARG:O	3:C:85:LEU:HG	1.73	0.89
9:W:691:ILE:HD12	9:W:697:MET:HB3	1.52	0.89
7:J:60:DA:H2''	7:J:61:DC:C5	2.08	0.89
9:W:376:LEU:HD13	9:W:380:GLN:HB3	1.54	0.89
9:W:1073:ILE:HG21	9:W:1110:LYS:HE2	1.53	0.89
3:G:47:ALA:HB3	3:G:48:PRO:HD3	1.54	0.89
1:A:88:ALA:HA	2:B:83:ALA:CB	2.02	0.89
3:G:84:GLN:NE2	3:G:102:ILE:HG13	1.88	0.89
9:W:471:PHE:HE1	9:W:481:LYS:HE2	1.38	0.89
8:N:45:PHE:CD1	8:N:67:LEU:CD2	2.56	0.89
1:A:84:PHE:CD1	2:B:81:VAL:HB	2.07	0.89
6:I:-37:DG:H2''	6:I:-36:DT:C5	2.07	0.89
9:W:474:ASN:CB	9:W:475:PRO:HD2	2.03	0.89
9:W:646:PHE:HA	9:W:649:LEU:HD12	1.53	0.89
9:W:638:THR:HB	9:W:667:ASN:ND2	1.87	0.88
1:A:88:ALA:HA	2:B:83:ALA:HB2	1.53	0.88
7:J:-25:DC:H2''	7:J:-24:DT:C6	2.06	0.88
8:O:54:ARG:HG2	8:O:58:ASP:HB2	1.53	0.88
1:A:48:LEU:HA	1:A:51:ILE:HD12	1.54	0.88
7:J:24:DC:C2'	7:J:25:DT:C7	2.50	0.88
7:J:14:DT:H2''	7:J:15:DT:C7	2.04	0.88
9:W:767:PHE:CE2	9:W:769:LEU:HD11	2.09	0.88
6:I:-28:DT:H2''	6:I:-27:DC:C6	2.08	0.88
9:W:348:PRO:HG2	9:W:483:MET:HB3	1.56	0.88
8:N:31:GLN:OE1	8:N:38:PRO:CG	2.22	0.88
3:G:26:PRO:O	3:G:30:VAL:HG22	1.72	0.88
6:I:45:DC:H2''	6:I:46:DA:N7	1.88	0.88
6:I:-37:DG:H2''	6:I:-36:DT:C7	2.04	0.87
1:A:120:MET:HB3	1:A:121:PRO:CD	2.04	0.87
6:I:24:DA:H5'	9:W:793:TRP:HZ2	1.40	0.87
7:J:14:DT:H2'	7:J:15:DT:H72	1.56	0.87
7:J:63:DG:OP2	9:W:478:LYS:HA	1.75	0.87
2:F:45:ARG:NH1	7:J:-4:DG:C4'	2.36	0.87
2:F:66:ILE:O	2:F:70:VAL:HG23	1.73	0.87
1:A:73:GLU:HG3	2:B:25:ASN:HD22	1.39	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:PHE:HA	2:F:98:TYR:HE1	1.31	0.87
7:J:-17:DT:C7	7:J:-16:DT:O4	2.23	0.87
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.38	0.87
9:W:182:VAL:HG11	9:W:245:TYR:CE2	2.10	0.87
9:W:436:THR:O	9:W:440:TRP:CD1	2.27	0.87
6:I:72:DT:H3	7:J:-72:DA:N6	1.72	0.86
9:W:1164:PRO:HD2	9:W:1176:LYS:HE3	1.57	0.86
3:G:103:ALA:C	3:G:104:GLN:OE1	2.18	0.86
9:W:436:THR:O	9:W:440:TRP:HD1	1.59	0.86
9:W:617:GLU:OE1	9:W:618:LEU:O	1.92	0.86
6:I:7:DC:N4	7:J:-7:DG:O6	2.06	0.86
7:J:-49:DG:H2''	7:J:-48:DC:C5	2.10	0.86
9:W:777:GLY:O	9:W:778:ILE:CG2	2.21	0.86
6:I:-35:DA:C8	6:I:-34:DG:C5	2.64	0.86
9:W:793:TRP:O	9:W:794:ASN:HB2	1.75	0.86
9:W:390:LEU:CD1	9:W:393:LYS:CD	2.53	0.86
9:W:1119:PHE:CE2	9:W:1129:ALA:HB2	2.10	0.86
7:J:-69:DG:H2''	7:J:-68:DA:N7	1.91	0.85
7:J:24:DC:H2''	7:J:25:DT:C7	2.06	0.85
2:B:26:ILE:CD1	2:B:59:LYS:HD3	2.06	0.85
7:J:-57:DT:H2''	7:J:-56:DG:C8	2.11	0.85
6:I:62:DT:N3	7:J:-62:DA:N6	2.04	0.85
2:B:58:LEU:HD23	2:B:62:LEU:CD1	2.07	0.85
6:I:15:DT:H2''	6:I:16:DA:C8	2.11	0.85
6:I:24:DA:H2''	6:I:25:DG:C8	2.12	0.85
8:N:45:PHE:HB3	8:N:59:TYR:HE2	1.33	0.85
9:W:1059:ALA:HB2	9:W:1132:LEU:HD21	1.58	0.85
7:J:14:DT:C2'	7:J:15:DT:C7	2.53	0.85
8:N:40:GLN:CG	8:N:72:ARG:NH2	2.36	0.85
3:C:26:PRO:HG3	4:D:37:TYR:CZ	2.11	0.85
2:F:17:ARG:HA	9:W:722:ARG:HH22	1.39	0.85
1:A:89:VAL:HG12	1:A:90:MET:CE	2.07	0.85
3:C:32:ARG:HD2	6:I:-44:DA:P	2.17	0.85
6:I:-35:DA:N7	6:I:-34:DG:C5	2.45	0.85
6:I:34:DT:C2'	6:I:35:DC:C5	2.60	0.85
9:W:295:ARG:CD	9:W:1198:ARG:NH2	2.39	0.85
9:W:786:VAL:CG2	9:W:816:VAL:HG22	2.06	0.85
4:H:113:LYS:O	4:H:117:LYS:HG3	1.77	0.84
7:J:-17:DT:C5	7:J:-16:DT:O4	2.29	0.84
6:I:-22:DA:H61	7:J:22:DT:H3	1.24	0.84
6:I:-4:DC:N3	7:J:4:DG:N2	2.25	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:457:MET:HG3	9:W:457:MET:O	1.77	0.84
9:W:720:MET:SD	9:W:721:VAL:N	2.49	0.84
6:I:-73:DC:C4	6:I:-72:DA:N6	2.46	0.84
7:J:78:DG:C6	7:J:79:DG:C6	2.65	0.84
6:I:-6:DT:H2''	6:I:-5:DA:N7	1.90	0.84
9:W:307:TYR:HD2	9:W:327:ILE:HD13	1.41	0.84
9:W:524:SER:O	9:W:528:SER:HB2	1.77	0.84
2:F:88:TYR:HH	4:H:80:TYR:HE1	1.22	0.84
9:W:681:MET:SD	9:W:682:THR:N	2.50	0.84
6:I:21:DC:C4	6:I:22:DC:N4	2.46	0.84
6:I:23:DA:C5	6:I:24:DA:N6	2.45	0.84
8:N:40:GLN:CG	8:N:72:ARG:HH21	1.89	0.84
3:C:77:ARG:HD3	6:I:-55:DG:OP1	1.77	0.84
7:J:51:DG:H2''	7:J:52:DC:OP2	1.75	0.84
3:C:39:TYR:CZ	4:D:71:ALA:HB1	2.13	0.84
2:F:17:ARG:CA	9:W:722:ARG:NH2	2.40	0.84
2:F:78:ARG:NH1	6:I:29:DA:OP2	2.10	0.84
9:W:518:LEU:HD11	9:W:555:LEU:HD12	1.53	0.84
9:W:207:CYS:HA	9:W:211:TYR:CD2	2.13	0.84
2:B:58:LEU:HD23	2:B:62:LEU:HD11	1.57	0.84
9:W:806:HIS:ND1	9:W:814:VAL:HG21	1.93	0.84
9:W:1132:LEU:HD12	9:W:1133:LEU:N	1.93	0.84
2:F:80:THR:OG1	6:I:28:DG:H5''	1.78	0.83
9:W:551:GLU:O	9:W:555:LEU:HD13	1.77	0.83
3:G:77:ARG:HD2	6:I:57:DA:C4'	2.06	0.83
2:F:88:TYR:OH	4:H:80:TYR:CE1	2.32	0.83
9:W:723:MET:HE3	9:W:789:PHE:CE2	2.14	0.83
9:W:481:LYS:HD2	9:W:483:MET:HE1	1.58	0.83
1:A:88:ALA:CA	2:B:83:ALA:HB2	2.09	0.83
7:J:14:DT:C2'	7:J:15:DT:H72	2.08	0.83
6:I:21:DC:OP1	9:W:523:SER:HA	1.79	0.83
8:N:45:PHE:HD1	8:N:67:LEU:HD23	1.41	0.82
7:J:-50:DT:H2''	7:J:-49:DG:C8	2.13	0.82
7:J:24:DC:H2'	7:J:25:DT:H71	1.59	0.82
9:W:182:VAL:HG11	9:W:245:TYR:CD2	2.13	0.82
3:C:31:HIS:HB2	3:C:48:PRO:HB3	1.61	0.82
3:C:42:ARG:HD3	7:J:38:DG:C4'	2.04	0.82
4:H:36:ILE:CD1	6:I:48:DG:H3'	2.10	0.82
7:J:19:DC:C5	7:J:20:DG:C6	2.67	0.82
9:W:602:VAL:HG13	9:W:808:ILE:HG23	1.61	0.82
8:N:37:PRO:HD2	8:N:40:GLN:NE2	1.94	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:345:LYS:HB2	9:W:1036:ALA:CB	2.09	0.82
9:W:348:PRO:HB3	9:W:425:ASN:O	1.80	0.82
9:W:387:MET:HE3	9:W:538:MET:HE2	1.61	0.82
9:W:1025:GLY:HA3	9:W:1139:LEU:HD21	1.60	0.82
2:F:75:HIS:ND1	4:H:93:THR:HG21	1.95	0.82
5:E:63:ARG:NH2	7:J:-13:DA:C5'	2.41	0.82
2:F:48:GLY:HA2	2:F:51:TYR:HE2	1.44	0.82
7:J:-48:DC:H2''	7:J:-47:DC:C5	2.13	0.82
9:W:591:GLN:HG3	9:W:592:PRO:HD3	1.60	0.82
9:W:615:ARG:HB3	9:W:822:LYS:CD	2.05	0.82
1:A:83:ARG:C	1:A:84:PHE:HD1	1.87	0.82
5:E:61:LEU:CD1	2:F:37:LEU:CD1	2.40	0.82
6:I:67:DA:N1	7:J:-67:DT:C2	2.48	0.82
7:J:-33:DG:H2''	7:J:-32:DT:O5'	1.78	0.82
7:J:24:DC:H2'	7:J:25:DT:C7	2.10	0.82
7:J:32:DG:C2'	7:J:33:DT:C7	2.55	0.82
9:W:476:ARG:NH1	9:W:480:LYS:O	2.13	0.82
3:C:26:PRO:HG3	4:D:37:TYR:CE2	2.15	0.82
7:J:-35:DG:H2''	7:J:-34:DA:C8	2.14	0.82
9:W:502:LEU:O	9:W:507:TRP:CZ3	2.32	0.82
9:W:1143:LYS:HD3	9:W:1187:PHE:CE1	2.14	0.82
8:N:45:PHE:CD1	8:N:67:LEU:HD23	2.15	0.81
9:W:1039:THR:HG22	9:W:1040:LEU:HD12	1.62	0.81
5:E:103:LEU:O	5:E:107:THR:HG23	1.80	0.81
7:J:-32:DT:H2''	7:J:-31:DA:H8	1.40	0.81
6:I:-22:DA:C5	6:I:-21:DC:C4	2.69	0.81
9:W:607:PRO:HB2	9:W:813:HIS:CA	2.11	0.81
9:W:794:ASN:OD1	9:W:795:PRO:CD	2.29	0.81
3:C:79:ILE:HG23	3:C:80:PRO:CD	2.11	0.81
5:E:134:ARG:NH1	5:E:135:ALA:HB3	1.95	0.81
4:H:30:ARG:HD2	7:J:-45:DG:OP1	1.79	0.81
7:J:-38:DA:H2''	7:J:-37:DG:C8	2.14	0.81
9:W:345:LYS:HB3	9:W:1036:ALA:HB3	1.33	0.81
7:J:-7:DG:H2''	7:J:-6:DG:N7	1.96	0.81
9:W:609:LYS:HD2	9:W:814:VAL:HG11	1.60	0.81
9:W:807:ARG:NH2	11:W:1302:ADP:O1B	2.13	0.81
1:A:73:GLU:HG3	2:B:22:LEU:O	1.80	0.81
9:W:807:ARG:HH22	11:W:1302:ADP:PB	2.03	0.81
9:W:1150:TYR:CE2	9:W:1157:PHE:HA	2.15	0.81
3:G:25:PHE:CD2	3:G:52:ALA:O	2.34	0.81
3:C:25:PHE:CG	3:C:26:PRO:HD2	2.16	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:-50:DT:H2''	7:J:-49:DG:H8	1.43	0.81
9:W:663:TYR:OH	9:W:672:VAL:HG11	1.81	0.81
7:J:69:DC:H2''	7:J:70:DT:H71	1.63	0.80
9:W:348:PRO:CG	9:W:483:MET:HB3	2.10	0.80
9:W:315:ASN:HD21	9:W:458:GLY:HA2	1.47	0.80
9:W:387:MET:CE	9:W:538:MET:HE2	2.12	0.80
1:A:95:ALA:HB2	2:B:97:LEU:HD11	1.62	0.80
6:I:5:DC:C2'	6:I:6:DC:C5	2.64	0.80
9:W:612:ARG:N	9:W:816:VAL:O	2.13	0.80
9:W:1246:VAL:CG1	9:W:1247:PRO:HA	2.11	0.80
2:F:17:ARG:CB	9:W:722:ARG:HH22	1.93	0.80
3:C:110:ASN:O	3:C:111:ILE:HD13	1.82	0.80
3:G:45:ALA:HB2	6:I:38:DT:P	2.20	0.80
1:A:76:GLN:OE1	2:B:21:VAL:HA	1.81	0.80
1:A:116:ARG:HH11	1:A:120:MET:HG2	1.42	0.80
1:A:132:GLY:O	3:C:99:ARG:NH1	2.14	0.80
6:I:17:DA:N6	7:J:-18:DG:O6	2.15	0.80
9:W:655:LEU:CD2	9:W:825:VAL:HB	2.11	0.80
3:C:100:VAL:HG21	2:F:98:TYR:HE2	1.46	0.80
2:B:30:THR:HB	6:I:-12:DC:P	2.22	0.80
5:E:42:ARG:H	5:E:43:PRO:HD2	1.45	0.80
5:E:122:LYS:O	5:E:125:GLN:N	2.14	0.80
7:J:-38:DA:N7	7:J:-37:DG:O6	2.15	0.79
7:J:-33:DG:C2'	7:J:-32:DT:O5'	2.30	0.79
9:W:1119:PHE:HE2	9:W:1129:ALA:HB2	1.46	0.79
1:A:70:LEU:HD13	2:B:25:ASN:CG	2.07	0.79
2:F:82:THR:HG22	2:F:84:MET:H	1.48	0.79
4:H:51:ILE:HD13	4:H:56:MET:CE	2.13	0.79
9:W:429:ILE:HG23	9:W:510:MET:SD	2.22	0.79
9:W:433:PRO:CD	9:W:513:ASP:HB3	2.13	0.79
9:W:474:ASN:HB2	9:W:475:PRO:CD	2.12	0.79
9:W:713:ARG:HA	9:W:765:PHE:HB2	1.64	0.79
1:A:63:ARG:HD2	6:I:-13:DA:OP1	1.83	0.79
7:J:42:DA:C2'	7:J:43:DA:O5'	2.30	0.79
3:G:51:LEU:HD21	4:H:91:ILE:HG12	1.63	0.79
6:I:43:DT:H2''	6:I:44:DC:O5'	1.81	0.79
9:W:254:GLN:HA	9:W:258:LEU:HB2	1.64	0.79
2:F:34:ILE:HD11	2:F:55:ARG:HH11	1.48	0.79
6:I:-30:DG:N7	6:I:-29:DC:C4	2.51	0.79
7:J:50:DG:H2''	7:J:51:DG:OP2	1.82	0.79
7:J:67:DT:H2''	7:J:68:DT:C7	2.13	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:813:HIS:O	9:W:814:VAL:CG2	2.31	0.79
3:G:50:TYR:O	3:G:54:VAL:HG23	1.83	0.79
9:W:419:ILE:CG2	9:W:451:LEU:HD11	2.11	0.79
3:G:51:LEU:HD21	4:H:91:ILE:CG2	2.13	0.79
7:J:20:DG:H4'	7:J:21:DG:OP1	1.82	0.79
6:I:-23:DC:C5	6:I:-22:DA:N7	2.51	0.78
6:I:55:DT:C4	7:J:-55:DA:N1	2.51	0.78
8:N:40:GLN:HG2	8:N:72:ARG:HH22	1.46	0.78
9:W:429:ILE:HB	9:W:507:TRP:CD1	2.18	0.78
3:G:80:PRO:HG3	4:H:55:ALA:HB2	1.65	0.78
7:J:19:DC:C2'	7:J:20:DG:C8	2.65	0.78
9:W:606:LEU:C	9:W:606:LEU:HD12	2.08	0.78
9:W:645:HIS:CE1	9:W:649:LEU:CD1	2.66	0.78
3:C:79:ILE:CG2	3:C:80:PRO:HD2	2.13	0.78
5:E:63:ARG:HH21	7:J:-13:DA:H5'	1.48	0.78
6:I:16:DA:N1	7:J:-17:DT:O4	2.16	0.78
9:W:177:HIS:CE1	9:W:217:TRP:CE2	2.71	0.78
9:W:345:LYS:HB2	9:W:1036:ALA:HB3	1.63	0.78
3:C:44:GLY:HA3	4:D:87:THR:HA	1.64	0.78
9:W:624:GLU:OE1	9:W:625:TYR:CD1	2.36	0.78
2:B:90:LEU:CD1	2:B:97:LEU:HD11	2.12	0.78
9:W:620:ASP:OD1	9:W:621:VAL:N	2.16	0.78
7:J:-25:DC:H2''	7:J:-24:DT:C5	2.17	0.78
8:N:45:PHE:HB2	8:N:67:LEU:HD22	1.66	0.78
5:E:72:ARG:NH2	7:J:-23:DT:P	2.57	0.78
2:F:17:ARG:CA	9:W:722:ARG:HH22	1.97	0.78
9:W:656:LYS:CE	9:W:826:GLU:HA	2.13	0.78
7:J:58:DG:H2''	7:J:59:DC:C5	2.18	0.78
3:C:34:LEU:HD23	3:C:39:TYR:CE2	2.19	0.77
4:D:121:ALA:O	4:D:122:LYS:HB2	1.83	0.77
2:F:75:HIS:HE2	4:H:90:GLU:CD	1.92	0.77
4:H:97:LEU:HD12	4:H:98:LEU:N	1.99	0.77
6:I:-12:DC:N4	6:I:-11:DG:O6	2.17	0.77
5:E:48:LEU:HA	5:E:51:ILE:HD12	1.66	0.77
2:F:47:SER:O	2:F:50:ILE:HG22	1.84	0.77
9:W:324:ALA:O	9:W:327:ILE:HG22	1.83	0.77
6:I:32:DA:H1'	6:I:33:DC:H5'	1.66	0.77
7:J:67:DT:H2''	7:J:68:DT:C5	2.20	0.77
9:W:345:LYS:CB	9:W:1036:ALA:HB1	1.99	0.77
6:I:66:DC:N4	7:J:-67:DT:O4	2.16	0.77
9:W:408:THR:HG23	9:W:440:TRP:CE3	2.19	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:474:ASN:HB3	9:W:475:PRO:CD	2.14	0.77
3:C:63:LEU:HD12	4:D:41:VAL:CG1	2.15	0.77
6:I:-38:DC:C5	6:I:-37:DG:O6	2.37	0.77
6:I:-13:DA:N6	7:J:12:DG:O6	2.18	0.77
7:J:14:DT:H2''	7:J:15:DT:C6	2.18	0.77
9:W:470:GLU:HG2	9:W:485:PHE:HE2	1.50	0.77
3:C:42:ARG:CD	7:J:38:DG:H4'	2.07	0.77
3:G:31:HIS:CD2	3:G:43:VAL:HG11	2.19	0.77
3:C:30:VAL:CG1	4:D:67:PHE:HE1	1.96	0.77
3:C:39:TYR:O	4:D:75:SER:OG	2.01	0.77
9:W:607:PRO:C	9:W:813:HIS:HA	2.09	0.77
7:J:-17:DT:H71	7:J:-16:DT:O4	1.83	0.77
1:A:84:PHE:CE1	2:B:81:VAL:CB	2.66	0.77
2:B:90:LEU:HD12	2:B:97:LEU:HD11	1.67	0.77
3:G:84:GLN:NE2	3:G:102:ILE:HG12	2.00	0.77
6:I:-30:DG:C5	6:I:-29:DC:C4	2.73	0.77
6:I:-23:DC:H42	6:I:-22:DA:N6	1.82	0.77
9:W:434:LEU:HD12	9:W:435:SER:N	1.99	0.77
6:I:-62:DC:O2	7:J:63:DG:N2	2.18	0.76
9:W:433:PRO:HG2	9:W:514:GLU:OE1	1.85	0.76
9:W:654:GLU:O	9:W:657:LYS:N	2.18	0.76
6:I:-6:DT:C5	6:I:-5:DA:N6	2.53	0.76
7:J:32:DG:H2'	7:J:33:DT:H72	1.67	0.76
9:W:350:TYR:HE1	9:W:1042:VAL:CG1	1.98	0.76
9:W:379:PHE:HE1	9:W:597:ARG:CD	1.97	0.76
8:N:45:PHE:CD1	8:N:67:LEU:HD21	2.19	0.76
9:W:432:VAL:HG11	9:W:440:TRP:CD1	2.21	0.76
5:E:74:ILE:HG21	2:F:59:LYS:HE3	1.65	0.76
6:I:-77:DC:OP2	9:W:1254[A]:ARG:NH2	2.18	0.76
9:W:398:ILE:HG23	9:W:539:LEU:CD1	2.10	0.76
1:A:89:VAL:HG12	1:A:90:MET:HE2	1.68	0.76
5:E:61:LEU:HD12	2:F:37:LEU:HD13	1.67	0.76
7:J:-37:DG:C2'	7:J:-36:DG:N7	2.46	0.76
7:J:-64:DA:H2'	7:J:-63:DT:C7	2.15	0.76
9:W:715:LEU:HD21	9:W:780:LEU:HD22	1.67	0.76
9:W:391:TRP:CE3	9:W:391:TRP:O	2.38	0.76
9:W:608:SER:N	9:W:813:HIS:HA	2.00	0.76
9:W:723:MET:HE3	9:W:789:PHE:HE2	1.49	0.76
3:C:65:LEU:HD23	3:C:90:ASP:OD2	1.85	0.76
6:I:15:DT:H2''	6:I:16:DA:H8	1.49	0.76
9:W:666:ASP:OD1	9:W:667:ASN:N	2.18	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:75:ALA:HB1	5:E:82:LEU:CD2	2.15	0.76
8:N:43:LEU:CB	8:N:50:LEU:CD1	2.64	0.76
3:C:46:GLY:C	4:D:88:SER:HB3	2.11	0.76
5:E:89:VAL:HA	5:E:92:LEU:HD12	1.68	0.76
9:W:613:ILE:O	9:W:614:LEU:HD12	1.87	0.75
6:I:-68:DG:H2''	6:I:-67:DA:C8	2.21	0.75
6:I:-3:DG:C6	7:J:4:DG:N2	2.55	0.75
7:J:-35:DG:C5	7:J:-34:DA:C6	2.74	0.75
9:W:376:LEU:HD13	9:W:380:GLN:CB	2.17	0.75
9:W:654:GLU:O	9:W:658:ALA:N	2.19	0.75
1:A:63:ARG:CZ	7:J:17:DA:H4'	2.16	0.75
6:I:-32:DC:H2''	6:I:-31:DA:C8	2.21	0.75
6:I:23:DA:N6	7:J:-22:DG:O6	2.18	0.75
9:W:200:THR:O	9:W:258:LEU:HD13	1.86	0.75
7:J:-11:DC:H2'	7:J:-10:DG:C8	2.22	0.75
8:N:28:ALA:O	8:N:31:GLN:HG2	1.87	0.75
3:C:63:LEU:HD13	4:D:42:LEU:N	2.01	0.75
4:D:36:ILE:HD13	7:J:48:DG:H3'	1.69	0.75
3:C:39:TYR:CE2	4:D:71:ALA:HB1	2.21	0.75
9:W:466:ILE:O	9:W:470:GLU:HB2	1.87	0.75
9:W:508:GLN:HB2	9:W:535:ALA:HB3	1.67	0.75
3:C:110:ASN:C	3:C:111:ILE:HD13	2.12	0.74
5:E:72:ARG:NH2	7:J:-23:DT:OP1	2.20	0.74
6:I:-28:DT:C2'	6:I:-27:DC:C5	2.69	0.74
9:W:385:ASN:O	9:W:389:PHE:HB2	1.87	0.74
9:W:1119:PHE:HE2	9:W:1129:ALA:CB	1.99	0.74
2:B:26:ILE:HD13	2:B:59:LYS:CD	2.14	0.74
2:F:17:ARG:HA	9:W:722:ARG:NH2	2.00	0.74
6:I:27:DG:H2''	6:I:28:DG:C8	2.22	0.74
9:W:180:ASP:HB2	9:W:218:THR:HA	1.68	0.74
9:W:617:GLU:CD	9:W:618:LEU:N	2.45	0.74
9:W:345:LYS:HE2	9:W:1037:ASP:CA	2.16	0.74
9:W:607:PRO:CG	9:W:811:LYS:C	2.56	0.74
7:J:4:DG:C2'	7:J:5:DT:C6	2.71	0.74
9:W:177:HIS:NE2	9:W:217:TRP:CG	2.55	0.74
6:I:-19:DG:H2''	6:I:-18:DC:C5	2.22	0.74
9:W:591:GLN:CG	9:W:592:PRO:HD3	2.17	0.74
2:F:45:ARG:CZ	7:J:-4:DG:H4'	2.18	0.74
3:G:25:PHE:CE1	3:G:56:GLU:HA	2.22	0.74
1:A:119:ILE:HD11	2:B:46:ILE:HG12	1.68	0.74
4:D:79:HIS:NE2	3:G:38:ASN:ND2	2.35	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:45:PHE:HB2	8:N:67:LEU:CD2	2.18	0.74
9:W:518:LEU:HD13	9:W:555:LEU:HD12	1.65	0.74
3:G:51:LEU:CD2	4:H:91:ILE:CG2	2.65	0.74
6:I:5:DC:H2''	6:I:6:DC:H5	1.52	0.74
6:I:67:DA:C2	7:J:-67:DT:O2	2.41	0.74
9:W:602:VAL:CG1	9:W:808:ILE:HG23	2.18	0.74
9:W:638:THR:HB	9:W:667:ASN:HD22	1.51	0.74
1:A:73:GLU:OE1	1:A:74:ILE:HD12	1.88	0.74
2:B:82:THR:HG22	2:B:84:MET:H	1.52	0.74
4:D:91:ILE:O	4:D:95:VAL:HG23	1.88	0.74
6:I:-23:DC:C4	6:I:-22:DA:N7	2.56	0.74
7:J:-57:DT:H2''	7:J:-56:DG:N7	2.02	0.74
8:O:54:ARG:CG	8:O:58:ASP:HB2	2.18	0.74
9:W:354:TYR:CE2	9:W:359:PRO:HG3	2.23	0.74
9:W:690:LEU:O	9:W:697:MET:SD	2.46	0.74
3:C:44:GLY:N	4:D:86:ILE:O	2.17	0.74
9:W:348:PRO:HG2	9:W:483:MET:CB	2.18	0.74
9:W:540:ILE:HD12	9:W:540:ILE:O	1.86	0.74
2:B:97:LEU:HD23	3:G:101:THR:CG2	2.18	0.73
9:W:607:PRO:HD3	9:W:811:LYS:HA	1.68	0.73
3:G:83:LEU:CD1	4:H:59:MET:SD	2.76	0.73
7:J:24:DC:C2'	7:J:25:DT:C5	2.71	0.73
9:W:586:LEU:HG	9:W:590:ILE:HD12	1.69	0.73
3:G:84:GLN:HE21	3:G:102:ILE:CG1	2.01	0.73
4:H:51:ILE:CD1	4:H:56:MET:HE3	2.19	0.73
9:W:624:GLU:OE1	9:W:625:TYR:CE1	2.41	0.73
6:I:-35:DA:N6	7:J:35:DT:C4	2.53	0.73
7:J:34:DC:C6	7:J:34:DC:H5'	2.23	0.73
1:A:42:ARG:O	1:A:45:THR:HG22	1.89	0.73
2:F:29:ILE:HG22	2:F:30:THR:N	2.01	0.73
7:J:19:DC:C6	7:J:20:DG:C6	2.76	0.73
8:N:43:LEU:HB3	8:N:50:LEU:CD1	2.17	0.73
1:A:41:TYR:HB3	1:A:45:THR:CG2	2.19	0.73
5:E:66:PRO:HB2	2:F:29:ILE:CG1	2.15	0.73
9:W:481:LYS:HD3	9:W:483:MET:HE1	1.68	0.73
3:C:63:LEU:CD1	4:D:41:VAL:HG12	2.17	0.73
2:F:48:GLY:HA2	2:F:51:TYR:CE2	2.23	0.73
6:I:-12:DC:C4	6:I:-11:DG:C6	2.76	0.73
1:A:95:ALA:CB	2:B:90:LEU:HD11	2.18	0.73
2:B:79:LYS:O	2:B:81:VAL:N	2.22	0.73
9:W:656:LYS:HE3	9:W:829:VAL:HG23	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:807:ARG:NH2	11:W:1302:ADP:PB	2.62	0.73
1:A:53:ARG:NH1	7:J:-65:DT:OP1	2.22	0.73
7:J:69:DC:H2''	7:J:70:DT:C7	2.19	0.73
3:G:88:ARG:O	3:G:94:ASN:ND2	2.21	0.72
6:I:-63:DC:O2	7:J:64:DG:N2	2.22	0.72
7:J:-25:DC:H2'	7:J:-24:DT:C7	2.10	0.72
9:W:1039:THR:HG22	9:W:1040:LEU:CD1	2.19	0.72
5:E:65:LEU:CD2	6:I:17:DA:OP2	2.36	0.72
5:E:63:ARG:CZ	6:I:17:DA:C5'	2.65	0.72
7:J:-49:DG:H2''	7:J:-48:DC:C6	2.24	0.72
9:W:1119:PHE:HE2	9:W:1129:ALA:CA	2.02	0.72
3:G:26:PRO:HD3	4:H:37:TYR:CD2	2.24	0.72
3:C:47:ALA:CB	4:D:91:ILE:HD11	2.19	0.72
6:I:34:DT:H2''	6:I:35:DC:H6	1.47	0.72
3:C:31:HIS:O	3:C:35:ARG:HG3	1.89	0.72
4:D:46:HIS:HB3	4:D:49:THR:OG1	1.90	0.72
3:G:96:LEU:HD12	4:H:100:PRO:HD3	1.70	0.72
9:W:298:LEU:HD11	9:W:304:GLN:HG2	1.70	0.72
2:F:35:ARG:HH21	2:F:39:ARG:HH22	1.37	0.72
9:W:608:SER:O	9:W:814:VAL:N	2.23	0.72
6:I:-12:DC:C4	6:I:-11:DG:O6	2.43	0.72
9:W:178:GLY:O	9:W:218:THR:OG1	2.05	0.72
5:E:65:LEU:H	5:E:66:PRO:CD	2.01	0.72
6:I:24:DA:H5'	9:W:793:TRP:CZ2	2.24	0.72
3:C:25:PHE:CD1	3:C:26:PRO:HD2	2.24	0.72
3:G:24:GLN:O	4:H:37:TYR:CD2	2.43	0.72
3:G:65:LEU:HD12	3:G:68:ASN:HB2	1.72	0.72
6:I:55:DT:N3	7:J:-55:DA:C2	2.49	0.71
7:J:23:DG:C8	7:J:24:DC:C5	2.79	0.71
3:C:80:PRO:HD3	4:D:55:ALA:HB2	1.71	0.71
5:E:62:ILE:HD13	2:F:33:ALA:O	1.89	0.71
1:A:73:GLU:HG3	2:B:25:ASN:ND2	2.03	0.71
2:F:84:MET:CE	2:F:101:GLY:O	2.39	0.71
6:I:-22:DA:N6	7:J:22:DT:H3	1.88	0.71
6:I:7:DC:H2''	6:I:8:DC:C6	2.25	0.71
7:J:4:DG:H2'	7:J:5:DT:C5	2.25	0.71
6:I:5:DC:H1'	6:I:6:DC:C5	2.25	0.71
7:J:-58:DC:H2'	7:J:-57:DT:H71	1.72	0.71
9:W:429:ILE:CG2	9:W:510:MET:SD	2.78	0.71
9:W:616:VAL:CG1	9:W:695:GLY:HA3	2.21	0.71
4:D:89:ARG:O	4:D:92:GLN:HB3	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:38:DG:C2	7:J:39:DA:C4	2.79	0.71
9:W:781:MET:HE1	11:W:1302:ADP:H4'	1.73	0.71
1:A:58:THR:HB	3:G:104:GLN:HB3	1.71	0.71
3:C:32:ARG:CD	6:I:44:DA:OP1	2.38	0.71
3:G:34:LEU:HD23	4:H:67:PHE:HZ	1.54	0.71
6:I:5:DC:H1'	6:I:6:DC:C6	2.26	0.71
9:W:482:THR:O	9:W:483:MET:HB2	1.91	0.71
9:W:532:PHE:O	9:W:533:LYS:C	2.33	0.71
3:G:25:PHE:CZ	3:G:56:GLU:HA	2.25	0.71
6:I:23:DA:N6	7:J:-23:DT:O4	2.18	0.71
9:W:518:LEU:CD1	9:W:555:LEU:HD11	2.20	0.71
1:A:100:LEU:HD23	2:B:37:LEU:CD1	2.19	0.71
2:B:66:ILE:O	2:B:70:VAL:HG23	1.90	0.71
7:J:60:DA:H2''	7:J:61:DC:C6	2.25	0.71
9:W:388:ALA:N	9:W:414:PHE:HE1	1.89	0.71
1:A:95:ALA:CB	2:B:90:LEU:CD1	2.69	0.70
3:G:97:LEU:HB3	3:G:100:VAL:CG2	2.20	0.70
6:I:-38:DC:N3	6:I:-37:DG:C6	2.59	0.70
6:I:-1:DG:N2	7:J:2:DG:C2	2.58	0.70
9:W:179:ILE:HD13	9:W:217:TRP:CZ3	2.26	0.70
2:B:63:GLU:O	2:B:66:ILE:HG13	1.90	0.70
9:W:229:THR:HG22	9:W:230:TYR:N	2.06	0.70
9:W:656:LYS:HA	9:W:825:VAL:HG13	1.73	0.70
9:W:768:LEU:HD12	9:W:768:LEU:O	1.91	0.70
3:C:65:LEU:HD22	3:C:90:ASP:OD2	1.90	0.70
5:E:63:ARG:HH11	6:I:17:DA:C5'	1.77	0.70
6:I:-3:DG:N7	6:I:-2:DC:N4	2.38	0.70
7:J:38:DG:N2	7:J:39:DA:N3	2.39	0.70
9:W:398:ILE:CG2	9:W:539:LEU:HD11	2.14	0.70
6:I:-35:DA:C5	6:I:-34:DG:C5	2.79	0.70
7:J:67:DT:H2''	7:J:68:DT:H71	1.72	0.70
8:N:45:PHE:CB	8:N:67:LEU:CD2	2.70	0.70
3:C:79:ILE:HG12	4:D:52:SER:CB	2.20	0.70
7:J:17:DA:H2''	7:J:18:DG:C8	2.26	0.70
9:W:431:VAL:O	9:W:431:VAL:HG13	1.92	0.70
9:W:1146:ILE:HG13	9:W:1150:TYR:HB2	1.71	0.70
7:J:-38:DA:C6	7:J:-37:DG:C6	2.79	0.70
9:W:627:LYS:O	9:W:630:LEU:HG	1.91	0.70
6:I:23:DA:H2''	6:I:24:DA:OP2	1.92	0.70
9:W:328:VAL:HG21	9:W:1201:PRO:HB2	1.74	0.70
9:W:474:ASN:HB3	9:W:475:PRO:HD3	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG21	7:J:9:DT:H3'	1.73	0.70
9:W:470:GLU:HG2	9:W:485:PHE:CZ	2.26	0.70
1:A:124:ILE:HD12	2:B:50:ILE:HG21	1.71	0.69
9:W:740:ARG:HB2	9:W:768:LEU:HD11	1.74	0.69
9:W:795:PRO:HG3	9:W:836:LYS:HB2	1.72	0.69
9:W:1143:LYS:HA	9:W:1187:PHE:HE1	1.57	0.69
1:A:47:ALA:O	1:A:51:ILE:HG13	1.92	0.69
6:I:-23:DC:H2''	6:I:-22:DA:C5'	2.22	0.69
6:I:22:DC:C2	7:J:-21:DG:N1	2.44	0.69
3:C:17:ARG:CD	6:I:-43:DT:OP1	2.40	0.69
4:D:109:SER:O	4:D:112:THR:HG22	1.92	0.69
6:I:-35:DA:N7	6:I:-34:DG:O6	2.25	0.69
7:J:-3:DA:H2''	7:J:-2:DC:C6	2.26	0.69
3:G:47:ALA:N	3:G:48:PRO:CD	2.54	0.69
4:H:30:ARG:HG2	4:H:32:GLU:OE2	1.92	0.69
4:H:114:ALA:HA	4:H:117:LYS:HD2	1.74	0.69
6:I:61:DA:N6	7:J:-62:DA:N6	2.41	0.69
7:J:26:DA:C5	7:J:27:DG:C6	2.80	0.69
2:B:98:TYR:HE1	4:H:62:PHE:CA	2.04	0.69
6:I:62:DT:O2	7:J:-62:DA:C2	2.45	0.69
6:I:62:DT:N3	7:J:-62:DA:C6	2.54	0.69
9:W:602:VAL:CG1	9:W:808:ILE:HD12	2.23	0.69
6:I:-23:DC:H2''	6:I:-22:DA:H5'	1.74	0.69
7:J:30:DC:C4	7:J:31:DT:C4	2.80	0.69
9:W:602:VAL:HG12	9:W:808:ILE:HD12	1.73	0.69
3:C:77:ARG:HH11	6:I:-55:DG:P	2.16	0.69
4:D:77:LEU:HD12	4:D:78:ALA:N	2.08	0.69
9:W:575:GLN:HB2	9:W:578:GLU:HB2	1.74	0.69
9:W:616:VAL:HG22	9:W:699:LEU:HD12	1.74	0.69
9:W:1192:GLY:HA2	9:W:1194:TRP:CH2	2.28	0.69
1:A:113:HIS:HB2	5:E:126:LEU:HD21	1.75	0.69
2:B:90:LEU:HD12	2:B:97:LEU:CD1	2.23	0.69
2:B:96:THR:O	3:G:101:THR:HG22	1.93	0.69
5:E:72:ARG:NH2	7:J:-23:DT:O5'	2.22	0.69
9:W:350:TYR:HE1	9:W:1042:VAL:HG13	1.58	0.69
9:W:380:GLN:O	9:W:384:ILE:HG13	1.93	0.69
9:W:430:ILE:CG1	9:W:511:ALA:HB3	2.23	0.69
1:A:104:PHE:CD2	2:B:38:ALA:HA	2.28	0.69
7:J:-64:DA:H2''	7:J:-63:DT:C6	2.29	0.69
9:W:616:VAL:CG2	9:W:699:LEU:HD12	2.22	0.69
4:D:51:ILE:O	4:D:51:ILE:HD12	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:25:PHE:HB3	3:G:52:ALA:HB1	1.74	0.68
9:W:184:ASN:OD1	9:W:185:HIS:N	2.25	0.68
9:W:471:PHE:CE1	9:W:481:LYS:HE2	2.24	0.68
3:G:97:LEU:HD22	3:G:100:VAL:HG11	1.74	0.68
6:I:-64:DC:H2''	6:I:-63:DC:C5	2.28	0.68
9:W:545:LEU:HD13	9:W:552:LEU:HD13	1.73	0.68
3:C:46:GLY:HA3	4:D:88:SER:CB	2.24	0.68
7:J:4:DG:H2'	7:J:5:DT:H71	1.73	0.68
9:W:181:ILE:HG22	9:W:182:VAL:N	2.08	0.68
6:I:5:DC:C4	7:J:-6:DG:O6	2.47	0.68
7:J:34:DC:C2'	7:J:35:DT:C6	2.76	0.68
9:W:357:GLN:HG3	9:W:358:ARG:H	1.58	0.68
9:W:1014:VAL:HG12	9:W:1124:VAL:CG2	2.23	0.68
1:A:63:ARG:NH2	7:J:17:DA:H4'	2.07	0.68
3:G:91:GLU:O	3:G:95:LYS:HD2	1.91	0.68
6:I:47:DG:C5	6:I:48:DG:C6	2.82	0.68
8:N:45:PHE:CG	8:N:67:LEU:HD21	2.28	0.68
9:W:607:PRO:CG	9:W:811:LYS:CA	2.72	0.68
2:B:68:ASP:OD1	2:B:72:TYR:HE1	1.77	0.68
2:F:48:GLY:O	2:F:51:TYR:CE2	2.46	0.68
3:G:34:LEU:HD23	4:H:67:PHE:CZ	2.28	0.68
9:W:263:THR:HG22	9:W:264:ALA:H	1.58	0.68
9:W:358:ARG:HD3	9:W:392:SER:O	1.94	0.68
2:F:84:MET:HE1	2:F:101:GLY:O	1.94	0.68
5:E:46:VAL:HG12	5:E:50:GLU:HG3	1.74	0.68
7:J:-38:DA:C2'	7:J:-37:DG:C8	2.77	0.68
9:W:377:ARG:NE	9:W:602:VAL:HG23	2.09	0.68
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.07	0.68
3:G:24:GLN:CD	4:H:41:VAL:HG12	2.18	0.68
6:I:62:DT:C4	7:J:-62:DA:N6	2.58	0.68
3:C:34:LEU:HD11	3:C:51:LEU:HD23	1.76	0.67
2:F:45:ARG:CZ	7:J:-4:DG:H5'	2.24	0.67
9:W:180:ASP:O	9:W:181:ILE:HG13	1.95	0.67
9:W:215:ILE:HD12	9:W:228:GLU:HB2	1.74	0.67
9:W:284:PHE:O	9:W:311:TRP:CD1	2.47	0.67
9:W:430:ILE:HG13	9:W:511:ALA:HB3	1.77	0.67
2:F:30:THR:OG1	2:F:33:ALA:HB2	1.94	0.67
7:J:-25:DC:C2	7:J:-24:DT:C4	2.81	0.67
9:W:491:THR:HB	9:W:494:TYR:CD2	2.29	0.67
9:W:608:SER:O	9:W:813:HIS:C	2.36	0.67
9:W:1039:THR:C	9:W:1040:LEU:HD12	2.20	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:655:LEU:HD21	9:W:825:VAL:HB	1.75	0.67
3:G:59:THR:O	3:G:63:LEU:HB2	1.95	0.67
6:I:-4:DC:H2''	6:I:-3:DG:C8	2.30	0.67
7:J:-33:DG:C5	7:J:-32:DT:C4	2.81	0.67
9:W:660:ASN:OD1	9:W:821:SER:HB2	1.94	0.67
9:W:660:ASN:CG	9:W:696:LYS:HZ1	2.02	0.67
3:C:67:GLY:HA2	3:C:78:ILE:HD11	1.77	0.67
6:I:67:DA:N6	7:J:-68:DA:N1	2.42	0.67
9:W:656:LYS:CD	9:W:826:GLU:HA	2.24	0.67
3:C:116:LEU:CD1	3:C:118:LYS:HB2	2.24	0.67
6:I:24:DA:H2''	6:I:25:DG:N7	2.10	0.67
9:W:614:LEU:HB2	9:W:819:LEU:HA	1.77	0.67
9:W:616:VAL:HG22	9:W:699:LEU:CD1	2.24	0.67
2:B:62:LEU:O	2:B:66:ILE:HG23	1.95	0.67
4:H:38:VAL:O	4:H:42:LEU:HG	1.94	0.67
4:H:95:VAL:HG13	4:H:99:LEU:HD13	1.76	0.67
8:N:45:PHE:CB	8:N:59:TYR:CE2	2.62	0.67
9:W:655:LEU:HD23	9:W:825:VAL:HB	1.75	0.67
9:W:419:ILE:CD1	9:W:451:LEU:HD13	2.24	0.67
6:I:-59:DT:C2	6:I:-58:DG:C2	2.83	0.67
9:W:214:LEU:HD21	9:W:225:ASN:HB2	1.77	0.67
4:D:45:VAL:O	4:D:46:HIS:ND1	2.27	0.67
4:D:65:ASP:OD2	2:F:98:TYR:OH	2.12	0.67
3:G:57:TYR:HH	4:H:106:HIS:HD1	1.41	0.67
9:W:1205:ILE:HD12	9:W:1208:LYS:HD2	1.77	0.67
1:A:100:LEU:CD2	2:B:37:LEU:CD1	2.70	0.66
3:C:46:GLY:CA	4:D:88:SER:HB3	2.25	0.66
5:E:134:ARG:HH12	5:E:135:ALA:HB3	1.58	0.66
3:G:97:LEU:HB3	3:G:100:VAL:HG21	1.77	0.66
7:J:-21:DG:C5	7:J:-20:DC:C4	2.83	0.66
9:W:189:THR:OG1	9:W:210:ASN:OD1	2.11	0.66
9:W:650:ASN:O	9:W:655:LEU:N	2.27	0.66
2:F:45:ARG:CZ	7:J:-4:DG:C5'	2.73	0.66
6:I:-72:DA:C2	7:J:73:DT:O2	2.48	0.66
7:J:-11:DC:H2''	7:J:-10:DG:C5'	2.24	0.66
7:J:20:DG:N2	7:J:21:DG:C6	2.64	0.66
9:W:415:ILE:HA	9:W:418:LEU:CD2	2.26	0.66
9:W:654:GLU:O	9:W:655:LEU:C	2.38	0.66
9:W:541:THR:HG23	9:W:543:THR:H	1.60	0.66
9:W:738:PHE:O	9:W:739:GLN:OE1	2.14	0.66
7:J:39:DA:H2''	7:J:40:DC:H5'	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:347:LEU:HB3	9:W:348:PRO:HD2	1.76	0.66
9:W:656:LYS:HA	9:W:825:VAL:CG1	2.25	0.66
5:E:48:LEU:HB3	5:E:52:ARG:HH12	1.61	0.66
2:F:29:ILE:CG2	2:F:30:THR:N	2.57	0.66
2:F:75:HIS:ND1	4:H:93:THR:CG2	2.58	0.66
3:G:77:ARG:HD3	6:I:58:DG:P	2.34	0.66
9:W:606:LEU:HD12	9:W:607:PRO:O	1.96	0.66
3:C:39:TYR:CZ	4:D:71:ALA:CB	2.78	0.66
3:C:41:GLU:HB3	4:D:84:SER:O	1.96	0.66
3:G:24:GLN:NE2	4:H:44:GLN:OE1	2.29	0.66
6:I:-7:DG:H2''	6:I:-6:DT:C5	2.31	0.66
9:W:345:LYS:HE2	9:W:1037:ASP:N	2.11	0.66
4:H:54:LYS:O	4:H:58:ILE:HG13	1.95	0.66
6:I:38:DT:H2'	6:I:39:DA:C8	2.30	0.66
9:W:419:ILE:HD12	9:W:451:LEU:HD13	1.78	0.66
9:W:655:LEU:HD23	9:W:825:VAL:CB	2.26	0.66
9:W:656:LYS:HE2	9:W:826:GLU:CA	2.23	0.66
1:A:65:LEU:CB	7:J:17:DA:H3'	2.26	0.66
6:I:-19:DG:H2''	6:I:-18:DC:H5	1.59	0.66
8:O:54:ARG:CG	8:O:58:ASP:CB	2.74	0.66
9:W:611:GLU:CG	9:W:816:VAL:CG1	2.74	0.66
9:W:1170:TRP:HE3	9:W:1174:TRP:NE1	1.94	0.66
3:C:40:ALA:HB3	4:D:86:ILE:HD12	1.74	0.66
7:J:4:DG:H2'	7:J:5:DT:H6	1.59	0.66
7:J:14:DT:H2''	7:J:15:DT:H73	1.76	0.66
9:W:307:TYR:CD2	9:W:327:ILE:HD13	2.27	0.66
9:W:1183:LEU:HD12	9:W:1184:ILE:N	2.11	0.66
4:D:78:ALA:O	4:D:83:ARG:O	2.13	0.66
5:E:69:ARG:HB3	2:F:24:ASP:CB	2.26	0.66
2:F:45:ARG:CZ	7:J:-4:DG:C4'	2.74	0.66
7:J:51:DG:C5	7:J:52:DC:C4	2.84	0.66
7:J:79:DG:H2''	7:J:80:DC:OP2	1.96	0.66
9:W:177:HIS:CE1	9:W:217:TRP:CD2	2.84	0.66
9:W:650:ASN:HA	9:W:654:GLU:CG	2.26	0.66
5:E:61:LEU:HD13	2:F:37:LEU:HA	0.70	0.65
7:J:34:DC:H2''	7:J:35:DT:C6	2.30	0.65
9:W:315:ASN:ND2	9:W:458:GLY:HA2	2.11	0.65
2:B:98:TYR:OH	4:H:65:ASP:HB3	1.97	0.65
3:G:45:ALA:HB2	6:I:38:DT:OP1	1.95	0.65
8:N:31:GLN:OE1	8:N:38:PRO:CB	2.44	0.65
9:W:290:ILE:O	9:W:341:ARG:NH2	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:660:ASN:CG	9:W:696:LYS:NZ	2.54	0.65
1:A:76:GLN:HG3	1:A:80:THR:HG22	1.78	0.65
7:J:-17:DT:C4	7:J:-16:DT:C4	2.84	0.65
7:J:33:DT:C2'	7:J:34:DC:H5	2.05	0.65
9:W:177:HIS:HE2	9:W:217:TRP:CG	2.13	0.65
9:W:599:LYS:C	9:W:601:ASP:N	2.54	0.65
9:W:1171:SER:HB3	9:W:1245:LYS:HE3	1.77	0.65
9:W:1180:GLU:O	9:W:1183:LEU:HG	1.96	0.65
4:H:84:SER:C	7:J:-34:DA:OP1	2.39	0.65
7:J:14:DT:H2''	7:J:15:DT:C5	2.31	0.65
7:J:23:DG:C8	7:J:24:DC:H5	2.13	0.65
4:D:70:ILE:HD13	4:D:98:LEU:CD1	2.27	0.65
7:J:68:DT:H2''	7:J:69:DC:C5	2.32	0.65
2:F:78:ARG:HH12	6:I:29:DA:P	2.19	0.65
1:A:60:LEU:HD13	1:A:93:GLN:HG2	1.77	0.65
2:B:68:ASP:OD2	2:B:89:ALA:HA	1.97	0.65
3:C:97:LEU:HB3	3:C:100:VAL:CG2	2.27	0.65
4:D:116:THR:O	4:D:119:THR:HG22	1.97	0.65
3:G:45:ALA:CB	6:I:38:DT:OP1	2.44	0.65
7:J:69:DC:H2''	7:J:70:DT:C5	2.32	0.65
6:I:23:DA:N1	7:J:-22:DG:C6	2.64	0.65
6:I:38:DT:C2'	6:I:39:DA:C8	2.80	0.65
7:J:-33:DG:H2''	7:J:-32:DT:C5'	2.27	0.65
9:W:391:TRP:HD1	9:W:414:PHE:CZ	2.14	0.65
1:A:52:ARG:HD2	3:G:111:ILE:HD11	1.79	0.65
2:F:88:TYR:OH	4:H:80:TYR:HE1	1.73	0.65
6:I:43:DT:C4	7:J:-43:DA:N1	2.65	0.65
9:W:720:MET:SD	9:W:720:MET:C	2.79	0.65
5:E:42:ARG:N	5:E:43:PRO:CD	2.56	0.65
7:J:19:DC:C2'	7:J:20:DG:N7	2.60	0.65
9:W:1099:PRO:HG2	9:W:1102:ASN:HB3	1.78	0.65
1:A:70:LEU:CD1	2:B:25:ASN:CG	2.70	0.64
4:D:121:ALA:O	4:D:122:LYS:CB	2.44	0.64
7:J:-48:DC:H2''	7:J:-47:DC:C6	2.32	0.64
8:N:8:LEU:HD21	8:N:69:LEU:O	1.97	0.64
9:W:437:MET:HE1	9:W:457:MET:SD	2.36	0.64
9:W:223:LEU:HD11	9:W:285:HIS:HA	1.79	0.64
9:W:525:LEU:HA	9:W:528:SER:HB3	1.77	0.64
2:B:30:THR:HB	6:I:-12:DC:OP2	1.96	0.64
3:C:112:GLN:NE2	5:E:108:ASN:CG	2.56	0.64
2:F:79:LYS:N	6:I:28:DG:OP1	2.29	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:56:DC:N4	7:J:-57:DT:O4	2.30	0.64
9:W:387:MET:CB	9:W:414:PHE:CE1	2.80	0.64
9:W:508:GLN:OE1	9:W:508:GLN:N	2.30	0.64
9:W:795:PRO:HG3	9:W:836:LYS:CB	2.26	0.64
1:A:65:LEU:HB3	7:J:17:DA:H3'	1.79	0.64
2:B:52:GLU:OE1	2:B:52:GLU:N	2.30	0.64
2:B:84:MET:CE	2:B:88:TYR:OH	2.43	0.64
6:I:21:DC:H2'	6:I:22:DC:C6	2.32	0.64
6:I:54:DG:H2'	6:I:55:DT:H72	1.79	0.64
7:J:-32:DT:C2'	7:J:-31:DA:C8	2.77	0.64
7:J:34:DC:H2''	7:J:35:DT:H6	1.63	0.64
9:W:402:GLU:CD	9:W:403:MET:N	2.56	0.64
9:W:1025:GLY:CA	9:W:1139:LEU:HD21	2.27	0.64
2:B:31:LYS:HB3	2:B:32:PRO:HD3	1.79	0.64
2:B:26:ILE:CD1	2:B:59:LYS:CD	2.76	0.64
6:I:5:DC:C1'	6:I:6:DC:C5	2.81	0.64
7:J:-17:DT:H2''	7:J:-16:DT:O5'	1.97	0.64
7:J:38:DG:C2	7:J:39:DA:C5	2.86	0.64
9:W:185:HIS:O	9:W:186:ARG:NH1	2.27	0.64
1:A:83:ARG:HB2	2:B:80:THR:OG1	1.98	0.64
7:J:-28:DC:C5	7:J:-27:DC:N4	2.66	0.64
1:A:46:VAL:O	1:A:50:GLU:HG3	1.98	0.64
1:A:88:ALA:HB2	2:B:83:ALA:N	2.13	0.64
3:G:67:GLY:CA	3:G:78:ILE:HD11	2.23	0.64
9:W:207:CYS:HA	9:W:211:TYR:HD2	1.62	0.64
9:W:660:ASN:CB	9:W:696:LYS:HZ2	2.11	0.64
2:F:76:ALA:O	2:F:77:LYS:CG	2.45	0.64
7:J:-9:DC:H2''	7:J:-8:DG:H8	1.63	0.64
9:W:362:GLU:N	9:W:362:GLU:OE1	2.30	0.64
9:W:387:MET:C	9:W:414:PHE:CE1	2.76	0.64
9:W:813:HIS:C	9:W:814:VAL:HG23	2.22	0.64
9:W:1143:LYS:HD3	9:W:1187:PHE:CD1	2.32	0.64
6:I:-3:DG:C5	6:I:-2:DC:C4	2.84	0.64
6:I:-3:DG:N1	7:J:4:DG:N2	2.46	0.64
9:W:473:THR:OG1	9:W:476:ARG:NH2	2.26	0.64
9:W:607:PRO:CD	9:W:810:GLN:O	2.45	0.64
9:W:612:ARG:O	9:W:817:TYR:HA	1.97	0.64
9:W:1013:GLU:HG2	9:W:1041:PRO:HG2	1.79	0.64
1:A:83:ARG:NH1	7:J:27:DG:H5'	2.14	0.63
2:F:35:ARG:HH12	6:I:8:DC:P	2.21	0.63
9:W:556:VAL:HG22	9:W:593:PHE:HE2	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1174:TRP:HE1	9:W:1247:PRO:HD3	1.63	0.63
7:J:-25:DC:H2''	7:J:-24:DT:H6	1.60	0.63
9:W:293:SER:HB3	9:W:307:TYR:CD1	2.33	0.63
9:W:317:ASP:OD1	9:W:318:GLU:N	2.31	0.63
9:W:371:ILE:HG13	9:W:371:ILE:O	1.98	0.63
9:W:510:MET:O	9:W:538:MET:HB3	1.98	0.63
9:W:1104:LEU:HD12	9:W:1105:THR:N	2.14	0.63
1:A:133:GLU:HA	3:C:99:ARG:HH22	1.63	0.63
6:I:-60:DG:N2	7:J:61:DC:O2	2.31	0.63
6:I:64:DT:H2''	6:I:65:DA:OP2	1.98	0.63
9:W:643:GLY:HA2	9:W:646:PHE:CE2	2.33	0.63
9:W:696:LYS:HG2	9:W:819:LEU:HD23	1.80	0.63
3:C:97:LEU:CD1	4:D:62:PHE:HE2	2.07	0.63
6:I:-22:DA:C4	6:I:-21:DC:C5	2.87	0.63
9:W:660:ASN:CB	9:W:696:LYS:NZ	2.62	0.63
4:D:76:ARG:NH2	4:D:80:TYR:OH	2.30	0.63
6:I:-84:DA:H2''	6:I:-83:DC:C5	2.33	0.63
7:J:-14:DA:H2''	7:J:-13:DA:C8	2.33	0.63
7:J:5:DT:H2''	7:J:6:DA:C8	2.34	0.63
1:A:100:LEU:HD22	2:B:37:LEU:HD13	1.79	0.63
2:F:45:ARG:HH11	7:J:-4:DG:H4'	1.58	0.63
6:I:33:DC:N4	7:J:-33:DG:N1	2.47	0.63
8:N:17:VAL:HG11	8:N:26:VAL:HG13	1.80	0.63
9:W:437:MET:CG	9:W:438:PRO:HD3	2.28	0.63
9:W:607:PRO:CG	9:W:811:LYS:HA	2.27	0.63
9:W:807:ARG:NH2	11:W:1302:ADP:O3B	2.30	0.63
3:C:112:GLN:HE22	5:E:108:ASN:CG	2.06	0.63
2:F:80:THR:OG1	6:I:28:DG:C5'	2.47	0.63
6:I:71:DA:C8	6:I:72:DT:C7	2.82	0.63
8:N:28:ALA:HA	8:N:31:GLN:HG2	1.80	0.63
9:W:391:TRP:O	9:W:391:TRP:HE3	1.82	0.63
9:W:1023:LYS:HZ2	9:W:1024:PHE:HE1	1.44	0.63
6:I:54:DG:C2'	6:I:55:DT:H72	2.28	0.63
9:W:348:PRO:HG2	9:W:483:MET:CG	2.29	0.63
9:W:654:GLU:OE2	9:W:658:ALA:HB2	1.98	0.63
2:B:59:LYS:O	2:B:63:GLU:HG3	1.99	0.63
3:G:116:LEU:HD12	3:G:117:PRO:HD3	1.80	0.63
6:I:-80:DG:C8	6:I:-79:DG:C6	2.87	0.63
7:J:-17:DT:H2'	7:J:-16:DT:C6	2.34	0.63
9:W:1070:ARG:NH2	9:W:1113:GLU:HG2	2.14	0.63
2:B:98:TYR:OH	4:H:65:ASP:CB	2.47	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-64:DC:H2''	6:I:-63:DC:C6	2.34	0.62
8:N:40:GLN:HA	8:N:72:ARG:HE	1.63	0.62
9:W:599:LYS:O	9:W:600:LYS:C	2.42	0.62
9:W:795:PRO:HD3	9:W:836:LYS:HD2	1.79	0.62
7:J:-38:DA:C4	7:J:-37:DG:C6	2.87	0.62
7:J:-19:DG:OP1	9:W:773:ALA:HB2	1.99	0.62
9:W:674:GLN:OE1	9:W:674:GLN:N	2.32	0.62
9:W:1043:LYS:HD2	9:W:1048:TYR:CE1	2.34	0.62
3:C:112:GLN:HE22	5:E:108:ASN:ND2	1.97	0.62
6:I:5:DC:N3	7:J:-6:DG:O6	2.33	0.62
7:J:-47:DC:H2''	7:J:-46:DT:C5	2.33	0.62
9:W:603:GLU:HG2	9:W:603:GLU:O	1.98	0.62
9:W:784:ASP:OD1	9:W:785:THR:N	2.32	0.62
9:W:656:LYS:HD2	9:W:826:GLU:HA	1.80	0.62
6:I:-35:DA:H2	7:J:36:DA:C2	2.18	0.62
7:J:-46:DT:OP2	7:J:-46:DT:H6	1.82	0.62
9:W:730:TYR:CD2	9:W:731:LEU:HD12	2.34	0.62
9:W:1098:GLN:OE1	9:W:1104:LEU:HD21	1.99	0.62
1:A:83:ARG:HD3	6:I:-24:DG:H4'	1.81	0.62
3:C:40:ALA:HB2	4:D:86:ILE:HD13	1.73	0.62
3:C:63:LEU:HD22	4:D:42:LEU:HB2	1.81	0.62
5:E:48:LEU:HB3	5:E:52:ARG:NH1	2.15	0.62
3:G:26:PRO:HB3	4:H:37:TYR:CZ	2.35	0.62
7:J:-25:DC:H2''	7:J:-24:DT:H73	1.81	0.62
7:J:37:DC:C2	7:J:38:DG:N7	2.67	0.62
9:W:781:MET:O	9:W:810:GLN:NE2	2.32	0.62
3:C:40:ALA:CB	4:D:86:ILE:HD13	2.25	0.62
3:C:47:ALA:HB1	4:D:91:ILE:HD11	1.81	0.62
6:I:23:DA:N1	7:J:-22:DG:C5	2.68	0.62
4:D:97:LEU:C	4:D:97:LEU:HD12	2.25	0.62
3:G:77:ARG:NH2	7:J:-54:DC:H5'	2.15	0.62
6:I:-8:DC:H2''	6:I:-7:DG:C8	2.33	0.62
6:I:9:DG:C5	6:I:10:DC:C4	2.88	0.62
6:I:47:DG:C6	6:I:48:DG:C6	2.88	0.62
9:W:313:ARG:NH2	9:W:751:ARG:NH2	2.48	0.62
3:C:100:VAL:HG21	2:F:98:TYR:CE2	2.33	0.62
4:D:36:ILE:HD11	7:J:48:DG:H5''	1.80	0.62
6:I:-72:DA:N1	7:J:73:DT:O2	2.33	0.62
6:I:23:DA:C6	6:I:24:DA:C6	2.88	0.62
2:B:50:ILE:O	2:B:54:THR:HG23	2.00	0.61
2:B:68:ASP:OD1	2:B:72:TYR:CE1	2.53	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:TYR:OH	4:H:65:ASP:CG	2.42	0.61
5:E:79:LYS:HD2	5:E:80:THR:H	1.65	0.61
5:E:121:PRO:O	2:F:53:GLU:OE1	2.18	0.61
8:N:45:PHE:CG	8:N:67:LEU:CD2	2.82	0.61
8:O:16:GLU:O	8:O:29:LYS:NZ	2.33	0.61
9:W:181:ILE:CG2	9:W:182:VAL:N	2.63	0.61
9:W:616:VAL:HG11	9:W:695:GLY:HA3	1.82	0.61
9:W:1170:TRP:HE3	9:W:1174:TRP:CD1	2.18	0.61
3:C:34:LEU:CD2	3:C:39:TYR:CZ	2.82	0.61
5:E:63:ARG:HD2	2:F:30:THR:HG23	1.82	0.61
6:I:33:DC:N4	7:J:-33:DG:C6	2.67	0.61
7:J:-35:DG:C4	7:J:-34:DA:C5	2.88	0.61
5:E:62:ILE:HA	2:F:33:ALA:HB1	1.83	0.61
6:I:-1:DG:N1	7:J:2:DG:C6	2.68	0.61
7:J:-33:DG:H2'	7:J:-32:DT:C6	2.34	0.61
9:W:241:ARG:O	9:W:244:ASN:OD1	2.18	0.61
9:W:379:PHE:CE1	9:W:597:ARG:CD	2.83	0.61
9:W:629:ILE:CG2	9:W:650:ASN:ND2	2.63	0.61
4:D:46:HIS:CB	4:D:49:THR:OG1	2.47	0.61
6:I:-20:DC:H2''	6:I:-19:DG:C8	2.35	0.61
9:W:379:PHE:CE1	9:W:597:ARG:NE	2.69	0.61
9:W:414:PHE:O	9:W:418:LEU:HD23	2.00	0.61
3:C:83:LEU:HD21	4:D:55:ALA:HB1	1.82	0.61
9:W:586:LEU:C	9:W:586:LEU:HD23	2.26	0.61
2:F:97:LEU:HD22	2:F:100:PHE:CD2	2.35	0.61
3:G:24:GLN:O	4:H:37:TYR:HD2	1.82	0.61
9:W:414:PHE:HE2	9:W:509:PHE:CZ	2.19	0.61
9:W:488:LEU:CD2	9:W:490:THR:HG22	2.30	0.61
4:H:85:THR:HG23	7:J:-34:DA:OP1	2.00	0.61
3:C:79:ILE:CG1	4:D:52:SER:HB3	2.29	0.61
6:I:-35:DA:C6	6:I:-34:DG:C6	2.89	0.61
7:J:-26:DC:H2''	7:J:-25:DC:C6	2.35	0.61
9:W:390:LEU:HD11	9:W:395:ASP:HB2	1.83	0.61
9:W:611:GLU:HA	9:W:816:VAL:HB	1.83	0.61
9:W:834:ARG:O	9:W:838:ILE:HG13	2.01	0.61
1:A:132:GLY:O	3:C:99:ARG:CZ	2.48	0.61
3:G:43:VAL:HB	6:I:39:DA:OP1	2.00	0.61
6:I:-39:DT:O4	7:J:38:DG:O6	2.18	0.61
7:J:-9:DC:H2''	7:J:-8:DG:C8	2.35	0.61
7:J:15:DT:O2	7:J:16:DA:C5	2.54	0.61
9:W:642:LYS:C	9:W:646:PHE:CE2	2.79	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:664:LEU:HG	9:W:664:LEU:O	2.01	0.61
9:W:1264:ARG:HH11	9:W:1264:ARG:HG3	1.65	0.61
7:J:-22:DG:C5'	9:W:649:LEU:HD21	2.31	0.60
9:W:609:LYS:HD3	9:W:806:HIS:CG	2.36	0.60
9:W:723:MET:HA	9:W:726:ILE:HD12	1.82	0.60
9:W:1059:ALA:CB	9:W:1132:LEU:HD11	2.31	0.60
3:C:23:LEU:HD13	3:C:53:ALA:HA	1.82	0.60
3:C:81:ARG:O	3:C:85:LEU:CG	2.47	0.60
2:F:50:ILE:O	2:F:54:THR:HG23	2.02	0.60
6:I:-8:DC:N3	6:I:-7:DG:C6	2.69	0.60
7:J:32:DG:H2''	7:J:33:DT:H73	1.79	0.60
7:J:78:DG:C5	7:J:79:DG:C6	2.89	0.60
9:W:1026:ASN:OD1	9:W:1028:LYS:HG2	2.01	0.60
2:B:45:ARG:HD3	7:J:8:DG:H5'	1.83	0.60
2:B:45:ARG:O	2:B:46:ILE:HG13	2.01	0.60
3:C:63:LEU:HD13	4:D:42:LEU:CA	2.31	0.60
6:I:9:DG:N7	6:I:10:DC:N4	2.49	0.60
7:J:15:DT:H2''	7:J:16:DA:C8	2.36	0.60
9:W:696:LYS:HE2	9:W:819:LEU:HB3	1.83	0.60
1:A:47:ALA:HB1	2:B:39:ARG:NH2	2.15	0.60
3:C:112:GLN:NE2	5:E:108:ASN:ND2	2.49	0.60
2:F:33:ALA:HA	2:F:36:ARG:HG3	1.84	0.60
7:J:-38:DA:C8	7:J:-37:DG:N7	2.69	0.60
9:W:607:PRO:CG	9:W:812:ASN:N	2.58	0.60
3:G:47:ALA:HB3	3:G:48:PRO:CD	2.31	0.60
6:I:-12:DC:H2'	6:I:-11:DG:H8	1.58	0.60
9:W:295:ARG:CD	9:W:1198:ARG:HH22	2.01	0.60
9:W:1192:GLY:HA2	9:W:1194:TRP:CZ3	2.36	0.60
1:A:62:ILE:HG22	1:A:63:ARG:N	2.15	0.60
2:B:73:THR:OG1	2:B:81:VAL:HG22	2.01	0.60
3:C:44:GLY:HA3	4:D:87:THR:CA	2.29	0.60
4:H:86:ILE:HG22	4:H:91:ILE:HD11	1.83	0.60
6:I:55:DT:O4	7:J:-55:DA:N1	2.34	0.60
7:J:32:DG:H2''	7:J:33:DT:C5	2.35	0.60
9:W:793:TRP:O	9:W:794:ASN:CB	2.48	0.60
6:I:-22:DA:C5	6:I:-21:DC:N4	2.70	0.60
6:I:23:DA:C5	6:I:24:DA:C6	2.90	0.60
7:J:-23:DT:H2''	7:J:-22:DG:H5'	1.83	0.60
4:D:36:ILE:HG23	7:J:49:DC:OP2	2.01	0.60
6:I:-25:DA:H1'	6:I:-24:DG:C8	2.37	0.60
7:J:-11:DC:H2''	7:J:-10:DG:O4'	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:GLN:NE2	5:E:80:THR:HA	2.17	0.60
3:G:115:LEU:C	3:G:115:LEU:HD12	2.26	0.60
4:H:98:LEU:HG	4:H:99:LEU:HD12	1.82	0.60
6:I:-14:DA:C2	6:I:-13:DA:C4	2.90	0.60
6:I:23:DA:C5	7:J:-22:DG:C6	2.90	0.60
8:N:45:PHE:CB	8:N:67:LEU:HD22	2.30	0.60
9:W:368:PRO:C	9:W:370:PHE:H	2.10	0.60
3:C:34:LEU:HD23	3:C:39:TYR:OH	2.01	0.60
3:C:71:ARG:HH12	4:D:49:THR:HG23	1.65	0.60
3:G:91:GLU:HB3	3:G:95:LYS:CE	2.29	0.60
2:F:29:ILE:HD13	2:F:55:ARG:NH2	2.17	0.59
6:I:-57:DC:H2''	6:I:-56:DC:C5	2.37	0.59
7:J:-17:DT:C6	7:J:-16:DT:C4	2.89	0.59
9:W:345:LYS:CG	9:W:1036:ALA:HB3	2.31	0.59
9:W:419:ILE:HD12	9:W:451:LEU:CD1	2.31	0.59
3:C:46:GLY:HA3	4:D:88:SER:OG	2.02	0.59
4:H:55:ALA:O	4:H:59:MET:HG2	2.01	0.59
6:I:-69:DA:H2''	6:I:-68:DG:C8	2.37	0.59
7:J:84:DG:H2''	7:J:85:DT:C5	2.37	0.59
8:N:31:GLN:OE1	8:N:38:PRO:HG3	2.02	0.59
9:W:210:ASN:O	9:W:211:TYR:CD1	2.55	0.59
9:W:350:TYR:CE1	9:W:1042:VAL:CG1	2.82	0.59
9:W:696:LYS:CG	9:W:819:LEU:HD23	2.32	0.59
9:W:767:PHE:CD2	9:W:769:LEU:HD11	2.37	0.59
2:F:84:MET:SD	2:F:101:GLY:HA3	2.42	0.59
6:I:-53:DG:N2	7:J:54:DT:O2	2.35	0.59
7:J:-38:DA:C4	7:J:-37:DG:C5	2.90	0.59
7:J:-50:DT:C2'	7:J:-49:DG:C8	2.85	0.59
5:E:34:ALA:HB1	5:E:38:ALA:HB3	1.84	0.59
6:I:-73:DC:N3	6:I:-72:DA:N6	2.49	0.59
7:J:61:DC:H2''	7:J:62:DC:H5''	1.84	0.59
9:W:208:LYS:HG2	9:W:230:TYR:CD2	2.38	0.59
4:H:78:ALA:O	4:H:83:ARG:N	2.35	0.59
6:I:-35:DA:N6	7:J:35:DT:N3	2.50	0.59
6:I:-11:DG:H2''	6:I:-10:DC:C6	2.38	0.59
7:J:-69:DG:C2'	7:J:-68:DA:N7	2.64	0.59
9:W:330:LEU:HD12	9:W:331:ALA:N	2.17	0.59
1:A:51:ILE:O	1:A:55:GLN:HG3	2.01	0.59
4:H:73:GLU:O	4:H:77:LEU:HD13	2.02	0.59
6:I:-3:DG:N7	6:I:-2:DC:C4	2.70	0.59
7:J:38:DG:N2	7:J:39:DA:C2	2.70	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:LEU:CD2	3:C:90:ASP:CG	2.75	0.59
6:I:-28:DT:H4'	6:I:-27:DC:OP1	2.02	0.59
6:I:54:DG:O6	7:J:-54:DC:N3	2.35	0.59
9:W:367:GLN:CG	9:W:371:ILE:HD11	2.33	0.59
9:W:388:ALA:HA	9:W:391:TRP:HB2	1.85	0.59
9:W:540:ILE:O	9:W:540:ILE:CG1	2.46	0.59
9:W:1164:PRO:CD	9:W:1176:LYS:HE3	2.29	0.59
5:E:66:PRO:CB	2:F:29:ILE:HG12	2.23	0.59
2:F:82:THR:HG22	2:F:84:MET:N	2.16	0.59
6:I:-43:DT:C4	6:I:-42:DT:O4	2.56	0.59
6:I:2:DG:C6	7:J:-3:DA:N6	2.70	0.59
9:W:379:PHE:CE1	9:W:597:ARG:HD2	2.24	0.59
9:W:390:LEU:HD12	9:W:393:LYS:HB2	1.84	0.59
9:W:655:LEU:O	9:W:659:SER:HB3	2.03	0.59
3:G:97:LEU:HD11	4:H:62:PHE:HE2	1.68	0.59
9:W:361:PHE:CE1	9:W:362:GLU:O	2.56	0.59
9:W:649:LEU:O	9:W:654:GLU:CB	2.51	0.59
1:A:108:ASN:ND2	2:B:42:GLY:O	2.36	0.58
1:A:116:ARG:NH1	1:A:120:MET:CG	2.64	0.58
2:B:30:THR:CG2	6:I:-12:DC:OP1	2.51	0.58
6:I:-30:DG:N7	6:I:-29:DC:C5	2.70	0.58
6:I:3:DT:O4	7:J:-4:DG:O6	2.20	0.58
7:J:-25:DC:C6	7:J:-24:DT:H72	2.38	0.58
7:J:14:DT:H2''	7:J:15:DT:H6	1.67	0.58
7:J:50:DG:C6	7:J:51:DG:C6	2.91	0.58
9:W:255:GLN:CG	9:W:255:GLN:O	2.50	0.58
1:A:73:GLU:OE1	1:A:74:ILE:CD1	2.51	0.58
6:I:23:DA:H2''	6:I:24:DA:C8	2.39	0.58
7:J:33:DT:C2'	7:J:34:DC:C5	2.81	0.58
9:W:589:ARG:O	9:W:593:PHE:HE1	1.86	0.58
9:W:593:PHE:O	9:W:594:ILE:HG12	2.03	0.58
9:W:628:ASN:OD1	9:W:633:ASN:ND2	2.36	0.58
9:W:656:LYS:HE3	9:W:829:VAL:HG21	1.85	0.58
9:W:795:PRO:O	9:W:796:GLN:HB2	2.02	0.58
6:I:63:DA:H2'	6:I:64:DT:H72	1.84	0.58
9:W:177:HIS:HE2	9:W:217:TRP:CD1	2.21	0.58
9:W:660:ASN:HB2	9:W:696:LYS:HZ2	1.69	0.58
9:W:786:VAL:HG22	9:W:816:VAL:HG22	1.85	0.58
5:E:50:GLU:HB3	5:E:54:TYR:CE2	2.38	0.58
2:F:15:ALA:CB	9:W:690:LEU:CD1	2.81	0.58
6:I:-35:DA:C6	6:I:-34:DG:N1	2.71	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:67:DA:C6	7:J:-68:DA:N1	2.71	0.58
9:W:206:ASN:O	9:W:210:ASN:N	2.36	0.58
9:W:386:TRP:HA	9:W:389:PHE:HB3	1.85	0.58
9:W:607:PRO:CG	9:W:813:HIS:H	2.15	0.58
2:B:58:LEU:HD21	2:B:62:LEU:HD11	1.85	0.58
9:W:357:GLN:HG3	9:W:358:ARG:N	2.18	0.58
9:W:1119:PHE:CD2	9:W:1129:ALA:HB2	2.39	0.58
6:I:-59:DT:C6	6:I:-58:DG:C6	2.91	0.58
6:I:-30:DG:N7	6:I:-29:DC:N4	2.52	0.58
7:J:-35:DG:C6	7:J:-34:DA:C6	2.90	0.58
9:W:660:ASN:HB3	9:W:696:LYS:CE	2.32	0.58
6:I:-77:DC:OP2	9:W:1254[B]:ARG:NH1	2.36	0.58
9:W:305:LEU:HD21	9:W:307:TYR:OH	2.03	0.58
3:C:31:HIS:NE2	3:C:35:ARG:HD2	2.19	0.58
3:G:55:LEU:O	3:G:59:THR:HG23	2.03	0.58
3:G:78:ILE:O	3:G:78:ILE:HG22	2.03	0.58
6:I:67:DA:N1	7:J:-67:DT:O2	2.36	0.58
7:J:34:DC:C2	7:J:35:DT:C4	2.92	0.58
8:N:50:LEU:HD23	8:N:59:TYR:CZ	2.39	0.58
9:W:540:ILE:O	9:W:540:ILE:CD1	2.51	0.58
6:I:-3:DG:C5	6:I:-2:DC:N3	2.72	0.58
7:J:4:DG:H2'	7:J:5:DT:C7	2.33	0.58
7:J:78:DG:C6	7:J:79:DG:O6	2.56	0.58
9:W:380:GLN:HG3	11:W:1302:ADP:N6	2.18	0.58
9:W:681:MET:HE3	9:W:682:THR:O	2.04	0.58
9:W:707:LEU:HD23	9:W:712:HIS:HB2	1.86	0.58
9:W:1059:ALA:CB	9:W:1132:LEU:HD21	2.32	0.58
3:C:34:LEU:HD23	3:C:39:TYR:CZ	2.39	0.58
4:H:36:ILE:HD13	6:I:48:DG:H3'	1.86	0.58
6:I:-28:DT:C6	6:I:-27:DC:N4	2.72	0.58
2:B:58:LEU:CD2	2:B:62:LEU:CD1	2.73	0.57
2:B:73:THR:CB	2:B:81:VAL:HG22	2.34	0.57
5:E:66:PRO:HA	2:F:23:ARG:O	2.03	0.57
4:H:87:THR:HG23	4:H:89:ARG:H	1.69	0.57
4:H:87:THR:O	4:H:91:ILE:HD12	2.04	0.57
9:W:402:GLU:HB3	9:W:405:LEU:HG	1.86	0.57
9:W:481:LYS:HG3	9:W:483:MET:HE3	0.71	0.57
1:A:123:ASP:OD1	5:E:113:HIS:NE2	2.18	0.57
6:I:-37:DG:H2''	6:I:-36:DT:H71	1.84	0.57
6:I:-35:DA:N6	7:J:35:DT:H3	2.02	0.57
6:I:67:DA:C6	7:J:-67:DT:N3	2.56	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1246:VAL:CG1	9:W:1247:PRO:CA	2.81	0.57
3:G:31:HIS:HD2	3:G:43:VAL:HG11	1.68	0.57
6:I:-66:DA:H2''	6:I:-65:DT:H71	1.85	0.57
7:J:-37:DG:C4	7:J:-36:DG:C6	2.91	0.57
7:J:-12:DA:H1'	7:J:-11:DC:H5'	1.86	0.57
7:J:19:DC:H2'	7:J:20:DG:N7	2.18	0.57
7:J:30:DC:C4	7:J:31:DT:O4	2.57	0.57
8:N:45:PHE:HB3	8:N:59:TYR:CZ	2.39	0.57
9:W:221:SER:HB3	9:W:311:TRP:CZ2	2.40	0.57
9:W:347:LEU:HD13	9:W:483:MET:O	2.04	0.57
9:W:361:PHE:CD1	9:W:362:GLU:N	2.72	0.57
9:W:626:TYR:CE1	9:W:824:THR:HG22	2.38	0.57
9:W:643:GLY:CA	9:W:646:PHE:CZ	2.80	0.57
3:G:53:ALA:O	3:G:56:GLU:HB3	2.05	0.57
3:G:84:GLN:HE22	3:G:102:ILE:HG12	1.68	0.57
4:H:36:ILE:CD1	6:I:49:DC:P	2.89	0.57
6:I:56:DC:N4	7:J:-57:DT:C4	2.72	0.57
9:W:483:MET:HE2	9:W:483:MET:HA	1.86	0.57
9:W:509:PHE:HZ	9:W:538:MET:CE	2.16	0.57
9:W:827:GLU:HG3	9:W:828:GLU:CD	2.30	0.57
6:I:54:DG:C6	7:J:-55:DA:N1	2.73	0.57
7:J:-38:DA:C6	7:J:-37:DG:O6	2.58	0.57
9:W:180:ASP:C	9:W:181:ILE:HG13	2.30	0.57
9:W:400:ALA:H	9:W:595:LEU:HB2	1.69	0.57
9:W:603:GLU:HA	9:W:606:LEU:HD23	1.86	0.57
9:W:770:SER:HB2	9:W:773:ALA:CB	2.27	0.57
1:A:99:TYR:HD1	1:A:100:LEU:HD12	1.69	0.57
4:H:84:SER:O	4:H:85:THR:HG23	2.04	0.57
6:I:-22:DA:C4	6:I:-21:DC:C4	2.92	0.57
6:I:24:DA:C5'	9:W:793:TRP:HZ2	2.15	0.57
5:E:118:THR:OG1	7:J:-3:DA:OP1	2.19	0.57
2:F:86:VAL:O	2:F:89:ALA:HB3	2.05	0.57
3:G:35:ARG:HG3	3:G:43:VAL:HG21	1.86	0.57
3:G:87:VAL:O	3:G:94:ASN:HB3	2.05	0.57
9:W:244:ASN:OD1	9:W:245:TYR:N	2.37	0.57
9:W:348:PRO:CD	9:W:483:MET:HB3	2.33	0.57
9:W:427:PRO:HA	9:W:486:ASN:HA	1.87	0.57
9:W:437:MET:HG2	9:W:438:PRO:HD3	1.87	0.57
5:E:46:VAL:O	5:E:49:ARG:N	2.37	0.57
3:G:90:ASP:HB2	3:G:93:LEU:HB2	1.86	0.57
4:H:97:LEU:HD12	4:H:97:LEU:C	2.29	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-50:DC:H2''	6:I:-49:DG:C8	2.39	0.57
7:J:-70:DC:H2''	7:J:-69:DG:C8	2.40	0.57
7:J:-11:DC:H2'	7:J:-10:DG:H8	1.69	0.57
7:J:51:DG:C8	7:J:52:DC:C5	2.92	0.57
7:J:78:DG:C2'	7:J:79:DG:C8	2.87	0.57
9:W:463:ARG:O	9:W:467:ARG:HG3	2.05	0.57
9:W:470:GLU:HA	9:W:485:PHE:HE2	1.69	0.57
9:W:650:ASN:C	9:W:654:GLU:HB3	2.30	0.57
9:W:730:TYR:HD2	9:W:731:LEU:HD12	1.69	0.57
3:C:63:LEU:CD1	4:D:41:VAL:CG1	2.79	0.57
5:E:63:ARG:HD2	2:F:30:THR:CG2	2.35	0.57
6:I:24:DA:C2'	6:I:25:DG:C8	2.88	0.57
6:I:55:DT:O4	7:J:-55:DA:C6	2.58	0.57
8:N:31:GLN:OE1	8:N:38:PRO:HB3	2.03	0.57
9:W:460:GLN:O	9:W:463:ARG:HB3	2.05	0.57
6:I:23:DA:H2''	6:I:24:DA:H8	1.70	0.57
9:W:387:MET:HB2	9:W:414:PHE:CE1	2.40	0.57
9:W:593:PHE:O	9:W:594:ILE:HD13	2.04	0.57
9:W:648:LEU:HA	9:W:651:ILE:HD12	1.86	0.57
9:W:781:MET:CE	11:W:1302:ADP:H4'	2.35	0.57
5:E:66:PRO:HG2	5:E:67:PHE:H	1.68	0.56
6:I:4:DC:H2''	6:I:5:DC:C6	2.40	0.56
6:I:33:DC:N4	7:J:-33:DG:H1	2.02	0.56
6:I:67:DA:C5	6:I:68:DT:N3	2.72	0.56
7:J:-25:DC:C2'	7:J:-24:DT:C5	2.83	0.56
9:W:183:ILE:HG23	9:W:281:PHE:CD2	2.40	0.56
9:W:347:LEU:CD2	9:W:483:MET:O	2.47	0.56
2:B:32:PRO:HD3	6:I:-12:DC:OP2	2.05	0.56
4:D:62:PHE:CA	2:F:98:TYR:CE1	2.76	0.56
2:F:39:ARG:O	2:F:42:GLY:N	2.38	0.56
3:G:97:LEU:HB3	3:G:100:VAL:HG22	1.87	0.56
7:J:-18:DG:O5'	9:W:434:LEU:HD21	2.04	0.56
9:W:181:ILE:CG2	9:W:182:VAL:H	2.18	0.56
9:W:183:ILE:HB	9:W:214:LEU:HD22	1.88	0.56
9:W:387:MET:C	9:W:414:PHE:HE1	2.12	0.56
9:W:723:MET:O	9:W:723:MET:SD	2.62	0.56
9:W:744:THR:HG22	9:W:744:THR:O	2.04	0.56
3:G:31:HIS:CD2	3:G:31:HIS:C	2.84	0.56
3:G:39:TYR:O	3:G:40:ALA:HB2	2.05	0.56
6:I:-47:DT:H2''	6:I:-46:DC:C4	2.41	0.56
6:I:54:DG:C6	7:J:-55:DA:C2	2.92	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:179:ILE:HD12	9:W:215:ILE:HG21	1.87	0.56
9:W:417:TRP:O	9:W:421:ALA:HB3	2.06	0.56
9:W:590:ILE:O	9:W:594:ILE:HG12	2.05	0.56
9:W:618:LEU:HG	9:W:622:GLN:CD	2.31	0.56
9:W:654:GLU:OE2	9:W:664:LEU:CD2	2.48	0.56
9:W:691:ILE:HD11	9:W:697:MET:O	2.05	0.56
9:W:741:LEU:HD22	9:W:769:LEU:HG	1.87	0.56
5:E:74:ILE:HG21	2:F:59:LYS:CE	2.33	0.56
5:E:122:LYS:O	5:E:123:ASP:C	2.49	0.56
2:F:75:HIS:CE1	4:H:90:GLU:HA	2.40	0.56
3:G:25:PHE:HA	4:H:37:TYR:CD2	2.40	0.56
7:J:-17:DT:C4	7:J:-16:DT:O4	2.59	0.56
9:W:643:GLY:N	9:W:646:PHE:CE2	2.74	0.56
9:W:754:ILE:HG12	9:W:778:ILE:HD11	1.87	0.56
9:W:263:THR:HG22	9:W:264:ALA:N	2.21	0.56
9:W:348:PRO:HD2	9:W:483:MET:HB3	1.86	0.56
9:W:681:MET:SD	9:W:682:THR:HG22	2.45	0.56
1:A:101:VAL:HG13	2:B:41:GLY:N	2.19	0.56
3:G:97:LEU:O	3:G:100:VAL:N	2.36	0.56
6:I:53:DT:H3	7:J:-53:DA:H61	1.54	0.56
9:W:291:ILE:HB	9:W:308:LEU:HD23	1.88	0.56
9:W:368:PRO:O	9:W:370:PHE:N	2.34	0.56
2:B:97:LEU:HD23	3:G:101:THR:HG21	1.87	0.56
4:D:70:ILE:CD1	4:D:98:LEU:CD1	2.84	0.56
5:E:89:VAL:HG13	5:E:90:MET:N	2.21	0.56
4:H:46:HIS:O	4:H:49:THR:HB	2.05	0.56
9:W:625:TYR:OH	9:W:667:ASN:O	2.20	0.56
6:I:-38:DC:H2''	6:I:-37:DG:OP2	2.06	0.56
6:I:-30:DG:O6	7:J:29:DG:C6	2.58	0.56
6:I:52:DG:H2'	6:I:53:DT:H71	1.88	0.56
6:I:57:DA:N6	7:J:-58:DC:N4	2.54	0.56
7:J:-70:DC:N3	7:J:-69:DG:C6	2.73	0.56
7:J:-35:DG:C2'	7:J:-34:DA:C8	2.86	0.56
7:J:5:DT:H2''	7:J:6:DA:N7	2.20	0.56
7:J:15:DT:C2	7:J:16:DA:N7	2.74	0.56
9:W:505:ILE:O	9:W:507:TRP:CE3	2.59	0.56
5:E:76:GLN:HE22	5:E:80:THR:HA	1.71	0.56
5:E:119:ILE:HG13	2:F:50:ILE:HD13	1.88	0.56
3:G:55:LEU:HA	3:G:58:LEU:HD12	1.85	0.56
7:J:23:DG:C4	7:J:24:DC:C5	2.93	0.56
9:W:717:PHE:CE1	9:W:769:LEU:CB	2.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1139:LEU:HD12	9:W:1140:LYS:N	2.21	0.56
1:A:88:ALA:CB	2:B:83:ALA:CA	2.84	0.56
4:D:119:THR:O	4:D:121:ALA:O	2.23	0.56
7:J:7:DC:H2''	7:J:8:DG:C8	2.41	0.56
9:W:476:ARG:HD2	9:W:480:LYS:HB2	1.88	0.56
9:W:518:LEU:HD12	9:W:555:LEU:HD11	1.88	0.56
9:W:601:ASP:C	9:W:603:GLU:H	2.14	0.56
9:W:1025:GLY:HA3	9:W:1139:LEU:CD2	2.34	0.56
1:A:65:LEU:HD13	7:J:17:DA:O5'	2.07	0.55
1:A:76:GLN:CG	1:A:80:THR:HG22	2.35	0.55
2:B:91:LYS:HD2	4:D:76:ARG:HH22	1.71	0.55
6:I:-1:DG:C2	7:J:2:DG:N1	2.74	0.55
7:J:-58:DC:H2''	7:J:-57:DT:O5'	2.06	0.55
8:N:3:ILE:HG12	8:N:17:VAL:HG22	1.88	0.55
8:N:43:LEU:HB3	8:N:50:LEU:HD11	1.87	0.55
7:J:31:DT:H2''	7:J:32:DG:H8	1.70	0.55
7:J:69:DC:C2'	7:J:70:DT:H71	2.36	0.55
6:I:23:DA:N6	6:I:24:DA:N6	2.54	0.55
6:I:27:DG:H2''	6:I:28:DG:N7	2.21	0.55
9:W:471:PHE:HE1	9:W:481:LYS:CE	2.14	0.55
9:W:663:TYR:OH	9:W:672:VAL:CG1	2.53	0.55
9:W:1029:GLU:HG2	9:W:1030:ILE:HG23	1.88	0.55
1:A:65:LEU:HB3	1:A:66:PRO:CD	2.31	0.55
7:J:4:DG:C2'	7:J:5:DT:H6	2.15	0.55
8:N:34:GLU:HB3	8:N:36:ILE:HD12	1.87	0.55
9:W:414:PHE:CE2	9:W:509:PHE:CZ	2.94	0.55
9:W:518:LEU:HD12	9:W:555:LEU:CD1	2.31	0.55
3:C:79:ILE:CG2	3:C:80:PRO:CD	2.79	0.55
2:F:84:MET:SD	2:F:101:GLY:O	2.64	0.55
6:I:61:DA:N6	7:J:-61:DT:H3	2.05	0.55
9:W:182:VAL:CG1	9:W:245:TYR:CE2	2.87	0.55
9:W:183:ILE:HD11	9:W:216:LYS:CE	2.36	0.55
9:W:295:ARG:CD	9:W:1198:ARG:HH21	2.18	0.55
1:A:85:GLN:HA	6:I:-24:DG:OP2	2.07	0.55
5:E:120:MET:C	2:F:50:ILE:HD12	2.32	0.55
4:H:51:ILE:CD1	4:H:56:MET:CE	2.83	0.55
6:I:-20:DC:N4	7:J:21:DG:H1	2.05	0.55
6:I:49:DC:N3	6:I:50:DA:C6	2.75	0.55
6:I:66:DC:H2''	6:I:67:DA:OP2	2.05	0.55
7:J:-44:DG:C6	7:J:-43:DA:C6	2.95	0.55
7:J:26:DA:H2''	7:J:27:DG:C8	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:-69:DG:C4	7:J:-68:DA:C6	2.95	0.55
9:W:417:TRP:O	9:W:417:TRP:CD1	2.60	0.55
1:A:65:LEU:HB2	7:J:18:DG:OP2	2.07	0.55
3:C:25:PHE:HD2	3:C:52:ALA:HB1	1.72	0.55
3:G:25:PHE:CZ	3:G:56:GLU:CA	2.89	0.55
3:G:80:PRO:HG3	4:H:55:ALA:CB	2.35	0.55
4:H:63:VAL:O	4:H:67:PHE:N	2.34	0.55
6:I:-56:DC:H2''	6:I:-55:DG:C8	2.41	0.55
6:I:43:DT:C2'	6:I:44:DC:O5'	2.55	0.55
8:N:28:ALA:C	8:N:31:GLN:HG2	2.32	0.55
9:W:1114:LYS:O	9:W:1115:LYS:HG2	2.07	0.55
9:W:1247:PRO:HB2	9:W:1251:HIS:HB2	1.89	0.55
1:A:85:GLN:HG2	6:I:-24:DG:P	2.47	0.55
6:I:-28:DT:C6	6:I:-27:DC:C4	2.95	0.55
7:J:14:DT:H2'	7:J:15:DT:C7	2.23	0.55
9:W:766:VAL:O	9:W:766:VAL:HG13	2.06	0.55
9:W:1014:VAL:HG12	9:W:1124:VAL:HG22	1.87	0.55
9:W:1132:LEU:HD12	9:W:1132:LEU:C	2.31	0.55
7:J:-35:DG:H2''	7:J:-34:DA:H8	1.69	0.55
8:N:28:ALA:HA	8:N:31:GLN:CD	2.32	0.55
9:W:429:ILE:HB	9:W:507:TRP:NE1	2.22	0.55
9:W:1157:PHE:CE2	9:W:1183:LEU:HD21	2.41	0.55
1:A:88:ALA:CB	2:B:83:ALA:N	2.70	0.54
3:C:25:PHE:CD2	3:C:26:PRO:HD2	2.41	0.54
4:D:81:ASN:O	4:D:82:LYS:HB2	2.06	0.54
6:I:-38:DC:C2	6:I:-37:DG:C5	2.95	0.54
6:I:-6:DT:C2'	6:I:-5:DA:N7	2.69	0.54
6:I:3:DT:H2''	6:I:4:DC:C5	2.42	0.54
6:I:58:DG:H2''	6:I:59:DA:C8	2.42	0.54
9:W:376:LEU:HD22	11:W:1302:ADP:N6	2.22	0.54
9:W:434:LEU:HD12	9:W:434:LEU:C	2.32	0.54
1:A:113:HIS:CB	5:E:126:LEU:HD21	2.37	0.54
5:E:85:GLN:NE2	2:F:82:THR:HA	2.22	0.54
3:G:102:ILE:O	3:G:103:ALA:C	2.50	0.54
6:I:-61:DG:H2''	6:I:-60:DG:C8	2.41	0.54
6:I:23:DA:C4	6:I:24:DA:C5	2.96	0.54
7:J:-69:DG:C5	7:J:-68:DA:N6	2.76	0.54
8:O:54:ARG:HG3	8:O:58:ASP:OD2	2.06	0.54
9:W:305:LEU:HD21	9:W:307:TYR:CZ	2.41	0.54
9:W:544:PRO:HG2	9:W:796:GLN:OE1	2.07	0.54
9:W:614:LEU:N	9:W:818:ARG:O	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:63:ARG:CZ	7:J:-13:DA:C5'	2.85	0.54
4:H:62:PHE:O	4:H:66:VAL:CG2	2.47	0.54
6:I:17:DA:N6	7:J:-18:DG:C6	2.75	0.54
6:I:21:DC:C5	6:I:22:DC:N4	2.76	0.54
9:W:295:ARG:HG2	9:W:303:SER:OG	2.07	0.54
9:W:633:ASN:OD1	9:W:633:ASN:N	2.37	0.54
5:E:119:ILE:HG23	2:F:43:VAL:HG21	1.88	0.54
6:I:5:DC:N3	7:J:-6:DG:C6	2.76	0.54
7:J:-55:DA:H2''	7:J:-54:DC:C6	2.43	0.54
7:J:17:DA:H2''	7:J:18:DG:H8	1.68	0.54
9:W:295:ARG:HD2	9:W:1198:ARG:HH21	1.66	0.54
9:W:311:TRP:HZ3	9:W:319:ALA:HA	1.71	0.54
9:W:433:PRO:HD3	9:W:513:ASP:CB	2.32	0.54
2:F:79:LYS:HB2	6:I:27:DG:H3'	1.90	0.54
6:I:-38:DC:N4	6:I:-37:DG:O6	2.41	0.54
6:I:47:DG:C5	6:I:48:DG:C5	2.95	0.54
9:W:476:ARG:HG2	9:W:480:LYS:C	2.33	0.54
9:W:717:PHE:CE1	9:W:769:LEU:HB3	2.43	0.54
9:W:786:VAL:HG23	9:W:786:VAL:O	2.08	0.54
1:A:45:THR:HG23	1:A:46:VAL:HG23	1.89	0.54
2:B:27:GLN:O	2:B:28:GLY:C	2.50	0.54
2:B:32:PRO:HA	2:B:35:ARG:NH1	2.23	0.54
3:C:46:GLY:CA	4:D:88:SER:CB	2.84	0.54
5:E:62:ILE:HG23	2:F:33:ALA:HB1	1.89	0.54
7:J:-16:DT:OP1	9:W:493:GLU:OE1	2.25	0.54
7:J:-1:DA:H2''	7:J:0:DG:H5'	1.88	0.54
9:W:359:PRO:HG2	9:W:422:ARG:HD2	1.89	0.54
9:W:486:ASN:OD1	9:W:487:VAL:N	2.41	0.54
9:W:1170:TRP:HB2	9:W:1174:TRP:HD1	1.72	0.54
1:A:46:VAL:HB	7:J:9:DT:OP1	2.08	0.54
1:A:100:LEU:HD22	2:B:37:LEU:CD1	2.37	0.54
5:E:50:GLU:HG2	5:E:53:ARG:HH21	1.72	0.54
7:J:-53:DA:H2''	7:J:-52:DC:H5'	1.89	0.54
7:J:34:DC:H2''	7:J:35:DT:O5'	2.07	0.54
9:W:220:GLU:OE1	9:W:220:GLU:HA	2.08	0.54
9:W:591:GLN:HG3	9:W:592:PRO:CD	2.33	0.54
9:W:593:PHE:O	9:W:594:ILE:CG1	2.56	0.54
5:E:65:LEU:HD22	6:I:17:DA:P	2.48	0.54
4:H:70:ILE:HD12	4:H:70:ILE:H	1.73	0.54
8:O:8:LEU:HD11	8:O:71:LEU:HG	1.89	0.54
9:W:586:LEU:HG	9:W:590:ILE:CD1	2.36	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:707:LEU:HD23	9:W:712:HIS:CB	2.38	0.54
9:W:767:PHE:CD2	9:W:769:LEU:CD1	2.91	0.54
9:W:1150:TYR:HD1	9:W:1156:LYS:CE	1.98	0.54
3:C:97:LEU:HD21	4:D:62:PHE:CE2	2.43	0.54
2:F:73:THR:OG1	2:F:81:VAL:HG22	2.08	0.54
6:I:-73:DC:N4	6:I:-72:DA:N6	2.55	0.54
6:I:-30:DG:C6	7:J:30:DC:N3	2.76	0.54
7:J:78:DG:H2''	7:J:79:DG:O5'	2.08	0.54
9:W:503:GLY:HA2	9:W:532:PHE:CD1	2.43	0.54
9:W:615:ARG:HD2	9:W:822:LYS:HG2	1.89	0.54
9:W:650:ASN:HA	9:W:654:GLU:HG2	1.90	0.54
3:G:24:GLN:HB3	4:H:40:LYS:HE3	1.90	0.54
3:G:34:LEU:HD21	4:H:67:PHE:HE1	1.73	0.54
4:H:97:LEU:HD12	4:H:98:LEU:CA	2.37	0.54
7:J:-65:DT:H2''	7:J:-64:DA:H8	1.72	0.54
9:W:229:THR:CG2	9:W:230:TYR:H	2.14	0.54
9:W:768:LEU:HD12	9:W:768:LEU:C	2.33	0.54
7:J:-38:DA:N7	7:J:-37:DG:C6	2.73	0.53
7:J:23:DG:C5	7:J:24:DC:C4	2.97	0.53
9:W:208:LYS:HG2	9:W:230:TYR:HD2	1.73	0.53
6:I:7:DC:H2''	6:I:8:DC:C5	2.43	0.53
9:W:377:ARG:HE	9:W:602:VAL:CG2	2.20	0.53
9:W:794:ASN:OD1	9:W:795:PRO:N	2.40	0.53
1:A:116:ARG:HG2	6:I:-3:DG:H5''	1.90	0.53
6:I:-35:DA:C2	7:J:36:DA:C2	2.96	0.53
7:J:-44:DG:C6	7:J:-43:DA:N6	2.77	0.53
9:W:183:ILE:HA	9:W:281:PHE:CE2	2.44	0.53
9:W:482:THR:O	9:W:483:MET:CB	2.56	0.53
9:W:611:GLU:HA	9:W:816:VAL:O	2.06	0.53
9:W:1055:MET:HA	9:W:1121:PHE:CE1	2.43	0.53
1:A:116:ARG:NH2	5:E:113:HIS:HE1	2.06	0.53
4:D:103:LEU:HD23	4:D:103:LEU:C	2.34	0.53
5:E:70:LEU:HD13	2:F:24:ASP:O	2.09	0.53
3:G:104:GLN:OE1	3:G:104:GLN:N	2.41	0.53
3:G:81:ARG:HG2	3:G:85:LEU:HD13	1.90	0.53
6:I:-43:DT:C2'	6:I:-42:DT:H71	2.39	0.53
6:I:57:DA:N6	7:J:-58:DC:H42	2.06	0.53
9:W:176:PHE:CD2	9:W:237:ARG:HD2	2.44	0.53
3:C:39:TYR:C	4:D:75:SER:HG	2.16	0.53
2:F:33:ALA:HA	2:F:36:ARG:CG	2.39	0.53
3:G:31:HIS:CD2	3:G:31:HIS:O	2.62	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:3:DT:H2''	6:I:4:DC:C6	2.42	0.53
6:I:61:DA:C6	7:J:-62:DA:N6	2.77	0.53
9:W:611:GLU:CG	9:W:816:VAL:HG12	2.32	0.53
9:W:715:LEU:HD21	9:W:780:LEU:CD2	2.38	0.53
3:C:97:LEU:HD21	4:D:62:PHE:HE2	1.73	0.53
6:I:-27:DC:H2''	6:I:-26:DT:H72	1.90	0.53
7:J:6:DA:C2'	7:J:7:DC:C5	2.83	0.53
6:I:67:DA:H1'	6:I:68:DT:O5'	2.08	0.53
9:W:626:TYR:CE1	9:W:655:LEU:HD11	2.44	0.53
5:E:72:ARG:HH12	7:J:-23:DT:H5''	1.74	0.53
6:I:-38:DC:N4	7:J:37:DC:H42	2.06	0.53
6:I:26:DG:C5	6:I:27:DG:C6	2.97	0.53
7:J:-58:DC:H2''	7:J:-57:DT:C6	2.43	0.53
3:C:51:LEU:HD11	4:D:70:ILE:HG21	1.90	0.53
3:C:97:LEU:HB3	3:C:100:VAL:HG22	1.91	0.53
4:D:36:ILE:CD1	7:J:48:DG:H5''	2.39	0.53
5:E:42:ARG:H	5:E:43:PRO:HD3	1.70	0.53
2:F:64:ASN:O	2:F:67:ARG:HB3	2.09	0.53
6:I:-3:DG:N1	7:J:4:DG:C2	2.77	0.53
7:J:-11:DC:N4	7:J:-10:DG:O6	2.42	0.53
9:W:387:MET:HB2	9:W:414:PHE:CD1	2.44	0.53
9:W:660:ASN:HB3	9:W:696:LYS:HE3	1.90	0.53
9:W:1013:GLU:CG	9:W:1041:PRO:HG2	2.39	0.53
3:C:32:ARG:NE	6:I:-44:DA:P	2.81	0.52
3:G:34:LEU:HD21	4:H:67:PHE:CE1	2.44	0.52
6:I:67:DA:H2	7:J:-67:DT:O2	1.87	0.52
7:J:17:DA:C2'	7:J:18:DG:C8	2.92	0.52
9:W:433:PRO:HG2	9:W:514:GLU:CD	2.34	0.52
1:A:95:ALA:HB2	2:B:90:LEU:CD1	2.37	0.52
3:C:77:ARG:HG3	4:D:51:ILE:N	2.23	0.52
5:E:100:LEU:HD13	2:F:37:LEU:CD2	2.40	0.52
2:F:64:ASN:OD1	2:F:65:VAL:N	2.42	0.52
2:F:75:HIS:HE1	4:H:90:GLU:HA	1.73	0.52
2:F:97:LEU:HD22	2:F:100:PHE:HD2	1.73	0.52
3:G:116:LEU:HD12	3:G:117:PRO:CD	2.38	0.52
6:I:-75:DC:H2'	6:I:-74:DC:C6	2.45	0.52
6:I:38:DT:H2''	6:I:39:DA:C8	2.43	0.52
7:J:-45:DG:N2	7:J:-44:DG:C2	2.77	0.52
7:J:58:DG:H2''	7:J:59:DC:H5	1.72	0.52
9:W:418:LEU:HD11	9:W:428:HIS:CE1	2.44	0.52
3:C:65:LEU:HD23	3:C:90:ASP:CG	2.32	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:76:ALA:O	2:F:77:LYS:HG3	2.10	0.52
4:H:93:THR:CG2	4:H:94:ALA:N	2.71	0.52
9:W:606:LEU:CD1	9:W:607:PRO:O	2.58	0.52
9:W:643:GLY:CA	9:W:646:PHE:CE2	2.92	0.52
9:W:1102:ASN:O	9:W:1105:THR:HG22	2.09	0.52
3:C:97:LEU:HD11	4:D:62:PHE:CD2	2.40	0.52
3:G:47:ALA:N	3:G:48:PRO:HD2	2.25	0.52
3:G:91:GLU:CB	3:G:95:LYS:HE3	2.31	0.52
6:I:5:DC:O3'	6:I:6:DC:C6	2.63	0.52
7:J:-37:DG:C2'	7:J:-36:DG:C8	2.85	0.52
7:J:-7:DG:H2''	7:J:-6:DG:C8	2.44	0.52
9:W:1171:SER:CB	9:W:1245:LYS:HE3	2.39	0.52
3:C:39:TYR:OH	4:D:71:ALA:CB	2.57	0.52
6:I:-74:DC:H1'	6:I:-73:DC:H5'	1.92	0.52
6:I:-69:DA:C2	7:J:71:DG:N2	2.78	0.52
6:I:23:DA:C5	7:J:-22:DG:O6	2.62	0.52
6:I:54:DG:H2''	6:I:55:DT:C7	2.39	0.52
6:I:57:DA:H61	7:J:-58:DC:N4	2.07	0.52
6:I:71:DA:C8	6:I:72:DT:H73	2.44	0.52
7:J:80:DC:O3'	7:J:81:DC:O4'	2.28	0.52
8:N:8:LEU:CD2	8:N:69:LEU:O	2.57	0.52
9:W:284:PHE:HE1	9:W:314:LEU:HD13	1.75	0.52
9:W:767:PHE:HE2	9:W:769:LEU:HD11	1.69	0.52
3:G:84:GLN:OE1	3:G:88:ARG:HG2	2.09	0.52
4:H:73:GLU:OE2	4:H:97:LEU:HD21	2.09	0.52
7:J:-17:DT:C4	7:J:-16:DT:N3	2.78	0.52
7:J:23:DG:C5	7:J:24:DC:C5	2.98	0.52
7:J:67:DT:C2'	7:J:68:DT:C7	2.87	0.52
9:W:284:PHE:CE1	9:W:314:LEU:HD22	2.44	0.52
2:F:76:ALA:O	2:F:77:LYS:HG2	2.09	0.52
3:G:35:ARG:CG	3:G:43:VAL:HG21	2.40	0.52
3:G:83:LEU:O	3:G:87:VAL:HG23	2.10	0.52
9:W:510:MET:HB3	9:W:537:ARG:HA	1.92	0.52
3:C:108:LEU:HD12	3:C:110:ASN:HB2	1.92	0.52
6:I:-58:DG:N1	7:J:58:DG:N1	2.57	0.52
6:I:-30:DG:O6	7:J:30:DC:N3	2.43	0.52
6:I:-3:DG:C8	6:I:-2:DC:C4	2.98	0.52
7:J:-6:DG:H2''	7:J:-5:DG:C8	2.45	0.52
7:J:69:DC:C2'	7:J:70:DT:C7	2.88	0.52
3:C:117:PRO:O	3:C:118:LYS:C	2.53	0.52
5:E:34:ALA:HA	5:E:38:ALA:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:47:DG:C8	6:I:48:DG:N7	2.78	0.52
7:J:30:DC:H2''	7:J:31:DT:O5'	2.09	0.52
8:N:28:ALA:CA	8:N:31:GLN:HG2	2.40	0.52
9:W:611:GLU:HG2	9:W:816:VAL:CB	2.39	0.52
1:A:70:LEU:HD13	2:B:25:ASN:OD1	2.09	0.52
2:B:65:VAL:HG23	2:B:66:ILE:N	2.24	0.52
2:B:98:TYR:CE1	4:H:62:PHE:CA	2.83	0.52
3:C:77:ARG:CD	6:I:-55:DG:OP1	2.56	0.52
5:E:121:PRO:HB2	2:F:53:GLU:OE2	2.09	0.52
3:G:77:ARG:HD2	6:I:57:DA:O3'	2.06	0.52
6:I:-12:DC:N3	6:I:-11:DG:C6	2.78	0.52
7:J:-44:DG:N1	7:J:-43:DA:C6	2.78	0.52
7:J:-30:DA:C8	7:J:-29:DT:C7	2.93	0.52
7:J:-8:DG:H2''	7:J:-7:DG:H8	1.71	0.52
7:J:15:DT:N3	7:J:16:DA:N6	2.57	0.52
7:J:78:DG:C5	7:J:79:DG:C5	2.98	0.52
9:W:350:TYR:CE1	9:W:1042:VAL:HG11	2.45	0.52
9:W:431:VAL:O	9:W:512:VAL:HA	2.09	0.52
9:W:593:PHE:O	9:W:594:ILE:CD1	2.58	0.52
9:W:718:SER:HB3	9:W:724:LEU:HD21	1.90	0.52
1:A:104:PHE:HD2	2:B:38:ALA:HA	1.74	0.51
3:C:32:ARG:NE	6:I:-44:DA:O5'	2.43	0.51
5:E:124:ILE:HD12	2:F:53:GLU:OE1	2.10	0.51
6:I:5:DC:O2	6:I:6:DC:N3	2.43	0.51
6:I:21:DC:C4	6:I:22:DC:C4	2.98	0.51
6:I:69:DC:C4	6:I:70:DG:O6	2.63	0.51
1:A:65:LEU:HD21	1:A:69:ARG:NE	2.24	0.51
3:C:23:LEU:CD1	3:C:53:ALA:HB2	2.39	0.51
5:E:62:ILE:HD11	2:F:37:LEU:HD22	1.92	0.51
6:I:-49:DG:H2''	6:I:-48:DC:C5	2.46	0.51
6:I:-40:DG:N2	7:J:40:DC:N3	2.57	0.51
6:I:-3:DG:H2''	6:I:-2:DC:O5'	2.11	0.51
7:J:-35:DG:C6	7:J:-34:DA:N1	2.78	0.51
9:W:515:ALA:H	9:W:541:THR:HB	1.76	0.51
9:W:729:ASP:O	9:W:733:ILE:HG12	2.10	0.51
9:W:1152:ASP:OD1	9:W:1153:ASP:N	2.44	0.51
9:W:1198:ARG:HB2	9:W:1209:ILE:HD13	1.92	0.51
5:E:63:ARG:HD3	6:I:17:DA:H5''	1.90	0.51
3:G:47:ALA:CB	3:G:48:PRO:HD3	2.33	0.51
7:J:-38:DA:C6	7:J:-37:DG:N1	2.78	0.51
9:W:415:ILE:HA	9:W:418:LEU:HD21	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:CG	2:B:25:ASN:HD22	2.18	0.51
2:B:75:HIS:HE1	4:D:89:ARG:HD3	1.75	0.51
6:I:-79:DG:N2	7:J:79:DG:H22	2.09	0.51
6:I:-79:DG:N2	7:J:79:DG:N2	2.58	0.51
6:I:-78:DC:H1'	6:I:-77:DC:H5'	1.90	0.51
6:I:-35:DA:C8	6:I:-34:DG:C8	2.98	0.51
7:J:-70:DC:H2'	7:J:-69:DG:N7	2.24	0.51
7:J:-64:DA:C2'	7:J:-63:DT:C7	2.89	0.51
7:J:24:DC:C2	7:J:25:DT:C4	2.98	0.51
9:W:293:SER:HB3	9:W:307:TYR:HD1	1.76	0.51
9:W:295:ARG:HH11	9:W:303:SER:CB	2.23	0.51
9:W:720:MET:SD	9:W:721:VAL:CG1	2.99	0.51
3:C:27:VAL:HG13	3:C:49:VAL:HA	1.92	0.51
3:C:63:LEU:HB3	4:D:42:LEU:CD1	2.41	0.51
3:G:76:THR:O	4:H:49:THR:HA	2.09	0.51
6:I:38:DT:H2'	6:I:39:DA:N7	2.25	0.51
7:J:-70:DC:C4	7:J:-69:DG:O6	2.64	0.51
7:J:-25:DC:C2'	7:J:-24:DT:C6	2.89	0.51
7:J:32:DG:H2''	7:J:33:DT:C6	2.45	0.51
9:W:183:ILE:HB	9:W:214:LEU:CD2	2.41	0.51
9:W:390:LEU:HD12	9:W:393:LYS:CB	2.40	0.51
9:W:415:ILE:O	9:W:419:ILE:HG13	2.10	0.51
9:W:517:ARG:O	9:W:519:LYS:N	2.44	0.51
9:W:595:LEU:HD13	9:W:597:ARG:HH22	1.76	0.51
9:W:622:GLN:NE2	9:W:659:SER:O	2.43	0.51
9:W:1017:LEU:HD12	9:W:1027:LEU:HD21	1.93	0.51
1:A:42:ARG:O	1:A:45:THR:CG2	2.59	0.51
2:B:30:THR:HB	6:I:-12:DC:OP1	2.11	0.51
3:G:54:VAL:O	3:G:58:LEU:HG	2.10	0.51
6:I:63:DA:H2''	6:I:64:DT:O5'	2.11	0.51
3:C:45:ALA:HB2	7:J:38:DG:OP1	2.11	0.51
6:I:-58:DG:H2''	6:I:-57:DC:C5	2.46	0.51
6:I:54:DG:H2''	6:I:55:DT:C6	2.46	0.51
7:J:38:DG:N2	7:J:39:DA:C4	2.79	0.51
8:N:28:ALA:HA	8:N:31:GLN:CG	2.40	0.51
8:N:40:GLN:HA	8:N:72:ARG:NE	2.23	0.51
9:W:380:GLN:OE1	9:W:410:GLN:HG3	2.10	0.51
9:W:518:LEU:HD11	9:W:555:LEU:HD11	1.81	0.51
9:W:800:GLN:O	9:W:803:ALA:N	2.41	0.51
1:A:40:ARG:HH12	7:J:8:DG:N2	2.07	0.51
2:F:15:ALA:HB3	9:W:690:LEU:HD11	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:-70:DC:H2''	7:J:-69:DG:O5'	2.09	0.51
7:J:-21:DG:C2'	7:J:-20:DC:O5'	2.50	0.51
7:J:37:DC:C2	7:J:38:DG:C5	2.98	0.51
9:W:516:HIS:HB3	9:W:543:THR:HB	1.93	0.51
9:W:645:HIS:HE1	9:W:649:LEU:HD11	1.63	0.51
9:W:764:ASP:OD1	9:W:764:ASP:O	2.29	0.51
9:W:799:LEU:O	9:W:802:MET:HG2	2.10	0.51
1:A:92:LEU:N	2:B:86:VAL:HG11	2.26	0.51
4:D:87:THR:HG23	4:D:89:ARG:H	1.75	0.51
6:I:61:DA:H61	7:J:-61:DT:H3	1.57	0.51
6:I:61:DA:N1	7:J:-61:DT:C2	2.79	0.51
7:J:-70:DC:C4	7:J:-69:DG:C6	2.99	0.51
7:J:15:DT:C2	7:J:16:DA:C5	2.99	0.51
7:J:41:DC:C2	7:J:42:DA:C8	2.99	0.51
9:W:268:GLU:O	9:W:272:MET:HB2	2.10	0.51
9:W:455:CYS:SG	9:W:456:TYR:N	2.84	0.51
9:W:458:GLY:HA3	9:W:462:SER:CB	2.41	0.51
9:W:795:PRO:CD	9:W:836:LYS:HD2	2.40	0.51
9:W:1118:LEU:C	9:W:1118:LEU:HD12	2.36	0.51
1:A:63:ARG:NH2	7:J:17:DA:C4'	2.74	0.51
1:A:83:ARG:O	2:B:80:THR:HA	2.11	0.51
2:B:62:LEU:O	2:B:65:VAL:CG2	2.59	0.51
2:B:62:LEU:O	2:B:65:VAL:HG22	2.11	0.51
7:J:38:DG:N3	7:J:39:DA:C5	2.79	0.51
9:W:328:VAL:CG2	9:W:1201:PRO:HB2	2.38	0.51
9:W:462:SER:O	9:W:463:ARG:C	2.54	0.51
3:C:31:HIS:HB2	3:C:48:PRO:CB	2.38	0.50
2:F:29:ILE:CG2	2:F:30:THR:H	2.24	0.50
4:H:70:ILE:HD12	4:H:70:ILE:N	2.26	0.50
6:I:-22:DA:C6	6:I:-21:DC:C4	3.00	0.50
6:I:-8:DC:C2	6:I:-7:DG:C5	2.99	0.50
6:I:61:DA:N1	7:J:-61:DT:O2	2.44	0.50
6:I:69:DC:H2''	6:I:70:DG:H8	1.76	0.50
7:J:-44:DG:N2	7:J:-43:DA:C2	2.78	0.50
7:J:-40:DC:C2'	7:J:-39:DT:H71	2.42	0.50
9:W:178:GLY:C	9:W:218:THR:HG1	2.14	0.50
9:W:1170:TRP:CZ3	9:W:1247:PRO:HG3	2.46	0.50
2:B:34:ILE:HD11	2:B:55:ARG:HE	1.76	0.50
6:I:19:DC:C2	6:I:20:DG:C8	2.99	0.50
6:I:22:DC:H3'	9:W:519:LYS:HE2	1.94	0.50
7:J:-70:DC:C2'	7:J:-69:DG:C8	2.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:31:DT:H2''	7:J:32:DG:C8	2.45	0.50
7:J:34:DC:H5'	7:J:34:DC:H6	1.74	0.50
9:W:408:THR:HG22	9:W:443:THR:HG21	1.92	0.50
3:C:97:LEU:CD1	4:D:62:PHE:CE2	2.72	0.50
5:E:120:MET:HE3	5:E:121:PRO:HD2	1.93	0.50
6:I:-28:DT:C2'	6:I:-27:DC:C6	2.91	0.50
6:I:15:DT:C2'	6:I:16:DA:C8	2.88	0.50
6:I:45:DC:H2''	6:I:46:DA:C8	2.46	0.50
9:W:1070:ARG:HH21	9:W:1113:GLU:HG2	1.76	0.50
3:C:63:LEU:HB3	4:D:42:LEU:HD12	1.94	0.50
5:E:50:GLU:HB3	5:E:54:TYR:HE2	1.76	0.50
6:I:-62:DC:H2''	6:I:-61:DG:C5'	2.41	0.50
6:I:-24:DG:H2''	6:I:-23:DC:OP2	2.11	0.50
6:I:21:DC:N4	6:I:22:DC:N4	2.58	0.50
6:I:67:DA:C6	7:J:-68:DA:C2	2.99	0.50
9:W:398:ILE:HG12	9:W:539:LEU:CD2	2.35	0.50
9:W:488:LEU:HD23	9:W:489:LEU:N	2.26	0.50
9:W:778:ILE:O	9:W:804:ARG:HD2	2.11	0.50
9:W:1099:PRO:O	9:W:1100:LYS:C	2.52	0.50
9:W:1102:ASN:OD1	9:W:1104:LEU:HG	2.12	0.50
3:G:96:LEU:HD12	4:H:100:PRO:CD	2.38	0.50
7:J:-22:DG:H4'	9:W:649:LEU:CD2	2.42	0.50
9:W:200:THR:HG22	9:W:201:VAL:HG23	1.92	0.50
9:W:611:GLU:OE2	9:W:818:ARG:HB2	2.11	0.50
9:W:1247:PRO:HB2	9:W:1251:HIS:CB	2.42	0.50
3:C:39:TYR:OH	4:D:71:ALA:HB3	2.12	0.50
3:G:32:ARG:HA	3:G:35:ARG:HE	1.76	0.50
4:H:35:ALA:HB1	4:H:56:MET:SD	2.52	0.50
4:H:51:ILE:HD13	4:H:56:MET:HB2	1.93	0.50
4:H:51:ILE:HD13	4:H:56:MET:SD	2.52	0.50
6:I:-13:DA:N6	7:J:12:DG:C6	2.79	0.50
9:W:207:CYS:HA	9:W:211:TYR:HB2	1.93	0.50
9:W:377:ARG:NE	9:W:602:VAL:CG2	2.75	0.50
9:W:387:MET:O	9:W:391:TRP:HB2	2.11	0.50
9:W:431:VAL:O	9:W:431:VAL:CG1	2.59	0.50
2:F:75:HIS:NE2	4:H:90:GLU:OE1	2.42	0.50
6:I:-45:DA:H2''	6:I:-44:DA:C8	2.47	0.50
7:J:-11:DC:C4	7:J:-10:DG:C6	3.00	0.50
7:J:78:DG:C4	7:J:79:DG:C5	3.00	0.50
7:J:81:DC:OP2	7:J:81:DC:C6	2.64	0.50
1:A:69:ARG:HB3	2:B:22:LEU:HD23	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LYS:HG2	1:A:115:LYS:O	2.11	0.50
3:G:25:PHE:CE2	3:G:55:LEU:HB2	2.47	0.50
9:W:177:HIS:NE2	9:W:217:TRP:CD2	2.80	0.50
9:W:370:PHE:CE1	9:W:417:TRP:HZ3	2.30	0.50
9:W:1034:LEU:O	9:W:1037:ASP:O	2.30	0.50
6:I:5:DC:H2''	6:I:6:DC:C6	2.43	0.49
6:I:69:DC:H2''	6:I:70:DG:C8	2.47	0.49
7:J:6:DA:H8	7:J:6:DA:OP2	1.94	0.49
7:J:55:DT:H2''	7:J:56:DC:C5	2.46	0.49
7:J:69:DC:H2''	7:J:70:DT:C6	2.47	0.49
9:W:602:VAL:HG13	9:W:602:VAL:O	2.11	0.49
9:W:611:GLU:CB	9:W:816:VAL:HB	2.42	0.49
9:W:1077:LEU:HD23	9:W:1107:LEU:HA	1.94	0.49
9:W:1145:LEU:HD21	9:W:1149:ASN:HD21	1.77	0.49
3:C:40:ALA:HB3	4:D:86:ILE:CD1	2.29	0.49
7:J:-11:DC:H2''	7:J:-10:DG:H5'	1.95	0.49
8:N:45:PHE:HB2	8:N:59:TYR:HE2	1.69	0.49
8:N:51:GLU:HB2	8:N:54:ARG:HG3	1.93	0.49
9:W:1124:VAL:HB	9:W:1127:LEU:HD11	1.94	0.49
3:G:26:PRO:HD3	4:H:37:TYR:CG	2.47	0.49
3:G:34:LEU:CD2	4:H:67:PHE:CZ	2.95	0.49
6:I:-14:DA:C2	6:I:-13:DA:C5	3.00	0.49
6:I:67:DA:N1	7:J:-68:DA:C2	2.80	0.49
9:W:417:TRP:O	9:W:417:TRP:CG	2.65	0.49
9:W:429:ILE:HG23	9:W:429:ILE:O	2.11	0.49
9:W:437:MET:CE	9:W:457:MET:SD	3.00	0.49
9:W:488:LEU:CD2	9:W:490:THR:CG2	2.90	0.49
9:W:523:SER:CB	9:W:526:TYR:CB	2.72	0.49
9:W:794:ASN:CG	9:W:795:PRO:HD2	2.33	0.49
9:W:1143:LYS:HA	9:W:1187:PHE:CE1	2.42	0.49
3:C:34:LEU:CD2	3:C:39:TYR:OH	2.61	0.49
3:C:77:ARG:HD3	6:I:-55:DG:P	2.52	0.49
3:C:102:ILE:HD11	4:D:58:ILE:CG2	2.42	0.49
7:J:34:DC:C2'	7:J:35:DT:C5	2.96	0.49
9:W:681:MET:SD	9:W:681:MET:C	2.95	0.49
6:I:-38:DC:H2''	6:I:-37:DG:C8	2.47	0.49
6:I:67:DA:N6	7:J:-68:DA:C5	2.79	0.49
8:O:54:ARG:CG	8:O:58:ASP:OD2	2.61	0.49
9:W:221:SER:HB3	9:W:311:TRP:CH2	2.48	0.49
9:W:359:PRO:O	9:W:360:ARG:C	2.52	0.49
9:W:387:MET:HB3	9:W:414:PHE:CE1	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:705:THR:O	9:W:708:LYS:HB3	2.12	0.49
1:A:116:ARG:HH21	5:E:113:HIS:HE1	1.58	0.49
3:C:23:LEU:HD11	3:C:53:ALA:HB2	1.94	0.49
3:C:116:LEU:C	3:C:116:LEU:HD12	2.38	0.49
4:H:87:THR:CG2	4:H:90:GLU:HG2	2.35	0.49
6:I:-73:DC:C2	7:J:74:DG:N2	2.80	0.49
6:I:-40:DG:H1	7:J:40:DC:H42	1.61	0.49
8:O:24:GLU:CD	8:O:53:GLY:H	2.20	0.49
9:W:717:PHE:CE1	9:W:769:LEU:HB2	2.47	0.49
5:E:69:ARG:CB	2:F:24:ASP:CB	2.90	0.49
2:F:34:ILE:O	2:F:37:LEU:HB3	2.12	0.49
6:I:-66:DA:H2''	6:I:-65:DT:C7	2.42	0.49
7:J:26:DA:C6	7:J:27:DG:C6	3.01	0.49
7:J:28:DA:H8	7:J:28:DA:OP2	1.95	0.49
9:W:508:GLN:HB2	9:W:535:ALA:CB	2.42	0.49
9:W:636:ALA:HA	9:W:640:GLY:HA2	1.95	0.49
1:A:88:ALA:HA	2:B:83:ALA:CA	2.43	0.49
6:I:21:DC:H2''	6:I:22:DC:H5'	1.95	0.49
7:J:14:DT:C2'	7:J:15:DT:H73	2.38	0.49
9:W:350:TYR:CE1	9:W:1042:VAL:HG13	2.43	0.49
9:W:415:ILE:HA	9:W:418:LEU:HD23	1.93	0.49
9:W:1094:LYS:HE2	9:W:1097:ASN:HB3	1.95	0.49
1:A:45:THR:O	1:A:49:ARG:HG3	2.12	0.49
6:I:-59:DT:C5	6:I:-58:DG:O6	2.66	0.49
7:J:-69:DG:C2'	7:J:-68:DA:C8	2.82	0.49
9:W:751:ARG:O	9:W:754:ILE:HG22	2.12	0.49
1:A:125:GLN:HG2	1:A:128:ARG:HH12	1.78	0.49
3:G:17:ARG:HD3	3:G:27:VAL:HG11	1.95	0.49
4:H:45:VAL:HG12	4:H:46:HIS:ND1	2.28	0.49
6:I:26:DG:N7	6:I:27:DG:C6	2.81	0.49
6:I:41:DT:C2	6:I:42:DC:C5	3.01	0.49
7:J:-21:DG:H2'	7:J:-20:DC:C6	2.48	0.49
7:J:38:DG:N3	7:J:39:DA:C4	2.81	0.49
9:W:387:MET:HE2	9:W:538:MET:HE2	1.92	0.49
9:W:507:TRP:O	9:W:534:VAL:HA	2.13	0.49
9:W:663:TYR:CE2	9:W:693:SER:HB3	2.48	0.49
9:W:828:GLU:OE1	9:W:828:GLU:N	2.41	0.49
9:W:1170:TRP:CE3	9:W:1174:TRP:CD1	2.99	0.49
5:E:122:LYS:C	5:E:124:ILE:N	2.68	0.48
6:I:-73:DC:C2	6:I:-72:DA:N7	2.81	0.48
6:I:5:DC:H1'	6:I:6:DC:C4	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:52:DC:H2''	7:J:53:DC:C5	2.48	0.48
1:A:88:ALA:CB	2:B:83:ALA:HA	2.43	0.48
4:H:51:ILE:CG1	4:H:56:MET:HE3	2.43	0.48
6:I:9:DG:C5	6:I:10:DC:N4	2.81	0.48
7:J:-48:DC:C2'	7:J:-47:DC:C5	2.91	0.48
7:J:-38:DA:H2''	7:J:-37:DG:OP2	2.14	0.48
8:N:4:PHE:CD1	8:N:64:GLU:HA	2.47	0.48
9:W:746:PRO:HB2	9:W:749:GLN:HG2	1.94	0.48
3:G:47:ALA:O	3:G:48:PRO:C	2.56	0.48
6:I:-11:DG:H2''	6:I:-10:DC:H6	1.78	0.48
6:I:54:DG:H2''	6:I:55:DT:H72	1.95	0.48
7:J:50:DG:C2'	7:J:51:DG:OP2	2.57	0.48
7:J:80:DC:O5'	7:J:80:DC:H6	1.96	0.48
1:A:42:ARG:HE	6:I:70:DG:P	2.36	0.48
1:A:104:PHE:CD2	2:B:38:ALA:CA	2.96	0.48
2:B:58:LEU:HD23	2:B:62:LEU:HD12	1.93	0.48
3:C:44:GLY:H	4:D:86:ILE:C	2.14	0.48
5:E:75:ALA:CB	5:E:82:LEU:CD2	2.88	0.48
3:G:65:LEU:HA	3:G:68:ASN:OD1	2.14	0.48
6:I:-63:DC:C2	7:J:64:DG:N2	2.82	0.48
6:I:-44:DA:N1	7:J:44:DT:O4	2.47	0.48
6:I:51:DC:C5	6:I:52:DG:N7	2.81	0.48
9:W:520:ASN:ND2	9:W:522:GLU:HB3	2.29	0.48
9:W:586:LEU:HD23	9:W:587:HIS:N	2.28	0.48
9:W:1056:MET:HE2	9:W:1133:LEU:HD23	1.95	0.48
5:E:104:PHE:HA	5:E:107:THR:OG1	2.14	0.48
3:G:26:PRO:HB3	4:H:37:TYR:OH	2.13	0.48
3:G:78:ILE:HD12	4:H:49:THR:CG2	2.44	0.48
7:J:-58:DC:H2'	7:J:-57:DT:C7	2.42	0.48
9:W:309:VAL:HG13	9:W:311:TRP:CH2	2.49	0.48
9:W:488:LEU:HD22	9:W:490:THR:CG2	2.44	0.48
6:I:-22:DA:N9	6:I:-21:DC:C5	2.82	0.48
7:J:58:DG:C2'	7:J:59:DC:C5	2.95	0.48
9:W:399:LEU:HG	9:W:595:LEU:HD12	1.95	0.48
1:A:68:GLN:O	1:A:72:ARG:HG2	2.14	0.48
1:A:70:LEU:HD13	2:B:25:ASN:CB	2.44	0.48
3:C:114:VAL:O	3:C:114:VAL:HG12	2.13	0.48
5:E:61:LEU:HD22	2:F:36:ARG:C	2.38	0.48
4:H:36:ILE:HD11	6:I:48:DG:H3'	1.90	0.48
6:I:7:DC:C2'	6:I:8:DC:C5	2.97	0.48
9:W:312:ARG:HD3	9:W:313:ARG:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:333:GLU:OE1	9:W:336:LYS:HE3	2.14	0.48
9:W:611:GLU:CA	9:W:816:VAL:HB	2.43	0.48
9:W:1114:LYS:O	9:W:1115:LYS:HD3	2.13	0.48
2:F:35:ARG:NH2	2:F:39:ARG:HH22	2.10	0.48
6:I:-23:DC:C4	6:I:-22:DA:C5	3.01	0.48
6:I:-23:DC:C6	6:I:-22:DA:C8	3.02	0.48
6:I:43:DT:O4	7:J:-43:DA:N1	2.47	0.48
7:J:52:DC:H2''	7:J:53:DC:C6	2.49	0.48
8:N:2:GLN:HE21	8:N:63:LYS:NZ	2.12	0.48
3:C:63:LEU:HD22	4:D:42:LEU:HD13	1.95	0.48
3:G:26:PRO:HB2	3:G:29:ARG:HB3	1.96	0.48
6:I:-35:DA:H2''	6:I:-34:DG:C8	2.49	0.48
6:I:40:DG:H1	7:J:-40:DC:H42	1.60	0.48
9:W:315:ASN:OD1	9:W:316:TYR:HD1	1.97	0.48
9:W:521:ALA:HA	9:W:526:TYR:CE2	2.49	0.48
4:D:55:ALA:HA	4:D:58:ILE:HD12	1.95	0.48
2:F:88:TYR:O	2:F:92:ARG:HG2	2.14	0.48
3:G:47:ALA:O	3:G:51:LEU:HG	2.14	0.48
6:I:-32:DC:H2''	6:I:-31:DA:H8	1.76	0.48
6:I:-22:DA:C8	6:I:-21:DC:C5	3.01	0.48
6:I:-1:DG:C2	7:J:2:DG:C2	3.02	0.48
9:W:376:LEU:HD22	11:W:1302:ADP:HN62	1.79	0.48
9:W:602:VAL:CG1	9:W:808:ILE:CG2	2.91	0.48
9:W:681:MET:HE1	9:W:682:THR:HG22	1.95	0.48
9:W:723:MET:SD	9:W:723:MET:C	2.97	0.48
1:A:65:LEU:HB2	7:J:17:DA:H3'	1.96	0.47
3:C:30:VAL:O	3:C:34:LEU:HG	2.13	0.47
3:G:25:PHE:HA	4:H:37:TYR:HD2	1.79	0.47
7:J:-8:DG:C2'	7:J:-7:DG:C8	2.89	0.47
7:J:33:DT:C2	7:J:34:DC:C4	3.02	0.47
9:W:214:LEU:HD21	9:W:225:ASN:CB	2.43	0.47
9:W:1070:ARG:O	9:W:1073:ILE:HG22	2.14	0.47
2:B:27:GLN:O	2:B:29:ILE:N	2.47	0.47
5:E:106:ASP:O	5:E:107:THR:C	2.56	0.47
3:G:103:ALA:HB1	3:G:104:GLN:OE1	2.13	0.47
6:I:-59:DT:H2''	6:I:-58:DG:C8	2.49	0.47
6:I:-38:DC:C5	6:I:-37:DG:C6	2.96	0.47
6:I:-8:DC:C2	6:I:-7:DG:C6	3.02	0.47
8:N:22:THR:OG1	8:N:25:ASN:ND2	2.46	0.47
9:W:793:TRP:CZ3	9:W:829:VAL:HG21	2.50	0.47
9:W:1047:LYS:O	9:W:1051:THR:HG23	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1073:ILE:CG2	9:W:1110:LYS:HE2	2.36	0.47
1:A:85:GLN:HG2	6:I:-24:DG:OP1	2.14	0.47
3:C:91:GLU:C	3:C:91:GLU:CD	2.82	0.47
2:F:51:TYR:O	2:F:54:THR:OG1	2.26	0.47
9:W:214:LEU:CD2	9:W:225:ASN:HB2	2.44	0.47
9:W:427:PRO:O	9:W:507:TRP:CD1	2.67	0.47
9:W:1145:LEU:HD23	9:W:1145:LEU:C	2.39	0.47
9:W:1205:ILE:HD12	9:W:1208:LYS:HB2	1.95	0.47
2:B:68:ASP:OD1	4:D:97:LEU:HD22	2.14	0.47
3:C:63:LEU:HD13	4:D:42:LEU:HA	1.96	0.47
6:I:49:DC:C2	6:I:50:DA:C5	3.02	0.47
7:J:-35:DG:C5	7:J:-34:DA:N6	2.82	0.47
8:N:43:LEU:O	8:N:50:LEU:HG	2.15	0.47
9:W:469:TYR:O	9:W:469:TYR:CG	2.66	0.47
9:W:525:LEU:HD12	9:W:525:LEU:O	2.14	0.47
9:W:649:LEU:O	9:W:654:GLU:HB2	2.13	0.47
9:W:663:TYR:OH	9:W:693:SER:HB2	2.14	0.47
9:W:754:ILE:HG12	9:W:778:ILE:CD1	2.44	0.47
9:W:1055:MET:HE3	9:W:1121:PHE:CD2	2.43	0.47
9:W:1067:GLU:C	9:W:1067:GLU:CD	2.83	0.47
9:W:1171:SER:HB3	9:W:1245:LYS:CE	2.44	0.47
1:A:64:LYS:N	7:J:18:DG:OP1	2.47	0.47
3:C:16:THR:N	3:C:19:SER:HB2	2.30	0.47
4:D:70:ILE:CD1	4:D:98:LEU:HD12	2.44	0.47
4:D:97:LEU:HD12	4:D:97:LEU:O	2.14	0.47
5:E:85:GLN:O	5:E:86:SER:C	2.58	0.47
6:I:-3:DG:C2'	6:I:-2:DC:C6	2.97	0.47
7:J:-53:DA:H2''	7:J:-52:DC:OP2	2.14	0.47
9:W:390:LEU:HD12	9:W:393:LYS:CG	2.44	0.47
9:W:614:LEU:CB	9:W:819:LEU:HA	2.44	0.47
3:C:60:ALA:HA	4:D:41:VAL:CG1	2.45	0.47
5:E:46:VAL:O	5:E:49:ARG:HB3	2.14	0.47
3:G:77:ARG:CG	6:I:58:DG:OP1	2.63	0.47
6:I:67:DA:C4	6:I:68:DT:C2	3.03	0.47
7:J:25:DT:OP2	7:J:25:DT:H6	1.98	0.47
7:J:26:DA:C4	7:J:27:DG:C5	3.03	0.47
9:W:221:SER:CB	9:W:311:TRP:CZ2	2.98	0.47
9:W:419:ILE:CD1	9:W:451:LEU:CD1	2.91	0.47
9:W:525:LEU:HA	9:W:528:SER:CB	2.43	0.47
9:W:681:MET:CE	9:W:682:THR:HG22	2.44	0.47
9:W:696:LYS:HB3	9:W:819:LEU:HD23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1157:PHE:CD2	9:W:1183:LEU:HD11	2.49	0.47
1:A:65:LEU:HD21	1:A:69:ARG:CZ	2.45	0.47
1:A:97:GLU:O	1:A:101:VAL:HG23	2.15	0.47
4:D:70:ILE:HD13	4:D:98:LEU:HD12	1.95	0.47
5:E:61:LEU:HD22	2:F:36:ARG:HB2	1.97	0.47
5:E:74:ILE:HG13	5:E:75:ALA:N	2.29	0.47
2:F:39:ARG:C	2:F:41:GLY:N	2.68	0.47
6:I:-62:DC:H2''	6:I:-61:DG:H5''	1.96	0.47
6:I:-59:DT:C5	6:I:-58:DG:C6	3.03	0.47
6:I:23:DA:C8	6:I:24:DA:N7	2.83	0.47
6:I:23:DA:N9	6:I:24:DA:N7	2.63	0.47
6:I:32:DA:H2''	6:I:33:DC:O5'	2.14	0.47
6:I:34:DT:C2'	6:I:35:DC:H5	2.24	0.47
6:I:34:DT:C2'	6:I:35:DC:C6	2.70	0.47
7:J:32:DG:C4	7:J:33:DT:C4	3.03	0.47
7:J:34:DC:C2'	7:J:35:DT:O5'	2.62	0.47
8:N:31:GLN:CD	8:N:38:PRO:HD3	2.36	0.47
8:N:31:GLN:HB2	8:N:36:ILE:O	2.14	0.47
9:W:298:LEU:HB2	9:W:302:THR:HG22	1.96	0.47
9:W:377:ARG:CD	9:W:602:VAL:HG23	2.44	0.47
9:W:399:LEU:HA	9:W:595:LEU:HD12	1.96	0.47
9:W:404:GLY:HA2	11:W:1302:ADP:O1B	2.15	0.47
9:W:469:TYR:O	9:W:469:TYR:CD2	2.68	0.47
9:W:602:VAL:HG11	9:W:808:ILE:CG2	2.45	0.47
9:W:655:LEU:CD2	9:W:825:VAL:CB	2.85	0.47
9:W:1055:MET:HB2	9:W:1121:PHE:CZ	2.50	0.47
9:W:1179:ASP:HA	9:W:1182:LEU:HD12	1.97	0.47
3:C:116:LEU:HD12	3:C:116:LEU:O	2.15	0.47
2:F:75:HIS:CE1	4:H:93:THR:CG2	2.98	0.47
6:I:8:DC:N3	7:J:-8:DG:N1	2.48	0.47
7:J:-52:DC:H2''	7:J:-51:DG:C8	2.50	0.47
7:J:59:DC:C4	7:J:60:DA:C6	3.03	0.47
7:J:65:DG:H2''	7:J:66:DA:C8	2.49	0.47
9:W:481:LYS:HD3	9:W:483:MET:CE	2.34	0.47
9:W:599:LYS:C	9:W:601:ASP:H	2.20	0.47
9:W:1174:TRP:NE1	9:W:1247:PRO:HD3	2.28	0.47
1:A:76:GLN:OE1	2:B:21:VAL:HG23	2.15	0.47
1:A:99:TYR:CD1	1:A:100:LEU:HD12	2.49	0.47
2:B:55:ARG:O	2:B:59:LYS:HG3	2.14	0.47
5:E:43:PRO:O	5:E:44:GLY:C	2.58	0.47
6:I:24:DA:C4	6:I:25:DG:C5	3.03	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:-47:DC:H2''	7:J:-46:DT:C7	2.45	0.47
7:J:-21:DG:C5	7:J:-20:DC:N4	2.83	0.47
9:W:177:HIS:HE1	9:W:217:TRP:CE2	2.29	0.47
9:W:410:GLN:O	9:W:414:PHE:HB2	2.15	0.47
9:W:488:LEU:HD22	9:W:490:THR:HG22	1.97	0.47
9:W:1197:ILE:O	9:W:1203:LEU:HD12	2.15	0.47
1:A:61:LEU:HD22	2:B:36:ARG:HD3	1.97	0.47
6:I:-66:DA:H2''	6:I:-65:DT:OP2	2.15	0.47
6:I:5:DC:C2'	6:I:6:DC:C6	2.98	0.47
9:W:326:ASP:HA	9:W:329:LYS:CB	2.44	0.47
9:W:380:GLN:HG3	11:W:1302:ADP:HN62	1.80	0.47
9:W:419:ILE:HD13	9:W:451:LEU:HD13	1.94	0.47
9:W:814:VAL:HG12	9:W:815:MET:N	2.29	0.47
2:B:50:ILE:O	2:B:50:ILE:HG22	2.14	0.46
5:E:75:ALA:CB	5:E:82:LEU:HD23	2.45	0.46
7:J:-46:DT:OP2	7:J:-46:DT:C6	2.67	0.46
7:J:-38:DA:H2''	7:J:-37:DG:O5'	2.15	0.46
7:J:-37:DG:H1'	7:J:-36:DG:C5	2.51	0.46
7:J:-21:DG:C8	7:J:-20:DC:C5	3.03	0.46
7:J:78:DG:C2'	7:J:79:DG:H8	2.27	0.46
9:W:284:PHE:CE1	9:W:314:LEU:HD13	2.50	0.46
9:W:305:LEU:HD21	9:W:307:TYR:CE1	2.50	0.46
9:W:556:VAL:HG22	9:W:593:PHE:CE2	2.47	0.46
9:W:618:LEU:HG	9:W:622:GLN:NE2	2.30	0.46
9:W:1059:ALA:HB1	9:W:1132:LEU:HD11	1.95	0.46
9:W:1070:ARG:HG3	9:W:1110:LYS:HE3	1.96	0.46
3:C:34:LEU:HD22	4:D:71:ALA:HB1	1.98	0.46
3:G:77:ARG:HD2	6:I:57:DA:C3'	2.45	0.46
3:G:101:THR:C	3:G:102:ILE:HD13	2.41	0.46
7:J:-38:DA:C8	7:J:-37:DG:C5	3.04	0.46
9:W:408:THR:CG2	9:W:443:THR:HG21	2.45	0.46
9:W:455:CYS:SG	9:W:489:LEU:HB2	2.55	0.46
9:W:1119:PHE:HE2	9:W:1129:ALA:HA	1.76	0.46
1:A:109:LEU:HD21	5:E:129:ARG:CZ	2.45	0.46
2:B:32:PRO:HA	2:B:35:ARG:HH12	1.80	0.46
5:E:64:LYS:O	5:E:64:LYS:HG2	2.14	0.46
6:I:-76:DG:N1	7:J:76:DG:N2	2.64	0.46
6:I:-73:DC:H2''	6:I:-72:DA:OP2	2.13	0.46
6:I:-37:DG:H4'	6:I:-36:DT:OP1	2.15	0.46
6:I:-4:DC:C2	7:J:4:DG:N2	2.78	0.46
6:I:20:DG:H2''	6:I:21:DC:O5'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:63:DA:C4	7:J:-62:DA:C2	3.03	0.46
8:N:28:ALA:O	8:N:31:GLN:CG	2.62	0.46
9:W:508:GLN:HA	9:W:535:ALA:H	1.80	0.46
9:W:517:ARG:HA	9:W:517:ARG:HD2	1.51	0.46
9:W:555:LEU:CD1	9:W:555:LEU:N	2.78	0.46
9:W:723:MET:O	9:W:726:ILE:HB	2.15	0.46
9:W:827:GLU:HG3	9:W:828:GLU:OE2	2.16	0.46
2:B:68:ASP:O	2:B:72:TYR:CD1	2.69	0.46
3:C:116:LEU:HD11	3:C:118:LYS:HB2	1.97	0.46
5:E:48:LEU:CB	5:E:52:ARG:HH12	2.27	0.46
3:G:25:PHE:HE2	3:G:55:LEU:HB2	1.81	0.46
9:W:183:ILE:HD11	9:W:216:LYS:HE2	1.97	0.46
9:W:330:LEU:HD12	9:W:331:ALA:CB	2.45	0.46
9:W:714:VAL:C	9:W:715:LEU:HD12	2.41	0.46
9:W:1018:TYR:OH	9:W:1128:ASN:HB2	2.16	0.46
9:W:1138:ASP:HB3	9:W:1260:LEU:CD2	2.27	0.46
3:C:97:LEU:HD22	3:C:100:VAL:HG21	1.97	0.46
3:G:88:ARG:C	3:G:94:ASN:HD22	2.22	0.46
6:I:-49:DG:H1'	6:I:-48:DC:C2	2.51	0.46
6:I:-30:DG:O6	7:J:29:DG:O6	2.33	0.46
6:I:54:DG:H2''	6:I:55:DT:C5	2.50	0.46
9:W:315:ASN:HD21	9:W:458:GLY:CA	2.22	0.46
9:W:509:PHE:CZ	9:W:538:MET:HE3	2.51	0.46
9:W:740:ARG:CB	9:W:768:LEU:HD11	2.44	0.46
9:W:1039:THR:O	9:W:1040:LEU:HD12	2.15	0.46
1:A:119:ILE:HG12	2:B:43:VAL:HG11	1.96	0.46
3:C:28:GLY:O	6:I:-44:DA:H5''	2.15	0.46
3:C:44:GLY:CA	4:D:87:THR:HA	2.41	0.46
2:F:34:ILE:HD11	2:F:55:ARG:HD2	1.96	0.46
3:G:24:GLN:NE2	4:H:41:VAL:HG12	2.30	0.46
6:I:-77:DC:P	9:W:1254[A]:ARG:HH21	2.36	0.46
7:J:-43:DA:H2''	7:J:-42:DG:H8	1.80	0.46
7:J:34:DC:C1'	7:J:35:DT:C6	2.98	0.46
7:J:68:DT:H2''	7:J:69:DC:C6	2.51	0.46
9:W:177:HIS:NE2	9:W:217:TRP:CD1	2.82	0.46
9:W:293:SER:HB3	9:W:307:TYR:CE1	2.50	0.46
9:W:347:LEU:O	9:W:425:ASN:ND2	2.49	0.46
9:W:1114:LYS:C	9:W:1115:LYS:HG2	2.41	0.46
9:W:1164:PRO:HB2	9:W:1259:LEU:HD21	1.98	0.46
1:A:60:LEU:HD13	1:A:93:GLN:CG	2.45	0.46
2:B:67:ARG:NH2	4:D:96:ARG:O	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:66:PRO:CG	5:E:67:PHE:H	2.29	0.46
3:G:24:GLN:CD	4:H:41:VAL:CG1	2.87	0.46
6:I:-58:DG:C8	6:I:-57:DC:N4	2.84	0.46
6:I:-3:DG:H2''	6:I:-2:DC:C6	2.50	0.46
6:I:10:DC:N3	7:J:-10:DG:O6	2.49	0.46
6:I:23:DA:N6	6:I:24:DA:H61	2.13	0.46
9:W:457:MET:O	9:W:457:MET:CG	2.52	0.46
9:W:688:ARG:O	9:W:691:ILE:HG22	2.15	0.46
9:W:1043:LYS:HD2	9:W:1048:TYR:CZ	2.50	0.46
1:A:88:ALA:HA	2:B:83:ALA:HA	1.98	0.46
5:E:119:ILE:HG21	5:E:119:ILE:HD13	1.76	0.46
2:F:75:HIS:O	2:F:75:HIS:CD2	2.69	0.46
6:I:-38:DC:N3	6:I:-37:DG:N1	2.64	0.46
6:I:-4:DC:N3	7:J:4:DG:C2	2.84	0.46
6:I:17:DA:C6	7:J:-18:DG:O6	2.68	0.46
6:I:69:DC:C4	6:I:70:DG:C6	3.03	0.46
7:J:34:DC:H2'	7:J:35:DT:C5	2.49	0.46
8:N:72:ARG:HG2	8:N:72:ARG:HH11	1.80	0.46
9:W:312:ARG:O	9:W:313:ARG:C	2.59	0.46
9:W:626:TYR:OH	9:W:824:THR:HA	2.16	0.46
9:W:696:LYS:CB	9:W:819:LEU:HD23	2.46	0.46
2:B:28:GLY:O	2:B:30:THR:HG23	2.16	0.46
4:D:77:LEU:HD11	4:D:90:GLU:HB3	1.96	0.46
5:E:50:GLU:O	5:E:54:TYR:CD2	2.69	0.46
5:E:88:ALA:O	5:E:92:LEU:HG	2.16	0.46
2:F:39:ARG:O	2:F:40:ARG:C	2.59	0.46
3:G:17:ARG:CD	3:G:27:VAL:HG11	2.45	0.46
3:G:24:GLN:NE2	4:H:44:GLN:CD	2.74	0.46
3:G:24:GLN:HE22	4:H:44:GLN:CD	2.24	0.46
3:G:36:LYS:O	3:G:36:LYS:HG2	2.16	0.46
6:I:43:DT:O4	7:J:-44:DG:O6	2.33	0.46
7:J:-44:DG:H2''	7:J:-43:DA:H5'	1.98	0.46
7:J:15:DT:O2	7:J:16:DA:N7	2.49	0.46
9:W:716:ILE:HD13	9:W:787:VAL:HB	1.98	0.46
9:W:722:ARG:O	9:W:726:ILE:HG13	2.16	0.46
9:W:775:GLY:O	9:W:804:ARG:NH2	2.48	0.46
3:C:88:ARG:HG3	3:C:108:LEU:HD23	1.98	0.46
5:E:124:ILE:HD11	2:F:50:ILE:HG12	1.98	0.46
6:I:24:DA:C4	6:I:25:DG:C6	3.03	0.46
1:A:59:GLU:CD	1:A:60:LEU:O	2.58	0.45
5:E:61:LEU:HD13	2:F:37:LEU:N	2.22	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:29:ARG:NH2	4:H:32:GLU:HB3	2.31	0.45
6:I:-73:DC:C2	6:I:-72:DA:C5	3.03	0.45
6:I:5:DC:O2	6:I:6:DC:C2	2.69	0.45
9:W:458:GLY:HA3	9:W:462:SER:HB2	1.96	0.45
9:W:470:GLU:HA	9:W:485:PHE:CE2	2.50	0.45
3:C:77:ARG:NH1	6:I:-55:DG:OP1	2.47	0.45
3:C:100:VAL:HG23	3:C:100:VAL:O	2.16	0.45
4:D:43:LYS:HD2	4:D:47:PRO:HA	1.97	0.45
5:E:61:LEU:HD22	2:F:36:ARG:CB	2.46	0.45
6:I:-59:DT:C2	6:I:-58:DG:N1	2.84	0.45
6:I:-29:DC:H2''	6:I:-28:DT:C6	2.52	0.45
6:I:29:DA:H2''	6:I:30:DT:OP2	2.16	0.45
9:W:351:SER:HB2	9:W:425:ASN:H	1.80	0.45
9:W:361:PHE:CG	9:W:362:GLU:N	2.84	0.45
9:W:371:ILE:HD12	9:W:374:GLY:O	2.16	0.45
9:W:545:LEU:HD13	9:W:552:LEU:CD1	2.42	0.45
1:A:65:LEU:HD22	7:J:17:DA:O5'	2.15	0.45
3:C:51:LEU:O	3:C:55:LEU:HG	2.16	0.45
4:H:104:ALA:O	4:H:108:VAL:HG23	2.16	0.45
6:I:23:DA:C2'	6:I:24:DA:C8	2.98	0.45
6:I:67:DA:H2''	6:I:68:DT:OP2	2.15	0.45
7:J:-27:DC:H2''	7:J:-26:DC:C5	2.50	0.45
7:J:20:DG:C4'	7:J:21:DG:OP1	2.59	0.45
7:J:51:DG:H1'	7:J:52:DC:H5'	1.99	0.45
9:W:202:PRO:HA	9:W:206:ASN:HD22	1.81	0.45
9:W:443:THR:HG22	9:W:443:THR:O	2.16	0.45
9:W:512:VAL:CG1	9:W:539:LEU:HA	2.47	0.45
9:W:720:MET:SD	9:W:721:VAL:HG13	2.56	0.45
9:W:738:PHE:HB3	9:W:766:VAL:HG13	1.98	0.45
9:W:1262:PHE:HD2	9:W:1263:LEU:HD12	1.80	0.45
2:F:62:LEU:O	2:F:66:ILE:HG12	2.16	0.45
6:I:-5:DA:H8	6:I:-5:DA:OP2	2.00	0.45
6:I:50:DA:C2	7:J:-49:DG:C2	3.05	0.45
6:I:62:DT:C2	6:I:63:DA:N7	2.84	0.45
7:J:37:DC:H2''	7:J:38:DG:OP2	2.16	0.45
9:W:1114:LYS:O	9:W:1115:LYS:CG	2.63	0.45
1:A:62:ILE:CG2	1:A:63:ARG:N	2.80	0.45
1:A:95:ALA:CB	2:B:90:LEU:HD13	2.46	0.45
5:E:63:ARG:CD	2:F:30:THR:HG21	2.47	0.45
5:E:121:PRO:HA	2:F:53:GLU:OE1	2.16	0.45
5:E:128:ARG:NH1	5:E:134:ARG:HB2	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:-59:DT:N3	6:I:-58:DG:N1	2.65	0.45
6:I:-43:DT:H2''	6:I:-42:DT:H71	1.99	0.45
6:I:36:DC:OP2	6:I:36:DC:H6	1.99	0.45
9:W:290:ILE:HB	9:W:338:PHE:CD1	2.52	0.45
9:W:432:VAL:CG1	9:W:440:TRP:NE1	2.79	0.45
9:W:577:GLU:OE1	9:W:577:GLU:N	2.49	0.45
9:W:810:GLN:OE1	9:W:812:ASN:HB2	2.16	0.45
1:A:40:ARG:NH2	7:J:9:DT:O2	2.49	0.45
1:A:73:GLU:CG	2:B:25:ASN:ND2	2.77	0.45
1:A:105:GLU:C	1:A:105:GLU:CD	2.84	0.45
2:B:60:VAL:O	2:B:64:ASN:ND2	2.49	0.45
3:C:25:PHE:HD2	3:C:52:ALA:CB	2.29	0.45
3:G:26:PRO:O	3:G:30:VAL:CG2	2.56	0.45
6:I:-57:DC:H2''	6:I:-56:DC:C6	2.51	0.45
9:W:601:ASP:C	9:W:603:GLU:N	2.74	0.45
9:W:656:LYS:NZ	9:W:829:VAL:HB	2.32	0.45
9:W:715:LEU:N	9:W:785:THR:O	2.49	0.45
9:W:1117:VAL:HG12	9:W:1129:ALA:HB3	1.98	0.45
9:W:1245:LYS:HD2	9:W:1245:LYS:HA	1.72	0.45
9:W:1252:LEU:HA	9:W:1255:ARG:HB2	1.98	0.45
1:A:125:GLN:HG2	1:A:128:ARG:HH22	1.81	0.45
3:G:77:ARG:CD	6:I:57:DA:C3'	2.95	0.45
6:I:-43:DT:H2'	6:I:-42:DT:H71	1.99	0.45
6:I:-28:DT:C6	6:I:-28:DT:OP2	2.70	0.45
6:I:67:DA:C5	6:I:68:DT:C4	3.05	0.45
7:J:38:DG:N1	7:J:39:DA:C6	2.85	0.45
8:N:23:ILE:HG13	8:N:56:LEU:HG	1.99	0.45
9:W:328:VAL:HG21	9:W:1201:PRO:CB	2.45	0.45
9:W:391:TRP:HD1	9:W:414:PHE:HZ	1.63	0.45
1:A:101:VAL:HG11	2:B:40:ARG:HB3	1.98	0.45
3:C:79:ILE:CG2	3:C:80:PRO:N	2.79	0.45
3:C:102:ILE:HD11	4:D:58:ILE:HG23	1.98	0.45
6:I:-31:DA:H2''	6:I:-30:DG:OP2	2.17	0.45
6:I:67:DA:C8	6:I:68:DT:C4	3.05	0.45
7:J:-44:DG:N1	7:J:-43:DA:N1	2.65	0.45
9:W:484:LYS:HA	9:W:484:LYS:HD2	1.55	0.45
9:W:607:PRO:HB2	9:W:813:HIS:HA	1.95	0.45
9:W:674:GLN:H	9:W:674:GLN:CD	2.25	0.45
9:W:770:SER:HB2	9:W:774:GLY:N	2.32	0.45
9:W:1146:ILE:HG21	9:W:1187:PHE:CE1	2.52	0.45
9:W:1262:PHE:CD2	9:W:1263:LEU:HD12	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:25:PHE:CE1	3:G:56:GLU:CA	2.95	0.45
3:G:111:ILE:HG23	3:G:115:LEU:HD11	1.99	0.45
4:H:99:LEU:HA	4:H:100:PRO:HD3	1.83	0.45
6:I:-83:DC:H2''	6:I:-82:DG:C8	2.52	0.45
6:I:-22:DA:C6	6:I:-21:DC:N4	2.84	0.45
8:N:56:LEU:HD22	8:N:61:ILE:HG21	1.99	0.45
2:F:25:ASN:OD1	2:F:26:ILE:N	2.50	0.45
3:G:17:ARG:O	3:G:20:ARG:N	2.50	0.45
6:I:13:DT:H2'	6:I:14:DT:H71	1.99	0.45
6:I:26:DG:H2''	6:I:27:DG:C8	2.51	0.45
7:J:46:DG:H4'	7:J:47:DA:OP1	2.17	0.45
9:W:417:TRP:O	9:W:421:ALA:CB	2.64	0.45
9:W:722:ARG:HD2	9:W:722:ARG:HA	1.83	0.45
9:W:1155:LEU:C	9:W:1157:PHE:H	2.24	0.45
6:I:49:DC:H2'	6:I:50:DA:C8	2.52	0.44
9:W:265:GLU:O	9:W:268:GLU:HB3	2.17	0.44
1:A:92:LEU:HD13	2:B:86:VAL:HG13	1.98	0.44
3:G:80:PRO:CG	4:H:55:ALA:HB2	2.43	0.44
4:H:116:THR:HG21	8:O:74:ARG:HH11	1.82	0.44
6:I:-35:DA:C2'	6:I:-34:DG:C8	3.00	0.44
6:I:53:DT:H3	7:J:-53:DA:N6	2.14	0.44
7:J:-25:DC:C2	7:J:-24:DT:C5	3.05	0.44
7:J:16:DA:C2	7:J:17:DA:C6	3.05	0.44
7:J:78:DG:H2'	7:J:79:DG:C8	2.52	0.44
9:W:767:PHE:CE2	9:W:769:LEU:CD1	2.92	0.44
3:G:25:PHE:CE1	3:G:56:GLU:CB	2.99	0.44
9:W:326:ASP:HA	9:W:329:LYS:HB2	1.99	0.44
9:W:450:ASP:OD1	9:W:450:ASP:N	2.50	0.44
2:B:98:TYR:OH	4:H:65:ASP:OD2	2.34	0.44
3:C:75:LYS:HG3	3:C:77:ARG:O	2.17	0.44
3:C:108:LEU:CD1	3:C:110:ASN:HB2	2.47	0.44
2:F:15:ALA:HB3	9:W:690:LEU:CD1	2.46	0.44
3:G:97:LEU:HD11	4:H:62:PHE:CE2	2.52	0.44
6:I:0:DC:C6	6:I:1:DT:H72	2.52	0.44
7:J:17:DA:C6	7:J:18:DG:C6	3.06	0.44
9:W:417:TRP:CE2	9:W:421:ALA:HB2	2.52	0.44
9:W:456:TYR:CD1	9:W:466:ILE:HG13	2.52	0.44
9:W:509:PHE:HZ	9:W:538:MET:HE3	1.82	0.44
9:W:656:LYS:HE2	9:W:826:GLU:C	2.42	0.44
9:W:1074:LEU:HD21	9:W:1110:LYS:HG3	2.00	0.44
9:W:1164:PRO:CB	9:W:1259:LEU:HD21	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:1302:ADP:H8	11:W:1302:ADP:O5'	2.01	0.44
5:E:62:ILE:CD1	2:F:33:ALA:O	2.62	0.44
5:E:66:PRO:CA	2:F:23:ARG:O	2.64	0.44
5:E:100:LEU:O	5:E:103:LEU:HB3	2.18	0.44
5:E:120:MET:CA	2:F:50:ILE:HD12	2.47	0.44
2:F:30:THR:OG1	2:F:33:ALA:CB	2.65	0.44
3:G:57:TYR:CE2	4:H:103:LEU:HD12	2.53	0.44
3:G:63:LEU:HD23	3:G:63:LEU:HA	1.69	0.44
6:I:-43:DT:C2	6:I:-42:DT:C4	3.06	0.44
6:I:21:DC:N4	6:I:22:DC:H42	2.15	0.44
6:I:22:DC:H5''	9:W:519:LYS:CD	2.48	0.44
7:J:-65:DT:H2''	7:J:-64:DA:C8	2.51	0.44
7:J:67:DT:H2''	7:J:68:DT:C6	2.51	0.44
9:W:312:ARG:HD3	9:W:313:ARG:H	1.82	0.44
9:W:418:LEU:HD11	9:W:428:HIS:NE2	2.32	0.44
4:D:81:ASN:O	4:D:82:LYS:CB	2.65	0.44
5:E:46:VAL:CG1	5:E:50:GLU:HG3	2.47	0.44
7:J:-43:DA:H2''	7:J:-42:DG:C8	2.53	0.44
7:J:-35:DG:C2	7:J:-34:DA:C2	3.06	0.44
9:W:284:PHE:CD1	9:W:314:LEU:HD22	2.52	0.44
9:W:432:VAL:HG11	9:W:440:TRP:NE1	2.33	0.44
9:W:1255:ARG:HD2	9:W:1255:ARG:HA	1.51	0.44
3:C:100:VAL:CG2	2:F:98:TYR:CE2	3.00	0.44
5:E:100:LEU:HB2	2:F:37:LEU:HD21	2.00	0.44
2:F:35:ARG:NH1	6:I:8:DC:OP2	2.47	0.44
6:I:-34:DG:N2	7:J:35:DT:C2	2.86	0.44
6:I:-4:DC:H2''	6:I:-3:DG:H8	1.81	0.44
6:I:18:DC:C4	6:I:19:DC:N4	2.86	0.44
9:W:580:GLU:HG3	9:W:581:GLU:N	2.32	0.44
9:W:724:LEU:HD22	9:W:768:LEU:HD13	2.00	0.44
3:C:26:PRO:HD3	4:D:37:TYR:CD1	2.53	0.44
6:I:24:DA:H1'	6:I:25:DG:C8	2.53	0.44
6:I:49:DC:C4	6:I:50:DA:N6	2.86	0.44
7:J:38:DG:H2''	7:J:39:DA:C8	2.53	0.44
9:W:437:MET:HG3	9:W:438:PRO:HD3	1.98	0.44
9:W:617:GLU:CD	9:W:618:LEU:H	2.24	0.44
9:W:1256:VAL:HG13	9:W:1257:ASP:N	2.32	0.44
1:A:88:ALA:HB1	2:B:83:ALA:HA	1.99	0.44
3:C:17:ARG:HD2	6:I:-43:DT:OP1	2.16	0.44
4:D:99:LEU:HD13	4:D:103:LEU:HD22	2.00	0.44
5:E:122:LYS:O	5:E:124:ILE:N	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:43:VAL:HG12	2:F:45:ARG:H	1.83	0.44
6:I:-77:DC:OP2	9:W:1251:HIS:CD2	2.71	0.44
7:J:20:DG:N2	7:J:21:DG:C5	2.86	0.44
7:J:38:DG:C2	7:J:39:DA:C6	3.05	0.44
7:J:51:DG:C5	7:J:52:DC:N3	2.86	0.44
7:J:67:DT:C2'	7:J:68:DT:H71	2.45	0.44
9:W:448:ALA:HA	9:W:449:PRO:HD2	1.83	0.44
9:W:691:ILE:HD12	9:W:691:ILE:HA	1.82	0.44
9:W:795:PRO:O	9:W:796:GLN:CB	2.63	0.44
1:A:113:HIS:CG	5:E:126:LEU:HD21	2.53	0.43
1:A:126:LEU:O	1:A:130:ILE:HG23	2.19	0.43
4:D:40:LYS:O	4:D:43:LYS:HB3	2.17	0.43
6:I:-59:DT:C4	6:I:-58:DG:N1	2.86	0.43
6:I:43:DT:N3	7:J:-43:DA:C2	2.69	0.43
6:I:67:DA:N6	7:J:-67:DT:C4	2.86	0.43
7:J:-64:DA:H2''	7:J:-63:DT:H6	1.76	0.43
7:J:-46:DT:H2''	7:J:-45:DG:C8	2.53	0.43
9:W:272:MET:O	9:W:275:GLU:HB3	2.17	0.43
9:W:348:PRO:HA	9:W:425:ASN:CB	2.48	0.43
2:F:100:PHE:HD1	2:F:100:PHE:HA	1.61	0.43
3:G:99:ARG:HD3	3:G:99:ARG:HA	1.75	0.43
7:J:-64:DA:C2'	7:J:-63:DT:C6	3.00	0.43
7:J:34:DC:C2'	7:J:35:DT:C7	2.77	0.43
7:J:38:DG:H2''	7:J:39:DA:H8	1.83	0.43
9:W:385:ASN:O	9:W:389:PHE:CB	2.60	0.43
9:W:502:LEU:HA	9:W:507:TRP:CH2	2.52	0.43
9:W:770:SER:O	9:W:774:GLY:HA3	2.18	0.43
2:B:30:THR:CB	6:I:-12:DC:P	3.00	0.43
2:B:33:ALA:HA	2:B:36:ARG:HG2	1.99	0.43
4:D:105:LYS:O	4:D:109:SER:OG	2.29	0.43
5:E:73:GLU:C	5:E:73:GLU:CD	2.86	0.43
5:E:118:THR:CB	7:J:-3:DA:OP1	2.66	0.43
5:E:120:MET:N	2:F:50:ILE:HD12	2.32	0.43
3:G:62:ILE:HG22	3:G:62:ILE:O	2.17	0.43
6:I:-3:DG:C2	7:J:4:DG:N2	2.86	0.43
6:I:67:DA:N7	6:I:68:DT:C4	2.86	0.43
7:J:-8:DG:H2''	7:J:-7:DG:N7	2.31	0.43
9:W:379:PHE:O	9:W:379:PHE:CG	2.70	0.43
9:W:418:LEU:HD12	9:W:418:LEU:O	2.18	0.43
1:A:76:GLN:HA	1:A:79:LYS:O	2.18	0.43
1:A:124:ILE:CD1	2:B:50:ILE:HG21	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:LEU:O	2:B:40:ARG:HB2	2.18	0.43
3:C:32:ARG:HD3	6:I:-44:DA:P	2.54	0.43
3:C:102:ILE:HG13	3:C:103:ALA:N	2.33	0.43
5:E:74:ILE:HD13	2:F:59:LYS:HE3	2.00	0.43
3:G:24:GLN:O	4:H:37:TYR:CE2	2.70	0.43
3:G:25:PHE:CD1	3:G:56:GLU:HB2	2.53	0.43
3:G:83:LEU:HD11	4:H:59:MET:SD	2.58	0.43
7:J:23:DG:N9	7:J:24:DC:C5	2.86	0.43
9:W:180:ASP:HB2	9:W:218:THR:CA	2.44	0.43
9:W:297:SER:HA	9:W:303:SER:HA	2.01	0.43
9:W:348:PRO:O	9:W:483:MET:HG3	2.19	0.43
9:W:630:LEU:C	9:W:630:LEU:HD12	2.44	0.43
9:W:654:GLU:HG3	9:W:658:ALA:HB3	2.00	0.43
9:W:706:ARG:HH11	9:W:706:ARG:HG2	1.83	0.43
9:W:1017:LEU:CD1	9:W:1027:LEU:HD21	2.48	0.43
9:W:1114:LYS:O	9:W:1115:LYS:CD	2.66	0.43
9:W:1146:ILE:HG23	9:W:1147:ASN:N	2.33	0.43
5:E:101:VAL:O	5:E:102:ALA:C	2.61	0.43
5:E:108:ASN:O	5:E:112:ILE:HG13	2.18	0.43
2:F:66:ILE:HG22	2:F:70:VAL:HG23	1.99	0.43
6:I:-45:DA:C2	6:I:-44:DA:C6	3.06	0.43
6:I:42:DC:C2'	6:I:43:DT:O5'	2.43	0.43
9:W:345:LYS:HG3	9:W:1033:GLU:O	2.19	0.43
9:W:606:LEU:C	9:W:606:LEU:CD1	2.82	0.43
9:W:613:ILE:C	9:W:614:LEU:HD12	2.42	0.43
9:W:643:GLY:HA2	9:W:646:PHE:CE1	2.48	0.43
1:A:54:TYR:HB3	2:B:40:ARG:HD3	2.00	0.43
2:B:32:PRO:CD	6:I:-12:DC:OP2	2.67	0.43
2:B:51:TYR:O	2:B:55:ARG:HG3	2.18	0.43
3:C:25:PHE:HB3	3:C:52:ALA:HB1	2.01	0.43
7:J:-70:DC:C2	7:J:-69:DG:C6	3.06	0.43
7:J:-62:DA:H2''	7:J:-61:DT:OP2	2.18	0.43
7:J:-22:DG:O5'	9:W:649:LEU:HD21	2.18	0.43
7:J:38:DG:C2	7:J:39:DA:C2	3.07	0.43
7:J:38:DG:C4	7:J:39:DA:C5	3.07	0.43
9:W:656:LYS:HE3	9:W:829:VAL:CB	2.47	0.43
9:W:1198:ARG:HB2	9:W:1209:ILE:CD1	2.48	0.43
4:D:87:THR:HG23	4:D:89:ARG:N	2.33	0.43
5:E:42:ARG:N	5:E:43:PRO:HD2	2.24	0.43
6:I:-67:DA:H2	7:J:68:DT:O2	2.01	0.43
6:I:52:DG:C5	6:I:53:DT:C4	3.07	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:298:LEU:N	9:W:302:THR:O	2.48	0.43
9:W:305:LEU:HB2	9:W:1199:ASP:CG	2.43	0.43
9:W:655:LEU:HG	9:W:825:VAL:CG1	2.48	0.43
9:W:656:LYS:CE	9:W:829:VAL:HB	2.49	0.43
9:W:738:PHE:HB3	9:W:766:VAL:CG1	2.49	0.43
9:W:800:GLN:C	9:W:803:ALA:H	2.25	0.43
1:A:81:ASP:O	1:A:81:ASP:CG	2.62	0.43
2:B:97:LEU:HD23	3:G:101:THR:HG23	1.99	0.43
3:C:25:PHE:CE1	3:C:26:PRO:HD2	2.52	0.43
6:I:-41:DG:C6	6:I:-40:DG:C6	3.06	0.43
6:I:61:DA:C5	6:I:62:DT:C4	3.07	0.43
9:W:609:LYS:HD3	9:W:806:HIS:CD2	2.53	0.43
9:W:1246:VAL:HG12	9:W:1247:PRO:CA	2.49	0.43
2:B:20:LYS:O	2:B:22:LEU:HD12	2.18	0.43
2:B:61:PHE:O	2:B:65:VAL:HG22	2.19	0.43
3:C:43:VAL:HG12	7:J:39:DA:OP2	2.19	0.43
6:I:-77:DC:OP2	9:W:1251:HIS:HD2	2.02	0.43
6:I:-16:DT:H1'	6:I:-15:DA:C8	2.54	0.43
7:J:5:DT:H6	7:J:5:DT:OP2	2.01	0.43
7:J:51:DG:N7	7:J:52:DC:N4	2.67	0.43
9:W:328:VAL:CG1	9:W:335:VAL:HG21	2.49	0.43
9:W:591:GLN:O	9:W:594:ILE:HB	2.18	0.43
9:W:646:PHE:HA	9:W:649:LEU:CD1	2.37	0.43
5:E:66:PRO:HG2	5:E:67:PHE:N	2.34	0.43
5:E:108:ASN:C	5:E:108:ASN:OD1	2.62	0.43
5:E:124:ILE:HD11	2:F:50:ILE:CG1	2.48	0.43
7:J:45:DT:H2''	7:J:46:DG:N7	2.34	0.43
9:W:284:PHE:O	9:W:311:TRP:HD1	2.00	0.43
9:W:361:PHE:CD2	9:W:422:ARG:NH2	2.78	0.43
9:W:505:ILE:HB	9:W:507:TRP:CZ3	2.53	0.43
9:W:1145:LEU:CD2	9:W:1149:ASN:HD21	2.32	0.43
1:A:65:LEU:N	7:J:18:DG:OP2	2.52	0.42
2:B:30:THR:OG1	2:B:32:PRO:HD2	2.19	0.42
2:B:99:GLY:O	2:B:100:PHE:CD1	2.72	0.42
5:E:61:LEU:O	2:F:36:ARG:HG3	2.19	0.42
5:E:65:LEU:N	5:E:66:PRO:HD2	2.12	0.42
2:F:16:LYS:O	9:W:729:ASP:CG	2.62	0.42
3:G:57:TYR:HE2	4:H:103:LEU:HD12	1.84	0.42
3:G:77:ARG:HH22	7:J:-54:DC:H5'	1.83	0.42
6:I:9:DG:N7	6:I:10:DC:C4	2.87	0.42
6:I:63:DA:C6	7:J:-62:DA:C6	3.06	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:-33:DG:C6	7:J:-32:DT:C4	3.07	0.42
7:J:-5:DG:H1'	7:J:-4:DG:C8	2.54	0.42
7:J:25:DT:H4'	7:J:26:DA:OP1	2.18	0.42
9:W:1259:LEU:HD23	9:W:1259:LEU:HA	1.84	0.42
6:I:-65:DT:H2''	6:I:-64:DC:C5	2.55	0.42
6:I:-23:DC:H2''	6:I:-22:DA:O5'	2.19	0.42
7:J:-30:DA:C8	7:J:-29:DT:H71	2.55	0.42
9:W:399:LEU:HB3	9:W:540:ILE:HG22	2.01	0.42
9:W:436:THR:O	9:W:436:THR:HG22	2.18	0.42
9:W:833:ALA:O	9:W:836:LYS:HB2	2.19	0.42
1:A:65:LEU:H	7:J:18:DG:P	2.42	0.42
2:F:48:GLY:CA	2:F:51:TYR:CE2	3.00	0.42
3:G:34:LEU:CD2	4:H:67:PHE:CE1	3.02	0.42
6:I:-67:DA:C2	6:I:-66:DA:C2	3.07	0.42
6:I:24:DA:C2	6:I:25:DG:C2	3.08	0.42
7:J:-9:DC:H6	7:J:-9:DC:H2'	1.70	0.42
8:N:37:PRO:HD2	8:N:40:GLN:HE22	1.80	0.42
9:W:207:CYS:CA	9:W:211:TYR:HD2	2.29	0.42
9:W:311:TRP:CZ3	9:W:319:ALA:HA	2.53	0.42
9:W:333:GLU:OE1	9:W:333:GLU:HA	2.19	0.42
9:W:607:PRO:CD	9:W:811:LYS:CA	2.84	0.42
9:W:649:LEU:O	9:W:654:GLU:HB3	2.18	0.42
9:W:656:LYS:HD3	9:W:825:VAL:HG13	2.00	0.42
9:W:1104:LEU:HD12	9:W:1104:LEU:C	2.43	0.42
9:W:1150:TYR:CD1	9:W:1156:LYS:HG3	2.54	0.42
9:W:1155:LEU:C	9:W:1157:PHE:N	2.77	0.42
2:B:90:LEU:HA	2:B:90:LEU:HD23	1.82	0.42
3:G:51:LEU:HD21	4:H:91:ILE:CG1	2.42	0.42
7:J:-51:DG:H2''	7:J:-50:DT:OP2	2.18	0.42
9:W:405:LEU:O	9:W:406:GLY:C	2.62	0.42
9:W:1119:PHE:CE2	9:W:1129:ALA:CB	2.82	0.42
2:B:80:THR:HG21	6:I:-24:DG:H5''	2.02	0.42
4:D:37:TYR:O	4:D:41:VAL:HG23	2.20	0.42
6:I:-28:DT:C5	6:I:-27:DC:N4	2.87	0.42
6:I:23:DA:C2	7:J:-22:DG:C5	3.08	0.42
6:I:45:DC:H1'	6:I:46:DA:C5	2.54	0.42
7:J:-44:DG:C2	7:J:-43:DA:C2	3.07	0.42
7:J:-14:DA:H2''	7:J:-13:DA:H8	1.80	0.42
7:J:-11:DC:N3	7:J:-10:DG:C6	2.87	0.42
9:W:1157:PHE:CE2	9:W:1183:LEU:CD2	3.03	0.42
2:B:32:PRO:HB3	2:B:35:ARG:HH22	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:GLY:HA3	4:D:88:SER:HB3	1.92	0.42
4:D:65:ASP:OD1	4:D:69:ARG:NH2	2.52	0.42
5:E:63:ARG:CD	2:F:30:THR:CG2	2.97	0.42
6:I:-35:DA:C6	7:J:35:DT:N3	2.83	0.42
6:I:26:DG:C8	6:I:27:DG:N7	2.88	0.42
7:J:-3:DA:H2''	7:J:-2:DC:H6	1.80	0.42
7:J:19:DC:C6	7:J:20:DG:C5	3.07	0.42
7:J:51:DG:N7	7:J:52:DC:C4	2.87	0.42
9:W:1256:VAL:CG2	9:W:1260:LEU:HD13	2.50	0.42
3:C:81:ARG:O	3:C:85:LEU:CD1	2.67	0.42
2:F:27:GLN:HG3	2:F:28:GLY:N	2.35	0.42
6:I:-28:DT:OP2	6:I:-28:DT:H6	2.02	0.42
7:J:-3:DA:C2'	7:J:-2:DC:C6	3.01	0.42
9:W:414:PHE:CD2	9:W:538:MET:CE	2.71	0.42
9:W:1066:GLU:C	9:W:1066:GLU:CD	2.88	0.42
9:W:1121:PHE:CD2	9:W:1121:PHE:O	2.73	0.42
1:A:83:ARG:HH12	7:J:27:DG:H5'	1.84	0.42
3:G:43:VAL:O	6:I:38:DT:O3'	2.38	0.42
3:G:70:ALA:HB2	3:G:78:ILE:HG13	2.02	0.42
6:I:71:DA:C8	6:I:72:DT:H71	2.54	0.42
9:W:305:LEU:CD2	9:W:307:TYR:OH	2.67	0.42
9:W:545:LEU:HB2	9:W:552:LEU:HD13	2.02	0.42
9:W:824:THR:O	9:W:827:GLU:HG2	2.20	0.42
9:W:1026:ASN:HA	9:W:1052:TYR:CZ	2.50	0.42
9:W:1157:PHE:CB	9:W:1184:ILE:HD11	2.50	0.42
9:W:1251:HIS:O	9:W:1255:ARG:HG2	2.19	0.42
1:A:99:TYR:CD1	1:A:99:TYR:C	2.97	0.42
2:B:26:ILE:HD12	2:B:26:ILE:HA	1.81	0.42
2:B:73:THR:HG22	2:B:78:ARG:O	2.19	0.42
3:G:79:ILE:O	3:G:82:HIS:HB2	2.20	0.42
4:H:109:SER:O	4:H:113:LYS:HG2	2.20	0.42
6:I:-23:DC:C6	6:I:-22:DA:N7	2.86	0.42
6:I:67:DA:C2	6:I:68:DT:O2	2.73	0.42
7:J:30:DC:C5	7:J:31:DT:C4	3.08	0.42
9:W:207:CYS:SG	9:W:211:TYR:HD2	2.42	0.42
9:W:379:PHE:O	9:W:379:PHE:CD2	2.73	0.42
9:W:512:VAL:HG13	9:W:539:LEU:HA	2.00	0.42
9:W:786:VAL:HG23	9:W:816:VAL:HG22	1.94	0.42
1:A:95:ALA:HB3	2:B:90:LEU:HD11	1.97	0.42
2:B:68:ASP:O	2:B:71:THR:HG22	2.19	0.42
3:C:75:LYS:HG2	3:C:82:HIS:HE1	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:88:ARG:HA	3:G:94:ASN:HB3	2.02	0.42
3:G:104:GLN:N	3:G:104:GLN:CD	2.77	0.42
4:H:98:LEU:CG	4:H:99:LEU:HD12	2.49	0.42
6:I:-3:DG:C6	6:I:-2:DC:N3	2.87	0.42
6:I:53:DT:H2''	6:I:54:DG:OP2	2.20	0.42
7:J:-66:DG:C5	7:J:-65:DT:C4	3.08	0.42
8:N:45:PHE:HB2	8:N:67:LEU:HD21	1.99	0.42
9:W:214:LEU:HD11	9:W:225:ASN:OD1	2.20	0.42
9:W:347:LEU:HD21	9:W:484:LYS:HD2	2.02	0.42
9:W:348:PRO:HA	9:W:425:ASN:HB2	2.02	0.42
9:W:370:PHE:HE1	9:W:417:TRP:HZ3	1.67	0.42
9:W:388:ALA:N	9:W:414:PHE:CE1	2.79	0.42
9:W:399:LEU:HD22	9:W:407:LYS:HD2	2.01	0.42
9:W:430:ILE:HG22	9:W:432:VAL:HG23	2.02	0.42
9:W:688:ARG:O	9:W:692:MET:HG2	2.19	0.42
9:W:1119:PHE:CE2	9:W:1129:ALA:HA	2.55	0.42
1:A:121:PRO:HG2	1:A:122:LYS:H	1.85	0.41
1:A:127:ALA:O	1:A:130:ILE:HG13	2.20	0.41
5:E:60:LEU:HD22	5:E:93:GLN:HG2	2.02	0.41
3:G:38:ASN:O	3:G:39:TYR:C	2.62	0.41
6:I:27:DG:C2'	6:I:28:DG:C8	3.00	0.41
7:J:59:DC:C4	7:J:60:DA:N1	2.88	0.41
9:W:654:GLU:C	9:W:656:LYS:N	2.76	0.41
9:W:1043:LYS:HB2	9:W:1048:TYR:CZ	2.55	0.41
9:W:1132:LEU:CD1	9:W:1133:LEU:HG	2.50	0.41
1:A:72:ARG:HB2	2:B:22:LEU:HD22	2.02	0.41
3:G:31:HIS:HD2	3:G:31:HIS:O	2.03	0.41
6:I:-38:DC:C2	6:I:-37:DG:C6	3.08	0.41
7:J:37:DC:O2	7:J:38:DG:C5	2.73	0.41
9:W:368:PRO:HA	9:W:369:PRO:HD3	1.94	0.41
9:W:470:GLU:CG	9:W:485:PHE:HE2	2.25	0.41
9:W:481:LYS:HD2	9:W:483:MET:CE	2.34	0.41
9:W:523:SER:O	9:W:526:TYR:HB3	2.20	0.41
9:W:606:LEU:HA	9:W:607:PRO:HD2	1.78	0.41
9:W:1157:PHE:HE2	9:W:1183:LEU:HD21	1.85	0.41
9:W:1163:THR:HA	9:W:1164:PRO:HD3	1.89	0.41
1:A:124:ILE:HD12	2:B:50:ILE:CG2	2.46	0.41
5:E:60:LEU:CD1	5:E:93:GLN:CD	2.75	0.41
6:I:-4:DC:C2'	6:I:-3:DG:C8	3.01	0.41
7:J:-3:DA:C5	7:J:-2:DC:C4	3.08	0.41
9:W:621:VAL:HG11	9:W:672:VAL:HB	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:626:TYR:O	9:W:630:LEU:HD23	2.21	0.41
9:W:656:LYS:HE2	9:W:826:GLU:O	2.21	0.41
9:W:720:MET:SD	9:W:721:VAL:HG12	2.61	0.41
9:W:798:ASP:HA	9:W:801:ALA:HB3	2.02	0.41
9:W:1094:LYS:HE2	9:W:1097:ASN:CB	2.50	0.41
2:F:33:ALA:C	2:F:36:ARG:HG2	2.45	0.41
2:F:47:SER:C	2:F:50:ILE:HG22	2.45	0.41
3:G:31:HIS:NE2	6:I:39:DA:OP1	2.52	0.41
6:I:-65:DT:H2''	6:I:-64:DC:C6	2.56	0.41
6:I:24:DA:C2'	6:I:25:DG:N7	2.82	0.41
6:I:63:DA:H2'	6:I:64:DT:C7	2.50	0.41
8:N:50:LEU:HD23	8:N:59:TYR:OH	2.20	0.41
9:W:754:ILE:HG12	9:W:778:ILE:HG12	2.01	0.41
2:B:84:MET:HE3	2:B:84:MET:HB3	1.53	0.41
6:I:49:DC:C2'	6:I:50:DA:C8	3.03	0.41
7:J:-33:DG:H2''	7:J:-32:DT:H5'	2.01	0.41
7:J:-11:DC:C2'	7:J:-10:DG:C8	2.99	0.41
8:O:71:LEU:HB3	8:O:72:ARG:H	1.69	0.41
1:A:60:LEU:HD13	1:A:93:GLN:NE2	2.36	0.41
1:A:83:ARG:HB3	2:B:80:THR:HG23	2.02	0.41
4:D:104:ALA:O	4:D:108:VAL:HG23	2.21	0.41
5:E:72:ARG:CZ	7:J:-23:DT:OP1	2.67	0.41
3:G:47:ALA:CB	3:G:48:PRO:CD	2.95	0.41
7:J:-38:DA:N9	7:J:-37:DG:C5	2.89	0.41
8:N:18:GLU:HA	8:N:19:PRO:HD3	1.90	0.41
8:O:43:LEU:HB3	8:O:50:LEU:HD12	2.02	0.41
9:W:514:GLU:HA	9:W:541:THR:OG1	2.20	0.41
3:C:112:GLN:CD	5:E:108:ASN:ND2	2.79	0.41
5:E:116:ARG:CZ	7:J:-2:DC:OP2	2.69	0.41
6:I:-23:DC:C2'	6:I:-22:DA:H5'	2.46	0.41
6:I:-1:DG:N2	7:J:2:DG:N3	2.69	0.41
7:J:-60:DA:H2''	7:J:-59:DT:OP2	2.21	0.41
7:J:26:DA:C8	7:J:27:DG:N7	2.88	0.41
9:W:347:LEU:HD22	9:W:484:LYS:HA	2.03	0.41
9:W:437:MET:HG3	9:W:438:PRO:CD	2.51	0.41
9:W:618:LEU:HD11	9:W:824:THR:HG23	2.02	0.41
9:W:696:LYS:NZ	9:W:789:PHE:O	2.50	0.41
9:W:1178:GLU:O	9:W:1182:LEU:HG	2.21	0.41
2:B:68:ASP:O	2:B:72:TYR:HD1	2.03	0.41
2:F:44:LYS:HG3	2:F:45:ARG:HG2	2.03	0.41
6:I:34:DT:H2'	6:I:35:DC:C5	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:17:DA:C5	7:J:18:DG:C6	3.08	0.41
7:J:78:DG:H2''	7:J:79:DG:C8	2.56	0.41
9:W:488:LEU:HD23	9:W:489:LEU:C	2.45	0.41
9:W:660:ASN:CB	9:W:696:LYS:CE	2.99	0.41
9:W:766:VAL:O	9:W:766:VAL:CG1	2.68	0.41
9:W:1139:LEU:HD12	9:W:1139:LEU:C	2.46	0.41
1:A:48:LEU:N	1:A:48:LEU:HD12	2.35	0.41
4:D:46:HIS:HB2	4:D:49:THR:CB	2.50	0.41
5:E:87:SER:O	5:E:88:ALA:C	2.63	0.41
2:F:40:ARG:HA	2:F:40:ARG:HD3	1.92	0.41
2:F:80:THR:HG1	6:I:28:DG:C5'	2.32	0.41
3:G:92:GLU:HA	3:G:95:LYS:HD2	2.02	0.41
3:G:97:LEU:C	3:G:99:ARG:N	2.78	0.41
6:I:-73:DC:N3	6:I:-72:DA:C6	2.89	0.41
6:I:-38:DC:H42	7:J:37:DC:H42	1.68	0.41
6:I:-6:DT:C6	6:I:-5:DA:N6	2.89	0.41
6:I:27:DG:O6	7:J:-28:DC:N4	2.54	0.41
6:I:61:DA:H2'	6:I:62:DT:H71	2.03	0.41
7:J:-17:DT:C6	7:J:-16:DT:C5	3.08	0.41
7:J:33:DT:C2	7:J:34:DC:N4	2.89	0.41
7:J:84:DG:H2''	7:J:85:DT:C7	2.51	0.41
9:W:505:ILE:O	9:W:507:TRP:CZ3	2.74	0.41
9:W:655:LEU:O	9:W:659:SER:CB	2.68	0.41
1:A:95:ALA:HB1	2:B:90:LEU:HD13	2.02	0.41
3:G:101:THR:O	3:G:102:ILE:HD13	2.21	0.41
3:G:103:ALA:O	3:G:104:GLN:C	2.64	0.41
4:H:93:THR:HG23	4:H:94:ALA:N	2.34	0.41
7:J:-40:DC:C2	7:J:-39:DT:C5	3.09	0.41
9:W:615:ARG:C	9:W:822:LYS:HE2	2.46	0.41
9:W:617:GLU:CD	9:W:617:GLU:C	2.89	0.41
1:A:88:ALA:CB	2:B:83:ALA:HB2	2.51	0.40
3:G:85:LEU:N	3:G:85:LEU:HD12	2.35	0.40
6:I:-30:DG:C5	6:I:-29:DC:N3	2.89	0.40
7:J:29:DG:H2''	7:J:30:DC:OP2	2.21	0.40
7:J:72:DA:H2''	7:J:73:DT:OP2	2.21	0.40
9:W:179:ILE:CD1	9:W:215:ILE:HG21	2.50	0.40
9:W:390:LEU:HD13	9:W:393:LYS:CD	2.32	0.40
9:W:414:PHE:CE2	9:W:509:PHE:HZ	2.39	0.40
9:W:589:ARG:O	9:W:592:PRO:HD2	2.21	0.40
9:W:1256:VAL:HG23	9:W:1260:LEU:HD13	2.02	0.40
2:B:40:ARG:HD2	2:B:40:ARG:HA	1.96	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:110:GLU:CD	4:D:110:GLU:C	2.89	0.40
6:I:-30:DG:H1'	6:I:-29:DC:O5'	2.21	0.40
6:I:-12:DC:N4	6:I:-11:DG:C6	2.86	0.40
6:I:-7:DG:H2''	6:I:-6:DT:C4	2.55	0.40
6:I:2:DG:H2''	6:I:3:DT:H72	2.03	0.40
6:I:27:DG:C2	6:I:28:DG:C2	3.09	0.40
6:I:36:DC:H2''	6:I:37:DC:H6	1.86	0.40
9:W:354:TYR:CZ	9:W:359:PRO:HG3	2.55	0.40
1:A:101:VAL:HG23	2:B:37:LEU:HD22	2.04	0.40
3:C:51:LEU:HD12	3:C:51:LEU:HA	1.77	0.40
3:G:17:ARG:HB3	3:G:27:VAL:HG11	2.03	0.40
6:I:71:DA:C5	6:I:72:DT:C4	3.10	0.40
7:J:-70:DC:C2	7:J:-69:DG:C5	3.09	0.40
7:J:48:DG:H2''	7:J:49:DC:H6	1.87	0.40
7:J:66:DA:H2''	7:J:67:DT:C6	2.57	0.40
8:N:17:VAL:HG11	8:N:26:VAL:CG1	2.49	0.40
8:N:45:PHE:CD2	8:N:59:TYR:CE2	3.09	0.40
9:W:259:ASP:O	9:W:262:VAL:HG12	2.22	0.40
9:W:376:LEU:HD13	9:W:380:GLN:HB2	2.02	0.40
9:W:401:ASP:OD1	9:W:597:ARG:NH2	2.54	0.40
9:W:525:LEU:HD12	9:W:525:LEU:C	2.45	0.40
9:W:560:MET:HB3	9:W:560:MET:HE2	1.71	0.40
9:W:1084:TYR:HE1	9:W:1093:ILE:HD12	1.86	0.40
9:W:1170:TRP:HH2	9:W:1255:ARG:CG	2.35	0.40
5:E:101:VAL:HG23	2:F:37:LEU:HD11	2.03	0.40
4:H:42:LEU:HD11	4:H:51:ILE:HG21	2.03	0.40
6:I:-35:DA:N6	6:I:-34:DG:N1	2.69	0.40
6:I:69:DC:N4	6:I:70:DG:O6	2.55	0.40
7:J:-38:DA:C5	7:J:-37:DG:C5	3.03	0.40
9:W:591:GLN:HG2	9:W:592:PRO:HD3	2.01	0.40
9:W:614:LEU:HD22	9:W:819:LEU:CD1	2.52	0.40
9:W:616:VAL:HG22	9:W:699:LEU:HD11	2.02	0.40
5:E:89:VAL:O	5:E:90:MET:C	2.63	0.40
6:I:5:DC:C2	6:I:6:DC:C4	3.09	0.40
8:O:54:ARG:HG2	8:O:58:ASP:CB	2.30	0.40
9:W:255:GLN:O	9:W:255:GLN:HG3	2.19	0.40
9:W:330:LEU:HD12	9:W:331:ALA:HB2	2.03	0.40
9:W:396:ASN:HD21	9:W:559:LEU:C	2.29	0.40
9:W:583:ILE:HA	9:W:586:LEU:HB3	2.03	0.40
9:W:745:VAL:HA	9:W:746:PRO:HD3	1.99	0.40
9:W:764:ASP:O	9:W:764:ASP:CG	2.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1025:GLY:O	9:W:1026:ASN:C	2.64	0.40
9:W:1074:LEU:HD23	9:W:1074:LEU:HA	1.87	0.40
9:W:1205:ILE:CD1	9:W:1208:LYS:HB2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	95/97 (98%)	87 (92%)	7 (7%)	1 (1%)	11	45
2	B	81/103 (79%)	69 (85%)	10 (12%)	2 (2%)	4	26
2	F	90/103 (87%)	85 (94%)	5 (6%)	0	100	100
3	C	101/130 (78%)	84 (83%)	13 (13%)	4 (4%)	2	18
3	G	103/130 (79%)	93 (90%)	10 (10%)	0	100	100
4	D	93/126 (74%)	85 (91%)	7 (8%)	1 (1%)	11	45
4	H	91/126 (72%)	81 (89%)	9 (10%)	1 (1%)	11	45
5	E	108/110 (98%)	94 (87%)	9 (8%)	5 (5%)	2	17
8	N	74/76 (97%)	74 (100%)	0	0	100	100
8	O	74/76 (97%)	70 (95%)	3 (4%)	1 (1%)	9	39
9	W	868/878 (99%)	783 (90%)	71 (8%)	14 (2%)	7	37
All	All	1778/1955 (91%)	1605 (90%)	144 (8%)	29 (2%)	10	37

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	82	LYS
5	E	42	ARG
9	W	474	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	W	600	LYS
9	W	602	VAL
9	W	778	ILE
9	W	794	ASN
3	C	17	ARG
9	W	221	SER
9	W	518	LEU
2	B	80	THR
5	E	47	ALA
5	E	63	ARG
5	E	65	LEU
9	W	459	ASN
9	W	483	MET
3	C	38	ASN
4	H	82	LYS
9	W	344	SER
9	W	427	PRO
1	A	121	PRO
3	C	46	GLY
3	C	80	PRO
5	E	38	ALA
9	W	369	PRO
8	O	75	GLY
2	B	81	VAL
9	W	540	ILE
9	W	181	ILE

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	
8	N	68/68 (100%)	63 (93%)	5 (7%)	13	34
8	O	68/68 (100%)	68 (100%)	0	100	100
9	W	787/789 (100%)	754 (96%)	33 (4%)	26	48
All	All	923/925 (100%)	885 (96%)	38 (4%)	28	49

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	N	9	THR
8	N	24	GLU
8	N	27	LYS
8	N	61	ILE
8	N	71	LEU
9	W	322	GLU
9	W	346	ILE
9	W	366	VAL
9	W	391	TRP
9	W	478	LYS
9	W	484	LYS
9	W	495	ILE
9	W	540	ILE
9	W	541	THR
9	W	598	LEU
9	W	602	VAL
9	W	606	LEU
9	W	613	ILE
9	W	631	THR
9	W	632	LYS
9	W	633	ASN
9	W	635	SER
9	W	645	HIS
9	W	652	MET
9	W	660	ASN
9	W	681	MET
9	W	703	LEU
9	W	720	MET
9	W	721	VAL
9	W	723	MET
9	W	731	LEU
9	W	739	GLN
9	W	799	LEU
9	W	1124	VAL
9	W	1132	LEU
9	W	1255	ARG
9	W	1263	LEU
9	W	1268	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
8	N	2	GLN
8	N	25	ASN
8	N	40	GLN
8	N	41	GLN
8	O	25	ASN
9	W	206	ASN
9	W	304	GLN
9	W	306	GLN
9	W	334	GLN
9	W	343	ASN
9	W	425	ASN
9	W	548	ASN
9	W	557	ASN
9	W	667	ASN
9	W	737	ASN
9	W	1147	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are 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
11	ADP	W	1302	10	28,29,29	1.92	6 (21%)	43,45,45	2.36	16 (37%)
10	BEF	W	1301	11	0,3,3	-	-	-		

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
11	ADP	W	1302	10	-	3/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	W	1302	ADP	C5-C4	5.59	1.49	1.39
11	W	1302	ADP	PA-O3A	4.97	1.64	1.59
11	W	1302	ADP	C5-C6	2.66	1.48	1.41
11	W	1302	ADP	C5-N7	-2.49	1.34	1.39
11	W	1302	ADP	C8-N7	2.43	1.36	1.31
11	W	1302	ADP	PB-O2B	-2.32	1.46	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	W	1302	ADP	C5-C4-N3	-6.33	118.00	126.72
11	W	1302	ADP	N3-C4-N9	5.32	136.21	127.17
11	W	1302	ADP	O3B-PB-O2B	4.21	123.57	107.80
11	W	1302	ADP	O3A-PA-O1A	4.09	123.00	110.70
11	W	1302	ADP	C4-C5-N7	-3.97	106.05	110.58
11	W	1302	ADP	C2-N3-C4	3.85	121.23	111.83
11	W	1302	ADP	C3'-C2'-C1'	3.70	108.47	101.46
11	W	1302	ADP	N3-C2-N1	-3.54	123.22	128.58
11	W	1302	ADP	C5-N7-C8	3.45	108.88	103.45
11	W	1302	ADP	O3A-PB-O1B	-2.94	95.56	111.04
11	W	1302	ADP	C4-N9-C8	2.60	108.47	105.74
11	W	1302	ADP	C6-C5-N7	2.50	136.91	132.09
11	W	1302	ADP	O5'-PA-O1A	-2.29	99.86	108.94
11	W	1302	ADP	N9-C8-N7	-2.23	110.78	113.94
11	W	1302	ADP	C4'-O4'-C1'	2.10	114.09	109.47
11	W	1302	ADP	C2-N1-C6	2.02	122.05	118.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

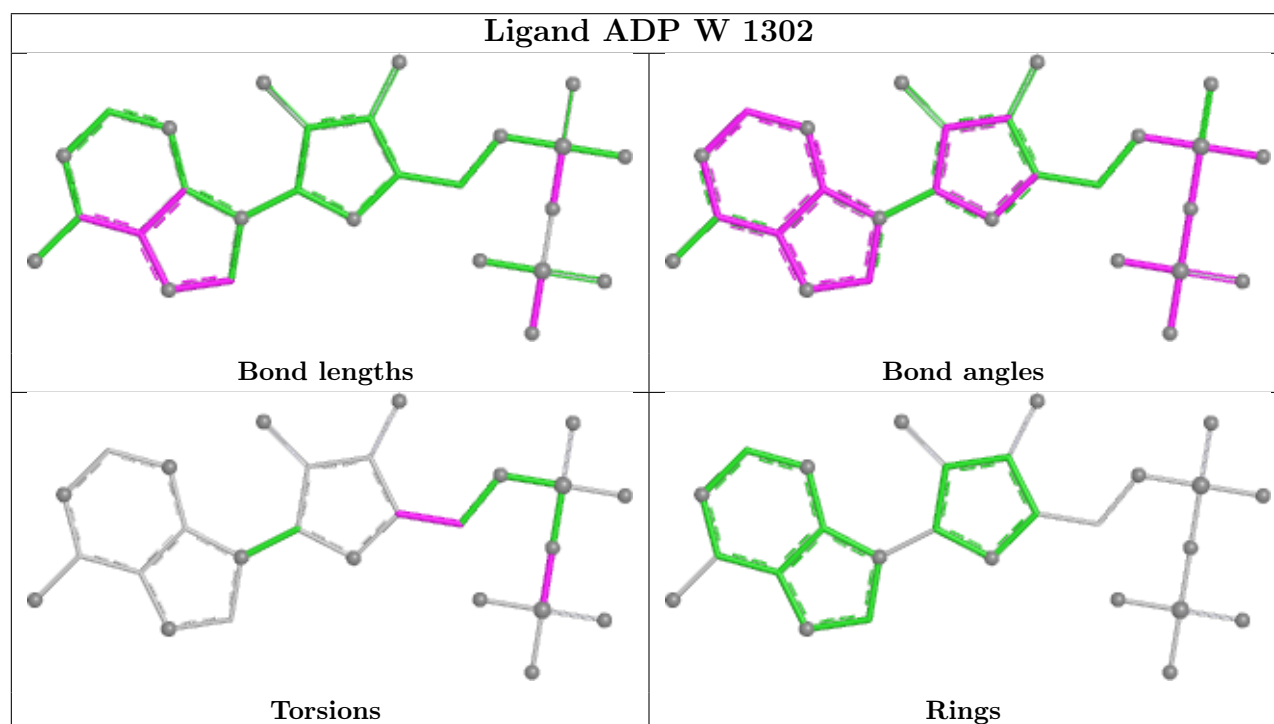
Mol	Chain	Res	Type	Atoms
11	W	1302	ADP	PA-O3A-PB-O2B
11	W	1302	ADP	O4'-C4'-C5'-O5'
11	W	1302	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	W	1302	ADP	12	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	W	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	841:TYR	C	1005:ASP	N	49.40
1	W	564:PHE	C	574:ASN	N	14.13
1	W	190:SER	C	199:LYS	N	11.85
1	W	676:PHE	C	681:MET	N	10.91
1	W	1211:LEU	C	1244:LYS	N	9.17

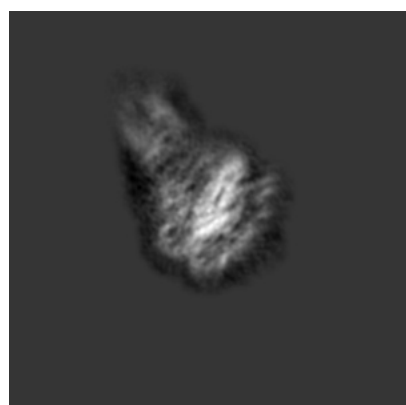
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4318. These allow visual inspection of the internal detail of the map and identification of artifacts.

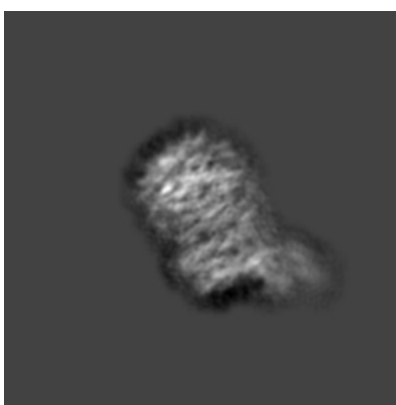
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

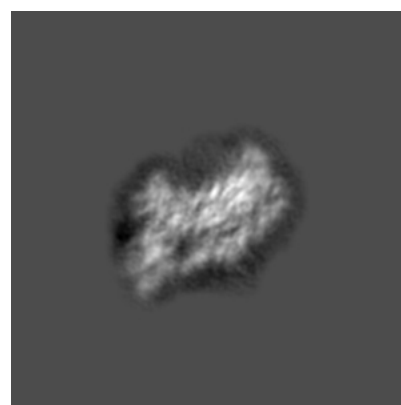
6.1.1 Primary map



X



Y

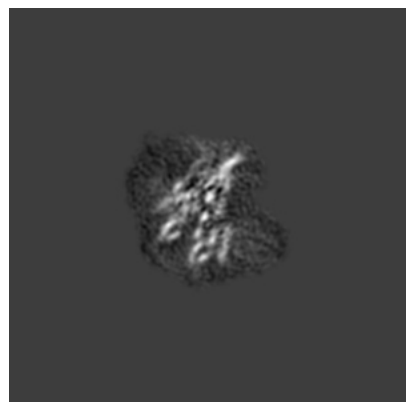


Z

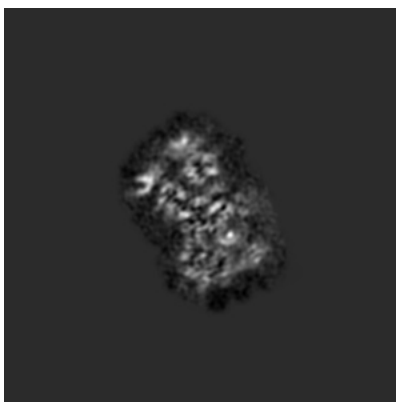
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

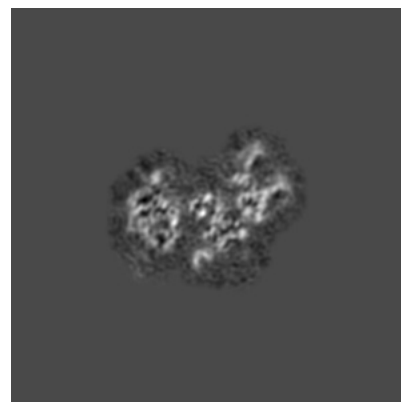
6.2.1 Primary map



X Index: 120



Y Index: 120

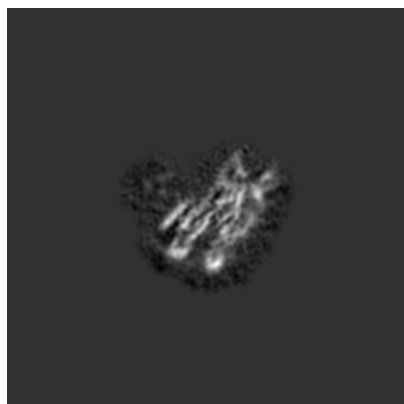


Z Index: 120

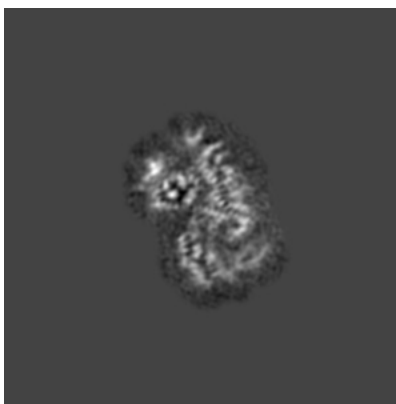
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

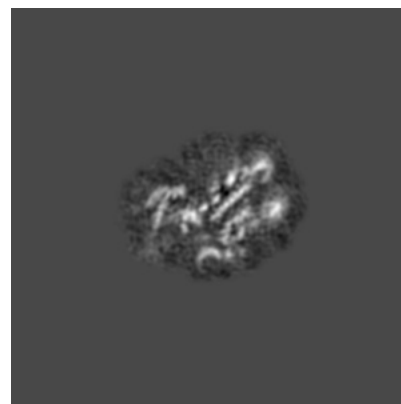
6.3.1 Primary map



X Index: 139



Y Index: 128



Z Index: 107

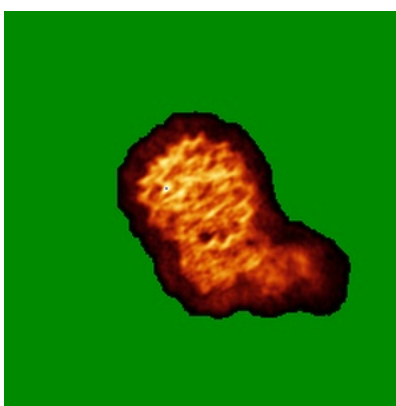
The images above show the largest variance slices of the map in three orthogonal directions.

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

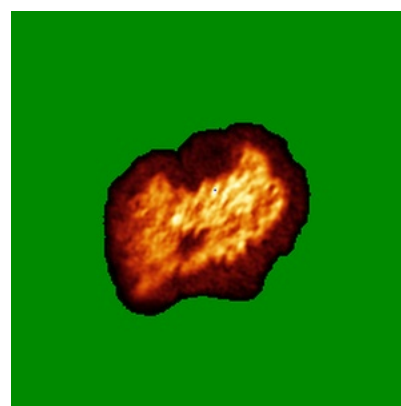
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

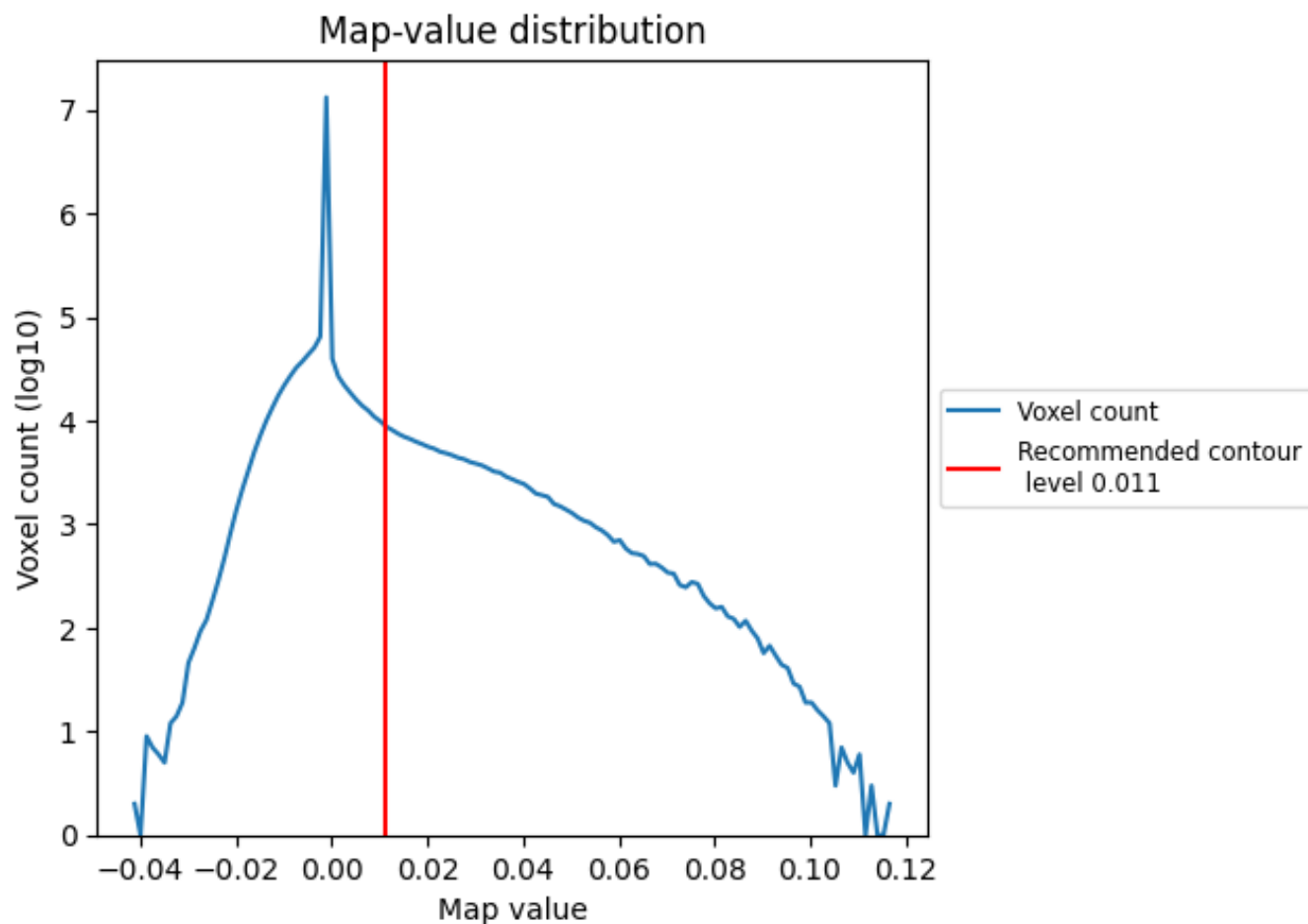
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

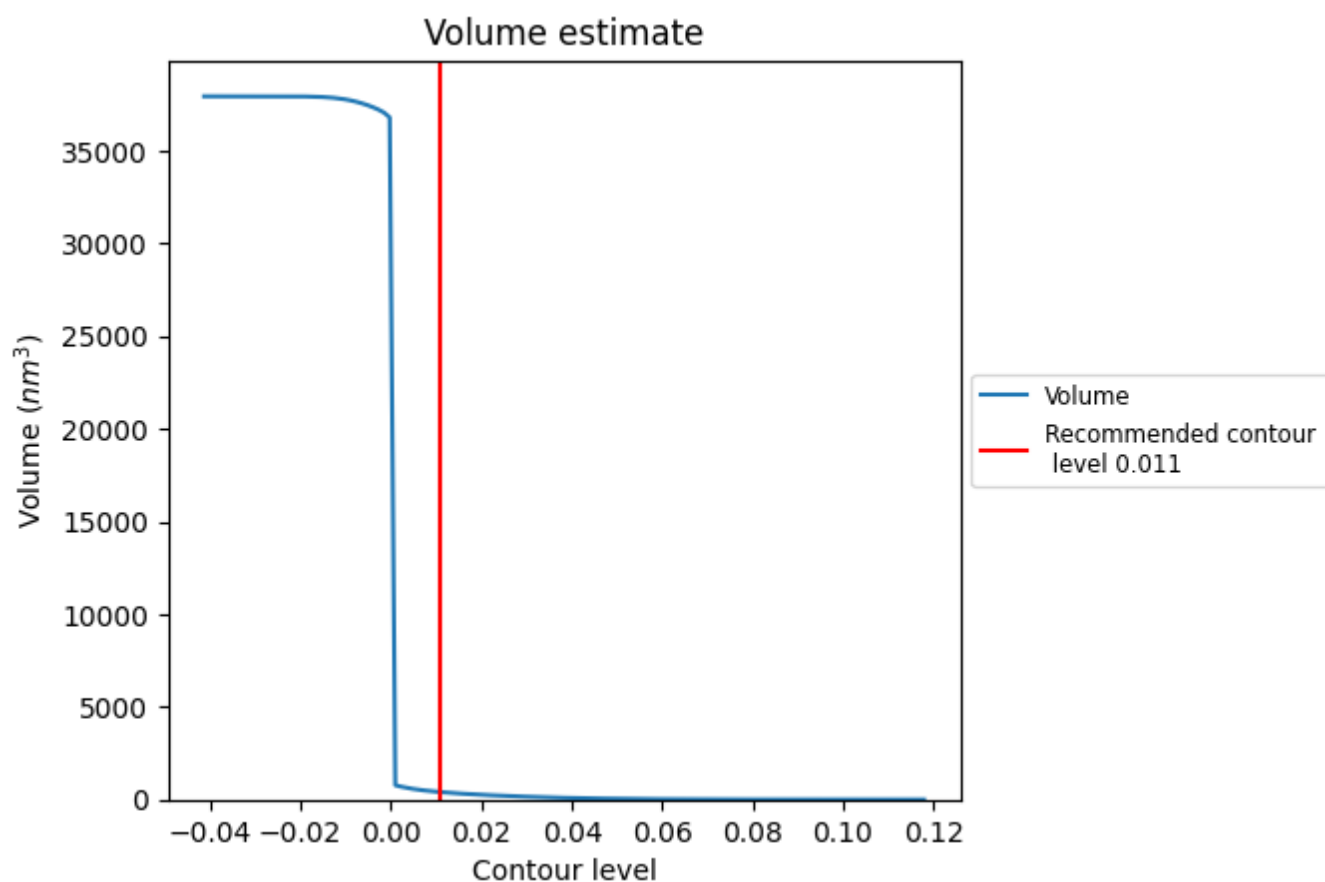
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

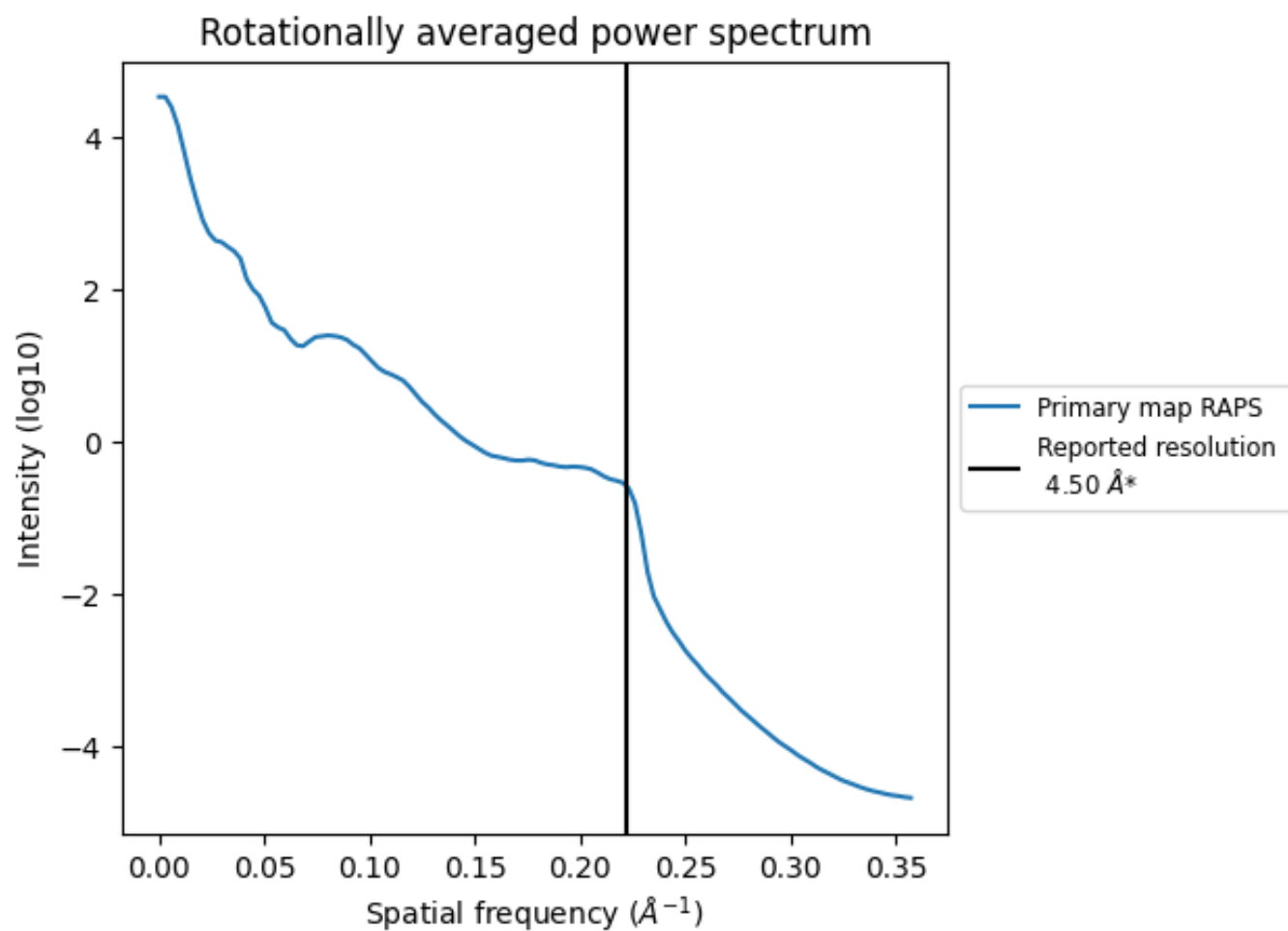
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 403 nm^3 ; this corresponds to an approximate mass of 364 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 ⓘ

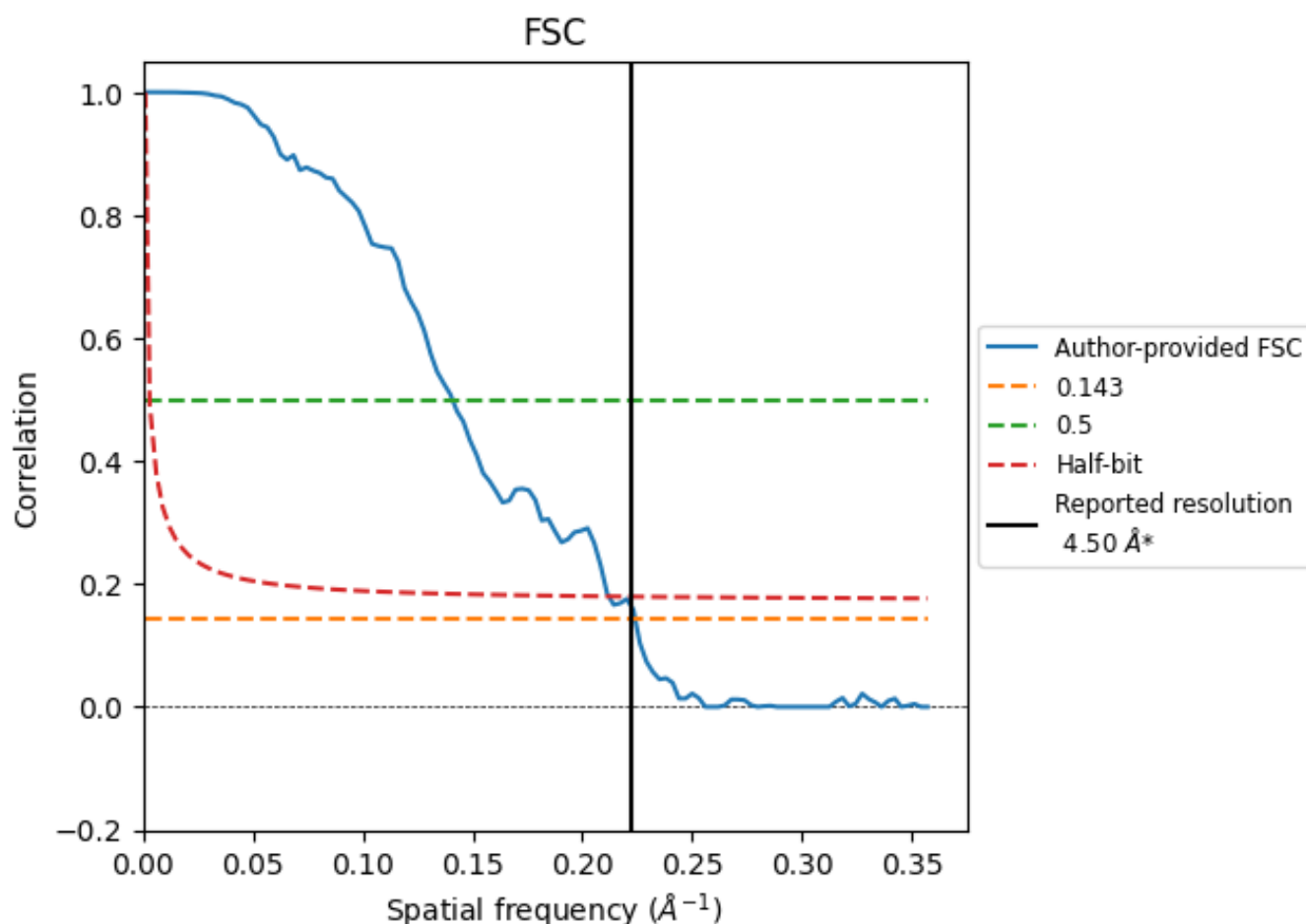


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

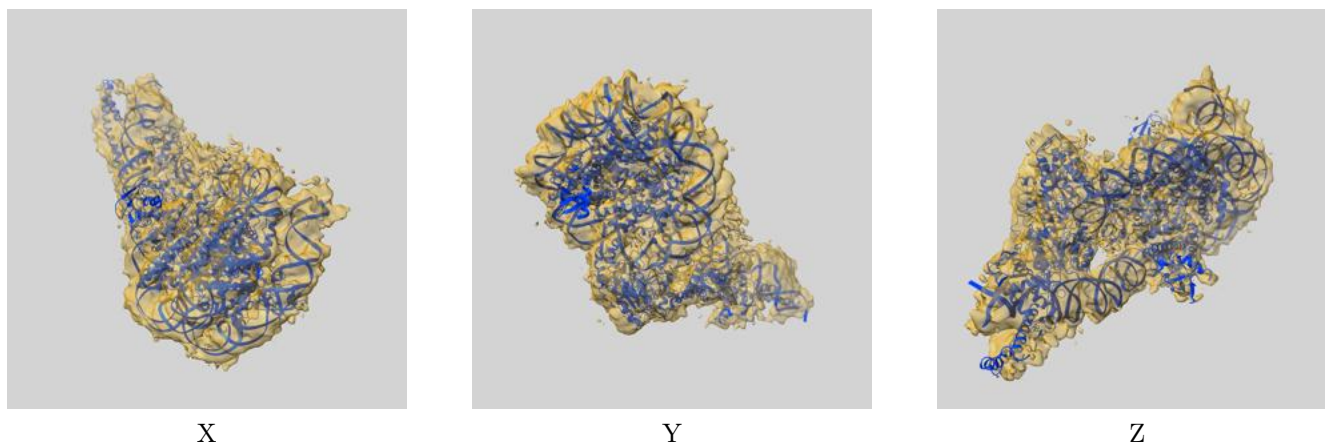
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.46	7.10	4.72
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

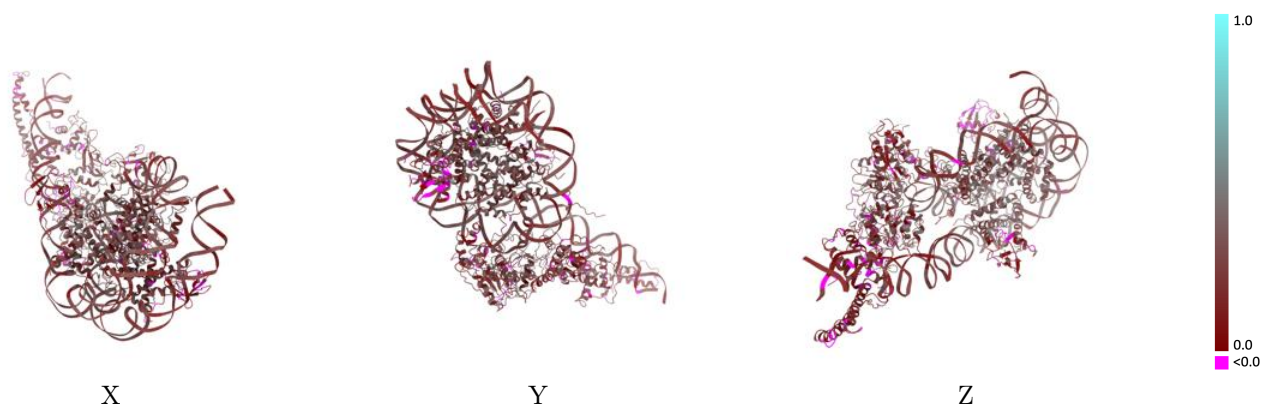
This section contains information regarding the fit between EMDB map EMD-4318 and PDB model 6FTX. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



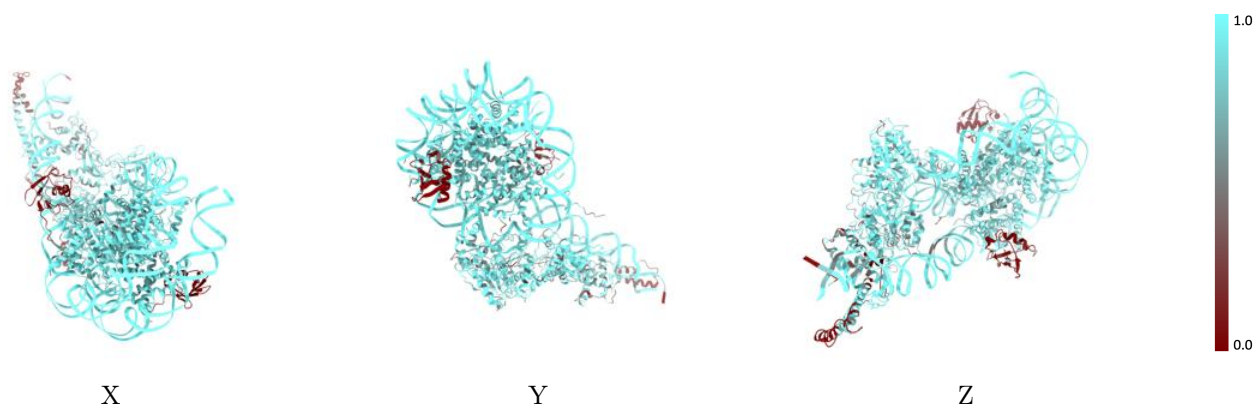
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



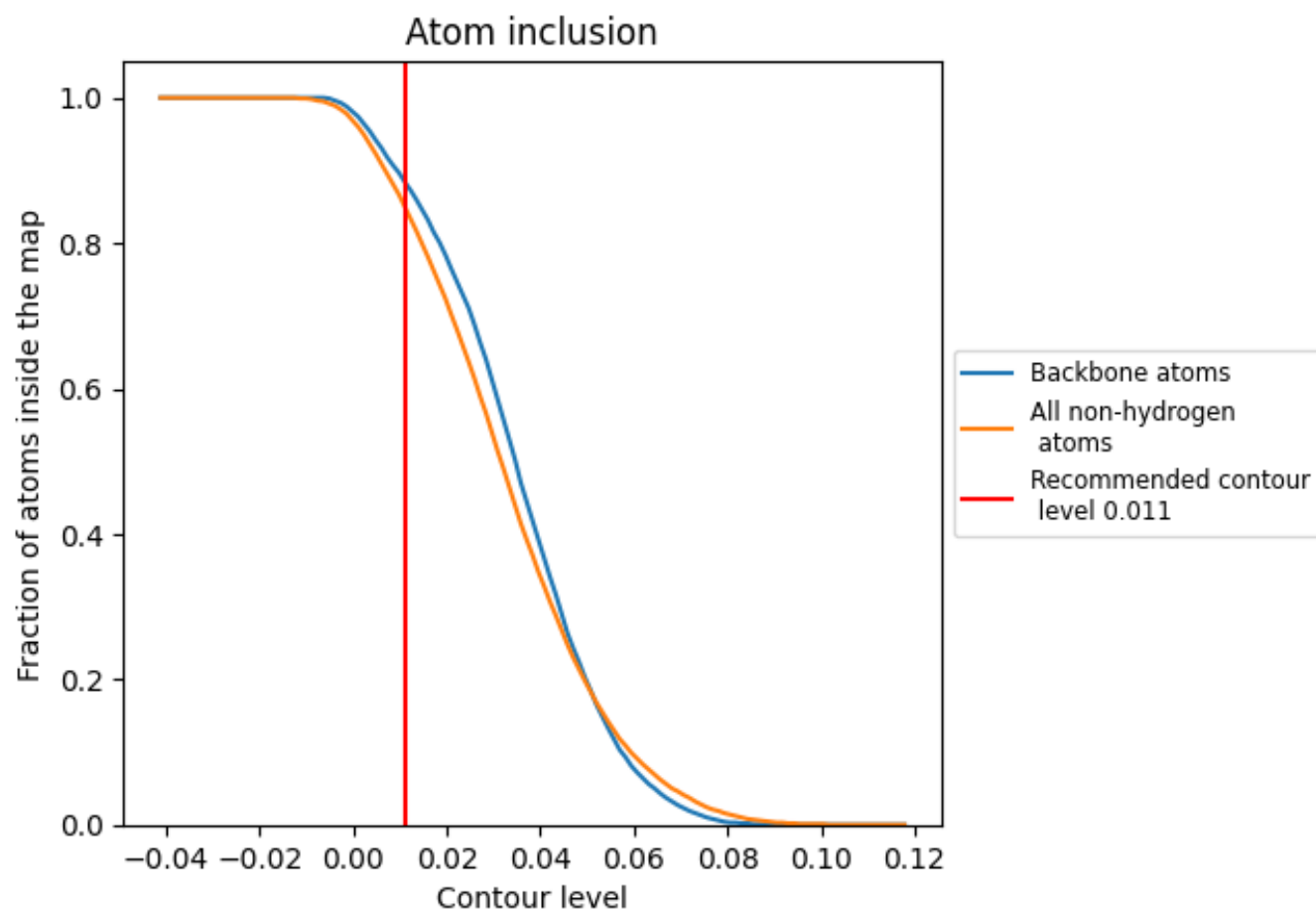
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 85% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8500	0.2300
A	0.9620	0.2600
B	0.9390	0.2750
C	0.8930	0.2760
D	0.9290	0.2790
E	0.8870	0.2670
F	0.8930	0.2510
G	0.9210	0.2810
H	0.9290	0.2700
I	0.9670	0.2470
J	0.9690	0.2480
N	0.1390	0.1150
O	0.0810	0.0360
W	0.8070	0.2070

