



Full wwPDB EM Validation Report ⓘ

Sep 24, 2024 – 01:34 pm BST

PDB ID : 8QKV
EMDB ID : EMD-18472
Title : SWR1-nucleosome complex in configuration 2
Authors : Jalal, A.S.B.; Wigley, D.B.
Deposited on : 2023-09-18
Resolution : 4.70 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.dev112
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

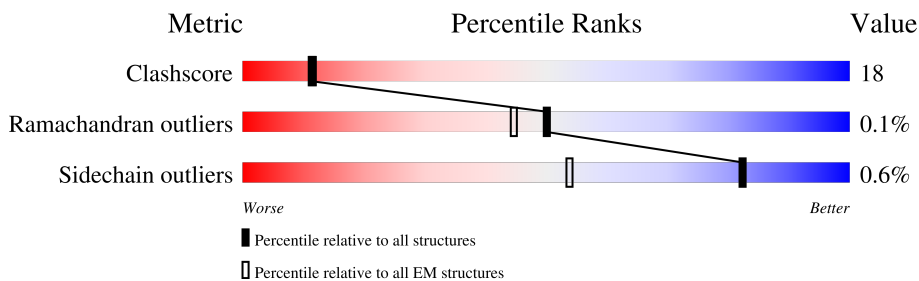
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	136	
1	B	136	
2	C	103	
2	D	103	
3	E	158	
3	F	158	
4	G	131	
4	H	131	

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Mol	Chain	Length	Quality of chain
5	I	194	41% 59%
6	J	194	30% 70%
7	Z	180	5% 73% 24%
8	M	1514	28% 17% 55%
9	R	438	60% 34% 6%
10	S	280	42% 24% 34%
11	T	463	60% 35% 5%
11	V	463	52% 41% 6%
11	X	463	57% 39% 5%
12	U	471	53% 38% 9%
12	W	471	50% 42% 8%
12	Y	471	62% 32% 5%

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
14	BEF	M	1602	-	-	X	-

2 Entry composition i

There are 16 unique types of molecules in this entry. The entry contains 45846 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
			Total	C	N	O		
1	B	97	796	506	152	138	0	0
1	A	97	796	506	152	138	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLU	ASP	conflict	UNP P61830
A	123	GLU	ASP	conflict	UNP P61830

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	C	82	651	410	126	115	0	0
2	D	80	638	401	124	113	0	0

- Molecule 3 is a protein called Histone H2A.2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	F	101	767	482	149	136	0	0
3	E	103	795	499	156	140	0	0

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	127	GLU	-	expression tag	UNP P04912
F	128	VAL	-	expression tag	UNP P04912
F	129	CYS	-	expression tag	UNP P04912

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Chain	Residue	Modelled	Actual	Comment	Reference
F	130	GLN	-	expression tag	UNP P04912
F	131	ASP	-	expression tag	UNP P04912
F	132	CYS	-	expression tag	UNP P04912
F	133	GLN	-	expression tag	UNP P04912
F	134	SER	-	expression tag	UNP P04912
F	135	PHE	-	expression tag	UNP P04912
F	136	SER	-	expression tag	UNP P04912
F	137	ARG	-	expression tag	UNP P04912
F	138	THR	-	expression tag	UNP P04912
F	139	VAL	-	expression tag	UNP P04912
F	140	ARG	-	expression tag	UNP P04912
F	141	THR	-	expression tag	UNP P04912
F	142	GLU	-	expression tag	UNP P04912
F	143	LEU	-	expression tag	UNP P04912
F	144	LYS	-	expression tag	UNP P04912
F	145	ARG	-	expression tag	UNP P04912
F	146	ASN	-	expression tag	UNP P04912
F	147	LYS	-	expression tag	UNP P04912
F	148	ALA	-	expression tag	UNP P04912
F	149	ASN	-	expression tag	UNP P04912
F	150	GLN	-	expression tag	UNP P04912
F	151	THR	-	expression tag	UNP P04912
F	152	PHE	-	expression tag	UNP P04912
F	153	LEU	-	expression tag	UNP P04912
F	154	SER	-	expression tag	UNP P04912
F	155	PHE	-	expression tag	UNP P04912
F	156	GLY	-	expression tag	UNP P04912
F	157	VAL	-	expression tag	UNP P04912
E	127	GLU	-	expression tag	UNP P04912
E	128	VAL	-	expression tag	UNP P04912
E	129	CYS	-	expression tag	UNP P04912
E	130	GLN	-	expression tag	UNP P04912
E	131	ASP	-	expression tag	UNP P04912
E	132	CYS	-	expression tag	UNP P04912
E	133	GLN	-	expression tag	UNP P04912
E	134	SER	-	expression tag	UNP P04912
E	135	PHE	-	expression tag	UNP P04912
E	136	SER	-	expression tag	UNP P04912
E	137	ARG	-	expression tag	UNP P04912
E	138	THR	-	expression tag	UNP P04912
E	139	VAL	-	expression tag	UNP P04912
E	140	ARG	-	expression tag	UNP P04912

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Chain	Residue	Modelled	Actual	Comment	Reference
E	141	THR	-	expression tag	UNP P04912
E	142	GLU	-	expression tag	UNP P04912
E	143	LEU	-	expression tag	UNP P04912
E	144	LYS	-	expression tag	UNP P04912
E	145	ARG	-	expression tag	UNP P04912
E	146	ASN	-	expression tag	UNP P04912
E	147	LYS	-	expression tag	UNP P04912
E	148	ALA	-	expression tag	UNP P04912
E	149	ASN	-	expression tag	UNP P04912
E	150	GLN	-	expression tag	UNP P04912
E	151	THR	-	expression tag	UNP P04912
E	152	PHE	-	expression tag	UNP P04912
E	153	LEU	-	expression tag	UNP P04912
E	154	SER	-	expression tag	UNP P04912
E	155	PHE	-	expression tag	UNP P04912
E	156	GLY	-	expression tag	UNP P04912
E	157	VAL	-	expression tag	UNP P04912

- Molecule 4 is a protein called Histone H2B.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	96	746	468	131	146	1	0	0
4	H	91	712	449	125	137	1	0	0

- Molecule 5 is a DNA chain called DNA (194-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	I	194	3960	1879	716	1171	194	0	0

- Molecule 6 is a DNA chain called DNA (194-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	J	194	3994	1888	755	1157	194	0	0

- Molecule 7 is a protein called Vacuolar protein sorting-associated protein 72.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Z	180	Total	C	N	O	S	0	0
			1367	854	248	262	3		

- Molecule 8 is a protein called Helicase SWR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	688	Total	C	N	O	S	0	0
			5398	3438	960	974	26		

- Molecule 9 is a protein called Actin-like protein ARP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	411	Total	C	N	O	S	0	0
			3335	2156	544	619	16		

- Molecule 10 is a protein called Vacuolar protein sorting-associated protein 71.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	185	Total	C	N	O	S	0	0
			1499	947	265	277	10		

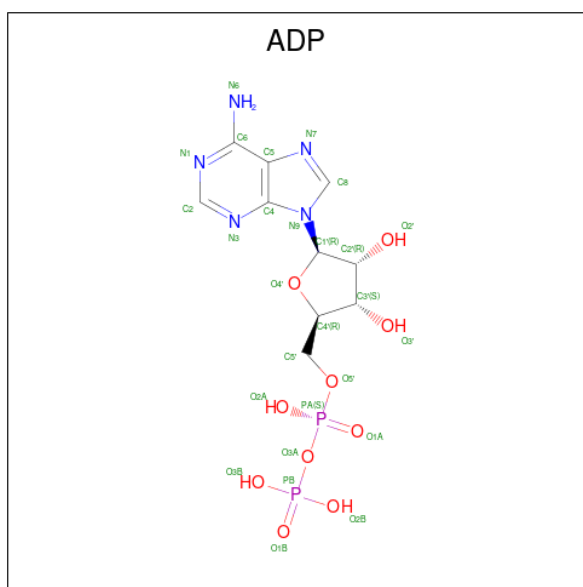
- Molecule 11 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	443	Total	C	N	O	S	0	0
			3391	2140	584	657	10		
11	V	434	Total	C	N	O	S	0	0
			3336	2107	574	645	10		
11	X	442	Total	C	N	O	S	0	0
			3397	2144	584	659	10		

- Molecule 12 is a protein called RuvB-like protein 2.

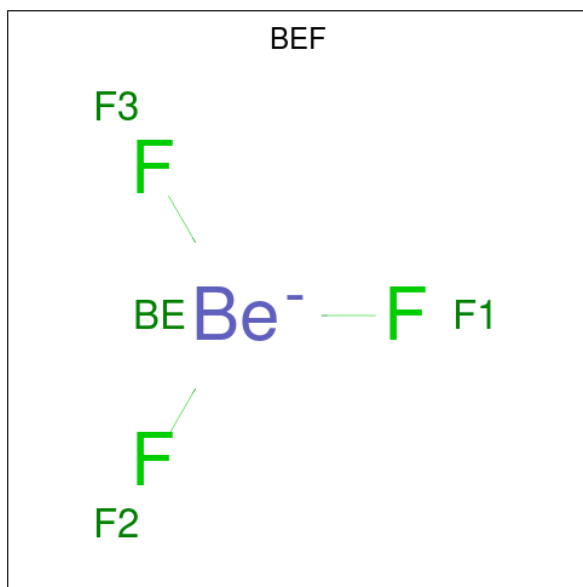
Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	430	Total	C	N	O	S	0	0
			3299	2063	570	655	11		
12	W	433	Total	C	N	O	S	0	0
			3325	2085	572	657	11		
12	Y	447	Total	C	N	O	S	0	0
			3410	2133	590	675	12		

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	M	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	R	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	T	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	U	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	V	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	W	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 14 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
14	M	1	4	1	3	0
14	R	1	4	1	3	0

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
15	M	1	1	1	0
15	R	1	1	1	0
15	T	1	1	1	0
15	U	1	1	1	0
15	V	1	1	1	0
15	W	1	1	1	0
15	X	1	1	1	0
15	Y	1	1	1	0

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

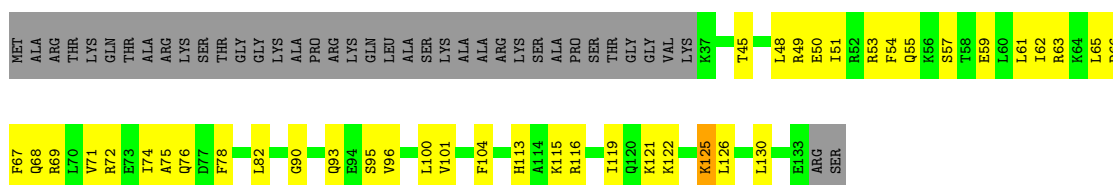
Mol	Chain	Residues	Atoms		AltConf
16	S	2	Total 2	Zn 2	0

3 Residue-property plots [i](#)

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.

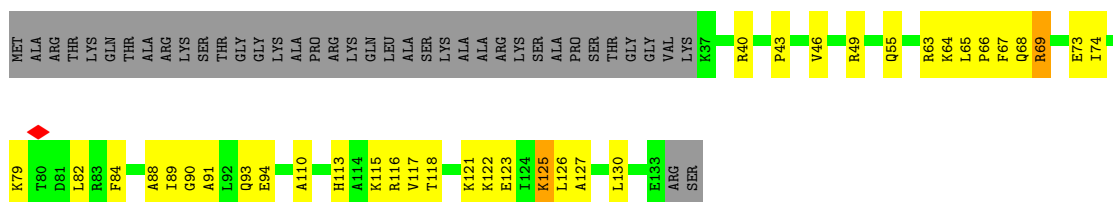
- Molecule 1: Histone H3

Chain B: 



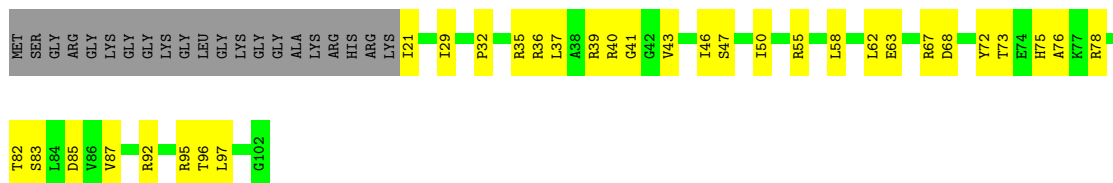
- Molecule 1: Histone H3

Chain A: 



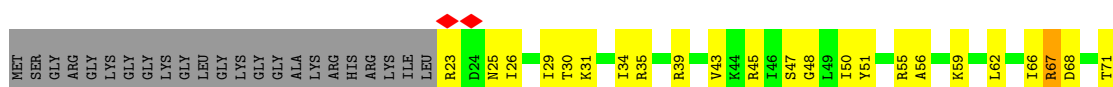
- Molecule 2: Histone H4

Chain C: 



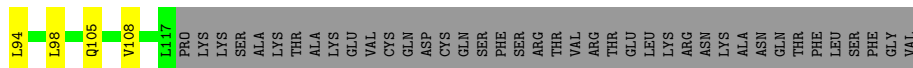
- Molecule 2: Histone H4

Chain D: 

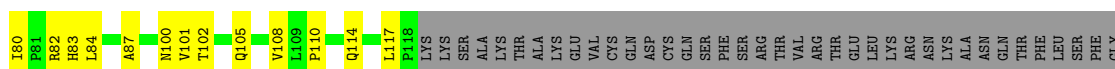




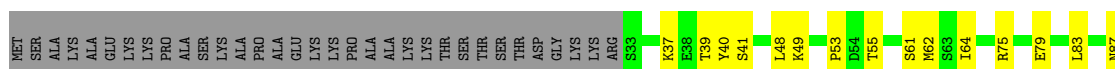
• Molecule 3: Histone H2A.2



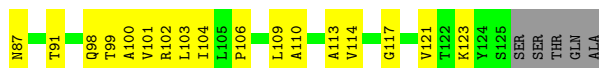
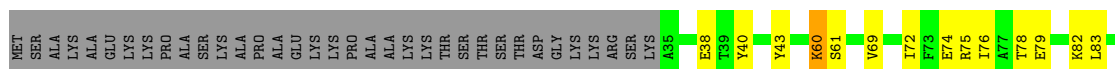
• Molecule 3: Histone H2A.2



• Molecule 4: Histone H2B.1



• Molecule 4: Histone H2B.1



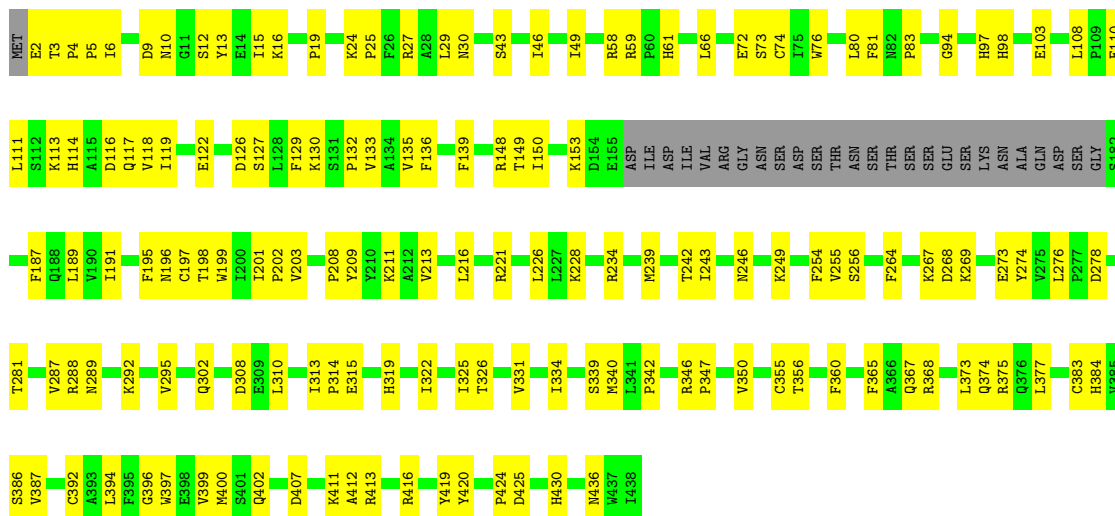
• Molecule 5: DNA (194-MER)



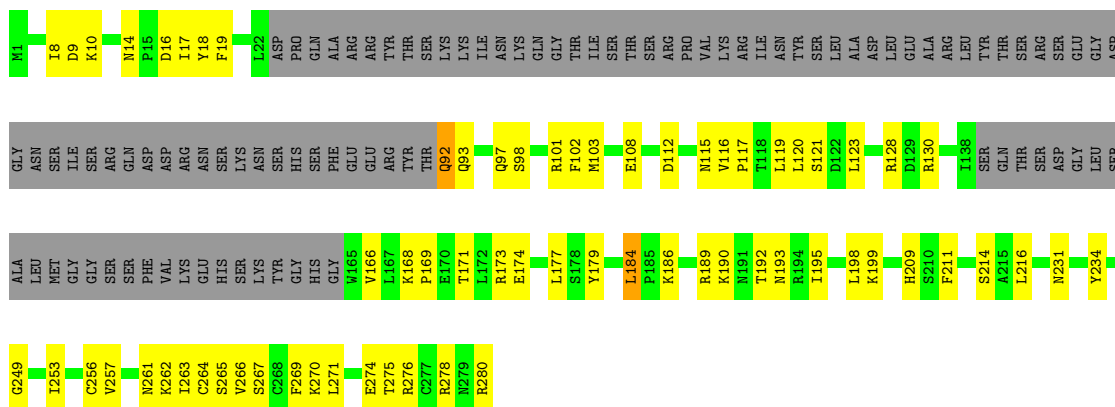
ALA	THR	R1313	C1217	L1128	A1015	K939	T862	S756	ASN	GLY	SER	ASP	TRP	HIS	ARG	ARG	LEU
MET	ASP	I1314	V1220	R1129	S1016	Q940	G853	V756	ARG	LEU	SER	VAL	ASN	MET	LEU	ASP	LEU
ARG	TYR	I1315	W1221	R1130	S1017	M841	T854	L757	ASP	SER	THR	LEU	MET	SER	LEU	THR	LYS
GLU	PHE	I1316	N1222	R1133	R1132	P942	L860	L758	ASP	ALA	THR	GLU	ALA	LYS	LEU	ARG	LYS
VAL	SER	I1318	M1223	R1134	K1019	K943	L861	M769	ILE	LEU	TYR	GLU	GLU	LYS	PHE	LEU	GLY
GLU	LYS	I1319	L1231	R1141	D1020	K944	E862	M768	ASP	PHE	ASP	ASP	ALA	LYS	ARG	GLY	ILE
ILE	LEU	S1323	L1232	D1142	R1023	Y945	L863	E761	VAL	GLY	SER	ASP	TYR	ASN	ASP	ASN	ASN
ASP	SER	I1328	A1234	L1143	T1024	E946	L867	F764	GLU	GLY	ASN	ASP	ARG	GLY	SER	GLY	GLY
ASN	VAL	I1329	F1235	L1144	L1025	E947	L868	P769	GLU	GLU	LYS	MET	ARG	THR	THR	LEU	ALA
ASP	ASP	M1329	P1236	T1145	L1026	H947	Y868	P768	ASP	GLU	ASP	LEU	LEU	LYS	LEU	ALA	ALA
ASP	PHE	L1330	D1237	T1146	L1027	H948	L869	P767	ASP	GLU	ASP	GLU	ARG	ALA	ALA	THR	LEU
ASP	LEU	A1333	K1238	K1147	Q1034	I948	L870	V773	GLU	SER	LYS	ASP	ASP	GLY	LYS	THR	TYR
GLU	GLY	D1334	Y1243	R1148	R1037	S954	L871	V772	THR	GLY	PHE	LEU	ASP	ILE	ASP	ASP	ASP
SER	SER	I1337	G1246	R1149	F1042	K955	T874	G779	LYS	ASP	THR	THR	GLU	ALA	ALA	ALA	LYS
GLU	GLU	F1338	G1247	V1150	F1043	R956	V875	G778	VAL	ASP	PRO	GLU	GLU	ARG	ARG	ARG	GLY
GLY	LEU	Y1338	K1247	K1151	L1045	Q957	Y876	Q782	GLN	LEU	PRO	GLU	GLU	ALA	ALA	THR	LYS
PRO	PRO	F1339	L1248	K1152	L1046	R958	L885	Q781	GLU	LEU	ASP	LEU	GLN	LYS	ALA	LEU	ASP
GLY	GLY	D1340	L1249	D1163	L1047	F959	A885	K792	GLU	ASP	ASP	GLU	GLN	ASP	ALA	LYS	ASP
LYS	GLU	S1341	Q1249	K1164	L1048	L960	ASP	P793	GLU	ASP	GLY	VAL	VAL	GLY	VAL	VAL	SER
ALA	ASN	D1342	K1250	K1165	L1049	Y961	ASP	D794	GLN	ASP	ASP	GLU	GLN	LYS	LYS	VAL	LEU
ALA	ALA	D1343	L1251	D1166	M1050	Y962	ASP	A795	LEU	SER	ASP	ASP	ARG	ASP	GLN	SER	GLN
GLU	SER	D1344	L1252	D1167	D1051	F964	ALA	A794	S682	GLU	GLU	GLU	GLU	VAL	VAL	GLN	PRO
GLY	GLY	K1349	L1253	K1168	K1052	M965	PHE	F798	LEU	GLU	GLU	GLU	GLU	ILE	ILE	ILE	PRO
GLY	GLY	Q1350	L1254	L1169	D1053	M966	GLN	C799	P689	PHE	THR	THR	GLY	GLN	GLN	GLN	ILE
GLY	ASP	Q1351	L1255	I1163	L1054	S966	TRP	R800	L692	TRP	SER	VAL	GLN	LYS	LYS	LYS	LYS
ASN	PRO	D1353	R1264	K1164	A1059	R967	PHE	V801	M695	GLN	ASP	ALA	GLN	HIS	HIS	HIS	GLY
LEU	LEU	R1354	I1267	K1165	K1064	Q969	GLY	S802	L696	GLN	SER	VAL	HIS	ASP	ASP	ASP	ILE
ASP	ASP	H1355	I1268	L1166	L1065	T970	ARG	Y803	L697	TRP	GLY	VAL	SER	GLY	GLY	GLY	LEU
ASP	ASP	R1357	T1272	R1169	L1066	K971	PRO	Q808	T698	PRO	THR	GLU	GLN	THR	VAL	VAL	THR
GLY	ASP	Q1360	L1273	R1174	T1067	A972	VAL	Q809	P699	GLY	GLY	ASP	ASP	VAL	VAL	ALA	ILE
ASP	ASP	T1361	V1274	R1177	V1068	A973	ASP	Q810	Q700	GLY	GLY	SER	LEU	GLY	GLY	ALA	ILE
TYR	VAL	R1362	L1275	I1177	K1069	N978	LYS	Y820	K701	ILE	ILE	VAL	PRO	GLY	ALA	ALA	THR
GLU	ALA	D1363	D1276	L1183	M1070	S981	ILE	V822	W706	GLU	GLU	GLU	GLU	GLU	ALA	ALA	TYR
THR	LYS	D1364	V1277	T1184	F1071	I982	THR	L823	L707	THR	GLY	GLU	THR	GLU	GLU	GLU	PRO
ALA	ASP	T1366	L1282	P1185	V1072	I983	GLY	L824	A708	LYS	THR	GLY	GLU	ARG	ARG	LYS	PRO
ALA	PRO	Y1367	G1286	K1187	E1073	V984	GLN	D824	S709	ASP	THR	ALA	LEU	LYS	ALA	ILE	ILE
VAL	ARG	R1368	Y1287	A1187	M1076	N984	ASN	E825	M713	GLN	SER	THR	GLU	LYS	LYS	LYS	SER
ASP	GLN	M1378	L1288	V1188	R1079	C985	PHE	A826	W706	VAL	THR	THR	GLU	GLU	GLU	GLU	GLY
GLU	GLU	Y1381	Y1289	V1188	E1080	M987	GLY	H827	L707	ASP	ASP	THR	GLN	GLU	GLU	GLU	PHE
TYR	GLY	K1381	M1290	K1189	R1079	Q988	GLN	N828	I718	ASN	ASN	LEU	GLN	GLY	GLY	GLY	TYR
MET	ARG	K1382	R1291	K1194	E1080	L989	ASP	H829	L719	ASN	ASN	ASP	ASN	THR	THR	ARG	GLU
ILE	LEU	A1383	L1292	L1199	L1085	L990	LYS	T831	A720	ALA	ALA	SER	GLN	GLN	HIS	HIS	GLY
PHE	ALA	K1386	D1293	M1101	M1101	R990	ASP	N831	D721	ALA	THR	VAL	VAL	VAL	VAL	VAL	GLN
ALA	ALA	R1387	T1296	M1200	F1104	K991	THR	F832	K727	THR	THR	GLY	GLY	GLY	ALA	ALA	ILE
ALA	ALA	Q1388	K1297	D1201	F1104	L998	GLU	S834	L738	PHE	GLY	LEU	GLN	GLN	GLN	GLN	GLN
ASP	ASP	L1389	L1298	G1206	S1107	F999	LEU	T835	L738	ARG	ALA	LEU	ARG	ARG	ARG	ARG	THR
TYR	GLY	D1390	E1207	E1207	M1108	E1000	R926	R836	K742	GLY	GLY	LEU	LEU	LEU	LEU	LEU	THR
TYR	TYR	T1394	M1208	M1208	G1114	V1001	R927	R837	E743	THR	THR	LEU	GLY	GLY	ALA	ALA	ALA
ASP	ASP	Q1395	T1209	T1209	G1114	R1002	R926	R838	M744	SER	SER	LEU	ASP	ASP	ASP	ASP	ASP
VAL	VAL	E1396	R1210	R1210	R1114	P1003	R926	R839	M744	PHE	PHE	GLY	GLY	GLY	GLY	GLY	GLY
LYS	LYS	E1396	R1211	R1211	M1118	I1004	L930	R843	L749	VAL	VAL	TYR	TYR	TYR	TYR	TYR	VAL
ALA	ALA	GLY	K1212	K1212	M1118	I1004	L930	R844	I750	HIS	HIS	GLY	GLY	GLY	GLY	GLY	ALA
ALA	ALA	ASP	V1213	V1213	M1124	L1005	R931	R844	I750	THR	THR	ASP	ASP	ASP	ASP	ASP	ASN
THR	LEU	THR	M1216	M1216	K1127	L1009	R936	R849	P753	GLN	GLN	SER	SER	SER	SER	SER	GLY
						L1010	E938		T754	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ILE

● Molecule 9: Actin-like protein ARP6

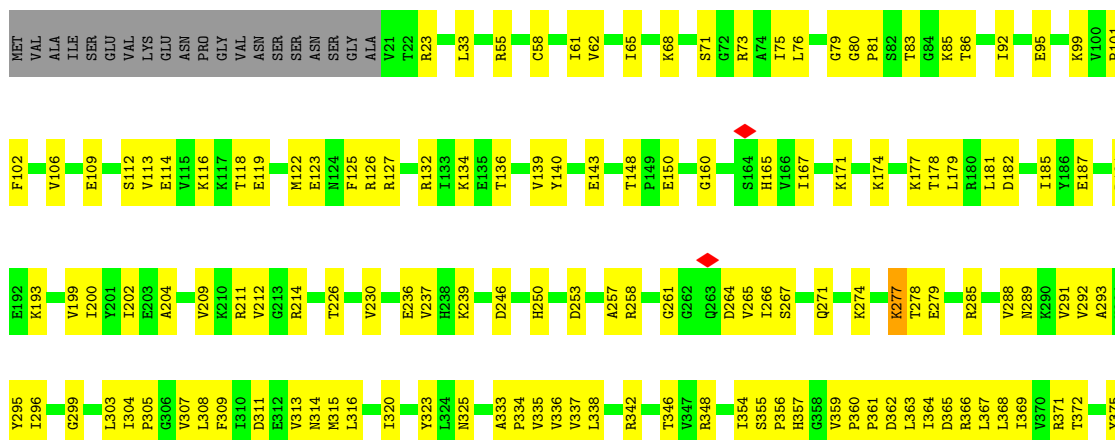


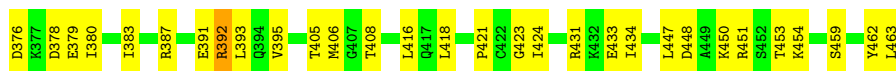


● Molecule 10: Vacuolar protein sorting-associated protein 71



● Molecule 11: RuvB-like protein 1





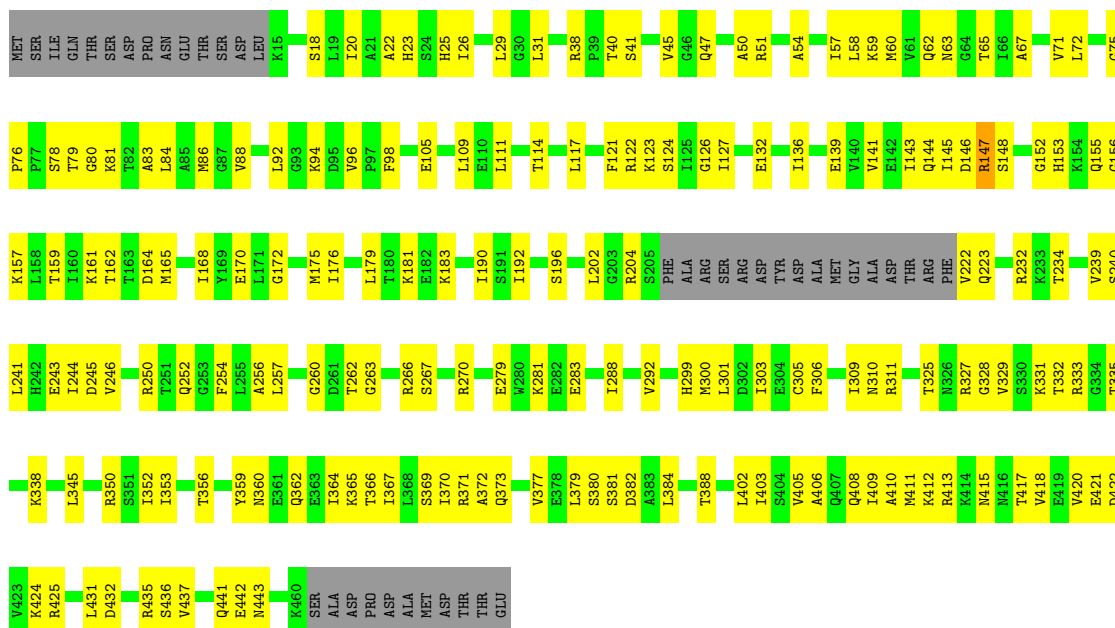
• Molecule 11: RuvB-like protein 1



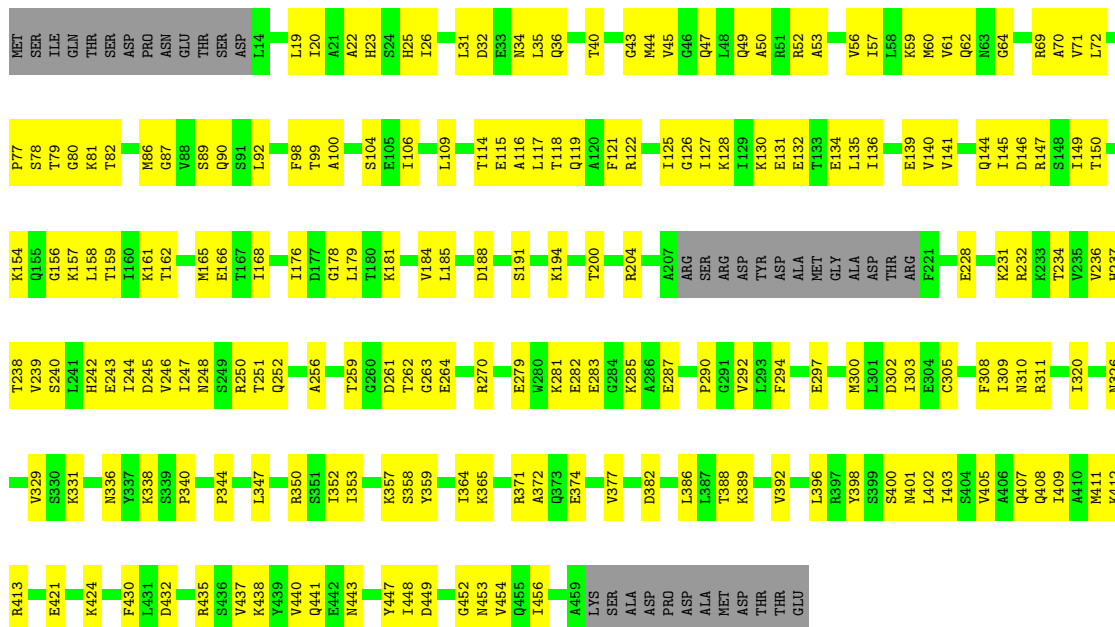
• Molecule 11: RuvB-like protein 1



• Molecule 12: RuvB-like protein 2



• Molecule 12: RuvB-like protein 2



• Molecule 12: RuvB-like protein 2



L111	S112	K113	T114	E115	Q119	R122	K123	S124	I125	G126	I127	K130	L135	I136	V141	K157	L158	T159	L160	K161	T162	M165	E166	T167	I168	L171	G172	M175	I176	V184	L185	A186	G187	D188	V189	I190	S191	I192	D193	K194	A195	S196	K201	R204	R208	
Y212	D213	A214	M215	G216	A217	D218	T219	R220	F221	Q223	L229	V236	H237	S240	L241	H242	E243	I244	D245	V246	I247	R250	G253	F254	L255	A256	L257	G263	R266	S267	E268	V269	R270	I273	K281	I288	L283	F294	V298	H299	M300	L301	D302	I303	E304	C305
F306	R311	D315	E316	P319	I320	V321	M322	M323	A324	T325	M326	R327	K331	T332	T335	K338	S339	P340	H341	P344	L345	D346	L347	L348	D349	R350	S351	I352	Y359	I364	I367	R371	E378	D382	L387	V392	L396	R397	M401	L402	I403					
Q408	I409	A410	M411	K414	M415	M416	T417	D432	R435	S436	V437	V440	Q446	Y447	I448	N453	V454	K460	SER	ALA	ASP	PRO	ASP	ALA	MET	ASP	THR	THR	GLU																	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33595	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00157	Depositor
Map size (\AA)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, ZN, 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	0.24	0/807	0.53	0/1081
1	B	0.24	0/807	0.55	0/1081
2	C	0.23	0/658	0.59	0/880
2	D	0.24	0/645	0.58	0/862
3	E	0.25	0/806	0.56	0/1091
3	F	0.25	0/777	0.52	0/1053
4	G	0.25	0/756	0.48	0/1017
4	H	0.26	0/722	0.51	0/972
5	I	0.54	0/4436	0.93	0/6841
6	J	0.54	0/4486	0.90	0/6925
7	Z	0.25	0/1385	0.51	0/1863
8	M	0.25	0/5495	0.52	1/7442 (0.0%)
9	R	0.25	0/3429	0.48	0/4650
10	S	0.24	0/1523	0.52	0/2052
11	T	0.25	0/3433	0.53	0/4646
11	V	0.24	0/3375	0.52	0/4565
11	X	0.24	0/3439	0.52	0/4652
12	U	0.25	0/3333	0.52	0/4492
12	W	0.25	0/3361	0.51	0/4530
12	Y	0.24	0/3447	0.50	0/4649
All	All	0.32	0/47120	0.62	1/65344 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	0	1
7	Z	0	1
10	S	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	T	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	953	LEU	CA-CB-CG	5.49	127.93	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	26	PHE	Peptide
10	S	211	PHE	Peptide
11	T	160	GLY	Peptide
7	Z	298	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	796	0	841	34	0
1	B	796	0	841	43	0
2	C	651	0	690	35	0
2	D	638	0	677	28	0
3	E	795	0	834	39	0
3	F	767	0	792	26	0
4	G	746	0	771	25	0
4	H	712	0	736	30	0
5	I	3960	0	2179	106	0
6	J	3994	0	2172	129	0
7	Z	1367	0	1291	40	0
8	M	5398	0	5352	215	0
9	R	3335	0	3256	109	0
10	S	1499	0	1544	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	T	3391	0	3513	139	0
11	V	3336	0	3474	167	0
11	X	3397	0	3533	157	0
12	U	3299	0	3387	137	0
12	W	3325	0	3410	155	0
12	Y	3410	0	3465	129	0
13	M	27	0	12	5	0
13	R	27	0	12	1	0
13	T	27	0	12	1	0
13	U	27	0	12	5	0
13	V	27	0	12	8	0
13	W	27	0	12	4	0
13	X	27	0	12	7	0
13	Y	27	0	12	5	0
14	M	4	0	0	2	0
14	R	4	0	0	1	0
15	M	1	0	0	0	0
15	R	1	0	0	0	0
15	T	1	0	0	0	0
15	U	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	X	1	0	0	0	0
15	Y	1	0	0	0	0
16	S	2	0	0	0	0
All	All	45846	0	42854	1560	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 18.

All (1560) 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)
10:S:92:GLN:N	10:S:92:GLN:HE21	1.36	1.20
10:S:92:GLN:N	10:S:92:GLN:NE2	2.16	0.92
5:I:-51:DC:O2	6:J:51:DG:N2	2.03	0.92
5:I:-51:DC:N3	6:J:51:DG:N1	2.23	0.85
8:M:758:LEU:HB3	8:M:1302:GLN:HG2	1.56	0.85
2:D:56:ALA:HA	2:D:59:LYS:HD2	1.57	0.84
5:I:10:DC:N3	6:J:-10:DG:N1	2.29	0.81
5:I:10:DC:O2	6:J:-10:DG:N2	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:68:DG:N1	6:J:68:DC:N3	2.26	0.80
12:U:156:GLY:HA3	12:U:176:ILE:HG21	1.64	0.80
11:X:201:TYR:HB3	11:X:210:LYS:HB3	1.65	0.78
11:T:315:MET:HA	11:T:348:ARG:HG3	1.66	0.77
6:J:58:DC:H5'	3:E:76:LYS:HG3	1.66	0.77
8:M:1222:ASN:H	11:V:191:ARG:HH22	1.30	0.77
11:T:274:LYS:HE2	12:Y:255:LEU:HD13	1.67	0.77
12:W:135:LEU:HD21	12:W:191:SER:HB3	1.66	0.76
11:V:316:LEU:HD13	11:V:320:ILE:HB	1.66	0.76
12:W:228:GLU:O	12:W:231:LYS:NZ	2.15	0.76
8:M:1357:ARG:HD2	13:M:1601:ADP:H4'	1.65	0.76
11:X:274:LYS:HG2	11:X:276:LYS:HE3	1.67	0.76
6:J:39:DA:H3'	3:E:36:ARG:HH21	1.49	0.75
11:T:278:THR:HG22	11:T:279:GLU:H	1.52	0.75
8:M:965:MET:O	8:M:969:GLN:NE2	2.20	0.75
12:U:59:LYS:O	12:U:63:ASN:HB2	1.86	0.75
12:U:38:ARG:HB2	12:U:41:SER:HB3	1.68	0.74
12:U:408:GLN:HA	12:U:411:MET:HG3	1.68	0.74
11:X:65:ILE:HG12	11:X:335:VAL:HG11	1.68	0.74
9:R:211:LYS:NZ	9:R:340:MET:SD	2.60	0.74
12:W:256:ALA:HB1	12:W:262:THR:HB	1.70	0.74
9:R:149:THR:HA	9:R:386:SER:HA	1.69	0.73
11:T:313:VAL:HG21	11:T:338:LEU:HD21	1.71	0.73
8:M:1328:ILE:HG12	8:M:1354:ARG:HD3	1.68	0.73
10:S:17:ILE:HG22	12:U:147:ARG:HH21	1.53	0.73
1:B:65:LEU:HG	5:I:17:DA:H5''	1.69	0.73
12:U:47:GLN:HB3	12:U:50:ALA:HB3	1.71	0.73
11:T:267:SER:O	11:T:271:GLN:NE2	2.21	0.72
12:W:87:GLY:HA2	12:W:90:GLN:HE21	1.54	0.72
11:X:84:GLY:HA3	13:X:501:ADP:H8	1.53	0.72
12:Y:115:GLU:O	12:Y:119:GLN:NE2	2.22	0.72
11:T:116:LYS:HD3	11:T:118:THR:H	1.52	0.72
1:B:119:ILE:HB	2:C:43:VAL:HG11	1.71	0.72
8:M:954:SER:H	8:M:957:GLN:HE21	1.37	0.72
12:U:425:ARG:NH2	11:V:56:GLU:OE1	2.23	0.71
9:R:58:ARG:HB3	10:S:166:VAL:HG13	1.72	0.71
5:I:48:DG:N3	5:I:49:DC:N4	2.36	0.71
11:T:309:PHE:HD1	11:T:337:VAL:HG23	1.54	0.71
3:F:108:VAL:H	1:A:55:GLN:HE22	1.37	0.71
5:I:20:DG:OP1	8:M:836:ARG:NH1	2.23	0.71
8:M:1208:ASN:OD1	11:T:191:ARG:NH1	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:203:VAL:HA	9:R:208:PRO:HA	1.73	0.71
7:Z:296:LEU:HD22	7:Z:588:GLU:HB3	1.73	0.71
12:U:126:GLY:HA2	12:U:240:SER:HA	1.73	0.71
12:W:311:ARG:O	12:W:311:ARG:NH1	2.24	0.71
4:H:102:ARG:HA	4:H:110:ALA:HB1	1.73	0.70
8:M:700:GLN:NE2	13:M:1601:ADP:N7	2.39	0.70
10:S:253:ILE:HA	10:S:262:LYS:HE2	1.72	0.70
11:T:200:ILE:HD11	11:T:209:VAL:HG13	1.72	0.70
11:T:127:ARG:NH2	12:U:267:SER:OG	2.23	0.70
11:V:43:ARG:HD3	11:V:44:VAL:HG23	1.73	0.70
11:V:124:ASN:HA	11:V:127:ARG:HD2	1.73	0.70
12:W:448:ILE:HG22	12:W:454:VAL:HB	1.73	0.70
11:V:185:ILE:HD11	11:V:202:ILE:HD11	1.74	0.70
12:W:126:GLY:HA2	12:W:240:SER:HA	1.73	0.70
12:U:18:SER:HA	11:V:331:ASN:HD21	1.56	0.70
8:M:1353:ASP:HA	8:M:1356:HIS:HB3	1.74	0.70
9:R:12:SER:O	9:R:59:ARG:NH1	2.24	0.69
12:U:406:ALA:HB1	12:U:418:VAL:HG11	1.74	0.69
1:B:74:ILE:HG21	2:C:62:LEU:HD21	1.74	0.69
12:Y:331:LYS:HA	12:Y:338:LYS:HA	1.75	0.69
11:V:76:LEU:HD22	11:V:367:LEU:HD22	1.73	0.69
8:M:828:ASN:O	8:M:836:ARG:NH2	2.26	0.69
2:C:95:ARG:HB2	3:E:101:VAL:HG23	1.76	0.68
5:I:100:DG:N2	6:J:-98:DA:OP1	2.26	0.68
12:Y:432:ASP:H	12:Y:435:ARG:HD3	1.58	0.68
11:T:80:GLY:O	11:T:85:LYS:NZ	2.26	0.68
1:B:101:VAL:HG11	3:E:108:VAL:HG21	1.76	0.68
2:C:97:LEU:HG	3:E:101:VAL:HB	1.76	0.68
8:M:1267:ILE:HG22	8:M:1337:ILE:HB	1.76	0.68
2:D:75:HIS:NE2	4:G:87:ASN:OD1	2.27	0.67
11:T:395:VAL:HG23	11:T:434:ILE:HB	1.75	0.67
11:V:126:ARG:HD2	11:V:250:HIS:HA	1.77	0.67
11:V:446:PHE:HB3	12:W:352:ILE:HD11	1.75	0.67
12:W:159:THR:HG23	12:W:168:ILE:HG13	1.76	0.67
6:J:-24:DT:H2''	6:J:-23:DT:H5'	1.77	0.67
8:M:1002:ARG:HD2	8:M:1003:PRO:HD2	1.77	0.67
3:E:72:ARG:NH2	3:E:76:LYS:O	2.28	0.67
9:R:58:ARG:HD2	10:S:166:VAL:HG22	1.76	0.67
11:X:88:LEU:O	11:X:92:ILE:HD12	1.95	0.67
11:V:96:LEU:HD22	11:V:100:VAL:HG11	1.77	0.67
12:W:421:GLU:HA	12:W:424:LYS:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:456:ILE:HD13	11:X:81:PRO:HG2	1.77	0.67
5:I:49:DC:H2''	5:I:50:DA:C8	2.30	0.67
7:Z:326:LYS:H	7:Z:327:PRO:HD2	1.59	0.67
11:T:289:ASN:HD21	12:Y:17:LEU:HG	1.60	0.66
12:Y:17:LEU:HD13	12:Y:19:LEU:HD13	1.77	0.66
1:A:116:ARG:NH2	1:A:123:GLU:OE2	2.28	0.66
12:U:23:HIS:HB3	12:U:86:MET:HG2	1.76	0.66
11:X:35:LEU:HD23	11:X:41:ALA:HB2	1.76	0.66
9:R:30:ASN:O	9:R:59:ARG:NH1	2.29	0.66
11:T:122:MET:HE3	11:T:323:TYR:HE2	1.59	0.66
12:W:100:ALA:HA	12:W:294:PHE:HB3	1.78	0.66
4:G:102:ARG:HA	4:G:110:ALA:HB1	1.76	0.66
8:M:1085:LEU:HD11	8:M:1108:ASN:HB3	1.78	0.66
12:U:58:LEU:HG	12:U:62:GLN:HE22	1.60	0.66
11:T:447:LEU:HB2	11:T:451:ARG:HG3	1.77	0.66
1:B:48:LEU:HG	3:E:117:LEU:HD13	1.76	0.66
11:T:361:PRO:HA	11:T:364:ILE:HG12	1.78	0.66
2:D:93:GLN:OE1	2:D:95:ARG:NH1	2.29	0.65
6:J:-92:DC:H2'	6:J:-91:DG:C8	2.31	0.65
8:M:854:THR:HG23	8:M:931:ARG:HH12	1.59	0.65
11:T:371:ARG:NH1	11:T:372:THR:O	2.28	0.65
12:U:408:GLN:HE21	11:V:60:VAL:HG13	1.61	0.65
6:J:-16:DT:H2''	6:J:-15:DA:C8	2.31	0.65
8:M:1067:CYS:SG	8:M:1133:ARG:NH1	2.68	0.65
12:U:327:ARG:NH2	12:U:329:VAL:O	2.29	0.65
11:T:106:VAL:HA	11:T:311:ASP:HB2	1.77	0.65
8:M:1286:GLY:HA3	12:W:232:ARG:HH12	1.60	0.65
6:J:64:DG:H1'	7:Z:225:ARG:HD2	1.78	0.65
11:V:387:ARG:HA	11:V:390:VAL:HG12	1.77	0.65
5:I:-68:DG:O6	6:J:68:DC:N4	2.15	0.65
12:W:386:LEU:HA	12:W:389:LYS:HG2	1.78	0.65
7:Z:234:HIS:HB3	8:M:793:PRO:HD2	1.79	0.65
8:M:953:LEU:HD23	8:M:958:ARG:HD2	1.79	0.64
8:M:1148:ARG:NH2	12:Y:250:ARG:O	2.30	0.64
11:T:139:VAL:HB	11:T:239:LYS:HB2	1.79	0.64
11:T:177:LYS:NZ	11:T:178:THR:O	2.30	0.64
11:X:42:LYS:HB3	11:X:45:GLU:HB2	1.77	0.64
9:R:126:ASP:HA	9:R:416:ARG:HE	1.61	0.64
8:M:1357:ARG:NH1	13:M:1601:ADP:O1B	2.29	0.64
8:M:1049:LEU:HA	8:M:1052:LYS:HZ3	1.62	0.64
11:V:314:ASN:HD22	11:V:342:ARG:HG2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:41:ALA:HB3	11:V:52:ILE:HG23	1.79	0.64
12:W:23:HIS:HB3	12:W:86:MET:HG2	1.80	0.64
11:T:132:ARG:HA	11:T:246:ASP:HA	1.80	0.64
6:J:-88:DA:H2''	6:J:-87:DC:C5	2.33	0.63
6:J:55:DC:H2''	6:J:56:DG:N7	2.13	0.63
11:T:387:ARG:NH2	13:T:501:ADP:O3'	2.31	0.63
8:M:829:ILE:HA	8:M:836:ARG:HH21	1.63	0.63
12:Y:159:THR:HG23	12:Y:168:ILE:HG12	1.80	0.63
12:U:241:LEU:HG	12:U:244:ILE:HD11	1.80	0.63
12:U:333:ARG:NH1	11:V:319:GLU:OE2	2.31	0.63
11:V:33:LEU:O	11:V:55:ARG:NH1	2.31	0.63
9:R:375:ARG:HH21	11:T:174:LYS:HB2	1.62	0.63
12:Y:247:ILE:HA	12:Y:253:GLY:HA3	1.80	0.63
6:J:83:DG:H2''	6:J:84:DG:N7	2.14	0.63
12:U:92:LEU:HD12	12:U:96:VAL:HG11	1.79	0.63
1:A:84:PHE:HB3	1:A:89:ILE:HD11	1.81	0.63
2:C:29:ILE:O	2:C:55:ARG:NH2	2.31	0.63
9:R:24:LYS:NZ	9:R:25:PRO:O	2.32	0.63
10:S:117:PRO:O	10:S:128:ARG:NH1	2.31	0.63
11:V:169:GLY:HA2	11:V:178:THR:HA	1.81	0.63
5:I:101:DT:H2''	5:I:102:DG:H5''	1.81	0.62
12:W:344:PRO:HG2	12:W:347:LEU:HD23	1.81	0.62
11:X:129:ILE:HD12	11:X:249:LEU:HD22	1.81	0.62
11:X:145:THR:N	11:X:169:GLY:O	2.31	0.62
2:C:73:THR:OG1	2:C:85:ASP:OD2	2.16	0.62
2:D:48:GLY:N	6:J:7:DC:OP1	2.32	0.62
3:E:30:ARG:HD3	3:E:33:ARG:HH21	1.64	0.62
2:D:45:ARG:HB3	1:A:118:THR:HG22	1.82	0.62
10:S:249:GLY:O	10:S:262:LYS:NZ	2.33	0.62
8:M:923:GLN:O	8:M:926:ARG:NH1	2.33	0.62
8:M:946:GLU:HA	8:M:1366:ILE:HB	1.82	0.62
8:M:764:PHE:HE2	8:M:800:ILE:HD11	1.64	0.62
9:R:198:THR:HB	9:R:216:LEU:HB3	1.82	0.62
12:U:202:LEU:HD11	12:U:223:GLN:HE21	1.63	0.62
12:U:415:ASN:ND2	12:U:417:THR:O	2.31	0.62
2:D:75:HIS:O	4:G:95:ARG:NH2	2.31	0.62
6:J:50:DG:H2''	6:J:51:DG:C8	2.35	0.62
10:S:119:LEU:HD13	10:S:209:HIS:NE2	2.14	0.62
11:V:361:PRO:HA	11:V:364:ILE:HG12	1.81	0.62
11:X:313:VAL:HG23	11:X:316:LEU:HD12	1.80	0.62
12:Y:24:SER:H	12:Y:371:ARG:HH12	1.45	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ARG:O	1:B:53:ARG:HG3	1.99	0.62
9:R:234:ARG:NH2	9:R:308:ASP:OD2	2.33	0.62
11:V:308:LEU:HB2	11:V:336:VAL:HG23	1.80	0.62
12:W:398:TYR:OH	12:W:430:PHE:O	2.17	0.62
12:Y:408:GLN:HA	12:Y:411:MET:HG3	1.82	0.62
5:I:-50:DC:N4	5:I:-49:DG:O6	2.33	0.62
10:S:195:ILE:HD13	10:S:198:LEU:HD12	1.82	0.62
11:T:448:ASP:OD1	11:T:451:ARG:HG2	1.99	0.62
12:U:145:ILE:HA	12:U:156:GLY:HA2	1.81	0.62
12:W:71:VAL:HG23	12:W:352:ILE:HG23	1.81	0.62
2:C:95:ARG:HG3	3:E:100:ASN:HB2	1.81	0.61
4:G:119:ARG:NH2	3:E:58:TYR:OH	2.33	0.61
6:J:45:DT:H2''	6:J:46:DG:N7	2.15	0.61
8:M:956:ARG:HD2	8:M:1002:ARG:HH11	1.65	0.61
12:Y:141:VAL:HG22	12:Y:161:LYS:HE3	1.82	0.61
5:I:55:DT:O4	6:J:-56:DG:N1	2.33	0.61
9:R:98:HIS:HD2	9:R:127:SER:HB2	1.65	0.61
4:G:48:LEU:HD21	4:G:55:THR:HB	1.82	0.61
11:X:166:VAL:N	11:X:181:LEU:O	2.31	0.61
9:R:110:GLU:O	9:R:114:HIS:ND1	2.34	0.61
9:R:347:PRO:HA	9:R:350:VAL:HG22	1.82	0.61
4:H:40:TYR:HA	4:H:43:TYR:HD2	1.66	0.61
11:T:308:LEU:HB3	11:T:336:VAL:HG22	1.82	0.61
12:W:409:ILE:HA	12:W:412:LYS:HE3	1.82	0.61
11:V:346:THR:HA	11:V:354:ILE:HA	1.82	0.61
12:W:413:ARG:NH1	12:W:421:GLU:OE2	2.30	0.61
11:X:264:ASP:O	11:X:267:SER:OG	2.13	0.61
12:Y:157:LYS:HD2	12:Y:168:ILE:HG22	1.83	0.61
1:B:63:ARG:HD3	6:J:-14:DA:H4'	1.83	0.61
8:M:830:LYS:HB2	8:M:862:GLU:HB2	1.82	0.61
9:R:288:ARG:NH1	9:R:295:VAL:O	2.34	0.61
11:T:368:LEU:HD21	12:Y:401:ASN:HB3	1.82	0.60
11:T:392:ARG:HH22	12:U:65:THR:HG21	1.65	0.60
12:U:25:HIS:CD2	12:U:26:ILE:HG23	2.36	0.60
5:I:99:DC:N4	6:J:-100:DC:O2	2.34	0.60
8:M:1267:ILE:HD11	8:M:1318:ILE:HG12	1.82	0.60
12:W:31:LEU:HD13	12:W:35:LEU:HA	1.83	0.60
12:W:130:LYS:HG3	12:W:236:VAL:HG22	1.82	0.60
8:M:1150:VAL:HG22	8:M:1152:TYR:H	1.65	0.60
11:V:384:ILE:HG23	11:V:419:LEU:HD11	1.83	0.60
12:W:408:GLN:HA	12:W:411:MET:HG3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:447:TYR:HH	11:X:345:THR:HG1	1.48	0.60
12:U:122:ARG:NH1	12:U:245:ASP:OD2	2.34	0.60
12:U:431:LEU:HB3	11:V:369:ILE:HD11	1.84	0.60
11:X:137:LYS:HE3	11:X:203:GLU:HB2	1.82	0.60
5:I:104:DC:H2'	5:I:105:DT:C6	2.35	0.60
8:M:778:GLY:HA3	8:M:782:GLN:HB2	1.84	0.60
9:R:430:HIS:O	9:R:436:ASN:ND2	2.35	0.60
12:W:329:VAL:HG22	12:W:340:PRO:HA	1.84	0.60
3:F:30:ARG:HD2	4:H:38:GLU:HG3	1.83	0.60
11:T:447:LEU:HA	11:T:451:ARG:HE	1.67	0.60
2:C:40:ARG:HH21	3:E:108:VAL:HG22	1.67	0.60
5:I:-77:DC:H2'	5:I:-76:DG:N7	2.17	0.60
11:T:356:PRO:HG3	12:Y:437:VAL:HG22	1.84	0.60
11:V:456:LEU:O	11:V:459:SER:OG	2.16	0.60
11:X:192:GLU:HG3	11:X:209:VAL:HB	1.84	0.59
11:T:33:LEU:O	11:T:55:ARG:NH1	2.35	0.59
11:V:395:VAL:HG22	11:V:434:ILE:HD12	1.84	0.59
11:X:58:CYS:HA	11:X:61:ILE:HD12	1.83	0.59
5:I:-59:DT:H5''	8:M:844:ASN:HD22	1.66	0.59
10:S:9:ASP:OD1	10:S:10:LYS:N	2.34	0.59
11:X:252:LEU:O	11:X:256:ASN:ND2	2.34	0.59
9:R:273:GLU:O	9:R:288:ARG:N	2.35	0.59
12:W:437:VAL:O	12:W:441:GLN:HG2	2.02	0.59
11:X:439:VAL:O	11:X:443:LYS:HG2	2.03	0.59
1:B:59:GLU:OE2	1:B:59:GLU:N	2.34	0.59
11:V:51:GLN:HB3	11:V:54:ALA:HB3	1.84	0.59
12:W:77:PRO:HG3	12:W:326:ASN:HD21	1.66	0.59
11:X:99:LYS:O	11:X:132:ARG:NH2	2.36	0.59
8:M:1272:THR:HA	8:M:1275:LEU:HD13	1.83	0.59
9:R:66:LEU:HD12	9:R:72:GLU:HG3	1.85	0.59
11:T:71:SER:OG	11:T:333:ALA:O	2.20	0.59
11:T:313:VAL:HG11	11:T:338:LEU:HG	1.84	0.59
12:W:132:GLU:HA	12:W:234:THR:HA	1.83	0.59
2:C:29:ILE:HD11	2:C:55:ARG:HG3	1.85	0.59
6:J:-15:DA:OP1	8:M:808:GLN:NE2	2.36	0.59
8:M:1174:ARG:HD2	8:M:1177:ILE:HD11	1.82	0.59
9:R:268:ASP:OD1	9:R:269:LYS:N	2.36	0.59
11:V:131:LEU:HD22	11:V:292:VAL:HG21	1.84	0.59
11:X:317:ASP:H	11:X:320:ILE:HD13	1.68	0.59
1:B:62:ILE:HD11	2:C:37:LEU:HD11	1.83	0.59
1:B:121:LYS:H	1:B:121:LYS:HD2	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-56:DC:H2''	5:I:-55:DG:C8	2.38	0.59
11:V:51:GLN:NE2	11:V:373:LEU:O	2.36	0.59
12:Y:47:GLN:HB3	12:Y:50:ALA:HB3	1.84	0.59
9:R:226:LEU:HD11	9:R:313:ILE:HG23	1.84	0.59
11:V:241:LYS:NZ	11:V:242:GLU:O	2.32	0.59
11:X:140:TYR:HB2	11:X:202:ILE:HB	1.84	0.59
12:Y:136:ILE:HD11	12:Y:194:LYS:HD3	1.83	0.59
5:I:105:DT:H4'	5:I:106:DT:H5'	1.83	0.59
8:M:1069:LYS:HD2	8:M:1072:VAL:HB	1.83	0.59
10:S:271:LEU:O	10:S:275:THR:OG1	2.21	0.59
12:W:32:ASP:OD1	12:W:36:GLN:N	2.32	0.59
9:R:377:LEU:HD21	9:R:383:CYS:HB2	1.84	0.58
12:U:332:THR:HG1	12:U:335:THR:HG1	1.51	0.58
11:V:203:GLU:OE1	11:V:206:THR:N	2.32	0.58
5:I:-18:DC:H2''	5:I:-17:DT:H5'	1.84	0.58
9:R:289:ASN:HB3	9:R:292:LYS:HG2	1.84	0.58
10:S:274:GLU:HA	10:S:280:ARG:HH21	1.68	0.58
9:R:9:ASP:HB2	9:R:16:LYS:HB3	1.84	0.58
10:S:103:MET:HG2	10:S:120:LEU:HD12	1.84	0.58
11:X:109:GLU:HB3	12:Y:114:THR:HG21	1.85	0.58
3:F:43:ARG:HB3	4:H:91:THR:HG23	1.85	0.58
6:J:-82:DA:H1'	6:J:-81:DG:C5	2.38	0.58
8:M:836:ARG:HA	8:M:839:ALA:HB3	1.85	0.58
2:D:39:ARG:NH1	2:D:43:VAL:O	2.36	0.58
4:G:102:ARG:HB3	4:G:114:VAL:HG21	1.84	0.58
9:R:407:ASP:O	9:R:411:LYS:NZ	2.35	0.58
11:V:424:ILE:HG21	12:W:59:LYS:HZ3	1.69	0.58
11:V:42:LYS:O	11:V:55:ARG:NH2	2.36	0.58
11:V:364:ILE:HA	11:V:367:LEU:HB2	1.86	0.58
11:X:321:PHE:HB3	11:X:363:LEU:HD11	1.84	0.58
12:Y:171:LEU:HD23	12:Y:176:ILE:HD13	1.84	0.58
12:Y:188:ASP:HA	12:Y:204:ARG:HA	1.84	0.58
12:Y:332:THR:OG1	12:Y:335:THR:OG1	2.21	0.58
12:Y:344:PRO:HG2	12:Y:347:LEU:HD23	1.86	0.58
12:W:139:GLU:N	12:W:161:LYS:O	2.34	0.58
12:Y:21:ALA:O	12:Y:371:ARG:NH2	2.28	0.58
12:U:45:VAL:O	13:U:501:ADP:N6	2.37	0.58
12:Y:44:MET:HB2	13:Y:501:ADP:HN62	1.67	0.58
11:T:264:ASP:OD1	11:T:265:VAL:N	2.37	0.58
11:V:109:GLU:HB3	12:W:114:THR:HG21	1.86	0.58
8:M:1169:ARG:NH1	11:X:256:ASN:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:134:LYS:NZ	11:T:136:THR:OG1	2.37	0.58
12:U:132:GLU:HB3	12:U:232:ARG:HH12	1.69	0.58
12:W:154:LYS:HB2	12:W:176:ILE:HD12	1.85	0.58
12:W:243:GLU:HA	12:W:246:VAL:HG22	1.86	0.58
12:W:191:SER:HB2	12:W:200:THR:HB	1.86	0.57
11:X:42:LYS:HD3	11:X:44:VAL:H	1.67	0.57
6:J:60:DC:H2''	6:J:61:DC:C5	2.39	0.57
8:M:1148:ARG:NH2	12:Y:247:ILE:O	2.37	0.57
8:M:1329:ASN:HA	8:M:1357:ARG:HH21	1.70	0.57
11:V:199:VAL:HG23	11:V:212:VAL:HB	1.84	0.57
12:W:47:GLN:HB3	12:W:50:ALA:HB3	1.86	0.57
11:X:226:THR:OG1	12:Y:196:SER:O	2.21	0.57
11:X:343:GLY:O	11:X:357:HIS:N	2.37	0.57
7:Z:312:GLN:HA	7:Z:315:LYS:HE3	1.86	0.57
11:T:140:TYR:HA	11:T:237:VAL:O	2.04	0.57
12:W:22:ALA:O	12:W:25:HIS:NE2	2.38	0.57
11:X:49:VAL:H	13:X:501:ADP:HN62	1.51	0.57
11:X:151:ASP:HA	11:X:163:ILE:HA	1.86	0.57
4:G:55:THR:HG23	3:E:72:ARG:HH12	1.69	0.57
8:M:837:TRP:HH2	8:M:868:TYR:HD2	1.53	0.57
8:M:953:LEU:HD12	8:M:957:GLN:NE2	2.18	0.57
12:U:331:LYS:HA	12:U:338:LYS:HA	1.86	0.57
12:Y:122:ARG:HH11	12:Y:241:LEU:HB3	1.69	0.57
6:J:42:DA:H2''	6:J:43:DA:C8	2.39	0.57
8:M:1297:LYS:O	8:M:1301:ARG:NH1	2.37	0.57
10:S:16:ASP:HB2	12:U:147:ARG:HG3	1.85	0.57
11:V:36:ASP:OD1	11:V:40:VAL:N	2.38	0.57
12:W:128:LYS:HD3	12:W:238:THR:HA	1.86	0.57
11:X:193:LYS:O	11:X:211:ARG:NH1	2.38	0.57
11:T:114:GLU:HB2	11:T:277:LYS:HE3	1.86	0.57
11:V:23:ARG:NH1	12:W:64:GLY:O	2.38	0.57
11:V:138:GLU:OE1	11:V:238:HIS:NE2	2.37	0.57
11:V:187:GLU:HG2	11:V:190:GLN:HE21	1.69	0.57
11:X:395:VAL:HG22	11:X:434:ILE:HD13	1.86	0.57
1:B:68:GLN:HA	1:B:71:VAL:HG12	1.87	0.57
3:F:53:THR:HA	3:F:56:LEU:HD12	1.86	0.57
5:I:58:DG:H2''	5:I:59:DA:N7	2.20	0.57
8:M:1133:ARG:NH2	12:Y:221:PHE:O	2.38	0.57
12:W:89:SER:HA	12:W:92:LEU:HD12	1.87	0.57
12:Y:448:ILE:HA	12:Y:454:VAL:HB	1.86	0.57
4:H:72:ILE:HD13	4:H:75:ARG:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:-24:DT:H2'	6:J:-23:DT:H71	1.87	0.57
8:M:803:TYR:OH	8:M:824:ASP:O	2.21	0.57
12:U:162:THR:HG23	12:U:164:ASP:H	1.69	0.57
11:V:196:ILE:O	11:V:214:ARG:NH2	2.37	0.57
11:V:413:ARG:HA	11:V:416:LEU:HD12	1.87	0.57
11:X:346:THR:HG22	11:X:354:ILE:HG12	1.85	0.57
11:X:406:MET:HA	11:X:409:GLU:HG2	1.87	0.56
8:M:1209:THR:HG23	11:T:191:ARG:NH1	2.19	0.56
10:S:14:ASN:ND2	10:S:16:ASP:OD1	2.38	0.56
7:Z:256:LEU:O	7:Z:260:LYS:NZ	2.33	0.56
1:A:64:LYS:NZ	1:A:68:GLN:OE1	2.38	0.56
9:R:116:ASP:OD1	9:R:419:TYR:OH	2.14	0.56
11:T:148:THR:O	11:T:167:ILE:N	2.35	0.56
12:U:121:PHE:O	12:U:124:SER:OG	2.23	0.56
12:U:267:SER:HA	12:U:270:ARG:HG3	1.86	0.56
11:V:139:VAL:HB	11:V:239:LYS:HB2	1.87	0.56
11:X:135:GLU:HB2	11:X:243:ILE:HB	1.87	0.56
5:I:-75:DC:H2''	5:I:-74:DC:C5	2.40	0.56
8:M:1069:LYS:HA	8:M:1072:VAL:HB	1.87	0.56
11:T:365:ASP:OD2	12:Y:397:ARG:NH2	2.36	0.56
12:U:76:PRO:O	12:U:81:LYS:NZ	2.37	0.56
2:D:90:LEU:HD22	2:D:95:ARG:HD2	1.87	0.56
3:F:91:ASP:HB3	3:F:94:LEU:HB2	1.88	0.56
9:R:339:SER:O	9:R:346:ARG:NH2	2.38	0.56
3:E:66:LEU:HB3	3:E:87:ALA:HB1	1.87	0.56
12:U:310:ASN:O	12:U:350:ARG:NH1	2.39	0.56
12:W:331:LYS:HE3	12:W:336:ASN:HA	1.87	0.56
5:I:-44:DA:H2'	5:I:-43:DT:H71	1.87	0.56
6:J:-56:DG:H1'	6:J:-55:DA:C8	2.41	0.56
12:U:204:ARG:O	12:U:222:VAL:N	2.39	0.56
11:V:282:GLU:OE1	11:V:285:ARG:NH2	2.39	0.56
11:V:384:ILE:HG21	11:V:403:LEU:HD13	1.87	0.56
12:W:80:GLY:HA2	13:W:501:ADP:H5'1	1.87	0.56
7:Z:590:LEU:HD23	12:W:185:LEU:HG	1.87	0.56
8:M:954:SER:H	8:M:957:GLN:NE2	2.04	0.56
11:T:405:THR:O	11:T:408:THR:OG1	2.19	0.56
11:V:286:GLN:HA	11:V:289:ASN:HD21	1.71	0.56
12:Y:135:LEU:HG	12:Y:193:ASP:HA	1.88	0.56
12:W:26:ILE:HA	12:W:43:GLY:HA3	1.87	0.56
2:C:75:HIS:NE2	4:H:87:ASN:OD1	2.39	0.56
2:C:76:ALA:O	2:C:78:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:76:LEU:HB2	11:T:338:LEU:HD22	1.87	0.56
12:U:420:VAL:HG12	12:U:424:LYS:HE2	1.88	0.56
11:V:248:THR:HG23	11:V:251:ASP:H	1.69	0.56
3:F:89:ARG:NH2	3:F:98:LEU:O	2.39	0.55
8:M:689:PRO:HA	8:M:692:LEU:HD12	1.88	0.55
8:M:1208:ASN:ND2	11:T:187:GLU:OE2	2.36	0.55
11:V:280:ILE:HG23	11:V:284:LEU:HD23	1.87	0.55
12:W:161:LYS:HB2	12:W:166:GLU:HG3	1.89	0.55
8:M:1267:ILE:HB	8:M:1339:TYR:HE2	1.70	0.55
9:R:5:PRO:HB3	9:R:98:HIS:HB2	1.88	0.55
12:W:259:THR:OG1	12:W:261:ASP:OD1	2.24	0.55
4:G:75:ARG:HH21	4:G:79:GLU:HB2	1.71	0.55
8:M:1378:ASN:HA	8:M:1381:LYS:HE3	1.88	0.55
12:W:20:ILE:HG22	11:X:73:ARG:HH22	1.71	0.55
4:G:75:ARG:NH2	4:G:79:GLU:OE1	2.39	0.55
12:U:281:LYS:HD3	12:U:288:ILE:HG23	1.89	0.55
2:D:34:ILE:HG21	2:D:51:TYR:HA	1.87	0.55
5:I:102:DG:C8	5:I:103:DT:H72	2.42	0.55
11:X:394:GLN:OE1	11:X:432:LYS:NZ	2.37	0.55
1:B:100:LEU:HD11	2:C:37:LEU:HD22	1.88	0.55
3:F:81:PRO:HB2	3:F:105:GLN:HB3	1.88	0.55
7:Z:202:ASN:OD1	7:Z:203:THR:N	2.40	0.55
10:S:264:CYS:SG	10:S:265:SER:N	2.80	0.55
12:U:136:ILE:HB	12:U:192:ILE:HB	1.89	0.55
1:B:45:THR:HG23	6:J:69:DT:H4'	1.88	0.55
3:F:55:VAL:HG22	4:H:113:ALA:HB1	1.89	0.55
7:Z:207:TYR:OH	3:E:69:ASN:OD1	2.04	0.55
8:M:1200:ASN:O	8:M:1210:ARG:NH1	2.40	0.55
10:S:112:ASP:HA	10:S:115:ASN:HD21	1.72	0.55
12:W:449:ASP:OD1	12:W:452:GLY:N	2.40	0.55
12:W:331:LYS:HA	12:W:338:LYS:HA	1.88	0.55
12:U:413:ARG:NH2	12:U:422:ASP:OD2	2.40	0.54
6:J:4:DG:H2''	6:J:5:DT:C5	2.42	0.54
11:T:71:SER:HB2	12:Y:19:LEU:HD23	1.88	0.54
12:W:44:MET:HA	13:W:501:ADP:N1	2.23	0.54
11:X:42:LYS:O	11:X:55:ARG:NH2	2.40	0.54
3:F:66:LEU:HB3	3:F:87:ALA:HB1	1.90	0.54
6:J:-46:DT:H2'	6:J:-45:DG:C8	2.42	0.54
9:R:27:ARG:HE	9:R:394:LEU:HD21	1.72	0.54
10:S:189:ARG:HH22	10:S:199:LYS:HB2	1.73	0.54
11:V:70:MET:SD	11:V:73:ARG:HB2	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:440:ASN:OD1	11:V:443:LYS:NZ	2.34	0.54
12:Y:243:GLU:HA	12:Y:257:LEU:HD21	1.89	0.54
8:M:1212:LYS:HD2	11:T:265:VAL:HG21	1.89	0.54
5:I:60:DT:H2''	5:I:61:DA:N7	2.23	0.54
6:J:-57:DT:O2	6:J:-56:DG:N1	2.40	0.54
6:J:-30:DA:H1'	6:J:-29:DT:H5'	1.89	0.54
9:R:148:ARG:O	9:R:387:VAL:N	2.40	0.54
10:S:189:ARG:NH2	10:S:199:LYS:HB2	2.23	0.54
11:V:168:VAL:O	11:V:179:LEU:N	2.36	0.54
4:H:100:ALA:O	4:H:104:ILE:HG12	2.07	0.54
8:M:988:GLN:HA	8:M:991:LYS:HG2	1.90	0.54
10:S:18:TYR:HB3	12:U:145:ILE:HD12	1.89	0.54
12:W:134:GLU:HA	12:W:232:ARG:HA	1.90	0.54
11:X:406:MET:HG2	11:X:443:LYS:HE3	1.90	0.54
3:F:52:LEU:O	3:F:56:LEU:HG	2.08	0.54
4:H:74:GLU:O	4:H:78:THR:HG23	2.08	0.54
6:J:82:DC:H2''	6:J:83:DG:C8	2.43	0.54
11:X:33:LEU:HD11	11:X:62:VAL:HG21	1.89	0.54
7:Z:257:ASP:OD1	7:Z:258:LYS:N	2.41	0.54
8:M:695:ASN:O	13:M:1601:ADP:N6	2.40	0.54
9:R:2:GLU:HG2	9:R:97:HIS:HA	1.90	0.54
9:R:153:LYS:HA	9:R:374:GLN:HG2	1.89	0.54
9:R:373:LEU:O	9:R:377:LEU:N	2.40	0.54
5:I:101:DT:H5''	7:Z:322:LYS:HD2	1.89	0.54
6:J:80:DC:H2''	6:J:81:DG:C8	2.43	0.54
8:M:1016:SER:HA	8:M:1019:LYS:HG2	1.90	0.54
8:M:1159:ASP:HA	8:M:1162:LEU:HB3	1.90	0.54
11:V:316:LEU:HB2	11:V:320:ILE:HD13	1.90	0.54
11:X:288:VAL:HA	11:X:291:VAL:HG22	1.90	0.54
4:G:116:GLU:O	4:G:119:ARG:HG3	2.08	0.53
8:M:758:LEU:O	8:M:761:GLU:HG3	2.08	0.53
8:M:1248:LEU:HD23	8:M:1251:LEU:HD23	1.90	0.53
11:X:106:VAL:HG12	11:X:108:SER:H	1.73	0.53
6:J:-61:DT:H2''	6:J:-60:DA:N7	2.24	0.53
8:M:1383:ALA:O	8:M:1388:GLN:N	2.40	0.53
9:R:274:TYR:HA	9:R:287:VAL:HA	1.89	0.53
11:V:386:ARG:O	11:V:389:THR:OG1	2.22	0.53
12:W:59:LYS:HA	12:W:62:GLN:HG3	1.89	0.53
2:C:29:ILE:HD13	2:C:58:LEU:HD13	1.89	0.53
4:H:106:PRO:HD2	4:H:109:LEU:HD12	1.89	0.53
10:S:16:ASP:OD1	10:S:16:ASP:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:211:ARG:HH22	11:T:214:ARG:HG2	1.73	0.53
11:X:331:ASN:OD1	11:X:332:ILE:HD12	2.08	0.53
5:I:72:DG:H2'	5:I:73:DT:H71	1.90	0.53
8:M:1034:GLN:HA	8:M:1037:ARG:HG2	1.90	0.53
12:U:40:THR:HA	12:U:45:VAL:HG12	1.90	0.53
12:U:256:ALA:HB1	12:U:262:THR:HG22	1.91	0.53
12:U:366:THR:O	12:U:370:ILE:HG12	2.09	0.53
12:Y:31:LEU:HD12	12:Y:55:GLY:HA3	1.90	0.53
1:B:115:LYS:HG2	1:A:122:LYS:HZ3	1.74	0.53
8:M:988:GLN:HG3	8:M:991:LYS:HE2	1.91	0.53
9:R:374:GLN:HA	9:R:377:LEU:HG	1.91	0.53
12:W:405:VAL:HB	12:W:408:GLN:HE21	1.72	0.53
11:X:198:ASP:HA	11:X:214:ARG:HA	1.90	0.53
11:X:253:ASP:OD1	11:X:288:VAL:HG11	2.08	0.53
12:W:365:LYS:HB2	12:W:388:THR:HG21	1.91	0.53
11:X:224:LEU:HD21	12:Y:192:ILE:HD13	1.90	0.53
8:M:1104:PHE:O	8:M:1107:SER:OG	2.19	0.53
8:M:1166:LEU:HA	8:M:1169:ARG:HD2	1.91	0.53
8:M:1209:THR:HG23	11:T:191:ARG:HH12	1.73	0.53
6:J:-89:DC:H2''	6:J:-88:DA:C8	2.44	0.53
6:J:29:DG:H2''	6:J:30:DC:C5	2.44	0.53
7:Z:298:THR:HB	7:Z:299:PRO:HD3	1.90	0.53
8:M:709:SER:O	8:M:713:ASN:ND2	2.36	0.53
8:M:1337:ILE:HG13	8:M:1367:TYR:HB2	1.91	0.53
11:V:272:LEU:HD13	11:X:269:MET:HG3	1.91	0.53
11:X:414:TYR:OH	11:X:446:PHE:O	2.25	0.53
5:I:96:DA:H2	6:J:-96:DT:H3	1.55	0.53
9:R:29:LEU:O	9:R:43:SER:OG	2.22	0.53
11:T:211:ARG:NH2	11:T:214:ARG:HG2	2.24	0.53
11:V:130:GLY:HA2	11:V:248:THR:HA	1.90	0.53
12:W:440:VAL:HA	12:W:443:ASN:HB2	1.90	0.53
11:X:166:VAL:O	11:X:181:LEU:N	2.39	0.53
11:X:293:ALA:HA	11:X:296:ILE:HG22	1.90	0.53
9:R:355:CYS:HB2	9:R:360:PHE:CG	2.44	0.53
11:X:328:LEU:HD21	11:X:366:ARG:HD3	1.91	0.53
11:X:341:ASN:OD1	11:X:342:ARG:NH1	2.42	0.53
8:M:1101:ASN:HA	9:R:187:PHE:HB2	1.89	0.52
9:R:256:SER:O	9:R:368:ARG:NH1	2.42	0.52
12:U:148:SER:N	12:U:152:GLY:O	2.41	0.52
12:W:402:LEU:HA	12:W:405:VAL:HG22	1.91	0.52
12:Y:71:VAL:HG23	12:Y:352:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-30:DG:N2	6:J:31:DT:O2	2.42	0.52
12:W:69:ARG:HB3	12:W:320:ILE:HD12	1.91	0.52
5:I:-7:DG:C8	5:I:-7:DG:H5'	2.45	0.52
9:R:113:LYS:HE3	9:R:424:PRO:HB2	1.90	0.52
11:T:65:ILE:HD11	11:T:305:PRO:HB2	1.92	0.52
12:U:246:VAL:HG11	12:U:257:LEU:HB2	1.92	0.52
12:Y:124:SER:HB2	12:Y:319:PRO:HG3	1.90	0.52
2:C:82:THR:HG23	2:C:85:ASP:H	1.73	0.52
7:Z:207:TYR:HD1	7:Z:210:LEU:HD12	1.74	0.52
9:R:25:PRO:HB3	9:R:397:TRP:CD2	2.45	0.52
12:U:409:ILE:HA	12:U:412:LYS:HD3	1.91	0.52
11:V:324:LEU:HA	11:V:327:ALA:HB3	1.91	0.52
12:Y:212:TYR:HB2	12:Y:215:MET:SD	2.50	0.52
12:Y:299:HIS:HB3	12:Y:325:THR:HG23	1.91	0.52
12:W:146:ASP:OD2	12:W:157:LYS:NZ	2.33	0.52
11:X:84:GLY:HA3	13:X:501:ADP:C8	2.41	0.52
6:J:-48:DC:H1'	6:J:-47:DC:C6	2.45	0.52
12:U:410:ALA:O	12:U:413:ARG:HG2	2.10	0.52
7:Z:599:TYR:HD1	11:X:159:TYR:HB2	1.74	0.52
8:M:698:THR:HA	8:M:701:LYS:HD2	1.90	0.52
8:M:957:GLN:NE2	8:M:1246:GLY:H	2.07	0.52
11:T:86:THR:OG1	12:U:311:ARG:NH1	2.43	0.52
12:U:20:ILE:HD11	11:V:70:MET:HA	1.92	0.52
11:V:114:GLU:HB2	11:V:276:LYS:HE2	1.91	0.52
11:X:130:GLY:HA2	11:X:248:THR:HA	1.92	0.52
11:T:462:TYR:HB2	12:U:328:GLY:HA3	1.91	0.52
11:X:86:THR:N	13:X:501:ADP:O1A	2.37	0.52
12:Y:244:ILE:HA	12:Y:247:ILE:HG12	1.90	0.52
6:J:-22:DG:H21	8:M:980:MET:HE2	1.75	0.52
9:R:201:ILE:HA	9:R:213:VAL:HG22	1.92	0.52
11:T:342:ARG:HB2	11:T:357:HIS:HA	1.92	0.52
11:T:463:LEU:HD22	12:U:76:PRO:HG3	1.91	0.52
12:U:123:LYS:NZ	12:U:243:GLU:OE2	2.42	0.52
12:W:398:TYR:HA	12:W:401:ASN:HD21	1.75	0.52
11:X:105:LEU:N	11:X:309:PHE:O	2.42	0.52
11:X:314:ASN:OD1	11:X:315:MET:N	2.43	0.52
11:X:413:ARG:NH2	13:X:501:ADP:O3A	2.43	0.52
12:Y:378:GLU:HG2	12:Y:417:THR:HA	1.91	0.52
5:I:56:DC:O2	6:J:-56:DG:N2	2.43	0.52
6:J:53:DC:H2''	6:J:54:DT:H73	1.91	0.52
7:Z:254:LEU:HD22	8:M:769:PRO:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:126:ARG:HD3	11:T:285:ARG:HH21	1.73	0.52
11:T:459:SER:HB3	11:T:463:LEU:H	1.74	0.51
12:U:437:VAL:O	12:U:441:GLN:HG3	2.10	0.51
11:V:86:THR:OG1	13:V:501:ADP:O1A	2.28	0.51
12:W:114:THR:O	12:W:118:THR:HG23	2.10	0.51
5:I:72:DG:H2''	5:I:73:DT:H5'	1.91	0.51
12:W:432:ASP:H	12:W:435:ARG:HD3	1.76	0.51
2:D:25:ASN:O	1:A:69:ARG:NH2	2.43	0.51
3:E:19:SER:OG	3:E:26:PHE:O	2.23	0.51
4:H:91:THR:N	6:J:-35:DG:OP1	2.44	0.51
11:T:393:LEU:HD21	11:T:423:GLY:HA3	1.93	0.51
2:C:29:ILE:O	2:C:29:ILE:HG13	2.11	0.51
2:D:25:ASN:ND2	1:A:73:GLU:OE2	2.38	0.51
5:I:-23:DC:H2''	5:I:-22:DA:C8	2.45	0.51
6:J:-96:DT:H2''	6:J:-95:DT:C5	2.45	0.51
7:Z:202:ASN:O	7:Z:206:VAL:HG23	2.11	0.51
8:M:1188:VAL:HG23	11:V:260:GLN:HB2	1.92	0.51
9:R:356:THR:HA	9:R:392:CYS:HB3	1.92	0.51
11:V:147:LEU:HD23	11:V:168:VAL:HG12	1.92	0.51
11:V:417:GLN:HB3	12:W:69:ARG:HH12	1.76	0.51
11:X:424:ILE:HG21	12:Y:56:VAL:HG13	1.92	0.51
4:H:103:LEU:HD12	4:H:104:ILE:HG23	1.92	0.51
5:I:27:DG:H2''	5:I:28:DG:C8	2.45	0.51
5:I:84:DG:H2''	5:I:85:DG:C8	2.46	0.51
11:T:109:GLU:HA	12:U:114:THR:HG21	1.92	0.51
11:T:253:ASP:OD2	11:T:285:ARG:NH2	2.44	0.51
4:H:60:LYS:HD2	4:H:61:SER:N	2.25	0.51
6:J:-53:DA:H2''	6:J:-52:DC:C5	2.46	0.51
6:J:78:DG:H2''	6:J:79:DC:H5'	1.93	0.51
8:M:810:GLN:HE22	8:M:843:PHE:HE1	1.57	0.51
8:M:1264:ARG:NH2	8:M:1310:THR:O	2.37	0.51
9:R:325:ILE:HD11	10:S:102:PHE:HB2	1.92	0.51
11:V:140:TYR:HB2	11:V:202:ILE:HG23	1.93	0.51
11:V:289:ASN:HA	11:V:292:VAL:HG12	1.91	0.51
11:V:459:SER:HB3	11:V:463:LEU:H	1.74	0.51
12:W:447:TYR:CE1	11:X:342:ARG:HA	2.45	0.51
11:X:456:LEU:HD11	12:Y:341:HIS:CD2	2.46	0.51
1:B:55:GLN:HG3	3:E:110:PRO:HD2	1.93	0.51
5:I:-16:DT:H2''	5:I:-15:DA:C8	2.46	0.51
11:V:75:ILE:O	11:V:337:VAL:HA	2.11	0.51
11:V:195:SER:N	11:V:198:ASP:OD2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:127:ILE:N	12:W:239:VAL:O	2.32	0.51
12:Y:190:ILE:HG22	12:Y:201:LYS:HA	1.92	0.51
2:D:47:SER:HB3	2:D:50:ILE:HG12	1.93	0.51
12:U:136:ILE:N	12:U:192:ILE:O	2.31	0.51
11:V:377:LYS:HG3	11:V:408:THR:HG21	1.93	0.51
2:D:78:ARG:HG2	2:D:80:THR:H	1.75	0.51
1:A:110:ALA:O	1:A:113:HIS:HB3	2.11	0.51
11:X:150:GLU:OE1	11:X:164:SER:OG	2.29	0.51
1:B:72:ARG:HB3	1:B:76:GLN:HE22	1.76	0.50
3:F:56:LEU:HD22	4:H:69:VAL:HG23	1.92	0.50
5:I:-37:DG:H1'	5:I:-36:DT:C6	2.46	0.50
1:A:66:PRO:O	1:A:69:ARG:NH1	2.44	0.50
9:R:196:ASN:OD1	9:R:221:ARG:NH2	2.40	0.50
11:T:139:VAL:N	11:T:239:LYS:O	2.37	0.50
11:T:289:ASN:ND2	12:Y:17:LEU:HG	2.25	0.50
12:U:305:CYS:O	12:U:309:ILE:HG12	2.10	0.50
11:V:308:LEU:HD11	11:V:334:PRO:HG2	1.92	0.50
3:F:22:ALA:HA	4:H:123:LYS:NZ	2.25	0.50
4:G:41:SER:OG	6:J:49:DC:OP1	2.24	0.50
6:J:-78:DC:H2''	6:J:-77:DA:C8	2.45	0.50
3:E:26:PHE:CZ	3:E:56:LEU:HD22	2.46	0.50
11:T:346:THR:HA	11:T:354:ILE:HA	1.93	0.50
8:M:960:LEU:HD21	8:M:998:LEU:HB3	1.93	0.50
8:M:1354:ARG:NH2	14:M:1602:BEF:F2	2.33	0.50
9:R:25:PRO:HB3	9:R:397:TRP:CE2	2.47	0.50
11:T:68:LYS:O	11:T:68:LYS:HG3	2.12	0.50
11:T:101:PRO:HD3	11:T:304:ILE:HD12	1.92	0.50
11:T:112:SER:OG	11:T:113:VAL:N	2.44	0.50
11:T:174:LYS:HE3	11:T:236:GLU:HG3	1.93	0.50
12:U:38:ARG:O	12:U:51:ARG:NH1	2.44	0.50
6:J:12:DG:H2''	6:J:13:DT:H5'	1.94	0.50
7:Z:311:GLU:HA	7:Z:314:ASN:HD21	1.75	0.50
8:M:822:VAL:HG22	8:M:849:LEU:HD23	1.92	0.50
12:U:256:ALA:O	12:U:260:GLY:N	2.44	0.50
12:U:380:SER:O	12:U:384:LEU:N	2.38	0.50
11:X:37:GLU:O	11:X:37:GLU:HG2	2.11	0.50
4:G:40:TYR:H	4:G:62:MET:HE2	1.76	0.50
5:I:57:DA:H2''	5:I:58:DG:C8	2.46	0.50
5:I:64:DT:H2''	5:I:65:DA:C8	2.47	0.50
5:I:66:DC:H5''	10:S:130:ARG:NH1	2.26	0.50
8:M:1334:ASP:OD2	8:M:1362:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:U:245:ASP:OD2	12:U:270:ARG:NH1	2.44	0.50
12:Y:359:TYR:OH	13:Y:501:ADP:N7	2.44	0.50
1:B:61:LEU:HD22	2:C:36:ARG:HD3	1.93	0.50
5:I:57:DA:H2''	5:I:58:DG:H8	1.77	0.50
6:J:-80:DT:H2''	6:J:-79:DA:C8	2.47	0.50
3:E:49:PRO:O	3:E:53:THR:HG23	2.11	0.50
8:M:1213:VAL:HA	8:M:1216:ASN:HD21	1.76	0.50
11:T:295:TYR:O	11:T:299:GLY:N	2.44	0.50
11:X:62:VAL:HA	11:X:65:ILE:HD12	1.94	0.50
5:I:-68:DG:N2	6:J:68:DC:O2	2.37	0.50
5:I:104:DC:H3'	5:I:105:DT:H2'	1.93	0.50
9:R:73:SER:HA	9:R:76:TRP:HE3	1.76	0.50
9:R:255:VAL:HG22	9:R:314:PRO:HB3	1.93	0.50
11:T:119:GLU:HG2	11:T:279:GLU:HA	1.94	0.50
11:V:200:ILE:HA	11:V:211:ARG:HA	1.94	0.50
11:V:453:THR:O	11:V:457:GLU:HG2	2.12	0.50
3:F:18:ARG:HA	3:F:21:LYS:HE3	1.94	0.50
5:I:100:DG:H2''	5:I:101:DT:C6	2.47	0.50
6:J:-105:DA:H2''	6:J:-104:DG:C8	2.47	0.50
8:M:1114:GLY:O	8:M:1118:MET:HG2	2.11	0.50
12:U:72:LEU:HD22	12:U:353:ILE:HG23	1.93	0.50
12:U:367:ILE:O	12:U:371:ARG:HG2	2.12	0.50
12:W:78:SER:HB2	12:W:396:LEU:HD21	1.93	0.50
11:X:51:GLN:HB3	11:X:54:ALA:HB3	1.94	0.50
11:X:66:LYS:HZ2	11:X:96:LEU:HD23	1.76	0.50
5:I:-5:DA:H5''	1:A:43:PRO:HG2	1.93	0.50
8:M:773:VAL:HG13	8:M:798:VAL:HG13	1.94	0.50
11:T:363:LEU:O	11:T:367:LEU:HD23	2.12	0.50
11:V:43:ARG:HH12	11:V:49:VAL:HB	1.77	0.50
11:V:285:ARG:O	11:V:289:ASN:ND2	2.45	0.50
12:W:19:LEU:HD23	11:X:71:SER:HB2	1.94	0.50
12:W:116:ALA:O	12:W:119:GLN:HG2	2.11	0.50
8:M:1023:ARG:HH22	12:U:196:SER:HB2	1.76	0.49
11:T:61:ILE:HD11	11:T:75:ILE:HD13	1.93	0.49
12:W:372:ALA:HB2	12:W:403:ILE:HD11	1.94	0.49
12:Y:204:ARG:N	12:Y:220:ARG:O	2.44	0.49
1:B:78:PHE:HZ	2:C:63:GLU:HG2	1.76	0.49
6:J:45:DT:H2''	6:J:46:DG:C8	2.47	0.49
8:M:968:ALA:O	8:M:972:ALA:N	2.45	0.49
8:M:1386:LYS:HE3	8:M:1390:ASP:H	1.77	0.49
9:R:189:LEU:HD11	9:R:334:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:58:CYS:O	11:T:62:VAL:HG23	2.12	0.49
11:V:387:ARG:HH11	11:V:419:LEU:HD12	1.77	0.49
2:C:47:SER:HB3	2:C:50:ILE:HG12	1.95	0.49
5:I:-36:DT:H4'	5:I:-35:DA:H5'	1.92	0.49
8:M:810:GLN:NE2	8:M:839:ALA:O	2.45	0.49
8:M:1166:LEU:HD13	11:X:259:PRO:HA	1.94	0.49
12:U:367:ILE:HB	12:U:371:ARG:HH12	1.77	0.49
11:V:378:ASP:OD1	11:V:379:GLU:N	2.45	0.49
12:W:145:ILE:HA	12:W:156:GLY:HA2	1.95	0.49
12:W:178:GLY:O	12:W:181:LYS:HG2	2.12	0.49
12:Y:315:ASP:OD1	12:Y:316:GLU:N	2.45	0.49
1:B:122:LYS:HZ3	1:A:115:LYS:HE3	1.77	0.49
2:D:62:LEU:HD11	1:A:67:PHE:CZ	2.48	0.49
8:M:753:PRO:HG2	8:M:756:VAL:CG1	2.42	0.49
10:S:93:GLN:O	10:S:97:GLN:HG2	2.12	0.49
11:T:378:ASP:OD1	11:T:378:ASP:N	2.44	0.49
12:U:139:GLU:HG2	12:U:161:LYS:O	2.13	0.49
11:V:106:VAL:HG12	11:V:108:SER:H	1.76	0.49
11:X:413:ARG:HH22	13:X:501:ADP:PA	2.34	0.49
11:X:453:THR:HA	11:X:456:LEU:HD12	1.94	0.49
4:H:72:ILE:O	4:H:76:ILE:HG22	2.12	0.49
5:I:3:DT:H2''	5:I:4:DC:C6	2.48	0.49
12:U:83:ALA:HB2	13:U:501:ADP:H2'	1.95	0.49
12:U:250:ARG:HG2	12:U:252:GLN:H	1.77	0.49
12:U:365:LYS:HG2	12:U:388:THR:HG21	1.95	0.49
12:U:402:LEU:HA	12:U:405:VAL:HG22	1.95	0.49
12:W:245:ASP:OD2	12:W:270:ARG:NE	2.40	0.49
8:M:1201:ASP:OD1	8:M:1201:ASP:N	2.46	0.49
8:M:1293:ASP:O	8:M:1296:THR:OG1	2.27	0.49
11:T:355:SER:OG	11:T:359:VAL:O	2.23	0.49
12:U:144:GLN:NE2	12:U:146:ASP:OD1	2.45	0.49
12:W:122:ARG:HE	12:W:242:HIS:HA	1.77	0.49
12:Y:127:ILE:HG12	12:Y:288:ILE:HG22	1.94	0.49
6:J:-31:DA:C8	6:J:-31:DA:H5'	2.47	0.49
8:M:1274:VAL:HA	8:M:1277:VAL:HG22	1.94	0.49
8:M:1353:ASP:CA	8:M:1356:HIS:HB3	2.42	0.49
12:U:80:GLY:N	13:U:501:ADP:O1B	2.44	0.49
12:U:157:LYS:HG3	12:U:170:GLU:HA	1.95	0.49
12:W:117:LEU:HD23	12:W:308:PHE:HD2	1.78	0.49
11:X:201:TYR:N	11:X:210:LYS:O	2.46	0.49
11:X:393:LEU:HD21	11:X:434:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LEU:HD13	1:A:127:ALA:HA	1.94	0.49
5:I:-10:DC:H2''	5:I:-9:DA:C8	2.48	0.49
6:J:-7:DG:H2''	6:J:-6:DG:N7	2.28	0.49
9:R:12:SER:HA	9:R:61:HIS:CG	2.48	0.49
11:T:313:VAL:HA	11:T:316:LEU:HD23	1.94	0.49
11:V:83:THR:N	13:V:501:ADP:O1B	2.46	0.49
1:B:67:PHE:CE2	1:B:93:GLN:HB3	2.47	0.49
6:J:-49:DG:H2''	6:J:-48:DC:O5'	2.12	0.49
6:J:25:DT:H2''	6:J:26:DA:C8	2.48	0.49
6:J:40:DC:OP1	3:E:36:ARG:NE	2.45	0.49
8:M:1221:SER:HA	11:V:191:ARG:NH1	2.27	0.49
12:U:377:VAL:HG21	12:U:403:ILE:HG12	1.94	0.49
11:V:138:GLU:HB2	11:V:204:ALA:HB3	1.93	0.49
5:I:23:DA:H1'	8:M:979:PHE:HZ	1.77	0.49
6:J:39:DA:P	3:E:32:HIS:HE2	2.36	0.49
6:J:52:DC:H2''	6:J:53:DC:C6	2.47	0.49
3:E:76:LYS:NZ	3:E:79:ILE:O	2.44	0.49
8:M:1206:GLY:O	8:M:1209:THR:OG1	2.31	0.49
11:T:292:VAL:O	11:T:296:ILE:HG23	2.13	0.49
12:U:111:LEU:HD11	12:U:263:GLY:HA2	1.95	0.49
12:U:117:LEU:HD23	12:U:309:ILE:HD11	1.95	0.49
12:U:143:ILE:HD13	12:U:179:LEU:HD11	1.94	0.49
11:V:313:VAL:HG11	11:V:338:LEU:HB3	1.94	0.49
11:X:23:ARG:HH12	12:Y:67:ALA:HB2	1.77	0.49
8:M:696:LEU:HD23	8:M:700:GLN:HB3	1.95	0.48
9:R:242:THR:O	9:R:246:ASN:ND2	2.46	0.48
12:Y:77:PRO:HB2	12:Y:397:ARG:HH22	1.78	0.48
5:I:-81:DC:H2''	5:I:-80:DG:C8	2.48	0.48
5:I:67:DA:H5'	5:I:67:DA:C8	2.47	0.48
6:J:31:DT:H2''	6:J:32:DG:C8	2.47	0.48
8:M:1142:ASP:OD1	8:M:1143:LEU:N	2.46	0.48
11:X:106:VAL:N	11:X:109:GLU:OE2	2.44	0.48
12:Y:440:VAL:HA	12:Y:447:TYR:CE2	2.48	0.48
6:J:-42:DG:H2''	6:J:-41:DA:C8	2.48	0.48
9:R:61:HIS:CE1	9:R:66:LEU:HB3	2.48	0.48
11:T:126:ARG:HD2	11:T:285:ARG:HE	1.78	0.48
12:W:447:TYR:OH	11:X:345:THR:OG1	2.21	0.48
12:Y:184:VAL:HG12	12:Y:186:ALA:H	1.76	0.48
12:Y:204:ARG:HB3	12:Y:208:ARG:HG3	1.95	0.48
6:J:31:DT:H2''	6:J:32:DG:N7	2.29	0.48
6:J:74:DG:C8	6:J:74:DG:H5'	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:985:CYS:O	8:M:989:LEU:HD23	2.13	0.48
8:M:1194:LYS:HD2	8:M:1199:LEU:HG	1.95	0.48
11:T:193:LYS:HA	11:T:193:LYS:HE2	1.95	0.48
11:V:79:GLY:O	11:V:85:LYS:NZ	2.46	0.48
12:W:131:GLU:OE2	12:W:237:HIS:NE2	2.45	0.48
12:W:188:ASP:HA	12:W:204:ARG:HA	1.94	0.48
11:X:352:ASP:N	11:X:352:ASP:OD1	2.46	0.48
12:Y:141:VAL:HB	12:Y:159:THR:HB	1.95	0.48
2:D:71:THR:O	4:G:102:ARG:NH2	2.46	0.48
5:I:-48:DC:H2''	5:I:-47:DT:C5	2.48	0.48
5:I:-20:DC:N4	5:I:-19:DG:O6	2.45	0.48
6:J:-35:DG:H5'	6:J:-35:DG:H8	1.79	0.48
6:J:49:DC:H2''	6:J:50:DG:C8	2.48	0.48
8:M:721:ASP:HB3	8:M:727:LYS:HD3	1.95	0.48
10:S:190:LYS:HB2	10:S:195:ILE:HG13	1.96	0.48
12:Y:29:LEU:HD21	12:Y:31:LEU:HD12	1.95	0.48
8:M:1328:ILE:HD12	8:M:1330:LEU:HD13	1.96	0.48
9:R:66:LEU:HD23	9:R:66:LEU:H	1.78	0.48
11:T:23:ARG:HH11	12:U:67:ALA:HB2	1.78	0.48
12:U:75:GLY:HA3	12:U:356:THR:HG22	1.94	0.48
11:V:285:ARG:HA	11:V:288:VAL:HG22	1.96	0.48
11:X:125:PHE:HZ	11:X:333:ALA:HA	1.78	0.48
12:Y:172:GLY:O	12:Y:176:ILE:N	2.39	0.48
3:F:47:GLY:HA3	4:H:121:VAL:HG22	1.95	0.48
12:Y:218:ASP:OD1	12:Y:218:ASP:N	2.46	0.48
6:J:77:DG:H2'	6:J:78:DG:H4'	1.95	0.48
7:Z:607:ASN:HB3	11:X:186:TYR:CE1	2.49	0.48
12:W:302:ASP:OD1	12:W:303:ILE:N	2.46	0.48
11:X:31:LYS:HB2	11:X:46:GLY:HA2	1.95	0.48
11:X:318:ILE:HA	11:X:321:PHE:HD2	1.78	0.48
4:H:79:GLU:OE2	4:H:100:ALA:HB1	2.14	0.48
5:I:52:DG:H1'	5:I:53:DT:H5'	1.95	0.48
5:I:54:DG:H2''	5:I:55:DT:O4'	2.13	0.48
7:Z:218:LYS:O	7:Z:222:GLU:N	2.46	0.48
8:M:1005:LEU:HB2	8:M:1234:ALA:HB3	1.95	0.48
11:T:424:ILE:HD13	12:U:59:LYS:HB3	1.94	0.48
11:V:375:TYR:HB3	11:V:379:GLU:HG3	1.95	0.48
12:W:250:ARG:HH22	12:W:262:THR:HA	1.79	0.48
12:W:371:ARG:HH12	12:W:400:SER:HB2	1.78	0.48
12:Y:410:ALA:O	12:Y:414:LYS:N	2.47	0.48
8:M:868:TYR:HE1	8:M:874:THR:HB	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:1054:LEU:HD21	8:M:1059:ALA:HB2	1.95	0.48
9:R:209:TYR:HE2	9:R:211:LYS:HZ2	1.62	0.48
12:U:141:VAL:HB	12:U:159:THR:HB	1.96	0.48
11:X:314:ASN:HB3	11:X:342:ARG:HG3	1.95	0.48
5:I:59:DA:H1'	5:I:60:DT:H5'	1.96	0.47
6:J:-25:DC:H2''	6:J:-24:DT:H5''	1.96	0.47
9:R:116:ASP:OD1	9:R:117:GLN:N	2.46	0.47
11:T:236:GLU:O	11:T:239:LYS:NZ	2.41	0.47
11:V:123:GLU:OE2	11:V:250:HIS:NE2	2.44	0.47
11:X:138:GLU:HG2	11:X:240:LYS:HD3	1.95	0.47
12:Y:219:THR:O	12:Y:220:ARG:NE	2.30	0.47
1:B:122:LYS:NZ	1:A:113:HIS:O	2.47	0.47
10:S:231:ASN:HD21	10:S:234:TYR:HD2	1.61	0.47
10:S:266:VAL:HG12	12:U:165:MET:SD	2.54	0.47
11:T:202:ILE:HG22	11:T:209:VAL:HG22	1.96	0.47
12:U:181:LYS:O	12:U:183:LYS:NZ	2.46	0.47
12:W:47:GLN:OE1	12:W:49:GLN:NE2	2.45	0.47
11:X:35:LEU:HD11	11:X:59:GLY:HA3	1.95	0.47
11:X:36:ASP:OD1	11:X:36:ASP:N	2.47	0.47
3:F:51:TYR:CD2	4:H:117:GLY:HA3	2.49	0.47
4:G:61:SER:HB2	3:E:79:ILE:HD13	1.96	0.47
5:I:-77:DC:H2'	5:I:-76:DG:C8	2.49	0.47
12:W:240:SER:O	12:W:243:GLU:HG2	2.14	0.47
11:X:41:ALA:N	11:X:56:GLU:OE2	2.47	0.47
6:J:-62:DA:H5'	6:J:-62:DA:C8	2.49	0.47
6:J:-22:DG:H21	8:M:980:MET:CE	2.26	0.47
11:V:189:ILE:HG13	11:V:209:VAL:HG11	1.96	0.47
11:V:422:CYS:SG	11:V:439:VAL:HG12	2.54	0.47
11:X:105:LEU:HB3	11:X:310:ILE:HG12	1.94	0.47
11:X:313:VAL:HG12	11:X:340:SER:HB2	1.95	0.47
1:B:113:HIS:CD2	1:A:126:LEU:HD22	2.49	0.47
4:H:98:GLN:HE21	4:H:114:VAL:CG1	2.26	0.47
7:Z:293:THR:O	7:Z:593:ARG:N	2.37	0.47
8:M:1249:GLN:NE2	12:W:283:GLU:OE2	2.47	0.47
8:M:1267:ILE:HB	8:M:1339:TYR:CE2	2.50	0.47
11:T:99:LYS:HE3	11:T:132:ARG:HH21	1.79	0.47
11:T:391:GLU:C	11:T:392:ARG:HD3	2.35	0.47
12:U:159:THR:HA	12:U:168:ILE:HA	1.96	0.47
12:W:262:THR:OG1	12:W:263:GLY:N	2.47	0.47
11:X:125:PHE:CZ	11:X:333:ALA:HA	2.50	0.47
12:Y:31:LEU:HD13	12:Y:35:LEU:HG	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:162:THR:OG1	12:Y:165:MET:O	2.19	0.47
4:G:64:ILE:HG21	3:E:84:LEU:HD11	1.95	0.47
4:H:79:GLU:HA	4:H:82:LYS:HG2	1.96	0.47
5:I:-51:DC:H2''	5:I:-50:DC:C5	2.50	0.47
11:V:28:THR:O	11:V:31:LYS:NZ	2.48	0.47
11:V:121:LEU:HA	11:V:124:ASN:HD21	1.80	0.47
12:Y:23:HIS:NE2	13:Y:501:ADP:H5'2	2.29	0.47
2:C:83:SER:O	2:C:87:VAL:HG23	2.14	0.47
6:J:-17:DT:H2'	6:J:-16:DT:H71	1.95	0.47
6:J:25:DT:H2''	6:J:26:DA:N7	2.29	0.47
1:A:121:LYS:HD2	1:A:121:LYS:H	1.80	0.47
8:M:1193:ARG:NE	11:V:261:GLY:O	2.35	0.47
9:R:331:VAL:HA	9:R:334:ILE:HG22	1.97	0.47
11:T:143:GLU:HG3	11:T:171:LYS:O	2.14	0.47
11:T:316:LEU:HD12	11:T:320:ILE:HG21	1.96	0.47
11:T:346:THR:O	11:T:348:ARG:NH1	2.47	0.47
11:T:450:LYS:O	11:T:454:LYS:HG2	2.14	0.47
11:V:84:GLY:N	13:V:501:ADP:O1B	2.48	0.47
11:V:121:LEU:HD23	11:V:323:TYR:HD2	1.79	0.47
12:W:141:VAL:HB	12:W:159:THR:HB	1.97	0.47
12:W:300:MET:HE3	11:X:319:GLU:HG2	1.97	0.47
11:X:386:ARG:HH12	11:X:387:ARG:HD2	1.79	0.47
12:Y:78:SER:HB2	12:Y:397:ARG:NE	2.30	0.47
5:I:37:DC:H2''	5:I:38:DT:H73	1.97	0.47
5:I:85:DG:H2''	5:I:86:DG:C8	2.50	0.47
6:J:-59:DT:H2''	6:J:-58:DC:C6	2.49	0.47
6:J:-7:DG:H2''	6:J:-6:DG:C8	2.50	0.47
6:J:8:DG:N2	1:A:40:ARG:HH22	2.12	0.47
8:M:826:ALA:H	8:M:852:THR:HB	1.79	0.47
8:M:1020:ASP:N	8:M:1020:ASP:OD1	2.48	0.47
8:M:1264:ARG:HB2	8:M:1333:ALA:HA	1.96	0.47
11:T:76:LEU:HD21	11:T:369:ILE:HG13	1.97	0.47
11:X:186:TYR:O	11:X:189:ILE:HG22	2.14	0.47
12:Y:113:LYS:NZ	12:Y:302:ASP:OD2	2.48	0.47
5:I:-68:DG:H2''	5:I:-67:DA:C8	2.50	0.47
5:I:-43:DT:H2''	5:I:-42:DT:H71	1.95	0.47
5:I:15:DT:H2''	5:I:16:DA:N7	2.30	0.47
6:J:-45:DG:H2''	6:J:-44:DG:H8	1.79	0.47
8:M:948:ILE:HG12	8:M:1368:ARG:HB3	1.97	0.47
10:S:17:ILE:HG22	12:U:147:ARG:NH2	2.24	0.47
12:U:382:ASP:N	12:U:382:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:202:ILE:HD13	11:V:209:VAL:HG12	1.96	0.47
2:C:35:ARG:HG3	2:C:46:ILE:HD13	1.97	0.47
5:I:-51:DC:C2	6:J:51:DG:N2	2.69	0.47
7:Z:586:GLY:O	7:Z:588:GLU:HB2	2.15	0.47
8:M:720:ALA:O	8:M:931:ARG:NE	2.40	0.47
9:R:46:ILE:O	9:R:49:ILE:HG12	2.15	0.47
9:R:150:ILE:HG21	9:R:367:GLN:HA	1.96	0.47
9:R:264:PHE:O	9:R:267:LYS:NZ	2.39	0.47
12:W:408:GLN:HG2	11:X:64:LEU:HD21	1.97	0.47
11:X:445:LEU:HD21	12:Y:52:ARG:HE	1.80	0.47
1:B:90:GLY:O	1:B:93:GLN:HG3	2.15	0.46
5:I:48:DG:H1'	5:I:49:DC:C5	2.50	0.46
8:M:756:VAL:HG13	8:M:760:TRP:CD1	2.50	0.46
9:R:255:VAL:HG21	9:R:365:PHE:HB2	1.98	0.46
11:V:135:GLU:O	11:V:243:ILE:N	2.38	0.46
12:W:382:ASP:OD1	12:W:382:ASP:N	2.48	0.46
6:J:77:DG:C3'	6:J:78:DG:H4'	2.46	0.46
1:A:46:VAL:O	1:A:49:ARG:HG2	2.15	0.46
7:Z:315:LYS:HA	7:Z:318:LYS:HG2	1.98	0.46
10:S:256:CYS:N	10:S:261:ASN:O	2.48	0.46
11:V:165:HIS:CE1	11:V:183:PRO:HD3	2.51	0.46
11:V:314:ASN:O	11:V:348:ARG:NH1	2.48	0.46
12:W:115:GLU:CD	12:W:264:GLU:H	2.18	0.46
12:W:140:VAL:HG13	12:W:158:LEU:HD11	1.96	0.46
12:Y:113:LYS:HD2	12:Y:304:GLU:HB2	1.97	0.46
4:G:39:THR:HG22	6:J:49:DC:H5''	1.97	0.46
1:A:91:ALA:O	1:A:94:GLU:HG3	2.16	0.46
8:M:1213:VAL:HA	8:M:1216:ASN:ND2	2.30	0.46
8:M:1348:ASP:OD1	8:M:1348:ASP:N	2.48	0.46
10:S:231:ASN:ND2	10:S:234:TYR:HB2	2.31	0.46
11:V:284:LEU:O	11:V:287:GLU:HG3	2.16	0.46
11:V:387:ARG:CD	11:V:416:LEU:HD22	2.45	0.46
12:W:69:ARG:NH2	12:W:70:ALA:O	2.43	0.46
11:X:265:VAL:O	11:X:269:MET:HG2	2.15	0.46
1:B:75:ALA:HB1	1:B:82:LEU:HD12	1.96	0.46
5:I:48:DG:H1'	5:I:49:DC:H5	1.80	0.46
1:A:63:ARG:HB2	1:A:66:PRO:HD2	1.98	0.46
9:R:94:GLY:HA2	9:R:97:HIS:ND1	2.30	0.46
9:R:289:ASN:HB3	9:R:292:LYS:HE3	1.97	0.46
12:W:117:LEU:HG	12:W:121:PHE:HE2	1.81	0.46
11:X:274:LYS:HE2	11:X:276:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:27:PRO:HD3	4:H:43:TYR:CG	2.51	0.46
5:I:79:DT:H2''	5:I:80:DA:C8	2.51	0.46
6:J:-35:DG:H5'	6:J:-35:DG:C8	2.50	0.46
7:Z:238:GLN:HE22	7:Z:241:ARG:HB2	1.80	0.46
12:W:80:GLY:N	13:W:501:ADP:O2B	2.49	0.46
12:W:261:ASP:OD1	12:W:261:ASP:N	2.44	0.46
12:Y:44:MET:HB2	13:Y:501:ADP:N6	2.30	0.46
3:F:51:TYR:HE1	4:H:101:VAL:HG21	1.81	0.46
3:F:51:TYR:CE1	4:H:101:VAL:HG21	2.51	0.46
5:I:68:DT:H2''	5:I:69:DC:C6	2.50	0.46
3:E:33:ARG:HA	3:E:36:ARG:HH11	1.79	0.46
9:R:399:VAL:HG23	9:R:402:GLN:HE21	1.80	0.46
10:S:184:LEU:O	10:S:186:LYS:NZ	2.49	0.46
12:U:442:GLU:HG2	12:U:443:ASN:ND2	2.31	0.46
12:Y:115:GLU:CD	12:Y:119:GLN:HE22	2.18	0.46
12:Y:301:LEU:HD23	12:Y:306:PHE:CE1	2.51	0.46
7:Z:202:ASN:O	7:Z:205:LYS:HG3	2.16	0.46
1:A:79:LYS:HB2	1:A:82:LEU:HD11	1.97	0.46
8:M:978:ASN:O	8:M:981:SER:OG	2.30	0.46
8:M:1045:LEU:HD21	11:T:291:VAL:HG11	1.98	0.46
8:M:1221:SER:HA	11:V:191:ARG:HH12	1.80	0.46
8:M:1340:ASP:OD1	8:M:1340:ASP:N	2.49	0.46
10:S:171:THR:HA	10:S:174:GLU:CD	2.36	0.46
11:T:102:PHE:HD1	11:T:307:VAL:HG23	1.80	0.46
11:T:366:ARG:HH21	12:Y:397:ARG:NH1	2.14	0.46
12:U:299:HIS:HB3	12:U:325:THR:HG23	1.98	0.46
11:V:182:ASP:HB3	11:V:185:ILE:HG22	1.97	0.46
11:V:264:ASP:O	11:V:267:SER:OG	2.22	0.46
11:V:387:ARG:O	11:V:391:GLU:HB2	2.16	0.46
12:W:435:ARG:O	12:W:438:LYS:HG2	2.15	0.46
5:I:53:DT:H1'	5:I:54:DG:C8	2.51	0.46
8:M:868:TYR:CE1	8:M:874:THR:HB	2.51	0.46
8:M:1004:ILE:HG23	8:M:1236:PRO:HD3	1.98	0.46
9:R:113:LYS:HD3	9:R:425:ASP:HA	1.97	0.46
12:W:310:ASN:HD21	12:W:347:LEU:HD22	1.81	0.46
12:Y:38:ARG:O	12:Y:51:ARG:NH2	2.49	0.46
1:B:57:SER:HB2	1:B:59:GLU:OE2	2.16	0.46
5:I:96:DA:H2''	5:I:97:DG:H2'	1.98	0.46
6:J:-107:DT:H2''	6:J:-106:DA:N7	2.31	0.46
6:J:33:DT:H2''	6:J:34:DC:C5	2.51	0.46
9:R:132:PRO:HG2	9:R:135:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:256:SER:OG	9:R:368:ARG:NH1	2.43	0.46
9:R:256:SER:OG	9:R:315:GLU:OE1	2.30	0.46
11:V:163:ILE:HG13	11:V:164:SER:H	1.81	0.46
11:V:417:GLN:HB3	12:W:69:ARG:NH1	2.31	0.46
12:W:40:THR:HG23	12:W:45:VAL:HG22	1.98	0.46
12:Y:266:ARG:HG3	12:Y:268:GLU:H	1.81	0.46
12:Y:281:LYS:HZ1	12:Y:288:ILE:HG12	1.81	0.46
12:Y:382:ASP:OD1	12:Y:382:ASP:N	2.48	0.46
4:G:64:ILE:HD13	3:E:84:LEU:HD13	1.97	0.45
8:M:1008:PHE:N	8:M:1186:SER:O	2.34	0.45
8:M:1254:LEU:HD12	8:M:1255:LEU:HD12	1.98	0.45
12:U:94:LYS:HD2	12:U:94:LYS:HA	1.72	0.45
12:U:279:GLU:O	12:U:283:GLU:HG3	2.15	0.45
11:V:121:LEU:HD22	11:V:320:ILE:HG23	1.98	0.45
11:V:412:LEU:O	11:V:416:LEU:HG	2.16	0.45
1:B:95:SER:HA	3:E:102:THR:HB	1.98	0.45
4:G:99:THR:O	4:G:102:ARG:HG2	2.16	0.45
7:Z:203:THR:HG21	3:E:69:ASN:ND2	2.32	0.45
8:M:1052:LYS:O	8:M:1141:ILE:HD12	2.15	0.45
8:M:1064:LYS:HG3	8:M:1065:LEU:HD12	1.97	0.45
8:M:1342:ASP:OD1	8:M:1342:ASP:N	2.44	0.45
10:S:267:SER:HA	10:S:270:LYS:HE3	1.97	0.45
11:V:33:LEU:HD21	11:V:55:ARG:O	2.16	0.45
11:X:106:VAL:HG21	12:Y:311:ARG:HG2	1.97	0.45
12:Y:30:GLY:O	12:Y:38:ARG:NH1	2.49	0.45
7:Z:311:GLU:HA	7:Z:314:ASN:ND2	2.32	0.45
8:M:955:LYS:HE3	12:W:279:GLU:HB2	1.98	0.45
9:R:98:HIS:CD2	9:R:127:SER:HB2	2.49	0.45
10:S:116:VAL:HG23	10:S:117:PRO:HD3	1.99	0.45
11:T:267:SER:OG	11:T:271:GLN:NE2	2.48	0.45
11:V:187:GLU:O	11:V:191:ARG:HG2	2.17	0.45
11:X:44:VAL:HG22	11:X:49:VAL:HG12	1.99	0.45
11:X:196:ILE:O	11:X:214:ARG:NH1	2.48	0.45
1:B:126:LEU:HD22	1:A:113:HIS:CG	2.51	0.45
5:I:-44:DA:H2''	5:I:-43:DT:H5'	1.99	0.45
5:I:5:DC:H2''	5:I:6:DC:C5	2.52	0.45
5:I:89:DG:H2''	5:I:90:DG:C8	2.52	0.45
11:T:431:ARG:HG2	11:T:433:GLU:H	1.80	0.45
12:W:25:HIS:CD2	12:W:371:ARG:HH21	2.35	0.45
12:W:25:HIS:ND1	12:W:26:ILE:HG23	2.32	0.45
12:W:179:LEU:HD12	12:W:184:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:80:ILE:HG12	3:F:83:HIS:CG	2.50	0.45
8:M:1129:ARG:HA	12:Y:220:ARG:NH1	2.32	0.45
9:R:254:PHE:CE1	9:R:310:LEU:HB3	2.51	0.45
11:T:181:LEU:HD22	11:T:185:ILE:HG21	1.97	0.45
12:U:105:GLU:OE1	12:U:105:GLU:N	2.41	0.45
12:U:232:ARG:HD2	12:U:232:ARG:HA	1.71	0.45
12:W:109:LEU:HD23	12:W:109:LEU:H	1.80	0.45
12:W:400:SER:O	12:W:403:ILE:HG22	2.17	0.45
2:C:72:TYR:HE1	4:H:103:LEU:HD13	1.82	0.45
3:F:56:LEU:HB3	4:H:69:VAL:HG23	1.98	0.45
8:M:707:LEU:HD21	8:M:719:LEU:HD22	1.98	0.45
9:R:72:GLU:HB3	9:R:76:TRP:CZ3	2.51	0.45
12:U:76:PRO:HD2	12:U:79:THR:HG21	1.99	0.45
12:U:157:LYS:HD2	12:U:170:GLU:HG2	1.97	0.45
12:U:332:THR:OG1	12:U:335:THR:OG1	2.28	0.45
11:V:82:SER:HA	13:V:501:ADP:H5'1	1.98	0.45
11:X:283:LYS:O	11:X:286:GLN:HG3	2.17	0.45
11:X:332:ILE:HG22	11:X:332:ILE:O	2.17	0.45
12:Y:165:MET:SD	12:Y:167:THR:HG23	2.57	0.45
3:F:59:LEU:O	3:F:63:ILE:HG12	2.17	0.45
5:I:-78:DC:C3'	5:I:-77:DC:H4'	2.47	0.45
6:J:-85:DC:H2''	6:J:-84:DC:C6	2.51	0.45
8:M:749:LEU:HA	8:M:799:CYS:O	2.17	0.45
10:S:276:ARG:HH12	10:S:278:ARG:HH21	1.62	0.45
11:T:406:MET:HE1	11:T:418:LEU:HD21	1.98	0.45
5:I:-36:DT:H1'	5:I:-35:DA:C4	2.51	0.45
6:J:58:DC:H2''	6:J:59:DA:H5'	1.98	0.45
7:Z:581:THR:OG1	7:Z:582:GLN:N	2.49	0.45
12:U:22:ALA:O	13:U:501:ADP:O2'	2.34	0.45
12:U:109:LEU:HD23	12:U:109:LEU:H	1.82	0.45
12:W:78:SER:HB2	12:W:396:LEU:CD2	2.46	0.45
11:X:51:GLN:NE2	11:X:373:LEU:O	2.50	0.45
11:X:187:GLU:O	11:X:191:ARG:HG2	2.17	0.45
12:Y:298:VAL:HG21	12:Y:323:MET:HG3	1.98	0.45
1:B:65:LEU:O	1:B:68:GLN:HG3	2.16	0.45
2:C:72:TYR:CE1	4:H:103:LEU:HD13	2.52	0.45
2:D:68:ASP:OD2	2:D:93:GLN:NE2	2.49	0.45
6:J:-38:DA:H1'	6:J:-37:DG:C4	2.52	0.45
6:J:15:DT:H1'	6:J:16:DA:O4'	2.17	0.45
6:J:54:DT:H2''	6:J:55:DC:OP2	2.15	0.45
7:Z:260:LYS:O	7:Z:264:VAL:HG22	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:10:ASN:HA	9:R:15:ILE:HG13	1.99	0.45
12:W:104:SER:N	12:W:297:GLU:OE2	2.48	0.45
12:W:447:TYR:HE1	11:X:342:ARG:HE	1.65	0.45
8:M:825:GLU:HB2	8:M:827:HIS:CE1	2.52	0.45
8:M:954:SER:HB3	8:M:957:GLN:HG2	1.98	0.45
8:M:975:ALA:HA	8:M:982:ILE:HD11	1.99	0.45
8:M:1005:LEU:HB3	8:M:1184:THR:HG21	1.98	0.45
8:M:1132:ARG:CZ	12:Y:217:ALA:HA	2.47	0.45
8:M:1231:LEU:HD12	12:W:251:THR:HG22	1.98	0.45
9:R:254:PHE:HE1	9:R:310:LEU:HD23	1.82	0.45
11:T:76:LEU:HD22	11:T:367:LEU:HB3	1.99	0.45
11:T:181:LEU:HD22	11:T:185:ILE:HD13	1.99	0.45
12:U:381:SER:HA	12:U:384:LEU:HD12	1.99	0.45
11:V:85:LYS:NZ	11:V:340:SER:O	2.41	0.45
11:X:281:THR:HG23	11:X:284:LEU:H	1.82	0.45
1:B:122:LYS:O	1:B:125:LYS:HG3	2.17	0.44
6:J:9:DT:H2''	6:J:10:DG:C8	2.52	0.44
9:R:74:CYS:HG	10:S:179:TYR:HH	1.62	0.44
12:U:31:LEU:O	12:U:38:ARG:NH1	2.46	0.44
11:X:310:ILE:HB	11:X:338:LEU:HD13	2.00	0.44
12:Y:299:HIS:CG	12:Y:327:ARG:HG3	2.51	0.44
2:C:76:ALA:HA	4:H:87:ASN:HD21	1.83	0.44
2:D:66:ILE:HG21	1:A:74:ILE:HG23	1.99	0.44
2:D:90:LEU:HD13	2:D:97:LEU:HD23	1.98	0.44
9:R:116:ASP:HA	9:R:119:ILE:HG12	1.99	0.44
12:U:79:THR:O	12:U:359:TYR:OH	2.35	0.44
11:V:106:VAL:O	11:V:109:GLU:HG3	2.17	0.44
12:W:56:VAL:O	12:W:60:MET:HG2	2.18	0.44
12:W:243:GLU:O	12:W:247:ILE:HG12	2.17	0.44
12:W:449:ASP:OD1	12:W:453:ASN:N	2.35	0.44
12:Y:303:ILE:HA	12:Y:306:PHE:HD2	1.83	0.44
3:F:51:TYR:O	3:F:55:VAL:HG23	2.17	0.44
5:I:-36:DT:H1'	5:I:-35:DA:C5	2.52	0.44
8:M:942:PRO:HB2	8:M:1363:ASP:HA	1.98	0.44
8:M:1291:ARG:NH2	8:M:1293:ASP:OD2	2.49	0.44
9:R:239:MET:SD	9:R:239:MET:N	2.91	0.44
9:R:399:VAL:O	9:R:402:GLN:HG3	2.17	0.44
10:S:263:ILE:HD12	10:S:269:PHE:HB2	1.98	0.44
11:T:126:ARG:NE	11:T:253:ASP:HB2	2.33	0.44
12:U:413:ARG:NH1	12:U:421:GLU:OE2	2.44	0.44
11:V:105:LEU:N	11:V:309:PHE:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:166:VAL:HG21	11:V:186:TYR:CE1	2.53	0.44
11:V:364:ILE:HA	11:V:367:LEU:HD12	1.98	0.44
12:W:117:LEU:HG	12:W:121:PHE:CE2	2.53	0.44
12:W:398:TYR:HA	12:W:401:ASN:ND2	2.32	0.44
11:X:330:SER:HB2	11:X:333:ALA:HB2	1.98	0.44
7:Z:293:THR:HG22	12:W:144:GLN:HA	1.99	0.44
1:A:122:LYS:HA	1:A:125:LYS:HG3	2.00	0.44
8:M:1251:LEU:HD12	8:M:1254:LEU:HD11	1.99	0.44
8:M:1382:LYS:HZ1	8:M:1394:ILE:HG23	1.81	0.44
10:S:174:GLU:HA	10:S:177:LEU:HG	1.98	0.44
11:T:68:LYS:HZ3	11:T:303:LEU:C	2.21	0.44
12:U:360:ASN:HD22	12:U:362:GLN:HE22	1.65	0.44
11:V:313:VAL:O	11:V:316:LEU:HG	2.18	0.44
11:V:421:PRO:O	11:V:424:ILE:HG22	2.18	0.44
11:V:447:LEU:HA	11:V:451:ARG:CZ	2.47	0.44
12:W:119:GLN:HB2	12:W:242:HIS:CE1	2.52	0.44
11:X:150:GLU:N	11:X:165:HIS:O	2.47	0.44
11:X:316:LEU:HD22	11:X:320:ILE:HG21	2.00	0.44
12:Y:136:ILE:HB	12:Y:192:ILE:HG23	1.99	0.44
5:I:88:DT:O4	6:J:-89:DC:N4	2.50	0.44
8:M:1216:ASN:O	8:M:1220:VAL:HG23	2.17	0.44
8:M:1350:GLN:O	8:M:1354:ARG:HG2	2.18	0.44
8:M:778:GLY:O	8:M:782:GLN:N	2.50	0.44
8:M:1070:ASN:O	8:M:1073:GLU:HG3	2.18	0.44
8:M:1183:LEU:HD22	12:W:248:ASN:HB3	1.98	0.44
11:T:143:GLU:HA	11:T:199:VAL:HA	1.99	0.44
6:J:-70:DG:H2''	6:J:-69:DG:N7	2.33	0.44
8:M:1015:ALA:HB1	12:U:254:PHE:HE2	1.82	0.44
8:M:1174:ARG:HA	8:M:1177:ILE:HG12	1.99	0.44
8:M:1354:ARG:HH21	8:M:1357:ARG:HH22	1.65	0.44
9:R:6:ILE:HD12	9:R:19:PRO:HA	2.00	0.44
9:R:103:GLU:HB3	9:R:130:LYS:HE3	1.98	0.44
11:T:76:LEU:HD23	11:T:368:LEU:O	2.18	0.44
12:U:300:MET:O	12:U:333:ARG:HD2	2.18	0.44
12:Y:387:LEU:HD22	12:Y:403:ILE:HD13	1.99	0.44
1:B:130:LEU:HD12	1:A:130:LEU:HD12	1.99	0.44
2:C:96:THR:H	3:E:101:VAL:HG21	1.83	0.44
2:D:30:THR:HG21	5:I:-13:DA:H4'	2.00	0.44
8:M:867:LEU:HD12	8:M:870:LEU:HD21	1.99	0.44
8:M:1025:LEU:HD13	12:U:244:ILE:HG22	2.00	0.44
11:T:125:PHE:HD1	11:T:334:PRO:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:286:GLN:HA	11:V:289:ASN:ND2	2.33	0.44
12:W:303:ILE:HD12	12:W:303:ILE:H	1.83	0.44
12:W:396:LEU:HD23	12:W:396:LEU:H	1.82	0.44
11:X:80:GLY:O	11:X:85:LYS:NZ	2.51	0.44
11:X:363:LEU:HD12	11:X:363:LEU:H	1.83	0.44
11:X:453:THR:HG22	12:Y:340:PRO:HB3	2.00	0.44
12:Y:23:HIS:CE1	13:Y:501:ADP:H5'2	2.53	0.44
12:Y:126:GLY:HA2	12:Y:240:SER:HA	2.00	0.44
12:Y:213:ASP:OD1	12:Y:214:ALA:N	2.50	0.44
6:J:27:DG:H2''	6:J:28:DA:C8	2.53	0.44
8:M:1210:ARG:HA	8:M:1213:VAL:HG22	2.00	0.44
9:R:197:CYS:SG	9:R:199:TRP:NE1	2.91	0.44
10:S:256:CYS:SG	10:S:257:VAL:N	2.91	0.44
11:T:126:ARG:HB3	11:T:250:HIS:HD2	1.82	0.44
12:U:58:LEU:HG	12:U:62:GLN:NE2	2.30	0.44
12:U:432:ASP:H	12:U:435:ARG:HD3	1.83	0.44
11:V:49:VAL:HG21	11:V:379:GLU:HB2	2.00	0.44
11:V:57:ALA:O	11:V:61:ILE:HG12	2.18	0.44
11:V:267:SER:O	11:V:271:GLN:HG3	2.18	0.44
11:X:55:ARG:HA	11:X:58:CYS:HB3	2.00	0.44
2:D:29:ILE:O	2:D:55:ARG:NH2	2.34	0.43
3:F:39:ASN:HB3	3:E:39:ASN:O	2.18	0.43
6:J:-63:DT:H2''	6:J:-62:DA:C8	2.53	0.43
8:M:825:GLU:HA	8:M:852:THR:HA	1.99	0.43
8:M:837:TRP:HD1	8:M:838:GLN:HG3	1.83	0.43
9:R:3:THR:OG1	9:R:4:PRO:HD3	2.17	0.43
9:R:191:ILE:HG13	9:R:355:CYS:HA	2.00	0.43
10:S:189:ARG:NH2	10:S:199:LYS:HE2	2.33	0.43
11:T:165:HIS:CE1	11:T:182:ASP:HA	2.53	0.43
12:U:132:GLU:HB3	12:U:232:ARG:NH1	2.31	0.43
12:U:183:LYS:HA	12:U:183:LYS:HD3	1.84	0.43
12:U:369:SER:O	12:U:373:GLN:OE1	2.36	0.43
11:V:198:ASP:OD1	11:V:214:ARG:NH1	2.51	0.43
11:X:234:LYS:O	11:X:239:LYS:NZ	2.42	0.43
11:X:425:LEU:O	11:X:428:THR:OG1	2.32	0.43
12:Y:172:GLY:N	12:Y:175:MET:HB2	2.33	0.43
1:B:45:THR:OG1	6:J:70:DC:OP1	2.36	0.43
1:B:119:ILE:HG22	2:C:46:ILE:HA	2.00	0.43
2:D:75:HIS:NE2	4:G:83:LEU:HG	2.34	0.43
5:I:77:DT:O4	6:J:-78:DC:N4	2.50	0.43
6:J:33:DT:H2''	6:J:34:DC:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:718:ILE:HD11	8:M:852:THR:HG22	2.00	0.43
8:M:792:LYS:O	8:M:795:ALA:HB2	2.18	0.43
8:M:1124:MET:HA	8:M:1127:LYS:HZ3	1.83	0.43
9:R:396:GLY:O	9:R:399:VAL:HG12	2.18	0.43
11:T:73:ARG:O	11:T:335:VAL:HA	2.18	0.43
11:T:261:GLY:HA2	11:T:271:GLN:NE2	2.33	0.43
11:X:83:THR:HG1	11:X:85:LYS:HZ3	1.61	0.43
11:X:137:LYS:HD2	11:X:137:LYS:HA	1.71	0.43
11:X:413:ARG:HG2	12:Y:350:ARG:HG3	2.00	0.43
1:B:69:ARG:HG2	2:C:21:ILE:HA	2.00	0.43
1:B:116:ARG:HB2	6:J:-3:DA:OP1	2.18	0.43
2:D:74:GLU:HB2	4:G:102:ARG:HH22	1.82	0.43
5:I:21:DC:OP2	8:M:833:ARG:NH2	2.44	0.43
6:J:17:DA:H5''	1:A:65:LEU:HB2	2.00	0.43
6:J:22:DT:H2''	6:J:23:DG:C8	2.52	0.43
7:Z:267:LYS:HE3	8:M:1303:ILE:HA	2.01	0.43
3:E:18:ARG:HB2	3:E:21:LYS:HE3	2.00	0.43
8:M:1142:ASP:HA	8:M:1145:THR:HG22	1.99	0.43
8:M:1249:GLN:NE2	12:W:283:GLU:O	2.51	0.43
9:R:276:LEU:HD22	9:R:302:GLN:HE21	1.83	0.43
11:T:418:LEU:C	11:T:421:PRO:HD2	2.38	0.43
11:V:121:LEU:HA	11:V:124:ASN:ND2	2.33	0.43
11:V:137:LYS:HG2	11:V:243:ILE:HD13	2.00	0.43
11:X:214:ARG:HB2	11:X:229:TYR:CD1	2.53	0.43
12:Y:244:ILE:HB	12:Y:273:ILE:HD11	2.00	0.43
12:Y:294:PHE:HA	12:Y:322:MET:HB3	2.01	0.43
1:B:104:PHE:HB3	2:C:41:GLY:HA3	2.00	0.43
5:I:25:DG:H2''	5:I:26:DG:H5'	2.00	0.43
6:J:-29:DT:H2''	6:J:-28:DC:C6	2.54	0.43
7:Z:217:ARG:HD2	7:Z:217:ARG:HA	1.87	0.43
13:M:1601:ADP:O3B	14:M:1602:BEF:F1	2.26	0.43
11:T:79:GLY:HA3	11:T:372:THR:HG22	2.00	0.43
12:U:281:LYS:HZ2	12:U:288:ILE:H	1.65	0.43
12:W:305:CYS:O	12:W:309:ILE:HG12	2.18	0.43
8:M:1067:CYS:HB3	12:Y:223:GLN:HG3	2.00	0.43
12:U:172:GLY:O	12:U:176:ILE:HG12	2.19	0.43
12:W:61:VAL:HG12	12:W:320:ILE:HG13	2.00	0.43
11:X:320:ILE:H	11:X:320:ILE:HD12	1.84	0.43
12:Y:367:ILE:HG21	12:Y:396:LEU:HD21	2.00	0.43
5:I:20:DG:P	8:M:831:ASN:HD22	2.42	0.43
6:J:-86:DC:H5'	6:J:-86:DC:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:18:DG:C8	6:J:18:DG:H5'	2.54	0.43
8:M:1143:LEU:HD21	12:Y:237:HIS:CG	2.54	0.43
12:U:153:HIS:O	12:U:155:GLN:NE2	2.51	0.43
12:U:345:LEU:HD11	12:Y:454:VAL:HG12	2.01	0.43
11:V:24:THR:OG1	11:V:27:HIS:O	2.37	0.43
11:V:76:LEU:HD23	11:V:368:LEU:O	2.17	0.43
11:X:421:PRO:HA	11:X:424:ILE:HG22	2.00	0.43
12:Y:130:LYS:HA	12:Y:236:VAL:HA	1.99	0.43
12:Y:321:VAL:HG12	12:Y:323:MET:SD	2.58	0.43
1:B:50:GLU:OE2	2:C:36:ARG:NH1	2.45	0.43
6:J:38:DG:H2''	6:J:39:DA:C8	2.54	0.43
6:J:58:DC:N3	6:J:59:DA:N6	2.66	0.43
8:M:738:LEU:HD22	8:M:820:TYR:CE2	2.53	0.43
8:M:930:LEU:HD12	8:M:930:LEU:HA	1.94	0.43
8:M:1143:LEU:O	8:M:1146:LYS:HG3	2.18	0.43
8:M:1293:ASP:HA	8:M:1323:SER:HB3	2.01	0.43
12:U:431:LEU:HB3	11:V:369:ILE:CD1	2.49	0.43
11:V:27:HIS:O	11:V:28:THR:OG1	2.35	0.43
11:V:274:LYS:HD2	11:V:274:LYS:O	2.19	0.43
4:G:37:LYS:HZ2	6:J:50:DG:P	2.42	0.43
4:G:103:LEU:HD12	4:G:104:ILE:HG23	2.00	0.43
5:I:-61:DG:N1	6:J:62:DG:O6	2.52	0.43
5:I:-53:DG:H2''	5:I:-52:DG:C8	2.54	0.43
5:I:101:DT:C2	5:I:102:DG:N7	2.87	0.43
7:Z:582:GLN:NE2	7:Z:583:THR:HG22	2.33	0.43
9:R:139:PHE:O	9:R:402:GLN:NE2	2.43	0.43
12:Y:110:GLU:HG2	12:Y:111:LEU:HG	2.00	0.43
8:M:1076:ASN:HA	8:M:1079:ARG:CD	2.48	0.43
11:T:376:ASP:O	11:T:380:ILE:HD12	2.19	0.43
12:U:29:LEU:HD11	12:U:88:VAL:HG22	2.00	0.43
11:V:134:LYS:HE2	11:V:300:VAL:HG13	2.01	0.43
2:C:68:ASP:CG	2:C:92:ARG:HH21	2.23	0.43
5:I:38:DT:H6	5:I:38:DT:H2'	1.61	0.43
7:Z:207:TYR:CD1	7:Z:210:LEU:HD12	2.54	0.43
1:A:66:PRO:HA	1:A:69:ARG:NE	2.34	0.43
8:M:834:SER:HB2	8:M:836:ARG:NH1	2.34	0.43
8:M:1217:CYS:HB3	11:V:265:VAL:HB	2.01	0.43
9:R:118:VAL:HA	9:R:122:GLU:OE1	2.19	0.43
10:S:214:SER:HB2	10:S:216:LEU:HG	2.00	0.43
11:T:140:TYR:CE2	11:T:204:ALA:HB2	2.54	0.43
12:U:132:GLU:HA	12:U:234:THR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:330:SER:OG	11:V:331:ASN:N	2.52	0.43
11:V:456:LEU:HD21	12:W:329:VAL:HG23	2.01	0.43
11:X:232:LEU:O	11:X:234:LYS:NZ	2.39	0.43
6:J:42:DA:H2''	6:J:43:DA:N7	2.34	0.42
8:M:998:LEU:C	8:M:1000:GLU:H	2.22	0.42
8:M:1237:ASP:OD1	8:M:1238:LYS:N	2.52	0.42
11:T:83:THR:O	11:T:375:TYR:OH	2.36	0.42
11:V:342:ARG:O	11:V:357:HIS:ND1	2.52	0.42
12:Y:97:PRO:HB2	12:Y:124:SER:O	2.19	0.42
8:M:750:ILE:HG13	8:M:822:VAL:HB	2.00	0.42
9:R:127:SER:HB3	9:R:413:ARG:HB2	2.00	0.42
11:T:342:ARG:HA	11:T:342:ARG:HD3	1.88	0.42
11:V:112:SER:OG	11:V:114:GLU:OE1	2.38	0.42
11:V:193:LYS:O	11:V:211:ARG:NH1	2.52	0.42
11:V:343:GLY:O	11:V:357:HIS:N	2.52	0.42
12:W:47:GLN:NE2	12:W:357:LYS:O	2.53	0.42
12:W:82:THR:OG1	13:W:501:ADP:O1A	2.29	0.42
11:X:44:VAL:HA	11:X:48:PHE:O	2.19	0.42
11:X:194:VAL:HG23	11:X:198:ASP:HB3	2.01	0.42
11:X:452:SER:HG	12:Y:341:HIS:HE2	1.62	0.42
2:D:31:LYS:HZ3	2:D:35:ARG:HH21	1.67	0.42
9:R:108:LEU:HD23	9:R:108:LEU:HA	1.92	0.42
9:R:246:ASN:HA	9:R:249:LYS:HG2	2.00	0.42
11:T:123:GLU:OE2	12:U:266:ARG:HD3	2.19	0.42
11:T:125:PHE:CD1	11:T:334:PRO:HD2	2.55	0.42
11:T:140:TYR:HE2	11:T:204:ALA:HB2	1.84	0.42
11:T:165:HIS:ND1	11:T:181:LEU:O	2.52	0.42
12:U:281:LYS:HZ3	12:U:288:ILE:HG12	1.84	0.42
12:U:303:ILE:HD13	12:U:335:THR:HG23	2.01	0.42
12:W:34:ASN:O	12:W:36:GLN:NE2	2.51	0.42
11:X:132:ARG:CZ	11:X:304:ILE:HD11	2.49	0.42
1:B:66:PRO:HG3	1:B:69:ARG:HH21	1.85	0.42
3:E:114:GLN:H	3:E:114:GLN:HG3	1.73	0.42
8:M:966:SER:O	8:M:970:THR:HG23	2.19	0.42
11:T:380:ILE:HA	11:T:383:ILE:HG12	2.01	0.42
11:T:391:GLU:O	11:T:392:ARG:HD3	2.19	0.42
12:W:194:LYS:HB2	12:W:194:LYS:HE2	1.89	0.42
11:X:190:GLN:O	11:X:193:LYS:HE3	2.19	0.42
4:G:49:LYS:HA	4:G:49:LYS:HD3	1.78	0.42
6:J:-76:DT:H2''	6:J:-75:DG:C8	2.54	0.42
9:R:288:ARG:HA	9:R:288:ARG:HD2	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:319:HIS:O	9:R:322:ILE:HG12	2.19	0.42
12:W:130:LYS:HZ2	12:W:287:GLU:HG3	1.85	0.42
11:X:316:LEU:HD13	11:X:320:ILE:HG21	2.02	0.42
12:Y:293:LEU:O	12:Y:322:MET:N	2.46	0.42
7:Z:298:THR:HB	7:Z:299:PRO:CD	2.49	0.42
1:A:90:GLY:O	1:A:93:GLN:HG2	2.18	0.42
8:M:754:THR:HG22	8:M:802:SER:HB2	2.02	0.42
8:M:936:ASP:OD1	8:M:937:VAL:N	2.53	0.42
8:M:1288:LEU:HG	8:M:1314:ILE:HG13	2.02	0.42
8:M:1290:MET:HE1	8:M:1307:ARG:HB2	2.01	0.42
9:R:6:ILE:HG22	9:R:98:HIS:O	2.20	0.42
11:T:314:ASN:HD22	11:T:342:ARG:HG3	1.83	0.42
12:U:372:ALA:HA	12:U:377:VAL:HB	2.01	0.42
11:X:53:GLU:OE1	11:X:53:GLU:N	2.43	0.42
11:X:424:ILE:HD12	11:X:424:ILE:HA	1.92	0.42
2:D:25:ASN:HD22	1:A:73:GLU:CD	2.22	0.42
5:I:66:DC:H2''	5:I:67:DA:C8	2.54	0.42
6:J:-66:DG:H1'	6:J:-65:DT:H5'	2.01	0.42
8:M:964:PHE:CZ	8:M:988:GLN:HB2	2.54	0.42
9:R:228:LYS:NZ	10:S:108:GLU:HG2	2.34	0.42
10:S:19:PHE:CE1	12:U:144:GLN:HG2	2.54	0.42
11:T:81:PRO:HG3	12:Y:448:ILE:HD11	2.02	0.42
12:U:98:PHE:HD1	12:U:292:VAL:HB	1.85	0.42
11:V:309:PHE:HD1	11:V:337:VAL:HG13	1.85	0.42
12:W:119:GLN:HB2	12:W:242:HIS:ND1	2.35	0.42
12:W:364:ILE:HD12	12:W:392:VAL:HG22	2.01	0.42
11:X:111:TYR:OH	11:X:348:ARG:NH1	2.52	0.42
11:X:236:GLU:O	11:X:239:LYS:NZ	2.52	0.42
12:Y:364:ILE:HD13	12:Y:392:VAL:HG12	2.01	0.42
3:F:74:ASN:HD22	3:F:83:HIS:CD2	2.37	0.42
5:I:-68:DG:C6	5:I:-67:DA:N6	2.87	0.42
6:J:35:DT:H2''	6:J:36:DA:N7	2.34	0.42
7:Z:253:ILE:HG13	7:Z:254:LEU:N	2.34	0.42
8:M:742:LYS:HZ3	8:M:744:ASN:HB3	1.85	0.42
8:M:1236:PRO:HD2	11:V:210:LYS:NZ	2.35	0.42
8:M:1303:ILE:HG13	8:M:1304:LEU:N	2.35	0.42
9:R:326:THR:O	9:R:326:THR:HG22	2.20	0.42
9:R:416:ARG:HB3	9:R:420:TYR:CE2	2.55	0.42
10:S:8:ILE:HB	11:V:178:THR:O	2.20	0.42
10:S:98:SER:O	10:S:101:ARG:HG2	2.20	0.42
12:W:19:LEU:H	11:X:331:ASN:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:125:ILE:HD13	12:W:290:PRO:HA	2.02	0.42
12:W:300:MET:HE1	11:X:319:GLU:HA	2.01	0.42
11:X:445:LEU:HD11	12:Y:52:ARG:NE	2.35	0.42
1:B:113:HIS:O	1:A:122:LYS:NZ	2.46	0.42
6:J:-106:DA:H2''	6:J:-105:DA:C8	2.55	0.42
8:M:925:LEU:HD13	8:M:929:LEU:HD13	2.01	0.42
8:M:1079:ARG:NH1	8:M:1080:GLU:HG2	2.34	0.42
9:R:278:ASP:HB3	9:R:281:THR:HG22	2.00	0.42
13:R:501:ADP:O3B	14:R:502:BEF:F2	2.28	0.42
11:T:167:ILE:HA	11:T:179:LEU:O	2.20	0.42
11:V:313:VAL:HG22	11:V:339:ALA:O	2.20	0.42
11:V:400:LEU:HA	11:V:403:LEU:HG	2.02	0.42
11:X:119:GLU:O	11:X:123:GLU:HG2	2.20	0.42
12:Y:302:ASP:OD1	12:Y:303:ILE:N	2.52	0.42
6:J:0:DG:C8	6:J:0:DG:H5'	2.55	0.42
8:M:926:ARG:HD3	8:M:927:PRO:HD3	2.01	0.42
8:M:961:TYR:O	8:M:965:MET:HG2	2.19	0.42
9:R:396:GLY:HA2	9:R:399:VAL:HG12	2.01	0.42
11:T:181:LEU:HD23	11:T:181:LEU:HA	1.87	0.42
11:V:212:VAL:HG12	11:V:230:VAL:HG21	2.01	0.42
12:W:106:ILE:HD11	12:W:117:LEU:HB2	2.01	0.42
11:X:48:PHE:HZ	11:X:91:ALA:HB2	1.85	0.42
11:X:49:VAL:HG11	11:X:382:THR:OG1	2.19	0.42
11:X:316:LEU:HD22	11:X:320:ILE:HG12	2.00	0.42
2:D:26:ILE:HG13	2:D:55:ARG:HD3	2.02	0.41
4:G:49:LYS:O	4:G:53:PRO:HG3	2.20	0.41
5:I:-55:DG:H2''	5:I:-54:DA:N7	2.35	0.41
8:M:1220:VAL:HA	11:X:263:GLN:HE22	1.85	0.41
10:S:267:SER:HA	10:S:270:LYS:HG2	2.02	0.41
11:V:56:GLU:O	11:V:60:VAL:HG23	2.19	0.41
11:V:375:TYR:OH	13:V:501:ADP:N7	2.39	0.41
11:X:66:LYS:NZ	11:X:96:LEU:HA	2.35	0.41
11:X:276:LYS:HZ1	12:Y:263:GLY:HA2	1.85	0.41
12:Y:115:GLU:OE2	12:Y:119:GLN:NE2	2.53	0.41
12:Y:270:ARG:O	12:Y:273:ILE:HG22	2.20	0.41
12:Y:345:LEU:HD23	12:Y:348:LEU:HD12	2.01	0.41
2:C:39:ARG:NH2	2:C:43:VAL:O	2.41	0.41
6:J:19:DC:H2''	6:J:20:DG:H8	1.84	0.41
3:E:76:LYS:HE2	3:E:78:ARG:HB2	2.02	0.41
8:M:1042:PHE:HE1	8:M:1132:ARG:HB2	1.85	0.41
11:T:288:VAL:HA	11:T:291:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:25:HIS:HB3	12:W:374:GLU:HG3	2.02	0.41
12:W:310:ASN:HD22	12:W:350:ARG:HD2	1.84	0.41
11:X:83:THR:OG1	11:X:85:LYS:NZ	2.39	0.41
12:Y:165:MET:SD	12:Y:166:GLU:N	2.93	0.41
3:F:92:ASP:OD1	3:F:92:ASP:N	2.53	0.41
5:I:-69:DA:H2''	5:I:-68:DG:H8	1.85	0.41
7:Z:250:LYS:HA	7:Z:253:ILE:HG12	2.03	0.41
7:Z:598:LEU:HD23	7:Z:598:LEU:HA	1.95	0.41
3:E:59:LEU:O	3:E:62:GLU:HG3	2.20	0.41
8:M:924:VAL:HA	8:M:926:ARG:HH11	1.85	0.41
9:R:13:TYR:HB2	9:R:195:PHE:CD2	2.54	0.41
9:R:342:PRO:O	9:R:346:ARG:HG3	2.21	0.41
11:T:293:ALA:O	11:T:296:ILE:HG12	2.20	0.41
12:U:301:LEU:HB3	12:U:306:PHE:CZ	2.55	0.41
11:V:75:ILE:HD12	11:V:368:LEU:O	2.21	0.41
11:V:149:PRO:HA	11:V:165:HIS:O	2.20	0.41
11:V:198:ASP:OD1	11:V:214:ARG:HG2	2.20	0.41
11:V:345:THR:C	11:V:354:ILE:HG13	2.41	0.41
11:V:360:PRO:HB2	11:V:362:ASP:OD1	2.20	0.41
12:Y:73:VAL:HG12	12:Y:323:MET:O	2.19	0.41
6:J:-50:DT:H2''	6:J:-49:DG:C8	2.55	0.41
6:J:11:DC:H2'	6:J:12:DG:C8	2.55	0.41
6:J:22:DT:H2''	6:J:23:DG:N7	2.35	0.41
6:J:35:DT:H2''	6:J:36:DA:C8	2.55	0.41
8:M:944:LYS:HE3	8:M:1356:HIS:HB2	2.03	0.41
8:M:1154:LYS:HG3	8:M:1155:SER:H	1.84	0.41
9:R:149:THR:HG1	9:R:384:HIS:CD2	2.39	0.41
9:R:202:PRO:HG2	9:R:209:TYR:HB3	2.03	0.41
10:S:119:LEU:HD12	10:S:123:LEU:HD23	2.01	0.41
11:T:58:CYS:HA	11:T:61:ILE:HD12	2.02	0.41
11:T:346:THR:HG22	11:T:354:ILE:HB	2.00	0.41
12:U:78:SER:N	13:U:501:ADP:O3B	2.53	0.41
11:V:313:VAL:HG11	11:V:338:LEU:HD22	2.03	0.41
12:W:244:ILE:HD12	12:W:244:ILE:H	1.85	0.41
12:W:279:GLU:O	12:W:282:GLU:HG3	2.21	0.41
11:X:133:ILE:HG13	11:X:245:GLN:HB3	2.02	0.41
11:X:452:SER:OG	12:Y:341:HIS:NE2	2.35	0.41
12:Y:229:LEU:HD12	12:Y:229:LEU:HA	1.86	0.41
1:B:51:ILE:HA	1:B:54:PHE:CE2	2.55	0.41
5:I:-72:DT:H2''	5:I:-71:DG:C8	2.55	0.41
7:Z:601:PHE:N	7:Z:602:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:42:GLN:NE2	3:E:43:ARG:HB2	2.35	0.41
8:M:984:ASN:HA	8:M:987:MET:CE	2.50	0.41
8:M:1298:ILE:HA	8:M:1301:ARG:HH11	1.85	0.41
12:U:54:ALA:HB2	12:U:84:LEU:HD11	2.01	0.41
12:U:121:PHE:CZ	12:U:309:ILE:HD12	2.55	0.41
12:U:241:LEU:HA	12:U:244:ILE:HG12	2.02	0.41
12:U:257:LEU:HD23	11:V:283:LYS:HE2	2.03	0.41
12:U:364:ILE:HA	12:U:367:ILE:HG12	2.03	0.41
12:U:379:LEU:HD23	12:U:384:LEU:HD23	2.01	0.41
11:V:67:ALA:O	11:V:69:LYS:NZ	2.44	0.41
12:W:154:LYS:HE2	12:W:176:ILE:HD12	2.03	0.41
12:W:409:ILE:O	12:W:412:LYS:HG2	2.20	0.41
11:X:413:ARG:HH12	13:X:501:ADP:H4'	1.84	0.41
1:B:116:ARG:NH2	1:B:122:LYS:HE2	2.36	0.41
5:I:-32:DC:C4	5:I:-31:DA:C6	3.08	0.41
8:M:706:TRP:HB2	8:M:930:LEU:HD21	2.03	0.41
8:M:1273:LYS:HA	8:M:1273:LYS:HD2	1.94	0.41
9:R:129:PHE:CE1	9:R:412:ALA:HB1	2.56	0.41
11:T:92:ILE:HA	11:T:95:GLU:HG3	2.03	0.41
12:W:79:THR:OG1	12:W:81:LYS:NZ	2.37	0.41
12:W:136:ILE:HG23	12:W:194:LYS:NZ	2.36	0.41
12:Y:32:ASP:OD1	12:Y:38:ARG:NH2	2.54	0.41
12:Y:245:ASP:OD1	12:Y:273:ILE:HG21	2.21	0.41
2:D:67:ARG:HG3	2:D:68:ASP:N	2.36	0.41
6:J:56:DG:C6	6:J:57:DG:C6	3.08	0.41
8:M:831:ASN:HB3	8:M:834:SER:HB3	2.03	0.41
11:T:375:TYR:HB3	11:T:379:GLU:HB3	2.02	0.41
11:V:48:PHE:HA	13:V:501:ADP:N1	2.35	0.41
11:V:362:ASP:OD1	11:V:362:ASP:N	2.53	0.41
12:W:377:VAL:HG21	12:W:407:GLN:HB2	2.01	0.41
12:Y:77:PRO:HB2	12:Y:397:ARG:NH2	2.36	0.41
1:B:65:LEU:HA	1:B:68:GLN:HG3	2.02	0.41
2:C:46:ILE:O	5:I:7:DC:H5''	2.20	0.41
4:H:79:GLU:O	4:H:83:LEU:HD23	2.20	0.41
6:J:-28:DC:H4'	6:J:-27:DC:H5'	2.02	0.41
6:J:51:DG:H2''	6:J:52:DC:C5	2.56	0.41
1:A:63:ARG:H	1:A:63:ARG:HG2	1.71	0.41
8:M:1165:PRO:HB3	11:X:260:GLN:NE2	2.36	0.41
9:R:133:VAL:HG13	9:R:400:MET:SD	2.61	0.41
11:T:325:ASN:ND2	11:T:362:ASP:OD2	2.54	0.41
11:V:121:LEU:HD23	11:V:323:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:342:ARG:HD3	11:V:345:THR:OG1	2.20	0.41
11:V:378:ASP:O	11:V:382:THR:HG23	2.21	0.41
11:X:416:LEU:O	11:X:419:LEU:HD22	2.21	0.41
12:Y:125:ILE:HG13	12:Y:241:LEU:HD13	2.03	0.41
12:Y:453:ASN:OD1	12:Y:453:ASN:N	2.52	0.41
2:C:32:PRO:HG2	6:J:-13:DA:H2'	2.02	0.41
3:F:80:ILE:HG12	3:F:83:HIS:ND1	2.36	0.41
4:G:100:ALA:O	4:G:104:ILE:HG12	2.20	0.41
5:I:-42:DT:H2''	5:I:-41:DG:C8	2.55	0.41
6:J:-19:DG:O5'	6:J:-19:DG:H8	2.04	0.41
8:M:753:PRO:HB3	8:M:825:GLU:OE2	2.21	0.41
8:M:955:LYS:NZ	12:W:283:GLU:OE1	2.53	0.41
8:M:1009:VAL:HG11	11:V:205:ASN:HB3	2.03	0.41
8:M:1067:CYS:HB2	8:M:1070:ASN:OD1	2.21	0.41
8:M:1282:LEU:HD23	8:M:1289:TYR:CG	2.56	0.41
9:R:16:LYS:HG2	9:R:397:TRP:HB2	2.02	0.41
9:R:313:ILE:HB	9:R:314:PRO:HD3	2.03	0.41
10:S:169:PRO:O	10:S:173:ARG:HG2	2.20	0.41
12:U:190:ILE:HG13	12:U:192:ILE:HD11	2.03	0.41
11:V:116:LYS:HB3	11:V:116:LYS:HE2	1.92	0.41
12:W:147:ARG:HB3	12:W:154:LYS:HB3	2.02	0.41
12:W:162:THR:HG23	12:W:165:MET:H	1.86	0.41
12:W:250:ARG:HG3	12:W:252:GLN:HG2	2.03	0.41
12:W:281:LYS:HE3	12:W:281:LYS:HB3	1.91	0.41
12:W:358:SER:OG	12:W:359:TYR:N	2.54	0.41
11:X:25:ALA:HB1	12:Y:68:GLY:HA3	2.03	0.41
11:X:74:ALA:HB3	11:X:367:LEU:HB3	2.03	0.41
11:X:171:LYS:HE2	11:X:171:LYS:HB2	1.94	0.41
11:X:311:ASP:HA	11:X:339:ALA:HB3	2.02	0.41
12:Y:303:ILE:HD13	12:Y:335:THR:HG23	2.03	0.41
12:Y:416:ASN:OD1	12:Y:417:THR:N	2.50	0.41
5:I:87:DG:H2''	5:I:88:DT:C6	2.56	0.41
6:J:-23:DT:H2''	6:J:-22:DG:C8	2.56	0.41
6:J:62:DG:H2''	6:J:63:DG:O5'	2.20	0.41
3:E:26:PHE:HZ	3:E:56:LEU:HD22	1.83	0.41
8:M:1124:MET:HG2	8:M:1127:LYS:HZ3	1.87	0.41
9:R:133:VAL:HA	9:R:136:PHE:HD2	1.85	0.41
9:R:243:ILE:HD12	9:R:243:ILE:H	1.86	0.41
11:T:116:LYS:NZ	11:T:118:THR:OG1	2.32	0.41
11:T:150:GLU:HG3	11:T:167:ILE:HD11	2.03	0.41
12:U:57:ILE:O	12:U:60:MET:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:194:VAL:HG12	11:V:211:ARG:HD2	2.02	0.41
11:V:243:ILE:HG22	11:V:245:GLN:H	1.86	0.41
11:X:216:ASP:HA	11:X:229:TYR:HB3	2.03	0.41
11:X:252:LEU:HG	11:X:256:ASN:HD21	1.86	0.41
2:D:86:VAL:HG21	1:A:88:ALA:O	2.21	0.40
7:Z:296:LEU:HB3	7:Z:588:GLU:HG2	2.03	0.40
3:E:74:ASN:OD1	3:E:82:ARG:NH1	2.53	0.40
8:M:1148:ARG:HA	8:M:1148:ARG:HD3	1.89	0.40
9:R:76:TRP:O	9:R:80:LEU:HG	2.21	0.40
9:R:81:PHE:O	9:R:83:PRO:HD3	2.21	0.40
11:T:212:VAL:HG12	11:T:230:VAL:HG11	2.02	0.40
12:W:72:LEU:HD23	12:W:353:ILE:HG12	2.03	0.40
12:Y:60:MET:CE	12:Y:66:ILE:HG22	2.51	0.40
5:I:-66:DA:C8	5:I:-66:DA:H5'	2.56	0.40
5:I:-12:DC:H2''	5:I:-11:DG:H8	1.86	0.40
8:M:860:LEU:HA	8:M:863:LEU:HD12	2.02	0.40
8:M:1243:TYR:CE1	12:W:285:LYS:HB2	2.55	0.40
8:M:1333:ALA:O	8:M:1360:GLN:NE2	2.47	0.40
11:T:257:ALA:O	11:T:258:ARG:NE	2.54	0.40
11:T:266:ILE:HG13	11:T:267:SER:N	2.36	0.40
12:U:71:VAL:HG23	12:U:352:ILE:HG13	2.02	0.40
12:W:36:GLN:HG3	12:W:52:ARG:HH22	1.86	0.40
11:X:223:ASP:N	11:X:223:ASP:OD1	2.52	0.40
12:Y:240:SER:OG	12:Y:241:LEU:N	2.54	0.40
5:I:8:DC:H2''	5:I:9:DG:C8	2.57	0.40
6:J:-92:DC:H2'	6:J:-91:DG:H8	1.83	0.40
6:J:-19:DG:H5''	8:M:1272:THR:HG23	2.03	0.40
3:E:76:LYS:HZ3	3:E:79:ILE:C	2.23	0.40
3:E:105:GLN:HG3	3:E:105:GLN:O	2.21	0.40
8:M:1008:PHE:CD2	8:M:1010:LEU:HB3	2.57	0.40
10:S:121:SER:HB3	10:S:128:ARG:HD2	2.03	0.40
10:S:192:THR:HG22	10:S:193:ASN:N	2.37	0.40
11:T:360:PRO:HB2	11:T:362:ASP:OD1	2.21	0.40
11:T:371:ARG:NH2	12:Y:446:GLN:OE1	2.54	0.40
12:U:127:ILE:N	12:U:239:VAL:O	2.38	0.40
11:V:49:VAL:H	13:V:501:ADP:HN62	1.69	0.40
11:V:166:VAL:HG21	11:V:186:TYR:CZ	2.56	0.40
12:W:156:GLY:C	12:W:157:LYS:HD3	2.41	0.40
11:X:66:LYS:HZ2	11:X:96:LEU:HA	1.86	0.40
1:B:96:VAL:HG21	2:C:58:LEU:HG	2.02	0.40
2:C:75:HIS:CE1	4:H:99:THR:HG1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:ARG:HG3	2:D:68:ASP:H	1.86	0.40
5:I:-69:DA:H2''	5:I:-68:DG:C8	2.55	0.40
5:I:-4:DC:H5''	1:A:117:VAL:HG21	2.03	0.40
5:I:66:DC:H5''	10:S:130:ARG:HD2	2.03	0.40
6:J:58:DC:H2''	6:J:59:DA:C8	2.57	0.40
3:E:80:ILE:HG12	3:E:83:HIS:CE1	2.56	0.40
8:M:954:SER:O	8:M:958:ARG:N	2.44	0.40
8:M:967:ARG:HH22	8:M:998:LEU:HD11	1.85	0.40
8:M:1163:ILE:O	8:M:1169:ARG:NH2	2.55	0.40
11:T:126:ARG:HH11	11:T:285:ARG:NE	2.19	0.40
11:T:226:THR:HG23	12:U:175:MET:SD	2.62	0.40
11:T:278:THR:HG22	11:T:279:GLU:N	2.27	0.40
12:U:436:SER:HB3	11:V:369:ILE:CD1	2.52	0.40
11:V:105:LEU:HB3	11:V:310:ILE:HG13	2.02	0.40
11:V:280:ILE:HD12	11:V:284:LEU:HD23	2.03	0.40
5:I:-56:DC:H2''	5:I:-55:DG:N7	2.36	0.40
5:I:23:DA:H1'	8:M:979:PHE:CZ	2.56	0.40
5:I:39:DA:H1'	5:I:40:DG:C8	2.57	0.40
5:I:100:DG:H1'	5:I:101:DT:O4'	2.22	0.40
6:J:73:DG:H2''	6:J:74:DG:C8	2.57	0.40
7:Z:195:LYS:HB3	7:Z:195:LYS:HE3	1.87	0.40
9:R:111:LEU:HD23	9:R:111:LEU:HA	1.93	0.40
10:S:168:LYS:HD3	10:S:168:LYS:HA	1.95	0.40
11:T:387:ARG:HG3	11:T:416:LEU:HD22	2.03	0.40
11:T:450:LYS:O	11:T:453:THR:HG22	2.21	0.40
11:V:30:ILE:HG12	11:V:48:PHE:CE1	2.56	0.40
11:V:413:ARG:HH21	13:V:501:ADP:H5'2	1.86	0.40
12:W:53:ALA:O	12:W:57:ILE:HG12	2.22	0.40
12:W:98:PHE:HD1	12:W:292:VAL:HB	1.87	0.40
12:W:99:THR:O	12:W:294:PHE:N	2.46	0.40
12:W:149:ILE:HG13	12:W:150:THR:N	2.36	0.40
11:X:383:ILE:HG23	11:X:386:ARG:HH21	1.86	0.40
12:Y:31:LEU:CD1	12:Y:55:GLY:HA3	2.50	0.40
12:Y:204:ARG:HD3	12:Y:208:ARG:HE	1.86	0.40
12:Y:267:SER:HA	12:Y:270:ARG:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
1	B	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
2	C	80/103 (78%)	75 (94%)	5 (6%)	0	100	100
2	D	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
3	E	101/158 (64%)	96 (95%)	5 (5%)	0	100	100
3	F	99/158 (63%)	96 (97%)	3 (3%)	0	100	100
4	G	94/131 (72%)	92 (98%)	2 (2%)	0	100	100
4	H	89/131 (68%)	84 (94%)	5 (6%)	0	100	100
7	Z	176/180 (98%)	157 (89%)	17 (10%)	2 (1%)	12	46
8	M	684/1514 (45%)	629 (92%)	54 (8%)	1 (0%)	48	83
9	R	407/438 (93%)	386 (95%)	21 (5%)	0	100	100
10	S	179/280 (64%)	163 (91%)	15 (8%)	1 (1%)	22	60
11	T	441/463 (95%)	412 (93%)	29 (7%)	0	100	100
11	V	430/463 (93%)	415 (96%)	15 (4%)	0	100	100
11	X	440/463 (95%)	425 (97%)	15 (3%)	0	100	100
12	U	426/471 (90%)	413 (97%)	13 (3%)	0	100	100
12	W	429/471 (91%)	420 (98%)	9 (2%)	0	100	100
12	Y	445/471 (94%)	430 (97%)	14 (3%)	1 (0%)	44	78
All	All	4788/6270 (76%)	4554 (95%)	229 (5%)	5 (0%)	50	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	Z	299	PRO
10	S	184	LEU
7	Z	326	LYS
12	Y	416	ASN

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Mol	Chain	Res	Type
8	M	972	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/113 (74%)	82 (98%)	2 (2%)	44	63
1	B	84/113 (74%)	83 (99%)	1 (1%)	67	79
2	C	68/81 (84%)	67 (98%)	1 (2%)	60	75
2	D	67/81 (83%)	65 (97%)	2 (3%)	36	56
3	E	82/124 (66%)	82 (100%)	0	100	100
3	F	77/124 (62%)	77 (100%)	0	100	100
4	G	83/109 (76%)	83 (100%)	0	100	100
4	H	78/109 (72%)	77 (99%)	1 (1%)	65	77
7	Z	134/171 (78%)	132 (98%)	2 (2%)	60	75
8	M	574/1376 (42%)	567 (99%)	7 (1%)	67	79
9	R	372/396 (94%)	372 (100%)	0	100	100
10	S	178/261 (68%)	177 (99%)	1 (1%)	84	88
11	T	371/391 (95%)	369 (100%)	2 (0%)	86	90
11	V	368/391 (94%)	365 (99%)	3 (1%)	79	85
11	X	374/391 (96%)	373 (100%)	1 (0%)	91	92
12	U	367/403 (91%)	366 (100%)	1 (0%)	91	92
12	W	369/403 (92%)	369 (100%)	0	100	100
12	Y	372/403 (92%)	372 (100%)	0	100	100
All	All	4102/5440 (75%)	4078 (99%)	24 (1%)	82	88

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	125	LYS

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Mol	Chain	Res	Type
2	C	67	ARG
2	D	23	ARG
2	D	67	ARG
4	H	60	LYS
7	Z	205	LYS
7	Z	216	LYS
1	A	69	ARG
1	A	125	LYS
8	M	833	ARG
8	M	836	ARG
8	M	926	ARG
8	M	1050	ASN
8	M	1079	ARG
8	M	1146	LYS
8	M	1313	ARG
10	S	92	GLN
11	T	277	LYS
11	T	392	ARG
12	U	147	ARG
11	V	43	ARG
11	V	274	LYS
11	V	283	LYS
11	X	161	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	74	ASN
4	H	87	ASN
4	H	98	GLN
8	M	810	GLN
8	M	957	GLN
8	M	969	GLN
8	M	1249	GLN
8	M	1352	GLN
9	R	246	ASN
11	T	271	GLN
11	T	289	ASN
12	U	360	ASN
12	U	408	GLN
12	W	90	GLN
12	W	310	ASN

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Mol	Chain	Res	Type
12	W	408	GLN
11	X	325	ASN
12	Y	119	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	ADP	Y	501	15	24,29,29	0.98	1 (4%)	29,45,45	1.44	4 (13%)
14	BEF	R	502	13	0,3,3	-	-	-	-	-
13	ADP	V	501	15	24,29,29	0.93	1 (4%)	29,45,45	1.50	4 (13%)
13	ADP	T	501	15	24,29,29	0.97	1 (4%)	29,45,45	1.48	4 (13%)
14	BEF	M	1602	-	0,3,3	-	-	-	-	-
13	ADP	M	1601	15	24,29,29	0.96	1 (4%)	29,45,45	1.41	4 (13%)
13	ADP	R	501	15,14	24,29,29	0.96	1 (4%)	29,45,45	1.46	4 (13%)
13	ADP	W	501	15	24,29,29	0.94	1 (4%)	29,45,45	1.47	5 (17%)
13	ADP	X	501	15	24,29,29	0.98	1 (4%)	29,45,45	1.38	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	ADP	U	501	15	24,29,29	0.97	1 (4%)	29,45,45	1.50	4 (13%)

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
13	ADP	Y	501	15	-	2/12/32/32	0/3/3/3
13	ADP	V	501	15	-	5/12/32/32	0/3/3/3
13	ADP	T	501	15	-	0/12/32/32	0/3/3/3
13	ADP	M	1601	15	-	5/12/32/32	0/3/3/3
13	ADP	R	501	15,14	-	4/12/32/32	0/3/3/3
13	ADP	W	501	15	-	6/12/32/32	0/3/3/3
13	ADP	X	501	15	-	1/12/32/32	0/3/3/3
13	ADP	U	501	15	-	1/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	W	501	ADP	C5-C4	2.58	1.47	1.40
13	X	501	ADP	C5-C4	2.58	1.47	1.40
13	U	501	ADP	C5-C4	2.51	1.47	1.40
13	T	501	ADP	C5-C4	2.51	1.47	1.40
13	V	501	ADP	C5-C4	2.50	1.47	1.40
13	R	501	ADP	C5-C4	2.49	1.47	1.40
13	M	1601	ADP	C5-C4	2.48	1.47	1.40
13	Y	501	ADP	C5-C4	2.48	1.47	1.40

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	U	501	ADP	PA-O3A-PB	-3.92	119.38	132.83
13	V	501	ADP	PA-O3A-PB	-3.85	119.60	132.83
13	W	501	ADP	C3'-C2'-C1'	3.70	106.55	100.98
13	T	501	ADP	PA-O3A-PB	-3.67	120.23	132.83
13	Y	501	ADP	PA-O3A-PB	-3.61	120.45	132.83
13	U	501	ADP	C3'-C2'-C1'	3.46	106.18	100.98
13	X	501	ADP	C3'-C2'-C1'	3.44	106.16	100.98
13	R	501	ADP	C3'-C2'-C1'	3.38	106.07	100.98
13	R	501	ADP	PA-O3A-PB	-3.36	121.30	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1601	ADP	C3'-C2'-C1'	3.34	106.01	100.98
13	W	501	ADP	N3-C2-N1	-3.25	123.59	128.68
13	T	501	ADP	C3'-C2'-C1'	3.23	105.84	100.98
13	M	1601	ADP	N3-C2-N1	-3.16	123.73	128.68
13	V	501	ADP	C3'-C2'-C1'	3.16	105.73	100.98
13	R	501	ADP	N3-C2-N1	-3.16	123.74	128.68
13	V	501	ADP	N3-C2-N1	-3.13	123.79	128.68
13	T	501	ADP	N3-C2-N1	-3.12	123.79	128.68
13	U	501	ADP	N3-C2-N1	-3.12	123.81	128.68
13	Y	501	ADP	N3-C2-N1	-3.09	123.86	128.68
13	Y	501	ADP	C3'-C2'-C1'	2.99	105.49	100.98
13	X	501	ADP	N3-C2-N1	-2.97	124.04	128.68
13	M	1601	ADP	PA-O3A-PB	-2.88	122.94	132.83
13	W	501	ADP	C4-C5-N7	-2.77	106.52	109.40
13	X	501	ADP	PA-O3A-PB	-2.75	123.40	132.83
13	M	1601	ADP	C4-C5-N7	-2.68	106.61	109.40
13	V	501	ADP	C4-C5-N7	-2.67	106.61	109.40
13	W	501	ADP	PA-O3A-PB	-2.67	123.68	132.83
13	T	501	ADP	C4-C5-N7	-2.66	106.63	109.40
13	R	501	ADP	C4-C5-N7	-2.63	106.66	109.40
13	U	501	ADP	C4-C5-N7	-2.56	106.73	109.40
13	Y	501	ADP	C4-C5-N7	-2.45	106.84	109.40
13	X	501	ADP	C4-C5-N7	-2.44	106.86	109.40
13	W	501	ADP	C2-N1-C6	2.06	122.27	118.75

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	M	1601	ADP	PB-O3A-PA-O5'
13	M	1601	ADP	C5'-O5'-PA-O2A
13	R	501	ADP	C5'-O5'-PA-O3A
13	R	501	ADP	C3'-C4'-C5'-O5'
13	V	501	ADP	C5'-O5'-PA-O3A
13	W	501	ADP	C5'-O5'-PA-O2A
13	Y	501	ADP	C5'-O5'-PA-O3A
13	R	501	ADP	O4'-C4'-C5'-O5'
13	V	501	ADP	O4'-C4'-C5'-O5'
13	W	501	ADP	PB-O3A-PA-O5'
13	V	501	ADP	C3'-C4'-C5'-O5'
13	M	1601	ADP	C5'-O5'-PA-O3A
13	W	501	ADP	C5'-O5'-PA-O3A

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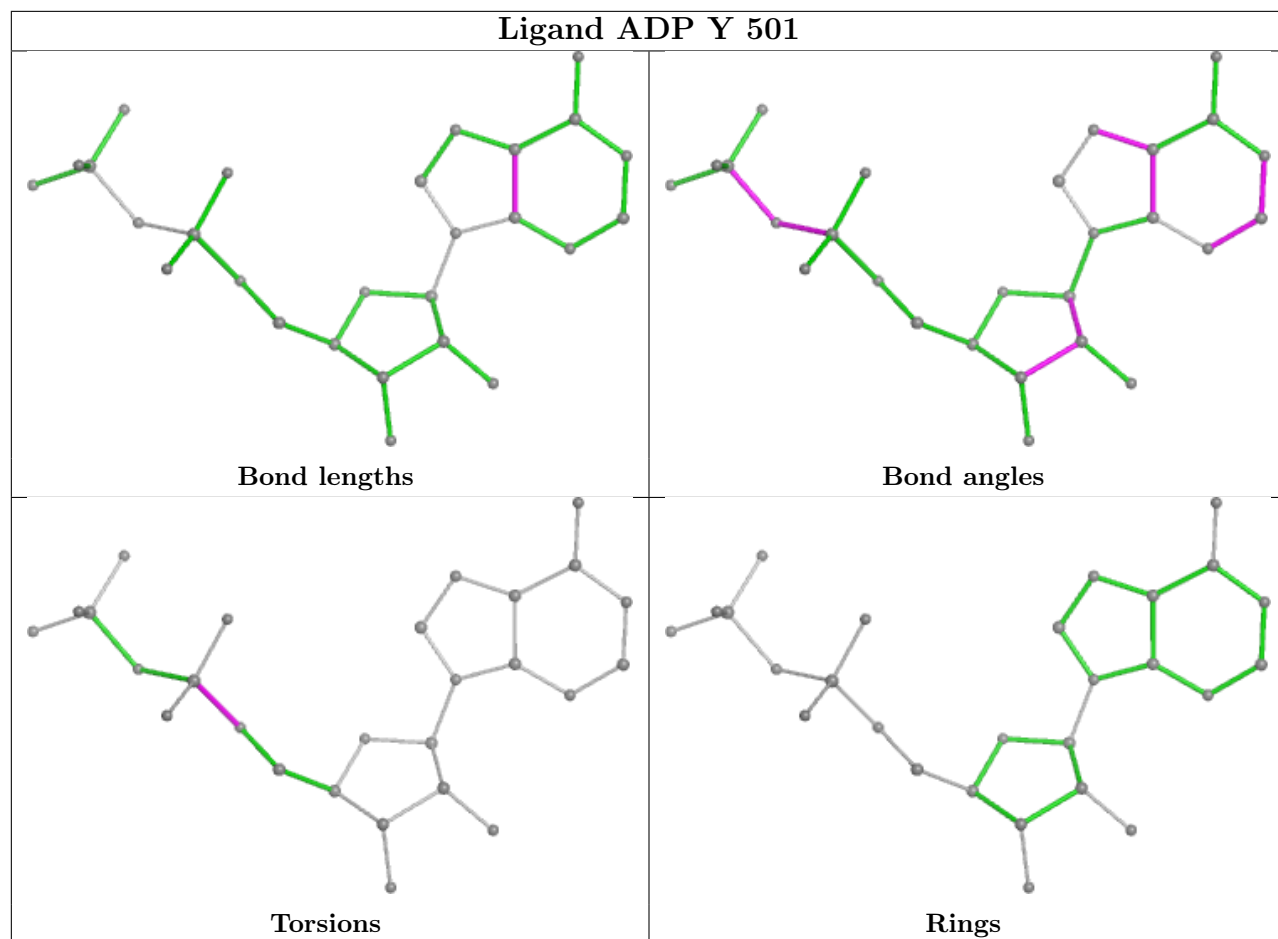
Mol	Chain	Res	Type	Atoms
13	W	501	ADP	O4'-C4'-C5'-O5'
13	M	1601	ADP	C5'-O5'-PA-O1A
13	R	501	ADP	C5'-O5'-PA-O1A
13	V	501	ADP	C5'-O5'-PA-O1A
13	V	501	ADP	C5'-O5'-PA-O2A
13	W	501	ADP	C5'-O5'-PA-O1A
13	Y	501	ADP	C5'-O5'-PA-O1A
13	M	1601	ADP	O4'-C4'-C5'-O5'
13	X	501	ADP	C5'-O5'-PA-O1A
13	U	501	ADP	O4'-C4'-C5'-O5'
13	W	501	ADP	C3'-C4'-C5'-O5'

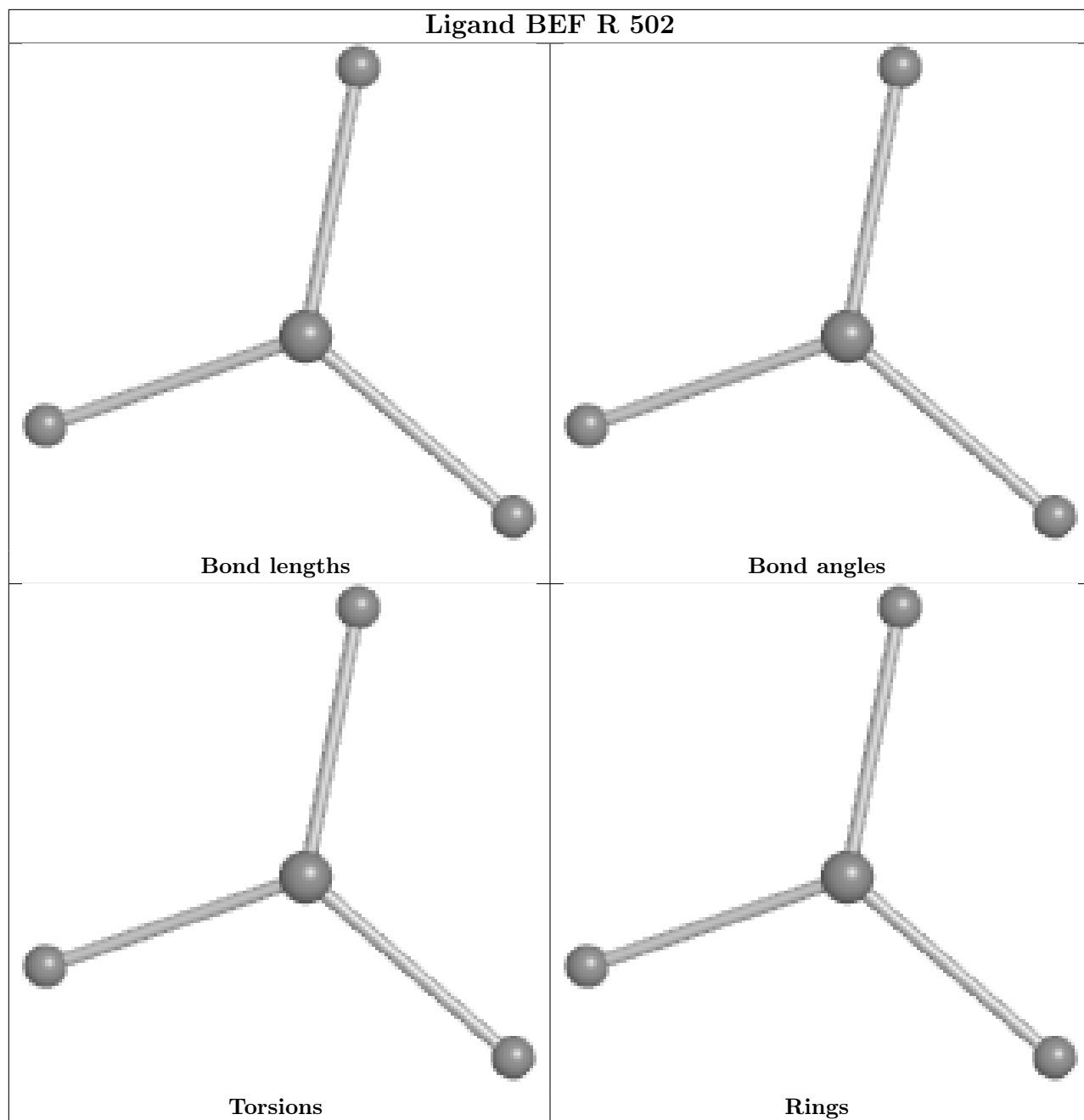
There are no ring outliers.

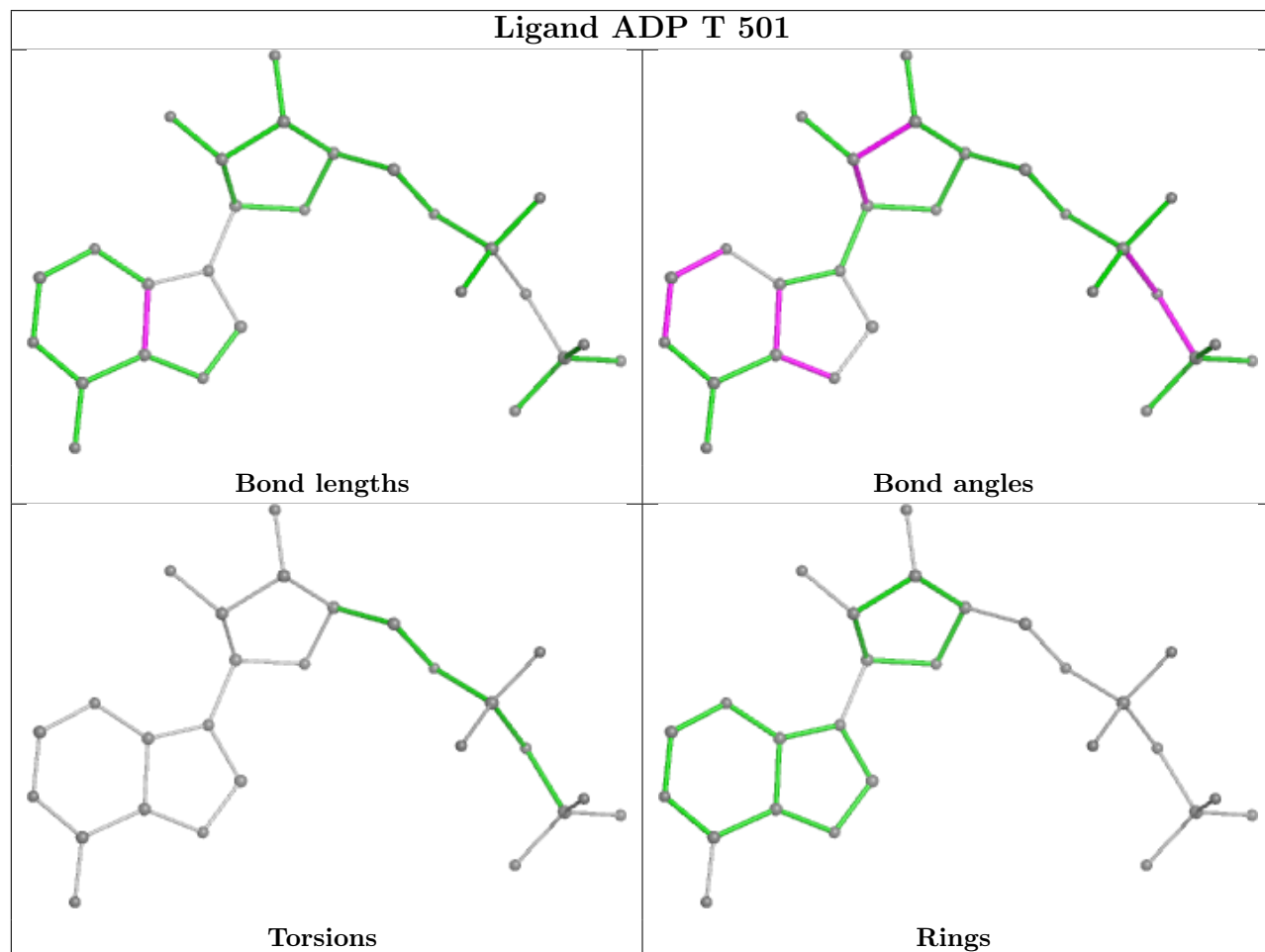
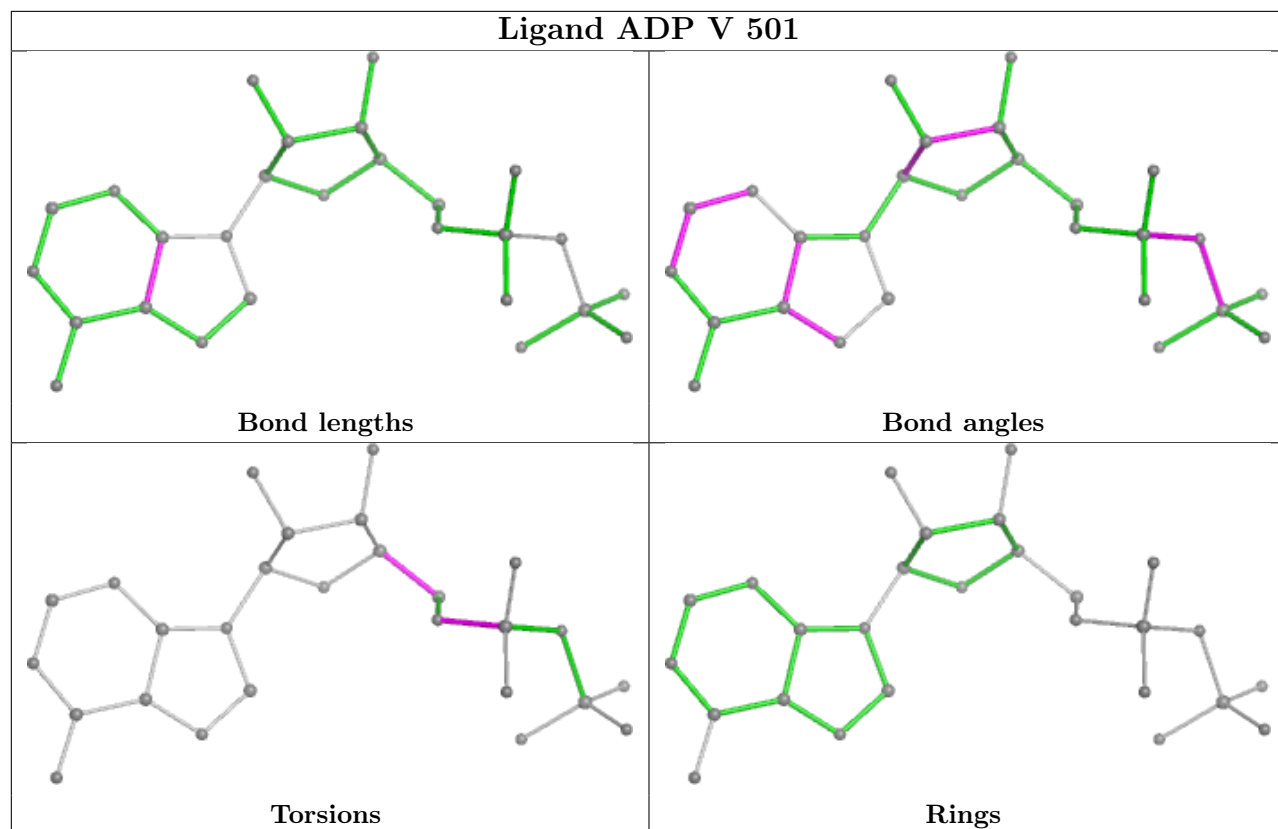
10 monomers are involved in 37 short contacts:

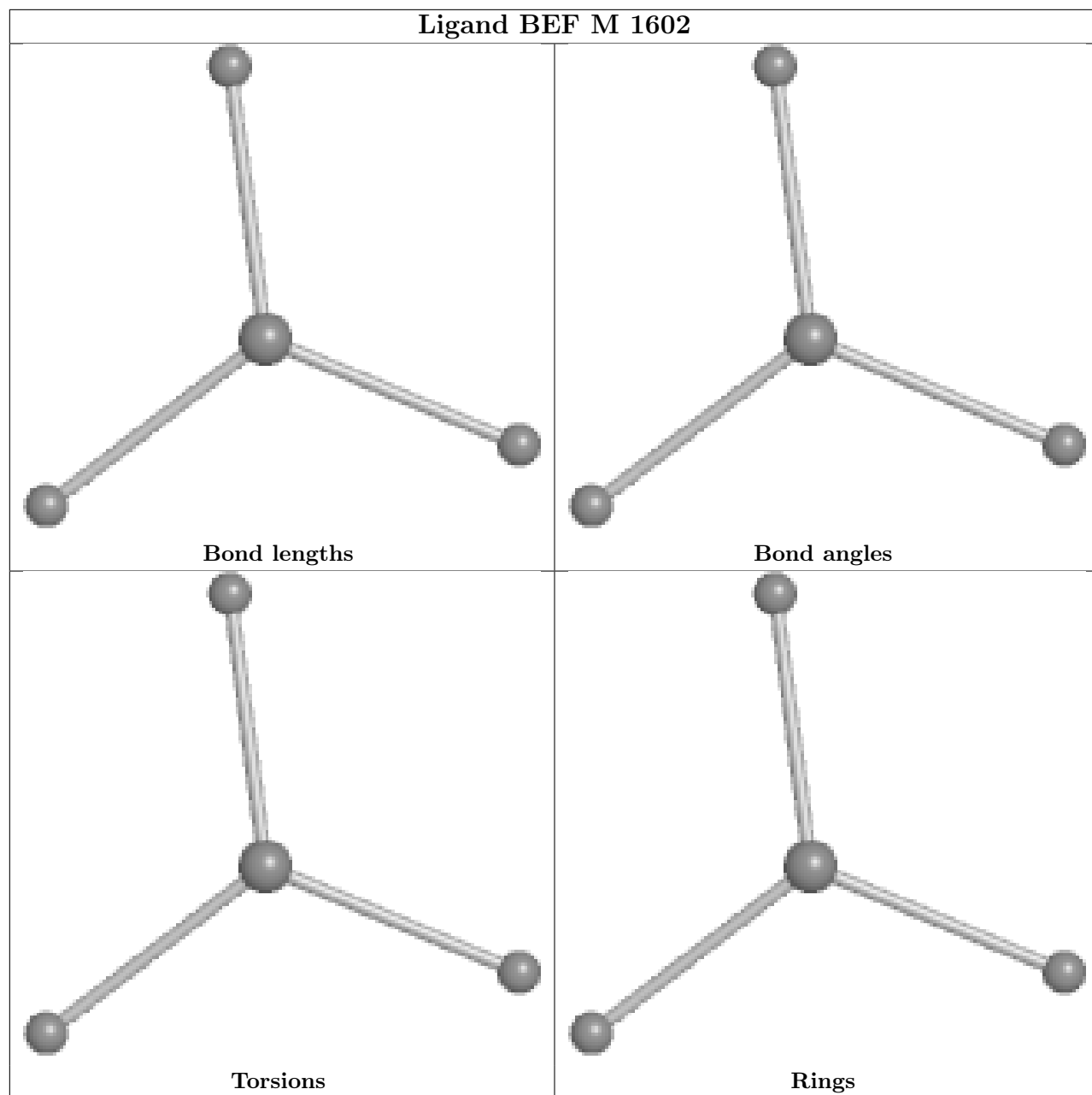
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	Y	501	ADP	5	0
14	R	502	BEF	1	0
13	V	501	ADP	8	0
13	T	501	ADP	1	0
14	M	1602	BEF	2	0
13	M	1601	ADP	5	0
13	R	501	ADP	1	0
13	W	501	ADP	4	0
13	X	501	ADP	7	0
13	U	501	ADP	5	0

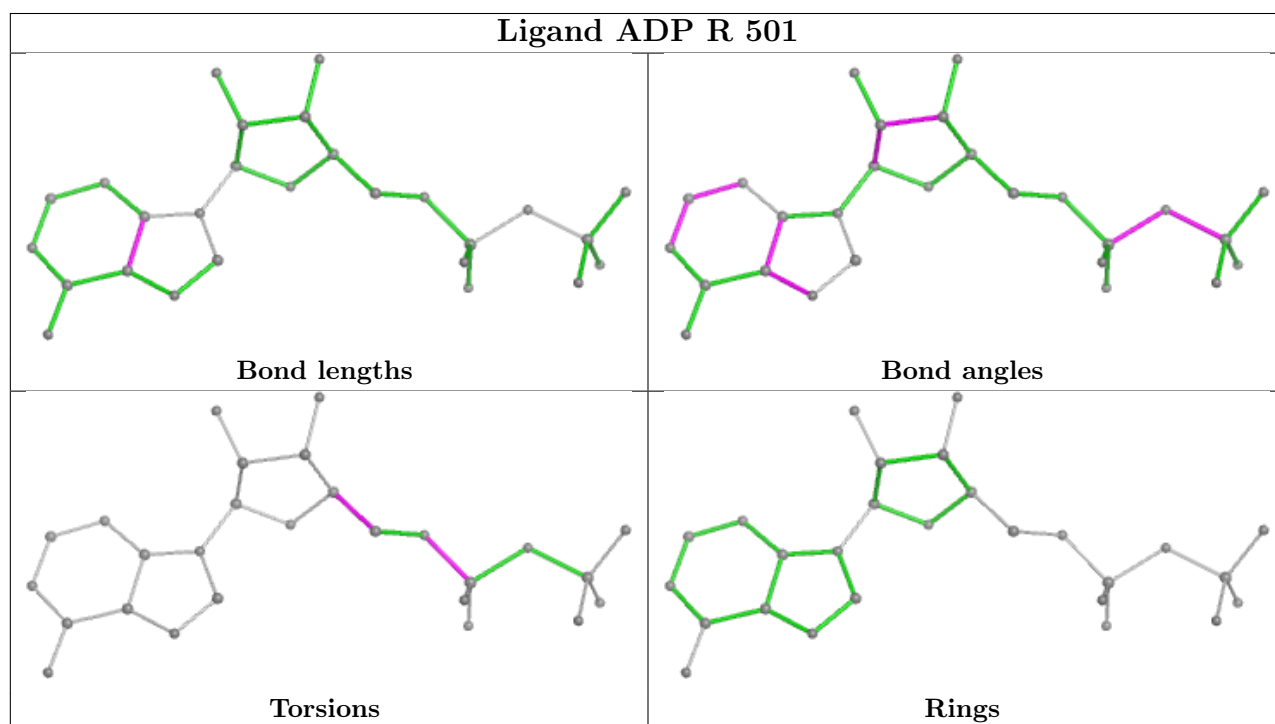
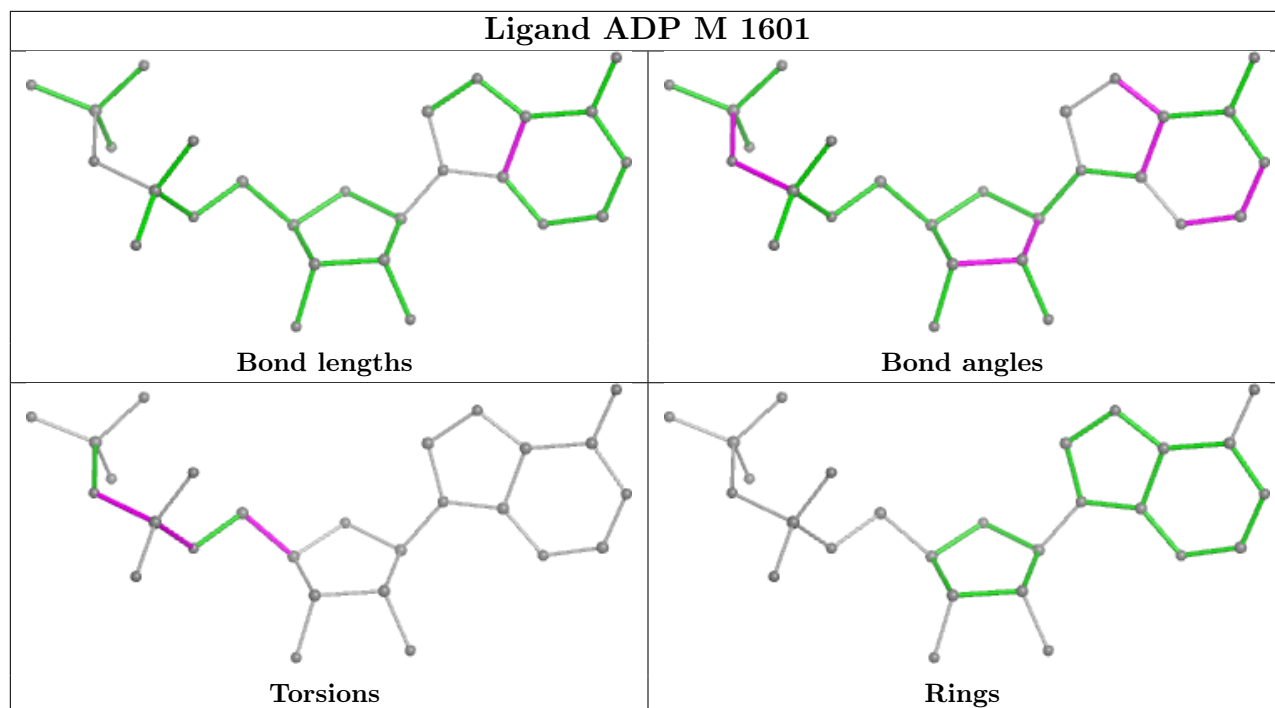
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

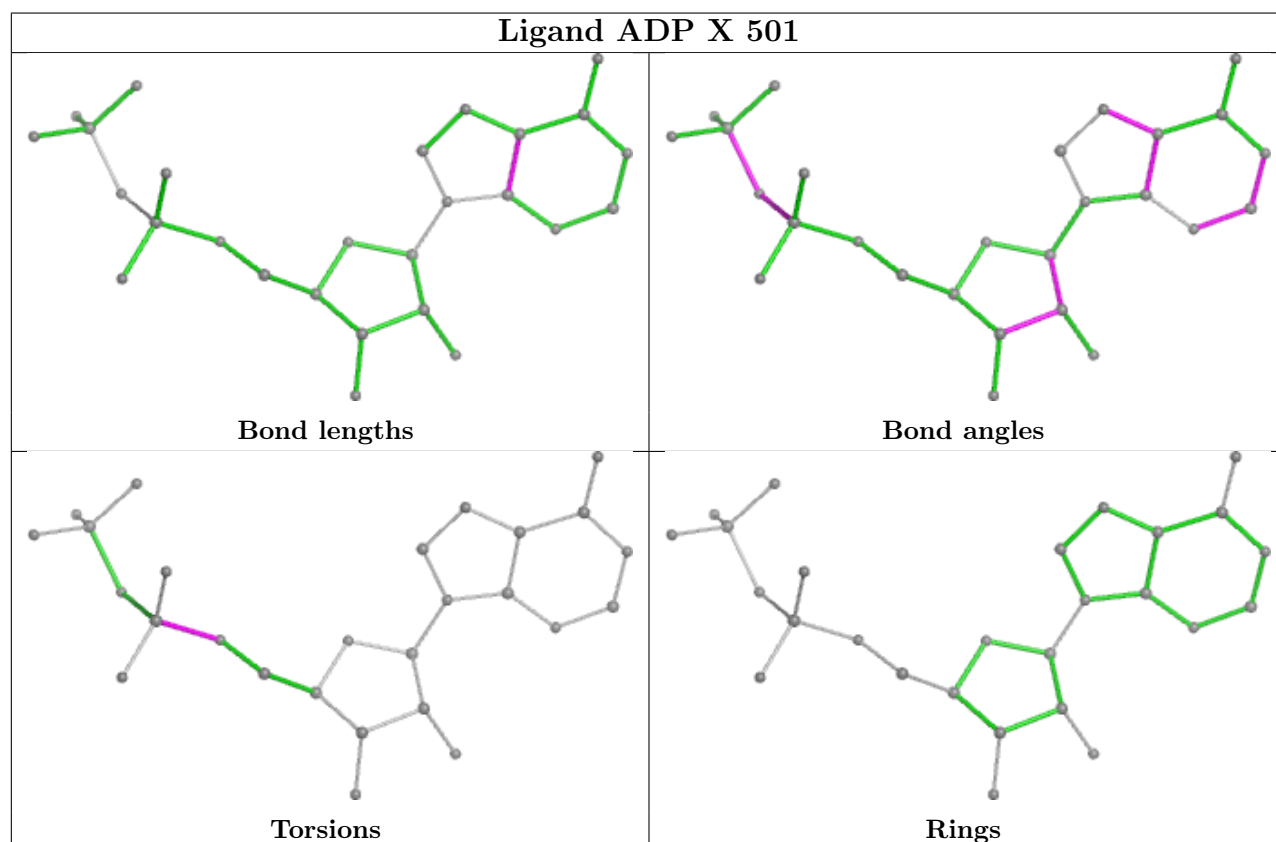
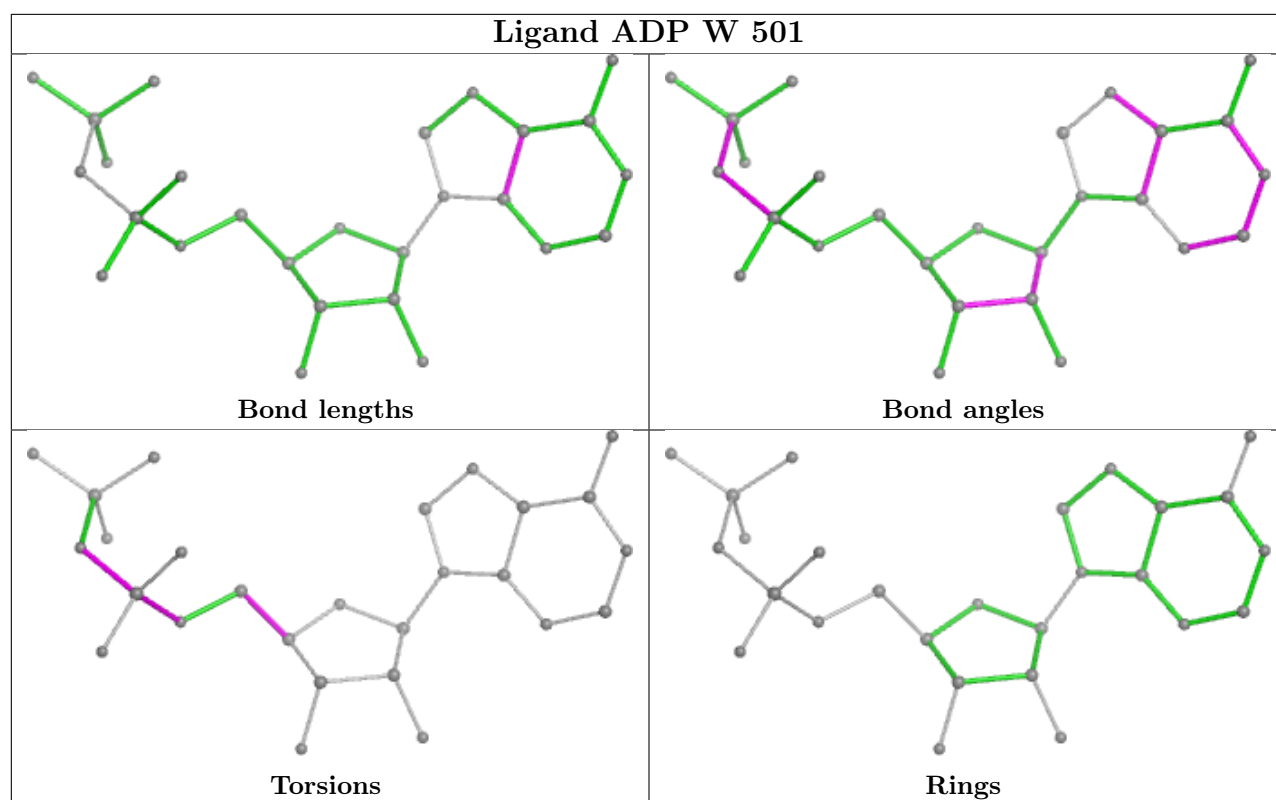


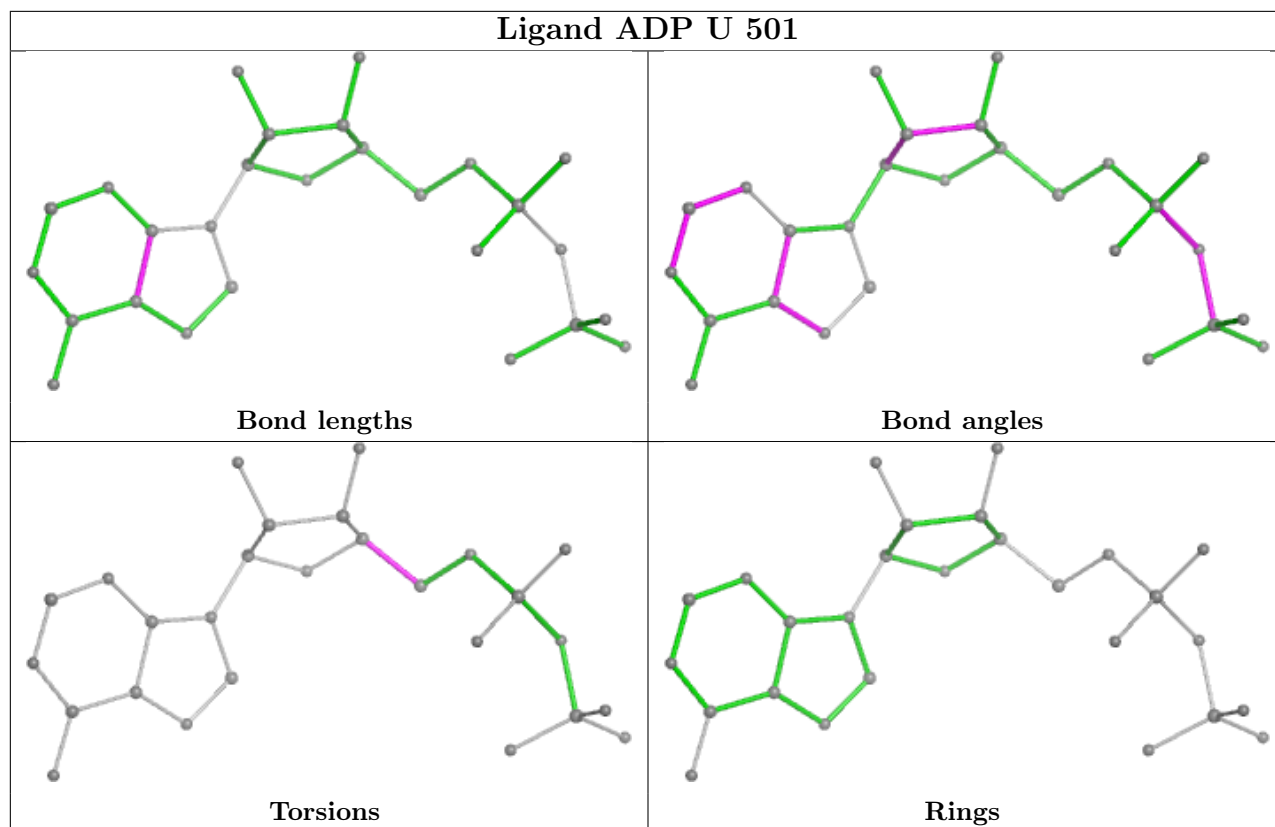












5.7 Other polymers [i](#)

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
7	Z	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	329:LYS	C	581:THR	N	57.91

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18472. These allow visual inspection of the internal detail of the map and identification of artifacts.

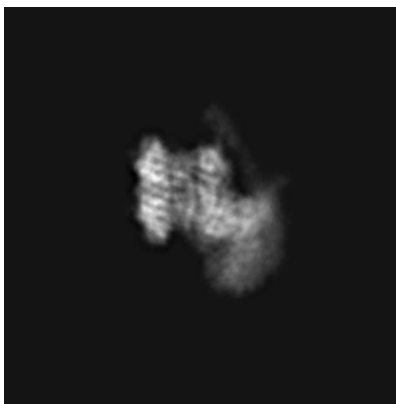
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

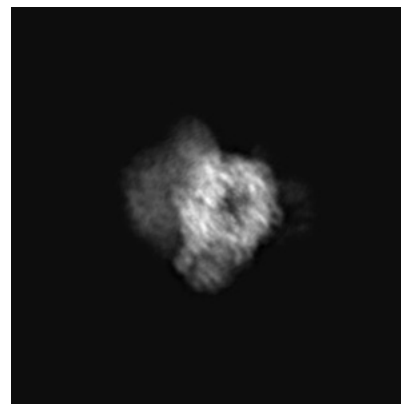
6.1.1 Primary map



X

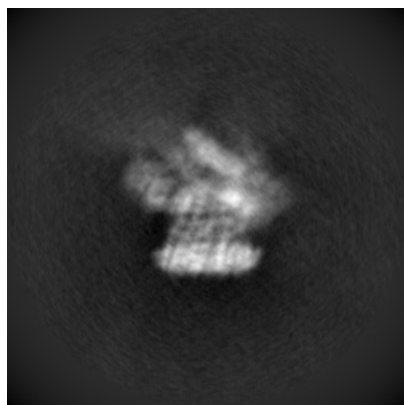


Y

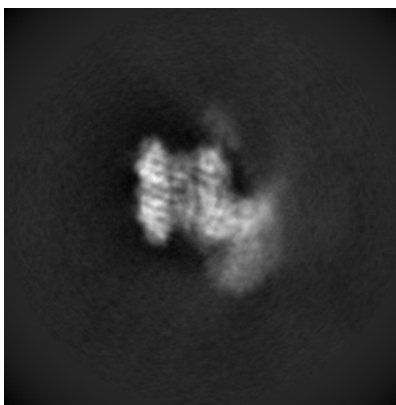


Z

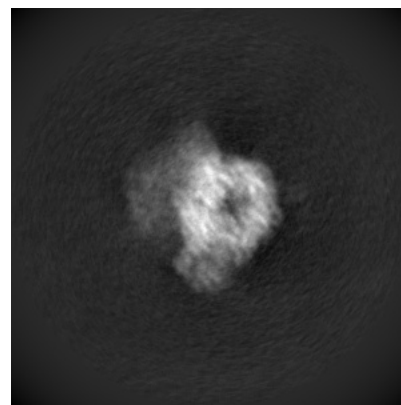
6.1.2 Raw map



X



Y

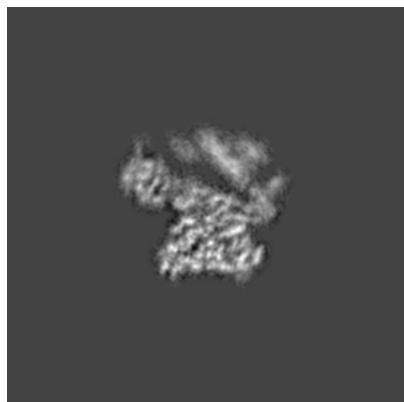


Z

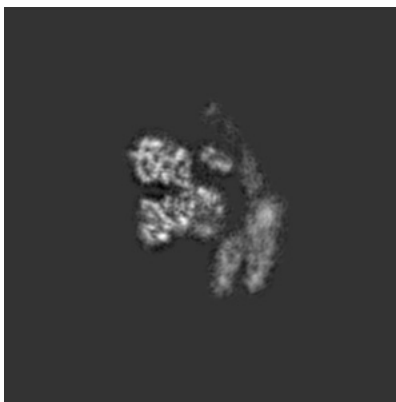
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

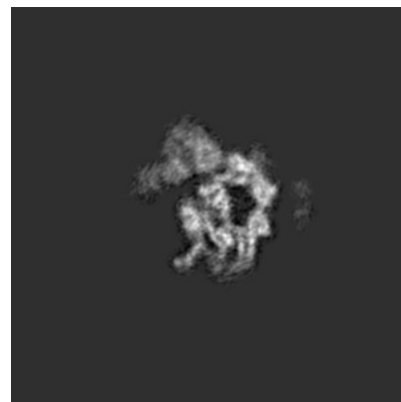
6.2.1 Primary map



X Index: 192

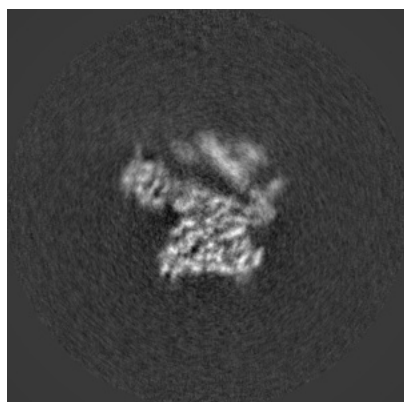


Y Index: 192

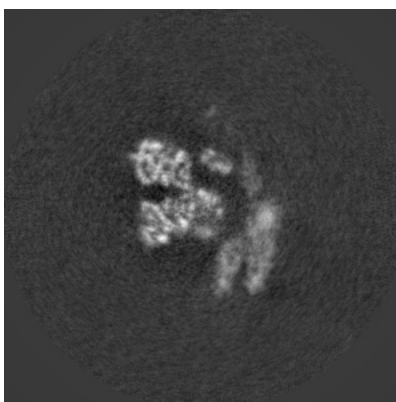


Z Index: 192

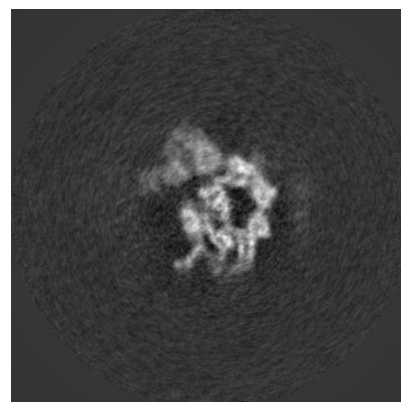
6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

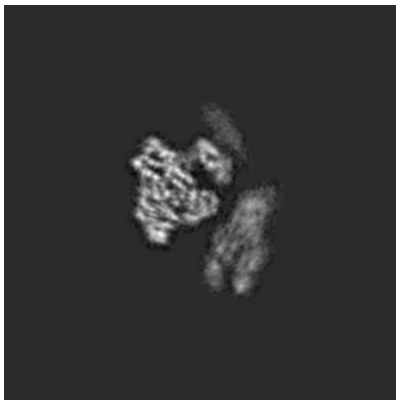
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

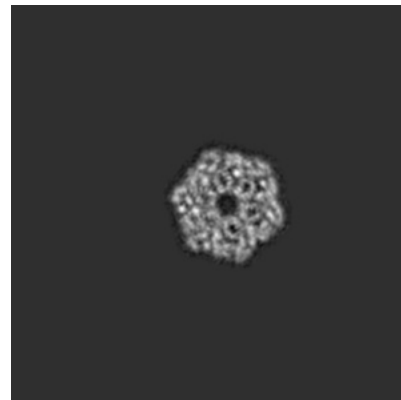
6.3.1 Primary map



X Index: 187

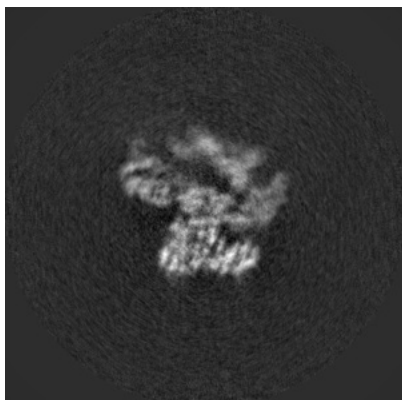


Y Index: 207

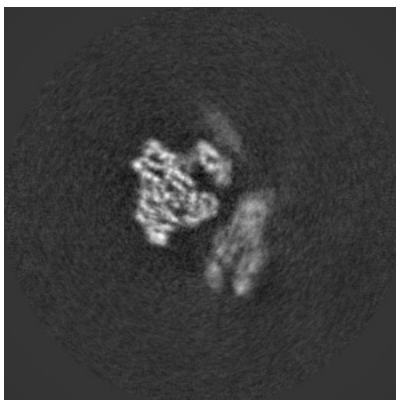


Z Index: 144

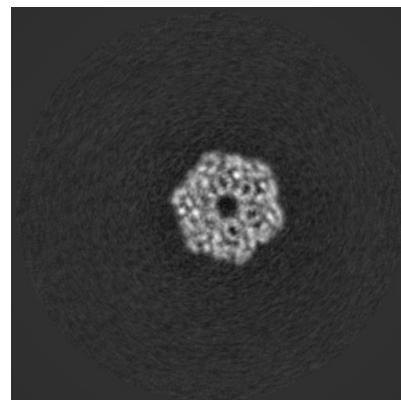
6.3.2 Raw map



X Index: 187



Y Index: 207

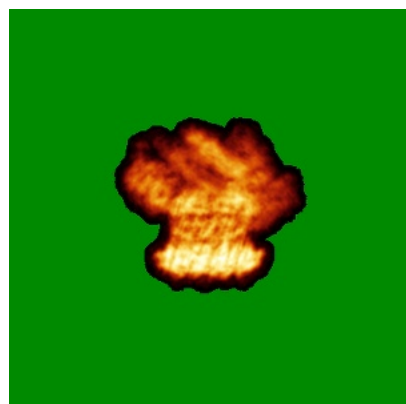


Z Index: 144

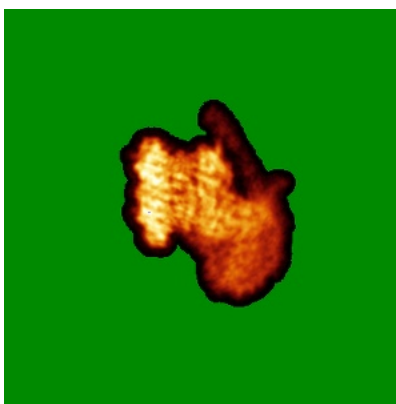
The images above show the largest variance slices of the map in three orthogonal directions.

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

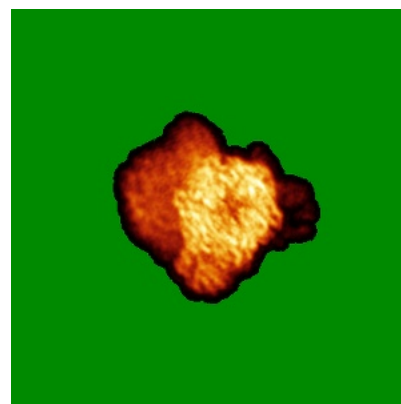
6.4.1 Primary map



X



Y

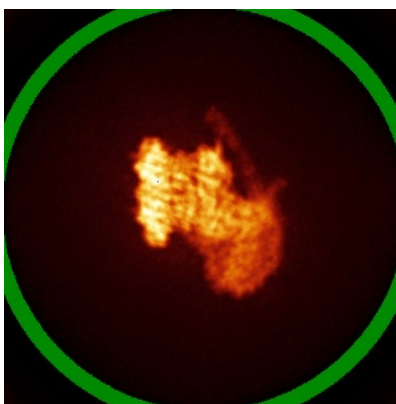


Z

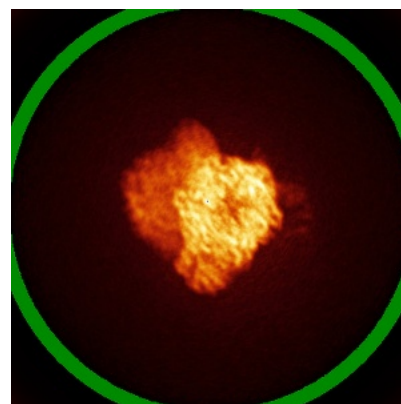
6.4.2 Raw map



X



Y



Z

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

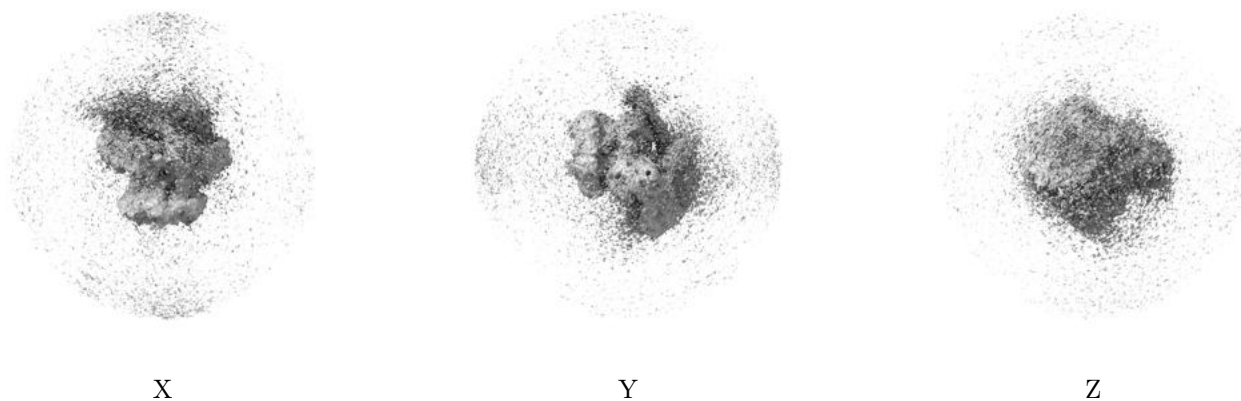
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00157. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

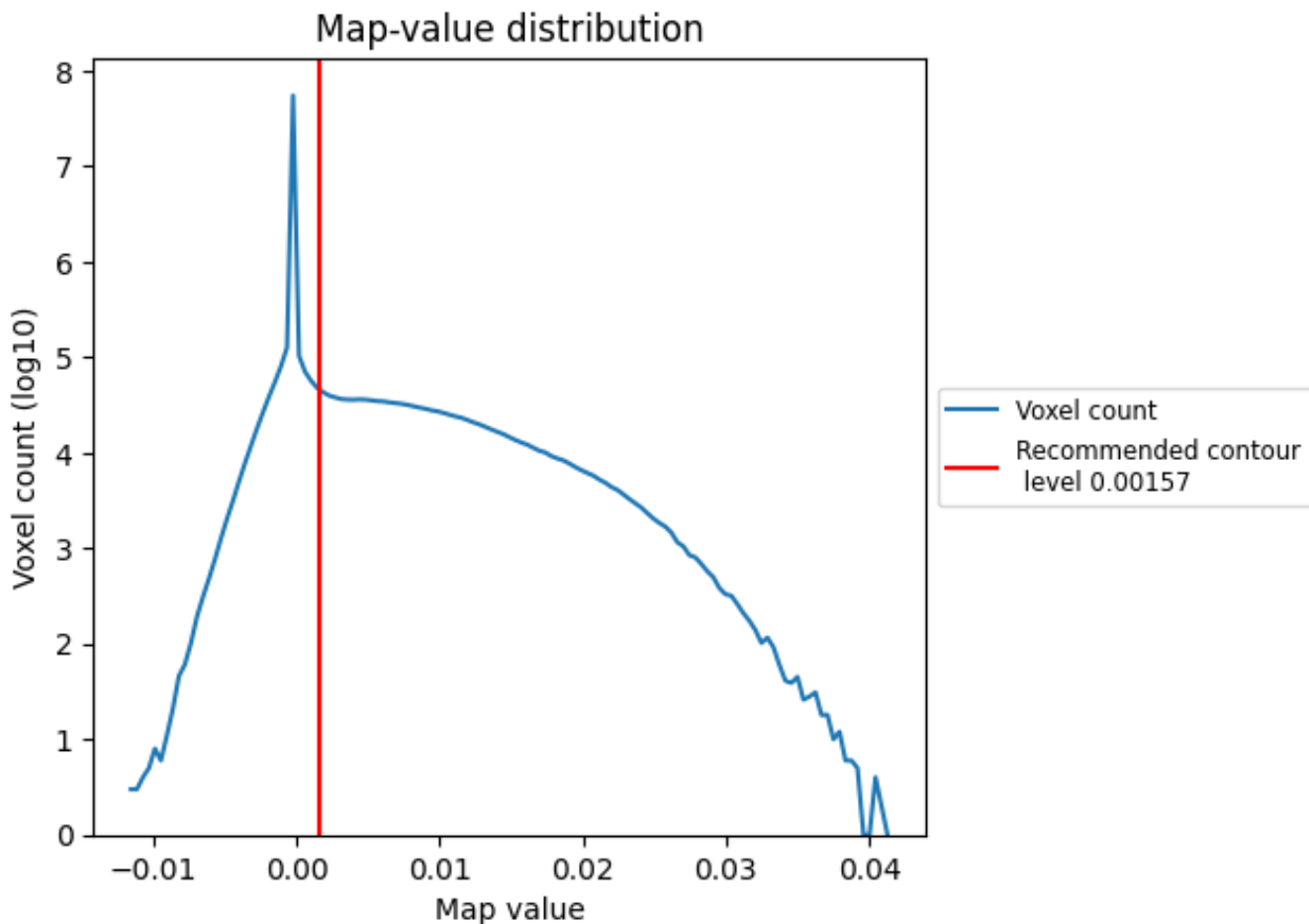
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

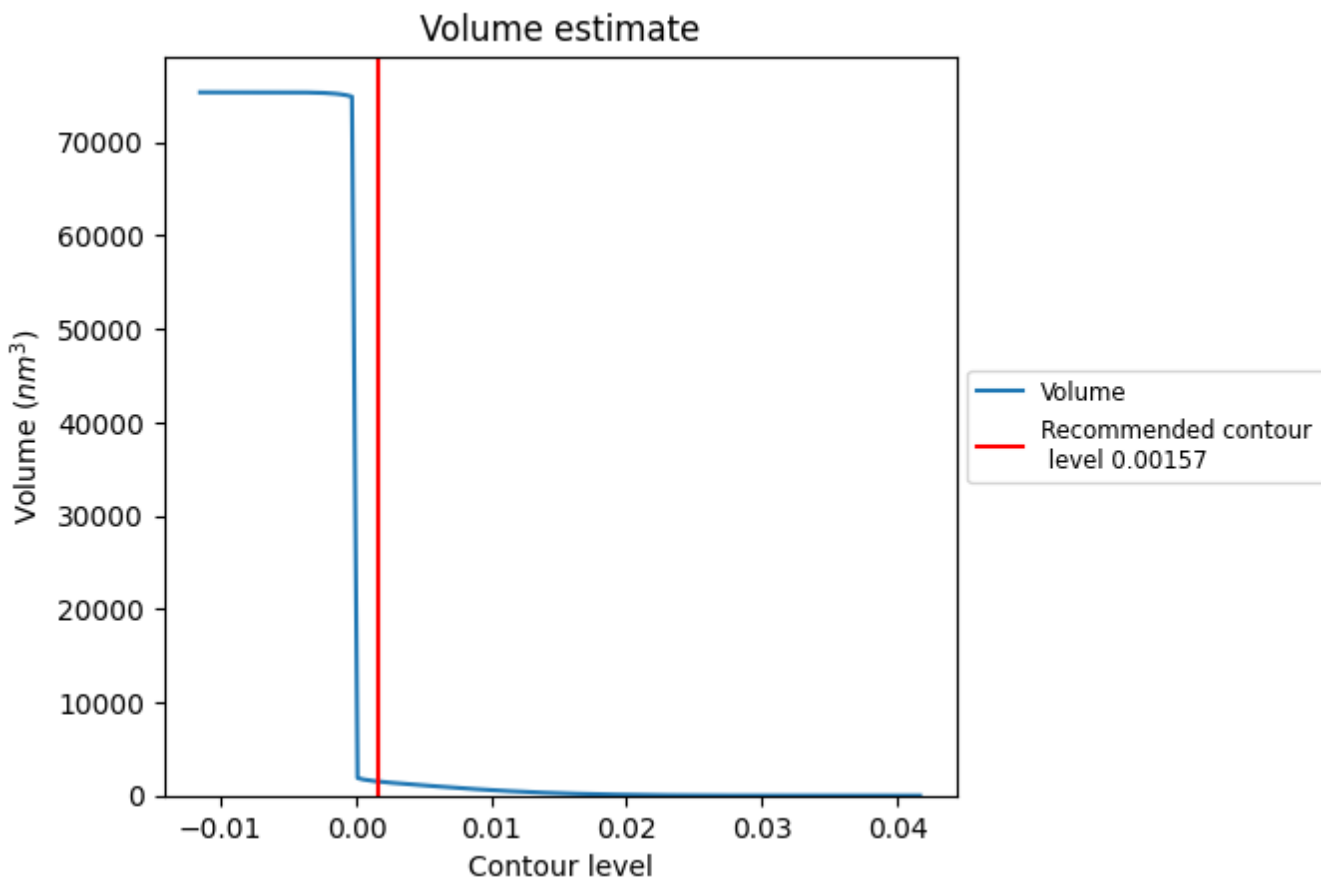
This section contains the results of statistical analysis of the map.

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.

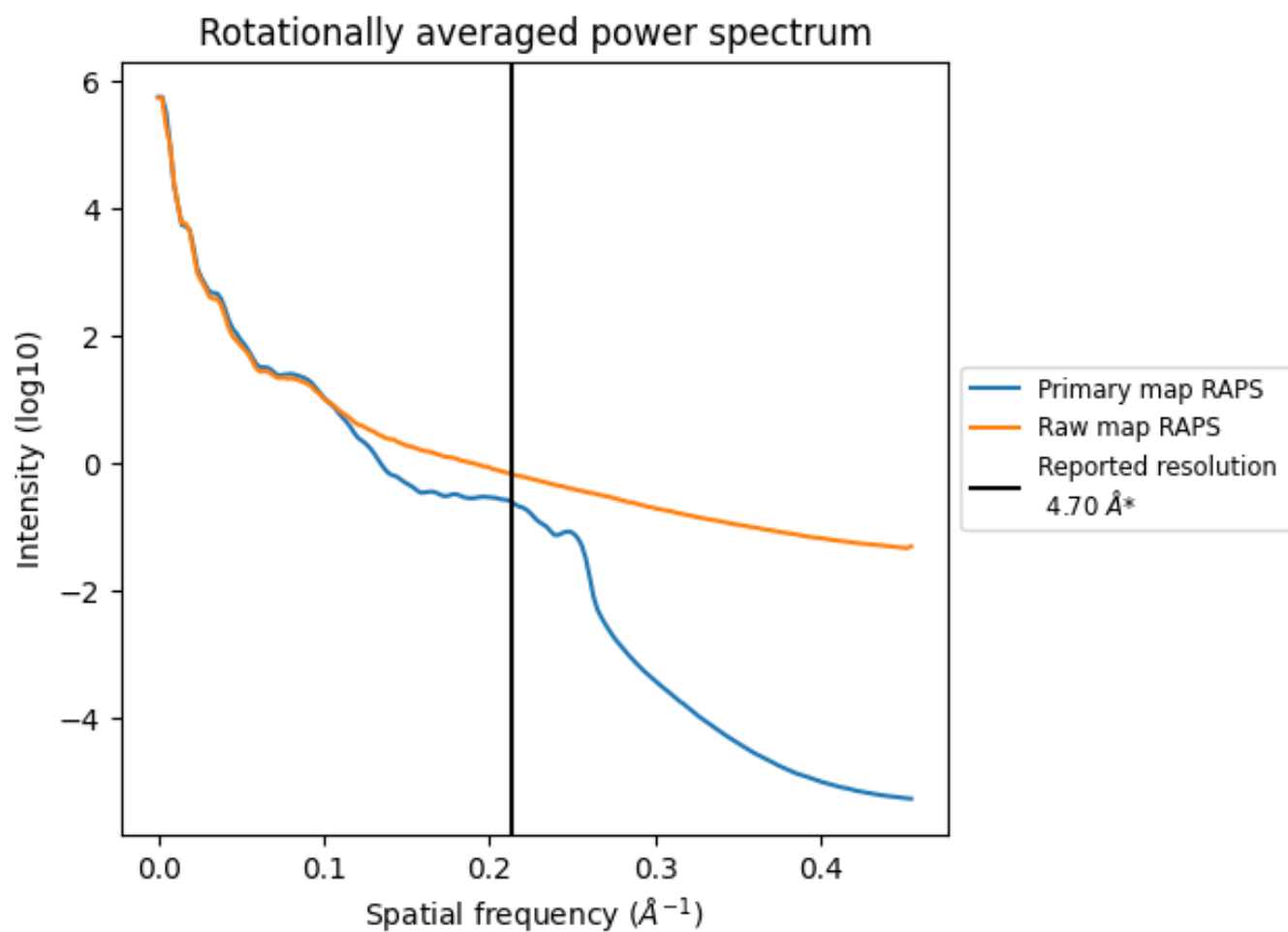
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1517 nm³; this corresponds to an approximate mass of 1370 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

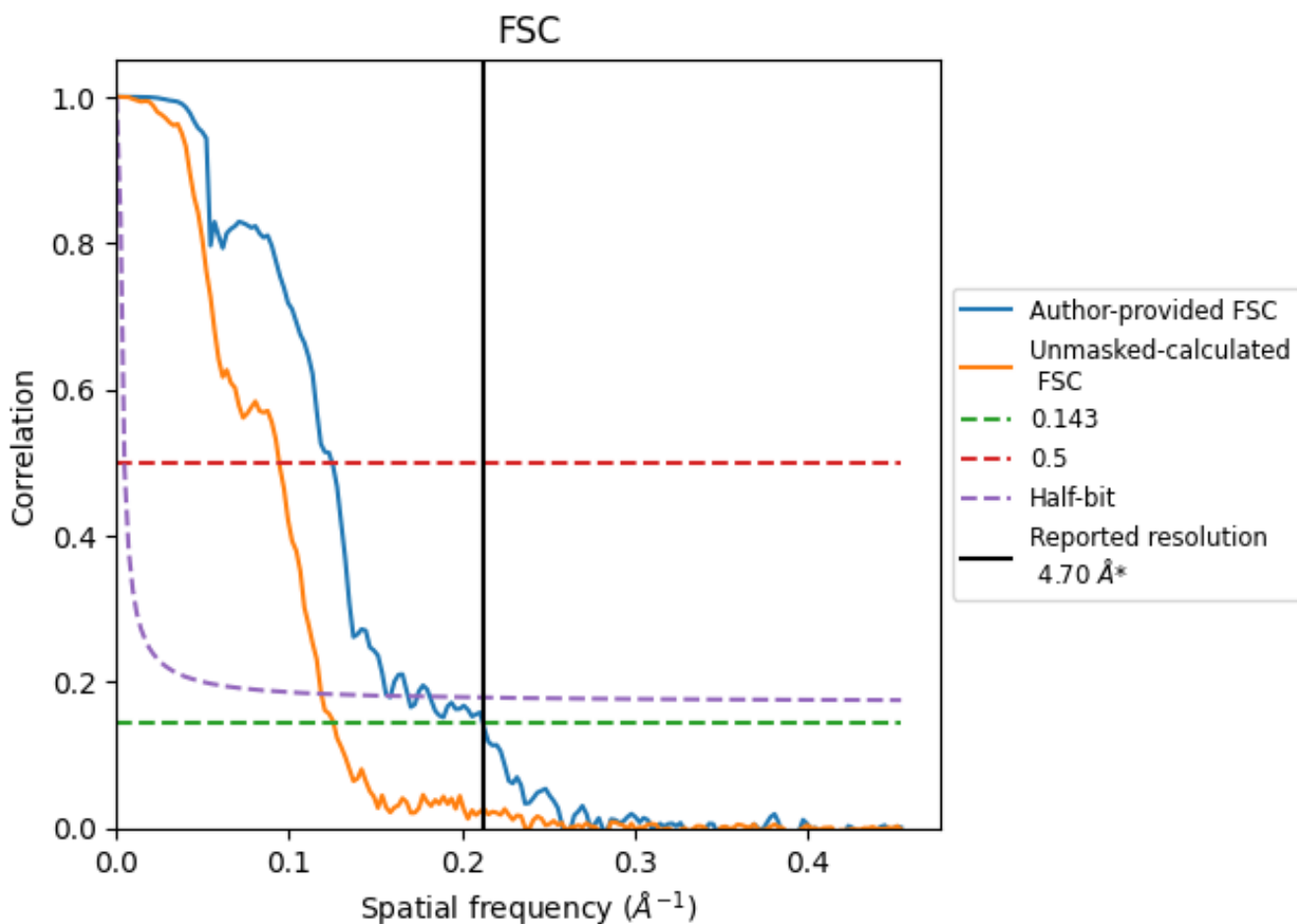


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 0.213 Å⁻¹

8.2 Resolution estimates [i](#)

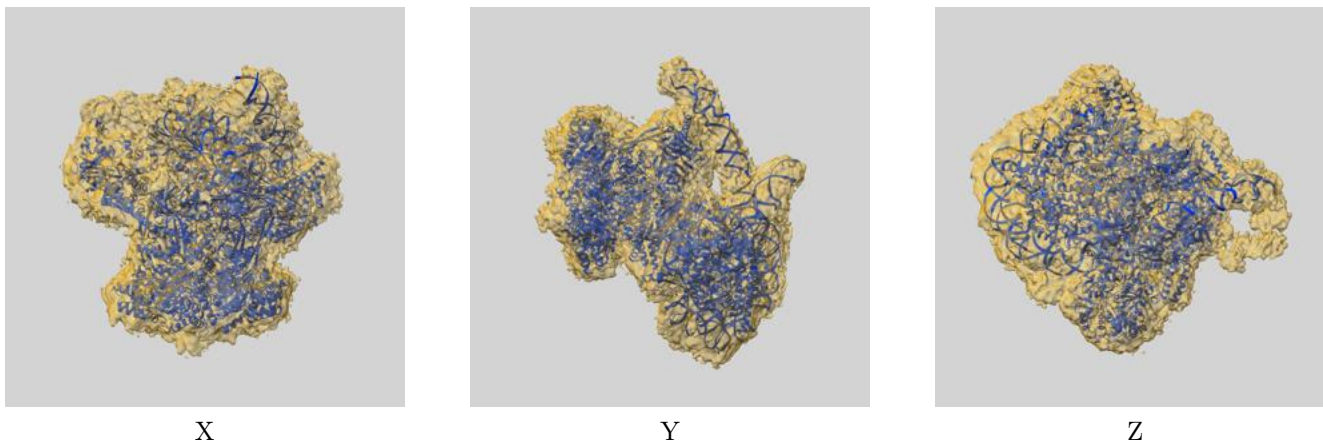
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.71	8.01	6.35
Unmasked-calculated*	7.95	10.60	8.42

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.95 differs from the reported value 4.7 by more than 10 %

9 Map-model fit [i](#)

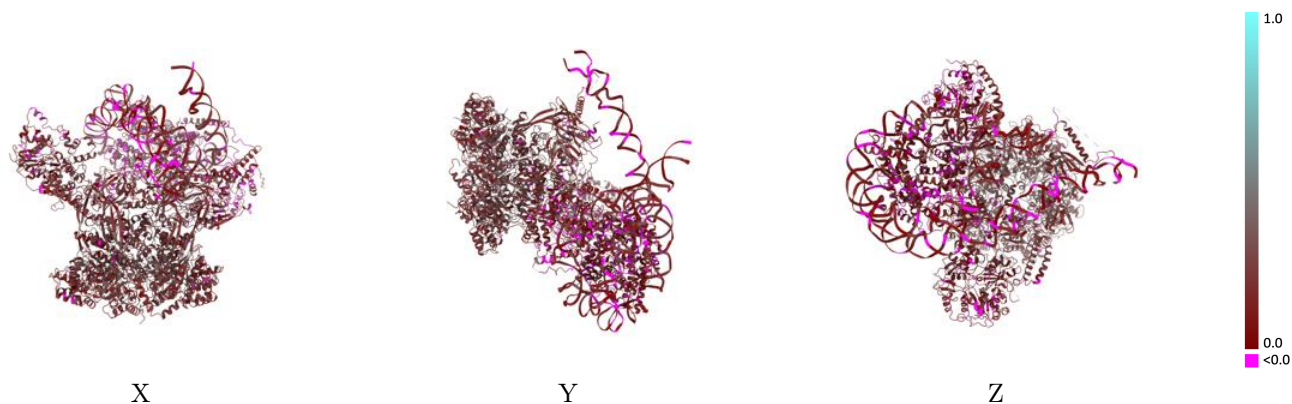
This section contains information regarding the fit between EMDB map EMD-18472 and PDB model 8QKV. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



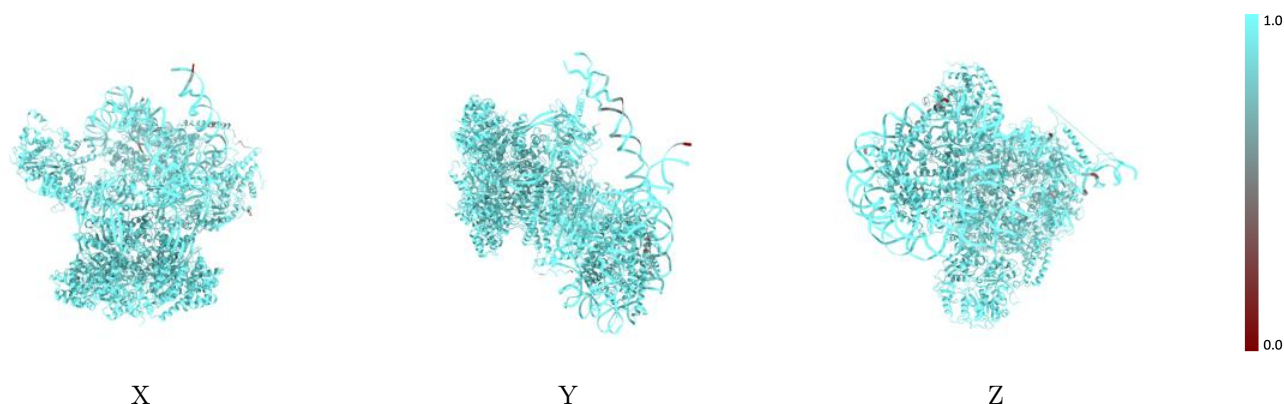
The images above show the 3D surface view of the map at the recommended contour level 0.00157 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



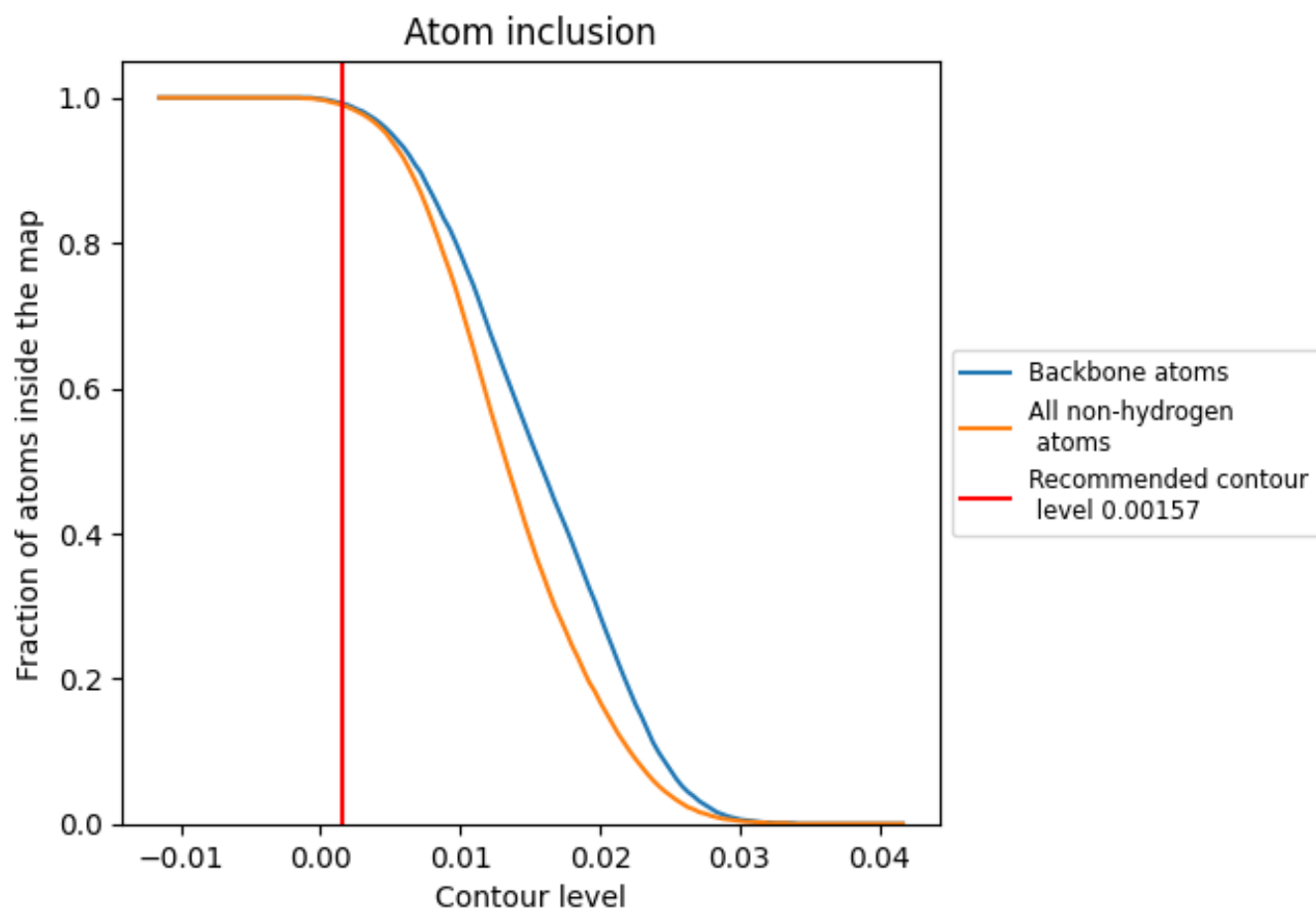
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00157).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.00157) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9900	 0.1850
A	 0.9870	 0.0990
B	 0.9970	 0.1270
C	 0.9980	 0.1380
D	 0.9790	 0.0630
E	 1.0000	 0.1340
F	 0.9890	 0.0960
G	 0.9900	 0.1180
H	 0.9970	 0.1260
I	 0.9720	 0.0980
J	 0.9720	 0.1160
M	 0.9910	 0.1810
R	 0.9960	 0.1810
S	 0.9940	 0.1710
T	 0.9930	 0.2280
U	 1.0000	 0.2460
V	 0.9990	 0.2470
W	 0.9990	 0.2450
X	 0.9990	 0.2430
Y	 0.9990	 0.2490
Z	 0.9340	 0.1360

