



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 09:38 PM UTC

PDB ID : 6J51 / pdb_00006j51
EMDB ID : EMD-0676
Title : RNA polymerase II elongation complex bound with Spt4/5 and foreign DNA, stalled at SHL(-1) of the nucleosome, weak Elf1 (+1 position)
Authors : Ehara, H.; Kujirai, T.; Fujino, Y.; Shirouzu, M.; Kurumizaka, H.; Sekine, S.
Deposited on : 2019-01-10
Resolution : 4.20 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:

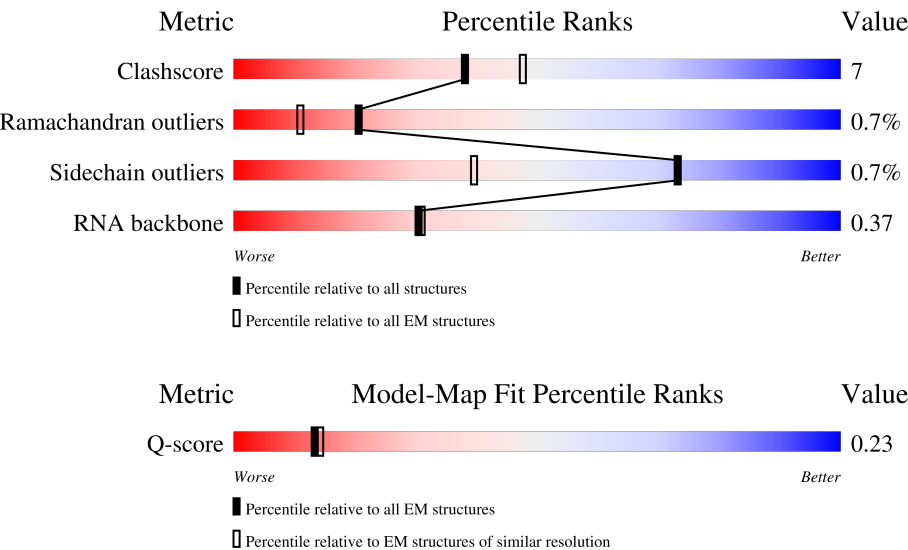
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.20 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	5410 (3.70 - 4.70)

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	1743	
2	B	1227	
3	C	304	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	186	
5	E	214	
6	F	155	
7	G	171	
8	H	145	
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	P	16	
14	T	198	
15	N	198	
16	M	113	
17	V	108	
18	W	911	
19	a	139	
19	e	139	
20	b	106	
20	f	106	
21	c	133	
21	g	133	
22	d	129	
22	h	129	
23	0	36	
24	1	36	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 47661 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1411	Total	C	N	O	S	0	0
			11116	7009	1937	2100	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1157	Total	C	N	O	S	0	0
			9228	5816	1630	1724	58		

- Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	263	Total	C	N	O	S	0	0
			2098	1319	354	413	12		

- Molecule 4 is a protein called RNA polymerase II subunit B32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	168	Total	C	N	O	S	0	0
			1314	812	237	263	2		

- Molecule 5 is a protein called RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1740	1094	312	324	10		

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			677	429	114	131	3		

- Molecule 7 is a protein called RNA polymerase II subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1324	858	214	247	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1052	671	169	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	111	Total	C	N	O	S	0	0
			917	565	161	180	11		

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			545	349	95	95	6		

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	113	Total	C	N	O	S	0	0
			932	599	160	169	4		

- Molecule 12 is a protein called RNA polymerase subunit ABC10-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	72	61	5		

- Molecule 13 is a RNA chain called RNA (5'-R(P*CP*CP*UP*GP*GP*UP*GP*UP*CP*UP*UP*GP*GP*GP*UP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	16	Total	C	N	O	P	0	0
			341	151	56	118	16		

- Molecule 14 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	127	Total	C	N	O	P	0	0
			2589	1227	486	750	126		

- Molecule 15 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	122	Total	C	N	O	P	0	0
			2509	1188	459	740	122		

- Molecule 16 is a protein called Transcription elongation factor 1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	64	Total	C	N	O	S	0	0
			505	318	82	99	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-2	GLY	-	expression tag	UNP C4QZ45
M	-1	PRO	-	expression tag	UNP C4QZ45
M	0	GLY	-	expression tag	UNP C4QZ45

- Molecule 17 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	102	Total	C	N	O	S	0	0
			792	492	143	150	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	7	MET	-	expression tag	UNP C4R0E6

- Molecule 18 is a protein called Protein that forms a complex with Spt4p.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	275	Total	C	N	O	S	0	0
			2226	1425	397	403	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-2	GLY	-	expression tag	UNP C4R370
W	-1	PRO	-	expression tag	UNP C4R370
W	0	GLY	-	expression tag	UNP C4R370

- Molecule 19 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	97	Total	C	N	O	S	0	0
			797	503	155	137	2		
19	e	97	Total	C	N	O	S	0	0
			796	501	155	138	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-3	GLY	-	expression tag	UNP P84243
a	-2	SER	-	expression tag	UNP P84243
a	-1	HIS	-	expression tag	UNP P84243
e	-3	GLY	-	expression tag	UNP P84243
e	-2	SER	-	expression tag	UNP P84243
e	-1	HIS	-	expression tag	UNP P84243

- Molecule 20 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
20	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

Continued on next page...

Continued from previous page...

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

- Molecule 21 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	c	103	Total	C	N	O	0	0
			796	502	155	139		
21	g	105	Total	C	N	O	0	0
			810	511	158	141		

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 22 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	d	95	Total	C	N	O	S	0	0
			746	468	136	140	2		
22	h	91	Total	C	N	O	S	0	0
			708	447	125	134	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 23 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	0	36	Total	C	N	O	P	0	0
			739	349	155	199	36		

- Molecule 24 is a DNA chain called DNA (36-MER).

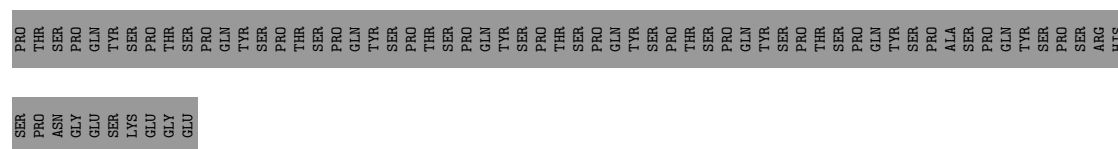
Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	36	Total	C	N	O	P	0	0
			737	354	114	233	36		

- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

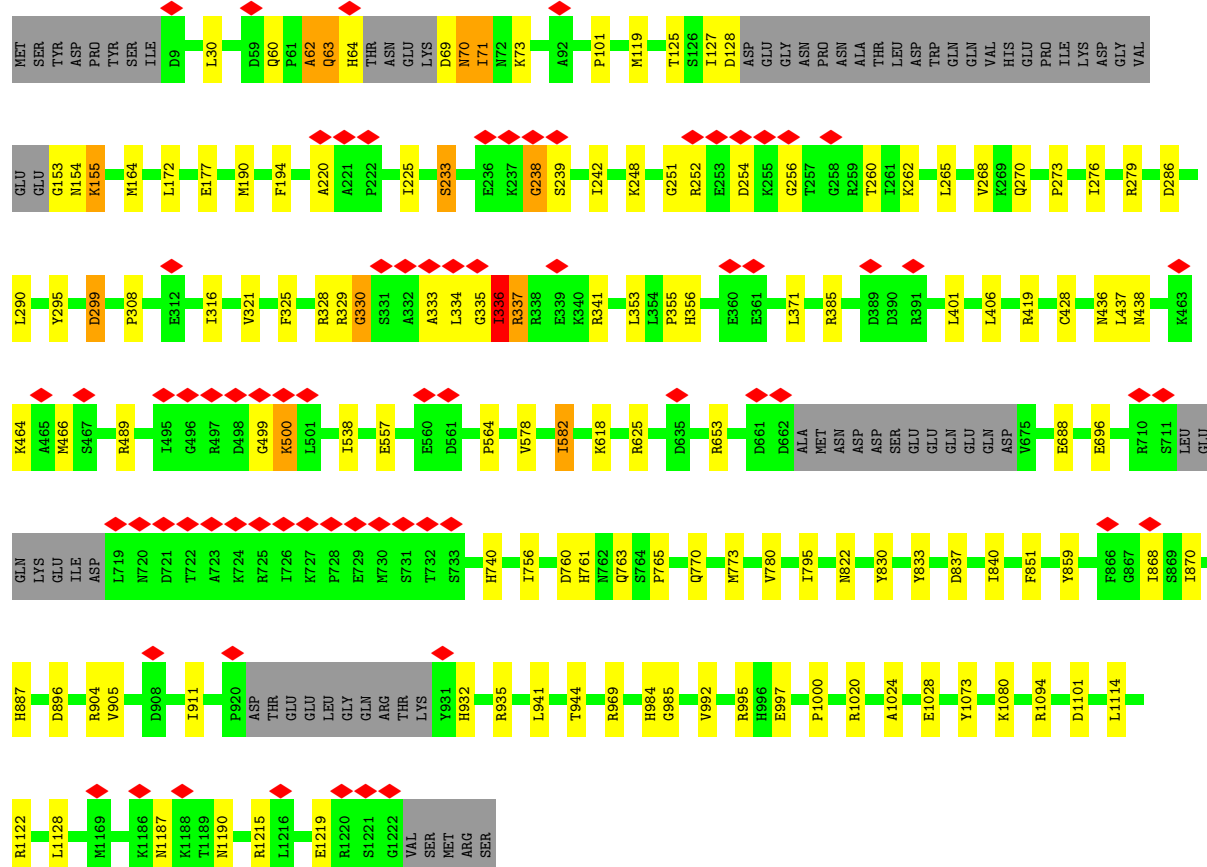
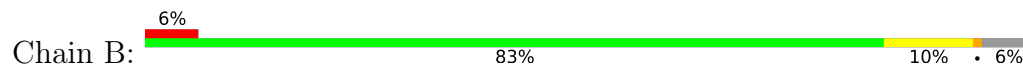
Mol	Chain	Residues	Atoms		AltConf
25	A	2	Total	Zn	0
			2	2	
25	B	1	Total	Zn	0
			1	1	
25	C	1	Total	Zn	0
			1	1	
25	I	2	Total	Zn	0
			2	2	
25	J	1	Total	Zn	0
			1	1	
25	L	1	Total	Zn	0
			1	1	
25	M	1	Total	Zn	0
			1	1	
25	V	1	Total	Zn	0
			1	1	

- Molecule 26 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

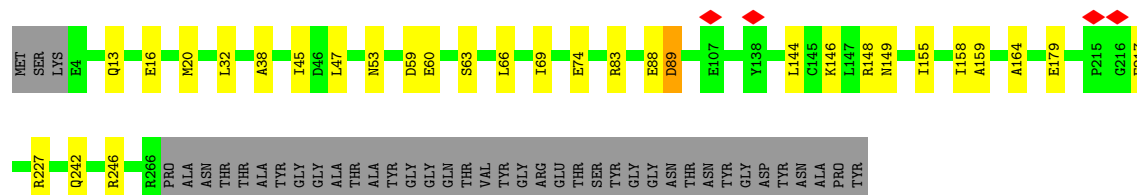
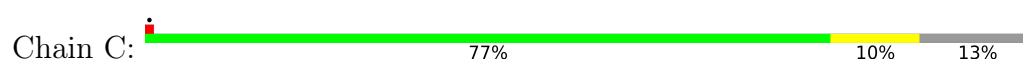
Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total	Mg	0
			1	1	



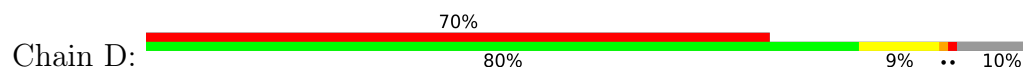
• Molecule 2: DNA-directed RNA polymerase subunit beta

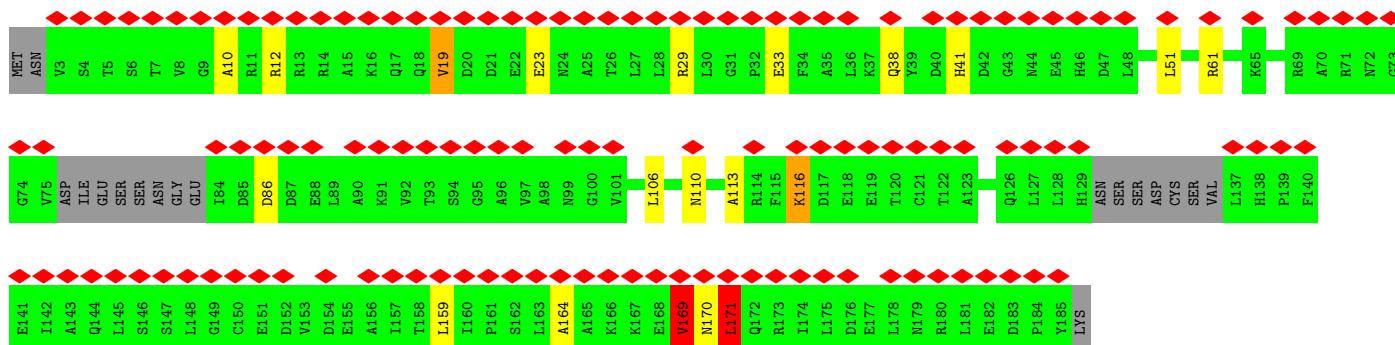


• Molecule 3: RNA polymerase II third largest subunit B44, part of central core



• Molecule 4: RNA polymerase II subunit B32





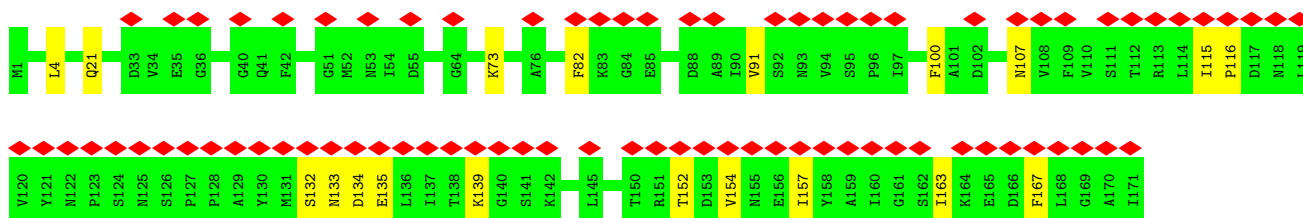
- Molecule 5: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III



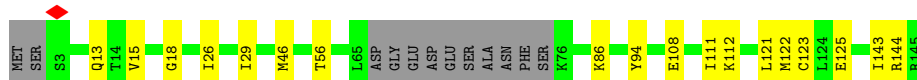
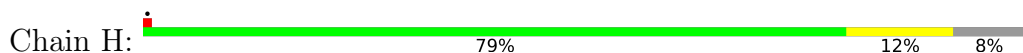
- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III



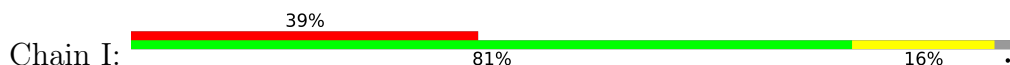
- Molecule 7: RNA polymerase II subunit

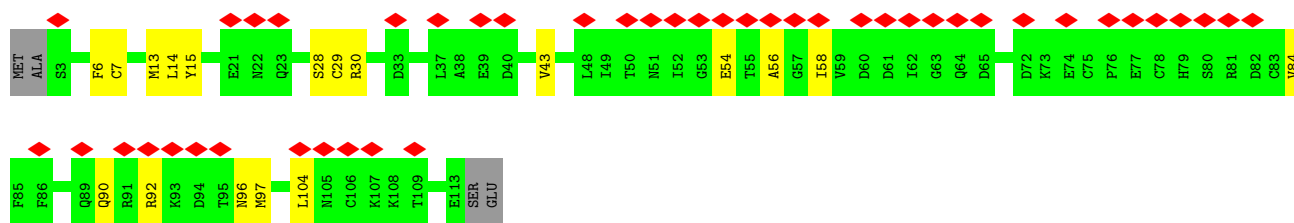


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

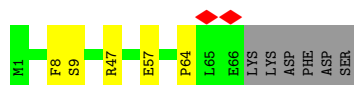
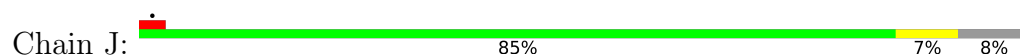


- Molecule 9: DNA-directed RNA polymerase subunit

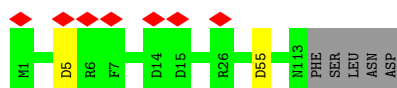




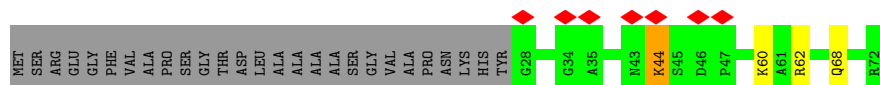
- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III



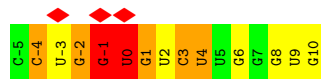
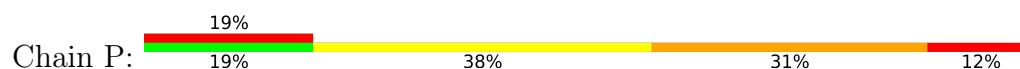
- Molecule 11: RNA polymerase II subunit B12.5



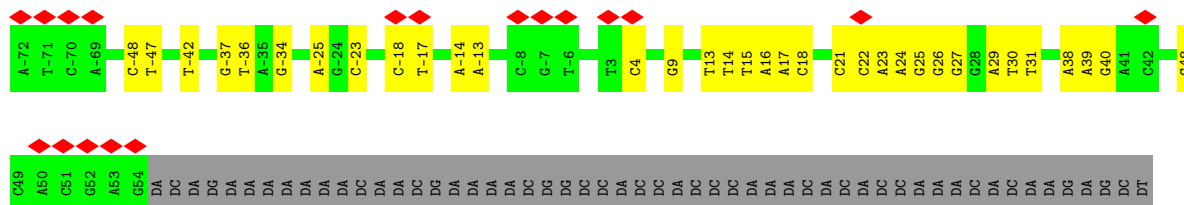
- Molecule 12: RNA polymerase subunit ABC10-alpha



- Molecule 13: RNA (5'-R(P*CP*CP*UP*GP*GP*UP*GP*UP*CP*UP*UP*GP*GP*GP*UP*G)-3')

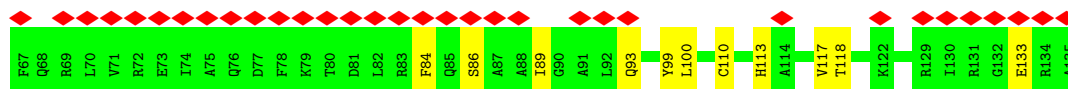
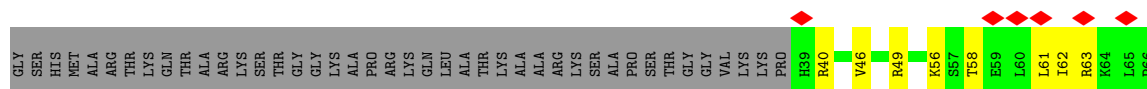


- Molecule 14: DNA (198-MER)

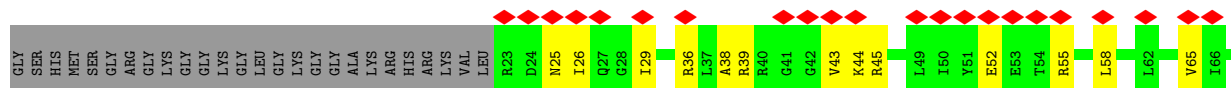




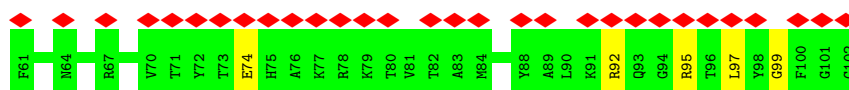
- Molecule 19: Histone H3.3



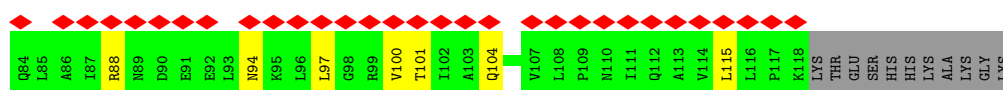
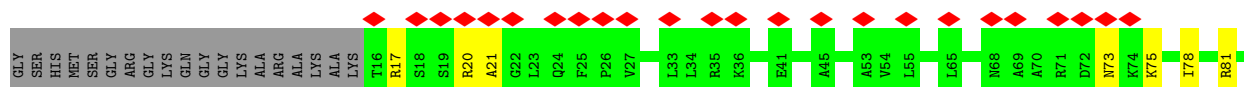
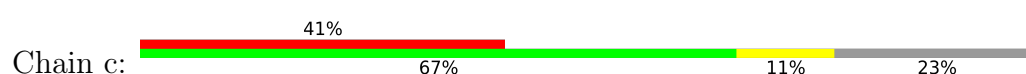
- Molecule 20: Histone H4



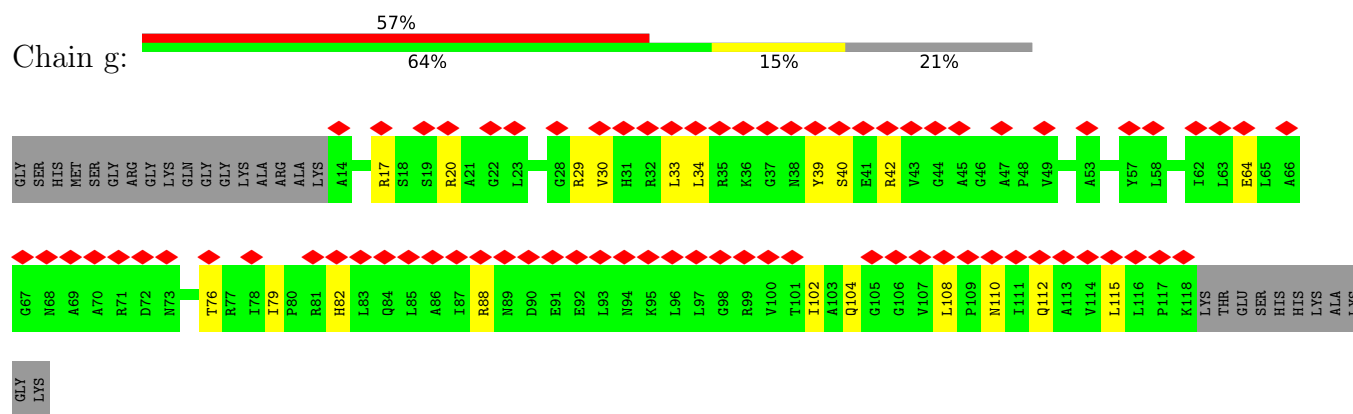
- Molecule 20: Histone H4



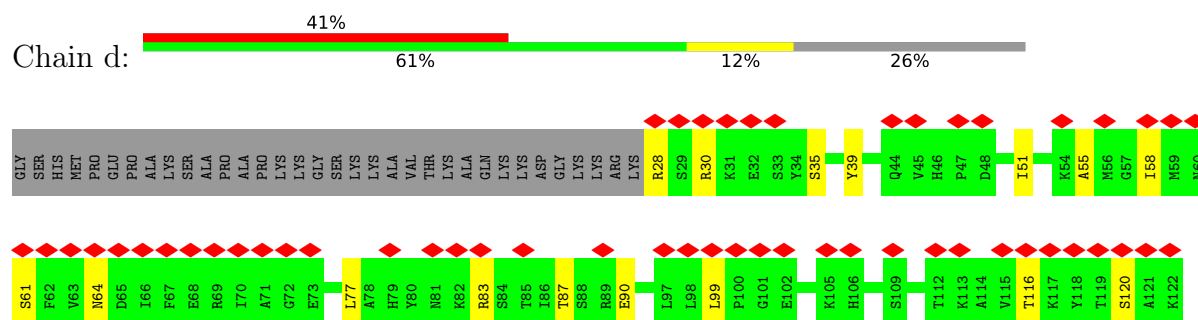
- Molecule 21: Histone H2A type 1-B/E



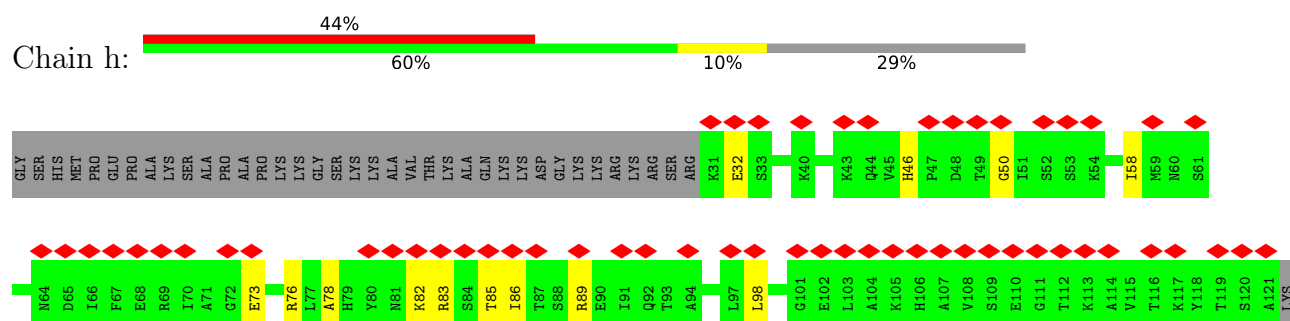
- Molecule 21: Histone H2A type 1-B/E



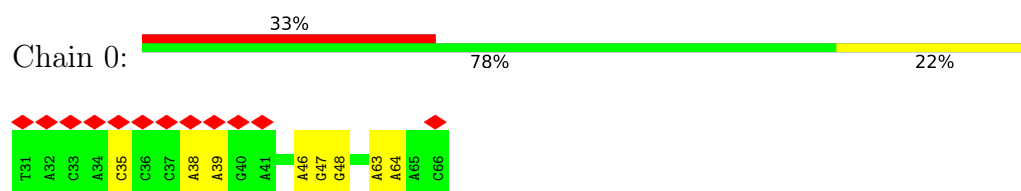
• Molecule 22: Histone H2B type 1-J



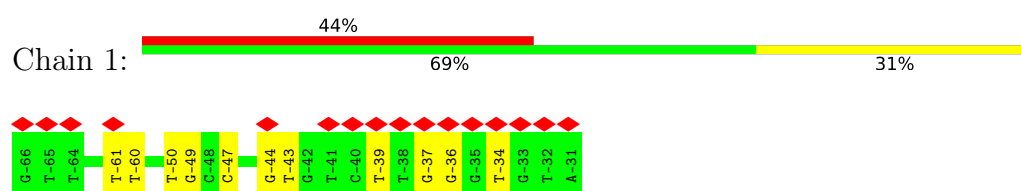
• Molecule 22: Histone H2B type 1-J



• Molecule 23: DNA (36-MER)



• Molecule 24: DNA (36-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	31784	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.024	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.016	Depositor
Map size ($\text{\AA}$)	357.6, 357.6, 357.6	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.49, 1.49, 1.49	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: ZN, MG

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	0.39	0/11322	0.74	3/15300 (0.0%)
2	B	0.43	0/9407	0.79	11/12685 (0.1%)
3	C	0.42	0/2139	0.76	4/2895 (0.1%)
4	D	0.30	0/1326	0.79	4/1788 (0.2%)
5	E	0.36	0/1772	0.73	0/2385
6	F	0.39	0/687	0.68	0/931
7	G	0.32	0/1353	0.79	2/1837 (0.1%)
8	H	0.36	0/1069	0.72	0/1444
9	I	0.32	0/934	0.89	4/1257 (0.3%)
10	J	0.46	0/554	0.80	0/742
11	K	0.40	0/953	0.73	0/1291
12	L	0.38	0/365	0.85	1/484 (0.2%)
13	P	0.95	5/379 (1.3%)	0.67	0/589
14	T	0.50	0/2905	0.65	0/4477
15	N	0.51	0/2812	0.67	0/4339
16	M	0.16	0/513	0.32	0/693
17	V	0.61	2/808 (0.2%)	0.91	1/1097 (0.1%)
18	W	0.50	2/2267 (0.1%)	0.86	5/3048 (0.2%)
19	a	0.38	0/809	0.74	0/1085
19	e	0.41	0/807	0.67	0/1081
20	b	0.41	0/645	0.76	0/862
20	f	0.40	0/626	0.70	0/837
21	c	0.41	0/806	0.65	0/1089
21	g	0.36	0/820	0.60	0/1107
22	d	0.41	0/757	0.66	0/1015
22	h	0.37	0/719	0.64	0/968
23	o	0.39	0/834	0.60	0/1282
24	l	0.41	0/820	0.63	0/1266
All	All	0.43	9/49208 (0.0%)	0.74	35/67874 (0.1%)

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
2	B	0	1
19	a	0	2
19	e	0	1
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	V	29	CYS	C-N	8.28	1.43	1.33
13	P	-2	G	C1'-N9	-7.52	1.36	1.48
13	P	-1	G	C1'-N9	-7.52	1.36	1.48
18	W	440	ILE	CA-C	-7.42	1.43	1.52
13	P	4	U	C1'-N1	6.92	1.58	1.48
17	V	63	ASN	C-N	-6.25	1.24	1.33
13	P	10	G	C1'-N9	-5.40	1.39	1.48
13	P	0	U	C1'-N1	5.36	1.55	1.47
18	W	307	LYS	C-N	-5.01	1.27	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	GLN	N-CA-C	-9.58	92.36	108.26
18	W	389	PRO	CA-N-CD	-8.94	99.49	112.00
2	B	63	GLN	N-CA-CB	-8.60	96.75	110.77
17	V	29	CYS	O-C-N	-8.23	114.31	121.31
18	W	388	ARG	CA-C-N	7.12	128.73	119.84
18	W	388	ARG	C-N-CA	7.12	128.73	119.84
2	B	336	ILE	CA-CB-CG2	6.97	122.35	110.50
7	G	133	ASN	CA-C-N	6.54	134.04	121.54
7	G	133	ASN	C-N-CA	6.54	134.04	121.54
4	D	170	ASN	CA-C-N	6.36	133.68	121.54
4	D	170	ASN	C-N-CA	6.36	133.68	121.54
2	B	238	GLY	CA-C-N	6.08	133.16	121.54
2	B	238	GLY	C-N-CA	6.08	133.16	121.54
2	B	60	GLN	CA-C-N	5.93	127.25	119.84
2	B	60	GLN	C-N-CA	5.93	127.25	119.84
1	A	1108	ASN	CA-C-N	5.71	132.25	121.97
1	A	1108	ASN	C-N-CA	5.71	132.25	121.97
1	A	473	LEU	CA-CB-CG	-5.69	96.37	116.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	330	GLY	N-CA-C	5.67	126.62	113.18
2	B	932	HIS	N-CA-C	-5.63	98.81	110.80
12	L	44	LYS	N-CA-C	5.55	122.63	110.80
3	C	88	GLU	CA-C-N	5.33	131.73	121.54
3	C	88	GLU	C-N-CA	5.33	131.73	121.54
4	D	169	VAL	CB-CA-C	5.21	119.83	111.29
4	D	169	VAL	CA-CB-CG1	5.20	119.23	110.40
9	I	58	ILE	CA-C-N	-5.16	115.02	122.45
9	I	58	ILE	C-N-CA	-5.16	115.02	122.45
3	C	89	ASP	CA-C-N	-5.15	111.69	122.03
3	C	89	ASP	C-N-CA	-5.15	111.69	122.03
2	B	499	GLY	N-CA-C	-5.10	101.09	113.18
18	W	306	TYR	CA-C-N	-5.07	112.60	120.31
18	W	306	TYR	C-N-CA	-5.07	112.60	120.31
2	B	336	ILE	CA-CB-CG1	5.05	118.98	110.40
9	I	54	GLU	CA-C-N	5.05	132.39	121.64
9	I	54	GLU	C-N-CA	5.05	132.39	121.64

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	336	ILE	Mainchain
19	a	42	ARG	Peptide
19	a	63	ARG	Peptide
19	e	63	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11116	0	11138	97	0
2	B	9228	0	9232	119	0
3	C	2098	0	2059	18	0
4	D	1314	0	1314	11	0
5	E	1740	0	1754	9	0
6	F	677	0	693	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1324	0	1342	11	0
8	H	1052	0	1050	9	0
9	I	917	0	868	9	0
10	J	545	0	561	4	0
11	K	932	0	944	2	0
12	L	359	0	358	3	0
13	P	341	0	170	20	0
14	T	2589	0	1420	87	0
15	N	2509	0	1373	102	0
16	M	505	0	496	25	0
17	V	792	0	757	7	0
18	W	2226	0	2273	142	0
19	a	797	0	835	23	0
19	e	796	0	832	16	0
20	b	638	0	676	19	0
20	f	619	0	659	16	0
21	c	796	0	848	10	0
21	g	810	0	866	14	0
22	d	746	0	771	12	0
22	h	708	0	727	12	0
23	0	739	0	398	5	0
24	1	737	0	415	8	0
25	A	2	0	0	0	0
25	B	1	0	0	0	0
25	C	1	0	0	0	0
25	I	2	0	0	0	0
25	J	1	0	0	0	0
25	L	1	0	0	0	0
25	M	1	0	0	0	0
25	V	1	0	0	0	0
26	A	1	0	0	0	0
All	All	47661	0	44829	649	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 7.

All (649) 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)
14:T:22:DC:C2	15:N:-22:DG:N2	1.86	1.43
14:T:22:DC:N3	15:N:-22:DG:N2	1.66	1.38

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:-25:DC:C2'	15:N:-24:DT:H72	1.64	1.27
14:T:22:DC:H2''	14:T:23:DA:C1'	1.66	1.24
1:A:288:HIS:CD2	18:W:299:PHE:CZ	2.26	1.23
18:W:409:ASP:HB2	18:W:413:PHE:CD2	1.73	1.23
15:N:-25:DC:C2'	15:N:-24:DT:C7	2.18	1.21
18:W:333:PHE:CD1	18:W:354:LEU:HD21	1.73	1.21
2:B:337:ARG:HD2	16:M:78:GLU:OE1	1.38	1.19
15:N:-25:DC:H2''	15:N:-24:DT:C7	1.73	1.18
14:T:22:DC:N4	15:N:-22:DG:H1	1.41	1.16
18:W:333:PHE:CG	18:W:354:LEU:HD21	1.80	1.14
14:T:27:DG:O6	15:N:-27:DC:N4	1.79	1.14
14:T:13:DT:H2''	14:T:14:DT:C6	1.83	1.14
14:T:22:DC:O2	15:N:-22:DG:N2	1.80	1.13
14:T:18:DC:O2	15:N:-18:DG:N2	1.79	1.13
14:T:22:DC:H2'	14:T:23:DA:C8	1.84	1.12
14:T:22:DC:N3	15:N:-22:DG:C2	2.16	1.11
18:W:409:ASP:HB2	18:W:413:PHE:HD2	1.04	1.11
1:A:976:ASP:O	1:A:977:ARG:HB2	1.51	1.10
14:T:25:DG:H2''	14:T:26:DG:H5'	1.10	1.09
18:W:352:LEU:HD11	18:W:435:LEU:HD11	1.31	1.09
18:W:399:ALA:HB1	18:W:406:ILE:HD11	1.27	1.08
18:W:332:LYS:HD2	18:W:389:PRO:HD3	1.24	1.06
2:B:419:ARG:HH11	15:N:-39:DT:H1'	1.13	1.05
15:N:-25:DC:H2''	15:N:-24:DT:H73	1.33	1.05
14:T:13:DT:H2'	14:T:14:DT:H72	1.36	1.05
14:T:13:DT:H2'	14:T:14:DT:C7	1.86	1.03
2:B:419:ARG:NH1	15:N:-39:DT:H1'	1.71	1.03
15:N:-25:DC:H2'	15:N:-24:DT:H72	1.39	1.03
18:W:320:LEU:HD22	18:W:432:LEU:CD1	1.89	1.02
14:T:48:DG:H5''	18:W:330:ASN:HD21	1.26	1.01
18:W:320:LEU:HD22	18:W:432:LEU:HD13	1.37	1.01
18:W:399:ALA:CB	18:W:406:ILE:HD11	1.90	1.01
1:A:288:HIS:CD2	18:W:299:PHE:CE1	2.48	1.01
15:N:24:DC:H2''	15:N:25:DT:C5	1.95	1.00
2:B:62:ALA:O	2:B:70:ASN:HA	1.62	1.00
14:T:22:DC:H42	15:N:-22:DG:H1	1.00	1.00
14:T:22:DC:N3	15:N:-22:DG:N1	2.11	0.99
18:W:396:GLU:OE2	18:W:414:VAL:HG23	1.64	0.98
14:T:22:DC:H2''	14:T:23:DA:N9	1.77	0.97
18:W:399:ALA:HB1	18:W:406:ILE:CD1	1.95	0.96
14:T:-25:DA:N1	15:N:25:DT:N3	2.12	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:22:DC:H2''	14:T:23:DA:O4'	1.65	0.95
18:W:409:ASP:CB	18:W:413:PHE:CD2	2.50	0.94
2:B:62:ALA:CB	2:B:71:ILE:CG2	2.46	0.94
1:A:286:PRO:CG	18:W:268:PHE:CZ	2.51	0.94
2:B:62:ALA:HB3	2:B:71:ILE:CG2	1.97	0.94
1:A:288:HIS:NE2	18:W:299:PHE:CZ	2.36	0.93
14:T:14:DT:H2''	14:T:15:DT:C5	2.03	0.93
2:B:337:ARG:CD	16:M:78:GLU:OE1	2.17	0.93
14:T:22:DC:C2'	14:T:23:DA:N9	2.31	0.93
18:W:409:ASP:CB	18:W:413:PHE:HD2	1.81	0.93
14:T:29:DA:H2''	14:T:30:DT:H71	1.49	0.92
15:N:-22:DG:H2''	15:N:-21:DG:C8	2.04	0.92
18:W:399:ALA:C	18:W:406:ILE:CD1	2.43	0.91
14:T:25:DG:C2'	14:T:26:DG:H5'	1.99	0.89
18:W:394:PHE:HE2	18:W:396:GLU:HG2	1.37	0.88
1:A:288:HIS:NE2	18:W:299:PHE:CE1	2.41	0.88
1:A:197:GLN:NE2	16:M:50:LYS:HB3	1.87	0.88
14:T:22:DC:C2'	14:T:23:DA:C8	2.57	0.88
17:V:85:ARG:NH1	17:V:87:ASP:OD1	2.07	0.88
14:T:13:DT:H2''	14:T:14:DT:H6	1.37	0.88
18:W:320:LEU:CD2	18:W:432:LEU:HD13	2.05	0.87
2:B:62:ALA:CB	2:B:71:ILE:HG23	2.03	0.87
14:T:24:DA:H2''	14:T:25:DG:H5''	1.57	0.86
18:W:333:PHE:CG	18:W:354:LEU:CD2	2.59	0.86
18:W:388:ARG:HB2	18:W:389:PRO:HD3	1.58	0.85
18:W:409:ASP:O	18:W:410:ARG:HG3	1.75	0.85
1:A:197:GLN:HE22	16:M:50:LYS:HB3	1.40	0.84
18:W:352:LEU:HD11	18:W:435:LEU:CD1	2.07	0.84
13:P:1:G:H2'	13:P:2:U:C6	2.13	0.84
18:W:357:ARG:C	18:W:389:PRO:HG2	2.02	0.84
14:T:29:DA:C2'	14:T:30:DT:H71	2.08	0.83
15:N:-25:DC:H2'	15:N:-24:DT:C7	1.99	0.83
15:N:-24:DT:C2	15:N:-23:DT:C5	2.67	0.83
18:W:332:LYS:HD2	18:W:388:ARG:HB2	1.59	0.83
2:B:62:ALA:HB3	2:B:71:ILE:HG22	1.59	0.83
2:B:500:LYS:H	2:B:500:LYS:HD3	1.42	0.82
1:A:286:PRO:HG2	18:W:268:PHE:CZ	2.14	0.82
18:W:329:LYS:HD2	18:W:436:ILE:HG13	1.59	0.82
18:W:399:ALA:C	18:W:406:ILE:HD11	2.02	0.82
14:T:13:DT:C2'	14:T:14:DT:C6	2.61	0.82
2:B:62:ALA:CB	2:B:71:ILE:HG22	2.09	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:-25:DC:C2'	15:N:-24:DT:H73	2.00	0.81
18:W:399:ALA:CB	18:W:406:ILE:CD1	2.55	0.80
18:W:357:ARG:HB3	18:W:389:PRO:HD2	1.64	0.80
16:M:33:SER:HA	16:M:50:LYS:HE2	1.63	0.80
2:B:328:ARG:HD3	16:M:68:ASP:OD1	1.81	0.80
1:A:286:PRO:HG2	18:W:268:PHE:CE2	2.16	0.79
15:N:-25:DC:C1'	15:N:-24:DT:H72	2.12	0.79
15:N:-40:DC:OP2	15:N:-40:DC:H2'	1.82	0.79
18:W:328:VAL:HA	18:W:435:LEU:HD23	1.64	0.79
15:N:-22:DG:C2'	15:N:-21:DG:C8	2.65	0.79
14:T:22:DC:C2'	14:T:23:DA:O4'	2.29	0.79
15:N:-24:DT:C2	15:N:-23:DT:C7	2.66	0.78
2:B:419:ARG:NH1	15:N:-39:DT:C1'	2.45	0.78
15:N:-22:DG:H2''	15:N:-21:DG:H8	1.46	0.78
2:B:328:ARG:CD	16:M:68:ASP:OD1	2.32	0.78
14:T:48:DG:H5''	18:W:330:ASN:ND2	1.99	0.77
15:N:-25:DC:N1	15:N:-24:DT:H72	1.98	0.77
14:T:22:DC:C5	14:T:23:DA:C6	2.71	0.77
18:W:319:LYS:O	18:W:320:LEU:CB	2.33	0.77
18:W:394:PHE:CE2	18:W:396:GLU:HG2	2.18	0.76
1:A:288:HIS:CE1	18:W:299:PHE:CE1	2.74	0.76
1:A:288:HIS:CE1	18:W:299:PHE:HE1	2.04	0.76
1:A:286:PRO:CD	18:W:268:PHE:CZ	2.69	0.75
15:N:-25:DC:C6	15:N:-24:DT:H72	2.21	0.75
14:T:13:DT:C2'	14:T:14:DT:C7	2.65	0.75
14:T:26:DG:O6	15:N:-26:DC:N4	2.15	0.74
18:W:396:GLU:OE2	18:W:414:VAL:CG2	2.36	0.73
14:T:22:DC:N4	15:N:-22:DG:N1	2.20	0.72
18:W:328:VAL:HG22	18:W:435:LEU:HD21	1.70	0.72
2:B:868:ILE:HG12	15:N:-46:DT:OP1	1.89	0.72
18:W:388:ARG:HB2	18:W:389:PRO:CD	2.19	0.72
22:h:83:ARG:HH21	24:l:-34:DT:H5''	1.55	0.71
1:A:45:ARG:O	1:A:45:ARG:HG2	1.88	0.71
16:M:52:CYS:O	16:M:53:ASN:HB2	1.90	0.71
15:N:-15:DA:H2''	15:N:-14:DA:C8	2.25	0.71
18:W:333:PHE:CD1	18:W:354:LEU:CD2	2.65	0.71
18:W:323:GLY:HA2	18:W:339:GLN:HE21	1.54	0.71
18:W:326:VAL:HG21	18:W:435:LEU:HD13	1.71	0.71
15:N:-41:DT:OP1	18:W:233:LEU:HD13	1.90	0.71
15:N:-40:DC:H1'	15:N:-39:DT:C7	2.20	0.70
14:T:25:DG:H2''	14:T:26:DG:C5'	2.06	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:21:DC:H2''	14:T:22:DC:H5''	1.72	0.70
2:B:71:ILE:HD12	2:B:127:ILE:HG23	1.73	0.70
15:N:-24:DT:O2	15:N:-23:DT:C5	2.44	0.70
2:B:500:LYS:HD3	2:B:500:LYS:N	2.06	0.70
15:N:24:DC:H2''	15:N:25:DT:C6	2.27	0.69
18:W:357:ARG:HB3	18:W:389:PRO:CD	2.22	0.69
15:N:-24:DT:O2	15:N:-23:DT:C6	2.45	0.69
1:A:1160:PRO:HB3	1:A:1190:GLN:HE21	1.56	0.69
14:T:18:DC:C2	15:N:-18:DG:N2	2.46	0.69
2:B:62:ALA:HB3	2:B:71:ILE:HG23	1.70	0.69
18:W:320:LEU:HD22	18:W:432:LEU:HD11	1.74	0.69
18:W:332:LYS:HG3	18:W:388:ARG:CB	2.22	0.69
1:A:14:VAL:H	1:A:1435:GLN:HE22	1.40	0.69
2:B:935:ARG:NH2	13:P:0:U:C4	2.61	0.68
18:W:357:ARG:HB3	18:W:389:PRO:HG2	1.75	0.68
18:W:399:ALA:CA	18:W:406:ILE:HD11	2.23	0.68
18:W:357:ARG:O	18:W:389:PRO:HG2	1.94	0.68
14:T:13:DT:C2'	14:T:14:DT:C5	2.77	0.68
18:W:329:LYS:CD	18:W:436:ILE:HG13	2.24	0.67
18:W:332:LYS:CD	18:W:388:ARG:HB2	2.24	0.67
12:L:68:GLN:HB3	18:W:784:ASN:HD21	1.61	0.66
14:T:14:DT:H2''	14:T:15:DT:H72	1.77	0.66
2:B:935:ARG:NH2	13:P:0:U:C5	2.62	0.66
18:W:329:LYS:HD2	18:W:436:ILE:CG1	2.25	0.66
18:W:409:ASP:O	18:W:410:ARG:CG	2.43	0.66
18:W:351:ARG:HG2	18:W:429:THR:HG22	1.78	0.66
2:B:335:GLY:HA2	16:M:74:ILE:HD13	1.78	0.66
1:A:243:PRO:O	1:A:248:ARG:NH1	2.28	0.65
7:G:132:SER:HB2	7:G:135:GLU:HB2	1.78	0.65
2:B:63:GLN:OE1	18:W:249:ALA:HA	1.96	0.65
2:B:70:ASN:O	2:B:127:ILE:HA	1.97	0.65
1:A:466:TYR:HB2	1:A:470:ARG:HH22	1.61	0.65
14:T:14:DT:H2''	14:T:15:DT:C7	2.27	0.65
18:W:409:ASP:CB	18:W:413:PHE:CE2	2.80	0.65
14:T:9:DG:N3	19:e:40:ARG:NH2	2.45	0.64
18:W:396:GLU:CD	18:W:414:VAL:CG2	2.70	0.64
18:W:352:LEU:CD1	18:W:435:LEU:HD11	2.19	0.64
14:T:22:DC:H2''	14:T:23:DA:H1'	1.76	0.64
2:B:896:ASP:OD2	12:L:60:LYS:NZ	2.31	0.64
1:A:197:GLN:HE22	16:M:50:LYS:CB	2.09	0.63
18:W:332:LYS:HG3	18:W:388:ARG:HB3	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLN:CD	16:M:50:LYS:HB3	2.24	0.63
14:T:39:DA:H2''	14:T:40:DG:H5''	1.80	0.63
2:B:63:GLN:OE1	18:W:249:ALA:CA	2.46	0.63
1:A:288:HIS:CG	18:W:299:PHE:CE1	2.87	0.63
15:N:24:DC:H2''	15:N:25:DT:C7	2.28	0.63
2:B:62:ALA:HB3	2:B:71:ILE:H	1.64	0.63
1:A:286:PRO:CG	18:W:268:PHE:CE2	2.80	0.62
19:a:116:ARG:NH1	19:a:118:THR:O	2.32	0.62
20:f:92:ARG:HH21	22:h:98:LEU:HA	1.65	0.62
18:W:328:VAL:HG22	18:W:435:LEU:CD2	2.30	0.62
18:W:329:LYS:CG	18:W:436:ILE:HG13	2.29	0.62
1:A:286:PRO:HD3	18:W:268:PHE:CZ	2.34	0.61
4:D:19:VAL:O	4:D:29:ARG:NH1	2.33	0.61
2:B:220:ALA:O	2:B:252:ARG:NH2	2.33	0.61
18:W:437:VAL:O	18:W:437:VAL:HG22	1.99	0.61
13:P:2:U:H6	13:P:2:U:O5'	1.82	0.61
4:D:159:LEU:HD21	7:G:167:PHE:HB2	1.81	0.61
5:E:118:SER:OG	15:N:-17:DT:OP1	2.18	0.61
15:N:-16:DT:H1'	15:N:-15:DA:H5'	1.82	0.61
14:T:13:DT:C2'	14:T:14:DT:H72	2.21	0.61
15:N:-24:DT:H2''	15:N:-23:DT:OP2	1.99	0.61
1:A:982:ASP:O	1:A:1041:ARG:NH2	2.33	0.61
9:I:29:CYS:SG	9:I:30:ARG:N	2.74	0.61
19:a:100:LEU:HD11	20:b:58:LEU:HD13	1.83	0.60
22:h:73:GLU:OE1	22:h:76:ARG:NH2	2.34	0.60
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.32	0.60
8:H:56:THR:HB	8:H:144:ARG:HB3	1.83	0.60
15:N:-21:DG:H2'	15:N:-20:DC:C5	2.36	0.60
17:V:44:ALA:O	17:V:48:GLU:HG2	2.01	0.60
14:T:22:DC:C3'	14:T:23:DA:O4'	2.50	0.60
14:T:-14:DA:O3'	19:a:63:ARG:NH2	2.35	0.60
19:e:118:THR:OG1	20:f:45:ARG:NH1	2.33	0.60
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.35	0.60
2:B:969:ARG:NH1	3:C:60:GLU:OE1	2.35	0.60
3:C:69:ILE:HD11	3:C:144:LEU:HD21	1.84	0.60
13:P:6:G:C2	14:T:38:DA:N1	2.70	0.60
21:c:88:ARG:NH1	21:c:94:ASN:OD1	2.35	0.60
5:E:85:PRO:HA	5:E:112:GLN:HB2	1.85	0.59
14:T:-42:DT:OP1	21:c:20:ARG:NH2	2.36	0.59
4:D:41:HIS:HB3	7:G:73:LYS:HD3	1.82	0.59
2:B:279:ARG:NH2	2:B:286:ASP:OD1	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:357:ARG:HB3	18:W:389:PRO:CG	2.31	0.59
18:W:394:PHE:HE2	18:W:396:GLU:CG	2.14	0.59
18:W:396:GLU:CD	18:W:414:VAL:HG21	2.27	0.59
18:W:413:PHE:CE1	18:W:420:GLU:HB3	2.38	0.59
21:g:29:ARG:NH2	22:h:32:GLU:OE1	2.35	0.59
2:B:328:ARG:HD3	16:M:68:ASP:HA	1.83	0.59
15:N:-3:DA:H5'	20:f:45:ARG:HH12	1.67	0.59
1:A:42:ASP:O	1:A:43:GLU:HG3	2.03	0.59
2:B:233:SER:HG	2:B:356:HIS:HD1	1.48	0.59
14:T:-25:DA:H2	15:N:25:DT:O2	1.85	0.59
15:N:49:DC:H4'	22:d:30:ARG:HD2	1.85	0.59
18:W:319:LYS:O	18:W:320:LEU:HB3	2.02	0.59
18:W:319:LYS:O	18:W:320:LEU:HB2	2.03	0.58
2:B:859:TYR:HD2	2:B:911:ILE:HD11	1.67	0.58
20:b:38:ALA:HB1	20:b:43:VAL:HB	1.84	0.58
8:H:112:LYS:HG2	8:H:125:GLU:HG2	1.85	0.58
18:W:389:PRO:HD2	18:W:389:PRO:O	2.04	0.58
18:W:328:VAL:HA	18:W:435:LEU:CD2	2.33	0.58
13:P:6:G:C2	14:T:38:DA:C2	2.90	0.58
15:N:-21:DG:H2''	15:N:-20:DC:C6	2.39	0.58
18:W:397:ALA:O	18:W:401:VAL:HG23	2.03	0.58
14:T:22:DC:C6	14:T:23:DA:C5	2.90	0.58
1:A:570:LYS:HB3	8:H:46:MET:HE1	1.86	0.58
2:B:295:TYR:HD1	2:B:564:PRO:HB3	1.69	0.58
2:B:337:ARG:HB2	16:M:75:ASP:OD1	2.03	0.58
18:W:399:ALA:O	18:W:406:ILE:CD1	2.50	0.58
5:E:84:GLU:OE1	5:E:91:THR:OG1	2.20	0.57
19:a:69:ARG:NH1	20:b:25:ASN:OD1	2.37	0.57
15:N:-39:DT:H6	15:N:-39:DT:O5'	1.88	0.57
22:d:35:SER:O	22:d:39:TYR:HB2	2.05	0.57
18:W:394:PHE:CE2	18:W:396:GLU:CG	2.86	0.57
2:B:328:ARG:HD2	16:M:68:ASP:OD1	2.02	0.57
18:W:409:ASP:HB2	18:W:413:PHE:CE2	2.35	0.57
18:W:332:LYS:CG	18:W:388:ARG:HB2	2.35	0.57
19:a:123:ASP:OD1	19:e:113:HIS:NE2	2.37	0.57
1:A:288:HIS:NE2	18:W:299:PHE:HZ	1.97	0.57
5:E:19:LYS:NZ	5:E:33:GLU:O	2.38	0.57
1:A:351:ARG:HB2	2:B:1128:LEU:HD11	1.87	0.56
2:B:935:ARG:NH2	13:P:0:U:O4	2.39	0.56
2:B:30:LEU:O	2:B:489:ARG:NH1	2.38	0.56
1:A:1201:ARG:NH2	1:A:1235:ALA:O	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:83:ARG:HG2	18:W:762:GLY:HA2	1.88	0.56
18:W:344:LEU:CD1	18:W:349:GLU:HB2	2.35	0.56
20:f:74:GLU:O	22:h:89:ARG:NH2	2.38	0.56
8:H:13:GLN:HE22	8:H:29:ILE:HD12	1.70	0.56
14:T:13:DT:C2	14:T:14:DT:C4	2.93	0.56
15:N:-21:DG:C2'	15:N:-20:DC:C5	2.88	0.56
20:f:38:ALA:HB1	20:f:43:VAL:HB	1.87	0.55
1:A:50:GLU:CD	18:W:444:LEU:HD11	2.31	0.55
13:P:8:G:C4	13:P:9:U:C5	2.94	0.55
14:T:30:DT:C4	14:T:31:DT:O4	2.60	0.55
2:B:268:VAL:HA	2:B:330:GLY:HA2	1.88	0.55
1:A:89:PRO:HB3	1:A:238:THR:HG22	1.87	0.55
2:B:822:ASN:O	10:J:47:ARG:NH1	2.40	0.55
2:B:760:ASP:OD1	2:B:760:ASP:N	2.38	0.55
14:T:29:DA:C2'	14:T:30:DT:C7	2.84	0.55
15:N:29:DG:OP1	20:b:78:ARG:NH1	2.40	0.55
2:B:62:ALA:HB2	2:B:71:ILE:HG23	1.89	0.54
19:a:62:ILE:O	19:a:93:GLN:NE2	2.40	0.54
2:B:334:LEU:HD22	16:M:67:ILE:CD1	2.36	0.54
15:N:-41:DT:OP1	18:W:233:LEU:CD1	2.55	0.54
2:B:270:GLN:HB3	2:B:329:ARG:HD3	1.89	0.54
2:B:904:ARG:NH1	18:W:782:LEU:O	2.41	0.54
21:c:115:LEU:HD22	19:e:117:VAL:HG13	1.90	0.54
17:V:43:GLN:NE2	17:V:47:ASN:OD1	2.39	0.54
18:W:352:LEU:HD11	18:W:435:LEU:HD21	1.90	0.54
19:e:62:ILE:O	19:e:93:GLN:NE2	2.41	0.54
10:J:8:PHE:HB2	10:J:47:ARG:HH22	1.73	0.54
14:T:-34:DG:H3'	22:d:83:ARG:HH21	1.73	0.54
3:C:74:GLU:O	3:C:246:ARG:NH2	2.33	0.53
18:W:409:ASP:OD2	18:W:415:THR:OG1	2.21	0.53
16:M:54:LEU:HD12	16:M:54:LEU:C	2.34	0.53
23:0:35:DC:N4	24:1:-36:DG:O6	2.41	0.53
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	1.91	0.53
1:A:1452:LEU:HD22	6:F:131:PRO:HB3	1.90	0.53
19:a:128:ARG:NH2	19:a:134:ARG:O	2.42	0.53
1:A:336:ARG:HH22	2:B:1114:LEU:HD21	1.74	0.53
1:A:50:GLU:OE1	18:W:444:LEU:HD11	2.09	0.53
3:C:20:MET:SD	3:C:227:ARG:NH2	2.75	0.53
22:d:55:ALA:HA	22:d:58:ILE:HD12	1.91	0.53
19:e:100:LEU:HD11	20:f:58:LEU:HD13	1.91	0.53
1:A:286:PRO:CD	18:W:268:PHE:CE1	2.92	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:90:GLN:HE21	9:I:92:ARG:HG3	1.74	0.52
21:c:81:ARG:NH1	19:e:56:LYS:O	2.41	0.52
1:A:409:ASP:OD1	1:A:409:ASP:N	2.40	0.52
2:B:333:ALA:HB3	2:B:336:ILE:HD11	1.92	0.52
18:W:772:GLU:OE2	18:W:774:ASN:ND2	2.42	0.52
2:B:944:THR:HG21	2:B:1122:ARG:HE	1.75	0.52
18:W:413:PHE:HZ	18:W:420:GLU:CD	2.17	0.52
14:T:48:DG:C5'	18:W:330:ASN:HD21	2.11	0.52
15:N:-17:DT:C6	15:N:-16:DT:H72	2.45	0.52
2:B:419:ARG:NH1	15:N:-39:DT:C2	2.73	0.52
15:N:28:DA:H3'	20:b:78:ARG:HD2	1.91	0.52
17:V:41:SER:HB2	17:V:45:THR:HB	1.91	0.52
1:A:227:GLU:OE1	1:A:231:ARG:NH1	2.44	0.51
19:a:45:THR:O	19:a:49:ARG:HB2	2.10	0.51
3:C:146:LYS:NZ	10:J:57:GLU:OE2	2.34	0.51
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.92	0.51
13:P:6:G:N2	14:T:38:DA:C2	2.79	0.51
2:B:316:ILE:HG23	2:B:321:VAL:HG23	1.92	0.51
22:d:61:SER:HA	22:d:64:ASN:HD22	1.75	0.51
15:N:-41:DT:H4'	15:N:-40:DC:O5'	2.08	0.51
1:A:1402:ARG:NH2	1:A:1420:GLU:OE1	2.43	0.51
2:B:62:ALA:HB1	2:B:71:ILE:HG22	1.89	0.51
16:M:25:CYS:SG	16:M:54:LEU:HD21	2.50	0.51
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	1.93	0.51
21:c:78:ILE:H	22:d:51:ILE:HA	1.76	0.51
1:A:354:ILE:HG22	1:A:469:PHE:HB2	1.93	0.51
7:G:100:PHE:HB3	7:G:107:ASN:HD21	1.75	0.50
14:T:29:DA:N6	15:N:-30:DA:N6	2.59	0.50
15:N:51:DG:OP1	22:d:28:ARG:NH1	2.45	0.50
22:d:58:ILE:HG12	20:f:99:GLY:HA2	1.93	0.50
2:B:63:GLN:OE1	18:W:249:ALA:HB1	2.11	0.50
2:B:260:THR:HG22	2:B:308:PRO:HB2	1.94	0.50
2:B:242:ILE:HG21	2:B:355:PRO:HG3	1.93	0.50
9:I:7:CYS:HB2	9:I:14:LEU:HD21	1.94	0.50
21:c:101:THR:HG23	20:f:97:LEU:HD13	1.93	0.50
1:A:1146:LYS:NZ	2:B:254:ASP:OD2	2.38	0.50
15:N:-22:DG:C5	15:N:-21:DG:C6	3.00	0.50
19:e:99:TYR:OH	19:e:133:GLU:OE2	2.29	0.50
20:f:29:ILE:HB	20:f:55:ARG:HE	1.77	0.50
19:a:79:LYS:HB3	19:a:82:LEU:HD11	1.93	0.50
4:D:33:GLU:O	4:D:38:GLN:NE2	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:113:ALA:O	4:D:116:LYS:NZ	2.44	0.50
14:T:22:DC:C5	14:T:23:DA:N6	2.80	0.50
18:W:409:ASP:C	18:W:410:ARG:HG3	2.37	0.50
2:B:62:ALA:HB3	2:B:71:ILE:N	2.26	0.50
2:B:859:TYR:HE2	2:B:941:LEU:HD12	1.77	0.50
2:B:1101:ASP:O	2:B:1122:ARG:NH1	2.45	0.50
18:W:332:LYS:HG3	18:W:388:ARG:HB2	1.93	0.50
18:W:349:GLU:HG2	18:W:431:ARG:HA	1.92	0.50
2:B:1187:ASN:HD21	2:B:1190:ASN:HB3	1.77	0.49
15:N:-44:DG:OP1	18:W:334:LYS:HE3	2.12	0.49
1:A:286:PRO:HG3	18:W:268:PHE:CZ	2.46	0.49
13:P:1:G:H2'	13:P:2:U:H6	1.75	0.49
14:T:29:DA:H2'	14:T:30:DT:H71	1.92	0.49
19:e:46:VAL:HG22	19:e:49:ARG:HH12	1.77	0.49
20:f:34:ILE:HA	20:f:37:LEU:HD12	1.94	0.49
23:0:63:DA:H2''	23:0:64:DA:H2'	1.93	0.49
18:W:357:ARG:CB	18:W:389:PRO:HG2	2.42	0.49
1:A:351:ARG:NE	1:A:487:GLU:OE1	2.44	0.49
14:T:-25:DA:C2	15:N:25:DT:O2	2.65	0.49
18:W:388:ARG:CB	18:W:389:PRO:CD	2.88	0.49
18:W:403:GLU:O	18:W:403:GLU:HG3	2.12	0.49
1:A:912:ASP:OD1	1:A:912:ASP:N	2.42	0.49
5:E:27:TYR:HA	5:E:63:PRO:HA	1.95	0.49
15:N:-22:DG:C6	15:N:-21:DG:C6	3.01	0.49
18:W:286:LEU:HD22	18:W:292:VAL:HG21	1.93	0.49
21:g:110:ASN:OD1	21:g:112:GLN:NE2	2.45	0.49
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.95	0.49
18:W:409:ASP:OD2	18:W:413:PHE:CE2	2.66	0.49
3:C:74:GLU:HG3	3:C:242:GLN:HE22	1.78	0.49
14:T:30:DT:H2'	14:T:31:DT:C6	2.48	0.49
17:V:28:GLY:HA3	17:V:33:ASP:CG	2.38	0.49
18:W:399:ALA:O	18:W:406:ILE:HD12	2.13	0.49
9:I:15:TYR:N	9:I:28:SER:O	2.37	0.49
15:N:-25:DC:C2	15:N:-24:DT:C5	3.01	0.49
15:N:-25:DC:H2''	15:N:-24:DT:C5	2.43	0.48
18:W:413:PHE:HE1	18:W:420:GLU:HB3	1.78	0.48
20:b:39:ARG:NH1	20:b:44:LYS:O	2.45	0.48
19:a:95:ALA:HB2	20:b:97:LEU:HD22	1.94	0.48
1:A:43:GLU:OE2	18:W:335:GLY:O	2.31	0.48
1:A:122:MET:HE1	1:A:138:VAL:HG13	1.96	0.48
1:A:841:ARG:NH2	1:A:1108:ASN:OD1	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:23:DA:C2	15:N:-22:DG:N2	2.81	0.48
1:A:285:SER:O	1:A:285:SER:OG	2.30	0.48
2:B:419:ARG:NH1	15:N:-39:DT:N1	2.58	0.48
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.46	0.48
21:g:30:VAL:HA	21:g:33:LEU:HD12	1.96	0.48
2:B:419:ARG:HH11	15:N:-39:DT:C1'	2.03	0.48
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.95	0.48
13:P:-4:C:H4'	13:P:-4:C:OP1	2.14	0.48
15:N:4:DG:H4'	15:N:5:DT:H5'	1.95	0.48
21:g:76:THR:HG22	22:h:50:GLY:H	1.79	0.48
1:A:283:ASP:OD1	1:A:283:ASP:N	2.46	0.48
13:P:8:G:C6	13:P:9:U:C4	3.02	0.48
19:a:126:LEU:HD21	19:e:110:CYS:HA	1.95	0.48
1:A:115:LEU:HB2	1:A:122:MET:HE2	1.96	0.48
1:A:1193:TRP:HZ3	9:I:43:VAL:HG21	1.79	0.48
2:B:780:VAL:HG22	2:B:795:ILE:HG23	1.95	0.48
3:C:13:GLN:HE21	3:C:16:GLU:HG2	1.79	0.48
1:A:113:LEU:O	1:A:165:ARG:NH2	2.47	0.48
21:g:79:ILE:HG12	21:g:82:HIS:CG	2.49	0.48
15:N:-24:DT:C2	15:N:-23:DT:H73	2.48	0.47
2:B:401:LEU:HD13	2:B:538:ILE:HG21	1.96	0.47
1:A:14:VAL:H	1:A:1435:GLN:NE2	2.10	0.47
3:C:47:LEU:HB2	3:C:158:ILE:HB	1.96	0.47
18:W:399:ALA:O	18:W:406:ILE:HD11	2.14	0.47
19:a:45:THR:O	19:a:49:ARG:CB	2.62	0.47
23:O:46:DA:N6	24:I:-47:DC:N3	2.63	0.47
1:A:254:ASP:OD1	1:A:254:ASP:N	2.48	0.47
1:A:1227:PHE:HB2	1:A:1245:ILE:HD11	1.97	0.47
19:a:61:LEU:HD22	20:b:36:ARG:HD2	1.95	0.47
19:e:61:LEU:HD22	20:f:36:ARG:HD2	1.97	0.47
19:e:86:SER:HA	19:e:89:ILE:HD12	1.95	0.47
2:B:273:PRO:HD2	2:B:276:ILE:HD12	1.96	0.47
5:E:142:ASN:HB3	5:E:145:HIS:HD2	1.80	0.47
17:V:91:PRO:HB2	17:V:93:ASP:OD1	2.14	0.47
20:b:29:ILE:HB	20:b:55:ARG:HE	1.79	0.47
5:E:189:LEU:HD13	5:E:213:CYS:HB2	1.97	0.47
13:P:-1:G:H2'	13:P:0:U:H5''	1.97	0.47
18:W:437:VAL:O	18:W:437:VAL:CG2	2.61	0.47
11:K:5:ASP:OD1	18:W:787:LYS:NZ	2.48	0.47
13:P:-1:G:H2'	13:P:-1:G:N3	2.30	0.47
14:T:22:DC:C4	14:T:23:DA:C6	3.03	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:-37:DG:H2''	24:1:-36:DG:C8	2.50	0.47
15:N:-24:DT:C2	15:N:-23:DT:H71	2.48	0.46
16:M:52:CYS:O	16:M:53:ASN:CB	2.62	0.46
18:W:308:ASP:HA	18:W:311:ARG:HG3	1.96	0.46
1:A:358:PRO:HD2	2:B:833:TYR:CE1	2.51	0.46
1:A:1109:VAL:HG13	1:A:1335:PHE:HE2	1.80	0.46
13:P:1:G:O2'	13:P:2:U:O4'	2.23	0.46
15:N:-22:DG:C2'	15:N:-21:DG:H8	2.15	0.46
2:B:63:GLN:OE1	18:W:249:ALA:CB	2.63	0.46
10:J:9:SER:OG	10:J:47:ARG:NH2	2.46	0.46
21:g:40:SER:OG	21:g:42:ARG:O	2.33	0.46
1:A:1459:ASP:OD1	1:A:1459:ASP:N	2.34	0.46
2:B:164:MET:HB2	2:B:194:PHE:HE1	1.81	0.46
2:B:225:ILE:HD13	2:B:248:LYS:HD3	1.97	0.46
14:T:27:DG:N2	15:N:-26:DC:O2	2.48	0.46
2:B:969:ARG:HH22	3:C:59:ASP:HB2	1.80	0.46
14:T:22:DC:C4	14:T:23:DA:N1	2.83	0.46
19:a:45:THR:HG22	19:a:49:ARG:HH11	1.81	0.46
20:b:99:GLY:HA2	22:h:58:ILE:HG12	1.97	0.46
1:A:979:LYS:O	1:A:980:ALA:C	2.58	0.46
18:W:265:ARG:HA	18:W:265:ARG:HD2	1.71	0.46
19:a:41:TYR:HE2	19:a:45:THR:H	1.64	0.46
21:c:97:LEU:HD22	21:c:100:VAL:HG21	1.98	0.46
14:T:25:DG:O6	15:N:-25:DC:N3	2.49	0.46
18:W:352:LEU:CD1	18:W:435:LEU:HD21	2.46	0.46
23:0:47:DG:H2''	23:0:48:DG:C8	2.51	0.46
2:B:299:ASP:OD2	2:B:385:ARG:NH1	2.37	0.46
8:H:94:TYR:HD2	8:H:143:ILE:HD12	1.80	0.46
14:T:-14:DA:H2''	14:T:-13:DA:H8	1.80	0.46
14:T:22:DC:C4	15:N:-22:DG:N1	2.51	0.46
4:D:51:LEU:HD11	7:G:4:LEU:HG	1.98	0.45
1:A:119:ASN:HB3	1:A:122:MET:HB3	1.98	0.45
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.36	0.45
19:e:99:TYR:HD1	20:f:95:ARG:HH22	1.64	0.45
18:W:322:ARG:HD3	18:W:342:GLU:HA	1.99	0.45
1:A:542:ILE:HD12	1:A:578:LEU:HD13	1.98	0.45
2:B:870:ILE:HG13	18:W:387:PHE:CZ	2.52	0.45
14:T:-23:DC:OP2	19:a:72:ARG:NH2	2.49	0.45
15:N:-21:DG:H2''	15:N:-20:DC:C5	2.51	0.45
22:d:116:THR:O	22:d:120:SER:OG	2.28	0.45
21:g:64:GLU:HA	22:h:46:HIS:HE1	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:90:LEU:HD23	20:b:90:LEU:HA	1.78	0.45
1:A:599:LEU:HD13	8:H:123:CYS:HB2	1.98	0.45
13:P:8:G:C6	13:P:9:U:O4	2.69	0.45
14:T:15:DT:H2''	14:T:16:DA:C8	2.52	0.45
1:A:1168:ASP:OD2	1:A:1196:ARG:NE	2.49	0.45
14:T:13:DT:H2'	14:T:14:DT:H73	1.90	0.45
2:B:265:LEU:HD22	2:B:353:LEU:HD13	1.99	0.45
15:N:3:DC:H2''	15:N:4:DG:C8	2.52	0.45
18:W:409:ASP:OD2	18:W:413:PHE:HE2	2.00	0.45
24:1:-61:DT:H2'	24:1:-60:DT:C6	2.52	0.45
1:A:1461:ALA:HB1	7:G:21:GLN:HB2	1.99	0.44
2:B:73:LYS:HG2	2:B:125:THR:HG22	1.99	0.44
2:B:325:PHE:CE1	16:M:63:LEU:HB3	2.52	0.44
2:B:371:LEU:HD23	2:B:371:LEU:HA	1.76	0.44
2:B:406:LEU:HD23	2:B:406:LEU:HA	1.87	0.44
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.52	0.44
2:B:1219:GLU:O	4:D:12:ARG:NH2	2.49	0.44
14:T:-18:DC:H1'	14:T:-17:DT:H5'	2.00	0.44
18:W:344:LEU:HD12	18:W:349:GLU:HB2	2.00	0.44
1:A:1153:GLU:OE1	1:A:1196:ARG:NH1	2.45	0.44
2:B:557:GLU:HB2	2:B:582:ILE:HD12	1.98	0.44
14:T:22:DC:C2'	14:T:23:DA:C4	3.00	0.44
15:N:17:DA:H2''	15:N:18:DG:H8	1.81	0.44
2:B:71:ILE:HG12	2:B:73:LYS:HE3	2.00	0.44
15:N:28:DA:H2''	15:N:29:DG:H8	1.82	0.44
19:e:40:ARG:HD2	19:e:40:ARG:HA	1.80	0.44
22:h:78:ALA:O	22:h:82:LYS:N	2.50	0.44
2:B:887:HIS:CE1	13:P:-2:G:C5	3.05	0.44
2:B:334:LEU:HD22	16:M:67:ILE:HD11	2.00	0.44
18:W:396:GLU:CD	18:W:414:VAL:HG23	2.30	0.44
18:W:442:PRO:HB2	18:W:447:LEU:CD1	2.48	0.44
1:A:286:PRO:O	1:A:288:HIS:N	2.50	0.44
2:B:276:ILE:HD11	16:M:63:LEU:HD21	2.00	0.44
19:a:48:LEU:HD13	19:a:51:ILE:HD12	1.99	0.44
2:B:935:ARG:CZ	13:P:0:U:O4	2.66	0.44
21:c:73:ASN:HB3	21:c:75:LYS:HD3	2.00	0.44
2:B:436:ASN:O	2:B:438:ASN:N	2.48	0.44
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.99	0.44
22:d:87:THR:OG1	22:d:90:GLU:OE1	2.29	0.44
7:G:116:PRO:HD2	7:G:163:ILE:HG13	1.99	0.43
11:K:55:ASP:OD1	11:K:55:ASP:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:-44:DG:H2'	24:1:-43:DT:H71	1.99	0.43
1:A:271:LEU:HD12	1:A:271:LEU:HA	1.86	0.43
2:B:1073:TYR:HE2	3:C:179:GLU:HA	1.83	0.43
3:C:45:ILE:HA	3:C:159:ALA:HA	1.99	0.43
3:C:148:ARG:HG2	3:C:149:ASN:H	1.83	0.43
6:F:79:ARG:NH1	6:F:150:GLU:OE2	2.48	0.43
15:N:15:DT:H2''	15:N:16:DA:C8	2.54	0.43
15:N:18:DG:OP1	19:a:64:LYS:N	2.52	0.43
21:g:17:ARG:HA	21:g:20:ARG:HB2	2.00	0.43
1:A:468:THR:OG1	1:A:470:ARG:NH1	2.52	0.43
2:B:64:HIS:O	2:B:64:HIS:CG	2.70	0.43
19:a:54:TYR:HD2	20:b:39:ARG:HB2	1.84	0.43
23:0:38:DA:H2''	23:0:39:DA:C8	2.53	0.43
21:c:17:ARG:O	21:c:21:ALA:N	2.50	0.43
22:h:85:THR:OG1	22:h:86:ILE:N	2.52	0.43
14:T:14:DT:C2'	14:T:15:DT:H72	2.48	0.43
15:N:-41:DT:H3'	15:N:-41:DT:H6	1.83	0.43
1:A:407:ILE:HG12	1:A:413:ARG:HG2	2.00	0.43
6:F:89:GLU:OE2	6:F:136:ARG:NE	2.51	0.43
4:D:23:GLU:HB3	7:G:82:PHE:HD1	1.83	0.43
1:A:891:ASP:HA	1:A:941:ARG:HH12	1.83	0.43
1:A:1445:ASP:HB3	1:A:1447:MET:HE3	2.01	0.43
2:B:334:LEU:HD22	16:M:67:ILE:HD13	2.00	0.43
14:T:14:DT:H2''	14:T:15:DT:C6	2.51	0.43
15:N:-27:DC:H2''	15:N:-26:DC:C6	2.54	0.43
15:N:62:DG:H1'	15:N:63:DG:H5'	2.01	0.43
18:W:792:PRO:HG2	18:W:795:PHE:CD2	2.54	0.43
5:E:160:LYS:NZ	5:E:192:GLY:O	2.44	0.43
13:P:3:C:H2'	13:P:4:U:O4'	2.19	0.43
15:N:-41:DT:H2''	15:N:-40:DC:C6	2.54	0.43
15:N:-40:DC:O3'	15:N:-39:DT:H71	2.19	0.43
2:B:154:ASN:OD1	2:B:155:LYS:N	2.45	0.43
20:b:26:ILE:HD11	20:b:55:ARG:HB3	2.01	0.43
12:L:60:LYS:HE3	12:L:60:LYS:HB3	1.81	0.42
14:T:13:DT:C6	14:T:14:DT:H72	2.54	0.42
18:W:344:LEU:HD11	18:W:349:GLU:HB2	2.00	0.42
1:A:240:LEU:HD12	1:A:240:LEU:HA	1.88	0.42
1:A:958:LEU:HD13	1:A:1023:LEU:HD22	2.01	0.42
2:B:761:HIS:HB2	2:B:1024:ALA:HB2	2.01	0.42
3:C:53:ASN:ND2	3:C:59:ASP:OD1	2.47	0.42
7:G:115:ILE:HG23	7:G:163:ILE:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:84:VAL:HG22	9:I:104:LEU:HD21	2.01	0.42
15:N:52:DC:H1'	15:N:53:DC:H5'	2.01	0.42
1:A:286:PRO:O	1:A:288:HIS:ND1	2.52	0.42
18:W:333:PHE:CD2	18:W:354:LEU:CD2	3.00	0.42
19:a:117:VAL:HG11	20:b:44:LYS:HD3	2.01	0.42
1:A:887:ILE:O	1:A:945:ARG:NH2	2.41	0.42
2:B:336:ILE:H	2:B:341:ARG:HH21	1.67	0.42
4:D:61:ARG:NH1	4:D:86:ASP:OD1	2.52	0.42
14:T:-13:DA:P	19:a:63:ARG:HH22	2.42	0.42
17:V:15:CYS:HB3	17:V:32:CYS:SG	2.59	0.42
18:W:421:TYR:HA	18:W:425:PHE:O	2.18	0.42
2:B:756:ILE:HG12	2:B:770:GLN:HG2	2.02	0.42
6:F:107:VAL:HG11	6:F:111:ILE:HD11	2.00	0.42
15:N:25:DT:H2''	15:N:26:DA:N7	2.35	0.42
21:c:104:GLN:OE1	19:e:58:THR:OG1	2.29	0.42
20:f:47:SER:OG	20:f:48:GLY:N	2.38	0.42
1:A:168:CYS:SG	1:A:170:ASN:ND2	2.93	0.42
1:A:615:PHE:HB3	8:H:121:LEU:HD21	2.01	0.42
14:T:-25:DA:C2	15:N:25:DT:C2	3.08	0.42
14:T:-25:DA:C2	15:N:25:DT:N3	2.77	0.42
20:b:38:ALA:O	20:b:43:VAL:N	2.46	0.42
2:B:70:ASN:HB2	2:B:128:ASP:O	2.18	0.42
2:B:251:GLY:HA2	2:B:256:GLY:HA3	2.02	0.42
14:T:-37:DG:H2''	14:T:-36:DT:C5	2.54	0.42
14:T:13:DT:N3	14:T:14:DT:C4	2.88	0.42
15:N:4:DG:H2''	15:N:5:DT:C5	2.55	0.42
1:A:292:GLU:OE1	18:W:271:HIS:HE1	2.02	0.42
1:A:341:LEU:HD23	1:A:341:LEU:HA	1.78	0.42
15:N:24:DC:C2'	15:N:25:DT:C7	2.97	0.42
20:f:38:ALA:O	20:f:42:GLY:N	2.52	0.42
20:b:65:VAL:HG13	20:b:90:LEU:HD21	2.01	0.42
21:g:34:LEU:HA	21:g:39:TYR:CD2	2.55	0.42
2:B:101:PRO:HG2	2:B:172:LEU:HD11	2.01	0.42
2:B:190:MET:SD	2:B:190:MET:N	2.86	0.42
14:T:-14:DA:H2''	14:T:-13:DA:C8	2.55	0.42
18:W:278:LYS:HD2	18:W:280:GLU:OE2	2.20	0.42
2:B:653:ARG:HE	2:B:653:ARG:HB3	1.71	0.41
5:E:189:LEU:HD11	5:E:195:VAL:HG13	2.01	0.41
7:G:152:THR:HA	7:G:157:ILE:HG22	2.02	0.41
9:I:96:ASN:OD1	9:I:97:MET:N	2.48	0.41
15:N:23:DG:H1'	15:N:24:DC:H5'	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:332:LYS:HE3	18:W:357:ARG:HB2	2.01	0.41
18:W:784:ASN:HB2	18:W:785:PRO:HD3	2.01	0.41
21:g:88:ARG:HB3	21:g:108:LEU:HD11	2.01	0.41
3:C:66:LEU:HD11	3:C:155:ILE:HD12	2.02	0.41
7:G:91:VAL:HG23	7:G:139:LYS:HA	2.01	0.41
24:1:-39:DT:H6	24:1:-39:DT:H2'	1.70	0.41
1:A:37:TYR:HA	1:A:38:PRO:HD3	1.89	0.41
1:A:781:ALA:N	2:B:696:GLU:OE2	2.45	0.41
1:A:1356:LEU:HD13	1:A:1371:MET:HE1	2.02	0.41
2:B:325:PHE:CZ	16:M:63:LEU:HD23	2.55	0.41
2:B:688:GLU:OE2	2:B:740:HIS:NE2	2.38	0.41
14:T:4:DC:N4	15:N:-5:DG:O6	2.53	0.41
15:N:-7:DG:H2''	15:N:-6:DG:N7	2.35	0.41
18:W:352:LEU:HD11	18:W:435:LEU:CD2	2.49	0.41
20:b:52:GLU:OE2	20:b:55:ARG:NH1	2.53	0.41
1:A:337:LEU:HA	1:A:337:LEU:HD23	1.77	0.41
15:N:-41:DT:C4'	15:N:-40:DC:O5'	2.69	0.41
16:M:60:ILE:HB	16:M:64:SER:OG	2.20	0.41
4:D:169:VAL:C	4:D:171:LEU:H	2.28	0.41
13:P:2:U:H2'	13:P:3:C:C6	2.56	0.41
18:W:389:PRO:CD	18:W:389:PRO:O	2.68	0.41
19:a:94:GLU:OE2	21:g:104:GLN:N	2.52	0.41
1:A:447:ARG:HB2	1:A:488:MET:HG2	2.03	0.41
2:B:262:LYS:HA	2:B:273:PRO:HA	2.03	0.41
14:T:-48:DC:H2''	14:T:-47:DT:H5'	2.03	0.41
14:T:16:DA:H2''	14:T:17:DA:C8	2.55	0.41
15:N:42:DA:H2''	15:N:43:DA:C8	2.56	0.41
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.88	0.41
1:A:970:GLN:HA	1:A:975:LEU:HB2	2.03	0.41
2:B:63:GLN:OE1	18:W:249:ALA:O	2.38	0.41
15:N:21:DG:H2'	15:N:22:DT:H71	2.01	0.41
1:A:181:LYS:HB3	1:A:202:LEU:HD11	2.03	0.41
1:A:844:LYS:HA	1:A:844:LYS:HD2	1.93	0.41
2:B:335:GLY:HA2	16:M:74:ILE:CD1	2.48	0.41
3:C:63:SER:HA	3:C:66:LEU:HD12	2.03	0.41
15:N:7:DC:H5'	20:b:45:ARG:HH21	1.86	0.41
18:W:229:VAL:HG21	18:W:286:LEU:HD11	2.03	0.41
20:f:32:PRO:HA	20:f:35:ARG:HB2	2.01	0.41
1:A:288:HIS:CD2	18:W:299:PHE:HZ	2.18	0.41
1:A:1444:PHE:CZ	6:F:89:GLU:HA	2.55	0.41
2:B:840:ILE:HG12	2:B:992:VAL:HG12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:904:ARG:HG2	2:B:905:VAL:N	2.36	0.41
2:B:1073:TYR:CE1	2:B:1080:LYS:HG2	2.55	0.41
3:C:32:LEU:HD12	3:C:32:LEU:HA	1.84	0.41
18:W:352:LEU:HD21	18:W:435:LEU:CD1	2.50	0.41
20:b:87:VAL:HG11	20:b:102:GLY:HA3	2.02	0.41
22:d:35:SER:O	22:d:39:TYR:CB	2.69	0.41
24:1:-50:DT:H2''	24:1:-49:DG:C8	2.55	0.41
1:A:84:MET:HE2	1:A:271:LEU:HD13	2.03	0.41
1:A:262:ASP:OD1	1:A:317:GLN:NE2	2.54	0.41
2:B:119:MET:O	2:B:153:GLY:N	2.53	0.41
1:A:122:MET:HE3	1:A:126:ILE:HD11	2.02	0.40
1:A:916:TYR:OH	1:A:983:LEU:O	2.28	0.40
18:W:228:GLY:HA3	18:W:299:PHE:CZ	2.55	0.40
18:W:322:ARG:CD	18:W:342:GLU:HG3	2.51	0.40
19:e:118:THR:HG1	20:f:45:ARG:HH11	1.67	0.40
21:g:76:THR:O	22:h:50:GLY:N	2.54	0.40
21:g:102:ILE:HG23	22:h:58:ILE:HG21	2.02	0.40
1:A:195:ASP:OD1	1:A:195:ASP:N	2.53	0.40
15:N:-41:DT:H2''	15:N:-40:DC:O5'	2.21	0.40
2:B:290:LEU:HD22	9:I:6:PHE:HZ	1.85	0.40
8:H:86:LYS:HE2	8:H:86:LYS:HB3	1.87	0.40
15:N:20:DG:H2''	15:N:21:DG:H5''	2.04	0.40
22:d:99:LEU:HD23	22:d:99:LEU:HA	1.90	0.40
1:A:883:THR:O	1:A:1027:ARG:NH2	2.52	0.40
2:B:625:ARG:HH11	2:B:625:ARG:HD2	1.73	0.40
2:B:859:TYR:CE2	2:B:941:LEU:HD12	2.57	0.40
4:D:106:LEU:O	4:D:110:ASN:N	2.53	0.40
9:I:13:MET:HE3	9:I:13:MET:HB2	1.89	0.40
19:a:48:LEU:HD11	21:g:115:LEU:HB3	2.03	0.40
2:B:71:ILE:O	2:B:73:LYS:HG3	2.20	0.40
2:B:464:LYS:NZ	15:N:-37:DG:N2	2.70	0.40
14:T:30:DT:C4	14:T:31:DT:C4	3.09	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	1399/1743 (80%)	1342 (96%)	47 (3%)	10 (1%)	18	54
2	B	1145/1227 (93%)	1082 (94%)	55 (5%)	8 (1%)	18	54
3	C	261/304 (86%)	253 (97%)	6 (2%)	2 (1%)	16	52
4	D	162/186 (87%)	149 (92%)	9 (6%)	4 (2%)	4	27
5	E	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
6	F	82/155 (53%)	80 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	159 (94%)	8 (5%)	2 (1%)	10	42
8	H	129/145 (89%)	125 (97%)	2 (2%)	2 (2%)	7	37
9	I	109/115 (95%)	102 (94%)	6 (6%)	1 (1%)	14	49
10	J	64/72 (89%)	61 (95%)	2 (3%)	1 (2%)	7	37
11	K	111/118 (94%)	110 (99%)	1 (1%)	0	100	100
12	L	43/72 (60%)	42 (98%)	0	1 (2%)	5	29
16	M	62/113 (55%)	58 (94%)	4 (6%)	0	100	100
17	V	100/108 (93%)	97 (97%)	3 (3%)	0	100	100
18	W	265/911 (29%)	246 (93%)	17 (6%)	2 (1%)	16	52
19	a	95/139 (68%)	85 (90%)	10 (10%)	0	100	100
19	e	95/139 (68%)	86 (90%)	9 (10%)	0	100	100
20	b	78/106 (74%)	74 (95%)	4 (5%)	0	100	100
20	f	76/106 (72%)	69 (91%)	7 (9%)	0	100	100
21	c	101/133 (76%)	92 (91%)	9 (9%)	0	100	100
21	g	103/133 (77%)	94 (91%)	9 (9%)	0	100	100
22	d	93/129 (72%)	91 (98%)	2 (2%)	0	100	100
22	h	89/129 (69%)	86 (97%)	3 (3%)	0	100	100
All	All	5042/6668 (76%)	4790 (95%)	219 (4%)	33 (1%)	20	54

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	GLU
1	A	287	GLN
1	A	960	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1109	VAL
2	B	155	LYS
2	B	239	SER
2	B	337	ARG
3	C	89	ASP
7	G	134	ASP
8	H	108	GLU
12	L	44	LYS
18	W	320	LEU
1	A	284	GLY
1	A	977	ARG
1	A	1223	SER
2	B	62	ALA
2	B	177	GLU
2	B	299	ASP
4	D	169	VAL
4	D	171	LEU
7	G	154	VAL
8	H	18	GLY
1	A	979	LYS
4	D	10	ALA
9	I	56	ALA
1	A	47	ARG
2	B	437	LEU
3	C	217	GLU
4	D	164	ALA
1	A	43	GLU
2	B	238	GLY
10	J	64	PRO
18	W	806	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1224/1528 (80%)	1218 (100%)	6 (0%)	81 81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	1012/1077 (94%)	1002 (99%)	10 (1%)	68	75
3	C	236/264 (89%)	236 (100%)	0	100	100
4	D	143/160 (89%)	140 (98%)	3 (2%)	47	65
5	E	196/197 (100%)	195 (100%)	1 (0%)	81	81
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	148 (100%)	0	100	100
8	H	120/130 (92%)	118 (98%)	2 (2%)	53	67
9	I	106/109 (97%)	106 (100%)	0	100	100
10	J	60/66 (91%)	60 (100%)	0	100	100
11	K	104/109 (95%)	104 (100%)	0	100	100
12	L	38/56 (68%)	37 (97%)	1 (3%)	40	61
16	M	61/99 (62%)	61 (100%)	0	100	100
17	V	86/92 (94%)	85 (99%)	1 (1%)	63	73
18	W	241/796 (30%)	236 (98%)	5 (2%)	47	65
19	a	83/112 (74%)	82 (99%)	1 (1%)	63	73
19	e	82/112 (73%)	81 (99%)	1 (1%)	63	73
20	b	65/81 (80%)	64 (98%)	1 (2%)	57	70
20	f	63/81 (78%)	63 (100%)	0	100	100
21	c	82/102 (80%)	82 (100%)	0	100	100
21	g	83/102 (81%)	83 (100%)	0	100	100
22	d	81/107 (76%)	80 (99%)	1 (1%)	63	73
22	h	77/107 (72%)	77 (100%)	0	100	100
All	All	4466/5772 (77%)	4433 (99%)	33 (1%)	73	78

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ARG
1	A	248	ARG
1	A	473	LEU
1	A	661	ASN
1	A	977	ARG
1	A	1459	ASP
2	B	69	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	70	ASN
2	B	71	ILE
2	B	233	SER
2	B	428	CYS
2	B	466	MET
2	B	500	LYS
2	B	578	VAL
2	B	582	ILE
2	B	618	LYS
4	D	19	VAL
4	D	116	LYS
4	D	171	LEU
5	E	131	ILE
8	H	111	ILE
8	H	122	MET
12	L	62	ARG
17	V	33	ASP
18	W	246	LYS
18	W	264	GLN
18	W	313	VAL
18	W	342	GLU
18	W	343	VAL
19	a	74	ILE
20	b	72	TYR
22	d	77	LEU
19	e	84	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	197	GLN
1	A	287	GLN
1	A	340	ASN
1	A	400	HIS
1	A	446	ASN
1	A	563	GLN
1	A	651	GLN
1	A	661	ASN
1	A	1190	GLN
1	A	1261	GLN
1	A	1435	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	735	HIS
2	B	842	ASN
2	B	887	HIS
2	B	1062	ASN
2	B	1097	HIS
2	B	1174	ASN
3	C	8	ASN
3	C	13	GLN
3	C	126	ASN
3	C	188	HIS
3	C	242	GLN
4	D	179	ASN
5	E	4	ASN
5	E	51	ASN
5	E	94	ASN
5	E	112	GLN
5	E	120	ASN
5	E	145	HIS
5	E	193	GLN
7	G	21	GLN
7	G	125	ASN
8	H	13	GLN
8	H	136	GLN
9	I	90	GLN
9	I	105	ASN
17	V	37	ASN
18	W	264	GLN
18	W	330	ASN
18	W	339	GLN
18	W	402	HIS
18	W	434	ASN
18	W	784	ASN
19	a	108	ASN
21	c	24	GLN
22	d	60	ASN
22	d	64	ASN
19	e	68	GLN
21	g	31	HIS
21	g	110	ASN
21	g	112	GLN
22	h	64	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	15/16 (93%)	6 (40%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	-4	C
13	P	-3	U
13	P	-1	G
13	P	0	U
13	P	1	G
13	P	3	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

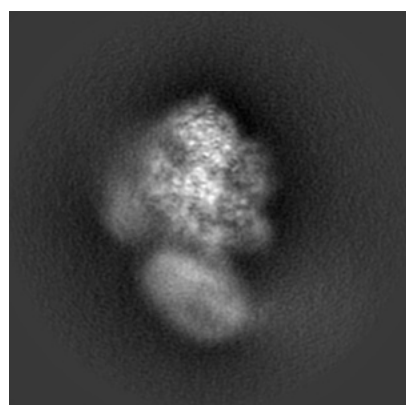
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0676. These allow visual inspection of the internal detail of the map and identification of artifacts.

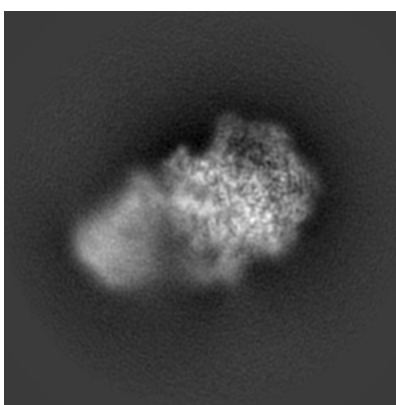
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

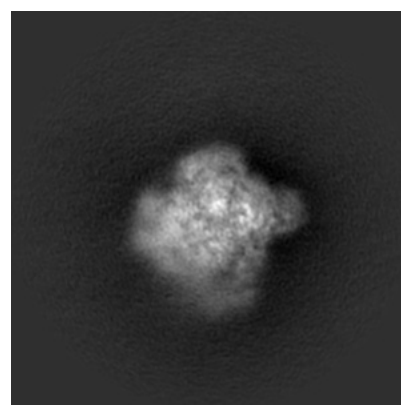
6.1.1 Primary map



X



Y

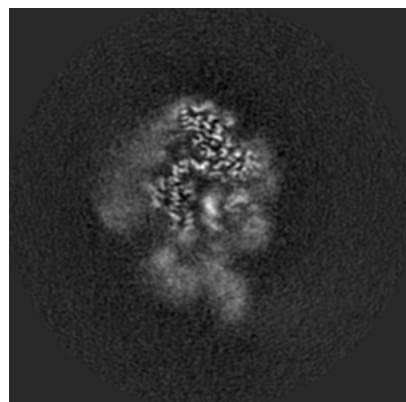


Z

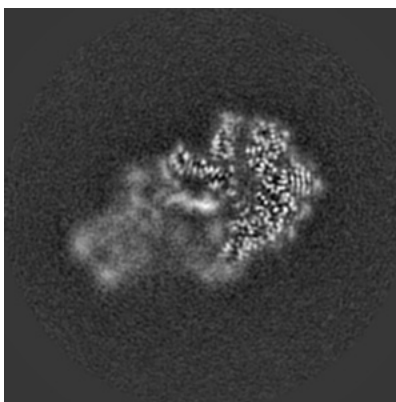
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

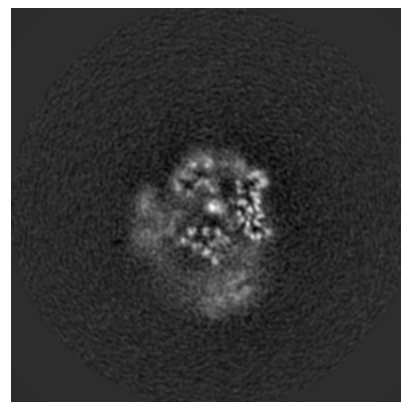
6.2.1 Primary map



X Index: 120



Y Index: 120

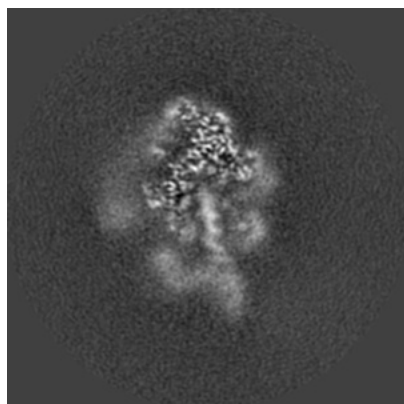


Z Index: 120

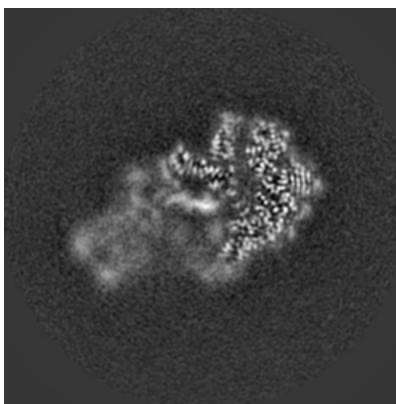
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

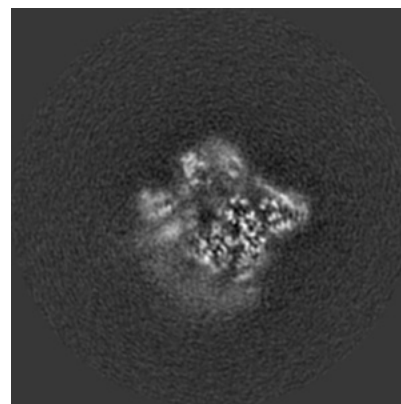
6.3.1 Primary map



X Index: 123



Y Index: 120

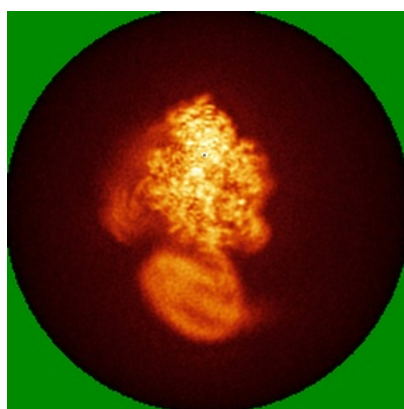


Z Index: 132

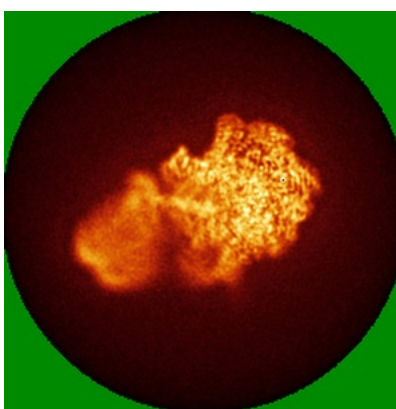
The images above show the largest variance slices of the map in three orthogonal directions.

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

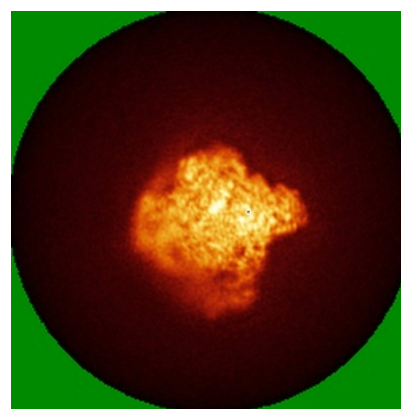
6.4.1 Primary map



X



Y

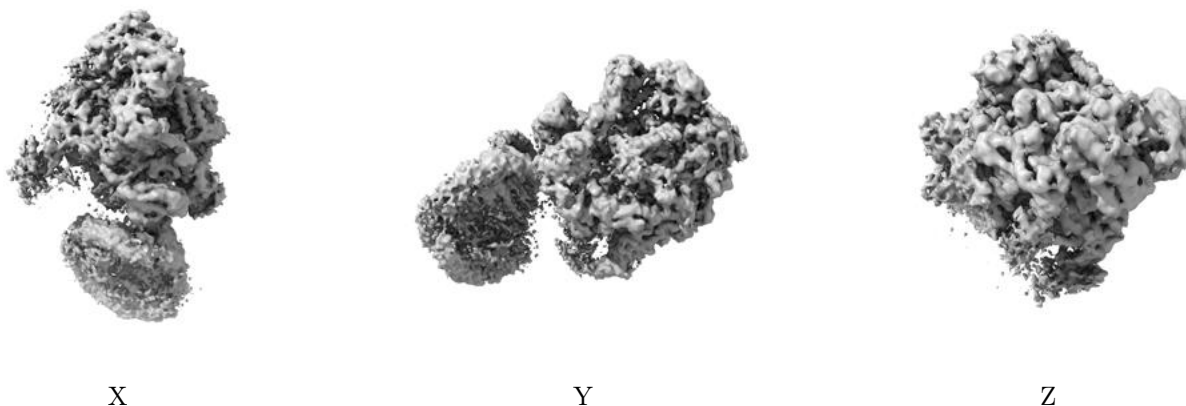


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

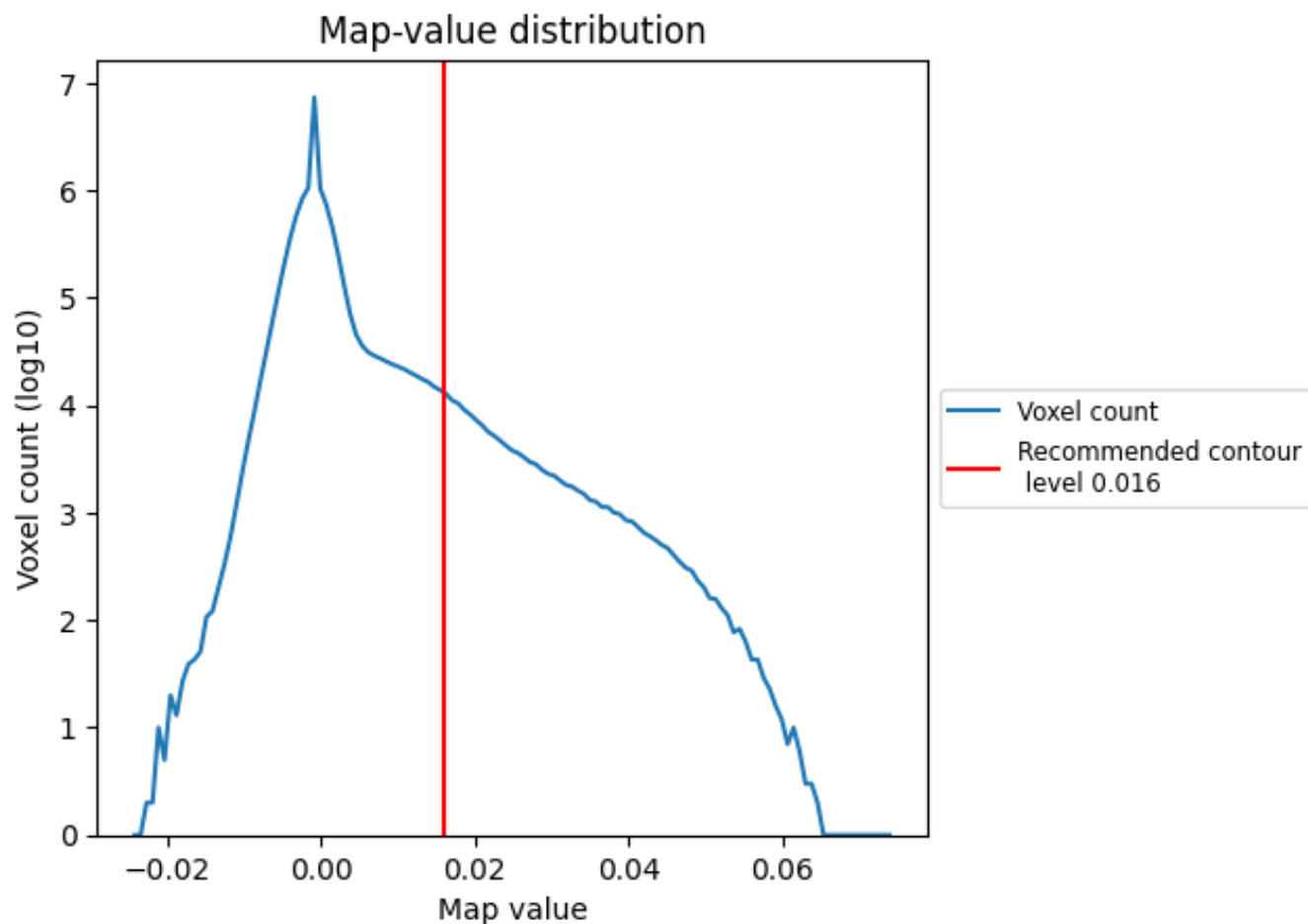
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

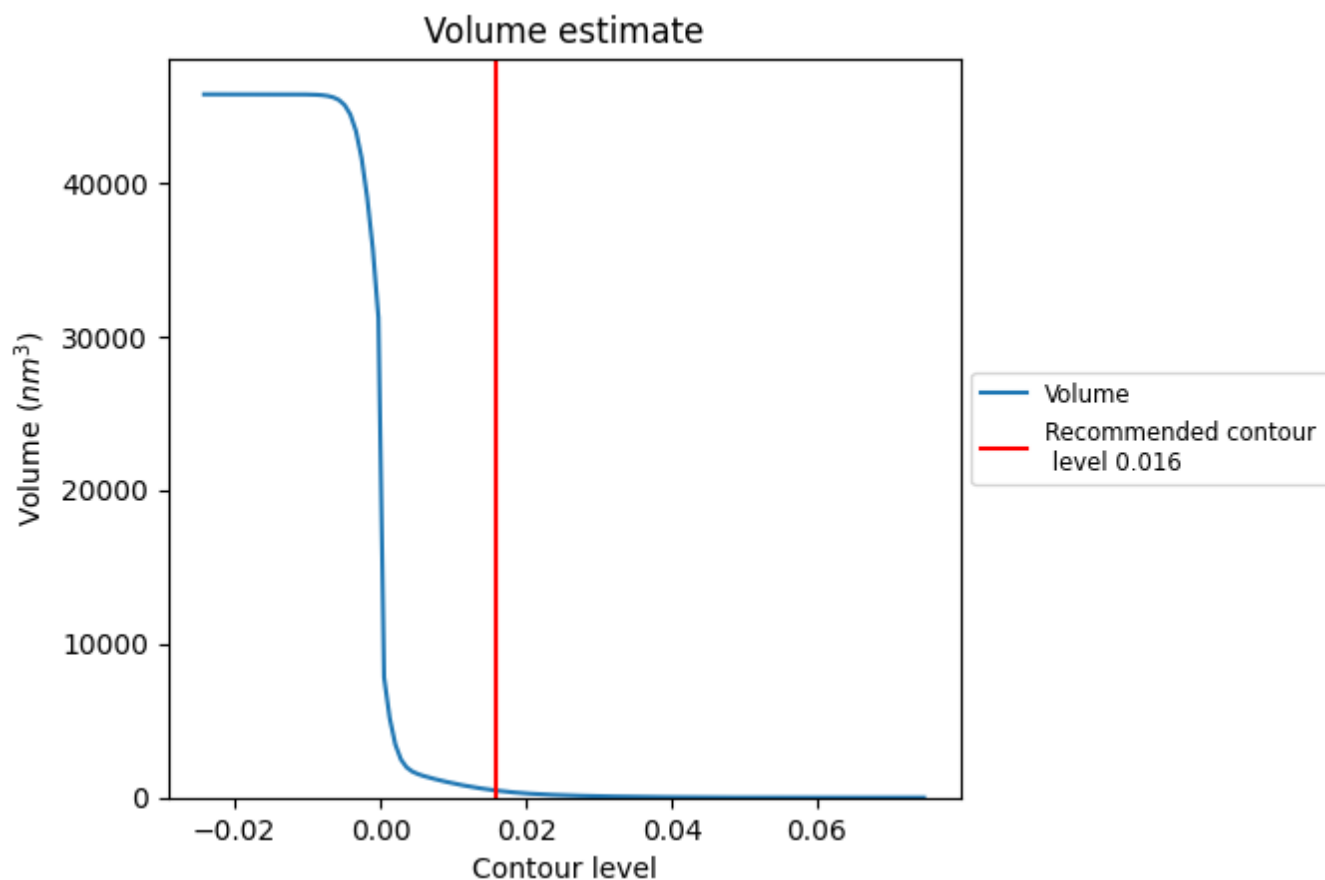
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

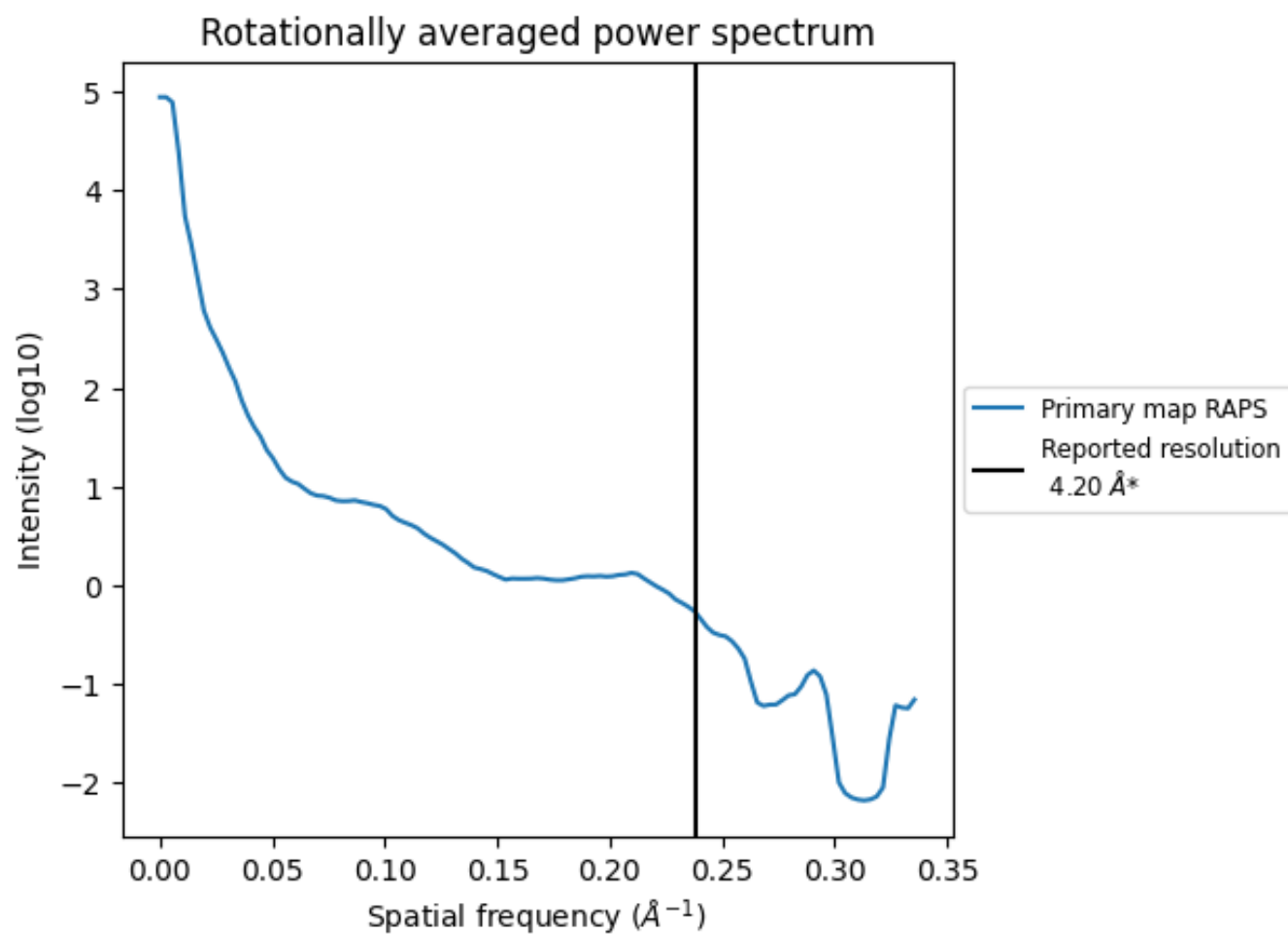
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 454 nm³; this corresponds to an approximate mass of 410 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 ⓘ

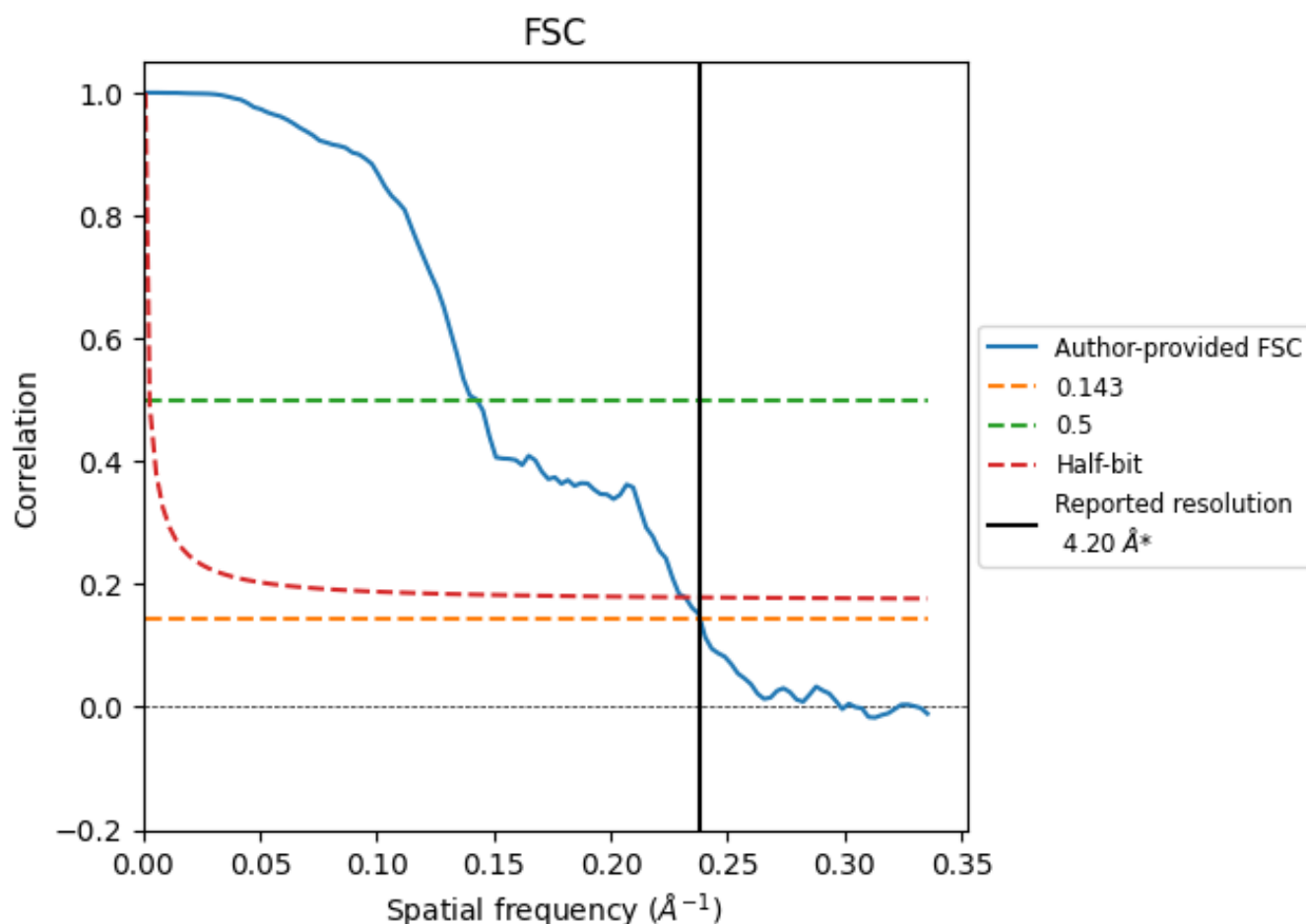


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

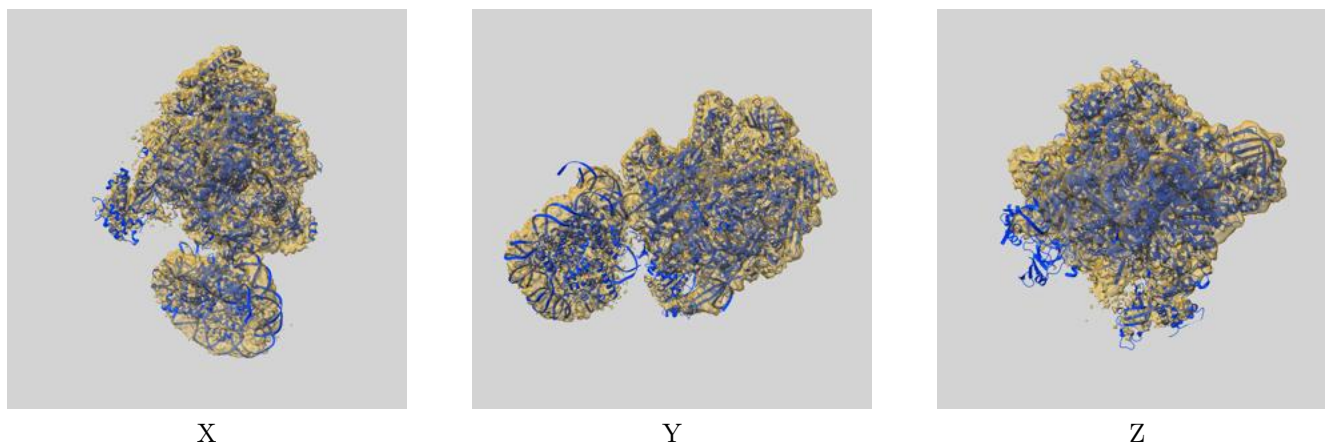
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.20	7.01	4.31
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

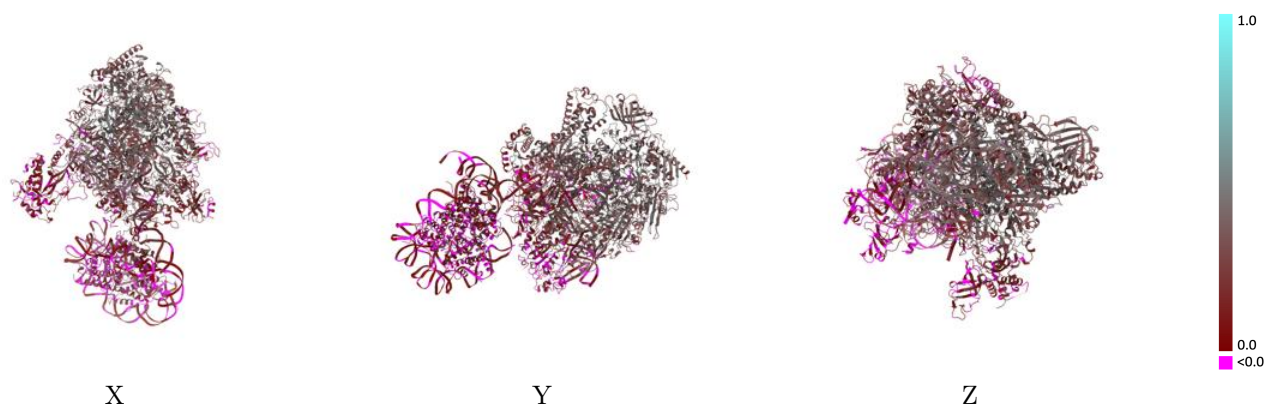
This section contains information regarding the fit between EMDB map EMD-0676 and PDB model 6J51. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



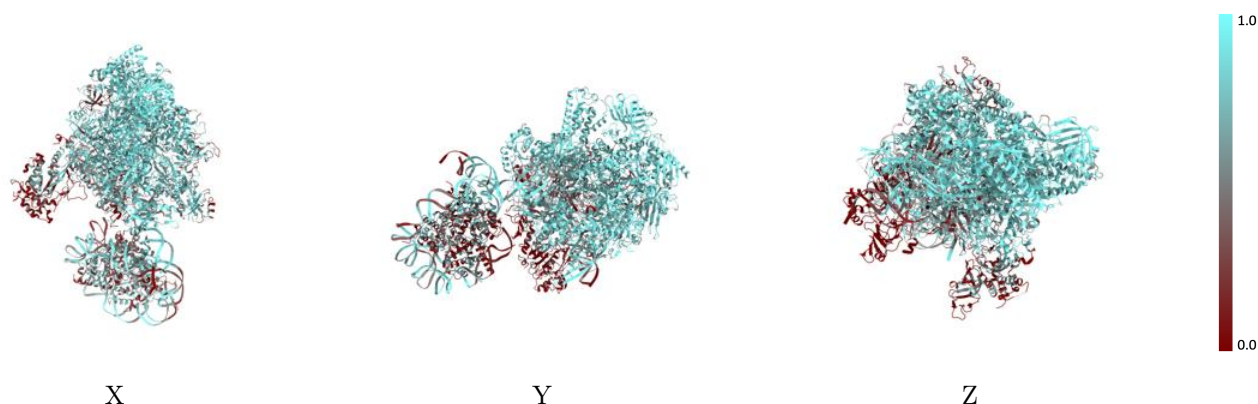
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



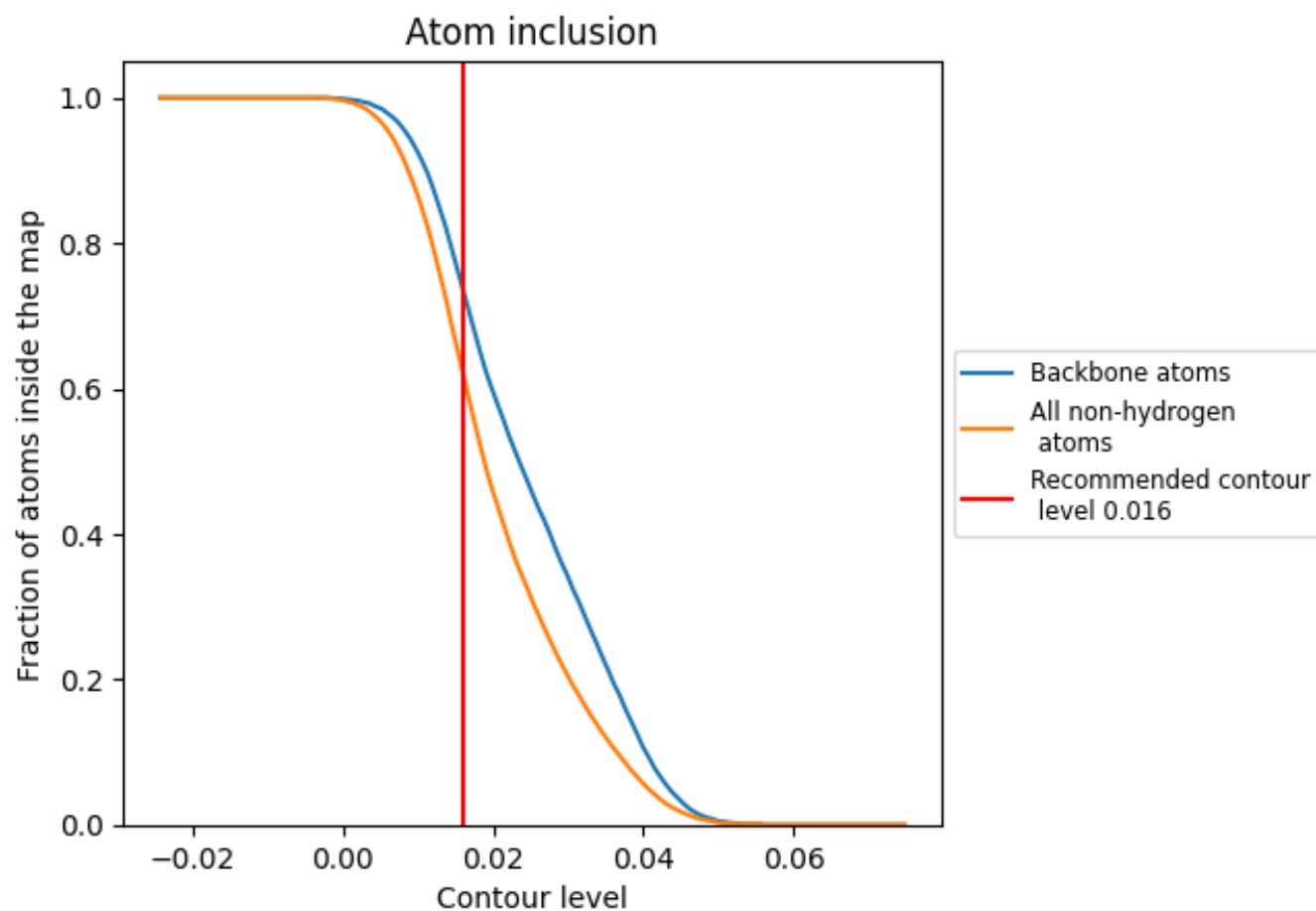
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 62% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6210	 0.2300
0	 0.4990	 0.0610
1	 0.4490	 0.0190
A	 0.7330	 0.3230
B	 0.7610	 0.3390
C	 0.8240	 0.3620
D	 0.1980	 0.0990
E	 0.7940	 0.3150
F	 0.8150	 0.3660
G	 0.4110	 0.1500
H	 0.8640	 0.3540
I	 0.4910	 0.1500
J	 0.8260	 0.3610
K	 0.7970	 0.3580
L	 0.7070	 0.2630
M	 0.0280	 0.0840
N	 0.6340	 0.0780
P	 0.7770	 0.2630
T	 0.7040	 0.1100
V	 0.1200	 0.0530
W	 0.1230	 0.0940
a	 0.3830	 0.0210
b	 0.4410	 0.0570
c	 0.4110	 0.0520
d	 0.3840	 0.0050
e	 0.5290	 0.1150
f	 0.4470	 0.1020
g	 0.2690	 0.0360
h	 0.3290	 0.0570

