



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:00 PM UTC

PDB ID : 8YNY / pdb_00008yny
EMDB ID : EMD-39431
Title : Structure of Cas9-sgRNA ribonucleoprotein bound to nucleosome
Authors : Nagamura, R.; Kujirai, T.; Kusakizako, T.; Hirano, H.; Kurumizaka, H.; Nureki, O.
Deposited on : 2024-03-12
Resolution : 4.52 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

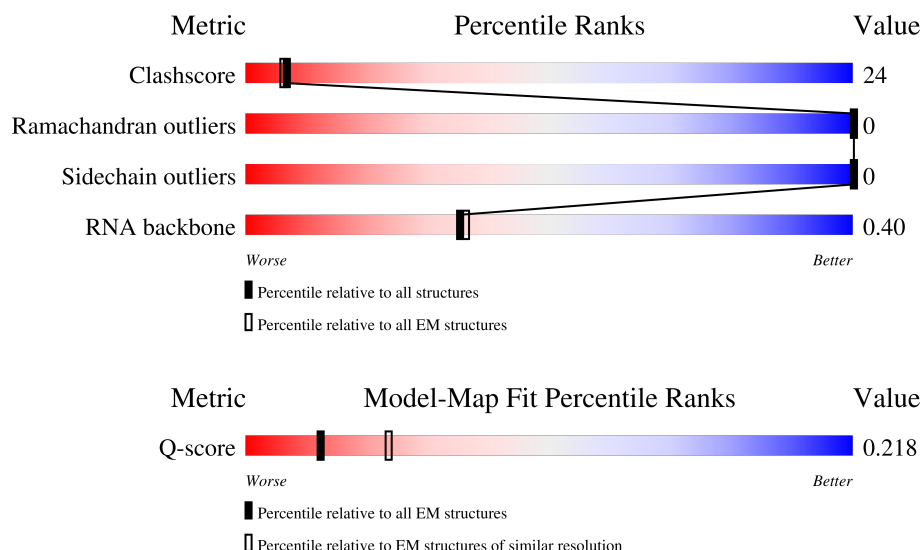
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.52 Å.

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



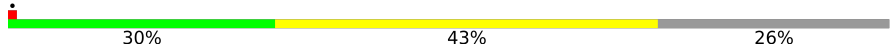
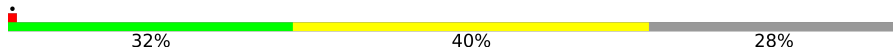
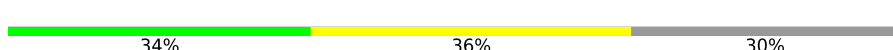
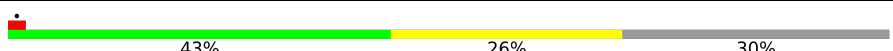
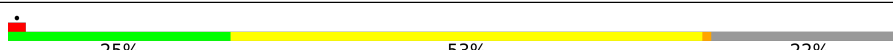
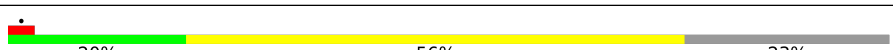
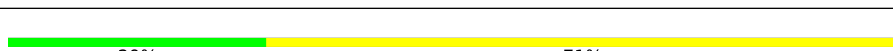
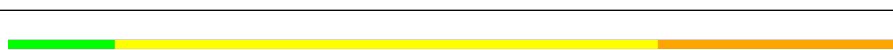
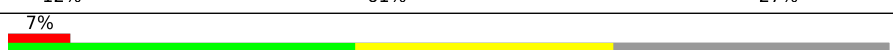
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2506 (4.02 - 5.02)

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	139	
1	E	139	
2	B	106	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	106	
3	C	133	
3	G	133	
4	D	129	
4	H	129	
5	I	175	
6	J	176	
7	K	17	
8	W	97	
9	X	1368	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21387 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 H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	91	Total	C	N	O	S	0	0
			743	468	141	130	4		
1	E	90	Total	C	N	O	S	0	0
			738	465	140	129	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P68431
A	-2	SER	-	expression tag	UNP P68431
A	-1	HIS	-	expression tag	UNP P68431
E	-3	GLY	-	expression tag	UNP P68431
E	-2	SER	-	expression tag	UNP P68431
E	-1	HIS	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	81	Total	C	N	O	S	0	0
			646	407	126	112	1		
2	F	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P62805
B	-2	SER	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
F	-3	GLY	-	expression tag	UNP P62805
F	-2	SER	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	96	Total	C	N	O	0	0
			743	466	146	131		
3	G	96	Total	C	N	O	0	0
			741	465	146	130		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP P04908
C	-2	SER	-	expression tag	UNP P04908
C	-1	HIS	-	expression tag	UNP P04908
G	-3	GLY	-	expression tag	UNP P04908
G	-2	SER	-	expression tag	UNP P04908
G	-1	HIS	-	expression tag	UNP P04908

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	90	Total	C	N	O	S	0	0
			699	441	123	133	2		
4	H	90	Total	C	N	O	S	0	0
			699	441	123	133	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP P06899
D	-5	SER	-	expression tag	UNP P06899
D	-4	HIS	-	expression tag	UNP P06899
H	-6	GLY	-	expression tag	UNP P06899
H	-5	SER	-	expression tag	UNP P06899
H	-4	HIS	-	expression tag	UNP P06899

- Molecule 5 is a DNA chain called DNA (175-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	137	Total	C	N	O	P	0	0
			2794	1324	512	821	137		

- Molecule 6 is a DNA chain called DNA (176-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	135	Total	C	N	O	P	0	0
			2783	1314	525	809	135		

- Molecule 7 is a DNA chain called DNA (17-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	17	Total	C	N	O	P	0	0
			351	166	65	103	17		

- Molecule 8 is a RNA chain called RNA (97-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	W	97	Total	C	N	O	P	0	0
			2072	927	376	672	97		

- Molecule 9 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	X	941	Total	C	N	O	S	0	0
			7759	4972	1352	1419	16		



N1308	K1222	L1144	GLY
I1309	G1223	V1145	GLU
I1310	N1224	V1146	THR
H1311	E1225	A1147	GLY
F1313	L1226		GLU
F1314		E1150	I1E
L1315	Y1232	K1151	W1073
L1316	V1233	G1152	D1074
L1317	N1234	K1153	D1075
L1318	F1235	S1154	
G1319	L1238	K1155	R1078
A1320	H1241	K1156	D1079
A1321	T1242	L1157	
A1322	GLU	K1161	V1083
A1323	LYS		R1084
F1324	LEU	V1085	V1085
K1325	LYS	I1166	L1087
Y1326	GLY	I1168	S1088
F1327	PER	M1169	M1089
S1328	SRP	E1170	P1090
	GLU	R1171	Q1091
	ASP		V1092
	ASN	F1174	M1093
I1331	E1253		I1094
D1332	Q1254	N1177	V1095
K1334			I1096
R1335	L1255	D1180	K1097
Y1336	Q1256	F1181	T1098
E1341	V1259	K1188	S1106
T1346	E1260		K1107
L1347	Q1261	K1191	E1108
I1348	H1262	S1192	S1109
S1351	Y1265	D1193	T1110
I1352	L1266	I1194	L1111
T1353		I1195	P1112
G1354	T1269	I1196	K1113
L1355	I1270	K1197	
E1356	E1271	L1198	A1121
E1357	T1272	P1199	
T1358	I1273	K1200	D1125
R1359		F1204	W1126
	F1276	E1205	D1127
	S1277	L1206	P1128
		E1207	K1129
LEU	V1280		K1130
GLY	I1281	N1208	G1131
GLY		G1209	G1132
ASP	M1286	R1210	G1133
	L1287	K1211	PHE
		R1212	D1135
	Y1294	M1213	S1136
		L1214	P1137
	K1300	A1215	T1138
	Q1305	S1216	V1139
	A1306		A1140
	E1307	E1219	Y1141
		L1220	S1142
		G1231	S1143

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.728	Depositor
Minimum map value	-0.205	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.517	Depositor
Map size ($\text{\AA}$)	304.5, 304.5, 304.5	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.5225, 1.5225, 1.5225	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.16	0/751	0.35	0/1006
1	E	0.17	0/746	0.35	0/998
2	B	0.18	0/653	0.30	0/873
2	F	0.20	0/626	0.38	0/837
3	C	0.20	0/752	0.37	0/1015
3	G	0.15	0/750	0.30	0/1011
4	D	0.29	0/710	0.42	0/957
4	H	0.17	0/710	0.36	0/957
5	I	0.34	0/3131	0.64	1/4826 (0.0%)
6	J	0.36	0/3125	0.64	1/4825 (0.0%)
7	K	0.25	0/393	0.42	0/605
8	W	0.21	0/2319	0.37	0/3612
9	X	0.13	0/7900	0.29	0/10605
All	All	0.23	0/22566	0.45	2/32127 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	17	DT	O3'-P-O5'	-5.69	95.46	104.00
6	J	20	DG	O3'-P-O5'	-5.29	96.07	104.00

There are no chirality outliers.

There are no planarity outliers.

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	743	0	782	57	0
1	E	738	0	777	66	0
2	B	646	0	687	52	0
2	F	619	0	659	56	0
3	C	743	0	784	97	0
3	G	741	0	785	46	0
4	D	699	0	714	70	0
4	H	699	0	714	48	0
5	I	2794	0	1535	113	0
6	J	2783	0	1512	119	0
7	K	351	0	192	19	0
8	W	2072	0	1045	117	0
9	X	7759	0	7901	320	0
All	All	21387	0	18087	957	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (957) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:CG2	3:G:81:ARG:HD3	1.48	1.40
9:X:5:TYR:CE1	9:X:22:THR:HG22	1.56	1.38
3:C:25:PHE:HE2	3:C:30:VAL:CG2	1.38	1.36
3:C:25:PHE:CE2	3:C:30:VAL:CG2	2.25	1.19
9:X:5:TYR:CE1	9:X:22:THR:CG2	2.30	1.14
1:E:118:THR:HG22	2:F:44:LYS:HB3	1.31	1.11
3:C:25:PHE:CE2	3:C:30:VAL:HG21	1.83	1.11
9:X:5:TYR:CE1	9:X:28:PRO:HG3	1.84	1.10
1:A:58:THR:HG21	3:G:81:ARG:HD3	1.22	1.10
3:C:25:PHE:HE2	3:C:30:VAL:HG21	0.94	1.09
3:C:88:ARG:CD	3:C:108:LEU:HB2	1.82	1.08
1:E:118:THR:HG21	2:F:45:ARG:HB3	1.32	1.04
1:A:58:THR:CG2	3:G:81:ARG:CD	2.37	1.03
3:C:88:ARG:HD2	3:C:108:LEU:HB2	1.03	1.03
3:C:25:PHE:CE2	3:C:30:VAL:HG23	1.97	0.98
9:X:5:TYR:HE1	9:X:28:PRO:HG3	1.19	0.96
1:A:58:THR:HG22	3:G:81:ARG:HD3	1.45	0.96
3:C:25:PHE:CD1	3:C:26:PRO:HD2	2.03	0.92
3:C:88:ARG:HD2	3:C:108:LEU:CB	1.98	0.92
9:X:5:TYR:CD1	9:X:22:THR:HG22	2.06	0.91
4:H:62:PHE:CZ	4:H:66:ILE:CD1	2.56	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:ILE:HG21	4:D:59:MET:HE1	1.54	0.88
9:X:5:TYR:HE1	9:X:22:THR:CG2	1.85	0.87
3:C:81:ARG:HB2	1:E:58:THR:HG21	1.57	0.86
9:X:5:TYR:CE1	9:X:28:PRO:CG	2.57	0.86
9:X:1308:ASN:ND2	9:X:1327:PHE:CE2	2.44	0.86
3:C:81:ARG:HD3	1:E:58:THR:CG2	2.08	0.83
4:H:62:PHE:CZ	4:H:66:ILE:HD11	2.15	0.82
3:G:28:GLY:HA3	6:J:-44:DG:H3'	1.61	0.81
3:C:88:ARG:HG2	3:C:108:LEU:HD12	1.61	0.81
1:E:118:THR:HG22	2:F:44:LYS:CB	2.12	0.79
4:H:62:PHE:CE2	4:H:66:ILE:HD11	2.18	0.79
3:C:88:ARG:CG	3:C:108:LEU:HD12	2.14	0.78
8:W:52:A:H1'	9:X:1169:MET:HE3	1.68	0.76
8:W:33:G:H3'	8:W:34:A:H5''	1.68	0.75
6:J:75:DT:H4'	9:X:1107:LYS:HD3	1.67	0.74
3:C:25:PHE:CD1	3:C:26:PRO:CD	2.71	0.74
1:E:116:ARG:NH1	6:J:-2:DC:OP2	2.21	0.73
3:C:25:PHE:CE1	3:C:26:PRO:HD2	2.23	0.73
3:C:16:THR:N	3:C:19:SER:HG	1.87	0.73
9:X:967:ARG:NE	9:X:972:PHE:O	2.22	0.72
3:C:88:ARG:HG2	3:C:108:LEU:CD1	2.19	0.72
9:X:162:ILE:HG12	9:X:444:LEU:HD12	1.72	0.72
4:H:62:PHE:CZ	4:H:66:ILE:HD12	2.25	0.71
2:F:75:HIS:NE2	4:H:90:GLU:HG2	2.06	0.71
9:X:469:SER:HB2	9:X:481:VAL:HG22	1.72	0.71
9:X:1206:LEU:HB2	9:X:1210:ARG:HB2	1.72	0.71
9:X:1308:ASN:ND2	9:X:1327:PHE:CD2	2.59	0.70
8:W:73:G:O2'	8:W:75:A:N7	2.24	0.70
9:X:1235:PHE:HE1	9:X:1259:VAL:HA	1.56	0.70
8:W:46:A:H2'	8:W:47:A:H8	1.57	0.70
9:X:1213:MET:HB2	9:X:1221:GLN:HB2	1.74	0.69
3:C:62:ILE:CG2	4:D:59:MET:HE1	2.22	0.69
3:G:84:GLN:OE1	3:G:88:ARG:NH1	2.25	0.69
5:I:5:DC:H2''	5:I:6:DA:C8	2.27	0.69
2:F:45:ARG:HE	5:I:89:DC:H5'	1.57	0.69
9:X:1308:ASN:ND2	9:X:1327:PHE:CZ	2.60	0.69
9:X:1323:ALA:HA	9:X:1331:ILE:O	1.93	0.69
1:E:102:GLY:O	1:E:131:ARG:NH2	2.26	0.68
3:C:25:PHE:CG	3:C:26:PRO:HD2	2.28	0.68
8:W:34:A:OP1	8:W:35:A:N6	2.25	0.68
9:X:9:LEU:O	9:X:990:ASN:ND2	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:TYR:HB3	4:D:75:SER:HB3	1.76	0.68
7:K:5:DG:H2'	7:K:6:DA:H8	1.60	0.67
8:W:69:A:H2'	8:W:70:C:C6	2.30	0.67
9:X:1235:PHE:HE2	9:X:1266:LEU:HB2	1.59	0.67
9:X:423:LEU:HD13	9:X:437:ARG:HG3	1.76	0.67
1:A:85:GLN:NE2	5:I:57:DG:OP1	2.25	0.67
2:B:48:GLY:HA2	2:B:51:TYR:HD2	1.59	0.67
3:G:51:LEU:HD13	4:H:70:ILE:HD13	1.77	0.67
6:J:3:DC:H2''	6:J:4:DG:C8	2.29	0.67
1:A:58:THR:HG21	3:G:81:ARG:CD	2.12	0.67
8:W:46:A:H2'	8:W:47:A:C8	2.30	0.67
9:X:925:ARG:HG2	9:X:927:ILE:HG22	1.77	0.67
8:W:33:G:N2	8:W:36:A:OP1	2.28	0.67
6:J:18:DG:H1'	6:J:19:DC:H5'	1.76	0.66
8:W:48:A:H2'	8:W:49:A:H8	1.60	0.66
3:C:17:ARG:HH21	3:C:28:GLY:HA2	1.59	0.66
5:I:12:DG:H1'	5:I:13:DA:H5'	1.77	0.66
4:D:95:VAL:HG13	4:D:99:LEU:HD12	1.78	0.65
1:A:126:LEU:HD11	1:E:109:LEU:HB3	1.77	0.65
3:C:76:THR:HG23	4:D:49:THR:HA	1.77	0.65
4:D:105:LYS:HA	4:D:108:VAL:HB	1.78	0.65
5:I:73:DC:H2''	5:I:74:DG:C8	2.32	0.65
9:X:393:LEU:HA	9:X:398:LEU:HD22	1.79	0.65
4:H:70:ILE:HD11	4:H:91:ILE:HG23	1.78	0.65
5:I:45:DT:H2''	5:I:46:DA:N7	2.12	0.65
8:W:70:C:H2'	8:W:71:U:C6	2.31	0.65
6:J:1:DC:H2''	6:J:2:DG:C8	2.31	0.65
7:K:7:DT:H5'	9:X:496:THR:HA	1.79	0.65
8:W:78:A:H2'	8:W:79:G:C8	2.33	0.65
1:E:83:ARG:HB2	2:F:80:THR:HG22	1.79	0.64
8:W:69:A:H2'	8:W:70:C:H6	1.61	0.64
6:J:64:DA:H2''	6:J:65:DT:H5'	1.78	0.64
8:W:3:C:H2'	8:W:4:G:C8	2.32	0.64
9:X:979:ASN:HD22	9:X:1225:GLU:HB3	1.63	0.64
9:X:1300:LYS:O	9:X:1305:GLN:NE2	2.25	0.64
3:C:25:PHE:CG	3:C:26:PRO:CD	2.81	0.64
6:J:-26:DC:H2''	6:J:-25:DC:C5	2.33	0.64
1:A:104:PHE:HE2	2:B:37:LEU:HB3	1.63	0.63
3:C:63:LEU:HD22	4:D:42:LEU:HD13	1.81	0.63
5:I:134:DT:H2''	5:I:135:DG:C8	2.33	0.63
6:J:37:DC:H2''	6:J:38:DG:C8	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:94:U:H2'	8:W:95:G:H8	1.62	0.63
6:J:-47:DC:H2''	6:J:-46:DT:C5	2.32	0.63
3:G:63:LEU:HD22	4:H:42:LEU:HD13	1.80	0.63
1:A:70:LEU:HD13	2:B:25:ASN:HB3	1.81	0.63
2:B:79:LYS:N	6:J:28:DA:OP1	2.32	0.62
9:X:627:GLU:O	9:X:655:ARG:NH1	2.32	0.62
9:X:1210:ARG:HG2	9:X:1280:VAL:HA	1.82	0.62
9:X:1204:PHE:HE2	9:X:1214:LEU:HB2	1.63	0.62
9:X:170:ILE:O	9:X:413:GLN:NE2	2.33	0.62
7:K:5:DG:H2'	7:K:6:DA:C8	2.35	0.62
9:X:558:LYS:HD2	9:X:586:ARG:HH12	1.65	0.62
8:W:10:U:H2'	8:W:11:A:C8	2.35	0.62
8:W:53:G:H2'	8:W:54:G:H8	1.65	0.62
9:X:138:LEU:HD21	9:X:153:LEU:HB3	1.81	0.62
8:W:29:G:H2'	8:W:30:C:C6	2.35	0.61
2:B:24:ASP:O	2:B:28:GLY:N	2.33	0.61
1:A:62:ILE:HD13	2:B:33:ALA:HB1	1.83	0.61
1:A:113:HIS:NE2	1:E:123:ASP:OD1	2.32	0.61
8:W:68:A:C8	9:X:1351:SER:HA	2.36	0.61
4:H:102:GLU:O	4:H:106:HIS:ND1	2.31	0.61
9:X:46:ASN:ND2	9:X:1089:MET:SD	2.73	0.61
9:X:324:ARG:HH11	9:X:400:ARG:HD3	1.66	0.61
3:G:88:ARG:HD3	3:G:108:LEU:HD12	1.82	0.61
1:A:66:PRO:HD3	6:J:17:DA:H5''	1.83	0.61
4:D:104:ALA:O	4:D:108:VAL:N	2.28	0.61
2:F:47:SER:HB3	2:F:50:ILE:HG12	1.81	0.61
9:X:999:LYS:HD2	9:X:1073:VAL:HA	1.83	0.61
9:X:557:ARG:HD3	9:X:595:HIS:HD2	1.65	0.61
1:A:72:ARG:O	1:A:76:GLN:HG2	2.00	0.60
3:C:108:LEU:O	1:E:55:GLN:NE2	2.34	0.60
1:E:116:ARG:NE	1:E:120:MET:SD	2.75	0.60
6:J:50:DG:H2''	6:J:51:DG:OP2	2.01	0.60
8:W:8:C:O2'	8:W:9:C:OP1	2.19	0.60
1:E:128:ARG:HH11	2:F:57:VAL:HG22	1.66	0.60
8:W:13:C:H2'	8:W:14:G:H8	1.67	0.60
9:X:48:ILE:O	9:X:1093:ASN:ND2	2.35	0.60
2:B:24:ASP:HB3	2:B:27:GLN:HB2	1.81	0.60
1:E:121:PRO:HB3	2:F:53:GLU:HG2	1.83	0.60
7:K:6:DA:H2'	7:K:7:DT:C6	2.36	0.60
9:X:28:PRO:HB2	9:X:47:LEU:HD12	1.82	0.60
9:X:1211:LYS:N	9:X:1224:ASN:OD1	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:-54:DC:H2''	6:J:-53:DA:C8	2.37	0.60
9:X:662:LEU:HB3	9:X:666:LEU:HD23	1.83	0.60
3:C:34:LEU:HD13	3:C:43:VAL:HG21	1.84	0.60
8:W:46:A:OP1	9:X:160:HIS:NE2	2.28	0.60
9:X:8:GLY:HA3	9:X:991:ALA:HB2	1.82	0.60
4:D:116:THR:O	4:D:120:SER:N	2.32	0.59
2:F:45:ARG:NE	5:I:89:DC:H5'	2.17	0.59
3:G:26:PRO:HG2	3:G:29:ARG:HB3	1.82	0.59
5:I:82:DT:H2''	5:I:83:DG:C8	2.38	0.59
1:A:72:ARG:HA	1:A:84:PHE:CZ	2.37	0.59
1:E:100:LEU:HD21	2:F:58:LEU:HB3	1.85	0.59
9:X:1216:SER:HB3	9:X:1219:GLU:HB2	1.83	0.59
1:A:79:LYS:NZ	1:A:80:THR:O	2.24	0.59
1:A:118:THR:HA	2:B:45:ARG:HB2	1.84	0.59
6:J:31:DT:H2''	6:J:32:DG:C8	2.38	0.59
8:W:48:A:H2'	8:W:49:A:C8	2.37	0.59
1:A:121:PRO:HB3	2:B:53:GLU:HG3	1.84	0.59
4:D:70:ILE:HD11	4:D:95:VAL:HG22	1.83	0.58
3:G:64:GLU:OE2	4:H:46:HIS:NE2	2.35	0.58
9:X:1086:VAL:HG13	9:X:1089:MET:HE2	1.84	0.58
8:W:42:A:O2'	8:W:43:G:OP1	2.20	0.58
8:W:60:C:H4'	9:X:456:ALA:HB2	1.85	0.58
8:W:16:G:OP1	9:X:74:ARG:NH2	2.21	0.58
4:D:83:ARG:NH2	5:I:48:DA:OP1	2.36	0.58
5:I:20:DG:H3'	9:X:1153:LYS:NZ	2.18	0.58
3:C:42:ARG:HG2	6:J:38:DG:H4'	1.85	0.58
6:J:30:DC:H2'	6:J:31:DT:H71	1.84	0.58
9:X:354:GLN:HB2	9:X:361:GLY:HA2	1.85	0.58
3:C:81:ARG:HD3	1:E:58:THR:HG22	1.83	0.58
5:I:103:DC:H2''	5:I:104:DA:C8	2.38	0.58
8:W:77:A:H2'	8:W:78:A:C8	2.38	0.58
8:W:88:A:N1	9:X:46:ASN:ND2	2.45	0.58
9:X:177:ASP:OD1	9:X:310:THR:OG1	2.22	0.58
9:X:749:LYS:HG2	9:X:753:ARG:HH22	1.68	0.58
9:X:979:ASN:O	9:X:982:HIS:ND1	2.31	0.58
8:W:15:C:H2'	8:W:16:G:H8	1.67	0.58
9:X:136:TYR:CD2	9:X:321:MET:HG2	2.38	0.58
4:D:103:LEU:O	4:D:106:HIS:HB2	2.03	0.57
8:W:81:G:N2	9:X:1357:GLU:O	2.37	0.57
9:X:1121:ALA:HB2	9:X:1128:PRO:HD3	1.86	0.57
6:J:51:DG:H2''	6:J:52:DC:OP2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:10:U:H2'	8:W:11:A:H8	1.67	0.57
8:W:23:U:H2'	8:W:24:U:H6	1.69	0.57
9:X:1209:GLY:O	9:X:1224:ASN:ND2	2.34	0.57
1:E:118:THR:CG2	2:F:45:ARG:HB3	2.21	0.57
2:F:46:ILE:N	5:I:89:DC:OP1	2.23	0.57
9:X:31:LYS:HG2	9:X:44:LYS:HB2	1.85	0.57
9:X:491:PHE:HD1	9:X:494:ARG:HH12	1.52	0.57
3:C:87:ILE:HD12	3:C:102:ILE:HD11	1.86	0.57
4:D:105:LYS:O	4:D:109:SER:N	2.29	0.57
4:H:62:PHE:CE1	4:H:66:ILE:HD12	2.39	0.57
6:J:-56:DG:H1'	6:J:-55:DA:C8	2.40	0.57
6:J:-7:DG:H2''	6:J:-6:DG:C8	2.40	0.57
9:X:20:VAL:O	9:X:27:VAL:HG23	2.05	0.57
1:A:121:PRO:HG2	2:B:49:LEU:HG	1.86	0.57
3:C:83:LEU:HD11	4:D:59:MET:HG2	1.86	0.57
6:J:-47:DC:H2''	6:J:-46:DT:C4	2.40	0.57
9:X:1095:VAL:HG21	9:X:1354:GLY:HA3	1.87	0.57
2:F:35:ARG:O	2:F:39:ARG:HG2	2.04	0.56
9:X:489:GLN:HG3	9:X:625:LEU:HD21	1.87	0.56
1:A:126:LEU:HB2	1:E:113:HIS:CE1	2.41	0.56
3:G:79:ILE:HG12	3:G:82:HIS:CG	2.40	0.56
9:X:21:ILE:HD11	9:X:995:THR:HG21	1.88	0.56
9:X:108:GLU:HA	9:X:111:LYS:HB2	1.87	0.56
1:A:61:LEU:HB2	2:B:37:LEU:HD22	1.88	0.56
1:E:91:ALA:HA	2:F:100:PHE:CE2	2.40	0.56
5:I:61:DC:H2''	5:I:62:DG:C8	2.41	0.56
2:B:39:ARG:NH2	2:B:44:LYS:O	2.39	0.56
9:X:586:ARG:HE	9:X:587:PHE:H	1.52	0.56
3:G:78:ILE:N	4:H:50:GLY:O	2.39	0.56
5:I:10:DC:H42	6:J:70:DA:H61	1.53	0.56
5:I:96:DT:H2''	5:I:97:DA:C8	2.41	0.56
5:I:100:DC:H2''	5:I:101:DG:C8	2.40	0.56
9:X:468:LYS:N	9:X:481:VAL:O	2.34	0.56
3:C:35:ARG:NH2	6:J:39:DA:OP1	2.38	0.56
3:C:34:LEU:HD21	3:C:48:PRO:HB3	1.88	0.56
3:C:88:ARG:CD	3:C:108:LEU:HD12	2.35	0.56
9:X:38:THR:HG21	9:X:1359:ARG:HG3	1.88	0.56
1:A:63:ARG:HH12	2:B:30:THR:HG21	1.70	0.56
3:G:31:HIS:CE1	3:G:35:ARG:HE	2.24	0.56
6:J:-39:DT:H2''	6:J:-38:DA:C8	2.41	0.56
9:X:464:TRP:NE1	9:X:491:PHE:HB2	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:PRO:HB3	4:D:58:ILE:HD12	1.88	0.56
2:F:62:LEU:O	2:F:66:ILE:HG22	2.06	0.56
5:I:116:DC:H2''	5:I:117:DC:C5	2.41	0.56
9:X:150:ASP:HB3	9:X:153:LEU:HG	1.87	0.56
9:X:90:MET:SD	9:X:95:ASP:HA	2.46	0.55
8:W:31:U:H3'	8:W:32:A:H8	1.72	0.55
9:X:954:LYS:HZ2	9:X:998:ILE:HD12	1.71	0.55
3:C:65:LEU:HB3	3:C:86:ALA:HB1	1.87	0.55
7:K:6:DA:H2'	7:K:7:DT:H6	1.71	0.55
9:X:97:PHE:HE1	9:X:118:ILE:HA	1.72	0.55
3:C:83:LEU:CD1	4:D:59:MET:SD	2.94	0.55
5:I:129:DG:H2''	5:I:130:DC:C5	2.41	0.55
9:X:508:LEU:HD21	9:X:664:ARG:HG3	1.88	0.55
9:X:756:PRO:HG2	9:X:953:VAL:HG11	1.88	0.55
6:J:-17:DT:H2'	6:J:-16:DT:C6	2.42	0.55
6:J:26:DA:H2''	6:J:27:DG:C8	2.40	0.55
9:X:343:LEU:HD13	9:X:383:MET:HG2	1.88	0.55
4:D:40:LYS:O	4:D:44:GLN:HG2	2.06	0.55
3:G:27:VAL:HG13	3:G:48:PRO:HB2	1.88	0.55
9:X:1262:HIS:HB3	9:X:1265:TYR:HB2	1.88	0.55
1:A:126:LEU:HD22	1:E:113:HIS:CG	2.42	0.55
1:E:121:PRO:HG2	2:F:49:LEU:HD23	1.88	0.55
9:X:342:GLN:HB2	9:X:383:MET:HE3	1.89	0.55
9:X:372:PHE:O	9:X:376:ILE:HG12	2.07	0.55
3:C:26:PRO:HG3	4:D:37:TYR:CZ	2.42	0.55
1:E:111:ALA:HA	1:E:116:ARG:HB3	1.89	0.55
9:X:494:ARG:O	9:X:496:THR:N	2.40	0.55
2:F:56:GLY:HA2	2:F:59:LYS:HE3	1.88	0.55
4:H:95:VAL:HG13	4:H:99:LEU:HD23	1.89	0.55
4:H:89:ARG:O	4:H:92:GLN:HG3	2.07	0.55
7:K:4:DC:H2'	7:K:5:DG:H8	1.72	0.55
3:G:78:ILE:HB	4:H:51:ILE:HA	1.89	0.54
5:I:108:DG:O6	6:J:-28:DC:N4	2.39	0.54
2:B:29:ILE:O	2:B:55:ARG:NH2	2.38	0.54
9:X:87:SER:HA	9:X:90:MET:HB3	1.89	0.54
9:X:1222:LYS:NZ	9:X:1315:LEU:O	2.39	0.54
9:X:1346:THR:HG21	9:X:1359:ARG:HH21	1.72	0.54
9:X:362:TYR:HA	9:X:367:ALA:HB3	1.89	0.54
1:A:122:LYS:O	1:E:113:HIS:NE2	2.41	0.54
3:C:18:SER:OG	3:C:23:LEU:O	2.25	0.54
3:C:71:ARG:HH21	4:D:46:HIS:CD2	2.26	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:ARG:NH2	1:E:133:GLU:OE1	2.39	0.54
8:W:94:U:H2'	8:W:95:G:C8	2.42	0.54
9:X:1157:LEU:HD21	9:X:1188:LYS:HD2	1.89	0.54
3:C:88:ARG:CD	3:C:108:LEU:CD1	2.85	0.54
9:X:1145:VAL:O	9:X:1161:LYS:HA	2.07	0.54
5:I:75:DT:H2''	5:I:76:DA:C8	2.43	0.54
3:C:18:SER:O	3:C:22:GLY:N	2.40	0.54
3:C:62:ILE:HG21	4:D:59:MET:CE	2.34	0.54
4:D:90:GLU:N	4:D:90:GLU:OE1	2.39	0.54
7:K:15:DG:N3	7:K:15:DG:H2'	2.22	0.54
9:X:628:ASP:HB3	9:X:631:MET:HB2	1.89	0.54
9:X:1348:ILE:HG12	9:X:1359:ARG:HB3	1.89	0.54
9:X:756:PRO:O	9:X:953:VAL:HG22	2.08	0.54
1:A:118:THR:HB	5:I:78:DG:H5''	1.89	0.54
6:J:24:DC:H2''	6:J:25:DT:C6	2.43	0.54
3:C:78:ILE:HG23	3:C:82:HIS:HB2	1.89	0.54
3:C:102:ILE:HG23	4:D:58:ILE:HD13	1.89	0.54
5:I:106:DG:H2''	5:I:107:DG:N7	2.23	0.53
9:X:1256:GLN:HE21	9:X:1260:GLU:HG3	1.73	0.53
5:I:67:DA:H1'	5:I:68:DA:H5'	1.89	0.53
8:W:5:G:H2'	8:W:6:A:H8	1.73	0.53
9:X:140:LYS:HA	9:X:143:VAL:HG12	1.89	0.53
2:F:66:ILE:HD12	2:F:69:ALA:HB3	1.91	0.53
3:G:43:VAL:HG23	4:H:86:ILE:HB	1.91	0.53
1:E:63:ARG:NH2	6:J:-13:DA:H5''	2.23	0.53
2:B:92:ARG:HG2	4:D:97:LEU:HD11	1.91	0.53
8:W:6:A:H2'	8:W:7:C:C6	2.44	0.53
8:W:14:G:N7	9:X:63:ARG:NH1	2.55	0.53
8:W:22:U:H2'	8:W:23:U:C6	2.43	0.53
8:W:53:G:H2'	8:W:54:G:C8	2.43	0.53
3:C:84:GLN:HA	3:C:102:ILE:HD12	1.89	0.53
2:F:75:HIS:NE2	4:H:90:GLU:CG	2.71	0.53
5:I:8:DG:O6	9:X:1335:ARG:NH1	2.39	0.53
8:W:13:C:H2'	8:W:14:G:C8	2.43	0.53
3:C:29:ARG:HH21	4:D:32:GLU:HG2	1.74	0.53
8:W:5:G:H2'	8:W:6:A:C8	2.43	0.53
9:X:133:PRO:HG2	9:X:137:HIS:CE1	2.44	0.53
8:W:15:C:H2'	8:W:16:G:C8	2.44	0.53
9:X:413:GLN:OE1	9:X:413:GLN:N	2.38	0.53
4:H:77:LEU:CD2	4:H:90:GLU:HG2	2.39	0.53
6:J:15:DT:H2''	6:J:16:DA:C5	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:49:GLY:HA3	9:X:1093:ASN:HB2	1.91	0.53
9:X:523:GLU:HG2	9:X:587:PHE:HD1	1.74	0.53
9:X:1177:ASN:ND2	9:X:1180:ASP:OD2	2.41	0.53
9:X:1310:ILE:HA	9:X:1313:PHE:CD2	2.44	0.53
6:J:-19:DG:H2''	6:J:-18:DG:C8	2.43	0.53
8:W:70:C:H2'	8:W:71:U:H6	1.74	0.53
9:X:373:TYR:HE2	9:X:396:GLU:HB2	1.74	0.53
8:W:21:G:H2'	8:W:22:U:H6	1.74	0.52
1:E:62:ILE:HG12	2:F:29:ILE:HD12	1.90	0.52
3:C:73:ASN:HD22	3:C:82:HIS:CD2	2.27	0.52
3:C:100:VAL:HA	2:F:96:THR:HG23	1.91	0.52
5:I:119:DT:H2''	5:I:120:DA:C8	2.44	0.52
8:W:4:G:H2'	8:W:5:G:H8	1.74	0.52
9:X:5:TYR:O	9:X:757:GLU:N	2.39	0.52
9:X:1198:LEU:HB3	9:X:1214:LEU:HD21	1.91	0.52
5:I:53:DT:H2''	5:I:54:DC:C6	2.44	0.52
5:I:109:DG:H2''	5:I:110:DA:H8	1.73	0.52
9:X:497:ASN:OD1	9:X:498:PHE:N	2.43	0.52
6:J:-37:DG:H2''	6:J:-36:DG:N7	2.25	0.52
9:X:1125:ASP:OD1	9:X:1125:ASP:N	2.35	0.52
6:J:-15:DA:H2''	6:J:-14:DA:C8	2.45	0.52
9:X:1235:PHE:CE2	9:X:1266:LEU:HB2	2.42	0.52
1:A:68:GLN:OE1	1:A:72:ARG:NE	2.42	0.52
1:A:69:ARG:NH1	6:J:17:DA:OP2	2.36	0.52
3:G:81:ARG:NH1	3:G:85:LEU:HD11	2.24	0.52
3:G:87:ILE:HD13	3:G:97:LEU:HD12	1.92	0.52
3:C:87:ILE:HD13	3:C:97:LEU:HD12	1.92	0.52
3:G:39:TYR:HB3	4:H:75:SER:HB2	1.92	0.51
9:X:410:ILE:HG23	9:X:414:ILE:HD11	1.92	0.51
5:I:39:DT:C2	5:I:40:DG:N7	2.78	0.51
6:J:-38:DA:H2''	6:J:-37:DG:C8	2.46	0.51
6:J:67:DC:H4'	6:J:68:DT:OP1	2.09	0.51
3:G:81:ARG:HG3	3:G:105:GLY:O	2.10	0.51
5:I:44:DG:H4'	5:I:45:DT:H5'	1.92	0.51
6:J:-16:DT:H2''	6:J:-15:DA:N7	2.25	0.51
4:D:104:ALA:O	4:D:107:ALA:HB3	2.10	0.51
3:G:18:SER:O	3:G:23:LEU:N	2.33	0.51
5:I:65:DT:H2''	5:I:66:DA:C5	2.45	0.51
8:W:4:G:H2'	8:W:5:G:C8	2.45	0.51
8:W:18:G:OP1	9:X:165:ARG:NE	2.22	0.51
9:X:128:TYR:HE1	9:X:138:LEU:HD22	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:751:MET:O	9:X:754:HIS:ND1	2.40	0.51
2:B:91:LYS:NZ	2:B:96:THR:OG1	2.44	0.51
5:I:127:DA:H2''	5:I:128:DG:N7	2.26	0.51
9:X:743:VAL:O	9:X:747:LEU:HG	2.11	0.51
3:C:25:PHE:HD2	3:C:52:ALA:CB	2.24	0.51
1:E:116:ARG:HH12	6:J:-3:DA:H3'	1.74	0.51
5:I:14:DG:H1'	5:I:15:DA:N7	2.26	0.51
8:W:95:G:H2'	8:W:96:C:C6	2.45	0.51
1:A:58:THR:HG23	3:G:81:ARG:CD	2.37	0.51
3:G:37:GLY:HA3	3:G:39:TYR:CE2	2.46	0.51
9:X:25:TYR:OH	9:X:1073:VAL:O	2.28	0.51
9:X:404:THR:H	9:X:407:ASN:ND2	2.09	0.51
2:B:92:ARG:NH2	4:D:98:LEU:HD13	2.26	0.51
6:J:-6:DG:H2''	6:J:-5:DG:C8	2.46	0.51
2:B:47:SER:HB3	2:B:50:ILE:HD13	1.92	0.50
7:K:17:DT:H4'	9:X:698:HIS:CD2	2.47	0.50
9:X:33:LYS:HE2	9:X:41:HIS:CD2	2.45	0.50
2:B:35:ARG:HE	2:B:51:TYR:HH	1.57	0.50
1:E:63:ARG:HD2	5:I:98:DA:H4'	1.94	0.50
3:C:35:ARG:HH22	6:J:39:DA:H3'	1.76	0.50
1:A:58:THR:HG22	3:G:81:ARG:CD	2.23	0.50
1:E:117:VAL:HB	6:J:-3:DA:OP2	2.12	0.50
9:X:54:ASP:OD1	9:X:54:ASP:N	2.45	0.50
4:D:117:LYS:O	4:D:120:SER:HB2	2.12	0.50
7:K:6:DA:H5''	9:X:659:TRP:HE1	1.77	0.50
4:D:84:SER:H	5:I:47:DG:P	2.35	0.50
2:F:39:ARG:NH1	2:F:44:LYS:O	2.43	0.50
4:H:36:ILE:HD13	5:I:129:DG:H3'	1.93	0.50
8:W:58:G:C6	8:W:60:C:C4	3.00	0.50
1:A:47:ALA:O	1:A:51:ILE:HG12	2.11	0.50
5:I:97:DA:H1'	5:I:98:DA:C8	2.47	0.50
6:J:5:DT:H2''	6:J:6:DA:C8	2.47	0.50
9:X:395:ARG:O	9:X:396:GLU:HG2	2.12	0.50
9:X:971:GLN:HA	9:X:973:TYR:CE2	2.46	0.50
3:C:79:ILE:HG13	3:C:80:PRO:HD2	1.94	0.50
9:X:449:PRO:HB2	9:X:452:VAL:HG23	1.94	0.50
1:A:126:LEU:HB2	1:E:113:HIS:NE2	2.28	0.49
3:C:32:ARG:HE	5:I:37:DA:P	2.35	0.49
8:W:83:C:OP1	9:X:30:LYS:NZ	2.38	0.49
9:X:82:LEU:HD13	9:X:162:ILE:HD12	1.92	0.49
2:B:75:HIS:HE1	4:D:77:LEU:HB3	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:47:A:C6	8:W:48:A:C6	3.00	0.49
9:X:421:ALA:O	9:X:425:ARG:HG2	2.11	0.49
3:C:88:ARG:CG	3:C:108:LEU:CD1	2.86	0.49
5:I:90:DG:C5	5:I:91:DC:C4	3.00	0.49
6:J:51:DG:OP2	6:J:51:DG:H2'	2.12	0.49
9:X:593:THR:O	9:X:597:LEU:HG	2.12	0.49
3:C:65:LEU:HA	3:C:68:ASN:HD21	1.77	0.49
1:E:79:LYS:HD3	1:E:82:LEU:HD11	1.93	0.49
8:W:29:G:H2'	8:W:30:C:H6	1.76	0.49
8:W:92:G:O6	9:X:44:LYS:NZ	2.40	0.49
9:X:1277:SER:O	9:X:1281:ILE:HG22	2.12	0.49
1:E:116:ARG:NH1	6:J:-3:DA:H3'	2.28	0.49
9:X:324:ARG:NH1	9:X:400:ARG:HD3	2.28	0.49
6:J:25:DT:H2''	6:J:26:DA:N7	2.27	0.49
9:X:137:HIS:HA	9:X:322:ILE:HD11	1.95	0.49
9:X:432:PHE:O	9:X:436:ASN:ND2	2.32	0.49
6:J:5:DT:H2''	6:J:6:DA:N7	2.28	0.49
8:W:89:G:H1	9:X:1272:GLN:CD	2.20	0.49
2:B:75:HIS:CE1	4:D:90:GLU:HB2	2.48	0.49
3:C:65:LEU:HA	3:C:68:ASN:ND2	2.28	0.49
8:W:52:A:N3	9:X:1169:MET:HG3	2.27	0.49
9:X:1002:PRO:O	9:X:1005:GLU:HG2	2.13	0.49
1:E:108:ASN:ND2	2:F:41:GLY:O	2.46	0.49
3:G:18:SER:OG	3:G:27:VAL:HG23	2.13	0.49
5:I:135:DG:H2''	5:I:136:DT:OP2	2.13	0.49
9:X:167:HIS:NE2	9:X:409:SER:O	2.36	0.49
2:B:67:ARG:O	2:B:71:THR:OG1	2.31	0.49
3:C:25:PHE:CZ	3:C:30:VAL:CG2	2.93	0.49
3:C:88:ARG:CD	3:C:108:LEU:CB	2.71	0.49
5:I:43:DC:H2''	5:I:44:DG:OP2	2.12	0.49
7:K:4:DC:H2'	7:K:5:DG:C8	2.47	0.49
9:X:1147:ALA:HB1	9:X:1188:LYS:O	2.12	0.49
1:A:97:GLU:O	1:A:101:VAL:HG23	2.13	0.48
8:W:20:C:H3'	8:W:21:G:H8	1.78	0.48
8:W:60:C:H2'	8:W:61:C:C6	2.47	0.48
9:X:90:MET:HG3	9:X:98:PHE:CZ	2.47	0.48
9:X:1144:LEU:HD13	9:X:1196:ILE:HD12	1.95	0.48
3:C:26:PRO:HG3	4:D:37:TYR:CE1	2.47	0.48
4:D:115:VAL:O	4:D:119:THR:N	2.34	0.48
2:F:58:LEU:O	2:F:62:LEU:HD23	2.13	0.48
5:I:16:DA:H2'	5:I:17:DT:H71	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:109:DG:H2''	5:I:110:DA:C8	2.48	0.48
6:J:-32:DT:H2''	6:J:-31:DA:C8	2.48	0.48
1:A:66:PRO:HB2	2:B:29:ILE:HD13	1.95	0.48
4:D:90:GLU:O	4:D:93:THR:OG1	2.25	0.48
8:W:20:C:H2'	8:W:21:G:O4'	2.13	0.48
9:X:310:THR:HG22	9:X:316:PRO:HB3	1.94	0.48
1:A:68:GLN:CD	1:A:72:ARG:HE	2.22	0.48
1:A:111:ALA:HB1	1:A:116:ARG:O	2.14	0.48
5:I:136:DT:H2''	5:I:137:DC:C5	2.48	0.48
6:J:39:DA:H1'	6:J:40:DC:H5'	1.94	0.48
8:W:23:U:H2'	8:W:24:U:C6	2.47	0.48
9:X:342:GLN:HB3	9:X:343:LEU:HD12	1.95	0.48
9:X:1210:ARG:NE	9:X:1280:VAL:O	2.33	0.48
4:H:62:PHE:CE2	4:H:66:ILE:CD1	2.90	0.48
6:J:61:DC:H2''	6:J:62:DG:N7	2.28	0.48
6:J:77:DG:H2'	6:J:78:DC:C6	2.47	0.48
8:W:12:U:H2'	8:W:13:C:H6	1.79	0.48
9:X:723:HIS:CE1	9:X:727:LEU:HD21	2.47	0.48
9:X:751:MET:HB3	9:X:754:HIS:HB2	1.96	0.48
3:C:83:LEU:HD11	4:D:59:MET:SD	2.53	0.48
5:I:115:DT:H2''	5:I:116:DC:C6	2.49	0.48
9:X:727:LEU:O	9:X:734:LYS:NZ	2.38	0.48
6:J:-43:DA:H2''	6:J:-42:DG:H8	1.79	0.48
9:X:1310:ILE:HA	9:X:1313:PHE:HD2	1.76	0.48
4:D:103:LEU:O	4:D:107:ALA:N	2.37	0.48
4:H:42:LEU:O	4:H:46:HIS:N	2.41	0.48
6:J:-21:DG:H2''	6:J:-20:DC:OP2	2.14	0.48
6:J:-2:DC:H2''	6:J:-1:DA:C8	2.48	0.48
4:H:88:SER:HA	4:H:91:ILE:HD13	1.96	0.48
6:J:-1:DA:H2''	6:J:0:DG:C8	2.49	0.48
9:X:11:ILE:HG23	9:X:16:VAL:HG22	1.96	0.48
9:X:60:GLU:CD	9:X:63:ARG:HH21	2.22	0.48
3:C:80:PRO:HG2	4:D:54:LYS:HB3	1.95	0.48
5:I:33:DC:N3	6:J:47:DA:N6	2.62	0.48
5:I:58:DC:H2''	5:I:59:DA:H8	1.79	0.48
8:W:20:C:C2	8:W:21:G:C8	3.02	0.48
8:W:34:A:H2'	8:W:34:A:N3	2.29	0.48
9:X:761:ILE:HD11	9:X:932:ALA:HB2	1.95	0.48
3:C:103:ALA:HB3	4:D:58:ILE:HD11	1.96	0.47
1:A:83:ARG:HH11	6:J:27:DG:H5'	1.79	0.47
9:X:35:LEU:HB2	9:X:1358:THR:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:724:ILE:HG21	9:X:738:LEU:HD12	1.95	0.47
9:X:963:VAL:O	9:X:967:ARG:HG3	2.14	0.47
9:X:1223:GLY:HA2	9:X:1318:LEU:HD12	1.95	0.47
9:X:1308:ASN:O	9:X:1312:LEU:HG	2.14	0.47
7:K:7:DT:H2'	7:K:8:DA:H8	1.79	0.47
9:X:1286:ASN:OD1	9:X:1287:LEU:N	2.47	0.47
2:B:39:ARG:NH1	2:B:43:VAL:O	2.47	0.47
1:E:83:ARG:O	2:F:81:VAL:N	2.45	0.47
6:J:-27:DC:H2''	6:J:-26:DC:C5	2.48	0.47
9:X:348:LYS:HB2	9:X:352:PHE:CE2	2.48	0.47
9:X:370:GLU:OE1	9:X:370:GLU:N	2.34	0.47
4:D:105:LYS:O	4:D:108:VAL:HB	2.14	0.47
9:X:7:ILE:O	9:X:759:ILE:HA	2.14	0.47
9:X:11:ILE:HG12	9:X:16:VAL:HG13	1.97	0.47
3:C:44:GLY:N	4:D:86:ILE:O	2.38	0.47
5:I:124:DT:H2''	5:I:125:DC:OP2	2.14	0.47
9:X:967:ARG:CZ	9:X:974:LYS:HB2	2.44	0.47
5:I:19:DC:H2''	5:I:20:DG:N7	2.30	0.47
7:K:14:DC:H2'	7:K:15:DG:H8	1.80	0.47
8:W:6:A:OP1	9:X:510:LYS:HE2	2.15	0.47
8:W:59:U:H3'	9:X:455:LEU:HD23	1.96	0.47
9:X:139:ARG:NH1	9:X:161:MET:HB3	2.30	0.47
9:X:615:ILE:O	9:X:619:ILE:HG13	2.15	0.47
9:X:636:LEU:HB2	9:X:648:MET:HE1	1.96	0.47
1:A:122:LYS:O	1:A:125:GLN:HG2	2.14	0.47
3:C:29:ARG:HG2	5:I:37:DA:OP1	2.14	0.47
3:C:32:ARG:NE	5:I:37:DA:OP2	2.45	0.47
3:G:81:ARG:HH11	3:G:85:LEU:HD21	1.80	0.47
5:I:44:DG:H1'	5:I:45:DT:C6	2.50	0.47
6:J:-38:DA:H2''	6:J:-37:DG:OP2	2.15	0.47
8:W:34:A:H3'	8:W:35:A:C8	2.50	0.47
1:E:122:LYS:HA	1:E:125:GLN:HE21	1.80	0.47
3:G:96:LEU:HD13	4:H:99:LEU:HD13	1.96	0.47
6:J:-28:DC:H2''	6:J:-27:DC:C6	2.49	0.47
7:K:2:DC:C2	7:K:3:DG:C8	3.03	0.47
8:W:54:G:H2'	8:W:55:C:C6	2.49	0.47
9:X:376:ILE:HA	9:X:379:ILE:HD12	1.95	0.47
9:X:632:ILE:O	9:X:636:LEU:HG	2.15	0.47
1:A:54:TYR:OH	2:B:36:ARG:HG2	2.15	0.47
5:I:108:DG:H2''	5:I:109:DG:C8	2.49	0.47
8:W:5:G:OP1	9:X:515:TYR:OH	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:12:U:H2'	8:W:13:C:C6	2.50	0.47
9:X:27:VAL:HG11	9:X:1089:MET:HE1	1.96	0.47
5:I:4:DC:H1'	5:I:5:DC:H5'	1.97	0.46
9:X:76:LYS:O	9:X:79:ILE:HG22	2.15	0.46
9:X:521:TYR:CZ	9:X:684:LYS:HA	2.51	0.46
9:X:730:SER:O	9:X:733:ILE:HG12	2.15	0.46
9:X:1075:ASP:N	9:X:1079:ASP:OD2	2.39	0.46
9:X:1226:LEU:HD13	9:X:1276:PHE:CD1	2.50	0.46
9:X:1265:TYR:O	9:X:1269:ILE:HG13	2.16	0.46
3:C:17:ARG:NH2	3:C:27:VAL:HG12	2.30	0.46
2:F:79:LYS:N	5:I:109:DG:OP1	2.49	0.46
3:G:40:SER:HB3	4:H:86:ILE:HD11	1.96	0.46
9:X:5:TYR:CE1	9:X:28:PRO:HG2	2.48	0.46
9:X:5:TYR:CD1	9:X:28:PRO:CG	2.98	0.46
1:A:65:LEU:HD22	6:J:17:DA:H2'	1.96	0.46
3:C:81:ARG:HD3	1:E:58:THR:HG23	1.93	0.46
2:F:75:HIS:CE1	4:H:77:LEU:HD21	2.51	0.46
9:X:619:ILE:HG12	9:X:639:TYR:CZ	2.50	0.46
9:X:1098:THR:HG22	9:X:1199:PRO:HB2	1.98	0.46
9:X:1192:LYS:HA	9:X:1195:ILE:HD12	1.96	0.46
2:B:75:HIS:CE1	4:D:77:LEU:HB3	2.50	0.46
3:C:100:VAL:HG11	2:F:98:TYR:CE2	2.50	0.46
1:E:100:LEU:HD13	2:F:37:LEU:HD13	1.97	0.46
3:G:50:TYR:O	3:G:54:VAL:HG23	2.16	0.46
5:I:7:DG:C2	5:I:8:DG:C6	3.04	0.46
6:J:21:DG:H2''	6:J:22:DT:OP2	2.16	0.46
7:K:7:DT:H2'	7:K:8:DA:C8	2.50	0.46
8:W:38:A:H2'	8:W:39:G:C8	2.51	0.46
8:W:68:A:C4	8:W:69:A:C8	3.04	0.46
9:X:86:PHE:HA	9:X:432:PHE:HE2	1.80	0.46
9:X:86:PHE:CZ	9:X:158:LEU:HD12	2.51	0.46
9:X:967:ARG:HA	9:X:972:PHE:HB2	1.98	0.46
9:X:1106:SER:HA	9:X:1137:PRO:HA	1.97	0.46
2:B:36:ARG:HH12	5:I:68:DA:P	2.39	0.46
2:F:72:TYR:CE1	4:H:77:LEU:HD12	2.51	0.46
5:I:130:DC:H2'	5:I:131:DA:C8	2.50	0.46
8:W:44:U:H5'	9:X:363:ILE:HD12	1.98	0.46
9:X:723:HIS:CE1	9:X:934:ILE:HD11	2.50	0.46
3:C:111:ILE:HG12	1:E:52:ARG:CZ	2.46	0.46
8:W:45:U:C2	8:W:46:A:C8	3.04	0.46
9:X:404:THR:H	9:X:407:ASN:HD21	1.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:ARG:HD2	3:C:108:LEU:HD12	1.98	0.46
1:E:102:GLY:O	1:E:105:GLU:HG2	2.15	0.46
6:J:-37:DG:H2''	6:J:-36:DG:C8	2.51	0.46
8:W:15:C:O2'	9:X:453:GLY:HA2	2.16	0.46
9:X:30:LYS:C	9:X:44:LYS:HG3	2.41	0.46
2:F:64:ASN:OD1	2:F:65:VAL:N	2.49	0.46
4:H:81:ASN:HD21	4:H:83:ARG:NH2	2.14	0.46
8:W:33:G:H3'	8:W:34:A:C5'	2.41	0.46
9:X:342:GLN:NE2	9:X:384:ASP:O	2.49	0.46
9:X:362:TYR:CZ	9:X:401:LYS:HG3	2.51	0.46
1:E:116:ARG:HH22	6:J:-3:DA:H3'	1.81	0.46
3:G:42:ARG:NH2	4:H:85:THR:OG1	2.49	0.46
5:I:7:DG:N1	5:I:8:DG:C6	2.84	0.46
7:K:12:DT:H2'	7:K:13:DC:C6	2.51	0.46
8:W:28:A:OP2	9:X:126:VAL:HG22	2.16	0.46
9:X:148:LYS:HE3	9:X:430:TYR:HE1	1.81	0.46
9:X:148:LYS:HB2	9:X:429:PHE:CD1	2.51	0.46
9:X:1232:TYR:CD2	9:X:1269:ILE:HG12	2.51	0.46
1:E:111:ALA:O	1:E:116:ARG:N	2.41	0.45
5:I:20:DG:H3'	9:X:1153:LYS:HZ1	1.80	0.45
5:I:37:DA:H2'	5:I:38:DT:H71	1.98	0.45
5:I:47:DG:H1'	5:I:48:DA:C8	2.51	0.45
5:I:53:DT:OP2	5:I:53:DT:H2'	2.16	0.45
9:X:651:LEU:HD23	9:X:654:ARG:NH2	2.32	0.45
9:X:760:VAL:HG22	9:X:956:ILE:HB	1.97	0.45
9:X:1086:VAL:O	9:X:1089:MET:HG2	2.15	0.45
5:I:52:DC:H2''	5:I:53:DT:OP2	2.15	0.45
5:I:98:DA:C4	5:I:99:DC:C5	3.05	0.45
6:J:6:DA:H2''	6:J:7:DC:C5	2.50	0.45
8:W:42:A:H3'	8:W:43:G:H8	1.81	0.45
3:C:110:ASN:H	1:E:55:GLN:NE2	2.15	0.45
1:E:72:ARG:NH2	6:J:-23:DT:OP2	2.49	0.45
5:I:65:DT:H4'	5:I:66:DA:H5'	1.98	0.45
6:J:31:DT:H2''	6:J:32:DG:H8	1.77	0.45
9:X:163:LYS:HE3	9:X:164:PHE:CE2	2.51	0.45
4:D:84:SER:HB2	5:I:46:DA:H3'	1.97	0.45
1:E:128:ARG:HD3	1:E:134:ARG:NH2	2.32	0.45
4:H:59:MET:O	4:H:63:VAL:HG23	2.17	0.45
8:W:75:A:H2'	8:W:76:A:O4'	2.15	0.45
9:X:89:GLU:O	9:X:93:VAL:HG23	2.15	0.45
3:C:24:GLN:NE2	4:D:40:LYS:HB3	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:THR:CG2	2:F:44:LYS:HB3	2.23	0.45
4:H:36:ILE:HG13	4:H:37:TYR:N	2.31	0.45
5:I:82:DT:H2''	5:I:83:DG:H8	1.79	0.45
6:J:38:DG:H2''	6:J:39:DA:C8	2.52	0.45
1:E:118:THR:HG22	2:F:45:ARG:H	1.81	0.45
9:X:148:LYS:HE3	9:X:430:TYR:CE1	2.52	0.45
1:A:128:ARG:NH1	2:B:57:VAL:HG22	2.32	0.45
5:I:8:DG:H1'	5:I:9:DC:H5'	1.99	0.45
5:I:51:DG:H2''	5:I:52:DC:OP2	2.17	0.45
8:W:7:C:H2'	8:W:8:C:C6	2.52	0.45
8:W:77:A:H2'	8:W:78:A:H8	1.80	0.45
9:X:995:THR:HA	9:X:998:ILE:HG12	1.99	0.45
1:A:78:PHE:CZ	2:B:67:ARG:HB2	2.52	0.45
5:I:96:DT:H2''	5:I:97:DA:N9	2.32	0.45
6:J:58:DC:H2''	6:J:59:DA:H8	1.82	0.45
8:W:22:U:C2	8:W:23:U:C5	3.05	0.45
8:W:48:A:C2	8:W:49:A:C5	3.04	0.45
2:B:76:ALA:O	2:B:78:ARG:HG3	2.17	0.45
4:D:36:ILE:HG13	4:D:37:TYR:N	2.31	0.45
5:I:50:DA:H2''	5:I:51:DG:H8	1.82	0.45
6:J:71:DG:C2	6:J:72:DG:C5	3.05	0.45
7:K:13:DC:H2'	7:K:14:DC:C6	2.52	0.45
8:W:40:C:C2	8:W:41:A:C8	3.05	0.45
9:X:651:LEU:HD23	9:X:654:ARG:HH22	1.82	0.45
9:X:1294:TYR:HA	9:X:1326:TYR:OH	2.17	0.45
3:C:79:ILE:HG22	3:C:82:HIS:CE1	2.53	0.45
4:H:92:GLN:OE1	4:H:96:ARG:NH2	2.50	0.45
5:I:103:DC:H2''	5:I:104:DA:H8	1.80	0.45
6:J:72:DG:C6	6:J:73:DC:C4	3.05	0.45
2:B:38:ALA:HB3	2:B:46:ILE:HD13	1.98	0.44
3:C:20:ARG:HE	5:I:39:DT:P	2.40	0.44
1:E:116:ARG:HG3	1:E:117:VAL:O	2.17	0.44
8:W:17:A:N7	9:X:71:ARG:NH1	2.65	0.44
3:C:87:ILE:HG21	3:C:97:LEU:HD12	1.99	0.44
1:E:96:CYS:SG	2:F:62:LEU:HD21	2.57	0.44
2:F:35:ARG:HG3	2:F:46:ILE:HD12	1.99	0.44
5:I:15:DA:H1'	5:I:16:DA:O4'	2.17	0.44
5:I:68:DA:H1'	5:I:69:DC:H5'	1.99	0.44
6:J:42:DA:H2''	6:J:43:DA:OP2	2.17	0.44
8:W:90:U:O4	9:X:1226:LEU:HD12	2.17	0.44
9:X:48:ILE:HD12	9:X:988:TYR:HB2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:X:496:THR:OG1	9:X:497:ASN:N	2.49	0.44
1:E:128:ARG:HB3	1:E:134:ARG:HB2	1.99	0.44
2:F:91:LYS:HD3	2:F:96:THR:HB	2.00	0.44
7:K:17:DT:H4'	9:X:698:HIS:HD2	1.82	0.44
9:X:384:ASP:HA	9:X:386:THR:HG21	1.98	0.44
1:A:70:LEU:O	1:A:74:ILE:HG12	2.17	0.44
5:I:59:DA:N6	6:J:23:DG:O6	2.50	0.44
6:J:37:DC:H2''	6:J:38:DG:N7	2.32	0.44
8:W:40:C:H2'	8:W:41:A:C8	2.52	0.44
9:X:504:ASN:OD1	9:X:505:GLU:N	2.51	0.44
1:A:116:ARG:HD3	5:I:78:DG:H3'	1.99	0.44
4:D:58:ILE:HG12	2:F:99:GLY:HA3	1.98	0.44
3:G:97:LEU:HD11	4:H:62:PHE:HE2	1.82	0.44
4:H:56:MET:HE3	4:H:60:ASN:HB2	1.99	0.44
8:W:53:G:C6	8:W:62:G:C6	3.06	0.44
9:X:107:VAL:O	9:X:111:LYS:N	2.46	0.44
9:X:150:ASP:OD2	9:X:152:ARG:NH2	2.51	0.44
9:X:398:LEU:HG	9:X:399:LEU:HG	2.00	0.44
9:X:485:GLY:HA2	9:X:631:MET:HE3	1.99	0.44
9:X:1043:MET:SD	9:X:1043:MET:N	2.90	0.44
3:C:50:TYR:HH	4:D:108:VAL:HG13	1.83	0.44
3:C:83:LEU:HD13	4:D:59:MET:SD	2.58	0.44
2:F:51:TYR:O	2:F:55:ARG:HG3	2.17	0.44
6:J:58:DC:H2''	6:J:59:DA:C8	2.53	0.44
8:W:21:G:H2'	8:W:22:U:C6	2.53	0.44
9:X:340:ARG:HD2	9:X:347:TYR:CD2	2.52	0.44
2:B:32:PRO:HA	2:B:35:ARG:HB3	2.00	0.44
6:J:-49:DG:H2''	6:J:-48:DC:C5	2.52	0.44
6:J:9:DT:H2''	6:J:10:DG:C8	2.53	0.44
8:W:52:A:N7	8:W:53:G:H1'	2.31	0.44
9:X:56:GLY:HA3	9:X:732:ALA:HA	1.99	0.44
9:X:1212:ARG:NE	9:X:1341:GLU:OE2	2.51	0.44
9:X:1314:THR:HA	9:X:1317:ASN:ND2	2.33	0.44
1:A:103:LEU:HD11	1:A:128:ARG:HG2	2.00	0.44
3:C:92:GLU:OE1	4:D:101:GLY:HA2	2.18	0.44
1:E:83:ARG:NH1	6:J:-23:DT:H5'	2.33	0.44
5:I:24:DC:H2''	5:I:25:DC:C5	2.53	0.44
6:J:71:DG:H3'	9:X:1332:ASP:OD2	2.17	0.44
9:X:1321:PRO:HG2	9:X:1334:LYS:O	2.18	0.44
1:E:118:THR:HG22	2:F:45:ARG:N	2.33	0.44
2:F:26:ILE:HD11	2:F:58:LEU:HD11	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:60:DC:C4	5:I:61:DC:N4	2.86	0.44
8:W:51:A:H2	8:W:62:G:C2	2.36	0.44
9:X:692:ASN:HB3	9:X:695:GLN:HG3	2.00	0.44
2:B:98:TYR:CD2	3:G:102:ILE:HG12	2.53	0.43
3:G:77:ARG:HH21	5:I:139:DG:H5'	1.83	0.43
6:J:-20:DC:H2''	6:J:-19:DG:H8	1.83	0.43
6:J:-7:DG:H2''	6:J:-6:DG:N7	2.32	0.43
9:X:106:LEU:HA	9:X:1131:TYR:HE2	1.83	0.43
9:X:952:GLU:HG2	9:X:953:VAL:HG23	1.99	0.43
3:C:84:GLN:OE1	3:C:102:ILE:HB	2.18	0.43
1:E:116:ARG:NH2	6:J:-3:DA:H3'	2.33	0.43
6:J:-46:DT:H2''	6:J:-45:DG:N7	2.33	0.43
6:J:9:DT:H2''	6:J:10:DG:H8	1.81	0.43
9:X:94:ASP:OD2	9:X:96:SER:OG	2.27	0.43
2:F:76:ALA:HB1	2:F:78:ARG:HE	1.83	0.43
5:I:89:DC:H2''	5:I:90:DG:C8	2.53	0.43
6:J:-54:DC:H2''	6:J:-53:DA:N7	2.33	0.43
6:J:-49:DG:H2'	6:J:-49:DG:OP2	2.18	0.43
7:K:3:DG:N3	7:K:3:DG:H2'	2.33	0.43
8:W:27:G:H4'	8:W:28:A:OP2	2.17	0.43
8:W:90:U:C2	9:X:1090:PRO:HB2	2.53	0.43
9:X:81:TYR:O	9:X:84:GLU:HG2	2.16	0.43
9:X:512:SER:HB3	9:X:515:TYR:HB2	2.00	0.43
9:X:1143:VAL:HG23	9:X:1166:ILE:HG13	2.00	0.43
2:F:75:HIS:HA	4:H:89:ARG:HH22	1.83	0.43
4:H:89:ARG:O	4:H:93:THR:HG22	2.18	0.43
8:W:18:G:H4'	9:X:166:GLY:O	2.18	0.43
8:W:26:A:H5''	9:X:115:ARG:HB2	2.00	0.43
8:W:91:C:H5	9:X:45:LYS:HA	1.83	0.43
3:G:51:LEU:O	3:G:55:LEU:HG	2.19	0.43
8:W:79:G:H2'	8:W:80:U:O4'	2.18	0.43
9:X:14:ASN:OD1	9:X:55:SER:OG	2.24	0.43
9:X:31:LYS:HA	9:X:44:LYS:HA	1.99	0.43
9:X:592:GLY:HA2	9:X:595:HIS:CD2	2.53	0.43
9:X:1084:ARG:HH12	9:X:1234:ASN:HD21	1.65	0.43
9:X:1128:PRO:HA	9:X:1132:GLY:O	2.18	0.43
2:B:88:TYR:CE2	4:D:80:TYR:HB3	2.54	0.43
3:C:16:THR:O	3:C:20:ARG:N	2.42	0.43
3:C:79:ILE:HG23	3:C:81:ARG:HB3	2.00	0.43
3:C:92:GLU:CD	4:D:101:GLY:HA2	2.43	0.43
2:F:92:ARG:CZ	4:H:97:LEU:HB3	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:57:A:H5''	9:X:457:ARG:HH21	1.84	0.43
8:W:68:A:OP1	9:X:1097:LYS:NZ	2.50	0.43
9:X:647:VAL:O	9:X:651:LEU:HG	2.18	0.43
9:X:1098:THR:HG23	9:X:1200:LYS:O	2.19	0.43
9:X:1167:THR:HG23	9:X:1170:GLU:H	1.84	0.43
2:F:83:ALA:O	2:F:86:VAL:HG12	2.18	0.43
2:F:90:LEU:HD13	2:F:97:LEU:HD22	2.01	0.43
9:X:368:SER:O	9:X:371:GLU:HG2	2.18	0.43
9:X:927:ILE:O	9:X:931:VAL:HG23	2.18	0.43
9:X:977:GLU:HG3	9:X:1310:ILE:HG23	2.00	0.43
1:A:61:LEU:O	2:B:36:ARG:NH2	2.52	0.43
4:D:43:LYS:HA	4:D:43:LYS:HD3	1.80	0.43
4:D:58:ILE:HA	2:F:99:GLY:HA2	2.00	0.43
1:E:96:CYS:O	1:E:100:LEU:HG	2.18	0.43
9:X:5:TYR:CD1	9:X:28:PRO:HG2	2.53	0.43
9:X:523:GLU:OE2	9:X:588:ASN:N	2.50	0.43
9:X:742:LYS:HD2	9:X:1352:ILE:HD12	2.01	0.43
3:G:91:GLU:OE1	3:G:91:GLU:N	2.38	0.43
5:I:88:DC:H2''	5:I:89:DC:C5	2.54	0.43
6:J:-24:DT:H2'	6:J:-23:DT:H71	2.00	0.43
8:W:73:G:C3'	8:W:74:A:H5''	2.49	0.43
9:X:27:VAL:O	9:X:27:VAL:HG13	2.18	0.43
2:B:72:TYR:CE2	4:D:77:LEU:HD21	2.54	0.43
4:D:78:ALA:O	4:D:83:ARG:N	2.52	0.43
1:E:118:THR:CG2	2:F:45:ARG:H	2.31	0.43
5:I:10:DC:N4	6:J:70:DA:H61	2.14	0.43
6:J:17:DA:H1'	6:J:18:DG:H5'	2.01	0.43
6:J:45:DT:H2'	6:J:46:DG:C8	2.54	0.43
8:W:30:C:H2'	8:W:31:U:C6	2.53	0.43
9:X:968:LYS:HA	9:X:973:TYR:CE1	2.54	0.43
1:A:107:THR:OG1	1:A:124:ILE:HG13	2.19	0.42
1:A:129:ARG:HH22	1:E:105:GLU:CD	2.27	0.42
2:B:48:GLY:HA2	2:B:51:TYR:CD2	2.47	0.42
2:B:77:LYS:NZ	5:I:48:DA:OP2	2.52	0.42
3:C:81:ARG:NH2	1:E:56:LYS:HA	2.34	0.42
4:D:103:LEU:HA	4:D:106:HIS:ND1	2.34	0.42
3:G:17:ARG:NH2	6:J:-43:DA:OP2	2.52	0.42
4:H:106:HIS:O	4:H:109:SER:OG	2.30	0.42
5:I:13:DA:H2''	5:I:14:DG:C8	2.54	0.42
6:J:-44:DG:H2''	6:J:-43:DA:H8	1.84	0.42
9:X:1238:LEU:HD22	9:X:1255:LYS:HG2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:LEU:HB3	2:B:95:ARG:O	2.18	0.42
3:C:83:LEU:CD2	4:D:59:MET:SD	3.07	0.42
4:D:77:LEU:HD13	4:D:77:LEU:HA	1.89	0.42
8:W:21:G:C8	8:W:21:G:OP2	2.72	0.42
8:W:40:C:H2'	8:W:41:A:H8	1.84	0.42
9:X:95:ASP:HB3	9:X:99:HIS:HE1	1.84	0.42
9:X:485:GLY:HA3	9:X:635:ARG:NH1	2.34	0.42
9:X:1207:GLU:CD	9:X:1207:GLU:H	2.27	0.42
1:A:50:GLU:HG3	1:A:54:TYR:CE2	2.54	0.42
4:D:42:LEU:HA	4:D:45:VAL:HG12	2.00	0.42
1:E:120:MET:HB2	1:E:122:LYS:HG2	2.02	0.42
3:G:24:GLN:HE22	4:H:44:GLN:HE22	1.67	0.42
5:I:20:DG:H3'	9:X:1153:LYS:HZ3	1.85	0.42
5:I:105:DA:H2''	5:I:106:DG:C8	2.54	0.42
6:J:-20:DC:H2''	6:J:-19:DG:C8	2.54	0.42
9:X:498:PHE:HB3	9:X:505:GLU:O	2.18	0.42
9:X:988:TYR:CE1	9:X:1086:VAL:HG21	2.54	0.42
1:A:96:CYS:O	1:A:100:LEU:HG	2.19	0.42
2:B:26:ILE:HD11	2:B:55:ARG:HA	2.02	0.42
2:B:39:ARG:HD3	2:B:39:ARG:HA	1.87	0.42
3:C:57:TYR:CD2	4:D:107:ALA:HB2	2.54	0.42
5:I:43:DC:H6	5:I:43:DC:H2'	1.63	0.42
5:I:84:DT:H2''	5:I:85:DC:C6	2.54	0.42
8:W:44:U:O3'	9:X:402:GLN:HG2	2.18	0.42
9:X:665:LYS:HE3	9:X:665:LYS:HB3	1.87	0.42
1:A:102:GLY:O	1:A:105:GLU:HG3	2.20	0.42
4:D:34:TYR:CD2	4:D:63:VAL:HG11	2.55	0.42
4:D:76:ARG:HB3	4:D:80:TYR:CE2	2.54	0.42
5:I:50:DA:H2''	5:I:51:DG:C8	2.55	0.42
5:I:62:DG:H2''	5:I:63:DC:H5	1.84	0.42
5:I:68:DA:C4	5:I:69:DC:C5	3.08	0.42
5:I:106:DG:N2	6:J:-24:DT:O2	2.52	0.42
9:X:96:SER:O	9:X:100:ARG:HG3	2.20	0.42
9:X:1306:ALA:O	9:X:1310:ILE:HG13	2.19	0.42
2:B:93:GLN:O	2:B:93:GLN:NE2	2.52	0.42
3:C:64:GLU:HG2	4:D:46:HIS:HE1	1.84	0.42
3:C:88:ARG:HD2	3:C:108:LEU:CD1	2.49	0.42
4:D:78:ALA:HA	4:D:83:ARG:HB2	2.02	0.42
3:G:71:ARG:HH22	3:G:76:THR:HA	1.84	0.42
8:W:73:G:H2'	8:W:74:A:H5''	2.02	0.42
9:X:1191:LYS:HD3	9:X:1194:LEU:HD12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:O	1:A:66:PRO:HD2	2.19	0.42
1:A:79:LYS:HE2	1:A:79:LYS:HB2	1.87	0.42
1:A:79:LYS:HZ2	1:A:82:LEU:HB2	1.85	0.42
2:B:66:ILE:HD13	2:B:66:ILE:HA	1.89	0.42
3:C:68:ASN:OD1	3:C:69:ALA:N	2.53	0.42
3:C:83:LEU:HD11	4:D:59:MET:CG	2.48	0.42
4:D:34:TYR:HD2	4:D:63:VAL:HG11	1.83	0.42
1:E:54:TYR:HA	1:E:57:SER:OG	2.20	0.42
1:E:66:PRO:HG3	5:I:98:DA:P	2.60	0.42
1:E:118:THR:CG2	2:F:45:ARG:N	2.83	0.42
5:I:8:DG:C2	5:I:9:DC:C2	3.08	0.42
5:I:16:DA:C2'	5:I:17:DT:H71	2.50	0.42
5:I:55:DT:H2''	5:I:56:DA:C8	2.55	0.42
6:J:-43:DA:H2''	6:J:-42:DG:C8	2.54	0.42
6:J:-24:DT:H2''	6:J:-23:DT:C6	2.55	0.42
6:J:28:DA:H8	6:J:28:DA:P	2.42	0.42
8:W:25:U:H2'	8:W:26:A:H8	1.85	0.42
8:W:42:A:H3'	8:W:43:G:C8	2.55	0.42
5:I:10:DC:H42	6:J:70:DA:N6	2.18	0.42
9:X:97:PHE:HD1	9:X:100:ARG:HH21	1.67	0.42
9:X:107:VAL:HG13	9:X:1131:TYR:CZ	2.55	0.42
3:G:77:ARG:HG2	4:H:50:GLY:HA3	2.02	0.42
4:H:93:THR:O	4:H:97:LEU:HG	2.19	0.42
6:J:64:DA:C2'	6:J:65:DT:H5'	2.49	0.42
9:X:1113:LYS:HD2	9:X:1130:LYS:HA	2.02	0.42
9:X:1141:TYR:HE1	9:X:1171:ARG:HD2	1.85	0.42
2:B:35:ARG:HB2	2:B:51:TYR:HH	1.84	0.42
3:C:25:PHE:HD2	3:C:52:ALA:HB1	1.85	0.42
5:I:7:DG:C6	5:I:8:DG:O6	2.73	0.42
5:I:109:DG:C6	5:I:110:DA:C6	3.08	0.42
6:J:-37:DG:OP2	6:J:-37:DG:H2'	2.20	0.42
6:J:-33:DG:H2''	6:J:-32:DT:OP2	2.20	0.42
9:X:5:TYR:CD1	9:X:22:THR:CG2	2.86	0.42
9:X:362:TYR:OH	9:X:401:LYS:N	2.48	0.42
9:X:679:ILE:HG23	9:X:696:LEU:HD13	2.01	0.42
9:X:1150:GLU:HB3	9:X:1155:LYS:HB3	2.02	0.42
9:X:1174:PHE:HD1	9:X:1181:PHE:CD2	2.38	0.42
1:A:83:ARG:HE	5:I:58:DC:H5'	1.85	0.41
6:J:61:DC:H2''	6:J:62:DG:C8	2.55	0.41
4:D:91:ILE:O	4:D:95:VAL:HG23	2.20	0.41
2:F:75:HIS:CD2	4:H:93:THR:HG21	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:53:DT:O2	6:J:29:DG:N2	2.53	0.41
5:I:89:DC:C2	5:I:90:DG:C5	3.08	0.41
6:J:69:DC:H2''	6:J:70:DA:C8	2.55	0.41
9:X:103:GLU:OE2	9:X:113:HIS:ND1	2.54	0.41
9:X:324:ARG:HD3	9:X:400:ARG:HB2	2.01	0.41
2:B:25:ASN:O	2:B:29:ILE:N	2.53	0.41
3:C:76:THR:CG2	4:D:49:THR:HA	2.47	0.41
3:C:79:ILE:H	3:C:82:HIS:CE1	2.38	0.41
2:F:25:ASN:HB2	2:F:26:ILE:H	1.67	0.41
8:W:11:A:H2'	8:W:12:U:H6	1.85	0.41
9:X:70:ARG:O	9:X:73:THR:OG1	2.34	0.41
9:X:128:TYR:CE1	9:X:138:LEU:HD22	2.53	0.41
9:X:498:PHE:C	9:X:507:VAL:HG23	2.45	0.41
9:X:521:TYR:CE1	9:X:684:LYS:HA	2.55	0.41
3:C:41:GLU:OE1	3:C:42:ARG:HB2	2.20	0.41
3:G:97:LEU:HD11	4:H:62:PHE:CE2	2.56	0.41
9:X:1222:LYS:HE3	9:X:1317:ASN:O	2.20	0.41
1:E:72:ARG:O	1:E:76:GLN:HG3	2.20	0.41
8:W:8:C:HO2'	8:W:9:C:P	2.40	0.41
9:X:737:ILE:HA	9:X:740:THR:HG22	2.02	0.41
6:J:-49:DG:H2''	6:J:-48:DC:C6	2.55	0.41
9:X:304:ASP:CG	9:X:305:ILE:HG13	2.45	0.41
9:X:379:ILE:H	9:X:379:ILE:HG13	1.69	0.41
9:X:979:ASN:ND2	9:X:1226:LEU:O	2.54	0.41
9:X:981:TYR:CD1	9:X:1092:VAL:HB	2.55	0.41
9:X:1083:VAL:O	9:X:1087:LEU:HG	2.21	0.41
2:B:38:ALA:O	2:B:43:VAL:HG12	2.20	0.41
3:C:44:GLY:HA2	6:J:38:DG:O5'	2.21	0.41
4:D:89:ARG:O	4:D:93:THR:HG23	2.21	0.41
1:E:97:GLU:HG2	2:F:37:LEU:HD21	2.03	0.41
2:F:31:LYS:HA	2:F:34:ILE:HD12	2.03	0.41
2:F:71:THR:HG22	4:H:93:THR:OG1	2.21	0.41
5:I:58:DC:C2'	5:I:59:DA:H8	2.33	0.41
6:J:-18:DG:OP2	6:J:-18:DG:H2'	2.20	0.41
8:W:50:U:H5''	8:W:51:A:H5'	2.03	0.41
9:X:338:LEU:HD12	9:X:338:LEU:HA	1.91	0.41
9:X:380:LEU:HD13	9:X:390:LEU:HA	2.03	0.41
9:X:404:THR:OG1	9:X:406:ASP:OD1	2.23	0.41
9:X:686:ASP:HB3	9:X:690:ASN:HA	2.03	0.41
9:X:737:ILE:O	9:X:740:THR:HG22	2.21	0.41
1:A:83:ARG:HD3	6:J:27:DG:H5'	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:PHE:CD2	3:C:52:ALA:CB	3.02	0.41
6:J:28:DA:C6	6:J:29:DG:C6	3.08	0.41
8:W:5:G:OP1	9:X:661:ARG:HG2	2.21	0.41
8:W:47:A:H2'	8:W:48:A:C8	2.56	0.41
8:W:85:C:H2'	8:W:86:C:H6	1.85	0.41
9:X:1146:VAL:HB	9:X:1161:LYS:HD3	2.02	0.41
1:A:72:ARG:HH12	5:I:58:DC:P	2.43	0.41
2:B:47:SER:OG	6:J:7:DC:OP1	2.22	0.41
2:B:72:TYR:CD2	4:D:77:LEU:HD11	2.56	0.41
2:B:76:ALA:HA	4:D:81:ASN:ND2	2.36	0.41
1:E:63:ARG:HH11	2:F:36:ARG:HH22	1.69	0.41
2:F:75:HIS:NE2	4:H:77:LEU:HD21	2.36	0.41
3:G:26:PRO:HG3	4:H:37:TYR:CZ	2.56	0.41
3:G:59:THR:HA	3:G:62:ILE:HG22	2.03	0.41
3:G:84:GLN:NE2	3:G:102:ILE:HB	2.35	0.41
5:I:13:DA:C6	5:I:14:DG:C2	3.09	0.41
6:J:-53:DA:H2''	6:J:-52:DC:OP2	2.20	0.41
6:J:-16:DT:H2''	6:J:-15:DA:C8	2.56	0.41
8:W:18:G:N3	8:W:18:G:H2'	2.36	0.41
8:W:50:U:H2'	9:X:72:TYR:HE2	1.86	0.41
8:W:58:G:H4'	9:X:457:ARG:HE	1.85	0.41
8:W:71:U:H2'	8:W:72:U:C6	2.56	0.41
9:X:5:TYR:CE1	9:X:22:THR:HG23	2.44	0.41
9:X:106:LEU:HA	9:X:1131:TYR:CE2	2.56	0.41
9:X:139:ARG:HH12	9:X:415:HIS:HD2	1.67	0.41
9:X:464:TRP:CE2	9:X:491:PHE:HB2	2.56	0.41
9:X:697:ILE:O	9:X:705:LYS:HD3	2.21	0.41
9:X:982:HIS:HA	9:X:985:HIS:ND1	2.36	0.41
9:X:1111:LEU:HD13	9:X:1111:LEU:HA	1.88	0.41
9:X:1215:ALA:HB2	9:X:1221:GLN:HG3	2.02	0.41
1:A:100:LEU:HD21	2:B:58:LEU:HD12	2.03	0.41
3:C:23:LEU:HD23	3:C:23:LEU:HA	1.89	0.41
1:E:79:LYS:HD3	1:E:82:LEU:HD21	2.03	0.41
1:E:128:ARG:HB2	1:E:134:ARG:HE	1.86	0.41
3:G:40:SER:HB3	4:H:86:ILE:CD1	2.51	0.41
4:H:42:LEU:HA	4:H:45:VAL:HG12	2.02	0.41
6:J:46:DG:H4'	6:J:47:DA:H5'	2.02	0.41
7:K:4:DC:H2''	9:X:450:TYR:CE2	2.56	0.41
9:X:136:TYR:CG	9:X:321:MET:HG2	2.56	0.41
9:X:335:LEU:O	9:X:339:VAL:HG22	2.21	0.41
9:X:1113:LYS:HB2	9:X:1129:LYS:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:5:DC:N4	6:J:75:DT:O4	2.55	0.40
5:I:26:DG:H1	6:J:55:DC:H42	1.69	0.40
5:I:99:DC:C4	5:I:100:DC:N4	2.89	0.40
6:J:38:DG:C4	6:J:39:DA:C5	3.09	0.40
8:W:42:A:HO2'	8:W:43:G:P	2.44	0.40
9:X:146:THR:HG22	9:X:425:ARG:HE	1.86	0.40
9:X:480:GLU:OE1	9:X:480:GLU:N	2.52	0.40
9:X:1127:ASP:OD2	9:X:1130:LYS:N	2.54	0.40
1:E:72:ARG:HH22	6:J:-23:DT:P	2.44	0.40
5:I:119:DT:H2''	5:I:120:DA:N7	2.36	0.40
6:J:-31:DA:H2''	6:J:-30:DA:OP2	2.21	0.40
6:J:-14:DA:H8	6:J:-14:DA:OP2	2.04	0.40
8:W:25:U:C2	8:W:26:A:C8	3.09	0.40
9:X:550:ASP:O	9:X:554:LYS:HB2	2.21	0.40
9:X:993:VAL:O	9:X:997:LEU:N	2.52	0.40
9:X:1219:GLU:HA	9:X:1336:TYR:O	2.21	0.40
9:X:1270:ILE:O	9:X:1273:ILE:HG22	2.21	0.40
9:X:1325:LYS:HD2	9:X:1328:ASP:HA	2.02	0.40
1:A:76:GLN:OE1	1:A:80:THR:HA	2.22	0.40
2:B:75:HIS:NE2	4:D:90:GLU:HB2	2.36	0.40
5:I:7:DG:C2	5:I:8:DG:C5	3.09	0.40
6:J:-37:DG:OP2	6:J:-37:DG:H8	2.04	0.40
9:X:1139:VAL:HG22	9:X:1140:ALA:O	2.22	0.40
2:B:35:ARG:HB2	2:B:51:TYR:OH	2.21	0.40
9:X:112:LYS:HB2	9:X:113:HIS:HD1	1.87	0.40
9:X:954:LYS:NZ	9:X:1005:GLU:OE1	2.31	0.40
5:I:117:DC:H2''	5:I:118:DC:C5	2.56	0.40
8:W:31:U:C2	8:W:32:A:N7	2.90	0.40
9:X:10:ASP:OD2	9:X:986:ASP:HB2	2.22	0.40
9:X:75:ARG:HD2	9:X:163:LYS:HG3	2.04	0.40
9:X:362:TYR:OH	9:X:401:LYS:HG3	2.22	0.40
9:X:644:ASP:HB2	9:X:647:VAL:HG23	2.03	0.40
9:X:1107:LYS:C	9:X:1109:SER:H	2.29	0.40
9:X:1351:SER:OG	9:X:1356:TYR:HB2	2.21	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	89/139 (64%)	89 (100%)	0	0	100	100
1	E	88/139 (63%)	86 (98%)	2 (2%)	0	100	100
2	B	79/106 (74%)	77 (98%)	2 (2%)	0	100	100
2	F	76/106 (72%)	74 (97%)	2 (3%)	0	100	100
3	C	94/133 (71%)	91 (97%)	3 (3%)	0	100	100
3	G	94/133 (71%)	94 (100%)	0	0	100	100
4	D	88/129 (68%)	85 (97%)	3 (3%)	0	100	100
4	H	88/129 (68%)	85 (97%)	3 (3%)	0	100	100
9	X	913/1368 (67%)	884 (97%)	29 (3%)	0	100	100
All	All	1609/2382 (68%)	1565 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	X	797/1227 (65%)	797 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
9	X	415	HIS
9	X	459	ASN
9	X	698	HIS
9	X	723	HIS
9	X	739	GLN
9	X	940	ASN
9	X	980	ASN
9	X	1234	ASN
9	X	1256	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	W	96/97 (98%)	27 (28%)	4 (4%)

All (27) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	W	9	C
8	W	18	G
8	W	21	G
8	W	22	U
8	W	23	U
8	W	28	A
8	W	29	G
8	W	31	U
8	W	32	A
8	W	35	A
8	W	37	U
8	W	38	A
8	W	42	A
8	W	43	G
8	W	44	U
8	W	45	U
8	W	51	A
8	W	59	U
8	W	68	A
8	W	69	A
8	W	74	A
8	W	75	A
8	W	81	G
8	W	82	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	W	87	G
8	W	89	G
8	W	91	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	W	8	C
8	W	27	G
8	W	42	A
8	W	68	A

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

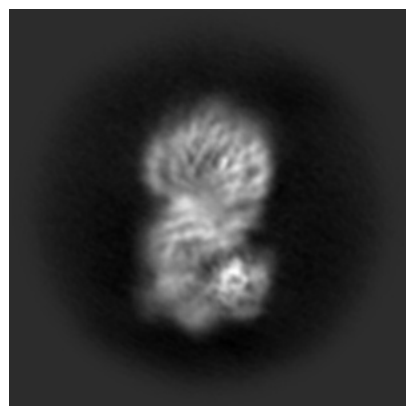
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39431. These allow visual inspection of the internal detail of the map and identification of artifacts.

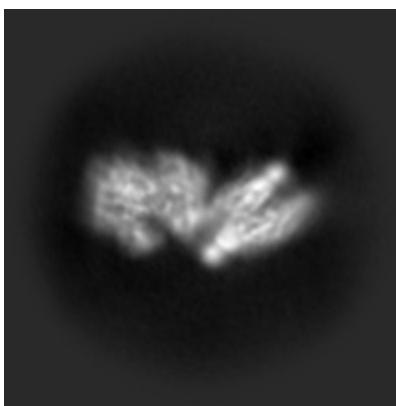
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

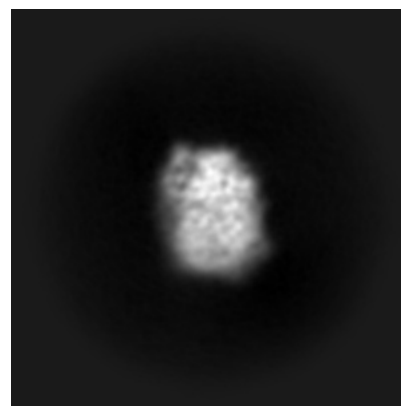
6.1.1 Primary map



X

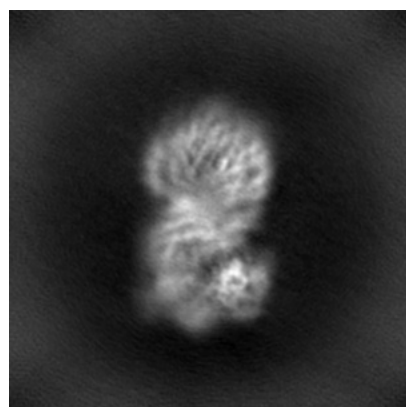


Y

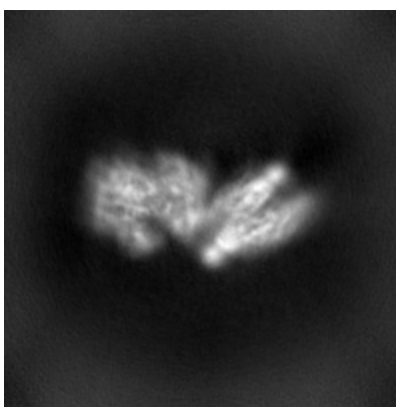


Z

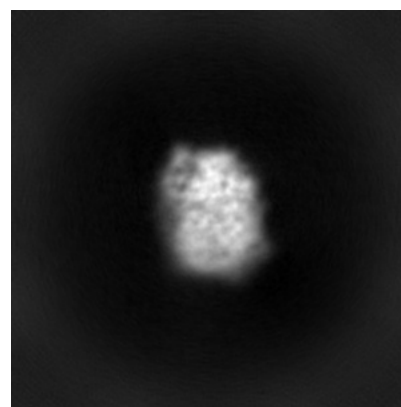
6.1.2 Raw map



X



Y

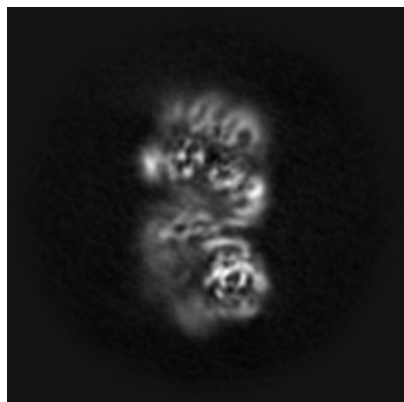


Z

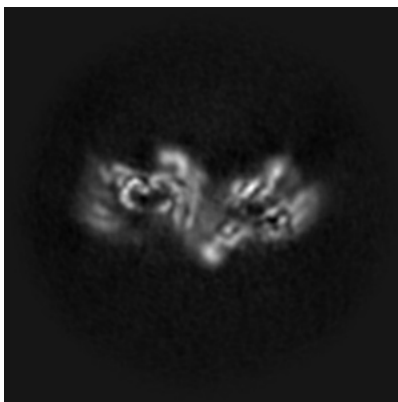
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

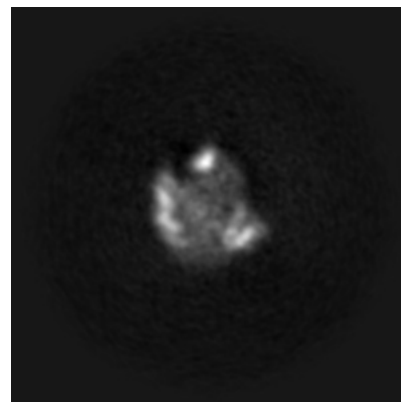
6.2.1 Primary map



X Index: 100

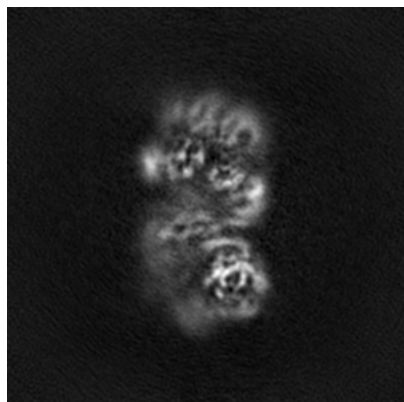


Y Index: 100

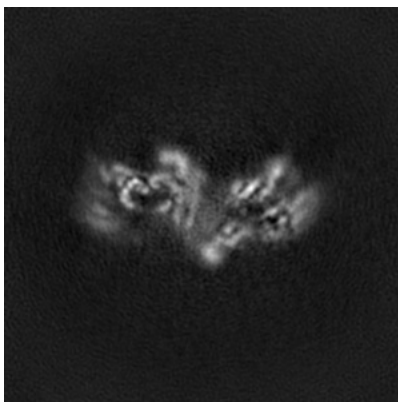


Z Index: 100

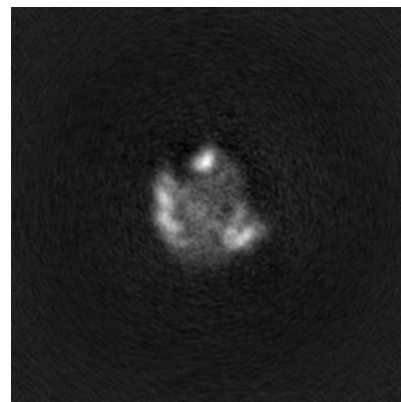
6.2.2 Raw map



X Index: 100



Y Index: 100

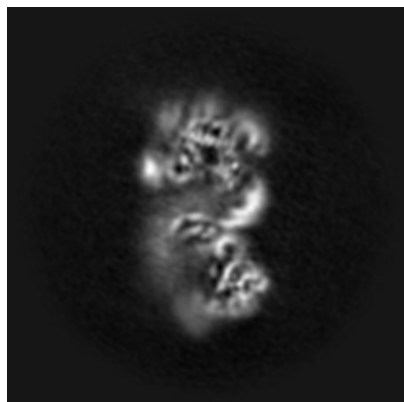


Z Index: 100

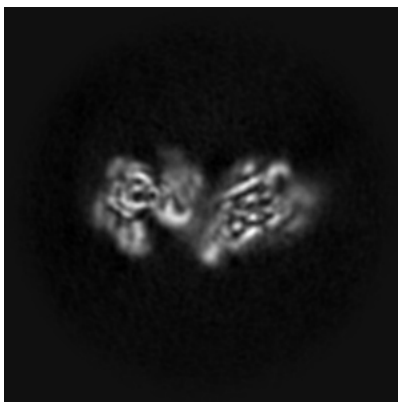
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

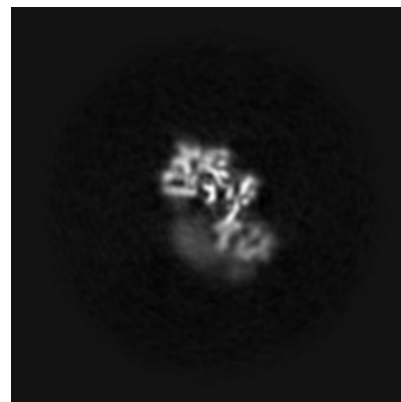
6.3.1 Primary map



X Index: 97

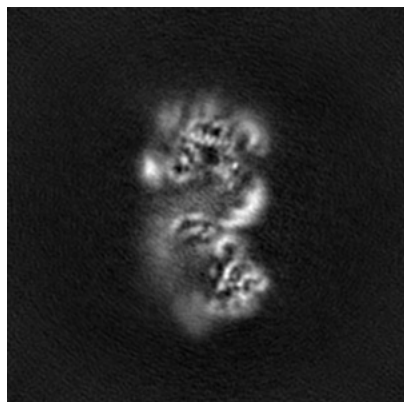


Y Index: 107

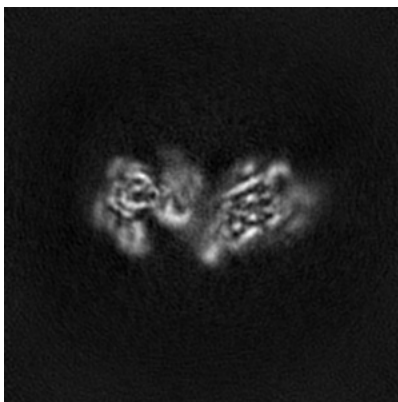


Z Index: 66

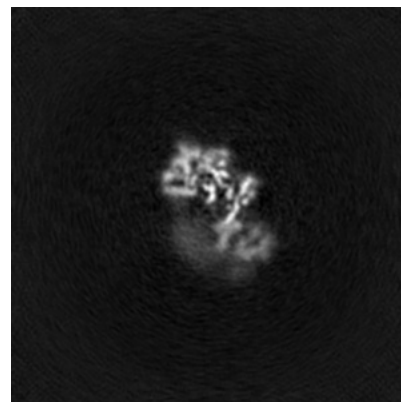
6.3.2 Raw map



X Index: 97



Y Index: 107

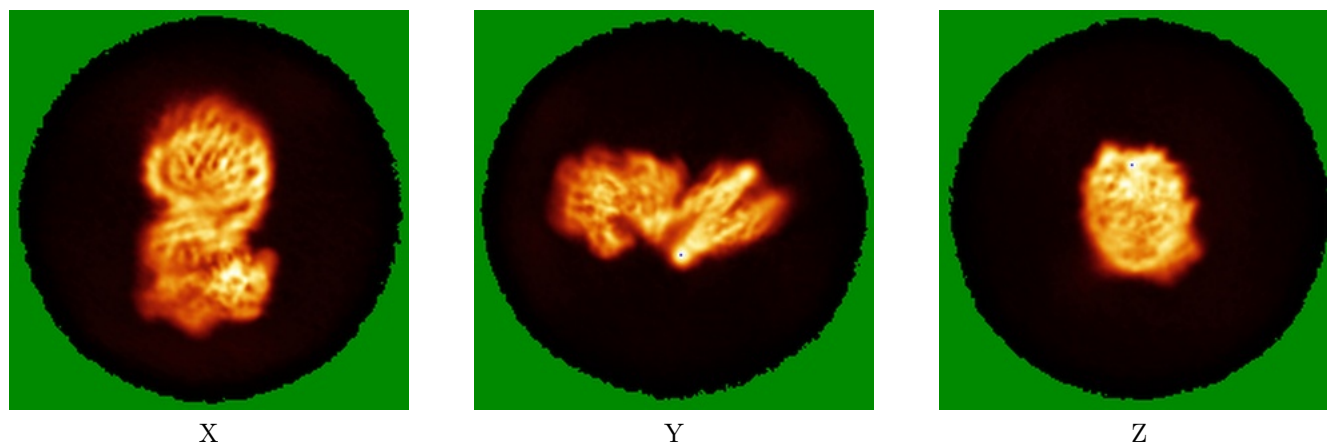


Z Index: 66

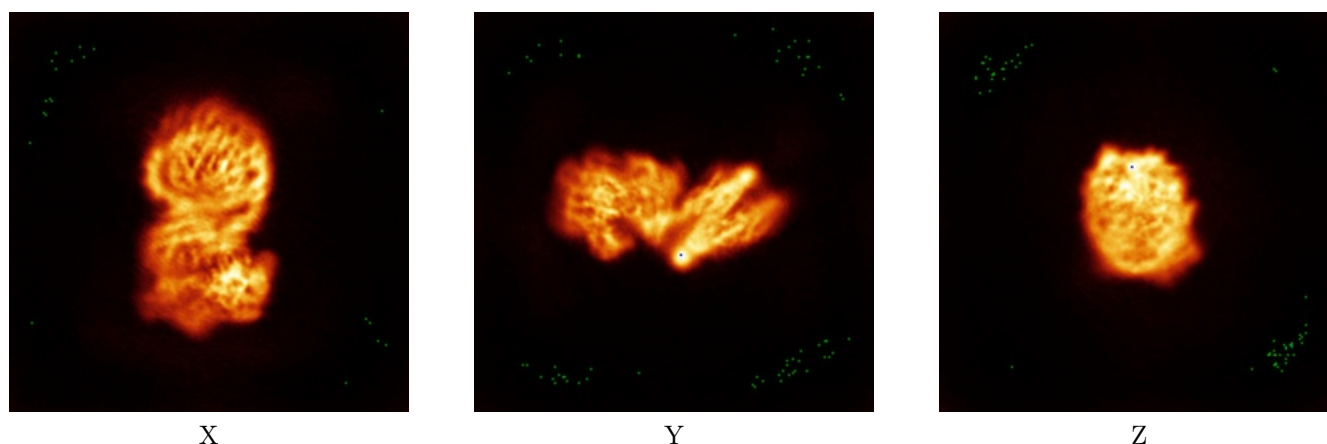
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

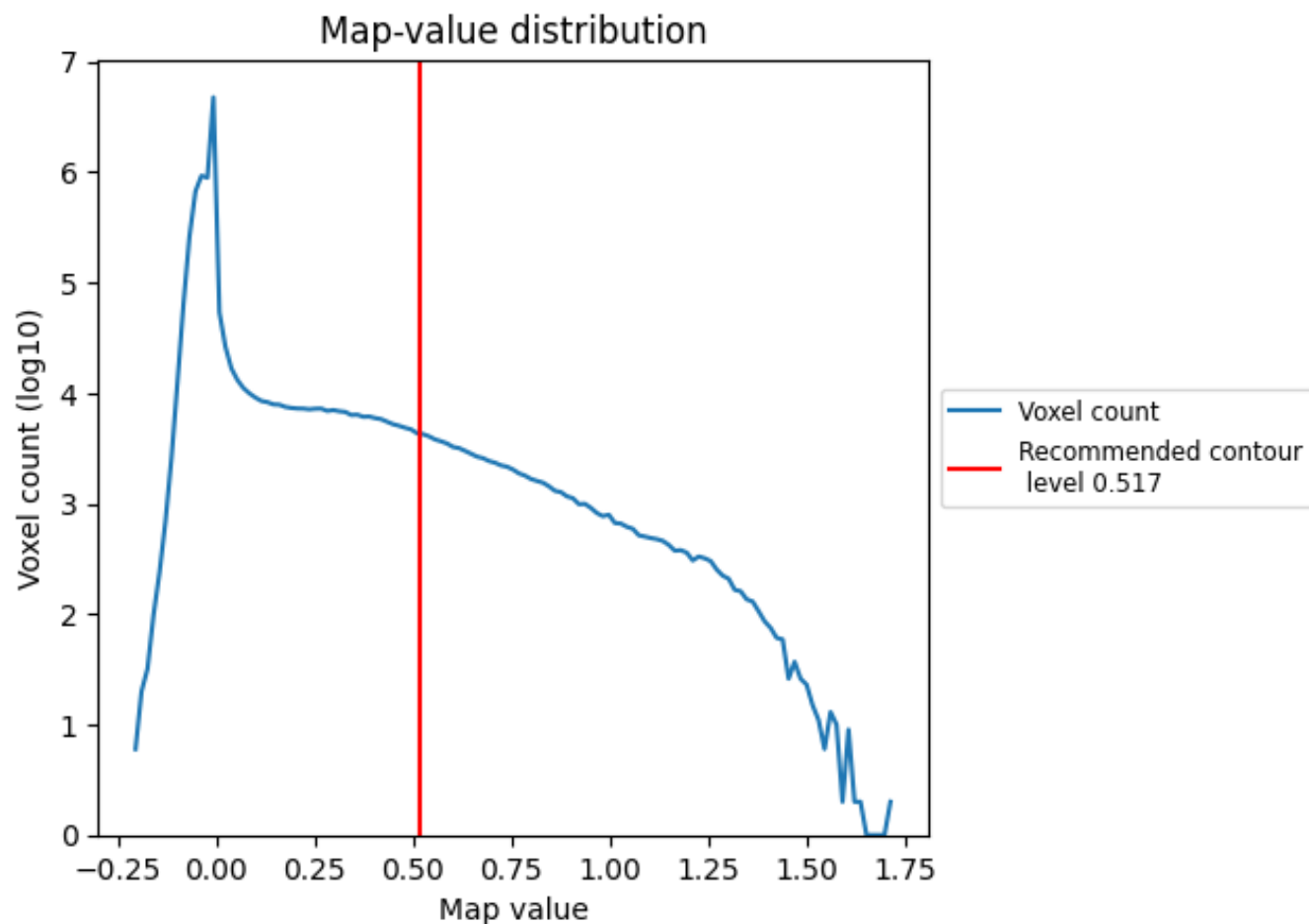
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

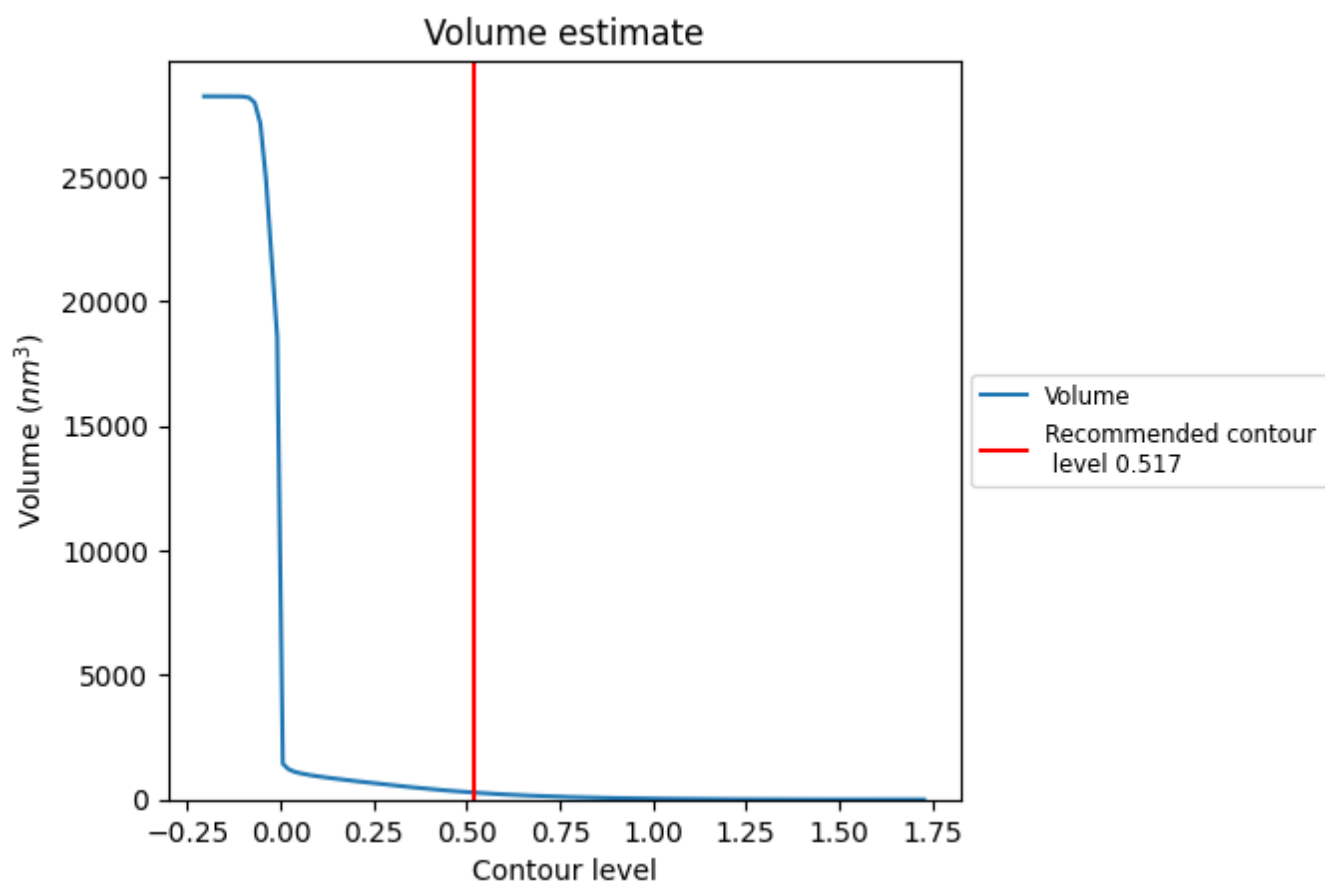
This section contains the results of statistical analysis of the map.

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.

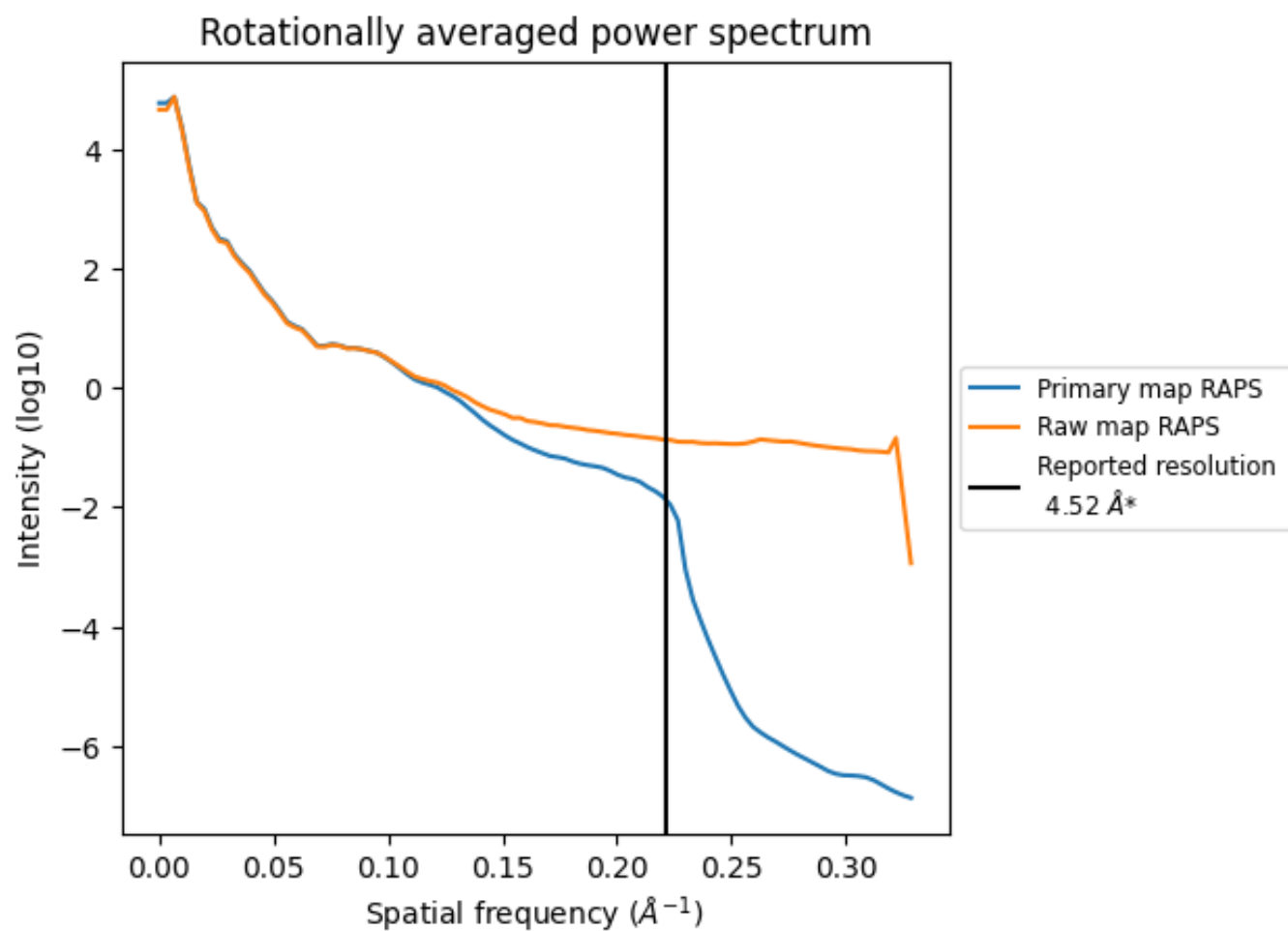
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 283 nm³; this corresponds to an approximate mass of 255 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

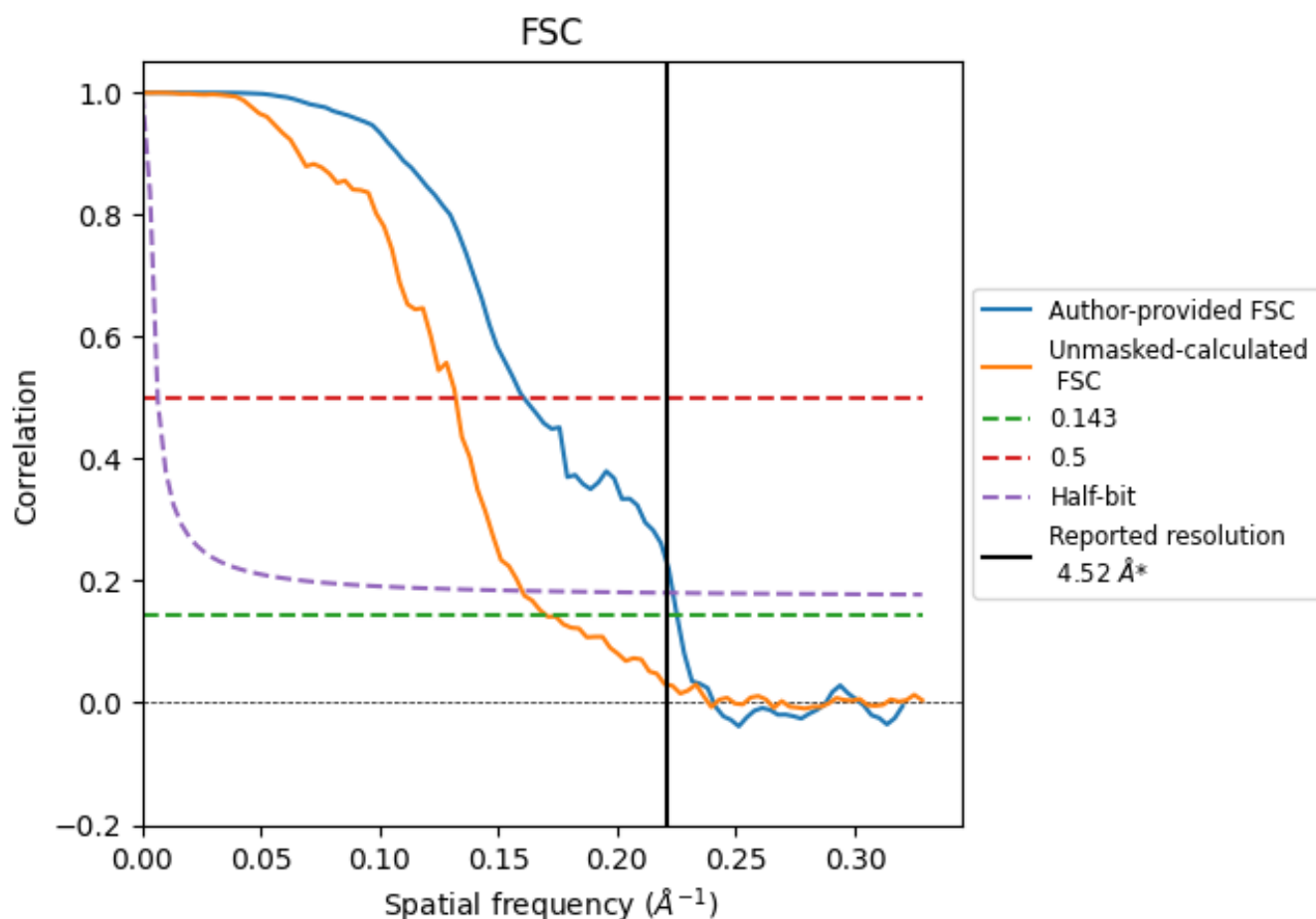


*Reported resolution corresponds to spatial frequency of $0.221 \text{ \AA}^{-1}$

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 0.221 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.52	-	-
Author-provided FSC curve	4.44	6.23	4.47
Unmasked-calculated*	5.88	7.58	6.25

*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 5.88 differs from the reported value 4.52 by more than 10 %

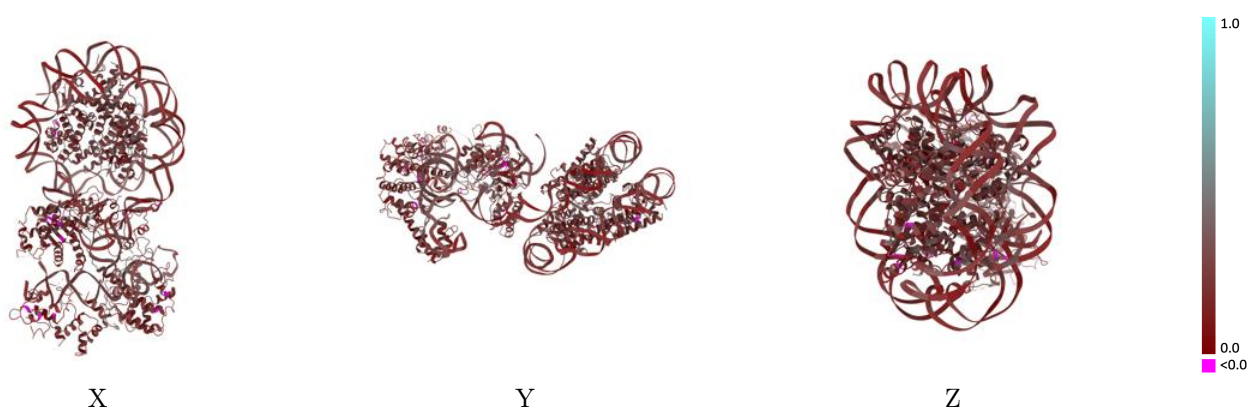
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39431 and PDB model 8YNY. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

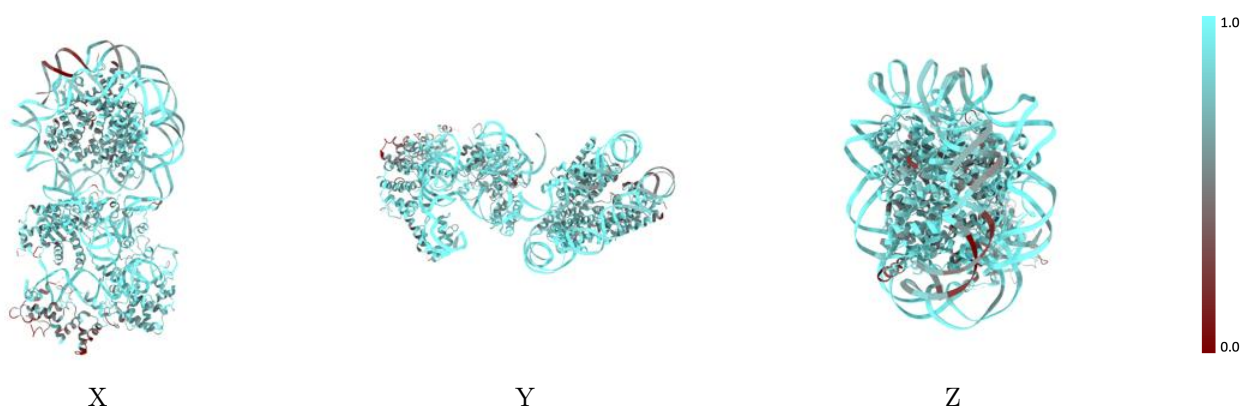
This section was not generated.

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



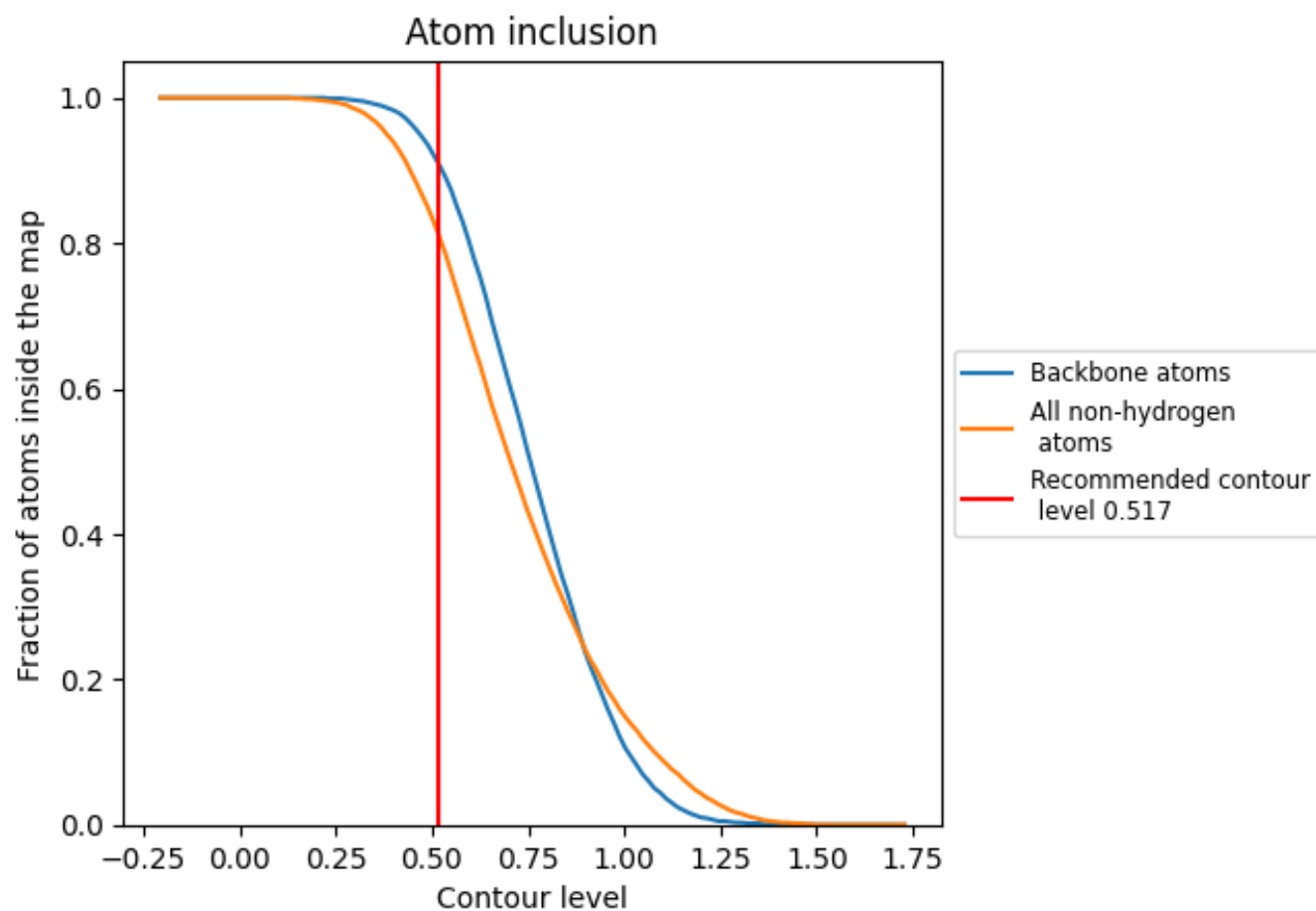
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.517).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 81% 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 (0.517) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8130	0.2180
A	0.7740	0.2070
B	0.7770	0.2230
C	0.8110	0.2350
D	0.8160	0.2520
E	0.8340	0.2180
F	0.8660	0.2260
G	0.7390	0.2270
H	0.7720	0.2260
I	0.8360	0.2060
J	0.8500	0.1970
K	0.9430	0.2760
W	0.9610	0.2720
X	0.7540	0.2070

1.0

0.0

<0.0