Full wwPDB EM Validation Report

Jul 16, 2025 – 04:25 PM JST

PDB ID	:	9II7 / pdb_00009ii7
EMDB ID	:	EMD-60593
Title	:	RNA polymerase II elongation complex stalled at SHL(-1) of the nucleosome containing histone variant H2A.B
Authors	:	Akatsu, M.; Kujirai, T.; Rina, H.; Ehara, H.; Takizawa, Y.; Sekine, S.; Kurumizaka, H.
Deposited on	:	2024-06-19
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

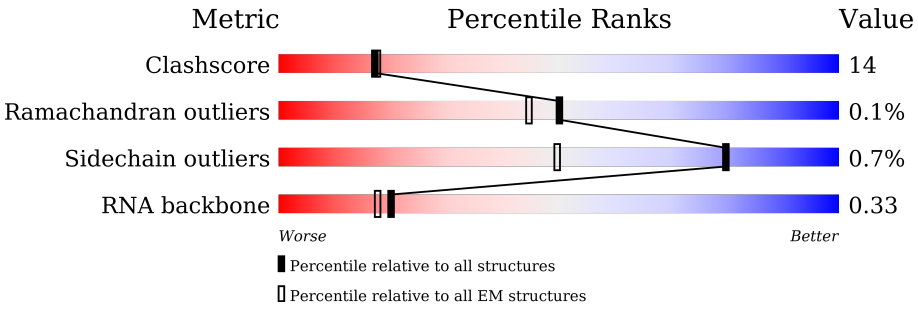
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

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



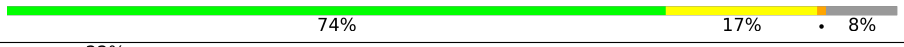
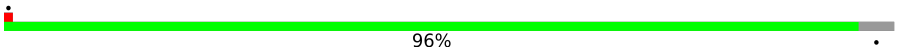
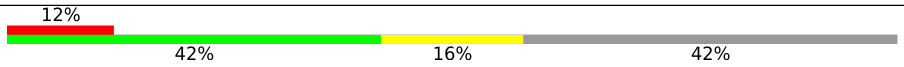
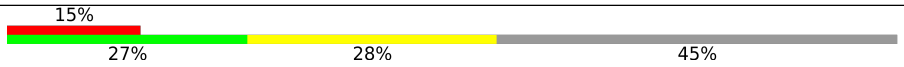
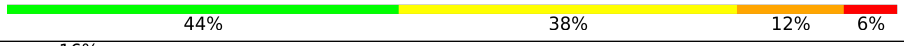
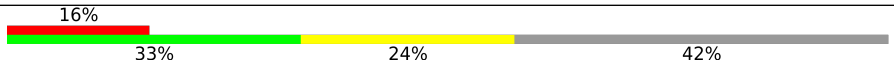
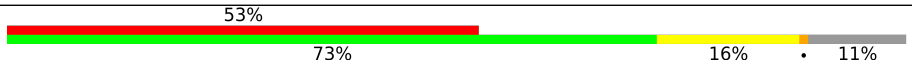
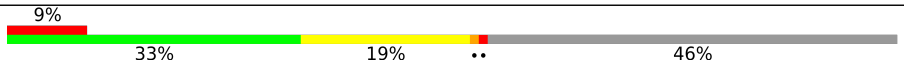
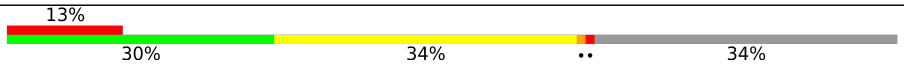
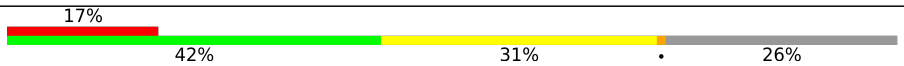
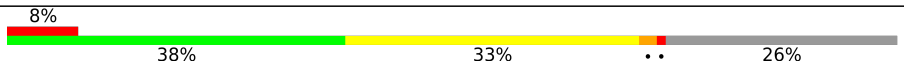
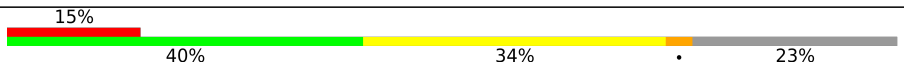
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 <=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	72% 8% 19%
2	B	1227	80% 15% 6%
3	C	304	73% 14% 13%
4	D	186	45% 72% 18% 10%
5	E	214	86% 13%
6	F	155	50% 5% 46%
7	G	171	26% 77% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	145	
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	M	110	
14	N	198	
15	P	16	
16	T	198	
17	V	114	
18	W	908	
19	a	136	
19	e	136	
20	b	103	
20	f	103	
21	c	115	
22	d	126	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 43686 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
			Total	C	N	O	S		
1	A	1412	11123	7014	1938	2101	70	0	0

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

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

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

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

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

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- 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 protein called Transcription elongation factor 1 homolog.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	109	Total	C	N	O	P	0	0
			2242	1061	412	660	109		

- Molecule 15 is a RNA chain called RNA (5'-R(P*CP*CP*CP*GP*GP*UP*GP*UP*CP*UP*UP*GP*GP*GP*UP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	16	Total	C	N	O	P	0	0
			341	151	57	117	16		

- Molecule 16 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	114	Total	C	N	O	P	0	0
			2326	1101	435	676	114		

- 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		

- Molecule 18 is a protein called Transcription elongation factor SPT5.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	74	Total	C	N	O	S	0	0
			595	379	110	104	2		
19	e	90	Total	C	N	O	S	0	0
			735	464	140	129	2		

- Molecule 20 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	76	Total 610	C 387	N 118	O 104	S 1	0	0
20	f	76	Total 610	C 387	N 118	O 104	S 1	0	0

- Molecule 21 is a protein called Histone H2A-Bbd type 2/3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	c	89	Total 699	C 436	N 127	O 135	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	d	88	Total 685	C 433	N 121	O 129	S 2	0	0

- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

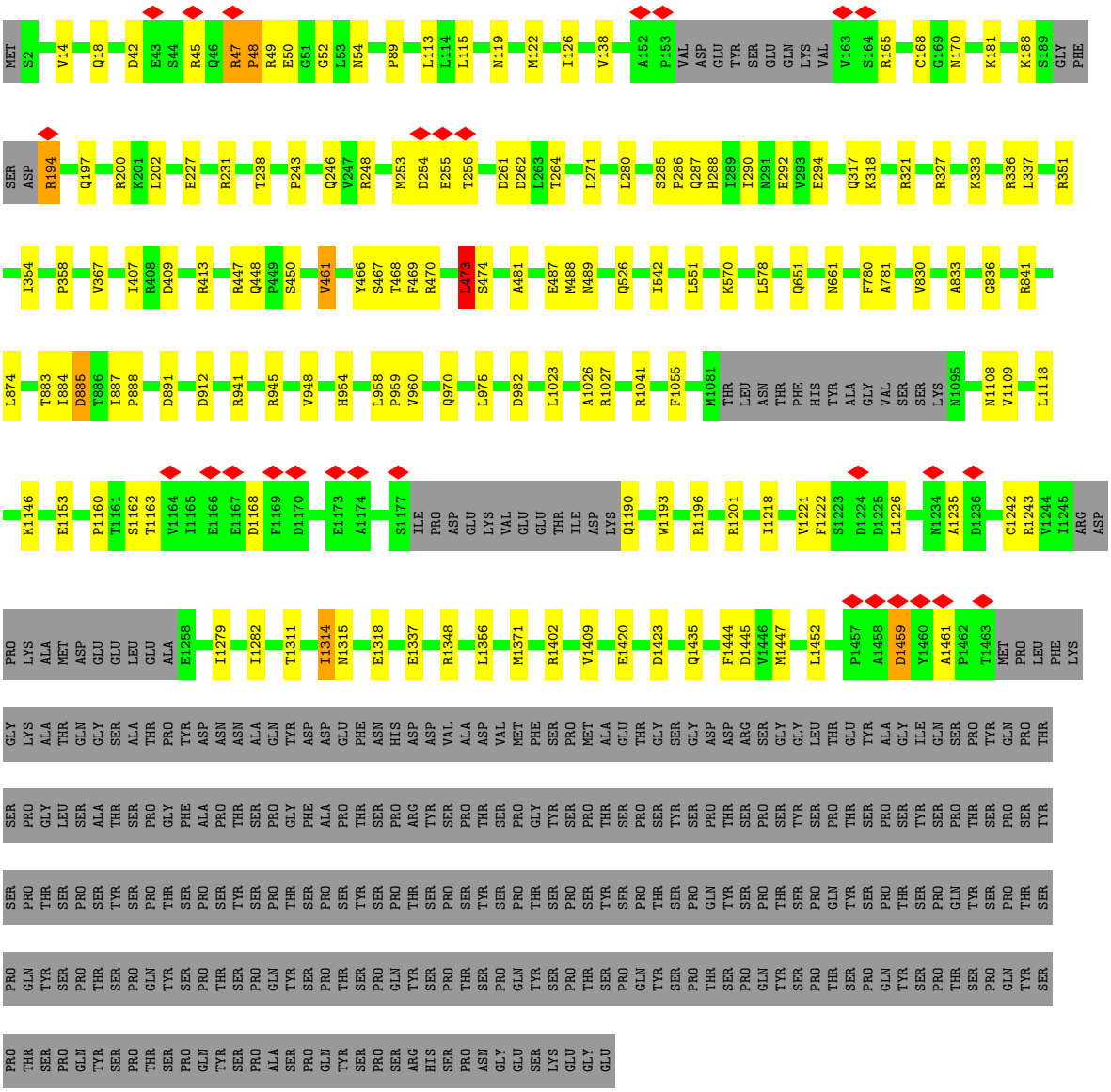
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
24	A	1	1	1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

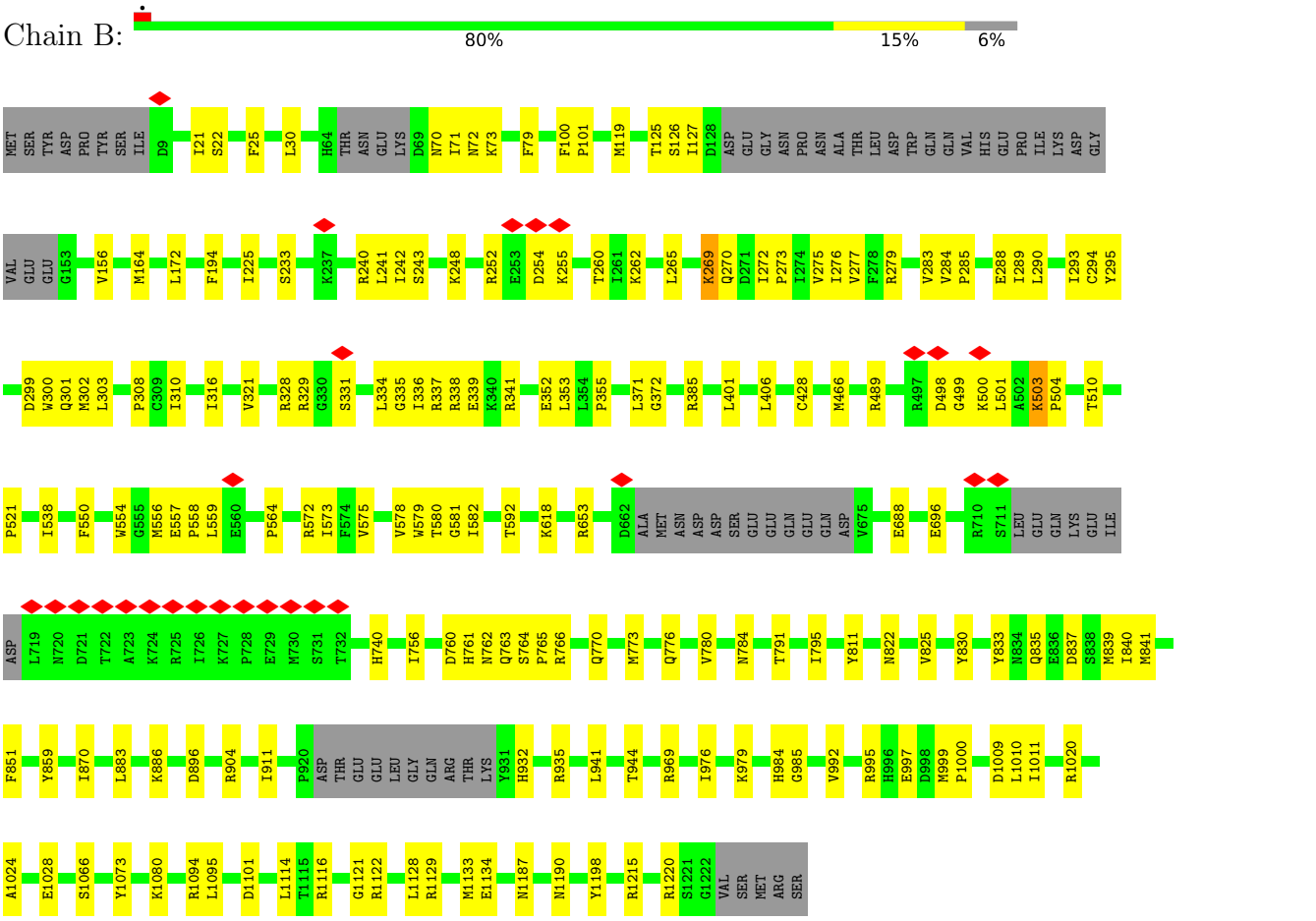
- Molecule 1: DNA-directed RNA polymerase subunit

Chain A:



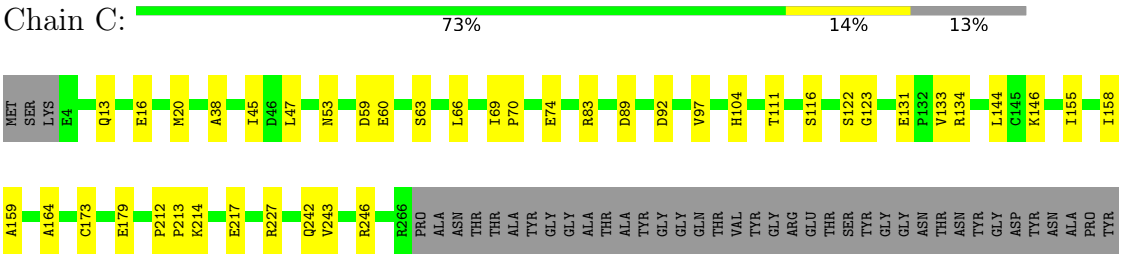
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:



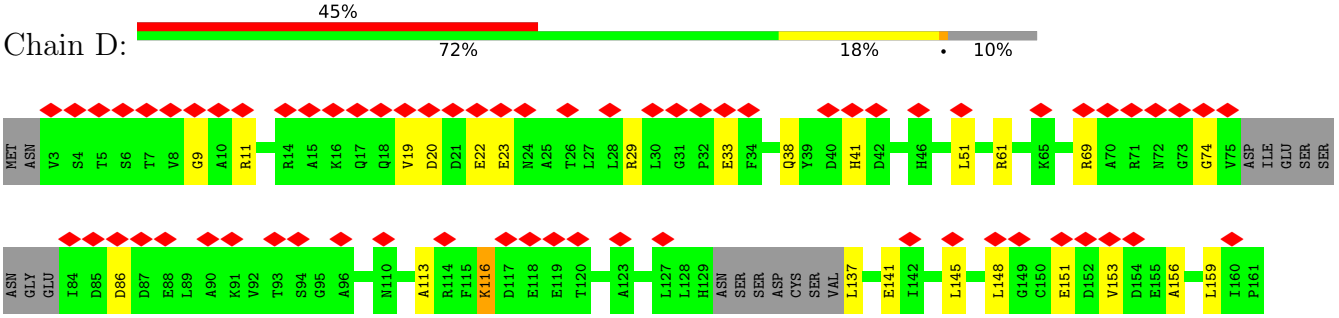
• Molecule 3: RNA polymerase II third largest subunit B44, part of central core

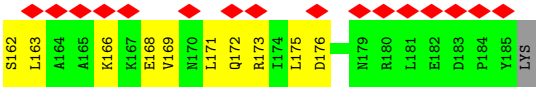
Chain C:



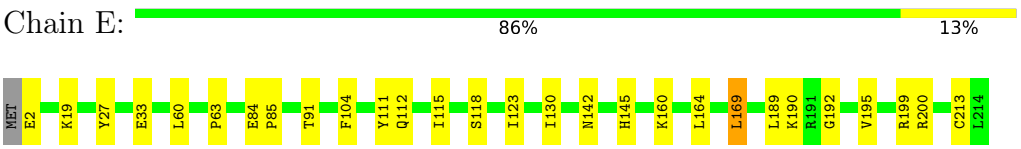
• Molecule 4: RNA polymerase II subunit B32

Chain D:

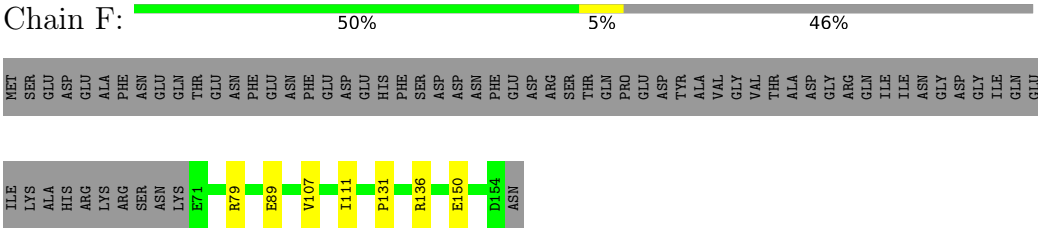




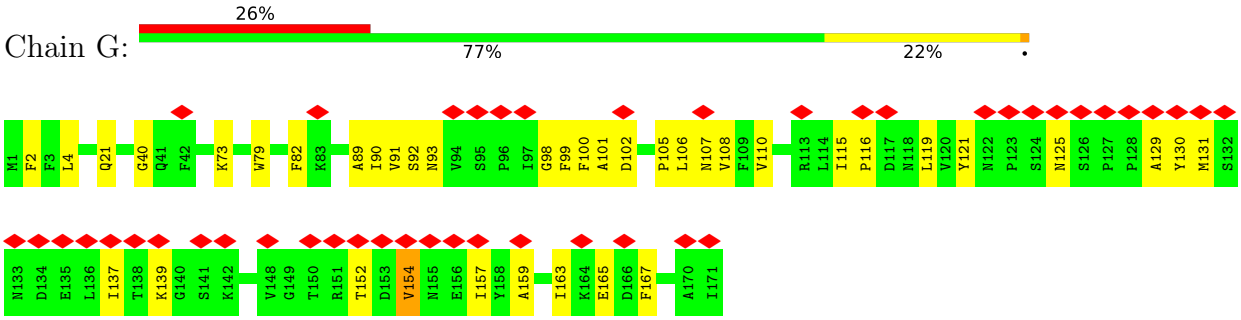
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



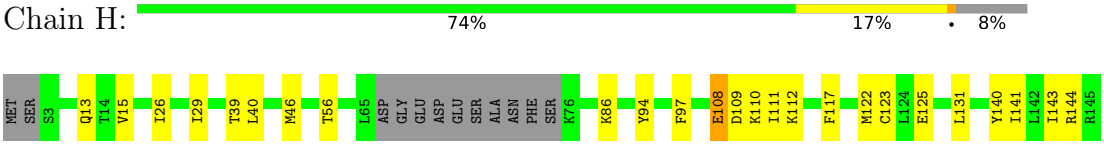
• Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III



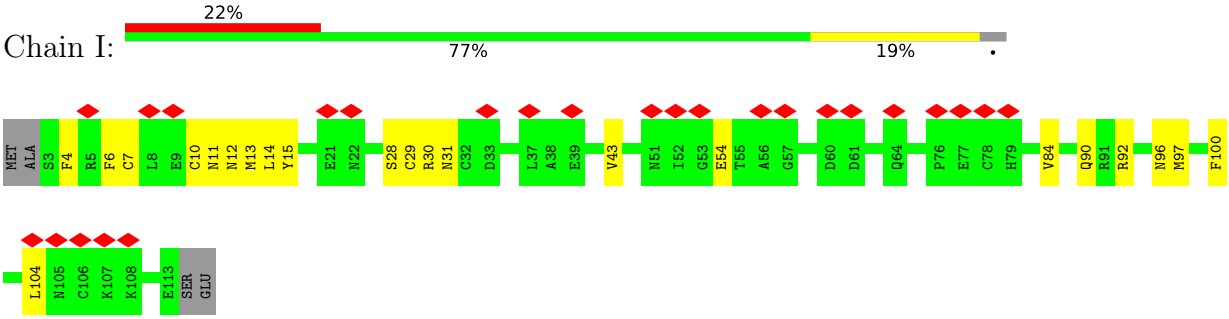
• Molecule 7: RNA polymerase II subunit



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

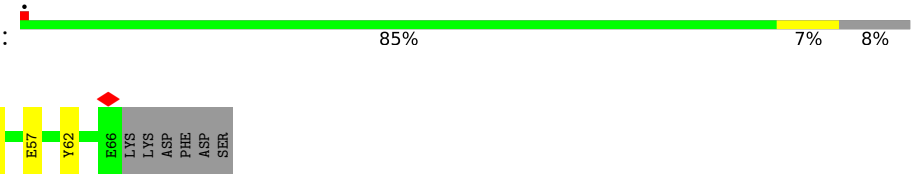


• Molecule 9: DNA-directed RNA polymerase subunit



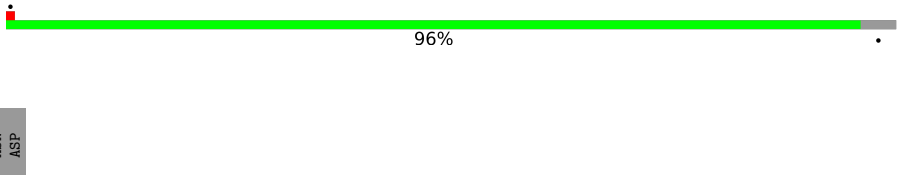
• Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

Chain J:



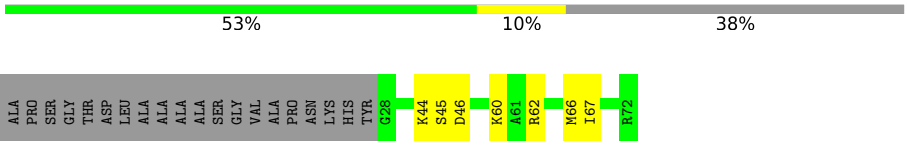
• Molecule 11: RNA polymerase II subunit B12.5

Chain K:



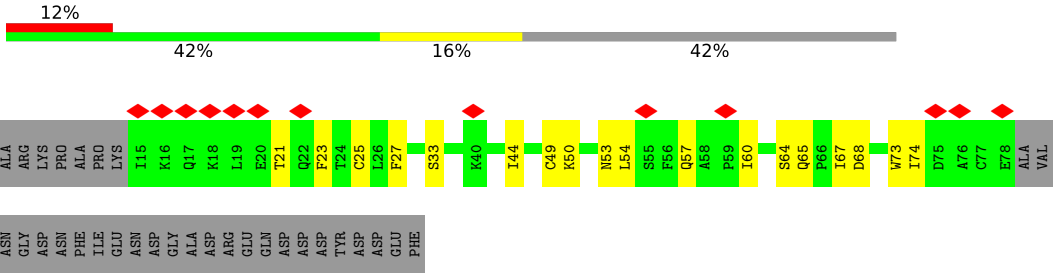
• Molecule 12: RNA polymerase subunit ABC10-alpha

Chain L:



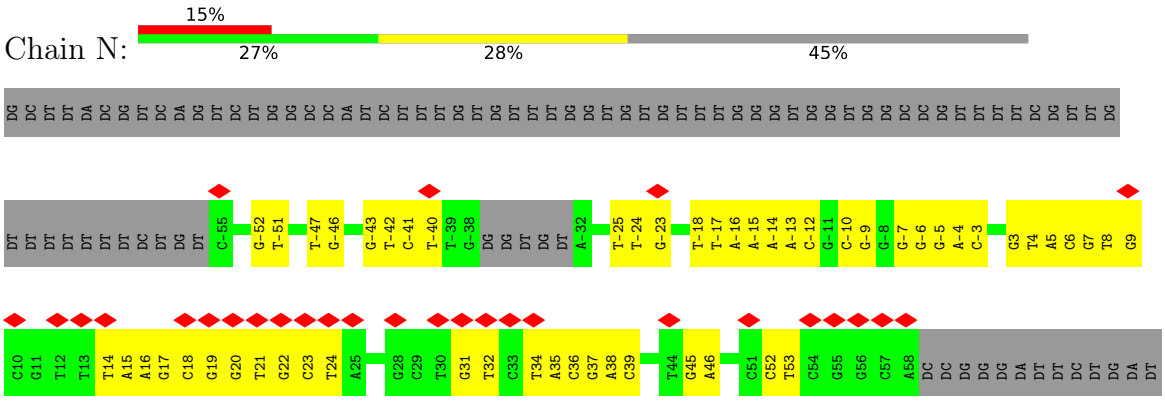
• Molecule 13: Transcription elongation factor 1 homolog

Chain M:



• Molecule 14: DNA (198-MER)

Chain N:

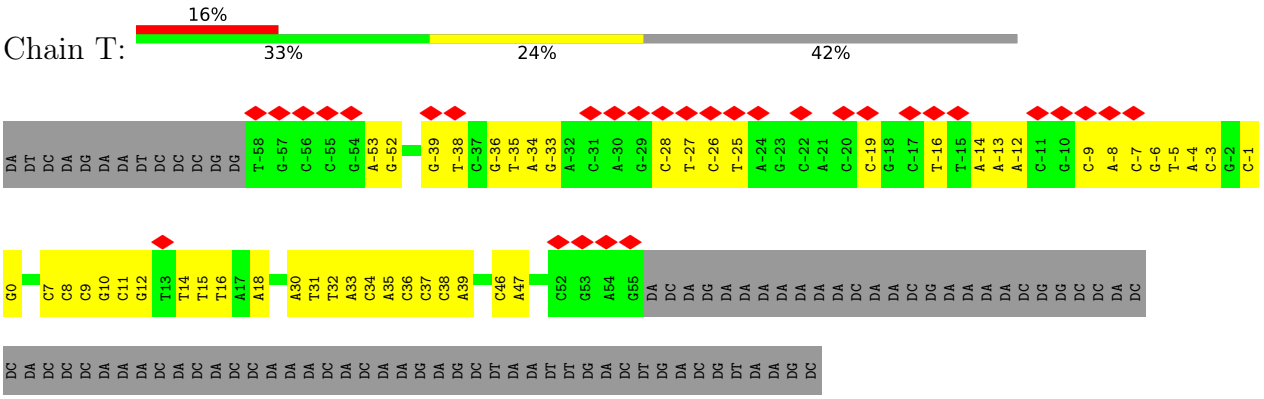


• Molecule 15: RNA (5'-R(P*CP*CP*CP*GP*GP*UP*GP*UP*CP*UP*UP*GP*GP*GP*UP*G)-3')

Chain P:

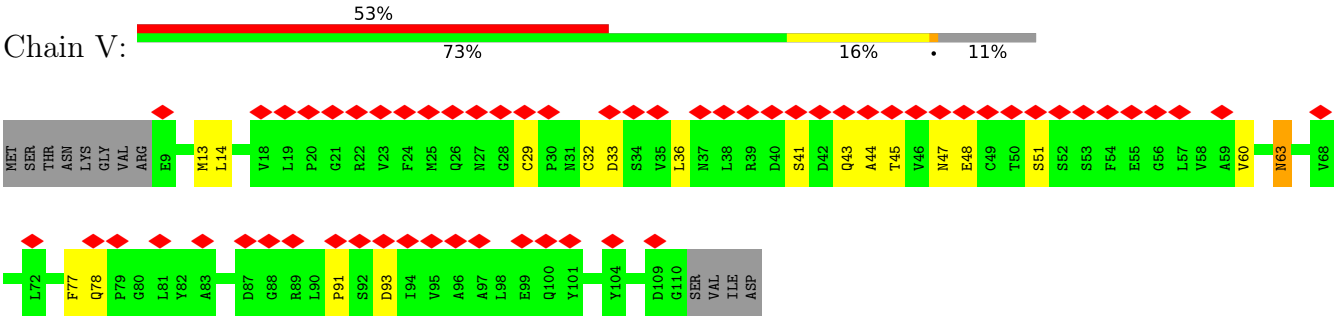
• Molecule 16: DNA (198-MER)

Chain T:



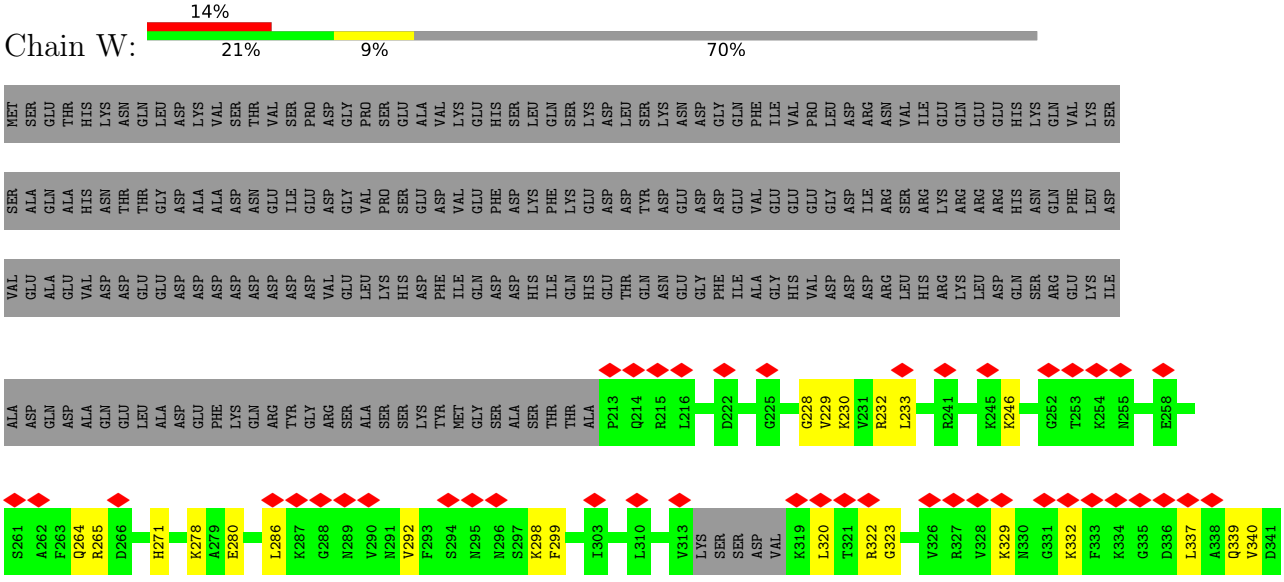
• Molecule 17: Transcription elongation factor SPT4

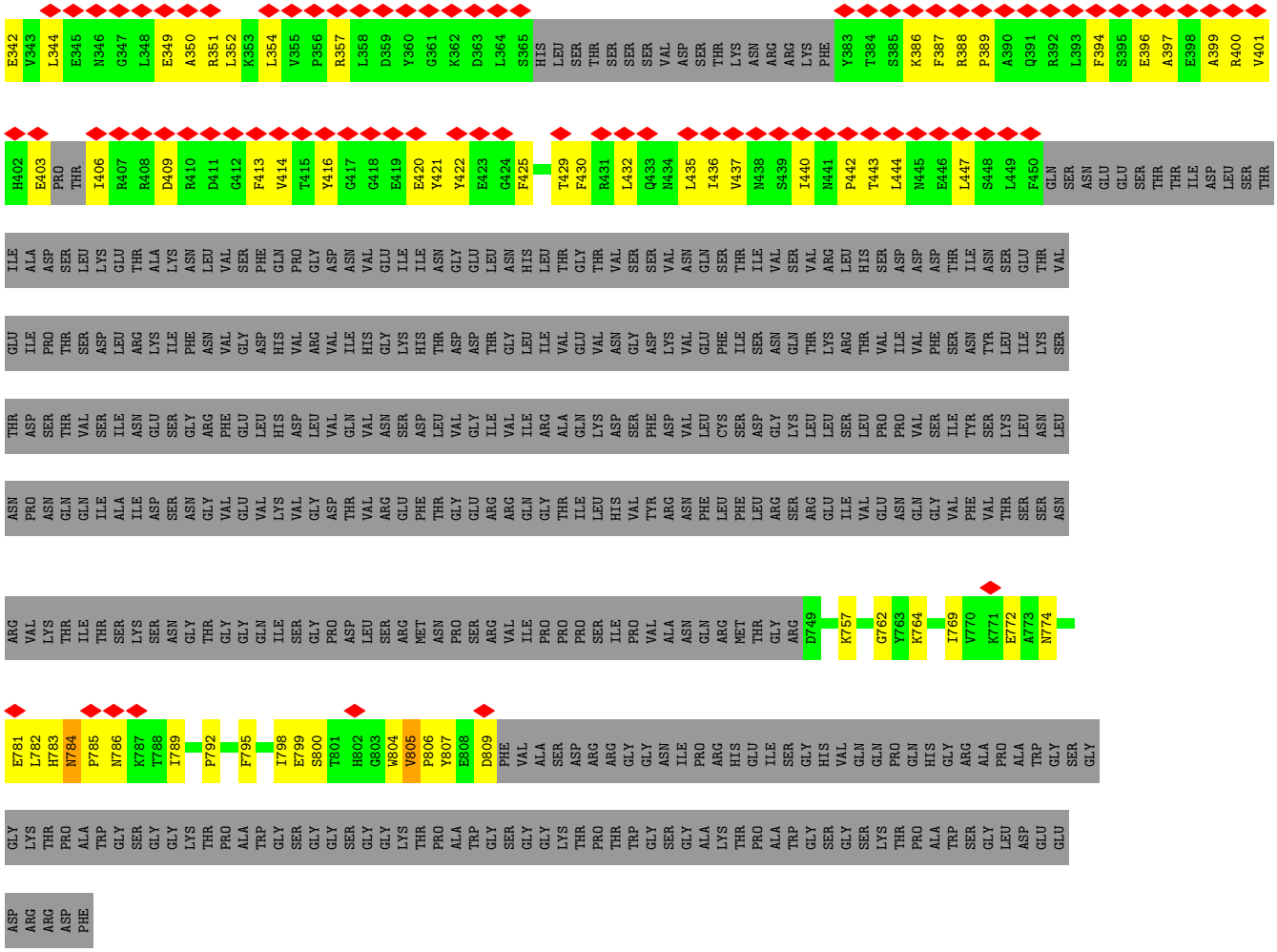
Chain V:



• Molecule 18: Transcription elongation factor SPT5

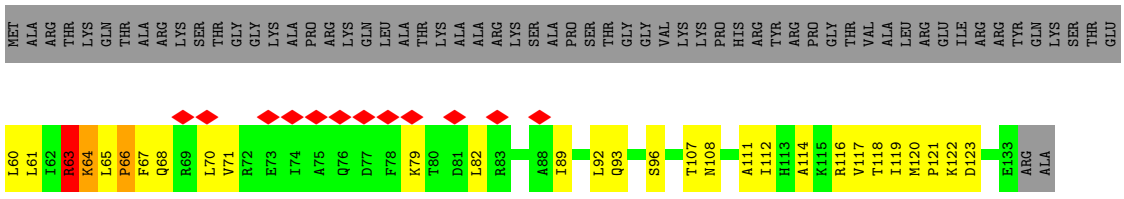
Chain W:





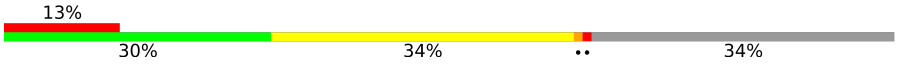
• Molecule 19: Histone H3.3

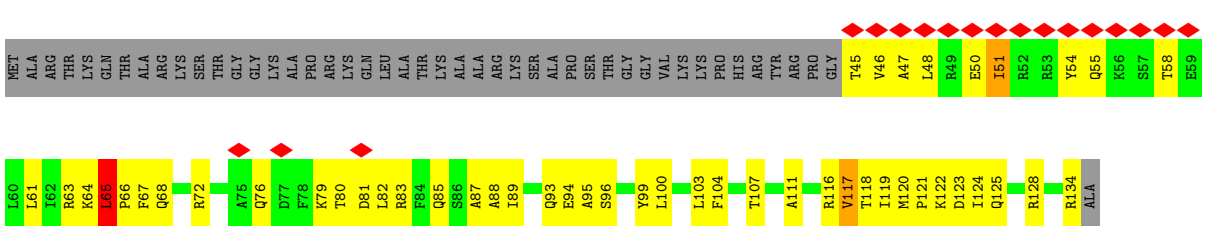
Chain a:



• Molecule 19: Histone H3.3

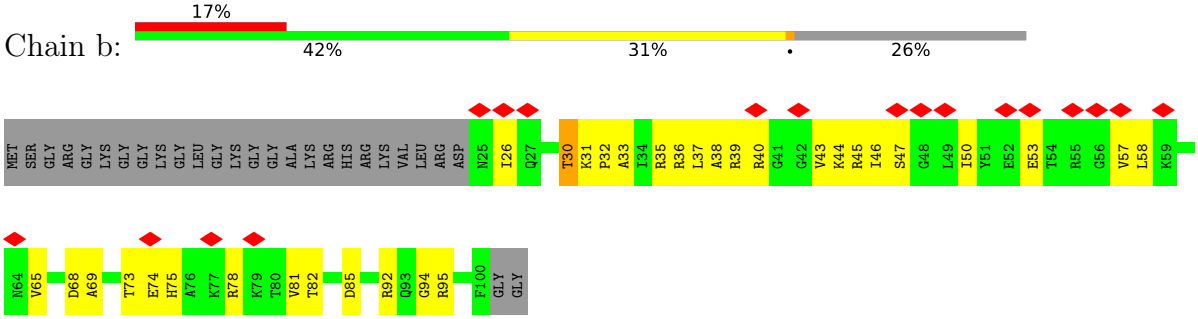
Chain e:





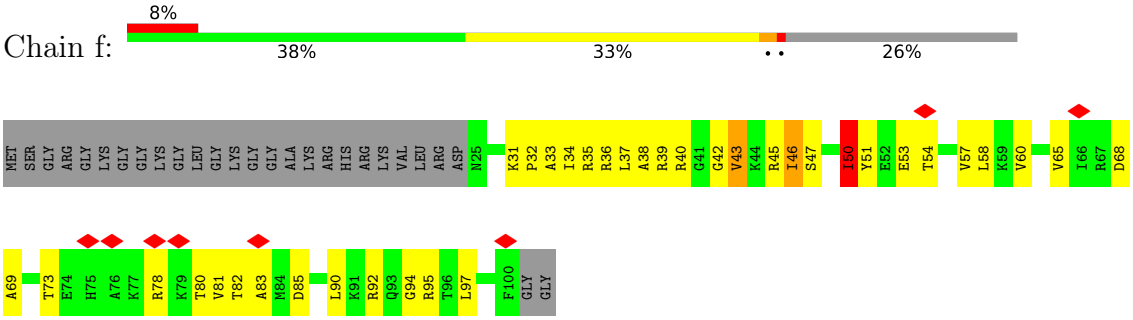
• Molecule 20: Histone H4

Chain b:



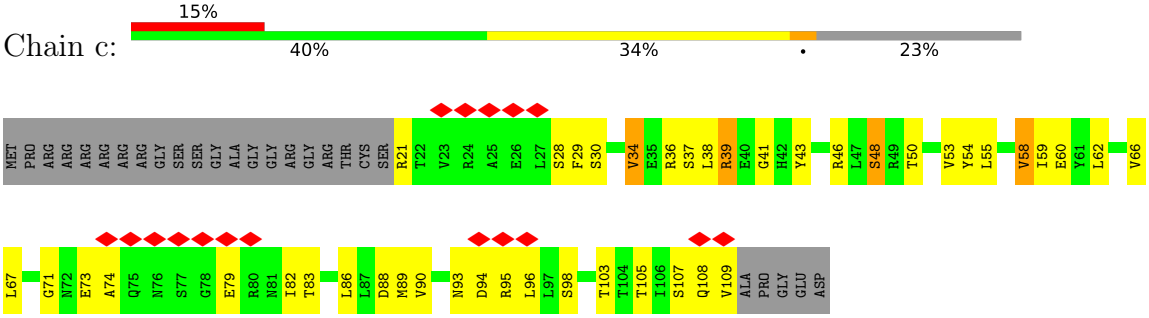
• Molecule 20: Histone H4

Chain f:



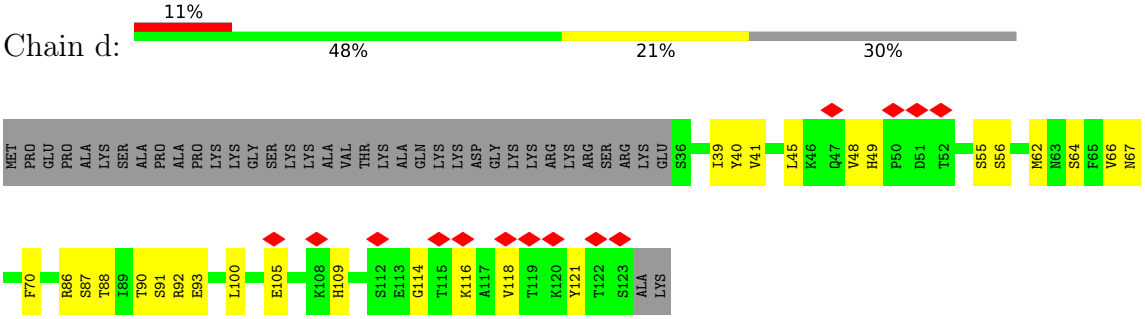
• Molecule 21: Histone H2A-Bbd type 2/3

Chain c:



• Molecule 22: Histone H2B type 1-J

Chain d:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	297456	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 ($e^-/Å^2$)	1.4	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.052	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00843	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.39	0/11329	0.75	6/15310 (0.0%)
2	B	0.42	0/9407	0.75	3/12685 (0.0%)
3	C	0.41	0/2139	0.71	0/2895
4	D	0.28	0/1326	0.75	1/1788 (0.1%)
5	E	0.36	0/1772	0.76	3/2385 (0.1%)
6	F	0.40	0/687	0.68	0/931
7	G	0.29	0/1353	0.78	2/1837 (0.1%)
8	H	0.35	0/1069	0.78	2/1444 (0.1%)
9	I	0.30	0/934	0.75	0/1257
10	J	0.44	0/554	0.76	0/742
11	K	0.40	0/953	0.73	0/1291
12	L	0.40	0/365	0.88	3/484 (0.6%)
13	M	0.27	0/513	0.51	0/693
14	N	0.15	0/2513	0.31	0/3877
15	P	0.18	0/379	0.41	1/589 (0.2%)
16	T	0.15	0/2609	0.29	0/4020
17	V	0.44	0/808	0.85	1/1097 (0.1%)
18	W	0.43	0/2267	0.80	0/3048
19	a	0.43	0/602	0.86	1/808 (0.1%)
19	e	0.34	0/743	0.85	4/996 (0.4%)
20	b	0.26	0/617	0.63	1/827 (0.1%)
20	f	0.28	0/617	0.71	1/827 (0.1%)
21	c	0.32	0/707	0.68	0/960
22	d	0.25	0/696	0.58	0/938
All	All	0.37	0/44959	0.70	29/61729 (0.0%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	45	SER	N-CA-C	8.85	120.93	111.28
1	A	47	ARG	CA-C-N	8.50	130.46	119.84
1	A	47	ARG	C-N-CA	8.50	130.46	119.84
8	H	109	ASP	N-CA-C	8.23	120.33	111.36
20	b	30	THR	N-CA-C	7.03	119.38	110.24
1	A	467	SER	N-CA-C	6.63	120.67	112.59
2	B	100	PHE	CA-C-N	6.62	128.12	119.84
2	B	100	PHE	C-N-CA	6.62	128.12	119.84
20	f	46	ILE	N-CA-C	6.47	117.20	107.75
19	a	63	ARG	CB-CA-C	5.89	118.64	110.16
19	e	80	THR	N-CA-C	5.77	118.63	110.50
4	D	9	GLY	N-CA-C	5.66	119.40	110.96
1	A	473	LEU	N-CA-C	5.64	119.26	112.38
17	V	63	ASN	N-CA-C	5.64	118.15	111.33
1	A	461	VAL	N-CA-C	5.64	116.33	108.89
7	G	165	GLU	N-CA-C	5.50	117.63	110.43
2	B	1066	SER	N-CA-C	5.47	119.06	112.38
8	H	110	LYS	N-CA-C	5.45	118.14	110.23
5	E	123	ILE	CA-C-N	-5.34	114.53	120.45
5	E	123	ILE	C-N-CA	-5.34	114.53	120.45
19	e	117	VAL	N-CA-C	-5.31	107.65	113.43
5	E	169	LEU	N-CA-C	5.28	118.16	109.72
19	e	65	LEU	CA-C-N	5.27	124.72	119.24
19	e	65	LEU	C-N-CA	5.27	124.72	119.24
15	P	9	U	OP1-P-O3'	5.23	123.69	108.00
7	G	98	GLY	N-CA-C	5.22	116.97	110.29
12	L	44	LYS	N-CA-C	5.16	116.91	111.28
12	L	46	ASP	N-CA-C	5.15	117.00	109.84
1	A	526	GLN	CB-CA-C	-5.10	110.71	116.63

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	11123	0	11147	180	0
2	B	9228	0	9232	218	0
3	C	2098	0	2059	41	0
4	D	1314	0	1314	44	0
5	E	1740	0	1754	26	0
6	F	677	0	693	6	0
7	G	1324	0	1342	56	0
8	H	1052	0	1050	23	0
9	I	917	0	867	37	0
10	J	545	0	561	6	0
11	K	932	0	944	0	0
12	L	359	0	358	5	0
13	M	505	0	497	38	0
14	N	2242	0	1226	73	0
15	P	341	0	172	13	0
16	T	2326	0	1274	80	0
17	V	792	0	758	14	0
18	W	2226	0	2273	135	0
19	a	595	0	626	84	0
19	e	735	0	775	91	0
20	b	610	0	653	56	0
20	f	610	0	653	92	0
21	c	699	0	712	56	0
22	d	685	0	703	32	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	M	1	0	0	0	0
23	V	1	0	0	0	0
24	A	1	0	0	0	0
All	All	43686	0	41643	1151	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 14.

All (1151) 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)
3:C:116:SER:OG	3:C:134:ARG:NH2	1.69	1.21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:112:ILE:HG12	19:a:117:VAL:HG22	1.26	1.18
3:C:116:SER:CB	3:C:134:ARG:HH12	1.58	1.16
19:e:120:MET:HB2	19:e:121:PRO:HD2	1.12	1.07
14:N:35:DA:C2	16:T:-34:DA:N1	2.25	1.04
3:C:116:SER:CA	3:C:134:ARG:HH12	1.72	1.02
19:a:111:ALA:O	19:a:116:ARG:N	1.92	1.02
3:C:116:SER:HB3	3:C:134:ARG:HH12	1.25	1.01
14:N:38:DA:H5'	21:c:46:ARG:HB3	1.43	0.99
2:B:503:LYS:HB2	2:B:504:PRO:HD3	1.41	0.99
19:a:118:THR:CG2	20:b:45:ARG:HB3	1.93	0.98
3:C:116:SER:HA	3:C:134:ARG:NH1	1.76	0.98
20:f:43:VAL:HG21	20:f:46:ILE:HD11	1.46	0.98
2:B:269:LYS:HE2	2:B:331:SER:HB3	1.46	0.97
18:W:396:GLU:OE2	18:W:414:VAL:HG23	1.63	0.97
19:e:103:LEU:CD2	20:f:57:VAL:HG11	1.95	0.97
19:e:134:ARG:HH11	20:f:60:VAL:HG21	1.30	0.97
4:D:145:LEU:HD21	4:D:163:LEU:HD11	1.44	0.96
2:B:575:VAL:O	2:B:578:VAL:HG12	1.64	0.96
2:B:101:PRO:HG2	2:B:172:LEU:HD11	1.46	0.96
3:C:116:SER:CA	3:C:134:ARG:NH1	2.27	0.96
7:G:108:VAL:HG13	7:G:159:ALA:O	1.66	0.96
18:W:399:ALA:HB1	18:W:406:ILE:HD11	1.46	0.96
19:e:107:THR:HG22	19:e:119:ILE:HG23	1.46	0.96
19:a:120:MET:HG2	19:a:121:PRO:HD2	1.45	0.96
19:e:107:THR:CG2	19:e:119:ILE:CG2	2.44	0.96
20:b:31:LYS:HE2	20:b:35:ARG:HH11	1.31	0.95
1:A:50:GLU:OE2	18:W:444:LEU:HD11	1.64	0.95
1:A:50:GLU:CD	18:W:444:LEU:HD11	1.89	0.95
19:e:65:LEU:HB2	19:e:66:PRO:HD3	1.48	0.95
19:e:120:MET:HB2	19:e:121:PRO:CD	1.96	0.95
20:f:43:VAL:HG21	20:f:46:ILE:CD1	1.95	0.95
19:a:116:ARG:NH1	19:a:122:LYS:HE3	1.82	0.95
1:A:1282:ILE:HG23	1:A:1311:THR:OG1	1.67	0.95
18:W:399:ALA:C	18:W:406:ILE:HD11	1.92	0.95
18:W:784:ASN:HB2	18:W:785:PRO:HD3	1.44	0.95
19:e:104:PHE:HE1	20:f:50:ILE:HD11	1.32	0.94
2:B:71:ILE:HD13	2:B:127:ILE:HG23	1.47	0.94
7:G:91:VAL:HA	7:G:100:PHE:O	1.66	0.94
19:a:116:ARG:HH12	19:a:122:LYS:HE3	1.32	0.94
3:C:116:SER:CB	3:C:134:ARG:NH1	2.30	0.94
1:A:830:VAL:HG13	2:B:500:LYS:CG	1.98	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:97:PHE:CD1	8:H:140:TYR:CZ	2.56	0.93
1:A:874:LEU:HD11	1:A:959:PRO:HG3	1.50	0.93
18:W:320:LEU:CD1	18:W:340:VAL:HG21	1.98	0.93
21:c:105:THR:CG2	20:f:95:ARG:HH11	1.81	0.93
19:a:111:ALA:O	19:a:116:ARG:CA	2.11	0.93
18:W:323:GLY:HA2	18:W:339:GLN:HE21	1.35	0.92
19:e:107:THR:HG22	19:e:119:ILE:CG2	1.99	0.92
2:B:839:MET:SD	2:B:1010:LEU:HD11	2.10	0.92
19:a:116:ARG:HH12	19:a:122:LYS:CE	1.83	0.92
1:A:830:VAL:HG13	2:B:500:LYS:HG3	1.47	0.91
20:f:38:ALA:O	20:f:43:VAL:HG13	1.68	0.91
9:I:10:CYS:SG	9:I:12:ASN:ND2	2.43	0.91
21:c:39:ARG:HG2	21:c:39:ARG:HH21	1.33	0.91
1:A:1226:LEU:HD11	1:A:1242:CYS:HB3	1.52	0.91
14:N:-42:DT:OP1	18:W:233:LEU:HD13	1.71	0.91
7:G:93:ASN:HB2	7:G:100:PHE:CD2	2.06	0.91
2:B:334:LEU:HD12	13:M:67:ILE:CD1	2.01	0.90
18:W:399:ALA:CB	18:W:406:ILE:HD11	2.01	0.90
19:a:118:THR:HG21	20:b:45:ARG:HB3	1.49	0.90
19:e:104:PHE:CE1	20:f:50:ILE:HD11	2.05	0.90
7:G:106:LEU:HD23	7:G:106:LEU:H	1.36	0.90
20:b:36:ARG:HG2	20:b:36:ARG:HH21	1.34	0.90
2:B:352:GLU:O	2:B:355:PRO:HD3	1.70	0.90
2:B:334:LEU:HD12	13:M:67:ILE:HD13	1.51	0.90
5:E:164:LEU:HD22	5:E:169:LEU:HD11	1.54	0.90
20:b:32:PRO:O	20:b:36:ARG:HG3	1.73	0.89
3:C:70:PRO:O	3:C:133:VAL:HG23	1.71	0.89
14:N:-4:DA:OP1	19:e:117:VAL:HG11	1.73	0.89
18:W:337:LEU:O	18:W:354:LEU:CD1	2.20	0.89
1:A:448:GLN:HE22	1:A:489:ASN:ND2	1.71	0.88
1:A:42:ASP:HB2	1:A:49:ARG:HB2	1.54	0.88
19:e:121:PRO:O	19:e:125:GLN:HG3	1.72	0.88
1:A:1118:LEU:HD11	1:A:1315:ASN:O	1.74	0.88
18:W:784:ASN:HB2	18:W:785:PRO:CD	2.03	0.88
18:W:399:ALA:C	18:W:406:ILE:CD1	2.47	0.87
18:W:413:PHE:CZ	18:W:420:GLU:HB3	2.08	0.87
1:A:448:GLN:HE22	1:A:489:ASN:HD22	1.20	0.87
21:c:54:TYR:O	21:c:58:VAL:HG12	1.75	0.87
8:H:97:PHE:CD1	8:H:140:TYR:CE2	2.62	0.87
1:A:887:ILE:HB	1:A:888:PRO:HD3	1.55	0.87
19:e:134:ARG:NH1	20:f:60:VAL:HG21	1.89	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:W:394:PHE:HE2	18:W:396:GLU:HG2	1.37	0.87
19:e:120:MET:CB	19:e:121:PRO:HD2	2.04	0.87
19:a:116:ARG:NH2	19:a:122:LYS:HE3	1.89	0.86
19:e:118:THR:HA	20:f:45:ARG:O	1.76	0.85
18:W:399:ALA:HB1	18:W:406:ILE:CD1	2.07	0.85
1:A:473:LEU:HD12	1:A:473:LEU:O	1.75	0.85
19:a:116:ARG:HH22	19:a:122:LYS:HE3	1.42	0.85
20:b:31:LYS:HE2	20:b:35:ARG:NH1	1.91	0.84
2:B:573:ILE:HB	2:B:581:GLY:O	1.77	0.84
2:B:503:LYS:CB	2:B:504:PRO:HD3	2.07	0.84
9:I:12:ASN:ND2	9:I:31:ASN:ND2	2.25	0.84
18:W:329:LYS:HD2	18:W:436:ILE:HG13	1.59	0.83
2:B:303:LEU:HD13	9:I:4:PHE:HD2	1.42	0.83
2:B:336:ILE:H	2:B:341:ARG:HH11	1.25	0.83
2:B:883:LEU:HB3	2:B:932:HIS:HE1	1.41	0.83
2:B:503:LYS:HB2	2:B:504:PRO:CD	2.09	0.83
1:A:1452:LEU:HD13	6:F:131:PRO:HA	1.60	0.83
2:B:572:ARG:HG2	2:B:579:TRP:HE1	1.42	0.83
9:I:6:PHE:CD1	9:I:13:MET:HA	2.13	0.83
19:a:111:ALA:CA	19:a:116:ARG:HB3	2.09	0.83
19:a:120:MET:HG2	19:a:121:PRO:CD	2.08	0.83
14:N:35:DA:H2	16:T:-34:DA:N1	1.73	0.83
1:A:1452:LEU:HD23	1:A:1452:LEU:O	1.80	0.82
19:e:95:ALA:HB2	20:f:90:LEU:HD11	1.60	0.82
9:I:7:CYS:O	9:I:11:ASN:HA	1.80	0.82
19:a:112:ILE:HG12	19:a:117:VAL:CG2	2.08	0.82
19:a:116:ARG:CZ	19:a:122:LYS:HE3	2.08	0.82
21:c:66:VAL:HG11	22:d:62:MET:HE1	1.60	0.82
19:e:107:THR:CG2	19:e:119:ILE:HG21	2.10	0.82
9:I:12:ASN:CG	9:I:31:ASN:ND2	2.38	0.81
1:A:473:LEU:O	1:A:473:LEU:CD1	2.27	0.81
18:W:805:VAL:HB	18:W:806:PRO:HD2	1.62	0.81
18:W:352:LEU:HD12	18:W:352:LEU:O	1.79	0.81
19:e:107:THR:CG2	19:e:119:ILE:HG23	2.05	0.81
13:M:54:LEU:HD12	13:M:54:LEU:O	1.80	0.81
18:W:399:ALA:CB	18:W:406:ILE:CD1	2.59	0.81
18:W:435:LEU:HD12	18:W:435:LEU:O	1.80	0.80
1:A:448:GLN:NE2	1:A:489:ASN:ND2	2.30	0.80
2:B:284:VAL:CG2	2:B:285:PRO:HD3	2.12	0.80
18:W:320:LEU:HD12	18:W:340:VAL:HG21	1.64	0.79
13:M:21:THR:HB	13:M:23:PHE:CD2	2.16	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:f:43:VAL:CG2	20:f:46:ILE:HD11	2.11	0.79
2:B:284:VAL:HG23	2:B:285:PRO:HD3	1.63	0.79
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.64	0.79
1:A:884:ILE:HD12	1:A:887:ILE:HD11	1.63	0.78
16:T:-6:DG:N2	20:b:45:ARG:HH22	1.81	0.78
2:B:337:ARG:HE	2:B:339:GLU:HB3	1.47	0.78
21:c:48:SER:HB3	22:d:90:THR:HA	1.65	0.78
2:B:269:LYS:CE	2:B:331:SER:HB3	2.13	0.78
1:A:253:MET:HA	15:P:1:G:N2	1.99	0.78
18:W:394:PHE:CE2	18:W:396:GLU:HG2	2.18	0.77
19:e:103:LEU:HD22	20:f:57:VAL:HG11	1.64	0.77
1:A:874:LEU:CD1	1:A:959:PRO:HG3	2.15	0.77
2:B:285:PRO:HG2	2:B:288:GLU:OE1	1.85	0.77
4:D:162:SER:O	4:D:166:LYS:HD3	1.84	0.77
7:G:106:LEU:CD1	7:G:157:ILE:CD1	2.62	0.77
7:G:157:ILE:O	7:G:157:ILE:HD12	1.84	0.77
5:E:164:LEU:HD22	5:E:169:LEU:CD1	2.14	0.77
3:C:214:LYS:HB2	3:C:217:GLU:HB2	1.65	0.77
20:f:47:SER:O	20:f:50:ILE:HG22	1.85	0.77
16:T:8:DC:P	20:f:35:ARG:HH22	2.07	0.77
2:B:334:LEU:H	2:B:334:LEU:HD22	1.50	0.76
3:C:116:SER:CB	3:C:134:ARG:HH22	1.97	0.76
13:M:44:ILE:HG23	13:M:57:GLN:HE21	1.50	0.76
5:E:111:TYR:CD1	5:E:115:ILE:HD11	2.20	0.76
1:A:447:ARG:HB2	1:A:488:MET:HE3	1.67	0.76
2:B:334:LEU:HD12	13:M:23:PHE:HE1	1.51	0.76
13:M:21:THR:HB	13:M:23:PHE:CE2	2.21	0.76
19:e:107:THR:HG21	19:e:119:ILE:HG21	1.66	0.76
19:e:111:ALA:HB2	19:e:123:ASP:OD2	1.85	0.75
20:f:38:ALA:HB1	20:f:43:VAL:HG11	1.67	0.75
16:T:-12:DA:P	20:b:30:THR:HG21	2.26	0.75
18:W:332:LYS:HD2	18:W:389:PRO:HD2	1.68	0.75
19:e:68:GLN:HG3	19:e:89:ILE:HD13	1.67	0.75
20:f:38:ALA:HB1	20:f:43:VAL:HG21	1.67	0.75
14:N:35:DA:C2	16:T:-34:DA:C2	2.75	0.75
7:G:89:ALA:HB1	7:G:101:ALA:HB1	1.68	0.74
17:V:13:MET:HE2	17:V:51:SER:HB2	1.69	0.74
19:a:111:ALA:O	19:a:116:ARG:CB	2.34	0.74
8:H:97:PHE:HD1	8:H:140:TYR:CE2	2.06	0.74
20:f:50:ILE:HD13	20:f:50:ILE:O	1.87	0.74
16:T:-6:DG:H21	20:b:45:ARG:HH22	1.32	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:LEU:CD1	13:M:67:ILE:HD13	2.17	0.74
2:B:559:LEU:HD22	2:B:579:TRP:CZ3	2.22	0.74
21:c:53:VAL:HG23	22:d:118:VAL:HG12	1.67	0.74
2:B:275:VAL:HG12	2:B:279:ARG:HE	1.52	0.74
8:H:97:PHE:CE1	8:H:140:TYR:CZ	2.76	0.74
19:e:65:LEU:N	19:e:65:LEU:HD13	2.02	0.74
2:B:572:ARG:CG	2:B:579:TRP:HE1	2.00	0.74
2:B:883:LEU:HB3	2:B:932:HIS:CE1	2.21	0.74
2:B:935:ARG:NH1	15:P:0:U:O4	2.21	0.74
18:W:230:LYS:HD3	18:W:271:HIS:NE2	2.03	0.74
4:D:22:GLU:OE1	4:D:22:GLU:N	2.19	0.74
4:D:173:ARG:NH2	4:D:173:ARG:HB2	2.03	0.74
1:A:887:ILE:HB	1:A:888:PRO:CD	2.17	0.73
7:G:106:LEU:HD11	7:G:157:ILE:CD1	2.19	0.73
2:B:498:ASP:HB3	16:T:32:DT:H3	1.52	0.73
2:B:503:LYS:CB	2:B:504:PRO:CD	2.66	0.73
18:W:332:LYS:HD2	18:W:389:PRO:CD	2.18	0.73
19:e:83:ARG:O	20:f:80:THR:HA	1.88	0.73
7:G:106:LEU:CD1	7:G:157:ILE:HD12	2.18	0.73
19:e:79:LYS:HB3	19:e:82:LEU:HD11	1.70	0.73
19:a:111:ALA:HA	19:a:116:ARG:HB3	1.71	0.73
21:c:36:ARG:HE	21:c:36:ARG:HA	1.54	0.73
22:d:105:GLU:HG2	22:d:109:HIS:CD2	2.24	0.73
4:D:172:GLN:HG3	4:D:176:ASP:OD2	1.89	0.72
18:W:396:GLU:OE2	18:W:414:VAL:CG2	2.36	0.72
21:c:105:THR:HG23	20:f:95:ARG:HH11	1.50	0.72
2:B:521:PRO:HB3	15:P:8:G:OP1	1.89	0.72
4:D:153:VAL:HG22	4:D:171:LEU:HB3	1.70	0.72
2:B:337:ARG:O	2:B:341:ARG:CB	2.37	0.72
2:B:935:ARG:NH1	15:P:0:U:C4	2.57	0.72
1:A:287:GLN:HE21	1:A:287:GLN:HA	1.55	0.72
2:B:25:PHE:CD2	2:B:811:TYR:CD1	2.77	0.72
9:I:12:ASN:CG	9:I:31:ASN:HD22	1.97	0.72
19:e:61:LEU:HD12	20:f:37:LEU:HD23	1.72	0.72
13:M:54:LEU:HD11	13:M:73:TRP:CH2	2.24	0.72
18:W:413:PHE:HD1	18:W:422:TYR:HB2	1.54	0.72
1:A:246:GLN:N	1:A:246:GLN:OE1	2.22	0.71
5:E:2:GLU:N	5:E:2:GLU:OE1	2.23	0.71
1:A:321:ARG:HA	2:B:466:MET:CE	2.20	0.71
9:I:12:ASN:ND2	9:I:31:ASN:HD22	1.85	0.71
18:W:320:LEU:HD11	18:W:340:VAL:HG21	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:ILE:HG21	9:I:13:MET:SD	2.30	0.71
16:T:18:DA:H5"	19:e:65:LEU:HG	1.71	0.71
7:G:93:ASN:H	7:G:100:PHE:HB2	1.53	0.71
3:C:116:SER:OG	3:C:134:ARG:CZ	2.38	0.71
19:e:128:ARG:HH12	19:e:134:ARG:HE	1.38	0.71
4:D:145:LEU:CD2	4:D:163:LEU:HD11	2.18	0.71
18:W:337:LEU:O	18:W:354:LEU:HD11	1.89	0.71
1:A:885:ASP:CG	1:A:1027:ARG:HE	1.98	0.71
1:A:833:ALA:HA	16:T:33:DA:C8	2.25	0.71
21:c:30:SER:O	21:c:34:VAL:HG22	1.91	0.71
2:B:285:PRO:HB2	2:B:288:GLU:HB2	1.73	0.70
19:e:85:GLN:CD	20:f:82:THR:HG22	2.15	0.70
1:A:1160:PRO:HB3	1:A:1190:GLN:HE21	1.56	0.70
2:B:272:ILE:HD13	2:B:277:VAL:HG12	1.74	0.70
2:B:1121:GLY:HA2	16:T:37:DC:OP1	1.92	0.70
14:N:7:DG:H4'	20:b:45:ARG:HG3	1.72	0.70
2:B:303:LEU:HD13	9:I:4:PHE:CD2	2.24	0.70
2:B:764:SER:HB3	2:B:765:PRO:HD3	1.74	0.70
19:e:88:ALA:HB2	20:f:81:VAL:O	1.92	0.70
2:B:336:ILE:HB	2:B:341:ARG:CZ	2.22	0.69
7:G:152:THR:HG22	7:G:154:VAL:H	1.57	0.69
19:a:112:ILE:CG1	19:a:117:VAL:HA	2.22	0.69
1:A:1452:LEU:HD23	1:A:1452:LEU:C	2.18	0.69
7:G:99:PHE:CZ	7:G:110:VAL:HG21	2.27	0.69
2:B:240:ARG:HD2	2:B:240:ARG:O	1.91	0.69
19:e:85:GLN:OE1	20:f:82:THR:HB	1.92	0.69
1:A:447:ARG:HB2	1:A:488:MET:HG2	1.73	0.69
2:B:336:ILE:HG22	2:B:341:ARG:HB2	1.74	0.69
9:I:6:PHE:HD1	9:I:13:MET:CA	2.05	0.69
21:c:55:LEU:O	21:c:59:ILE:HG13	1.92	0.69
19:a:65:LEU:HD13	19:a:65:LEU:O	1.92	0.69
19:a:112:ILE:HG13	19:a:117:VAL:HA	1.72	0.69
16:T:-12:DA:OP1	20:b:30:THR:CG2	2.40	0.69
1:A:318:LYS:CD	14:N:-43:DG:H1	2.06	0.69
2:B:1134:GLU:OE1	2:B:1134:GLU:N	2.23	0.69
14:N:-3:DC:OP2	19:e:116:ARG:HG2	1.92	0.69
19:e:88:ALA:CB	20:f:81:VAL:O	2.40	0.69
2:B:233:SER:O	2:B:241:LEU:HD12	1.93	0.69
7:G:91:VAL:CA	7:G:100:PHE:O	2.40	0.69
7:G:106:LEU:HD11	7:G:157:ILE:HD11	1.75	0.69
2:B:233:SER:OG	2:B:355:PRO:HG2	1.91	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:21:THR:CB	13:M:23:PHE:CD2	2.76	0.68
19:e:65:LEU:HD13	19:e:65:LEU:H	1.57	0.68
2:B:336:ILE:H	2:B:341:ARG:NH1	1.91	0.68
3:C:89:ASP:O	18:W:764:LYS:HE3	1.94	0.68
9:I:6:PHE:CD1	9:I:13:MET:CA	2.76	0.68
1:A:885:ASP:OD2	1:A:1027:ARG:CD	2.41	0.68
19:a:112:ILE:CG1	19:a:117:VAL:HG22	2.17	0.68
21:c:66:VAL:CG1	22:d:62:MET:HE1	2.24	0.68
22:d:105:GLU:HG2	22:d:109:HIS:HD2	1.57	0.68
13:M:33:SER:HA	13:M:50:LYS:HE2	1.75	0.68
7:G:100:PHE:HB3	7:G:107:ASN:HD21	1.59	0.68
8:H:111:ILE:HG22	8:H:131:LEU:HD12	1.75	0.68
18:W:357:ARG:C	18:W:389:PRO:HG2	2.19	0.68
1:A:1348:ARG:HD3	1:A:1348:ARG:C	2.19	0.67
18:W:332:LYS:HG3	18:W:388:ARG:CB	2.23	0.67
2:B:839:MET:HB2	2:B:1011:ILE:O	1.94	0.67
7:G:106:LEU:CD1	7:G:157:ILE:HD11	2.23	0.67
16:T:-34:DA:H5"	22:d:87:SER:CB	2.24	0.67
18:W:337:LEU:O	18:W:354:LEU:HD13	1.92	0.67
1:A:14:VAL:H	1:A:1435:GLN:HE22	1.40	0.67
1:A:448:GLN:OE1	1:A:448:GLN:N	2.26	0.67
2:B:337:ARG:O	2:B:341:ARG:HB2	1.94	0.67
17:V:60:VAL:HG12	17:V:63:ASN:OD1	1.94	0.67
20:f:53:GLU:O	20:f:57:VAL:HG23	1.93	0.67
8:H:108:GLU:N	8:H:108:GLU:OE1	2.28	0.67
14:N:-42:DT:OP1	18:W:233:LEU:CD1	2.42	0.67
16:T:-13:DA:C5'	19:a:63:ARG:HD3	2.24	0.67
1:A:1348:ARG:HD3	1:A:1348:ARG:O	1.95	0.66
2:B:582:ILE:HD12	2:B:582:ILE:O	1.94	0.66
2:B:337:ARG:NE	2:B:339:GLU:HB3	2.10	0.66
14:N:17:DG:N2	16:T:-16:DT:C2	2.63	0.66
18:W:329:LYS:HD2	18:W:436:ILE:CG1	2.25	0.66
18:W:342:GLU:HB2	18:W:351:ARG:HB2	1.77	0.66
18:W:351:ARG:HG2	18:W:429:THR:HG22	1.78	0.66
18:W:399:ALA:CA	18:W:406:ILE:HD11	2.26	0.66
16:T:-12:DA:OP1	20:b:30:THR:HG21	1.94	0.66
7:G:79:TRP:CZ3	7:G:105:PRO:HD2	2.30	0.66
18:W:332:LYS:HG3	18:W:388:ARG:HB3	1.76	0.66
21:c:108:GLN:NE2	19:e:58:THR:HG21	2.11	0.66
20:f:34:ILE:HB	20:f:51:TYR:CD1	2.31	0.66
1:A:321:ARG:HA	2:B:466:MET:HE1	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:6:PHE:CE1	9:I:13:MET:HB3	2.31	0.65
19:a:119:ILE:HD13	20:b:43:VAL:HG21	1.78	0.65
4:D:145:LEU:HD11	4:D:163:LEU:HD21	1.79	0.65
19:a:63:ARG:HB2	19:a:66:PRO:HD2	1.77	0.65
19:a:107:THR:HG22	19:a:119:ILE:HG22	1.79	0.65
1:A:833:ALA:HA	16:T:33:DA:H8	1.61	0.65
16:T:-6:DG:N2	20:b:45:ARG:NH2	2.44	0.65
18:W:329:LYS:CD	18:W:436:ILE:HG13	2.24	0.65
18:W:798:ILE:HD11	18:W:807:TYR:CD2	2.31	0.65
19:a:107:THR:CG2	19:a:119:ILE:HB	2.27	0.65
4:D:19:VAL:O	4:D:29:ARG:NH2	2.30	0.65
19:a:67:PHE:O	19:a:71:VAL:HG23	1.96	0.65
18:W:352:LEU:HD21	18:W:430:PHE:CD1	2.31	0.65
1:A:1226:LEU:HD12	1:A:1243:ARG:O	1.96	0.65
2:B:294:CYS:SG	2:B:302:MET:SD	2.88	0.65
2:B:582:ILE:HD12	2:B:582:ILE:C	2.21	0.65
18:W:805:VAL:HB	18:W:806:PRO:CD	2.26	0.65
7:G:93:ASN:CB	7:G:100:PHE:CD2	2.79	0.65
18:W:396:GLU:CD	18:W:414:VAL:CG2	2.70	0.65
19:a:118:THR:HG22	20:b:45:ARG:HB3	1.78	0.65
1:A:1279:ILE:CG2	1:A:1315:ASN:ND2	2.60	0.64
3:C:116:SER:HB3	3:C:134:ARG:NH1	2.01	0.64
4:D:171:LEU:HD23	4:D:171:LEU:O	1.98	0.64
16:T:-12:DA:OP2	20:b:30:THR:HB	1.96	0.64
18:W:800:SER:HB3	18:W:805:VAL:CG2	2.26	0.64
19:a:65:LEU:HD13	19:a:65:LEU:C	2.22	0.64
2:B:896:ASP:OD2	12:L:60:LYS:NZ	2.31	0.64
2:B:70:ASN:O	2:B:127:ILE:HA	1.97	0.64
7:G:129:ALA:HB1	7:G:137:ILE:O	1.98	0.64
1:A:248:ARG:HD2	1:A:264:THR:OG1	1.98	0.64
20:b:74:GLU:O	22:d:92:ARG:NH1	2.31	0.64
20:f:50:ILE:HD13	20:f:50:ILE:C	2.22	0.64
1:A:450:SER:O	2:B:1133:MET:HE2	1.97	0.64
4:D:11:ARG:O	4:D:11:ARG:HG2	1.97	0.64
18:W:784:ASN:CB	18:W:785:PRO:CD	2.76	0.64
20:f:38:ALA:HB1	20:f:43:VAL:CG2	2.27	0.64
14:N:-3:DC:P	19:e:116:ARG:HG2	2.37	0.64
20:f:46:ILE:HG22	20:f:50:ILE:HG21	1.79	0.64
9:I:12:ASN:ND2	9:I:31:ASN:HB2	2.13	0.64
19:e:107:THR:HG21	19:e:119:ILE:CG2	2.21	0.64
1:A:780:PHE:CZ	2:B:510:THR:HA	2.34	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:c:39:ARG:HG2	21:c:39:ARG:NH2	2.09	0.63
4:D:137:LEU:HD12	4:D:137:LEU:N	2.13	0.63
21:c:105:THR:HG23	20:f:95:ARG:NH1	2.13	0.63
14:N:34:DT:O2	16:T:-33:DG:N2	2.30	0.63
20:b:36:ARG:HG2	20:b:36:ARG:NH2	2.10	0.63
1:A:367:VAL:CG2	1:A:461:VAL:HG13	2.28	0.63
18:W:437:VAL:O	18:W:437:VAL:HG22	1.99	0.63
18:W:329:LYS:CG	18:W:436:ILE:HG13	2.29	0.63
20:f:38:ALA:HB1	20:f:43:VAL:CG1	2.28	0.63
4:D:171:LEU:CD2	4:D:175:LEU:HG	2.28	0.63
16:T:8:DC:OP2	20:f:35:ARG:NH2	2.32	0.63
13:M:21:THR:HG1	13:M:23:PHE:HD2	1.46	0.63
13:M:44:ILE:CG2	13:M:57:GLN:HE21	2.11	0.62
18:W:352:LEU:HD12	18:W:352:LEU:C	2.24	0.62
2:B:336:ILE:HG21	2:B:341:ARG:HA	1.81	0.62
20:b:73:THR:HG21	20:b:81:VAL:HG22	1.80	0.62
2:B:334:LEU:CD1	13:M:67:ILE:CD1	2.75	0.62
20:f:73:THR:HG21	20:f:81:VAL:HG22	1.80	0.62
4:D:159:LEU:HD21	7:G:167:PHE:HB2	1.80	0.62
4:D:19:VAL:O	4:D:19:VAL:HG12	1.99	0.62
16:T:-34:DA:H5”	22:d:87:SER:HB2	1.82	0.62
19:a:65:LEU:HB3	19:a:66:PRO:HD3	1.82	0.62
1:A:318:LYS:HD2	14:N:-43:DG:H1	1.64	0.62
1:A:982:ASP:O	1:A:1041:ARG:NH1	2.33	0.62
19:a:107:THR:HG22	19:a:119:ILE:CG2	2.30	0.62
1:A:333:LYS:HE2	16:T:34:DC:OP1	2.00	0.61
21:c:29:PHE:CD1	22:d:40:TYR:HB3	2.35	0.61
3:C:89:ASP:O	18:W:764:LYS:CE	2.48	0.61
16:T:-9:DC:H2”	16:T:-8:DA:C8	2.35	0.61
2:B:837:ASP:OD2	2:B:1020:ARG:NH1	2.32	0.61
22:d:90:THR:HG22	22:d:91:SER:H	1.65	0.61
14:N:-4:DA:OP1	19:e:117:VAL:CG1	2.46	0.61
1:A:1459:ASP:OD1	1:A:1459:ASP:N	2.34	0.61
2:B:233:SER:OG	2:B:355:PRO:CG	2.48	0.61
2:B:554:TRP:CZ2	2:B:592:THR:HG21	2.36	0.61
2:B:336:ILE:HB	2:B:341:ARG:NH1	2.16	0.61
17:V:44:ALA:O	17:V:48:GLU:HG2	2.01	0.61
2:B:283:VAL:HG23	2:B:283:VAL:O	2.00	0.61
8:H:56:THR:HB	8:H:144:ARG:HB3	1.83	0.61
13:M:54:LEU:HD12	13:M:54:LEU:C	2.25	0.61
14:N:-12:DC:H4’	14:N:-12:DC:OP1	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:0:U:H4'	15:P:1:G:H5'	1.82	0.61
21:c:105:THR:CG2	20:f:95:ARG:NH1	2.59	0.61
1:A:836:GLY:HA3	16:T:33:DA:H1'	1.81	0.61
9:I:29:CYS:SG	9:I:30:ARG:N	2.74	0.61
2:B:284:VAL:N	2:B:285:PRO:CD	2.63	0.60
8:H:111:ILE:HG22	8:H:111:ILE:O	1.99	0.60
7:G:115:ILE:HG23	7:G:163:ILE:HD11	1.82	0.60
20:b:92:ARG:NH1	22:d:100:LEU:O	2.34	0.60
9:I:6:PHE:HD1	9:I:13:MET:HA	1.60	0.60
18:W:799:GLU:HB3	18:W:804:TRP:CZ3	2.35	0.60
1:A:50:GLU:OE2	18:W:444:LEU:CD1	2.44	0.60
1:A:448:GLN:NE2	1:A:489:ASN:HD22	1.95	0.60
1:A:1109:VAL:O	1:A:1109:VAL:HG12	2.01	0.60
7:G:99:PHE:CE2	7:G:110:VAL:HB	2.35	0.60
7:G:106:LEU:HD23	7:G:106:LEU:N	2.12	0.60
18:W:413:PHE:CD1	18:W:422:TYR:HB2	2.35	0.60
19:a:120:MET:C	20:b:50:ILE:HD11	2.26	0.60
21:c:21:ARG:HD2	22:d:121:TYR:CE1	2.36	0.60
2:B:334:LEU:HD22	2:B:334:LEU:N	2.17	0.60
1:A:194:ARG:HE	1:A:194:ARG:N	2.00	0.60
1:A:885:ASP:HB2	1:A:1026:ALA:HB1	1.83	0.60
19:a:111:ALA:C	19:a:116:ARG:HB3	2.26	0.60
2:B:995:ARG:NH2	2:B:997:GLU:OE2	2.35	0.60
16:T:-6:DG:H21	20:b:45:ARG:NH2	2.00	0.60
1:A:1279:ILE:HG22	1:A:1315:ASN:ND2	2.17	0.59
2:B:859:TYR:HD2	2:B:911:ILE:HD11	1.67	0.59
2:B:969:ARG:NH2	3:C:60:GLU:OE1	2.35	0.59
3:C:116:SER:CB	3:C:134:ARG:NH2	2.59	0.59
7:G:154:VAL:O	7:G:154:VAL:HG12	2.02	0.59
18:W:396:GLU:CD	18:W:414:VAL:HG21	2.27	0.59
20:b:36:ARG:HH21	20:b:36:ARG:CG	2.11	0.59
19:e:103:LEU:HD21	20:f:57:VAL:HG11	1.81	0.59
1:A:253:MET:HA	15:P:1:G:C2	2.36	0.59
2:B:71:ILE:HG23	2:B:71:ILE:O	2.01	0.59
4:D:41:HIS:HB3	7:G:73:LYS:HD3	1.82	0.59
18:W:344:LEU:HG	18:W:349:GLU:HB2	1.84	0.59
19:a:120:MET:CA	20:b:50:ILE:HD11	2.33	0.59
7:G:137:ILE:O	7:G:137:ILE:HG22	2.02	0.59
21:c:39:ARG:HH21	21:c:39:ARG:CG	2.12	0.59
2:B:334:LEU:H	2:B:334:LEU:CD2	2.15	0.59
5:E:85:PRO:HA	5:E:112:GLN:HB2	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ARG:HG3	1:A:248:ARG:O	2.01	0.59
1:A:1279:ILE:HG22	1:A:1315:ASN:HD22	1.67	0.59
18:W:781:GLU:HG3	18:W:781:GLU:O	2.03	0.59
13:M:44:ILE:CG2	13:M:57:GLN:NE2	2.66	0.59
18:W:394:PHE:CE2	18:W:396:GLU:CG	2.86	0.58
18:W:397:ALA:O	18:W:401:VAL:HG23	2.03	0.58
1:A:466:TYR:CG	2:B:976:ILE:HD12	2.37	0.58
3:C:69:ILE:HD11	3:C:144:LEU:HD21	1.84	0.58
3:C:116:SER:CB	3:C:134:ARG:CZ	2.81	0.58
2:B:336:ILE:N	2:B:341:ARG:HH11	1.98	0.58
7:G:102:ASP:OD1	7:G:107:ASN:HB2	2.03	0.58
17:V:63:ASN:HD22	17:V:77:PHE:C	2.11	0.58
19:e:54:TYR:OH	20:f:36:ARG:CD	2.51	0.58
2:B:233:SER:OG	2:B:355:PRO:HD2	2.04	0.58
13:M:21:THR:OG1	13:M:23:PHE:HD2	1.85	0.58
16:T:-12:DA:P	20:b:30:THR:CG2	2.91	0.58
19:a:107:THR:HG21	19:a:119:ILE:HB	1.86	0.58
21:c:48:SER:CB	22:d:90:THR:HA	2.31	0.58
7:G:106:LEU:HD13	7:G:157:ILE:CD1	2.34	0.58
13:M:27:PHE:CD1	13:M:54:LEU:HD22	2.39	0.58
16:T:-28:DC:H2"	16:T:-27:DT:C5	2.39	0.58
18:W:413:PHE:HZ	18:W:420:GLU:CD	2.11	0.58
20:b:69:ALA:O	20:b:73:THR:HG23	2.04	0.58
5:E:84:GLU:OE1	5:E:91:THR:OG1	2.20	0.58
8:H:97:PHE:HD1	8:H:140:TYR:CZ	2.18	0.58
18:W:352:LEU:HD21	18:W:430:PHE:CE1	2.39	0.58
3:C:92:ASP:OD1	3:C:123:GLY:O	2.22	0.58
3:C:146:LYS:NZ	10:J:57:GLU:OE2	2.34	0.58
14:N:19:DG:H1	16:T:-19:DC:H42	1.50	0.58
21:c:55:LEU:HA	21:c:58:VAL:CG1	2.33	0.58
14:N:-13:DA:H3'	14:N:-12:DC:H5"	1.85	0.57
1:A:887:ILE:O	1:A:945:ARG:NH1	2.34	0.57
1:A:290:ILE:HG23	1:A:294:GLU:CD	2.29	0.57
14:N:-46:DG:OP1	18:W:386:LYS:HE3	2.04	0.57
20:f:43:VAL:CG2	20:f:46:ILE:CD1	2.76	0.57
20:f:69:ALA:O	20:f:73:THR:HG23	2.03	0.57
1:A:960:VAL:HG12	1:A:960:VAL:O	2.03	0.57
2:B:335:GLY:HA2	13:M:74:ILE:HD13	1.84	0.57
4:D:141:GLU:CD	4:D:166:LYS:NZ	2.63	0.57
4:D:173:ARG:HB2	4:D:173:ARG:HH21	1.68	0.57
1:A:466:TYR:HB2	1:A:470:ARG:HH12	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:TYR:HD1	2:B:564:PRO:HB3	1.69	0.57
9:I:6:PHE:HD1	9:I:13:MET:N	2.03	0.57
1:A:570:LYS:HB3	8:H:46:MET:HE1	1.86	0.57
19:e:128:ARG:NE	20:f:57:VAL:HG22	2.18	0.57
16:T:-3:DC:OP1	19:a:118:THR:OG1	2.21	0.57
1:A:841:ARG:NH1	1:A:1108:ASN:OD1	2.37	0.57
17:V:13:MET:CE	17:V:51:SER:HB2	2.35	0.57
17:V:32:CYS:O	17:V:36:LEU:HB2	2.05	0.57
20:f:34:ILE:CG2	20:f:51:TYR:HD1	2.18	0.57
2:B:466:MET:N	2:B:466:MET:SD	2.77	0.56
19:a:111:ALA:O	19:a:116:ARG:HB3	2.04	0.56
1:A:1452:LEU:HD22	6:F:131:PRO:HB3	1.86	0.56
4:D:20:ASP:HA	4:D:29:ARG:CZ	2.35	0.56
18:W:388:ARG:HB2	18:W:389:PRO:HD2	1.87	0.56
21:c:30:SER:O	21:c:34:VAL:CG2	2.53	0.56
20:f:38:ALA:C	20:f:43:VAL:HG13	2.28	0.56
1:A:89:PRO:HB3	1:A:238:THR:HG22	1.87	0.56
2:B:578:VAL:HG13	2:B:580:THR:HG23	1.87	0.56
4:D:171:LEU:HD23	4:D:175:LEU:HG	1.86	0.56
2:B:337:ARG:HH11	2:B:339:GLU:CD	2.14	0.56
3:C:20:MET:SD	3:C:227:ARG:NH1	2.75	0.56
13:M:44:ILE:HG23	13:M:57:GLN:NE2	2.20	0.56
14:N:-3:DC:OP1	19:e:118:THR:HG22	2.05	0.56
2:B:30:LEU:O	2:B:489:ARG:NH2	2.38	0.56
1:A:1201:ARG:NH1	1:A:1235:ALA:O	2.39	0.56
3:C:83:ARG:HG2	18:W:762:GLY:HA2	1.88	0.56
14:N:35:DA:H2	16:T:-34:DA:C2	2.21	0.56
21:c:71:GLY:HA3	22:d:49:HIS:CD2	2.41	0.56
19:e:107:THR:HG22	19:e:119:ILE:HG21	1.81	0.56
2:B:336:ILE:CG2	2:B:341:ARG:HA	2.36	0.56
8:H:13:GLN:HE22	8:H:29:ILE:HD12	1.70	0.56
14:N:31:DG:H2'	14:N:32:DT:C6	2.41	0.56
18:W:784:ASN:CB	18:W:785:PRO:HD3	2.27	0.56
19:a:116:ARG:HH12	19:a:122:LYS:CD	2.19	0.55
19:e:134:ARG:NH1	20:f:60:VAL:CG2	2.65	0.55
2:B:498:ASP:OD2	16:T:32:DT:O4	2.25	0.55
2:B:822:ASN:O	10:J:47:ARG:NH2	2.39	0.55
19:e:85:GLN:NE2	20:f:82:THR:HG22	2.20	0.55
21:c:73:GLU:HG3	21:c:90:VAL:HG12	1.88	0.55
7:G:79:TRP:HZ3	7:G:106:LEU:CD2	2.19	0.55
18:W:413:PHE:CE1	18:W:420:GLU:HB3	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:VAL:CG1	2:B:500:LYS:HG3	2.28	0.55
4:D:141:GLU:CD	4:D:166:LYS:HZ2	2.15	0.55
22:d:45:LEU:HA	22:d:48:VAL:HG12	1.89	0.55
12:L:62:ARG:NH1	12:L:67:ILE:HD12	2.22	0.55
19:e:65:LEU:N	19:e:65:LEU:CD1	2.68	0.55
2:B:1129:ARG:NE	16:T:35:DA:OP1	2.39	0.55
1:A:351:ARG:HB2	2:B:1128:LEU:HD11	1.87	0.55
16:T:-33:DG:P	22:d:86:ARG:HH21	2.31	0.55
20:f:34:ILE:HG21	20:f:51:TYR:HD1	1.72	0.55
3:C:74:GLU:O	3:C:246:ARG:NH1	2.33	0.54
13:M:25:CYS:SG	13:M:54:LEU:HD21	2.46	0.54
19:a:119:ILE:HG12	20:b:43:VAL:HG11	1.90	0.54
1:A:287:GLN:HA	1:A:287:GLN:NE2	2.22	0.54
18:W:388:ARG:HB2	18:W:389:PRO:CD	2.37	0.54
7:G:106:LEU:H	7:G:106:LEU:CD2	2.17	0.54
18:W:800:SER:CB	18:W:805:VAL:CG2	2.84	0.54
2:B:71:ILE:HD12	2:B:126:SER:C	2.32	0.54
19:a:116:ARG:HH22	19:a:122:LYS:CE	2.16	0.54
21:c:107:SER:O	19:e:94:GLU:OE1	2.25	0.54
2:B:279:ARG:HB3	2:B:284:VAL:HG12	1.89	0.54
18:W:394:PHE:HE2	18:W:396:GLU:CG	2.14	0.54
2:B:303:LEU:HB3	9:I:4:PHE:CE2	2.43	0.54
1:A:290:ILE:CG2	1:A:294:GLU:CD	2.81	0.54
1:A:830:VAL:HG13	2:B:500:LYS:CD	2.38	0.54
2:B:559:LEU:HD22	2:B:579:TRP:CH2	2.43	0.54
14:N:35:DA:N3	16:T:-34:DA:C2	2.75	0.54
16:T:-13:DA:H5'	19:a:63:ARG:HD3	1.89	0.54
16:T:-12:DA:OP1	20:b:30:THR:HG22	2.08	0.54
21:c:36:ARG:HH11	21:c:39:ARG:HG2	1.73	0.54
21:c:82:ILE:HA	21:c:86:LEU:HD12	1.88	0.54
1:A:321:ARG:HA	2:B:466:MET:HE2	1.89	0.54
1:A:409:ASP:OD1	1:A:409:ASP:N	2.41	0.54
1:A:885:ASP:OD2	1:A:1027:ARG:HD3	2.08	0.54
2:B:22:SER:HA	2:B:811:TYR:HE1	1.73	0.54
2:B:760:ASP:OD1	2:B:760:ASP:N	2.38	0.54
14:N:7:DG:P	20:b:47:SER:HA	2.46	0.54
14:N:7:DG:O4'	20:b:45:ARG:NH2	2.40	0.54
19:e:121:PRO:O	19:e:125:GLN:CG	2.53	0.54
2:B:776:GLN:NE2	15:P:8:G:O2'	2.40	0.54
9:I:12:ASN:HD22	9:I:31:ASN:HB2	1.72	0.54
13:M:54:LEU:HD11	13:M:73:TRP:CZ2	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-40:DT:OP1	18:W:232:ARG:HD2	2.08	0.54
7:G:89:ALA:CB	7:G:101:ALA:HB1	2.38	0.53
7:G:130:TYR:HB2	7:G:137:ILE:HD12	1.90	0.53
15:P:8:G:N2	16:T:37:DC:C2	2.76	0.53
19:a:120:MET:HA	20:b:50:ILE:HD11	1.90	0.53
2:B:762:ASN:HD21	2:B:1024:ALA:HB3	1.73	0.53
19:e:87:ALA:C	20:f:83:ALA:HB2	2.33	0.53
1:A:830:VAL:CG1	2:B:500:LYS:HB3	2.38	0.53
19:a:108:ASN:C	19:a:108:ASN:HD22	2.15	0.53
21:c:37:SER:OG	22:d:70:PHE:CZ	2.62	0.53
20:f:68:ASP:OD2	20:f:92:ARG:NH2	2.42	0.53
19:a:111:ALA:CB	19:a:116:ARG:HB3	2.39	0.53
20:f:33:ALA:O	20:f:37:LEU:HG	2.09	0.53
20:b:68:ASP:OD2	20:b:92:ARG:NH2	2.42	0.53
2:B:284:VAL:N	2:B:285:PRO:HD2	2.23	0.53
2:B:791:THR:HG21	16:T:39:DA:H5"	1.89	0.53
18:W:320:LEU:HD11	18:W:340:VAL:CG2	2.37	0.53
1:A:336:ARG:HH12	2:B:1114:LEU:HD21	1.74	0.53
1:A:367:VAL:HG21	1:A:461:VAL:HG13	1.88	0.53
1:A:448:GLN:CD	1:A:489:ASN:ND2	2.67	0.53
2:B:336:ILE:HB	2:B:341:ARG:NE	2.23	0.53
19:a:111:ALA:HB1	19:a:116:ARG:C	2.31	0.53
21:c:95:ARG:HA	21:c:98:SER:OG	2.09	0.53
10:J:8:PHE:HB2	10:J:47:ARG:HH12	1.73	0.53
2:B:290:LEU:HD22	9:I:6:PHE:HZ	1.74	0.53
19:a:64:LYS:H	19:a:64:LYS:HD2	1.73	0.53
18:W:352:LEU:CD2	18:W:430:PHE:CD1	2.92	0.52
18:W:399:ALA:O	18:W:406:ILE:HD11	2.08	0.52
19:a:107:THR:HG22	19:a:119:ILE:HB	1.91	0.52
1:A:473:LEU:O	1:A:473:LEU:HD13	2.06	0.52
1:A:912:ASP:OD1	1:A:912:ASP:N	2.42	0.52
2:B:71:ILE:HD13	2:B:127:ILE:CG2	2.31	0.52
16:T:34:DC:H2'	16:T:35:DA:H8	1.74	0.52
17:V:41:SER:HB2	17:V:45:THR:HB	1.91	0.52
5:E:130:ILE:CD1	5:E:190:LYS:HD3	2.40	0.52
8:H:122:MET:SD	8:H:141:ILE:HD12	2.49	0.52
17:V:43:GLN:NE2	17:V:47:ASN:OD1	2.39	0.52
1:A:1118:LEU:HB2	1:A:1311:THR:HG22	1.92	0.52
18:W:772:GLU:OE2	18:W:774:ASN:ND2	2.42	0.52
20:b:36:ARG:NH2	20:b:36:ARG:CG	2.72	0.52
21:c:74:ALA:O	21:c:79:GLU:N	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-17:DT:H2"	14:N:-16:DA:C8	2.45	0.52
18:W:413:PHE:HZ	18:W:420:GLU:HB3	1.68	0.52
19:e:65:LEU:HB2	19:e:66:PRO:CD	2.30	0.52
19:e:85:GLN:HG3	20:f:80:THR:HG22	1.90	0.52
2:B:25:PHE:HD2	2:B:811:TYR:CD1	2.25	0.52
2:B:944:THR:HG21	2:B:1122:ARG:HE	1.75	0.52
18:W:800:SER:HB3	18:W:805:VAL:HG21	1.90	0.52
18:W:805:VAL:CB	18:W:806:PRO:CD	2.87	0.52
2:B:21:ILE:HG22	2:B:811:TYR:CZ	2.45	0.52
7:G:79:TRP:HZ3	7:G:106:LEU:HD21	1.75	0.52
7:G:93:ASN:N	7:G:100:PHE:HB2	2.23	0.52
9:I:90:GLN:HE21	9:I:92:ARG:HG3	1.74	0.52
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	1.91	0.52
18:W:399:ALA:CB	18:W:406:ILE:HD13	2.39	0.52
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	1.92	0.52
1:A:318:LYS:CD	14:N:-43:DG:N1	2.73	0.52
2:B:316:ILE:HG23	2:B:321:VAL:HG23	1.92	0.52
18:W:798:ILE:HD12	18:W:807:TYR:HA	1.91	0.52
20:f:34:ILE:CG2	20:f:51:TYR:CD1	2.93	0.52
2:B:101:PRO:HG2	2:B:172:LEU:CD1	2.29	0.51
9:I:6:PHE:HE1	9:I:13:MET:HB3	1.74	0.51
14:N:-46:DG:OP1	18:W:386:LYS:CE	2.58	0.51
1:A:292:GLU:OE1	18:W:271:HIS:HE1	1.93	0.51
14:N:7:DG:OP1	20:b:47:SER:HA	2.09	0.51
18:W:409:ASP:HB2	18:W:413:PHE:HD2	1.76	0.51
1:A:948:VAL:O	5:E:200:ARG:HD2	2.11	0.51
4:D:113:ALA:O	4:D:116:LYS:NZ	2.44	0.51
5:E:60:LEU:HD13	5:E:104:PHE:HE1	1.75	0.51
1:A:1348:ARG:HG3	5:E:199:ARG:HH22	1.74	0.51
5:E:111:TYR:CD1	5:E:115:ILE:CD1	2.92	0.51
8:H:117:PHE:HE2	8:H:122:MET:CB	2.24	0.51
14:N:-7:DG:N2	16:T:8:DC:N3	2.58	0.51
19:a:63:ARG:HH11	20:b:30:THR:CG2	2.24	0.51
2:B:762:ASN:ND2	2:B:1024:ALA:HB3	2.25	0.51
13:M:49:CYS:HB3	13:M:53:ASN:HA	1.90	0.51
18:W:769:ILE:HB	18:W:781:GLU:CG	2.40	0.51
20:b:53:GLU:O	20:b:57:VAL:HG23	2.10	0.51
21:c:38:LEU:CD2	22:d:70:PHE:CZ	2.94	0.51
21:c:38:LEU:HD23	22:d:70:PHE:CZ	2.45	0.51
4:D:166:LYS:HD2	4:D:166:LYS:N	2.26	0.51
1:A:1402:ARG:NH1	1:A:1420:GLU:OE1	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:ILE:HG22	2:B:341:ARG:CB	2.40	0.51
4:D:145:LEU:HD21	4:D:163:LEU:CD1	2.29	0.51
20:f:34:ILE:CB	20:f:51:TYR:HD1	2.24	0.51
1:A:354:ILE:HG22	1:A:469:PHE:HB2	1.93	0.51
2:B:336:ILE:CG2	2:B:341:ARG:CA	2.89	0.51
20:b:75:HIS:O	22:d:92:ARG:NH2	2.28	0.51
2:B:260:THR:HG22	2:B:308:PRO:HB2	1.93	0.51
2:B:904:ARG:HH12	18:W:786:ASN:HA	1.76	0.51
7:G:119:LEU:HD22	7:G:137:ILE:CD1	2.41	0.51
14:N:21:DT:H2"	14:N:22:DG:H8	1.75	0.51
18:W:413:PHE:CZ	18:W:420:GLU:CB	2.88	0.51
2:B:301:GLN:C	2:B:303:LEU:H	2.18	0.51
14:N:52:DC:H4'	14:N:53:DT:OP2	2.10	0.51
18:W:357:ARG:HB3	18:W:389:PRO:HG2	1.93	0.51
19:e:45:THR:HA	19:e:48:LEU:HD12	1.91	0.50
1:A:285:SER:HB2	1:A:290:ILE:HG13	1.93	0.50
13:M:33:SER:HA	13:M:50:LYS:CE	2.41	0.50
19:a:67:PHE:CE2	19:a:92:LEU:HB3	2.45	0.50
19:e:95:ALA:HB1	20:f:90:LEU:HD21	1.93	0.50
1:A:885:ASP:OD2	1:A:1027:ARG:HG2	2.11	0.50
4:D:145:LEU:HD21	4:D:163:LEU:HD21	1.92	0.50
7:G:91:VAL:HA	7:G:101:ALA:HA	1.94	0.50
18:W:769:ILE:HB	18:W:781:GLU:OE2	2.12	0.50
2:B:337:ARG:O	2:B:341:ARG:HB3	2.11	0.50
18:W:396:GLU:CD	18:W:414:VAL:HG23	2.30	0.50
19:a:67:PHE:CZ	19:a:92:LEU:C	2.89	0.50
19:e:64:LYS:HD2	19:e:64:LYS:N	2.26	0.50
20:f:47:SER:O	20:f:50:ILE:CG2	2.57	0.50
1:A:227:GLU:OE1	1:A:231:ARG:NH2	2.44	0.50
1:A:780:PHE:CE2	2:B:510:THR:HG22	2.47	0.50
4:D:33:GLU:O	4:D:38:GLN:NE2	2.45	0.50
13:M:21:THR:CB	13:M:23:PHE:HD2	2.24	0.50
14:N:7:DG:H2"	14:N:8:DT:C5	2.46	0.50
14:N:35:DA:H2	16:T:-34:DA:C6	2.26	0.50
19:a:67:PHE:CZ	19:a:92:LEU:HB3	2.47	0.50
19:e:55:GLN:HG2	20:f:40:ARG:O	2.11	0.50
19:e:100:LEU:HD22	20:f:54:THR:HG23	1.94	0.50
20:f:34:ILE:HB	20:f:51:TYR:HD1	1.75	0.50
14:N:7:DG:H4'	20:b:45:ARG:CG	2.40	0.50
16:T:14:DT:OP2	16:T:14:DT:H2'	2.12	0.50
18:W:432:LEU:C	18:W:432:LEU:HD12	2.37	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:75:HIS:NE2	22:d:93:GLU:HG3	2.26	0.50
2:B:859:TYR:HE2	2:B:941:LEU:HD12	1.77	0.50
7:G:93:ASN:CB	7:G:100:PHE:HD2	2.24	0.50
19:a:107:THR:HG22	19:a:119:ILE:CB	2.42	0.50
2:B:556:MET:SD	2:B:581:GLY:HA3	2.52	0.50
9:I:7:CYS:HB2	9:I:14:LEU:CD1	2.41	0.50
9:I:7:CYS:HB2	9:I:14:LEU:HD11	1.94	0.50
14:N:17:DG:N2	16:T:-16:DT:O2	2.45	0.50
18:W:286:LEU:HD22	18:W:292:VAL:HG21	1.93	0.50
2:B:302:MET:O	2:B:302:MET:HG2	2.12	0.50
3:C:74:GLU:HG3	3:C:242:GLN:HE22	1.77	0.50
19:a:116:ARG:NH1	19:a:122:LYS:CE	2.54	0.50
21:c:103:THR:HA	20:f:95:ARG:NH2	2.27	0.50
19:e:96:SER:HB3	20:f:58:LEU:HD11	1.94	0.50
19:e:104:PHE:HZ	20:f:34:ILE:HG23	1.75	0.50
1:A:830:VAL:HG13	2:B:500:LYS:CB	2.41	0.49
2:B:336:ILE:HG22	2:B:341:ARG:CA	2.42	0.49
4:D:137:LEU:N	4:D:137:LEU:CD1	2.74	0.49
9:I:15:TYR:N	9:I:28:SER:O	2.37	0.49
21:c:53:VAL:CG2	22:d:118:VAL:HG12	2.39	0.49
1:A:1348:ARG:CG	5:E:199:ARG:HH22	2.25	0.49
4:D:141:GLU:OE1	4:D:166:LYS:HG2	2.12	0.49
17:V:29:CYS:O	17:V:33:ASP:N	2.45	0.49
18:W:800:SER:OG	18:W:809:ASP:OD2	2.25	0.49
21:c:46:ARG:O	22:d:88:THR:HA	2.11	0.49
19:e:48:LEU:HA	19:e:51:ILE:HG23	1.93	0.49
1:A:351:ARG:NE	1:A:487:GLU:OE1	2.44	0.49
2:B:242:ILE:HG21	2:B:355:PRO:HG3	1.93	0.49
2:B:1101:ASP:O	2:B:1122:ARG:NH2	2.45	0.49
18:W:403:GLU:O	18:W:403:GLU:HG3	2.12	0.49
19:a:118:THR:HB	20:b:45:ARG:O	2.12	0.49
19:e:68:GLN:HG2	19:e:72:ARG:HE	1.77	0.49
19:e:99:TYR:OH	20:f:57:VAL:CG1	2.61	0.49
18:W:332:LYS:HD2	18:W:389:PRO:HD3	1.92	0.49
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.95	0.49
18:W:357:ARG:O	18:W:389:PRO:HG2	2.12	0.49
21:c:39:ARG:NH2	21:c:39:ARG:CG	2.73	0.49
19:e:124:ILE:HD11	20:f:50:ILE:HG12	1.95	0.49
4:D:141:GLU:OE1	4:D:166:LYS:NZ	2.41	0.49
14:N:-47:DT:H2"	14:N:-46:DG:C8	2.46	0.49
1:A:47:ARG:O	1:A:47:ARG:HG2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:LEU:CD1	13:M:23:PHE:HE1	2.24	0.49
2:B:851:PHE:O	2:B:1094:ARG:NH2	2.46	0.49
19:a:79:LYS:HD3	19:a:82:LEU:HD21	1.94	0.49
1:A:1452:LEU:C	1:A:1452:LEU:CD2	2.86	0.49
2:B:1122:ARG:N	16:T:37:DC:OP1	2.37	0.49
8:H:15:VAL:HG22	8:H:26:ILE:HG22	1.95	0.49
8:H:112:LYS:HG2	8:H:125:GLU:HG2	1.95	0.49
13:M:21:THR:CB	13:M:23:PHE:CE2	2.94	0.49
2:B:886:LYS:HD3	15:P:-1:G:H1	1.78	0.49
2:B:1187:ASN:HD21	2:B:1190:ASN:HB3	1.78	0.49
17:V:63:ASN:ND2	17:V:77:PHE:O	2.45	0.49
18:W:320:LEU:O	18:W:320:LEU:HG	2.12	0.49
18:W:769:ILE:O	18:W:781:GLU:HG2	2.12	0.49
1:A:49:ARG:HH22	18:W:443:THR:HG22	1.77	0.49
19:e:85:GLN:OE1	20:f:82:THR:CB	2.58	0.49
20:f:34:ILE:HD13	20:f:51:TYR:HA	1.94	0.49
1:A:14:VAL:H	1:A:1435:GLN:NE2	2.09	0.48
1:A:188:LYS:HB2	19:e:83:ARG:HH12	1.76	0.48
1:A:887:ILE:CB	1:A:888:PRO:CD	2.84	0.48
2:B:780:VAL:HG22	2:B:795:ILE:HG23	1.95	0.48
14:N:-15:DA:H2"	14:N:-14:DA:C8	2.47	0.48
2:B:300:TRP:H	2:B:300:TRP:CD1	2.31	0.48
14:N:6:DC:H2"	14:N:7:DG:H8	1.78	0.48
20:b:39:ARG:HH22	20:b:44:LYS:HA	1.78	0.48
1:A:194:ARG:N	1:A:194:ARG:NE	2.60	0.48
2:B:284:VAL:HG23	2:B:285:PRO:CD	2.39	0.48
7:G:106:LEU:N	7:G:106:LEU:CD2	2.76	0.48
14:N:16:DA:N1	16:T:-16:DT:C4	2.81	0.48
18:W:437:VAL:O	18:W:437:VAL:CG2	2.61	0.48
19:a:65:LEU:C	19:a:65:LEU:CD1	2.86	0.48
19:a:112:ILE:HG12	19:a:117:VAL:HA	1.92	0.48
2:B:338:ARG:HD3	2:B:338:ARG:C	2.39	0.48
7:G:130:TYR:HD2	7:G:137:ILE:HG21	1.78	0.48
9:I:12:ASN:ND2	9:I:31:ASN:CG	2.70	0.48
19:a:60:LEU:HB2	19:a:64:LYS:HE2	1.95	0.48
19:a:61:LEU:HD11	20:b:40:ARG:NE	2.28	0.48
2:B:575:VAL:O	2:B:578:VAL:CG1	2.50	0.48
14:N:35:DA:C2	16:T:-34:DA:C6	2.99	0.48
20:f:38:ALA:CB	20:f:46:ILE:CD1	2.91	0.48
2:B:1116:ARG:HD2	2:B:1198:TYR:CE1	2.48	0.48
3:C:47:LEU:HB2	3:C:158:ILE:HB	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:TRP:HZ3	9:I:43:VAL:HG21	1.79	0.48
19:a:67:PHE:HE2	19:a:92:LEU:CB	2.26	0.48
21:c:67:LEU:HD11	22:d:41:VAL:HG13	1.95	0.48
1:A:115:LEU:HB2	1:A:122:MET:HE2	1.96	0.48
16:T:7:DC:C2	16:T:8:DC:H5	2.31	0.48
21:c:109:VAL:HG13	21:c:109:VAL:O	2.13	0.48
19:e:67:PHE:CZ	19:e:93:GLN:HA	2.48	0.48
1:A:113:LEU:O	1:A:165:ARG:NH1	2.47	0.48
8:H:117:PHE:HE2	8:H:122:MET:HB2	1.77	0.48
14:N:23:DC:H2"	14:N:24:DT:C6	2.48	0.48
1:A:122:MET:HE1	1:A:138:VAL:HG13	1.96	0.48
2:B:1009:ASP:OD1	10:J:9:SER:HA	2.14	0.48
19:a:111:ALA:HB1	19:a:116:ARG:HB3	1.94	0.48
1:A:448:GLN:CD	1:A:489:ASN:HD21	2.22	0.47
3:C:131:GLU:OE1	3:C:131:GLU:HA	2.14	0.47
4:D:141:GLU:CD	4:D:166:LYS:HG2	2.39	0.47
4:D:166:LYS:HB3	4:D:168:GLU:HG2	1.95	0.47
2:B:233:SER:OG	2:B:355:PRO:CD	2.62	0.47
2:B:334:LEU:HD12	13:M:67:ILE:HD11	1.90	0.47
2:B:841:MET:HE2	2:B:1010:LEU:HD12	1.96	0.47
3:C:173:CYS:SG	3:C:243:VAL:HG11	2.54	0.47
19:e:47:ALA:O	19:e:51:ILE:CG2	2.62	0.47
1:A:885:ASP:OD2	1:A:1027:ARG:CG	2.62	0.47
1:A:885:ASP:OD2	1:A:1027:ARG:NE	2.47	0.47
21:c:55:LEU:HA	21:c:58:VAL:HG12	1.96	0.47
2:B:240:ARG:HD2	2:B:240:ARG:C	2.38	0.47
2:B:401:LEU:HD13	2:B:538:ILE:HG21	1.96	0.47
5:E:189:LEU:HD13	5:E:213:CYS:HB2	1.97	0.47
14:N:6:DC:H2"	14:N:7:DG:C8	2.49	0.47
19:e:120:MET:HE2	19:e:122:LYS:HE2	1.95	0.47
1:A:447:ARG:HB2	1:A:488:MET:CE	2.42	0.47
2:B:25:PHE:HD2	2:B:811:TYR:CE1	2.32	0.47
17:V:60:VAL:CG1	17:V:63:ASN:OD1	2.61	0.47
1:A:1348:ARG:C	1:A:1348:ARG:CD	2.86	0.47
15:P:9:U:H2'	15:P:9:U:O2	2.14	0.47
18:W:399:ALA:HB3	18:W:406:ILE:HD13	1.97	0.47
2:B:572:ARG:CG	2:B:579:TRP:NE1	2.74	0.47
2:B:969:ARG:HH12	3:C:59:ASP:HB2	1.80	0.47
5:E:27:TYR:HA	5:E:63:PRO:HA	1.95	0.47
5:E:142:ASN:HB3	5:E:145:HIS:HD2	1.80	0.47
13:M:44:ILE:HG21	13:M:57:GLN:NE2	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:16:DA:H2"	14:N:17:DG:C8	2.50	0.47
15:P:8:G:N2	16:T:37:DC:O2	2.48	0.47
17:V:91:PRO:HB2	17:V:93:ASP:OD1	2.14	0.47
18:W:332:LYS:HG3	18:W:388:ARG:HB2	1.95	0.47
19:a:70:LEU:CD2	20:b:26:ILE:HD12	2.45	0.47
19:e:120:MET:CE	19:e:122:LYS:HE2	2.45	0.47
20:f:43:VAL:HG21	20:f:46:ILE:CG1	2.44	0.47
14:N:8:DT:H2"	14:N:9:DG:N7	2.29	0.47
19:a:64:LYS:HA	19:a:93:GLN:OE1	2.14	0.47
21:c:89:MET:O	21:c:93:ASN:ND2	2.48	0.47
1:A:448:GLN:OE1	1:A:489:ASN:ND2	2.48	0.47
1:A:887:ILE:HD12	1:A:954:HIS:HA	1.95	0.47
14:N:20:DG:H2"	14:N:21:DT:OP2	2.15	0.47
19:e:47:ALA:O	19:e:51:ILE:HG22	2.14	0.47
19:e:51:ILE:HB	20:f:39:ARG:O	2.15	0.47
19:e:100:LEU:HD11	20:f:58:LEU:HD22	1.96	0.47
20:f:38:ALA:CB	20:f:43:VAL:HG11	2.41	0.47
3:C:13:GLN:HE21	3:C:16:GLU:HG2	1.79	0.47
3:C:70:PRO:HB2	3:C:133:VAL:HG21	1.97	0.47
4:D:141:GLU:OE2	4:D:166:LYS:HG2	2.15	0.47
18:W:344:LEU:HD23	18:W:350:ALA:N	2.30	0.47
2:B:270:GLN:HB3	2:B:329:ARG:NH2	2.29	0.46
7:G:99:PHE:CE2	7:G:110:VAL:CB	2.98	0.46
10:J:9:SER:OG	10:J:47:ARG:NH1	2.47	0.46
14:N:39:DC:H5'	14:N:39:DC:C6	2.50	0.46
19:a:63:ARG:HH11	20:b:30:THR:HG23	1.81	0.46
19:e:76:GLN:OE1	19:e:81:ASP:N	2.48	0.46
2:B:164:MET:HB2	2:B:194:PHE:HE1	1.80	0.46
2:B:335:GLY:HA2	13:M:74:ILE:CD1	2.46	0.46
2:B:572:ARG:HG2	2:B:579:TRP:NE1	2.20	0.46
7:G:106:LEU:HD13	7:G:157:ILE:HD11	1.95	0.46
1:A:473:LEU:HG	2:B:835:GLN:OE1	2.15	0.46
2:B:119:MET:SD	2:B:156:VAL:HG21	2.56	0.46
2:B:839:MET:SD	2:B:1010:LEU:HD21	2.55	0.46
16:T:-14:DA:H2"	16:T:-13:DA:H8	1.80	0.46
16:T:37:DC:H2'	16:T:38:DC:C6	2.51	0.46
1:A:194:ARG:HA	19:e:72:ARG:CZ	2.45	0.46
2:B:284:VAL:HG22	2:B:285:PRO:HD3	1.94	0.46
2:B:521:PRO:CB	15:P:8:G:OP1	2.62	0.46
19:a:65:LEU:HB3	19:a:66:PRO:CD	2.44	0.46
20:b:33:ALA:O	20:b:37:LEU:HG	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:c:83:THR:HG22	21:c:86:LEU:HG	1.97	0.46
1:A:358:PRO:HD2	2:B:833:TYR:CE1	2.51	0.46
1:A:1118:LEU:HB2	1:A:1311:THR:CG2	2.46	0.46
2:B:272:ILE:HD13	2:B:277:VAL:CG1	2.44	0.46
4:D:20:ASP:OD1	4:D:29:ARG:NH1	2.48	0.46
5:E:2:GLU:N	5:E:2:GLU:CD	2.73	0.46
7:G:2:PHE:CG	7:G:79:TRP:HD1	2.34	0.46
19:a:63:ARG:CG	19:a:66:PRO:HG2	2.45	0.46
19:e:63:ARG:HB2	19:e:66:PRO:HG2	1.97	0.46
1:A:45:ARG:O	1:A:45:ARG:HG2	2.16	0.46
7:G:93:ASN:HB2	7:G:100:PHE:HD2	1.74	0.46
16:T:-36:DG:H2"	16:T:-35:DT:C5	2.50	0.46
16:T:36:DC:H2'	16:T:37:DC:C6	2.51	0.46
18:W:435:LEU:HD12	18:W:435:LEU:C	2.40	0.46
1:A:1282:ILE:HG23	1:A:1311:THR:HG1	1.73	0.46
7:G:92:SER:OG	7:G:100:PHE:HB3	2.15	0.46
14:N:19:DG:N1	14:N:20:DG:O6	2.48	0.46
21:c:103:THR:HB	20:f:94:GLY:O	2.15	0.46
1:A:836:GLY:HA3	16:T:33:DA:C1'	2.46	0.46
14:N:-41:DC:OP2	14:N:-41:DC:H2'	2.16	0.46
18:W:352:LEU:C	18:W:352:LEU:CD1	2.89	0.46
2:B:303:LEU:CB	9:I:4:PHE:CE2	2.99	0.46
2:B:825:VAL:HA	2:B:1010:LEU:O	2.16	0.46
20:f:32:PRO:O	20:f:36:ARG:HG3	2.16	0.46
20:f:34:ILE:CB	20:f:51:TYR:CD1	2.98	0.46
1:A:248:ARG:HB2	1:A:261:ASP:HB3	1.97	0.45
5:E:60:LEU:HD13	5:E:104:PHE:CE1	2.50	0.45
1:A:1168:ASP:OD2	1:A:1196:ARG:NE	2.49	0.45
2:B:273:PRO:HD2	2:B:276:ILE:HD12	1.97	0.45
9:I:14:LEU:HD11	9:I:29:CYS:HB2	1.97	0.45
13:M:27:PHE:HB2	13:M:54:LEU:HD23	1.99	0.45
16:T:46:DC:H2"	16:T:47:DA:C8	2.51	0.45
18:W:298:LYS:O	18:W:298:LYS:HG3	2.17	0.45
2:B:72:ASN:HB2	2:B:126:SER:OG	2.16	0.45
8:H:94:TYR:HD2	8:H:143:ILE:HD12	1.80	0.45
14:N:18:DC:OP1	19:a:64:LYS:NZ	2.49	0.45
18:W:406:ILE:HG12	18:W:416:TYR:HD1	1.82	0.45
20:b:94:GLY:O	20:b:95:ARG:HD2	2.16	0.45
2:B:225:ILE:HD13	2:B:248:LYS:HD3	1.98	0.45
9:I:12:ASN:ND2	9:I:31:ASN:CB	2.78	0.45
14:N:-46:DG:OP1	18:W:386:LYS:HD2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:9:DC:C2	16:T:10:DG:N7	2.84	0.45
16:T:34:DC:H2'	16:T:35:DA:C8	2.51	0.45
21:c:105:THR:O	20:f:97:LEU:HD12	2.16	0.45
5:E:160:LYS:NZ	5:E:192:GLY:O	2.44	0.45
19:a:108:ASN:C	19:a:108:ASN:ND2	2.73	0.45
2:B:337:ARG:O	2:B:341:ARG:N	2.42	0.45
4:D:168:GLU:OE2	4:D:168:GLU:HA	2.17	0.45
14:N:7:DG:C4'	20:b:45:ARG:HH21	2.30	0.45
2:B:550:PHE:O	2:B:554:TRP:HD1	2.00	0.45
2:B:559:LEU:HG	2:B:580:THR:O	2.17	0.45
4:D:51:LEU:HD11	7:G:4:LEU:HG	1.99	0.45
4:D:151:GLU:C	4:D:175:LEU:HD13	2.42	0.45
19:e:79:LYS:HB3	19:e:82:LEU:CD1	2.44	0.45
6:F:79:ARG:NH2	6:F:150:GLU:OE2	2.48	0.45
16:T:-3:DC:P	19:a:118:THR:OG1	2.75	0.45
18:W:782:LEU:HD11	18:W:789:ILE:HD13	1.99	0.45
19:e:54:TYR:OH	20:f:36:ARG:HG2	2.16	0.45
20:f:73:THR:HG22	20:f:85:ASP:OD2	2.17	0.45
19:a:67:PHE:CE2	19:a:92:LEU:CB	2.99	0.45
19:e:95:ALA:HB2	20:f:90:LEU:CD1	2.38	0.45
19:e:104:PHE:CZ	20:f:50:ILE:HD11	2.49	0.45
20:f:31:LYS:HG3	20:f:51:TYR:CE2	2.52	0.45
18:W:436:ILE:O	18:W:440:ILE:HD11	2.17	0.44
21:c:62:LEU:O	21:c:66:VAL:HG12	2.17	0.44
19:e:107:THR:HG23	19:e:123:ASP:CB	2.47	0.44
20:f:34:ILE:HG21	20:f:51:TYR:CD1	2.50	0.44
20:f:94:GLY:O	20:f:95:ARG:HD2	2.17	0.44
20:b:30:THR:HB	20:b:32:PRO:HD2	1.99	0.44
1:A:119:ASN:HB3	1:A:122:MET:HB3	1.98	0.44
1:A:1221:VAL:HG23	1:A:1222:PHE:CD2	2.52	0.44
16:T:15:DT:H2'	16:T:16:DT:H71	1.98	0.44
3:C:45:ILE:HA	3:C:159:ALA:HA	1.99	0.44
4:D:156:ALA:CB	4:D:171:LEU:HD11	2.48	0.44
5:E:164:LEU:CD2	5:E:169:LEU:HD11	2.36	0.44
7:G:116:PRO:HD2	7:G:163:ILE:HG13	1.98	0.44
18:W:800:SER:CB	18:W:805:VAL:HG21	2.47	0.44
19:a:107:THR:HG23	19:a:123:ASP:HB2	1.99	0.44
21:c:41:GLY:HA3	21:c:43:TYR:CE2	2.53	0.44
19:e:63:ARG:HA	19:e:63:ARG:HD3	1.67	0.44
1:A:318:LYS:HD3	14:N:-43:DG:H1	1.80	0.44
2:B:336:ILE:CG2	2:B:341:ARG:HB2	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:92:SER:N	7:G:100:PHE:O	2.50	0.44
19:e:118:THR:O	19:e:118:THR:HG23	2.17	0.44
1:A:542:ILE:HD12	1:A:578:LEU:HD13	1.98	0.44
2:B:265:LEU:HD22	2:B:353:LEU:HD13	1.99	0.44
14:N:-46:DG:P	18:W:386:LYS:HE3	2.58	0.44
16:T:-36:DG:C8	16:T:-36:DG:OP2	2.70	0.44
1:A:781:ALA:N	2:B:696:GLU:OE2	2.45	0.44
1:A:1153:GLU:OE1	1:A:1196:ARG:NH2	2.44	0.44
1:A:1461:ALA:HB1	7:G:21:GLN:HB2	1.99	0.44
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.52	0.44
4:D:171:LEU:HD22	4:D:175:LEU:CD1	2.48	0.44
9:I:13:MET:HG3	9:I:13:MET:O	2.17	0.44
13:M:49:CYS:HB3	13:M:53:ASN:CA	2.48	0.44
20:b:73:THR:HG22	20:b:85:ASP:OD2	2.17	0.44
1:A:447:ARG:CD	1:A:481:ALA:HB2	2.47	0.44
1:A:1146:LYS:NZ	2:B:254:ASP:OD2	2.38	0.44
2:B:371:LEU:HD23	2:B:371:LEU:HA	1.76	0.44
2:B:870:ILE:HG13	18:W:387:PHE:CZ	2.52	0.44
3:C:97:VAL:HB	3:C:122:SER:OG	2.17	0.44
14:N:-24:DT:H2"	14:N:-23:DG:H8	1.83	0.44
18:W:400:ARG:N	18:W:406:ILE:CD1	2.81	0.44
21:c:28:SER:H	21:c:60:GLU:CD	2.25	0.44
2:B:653:ARG:HE	2:B:653:ARG:HB3	1.70	0.44
13:M:27:PHE:CD1	13:M:54:LEU:CD2	3.01	0.44
16:T:-12:DA:OP2	20:b:30:THR:CB	2.63	0.44
18:W:406:ILE:HG12	18:W:416:TYR:CD1	2.53	0.44
21:c:88:ASP:OD2	21:c:108:GLN:NE2	2.51	0.44
1:A:243:PRO:HG2	1:A:248:ARG:NH2	2.33	0.43
1:A:271:LEU:HD12	1:A:271:LEU:HA	1.87	0.43
1:A:1348:ARG:CD	5:E:199:ARG:HH22	2.31	0.43
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.99	0.43
3:C:89:ASP:O	18:W:764:LYS:HE2	2.18	0.43
5:E:19:LYS:NZ	5:E:33:GLU:O	2.38	0.43
18:W:332:LYS:CG	18:W:388:ARG:HB2	2.48	0.43
19:a:64:LYS:H	19:a:64:LYS:CD	2.31	0.43
19:a:67:PHE:HE2	19:a:92:LEU:HB2	1.83	0.43
7:G:99:PHE:CZ	7:G:110:VAL:CG2	2.98	0.43
7:G:108:VAL:HG13	7:G:159:ALA:C	2.40	0.43
9:I:54:GLU:HG2	9:I:100:PHE:CE2	2.53	0.43
14:N:3:DG:H2"	14:N:4:DT:C5	2.52	0.43
20:f:43:VAL:CG2	20:f:46:ILE:HG12	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:LYS:HG2	2:B:125:THR:HG22	1.99	0.43
7:G:40:GLY:HA3	7:G:152:THR:HG21	2.00	0.43
7:G:90:ILE:O	7:G:101:ALA:HA	2.17	0.43
14:N:23:DC:H2"	14:N:24:DT:C5	2.53	0.43
1:A:287:GLN:HE21	1:A:287:GLN:CA	2.21	0.43
1:A:407:ILE:HG12	1:A:413:ARG:HG2	2.00	0.43
19:e:104:PHE:CZ	20:f:34:ILE:HG23	2.53	0.43
19:e:118:THR:O	19:e:118:THR:CG2	2.66	0.43
1:A:255:GLU:HB3	1:A:256:THR:H	1.64	0.43
9:I:54:GLU:HG2	9:I:100:PHE:HE2	1.83	0.43
1:A:254:ASP:OD1	1:A:254:ASP:N	2.51	0.43
2:B:501:LEU:HD12	2:B:501:LEU:N	2.34	0.43
12:L:67:ILE:CG2	18:W:783:HIS:CE1	3.02	0.43
16:T:-3:DC:P	19:a:118:THR:HG1	2.42	0.43
17:V:14:LEU:HD23	17:V:32:CYS:CB	2.49	0.43
21:c:83:THR:HG23	21:c:86:LEU:H	1.83	0.43
1:A:1314:ILE:HG13	1:A:1337:GLU:OE1	2.18	0.43
1:A:1445:ASP:HB3	1:A:1447:MET:HE3	2.01	0.43
2:B:285:PRO:CG	2:B:288:GLU:OE1	2.59	0.43
2:B:498:ASP:CB	16:T:32:DT:H3	2.24	0.43
2:B:784:ASN:HB3	10:J:62:TYR:CZ	2.53	0.43
7:G:121:TYR:HA	7:G:130:TYR:CE1	2.53	0.43
13:M:54:LEU:CD1	13:M:73:TRP:CZ2	3.02	0.43
19:a:111:ALA:C	19:a:116:ARG:CB	2.90	0.43
21:c:36:ARG:HA	21:c:36:ARG:NE	2.28	0.43
2:B:761:HIS:HB2	2:B:1024:ALA:HB2	2.01	0.43
18:W:442:PRO:HB2	18:W:447:LEU:CD1	2.48	0.43
19:a:68:GLN:HG3	19:a:89:ILE:HD12	2.00	0.43
22:d:64:SER:HA	22:d:67:ASN:ND2	2.34	0.43
1:A:286:PRO:HG2	1:A:288:HIS:CE1	2.54	0.43
1:A:1423:ASP:O	2:B:1220:ARG:NH2	2.51	0.43
2:B:285:PRO:O	2:B:289:ILE:HG13	2.19	0.43
22:d:39:ILE:HD12	22:d:39:ILE:N	2.34	0.43
1:A:318:LYS:HD3	14:N:-43:DG:N1	2.34	0.43
2:B:554:TRP:CE2	2:B:592:THR:HG21	2.54	0.43
2:B:979:LYS:HE2	2:B:1095:LEU:HD12	1.99	0.43
4:D:23:GLU:HB3	7:G:82:PHE:HD2	1.83	0.43
5:E:111:TYR:CE1	5:E:115:ILE:CD1	3.02	0.43
18:W:421:TYR:HA	18:W:425:PHE:O	2.19	0.43
1:A:468:THR:OG1	1:A:470:ARG:NH2	2.52	0.42
2:B:329:ARG:NH2	13:M:65:GLN:HE22	2.16	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:688:GLU:OE2	2:B:740:HIS:NE2	2.38	0.42
4:D:61:ARG:NH2	4:D:86:ASP:OD1	2.52	0.42
2:B:406:LEU:HD23	2:B:406:LEU:HA	1.87	0.42
7:G:91:VAL:HG23	7:G:139:LYS:HA	2.01	0.42
14:N:36:DC:H2"	14:N:37:DG:N7	2.34	0.42
18:W:805:VAL:CB	18:W:806:PRO:HD2	2.37	0.42
2:B:21:ILE:HG22	2:B:811:TYR:OH	2.20	0.42
2:B:1073:TYR:HE2	3:C:179:GLU:HA	1.83	0.42
7:G:125:ASN:OD1	7:G:131:MET:SD	2.77	0.42
12:L:66:MET:HE2	12:L:66:MET:HB3	1.91	0.42
14:N:14:DT:H2"	14:N:15:DA:C8	2.55	0.42
14:N:36:DC:H2"	14:N:37:DG:C8	2.55	0.42
16:T:-39:DG:H2"	16:T:-38:DT:OP2	2.19	0.42
16:T:-14:DA:H2"	16:T:-13:DA:C8	2.53	0.42
18:W:413:PHE:HZ	18:W:420:GLU:CB	2.31	0.42
19:a:61:LEU:HD11	20:b:40:ARG:CZ	2.49	0.42
21:c:29:PHE:HE2	21:c:59:ILE:HG22	1.83	0.42
1:A:285:SER:HB2	1:A:290:ILE:CD1	2.49	0.42
1:A:830:VAL:CG1	2:B:500:LYS:CB	2.98	0.42
2:B:233:SER:N	2:B:243:SER:O	2.49	0.42
4:D:148:LEU:HD23	4:D:148:LEU:HA	1.81	0.42
14:N:-46:DG:OP1	18:W:386:LYS:CD	2.67	0.42
16:T:-26:DC:H2"	16:T:-25:DT:C6	2.54	0.42
16:T:-13:DA:H5"	19:a:63:ARG:HD3	2.00	0.42
18:W:792:PRO:HG2	18:W:795:PHE:CD1	2.54	0.42
21:c:94:ASP:C	21:c:96:LEU:N	2.77	0.42
2:B:328:ARG:HD3	13:M:68:ASP:HA	2.00	0.42
2:B:839:MET:SD	2:B:1010:LEU:CD1	2.97	0.42
3:C:53:ASN:ND2	3:C:59:ASP:OD1	2.47	0.42
3:C:116:SER:C	3:C:134:ARG:HH12	2.26	0.42
5:E:189:LEU:HD11	5:E:195:VAL:HG13	2.01	0.42
16:T:-1:DC:C2	16:T:0:DG:N7	2.88	0.42
18:W:322:ARG:HA	18:W:340:VAL:O	2.18	0.42
18:W:342:GLU:O	18:W:350:ALA:HB1	2.20	0.42
21:c:29:PHE:CE1	22:d:40:TYR:HB3	2.54	0.42
22:d:90:THR:HG22	22:d:91:SER:N	2.33	0.42
19:e:88:ALA:HB2	20:f:82:THR:C	2.44	0.42
1:A:884:ILE:HD12	1:A:887:ILE:CD1	2.44	0.42
1:A:960:VAL:CG2	1:A:1055:PHE:HA	2.49	0.42
8:H:97:PHE:CE1	8:H:140:TYR:CE1	3.07	0.42
14:N:-6:DG:H2"	14:N:-5:DG:N7	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:11:DC:H2"	16:T:12:DG:C8	2.55	0.42
20:b:78:ARG:NH2	20:b:82:THR:HG23	2.35	0.42
1:A:168:CYS:SG	1:A:170:ASN:ND2	2.93	0.42
1:A:891:ASP:HA	1:A:941:ARG:HH22	1.83	0.42
9:I:84:VAL:HG22	9:I:104:LEU:HD21	2.01	0.42
17:V:63:ASN:HD21	17:V:78:GLN:C	2.28	0.42
18:W:344:LEU:HD23	18:W:350:ALA:CA	2.50	0.42
21:c:55:LEU:O	21:c:58:VAL:HG13	2.20	0.42
19:e:119:ILE:HA	19:e:123:ASP:OD2	2.19	0.42
20:f:38:ALA:CB	20:f:46:ILE:HD13	2.49	0.42
1:A:473:LEU:CD1	1:A:473:LEU:C	2.88	0.42
1:A:1218:ILE:HG23	1:A:1222:PHE:CD2	2.55	0.42
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.36	0.42
13:M:60:ILE:HB	13:M:64:SER:OG	2.20	0.42
16:T:37:DC:H2'	16:T:38:DC:H6	1.84	0.42
18:W:230:LYS:NZ	18:W:271:HIS:NE2	2.63	0.42
19:e:54:TYR:CE1	20:f:36:ARG:HD2	2.55	0.42
1:A:447:ARG:CB	1:A:488:MET:HG2	2.45	0.42
6:F:107:VAL:HG11	6:F:111:ILE:HD11	2.01	0.42
8:H:86:LYS:HE2	8:H:86:LYS:HB3	1.87	0.42
16:T:-26:DC:H2"	16:T:-25:DT:C2	2.54	0.42
18:W:228:GLY:HA3	18:W:299:PHE:CZ	2.55	0.42
19:a:111:ALA:HB1	19:a:116:ARG:CB	2.49	0.42
19:e:88:ALA:HA	20:f:83:ALA:HA	2.02	0.42
1:A:448:GLN:NE2	1:A:489:ASN:HD21	2.13	0.42
2:B:303:LEU:CB	9:I:4:PHE:HE2	2.32	0.42
2:B:303:LEU:HB2	9:I:4:PHE:HE2	1.83	0.42
2:B:999:MET:HE1	2:B:1011:ILE:CD1	2.49	0.42
4:D:20:ASP:HA	4:D:29:ARG:NH2	2.34	0.42
16:T:-8:DA:H2"	16:T:-7:DC:C2	2.55	0.42
19:a:96:SER:HB3	20:b:58:LEU:HD11	2.01	0.42
19:a:116:ARG:HH12	19:a:122:LYS:HD2	1.85	0.42
1:A:47:ARG:HA	1:A:48:PRO:HD2	1.79	0.41
1:A:122:MET:HE3	1:A:126:ILE:HD11	2.02	0.41
1:A:197:GLN:HE21	1:A:197:GLN:HA	1.84	0.41
1:A:958:LEU:HD13	1:A:1023:LEU:HD22	2.01	0.41
1:A:1444:PHE:CZ	6:F:89:GLU:HA	2.55	0.41
2:B:499:GLY:C	2:B:501:LEU:HD13	2.45	0.41
6:F:89:GLU:OE2	6:F:136:ARG:NE	2.51	0.41
14:N:-52:DG:H2'	14:N:-51:DT:H71	2.02	0.41
1:A:285:SER:HB2	1:A:290:ILE:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:756:ILE:HG12	2:B:770:GLN:HG2	2.02	0.41
8:H:97:PHE:CE1	8:H:140:TYR:OH	2.72	0.41
1:A:1356:LEU:HD13	1:A:1371:MET:HE1	2.03	0.41
3:C:66:LEU:HD11	3:C:155:ILE:HD12	2.02	0.41
4:D:171:LEU:HD22	4:D:175:LEU:HD11	2.01	0.41
8:H:39:THR:HB	8:H:123:CYS:HB3	2.02	0.41
15:P:2:U:H2'	15:P:3:C:C6	2.55	0.41
16:T:-5:DT:H2"	16:T:-4:DA:C8	2.55	0.41
16:T:8:DC:OP2	20:f:35:ARG:NH1	2.53	0.41
18:W:230:LYS:CD	18:W:271:HIS:NE2	2.81	0.41
22:d:55:SER:OG	22:d:56:SER:N	2.52	0.41
20:f:78:ARG:NH2	20:f:82:THR:HG23	2.35	0.41
1:A:883:THR:O	1:A:1027:ARG:NH1	2.52	0.41
2:B:762:ASN:OD1	2:B:1024:ALA:HB3	2.20	0.41
14:N:-25:DT:H5'	14:N:-25:DT:C6	2.55	0.41
19:e:61:LEU:HD21	20:f:40:ARG:NH1	2.36	0.41
3:C:212:PRO:HA	3:C:213:PRO:HD3	1.89	0.41
9:I:96:ASN:OD1	9:I:97:MET:N	2.48	0.41
20:f:43:VAL:CG2	20:f:46:ILE:CG1	2.98	0.41
1:A:197:GLN:HA	1:A:197:GLN:NE2	2.35	0.41
2:B:252:ARG:N	2:B:255:LYS:O	2.53	0.41
2:B:262:LYS:HA	2:B:273:PRO:HA	2.03	0.41
2:B:1073:TYR:CE1	2:B:1080:LYS:HG2	2.55	0.41
16:T:14:DT:H2"	16:T:15:DT:C5	2.56	0.41
2:B:840:ILE:HG12	2:B:992:VAL:HG12	2.03	0.41
8:H:40:LEU:CD1	8:H:122:MET:HB2	2.51	0.41
8:H:111:ILE:HD13	8:H:111:ILE:HA	1.93	0.41
16:T:8:DC:C2	16:T:9:DC:C5	3.08	0.41
18:W:413:PHE:CZ	18:W:420:GLU:CG	3.04	0.41
1:A:970:GLN:HA	1:A:975:LEU:HB2	2.03	0.41
3:C:63:SER:HA	3:C:66:LEU:HD12	2.03	0.41
14:N:16:DA:N1	16:T:-16:DT:O4	2.54	0.41
16:T:-53:DA:H2"	16:T:-52:DG:C8	2.56	0.41
1:A:49:ARG:NH2	18:W:443:THR:HG22	2.36	0.41
1:A:181:LYS:HB3	1:A:202:LEU:HD11	2.03	0.41
1:A:447:ARG:CB	1:A:488:MET:HE3	2.44	0.41
1:A:1162:SER:OG	1:A:1163:THR:N	2.49	0.41
1:A:1348:ARG:HD2	5:E:199:ARG:NH2	2.36	0.41
2:B:299:ASP:CG	2:B:385:ARG:HH12	2.29	0.41
2:B:334:LEU:CD1	13:M:67:ILE:HD11	2.51	0.41
2:B:572:ARG:CB	2:B:579:TRP:HE1	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:572:ARG:HA	2:B:582:ILE:HG22	2.02	0.41
2:B:999:MET:HE1	2:B:1011:ILE:HD11	2.02	0.41
3:C:104:HIS:ND1	3:C:111:THR:OG1	2.38	0.41
4:D:69:ARG:HG2	4:D:74:GLY:HA2	2.03	0.41
5:E:169:LEU:O	5:E:169:LEU:HD12	2.20	0.41
12:L:60:LYS:HB3	12:L:60:LYS:HE3	1.81	0.41
14:N:-10:DC:H1'	14:N:-9:DG:C8	2.56	0.41
14:N:18:DC:H6	14:N:18:DC:H2'	1.70	0.41
18:W:340:VAL:O	18:W:340:VAL:HG12	2.20	0.41
18:W:757:LYS:HD3	18:W:804:TRP:CE2	2.56	0.41
21:c:54:TYR:CD1	22:d:114:GLY:C	2.99	0.41
1:A:52:GLY:C	1:A:54:ASN:N	2.78	0.41
1:A:1315:ASN:HD21	1:A:1318:GLU:HB2	1.86	0.41
14:N:5:DA:H1'	14:N:6:DC:O4'	2.21	0.41
18:W:278:LYS:HD2	18:W:280:GLU:OE2	2.20	0.41
19:a:114:ALA:C	19:a:116:ARG:N	2.78	0.41
20:b:38:ALA:HB3	20:b:46:ILE:HD11	2.03	0.41
19:e:124:ILE:HG21	20:f:53:GLU:HG3	2.01	0.41
2:B:557:GLU:HA	2:B:558:PRO:HD3	1.89	0.40
22:d:62:MET:O	22:d:66:VAL:HG23	2.22	0.40
1:A:42:ASP:HB2	1:A:49:ARG:CB	2.39	0.40
1:A:474:SER:OG	1:A:651:GLN:NE2	2.55	0.40
5:E:118:SER:OG	14:N:-18:DT:H5"	2.20	0.40
14:N:45:DG:H2"	14:N:46:DA:C8	2.55	0.40
16:T:8:DC:H6	16:T:8:DC:H5'	1.87	0.40
19:e:51:ILE:HD12	20:f:42:GLY:HA2	2.02	0.40
1:A:262:ASP:OD1	1:A:317:GLN:NE2	2.54	0.40
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.77	0.40
1:A:473:LEU:HD21	2:B:835:GLN:HB2	2.03	0.40
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.88	0.40
2:B:766:ARG:HA	2:B:766:ARG:HD3	1.90	0.40
14:N:7:DG:H2"	14:N:8:DT:C4	2.56	0.40
18:W:265:ARG:HD2	18:W:265:ARG:HA	1.71	0.40
19:a:63:ARG:NH1	20:b:30:THR:CG2	2.84	0.40
21:c:94:ASP:O	21:c:96:LEU:N	2.55	0.40
19:e:46:VAL:O	19:e:50:GLU:HG3	2.21	0.40
20:f:53:GLU:O	20:f:57:VAL:N	2.54	0.40
2:B:79:PHE:HE1	2:B:119:MET:HE3	1.86	0.40
2:B:293:ILE:HG12	2:B:372:GLY:HA2	2.03	0.40
16:T:30:DA:H2'	16:T:31:DT:C6	2.57	0.40
18:W:229:VAL:HG21	18:W:286:LEU:HD11	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:70:LEU:HD21	20:b:26:ILE:HD12	2.04	0.40
21:c:50:THR:O	21:c:53:VAL:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1400/1743 (80%)	1345 (96%)	54 (4%)	1 (0%)	48 79
2	B	1145/1227 (93%)	1086 (95%)	57 (5%)	2 (0%)	44 75
3	C	261/304 (86%)	255 (98%)	6 (2%)	0	100 100
4	D	162/186 (87%)	155 (96%)	7 (4%)	0	100 100
5	E	211/214 (99%)	208 (99%)	3 (1%)	0	100 100
6	F	82/155 (53%)	80 (98%)	2 (2%)	0	100 100
7	G	169/171 (99%)	163 (96%)	5 (3%)	1 (1%)	22 56
8	H	129/145 (89%)	126 (98%)	3 (2%)	0	100 100
9	I	109/115 (95%)	102 (94%)	7 (6%)	0	100 100
10	J	64/72 (89%)	63 (98%)	1 (2%)	0	100 100
11	K	111/118 (94%)	110 (99%)	1 (1%)	0	100 100
12	L	43/72 (60%)	43 (100%)	0	0	100 100
13	M	62/110 (56%)	59 (95%)	3 (5%)	0	100 100
17	V	100/114 (88%)	97 (97%)	3 (3%)	0	100 100
18	W	265/908 (29%)	249 (94%)	15 (6%)	1 (0%)	30 64
19	a	72/136 (53%)	70 (97%)	2 (3%)	0	100 100
19	e	88/136 (65%)	86 (98%)	2 (2%)	0	100 100
20	b	74/103 (72%)	71 (96%)	3 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	f	74/103 (72%)	70 (95%)	3 (4%)	1 (1%)	9 40
21	c	87/115 (76%)	83 (95%)	4 (5%)	0	100 100
22	d	86/126 (68%)	85 (99%)	1 (1%)	0	100 100
All	All	4794/6373 (75%)	4606 (96%)	182 (4%)	6 (0%)	50 79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	PRO
2	B	503	LYS
7	G	154	VAL
2	B	269	LYS
18	W	784	ASN
20	f	50	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1225/1528 (80%)	1217 (99%)	8 (1%)	81 89
2	B	1012/1077 (94%)	1010 (100%)	2 (0%)	92 97
3	C	236/264 (89%)	236 (100%)	0	100 100
4	D	143/160 (89%)	141 (99%)	2 (1%)	62 79
5	E	196/197 (100%)	196 (100%)	0	100 100
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%)	119 (99%)	1 (1%)	79 88
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%)	38 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	61/98 (62%)	61 (100%)	0	100	100
17	V	86/97 (89%)	86 (100%)	0	100	100
18	W	241/795 (30%)	238 (99%)	3 (1%)	67	82
19	a	62/110 (56%)	59 (95%)	3 (5%)	21	50
19	e	77/110 (70%)	75 (97%)	2 (3%)	41	66
20	b	63/79 (80%)	62 (98%)	1 (2%)	58	76
20	f	63/79 (80%)	60 (95%)	3 (5%)	21	50
21	c	78/96 (81%)	74 (95%)	4 (5%)	20	48
22	d	75/105 (71%)	74 (99%)	1 (1%)	65	81
All	All	4269/5550 (77%)	4239 (99%)	30 (1%)	80	89

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	ARG
1	A	200	ARG
1	A	280	LEU
1	A	473	LEU
1	A	661	ASN
1	A	885	ASP
1	A	1314	ILE
1	A	1459	ASP
2	B	428	CYS
2	B	618	LYS
4	D	116	LYS
4	D	169	VAL
8	H	108	GLU
18	W	246	LYS
18	W	264	GLN
18	W	805	VAL
19	a	63	ARG
19	a	64	LYS
19	a	66	PRO
20	b	65	VAL
21	c	34	VAL
21	c	39	ARG
21	c	48	SER
21	c	58	VAL
22	d	116	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	e	51	ILE
19	e	65	LEU
20	f	43	VAL
20	f	50	ILE
20	f	65	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	197	GLN
1	A	287	GLN
1	A	291	ASN
1	A	400	HIS
1	A	452	HIS
1	A	489	ASN
1	A	518	ASN
1	A	563	GLN
1	A	651	GLN
1	A	661	ASN
1	A	787	HIS
1	A	954	HIS
1	A	1190	GLN
1	A	1261	GLN
1	A	1315	ASN
1	A	1435	GLN
2	B	64	HIS
2	B	102	GLN
2	B	438	ASN
2	B	524	GLN
2	B	735	HIS
2	B	776	GLN
2	B	794	ASN
2	B	842	ASN
2	B	932	HIS
2	B	1062	ASN
2	B	1174	ASN
3	C	8	ASN
3	C	13	GLN
3	C	188	HIS
3	C	242	GLN
4	D	179	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	4	ASN
5	E	51	ASN
5	E	94	ASN
5	E	103	ASN
5	E	112	GLN
5	E	145	HIS
5	E	193	GLN
7	G	21	GLN
8	H	13	GLN
8	H	136	GLN
9	I	12	ASN
9	I	31	ASN
9	I	90	GLN
9	I	105	ASN
13	M	57	GLN
13	M	65	GLN
18	W	264	GLN
18	W	339	GLN
18	W	402	HIS
18	W	434	ASN
19	a	108	ASN
20	b	75	HIS
21	c	72	ASN
22	d	49	HIS
22	d	84	ASN
22	d	109	HIS
19	e	113	HIS
20	f	75	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	15/16 (93%)	5 (33%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	-4	C
15	P	0	U
15	P	8	G
15	P	9	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	P	10	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

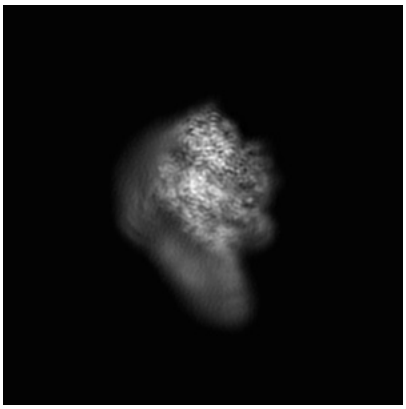
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60593. These allow visual inspection of the internal detail of the map and identification of artifacts.

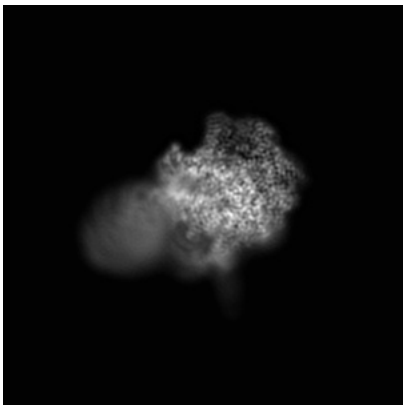
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

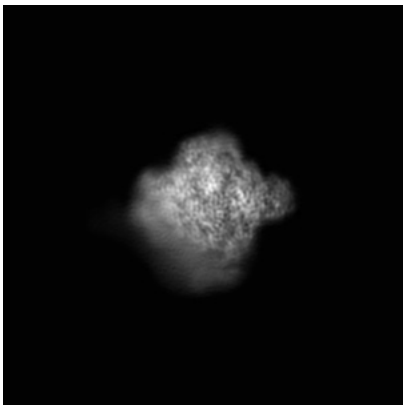
6.1.1 Primary map



X

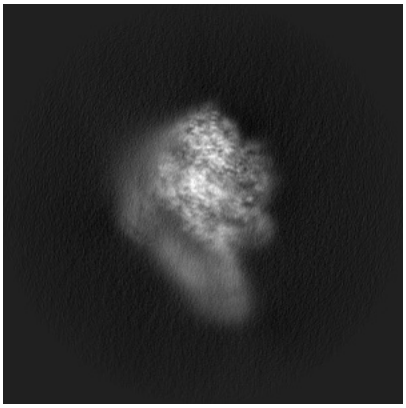


Y

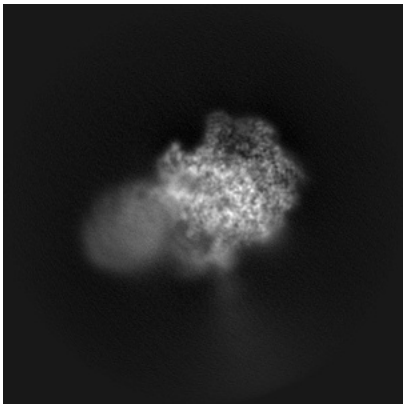


Z

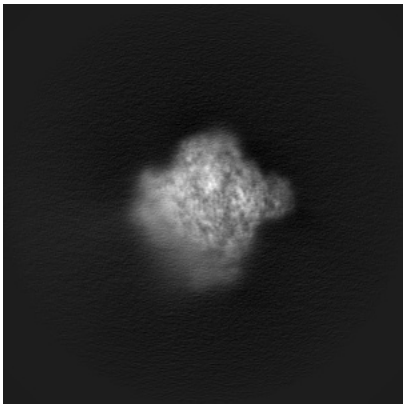
6.1.2 Raw map



X



Y

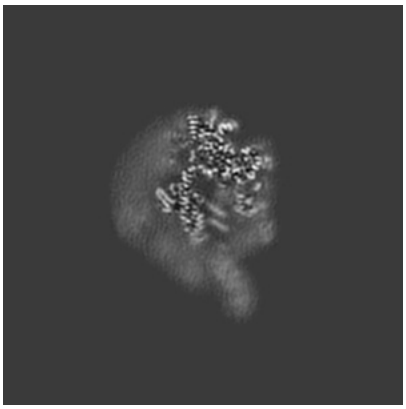


Z

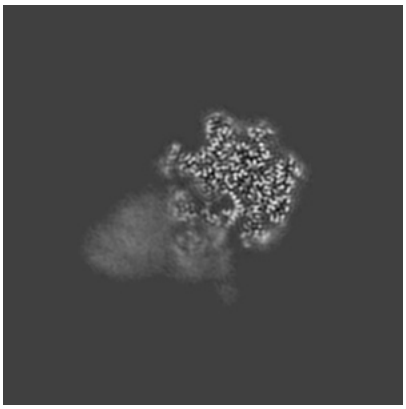
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

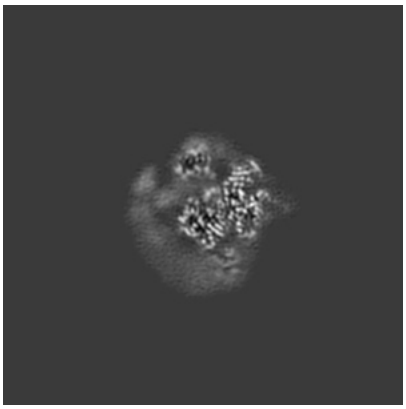
6.2.1 Primary map



X Index: 180

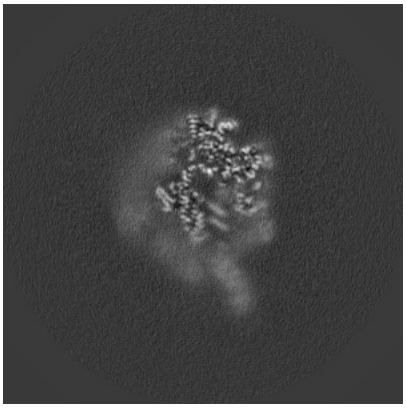


Y Index: 180

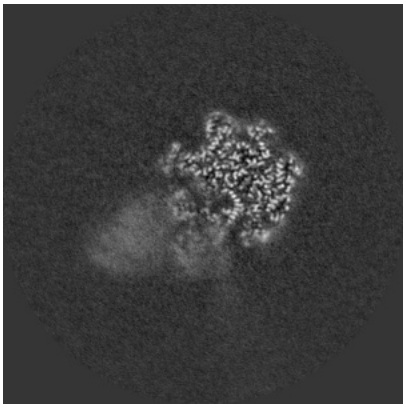


Z Index: 180

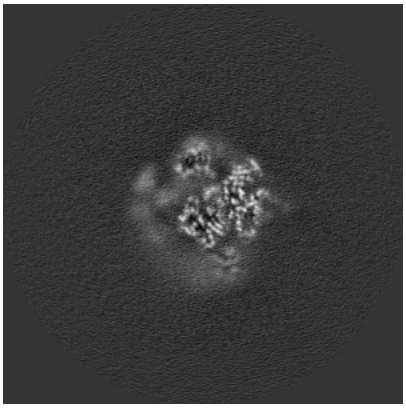
6.2.2 Raw map



X Index: 180



Y Index: 180

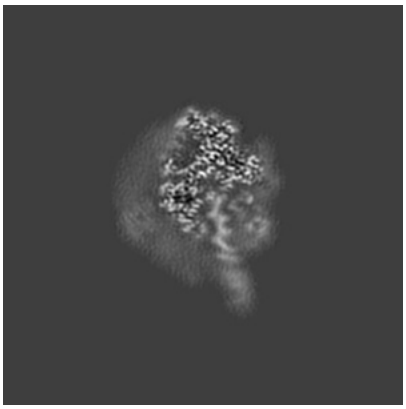


Z Index: 180

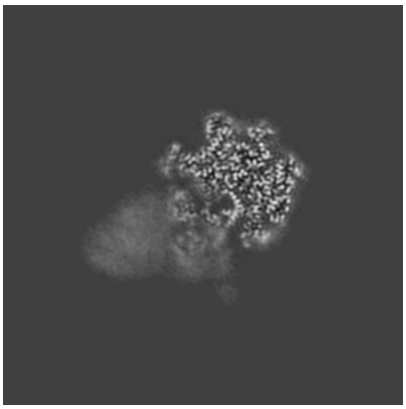
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

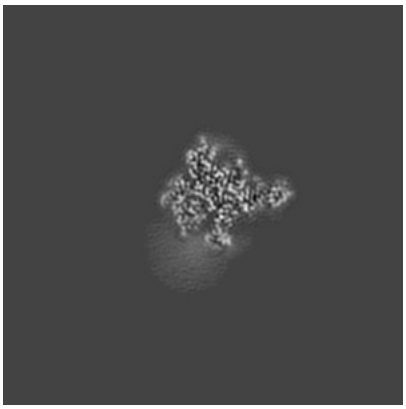
6.3.1 Primary map



X Index: 187

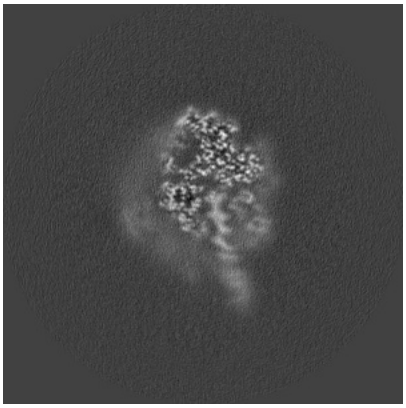


Y Index: 180

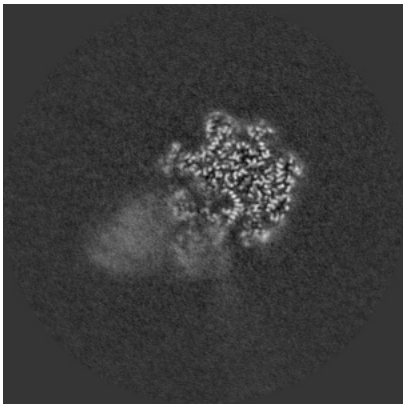


Z Index: 221

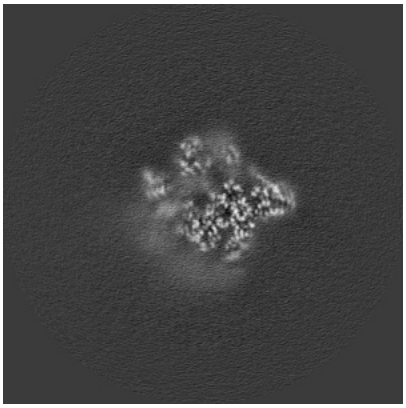
6.3.2 Raw map



X Index: 186



Y Index: 180

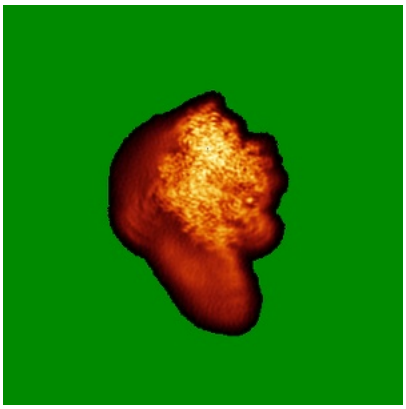


Z Index: 191

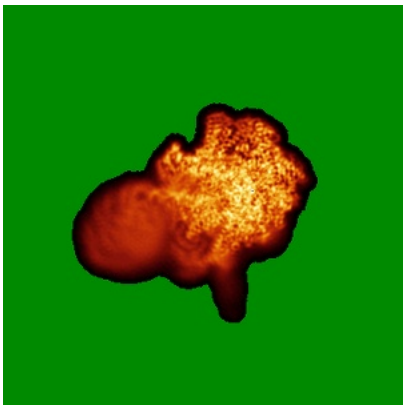
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

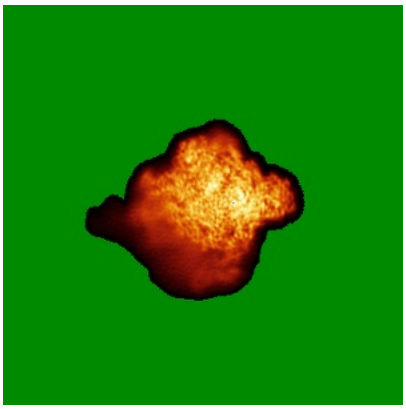
6.4.1 Primary map



X

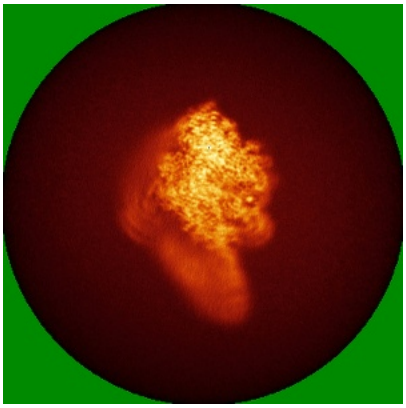


Y

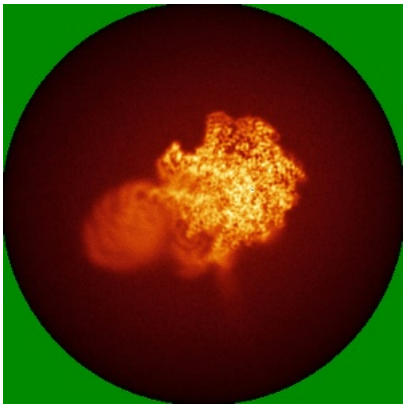


Z

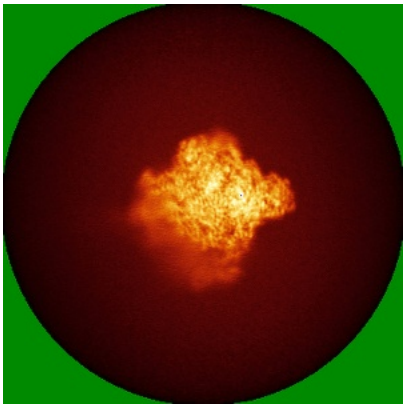
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00843. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

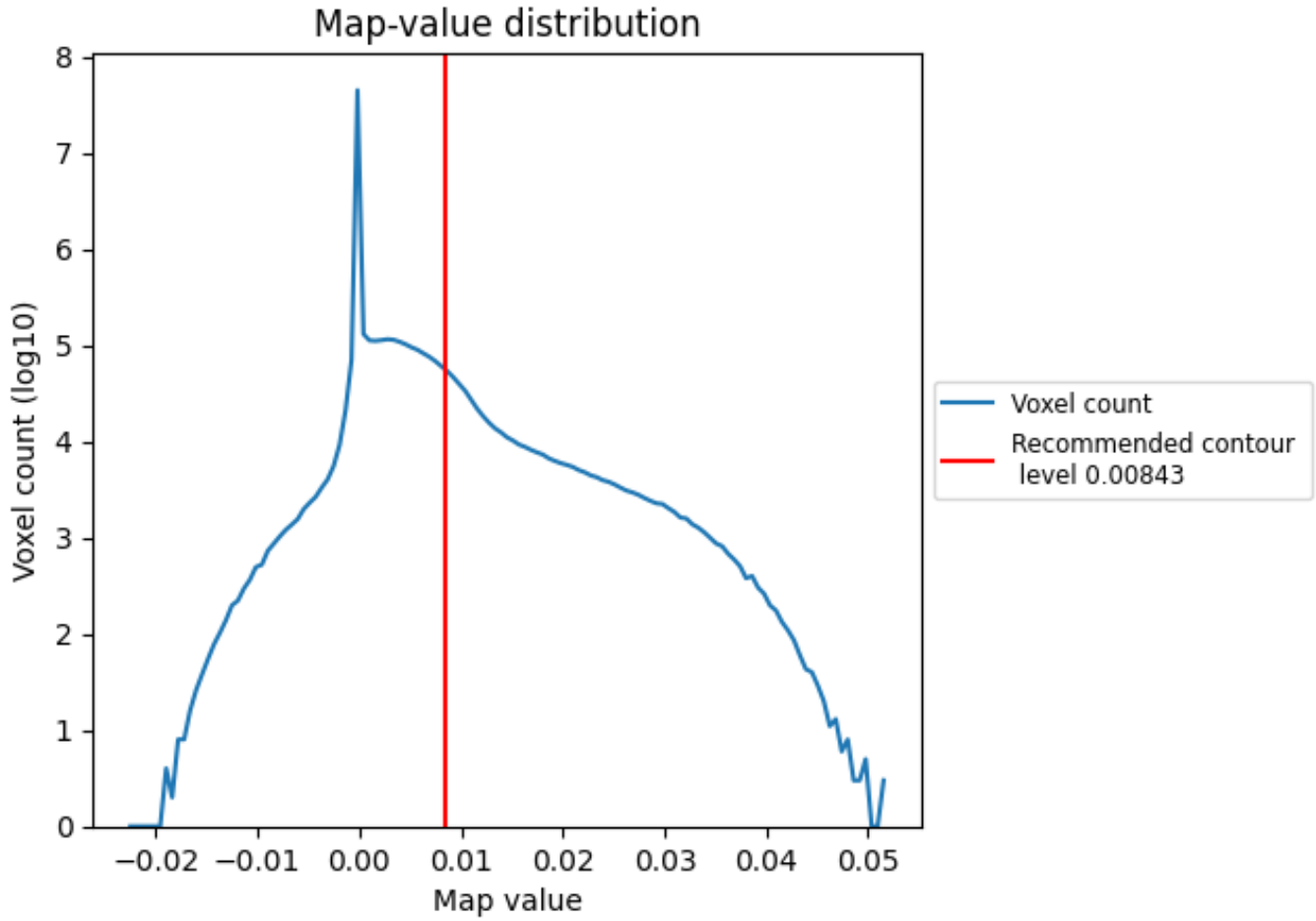
6.6 Mask visualisation (i)

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

7 Map analysis

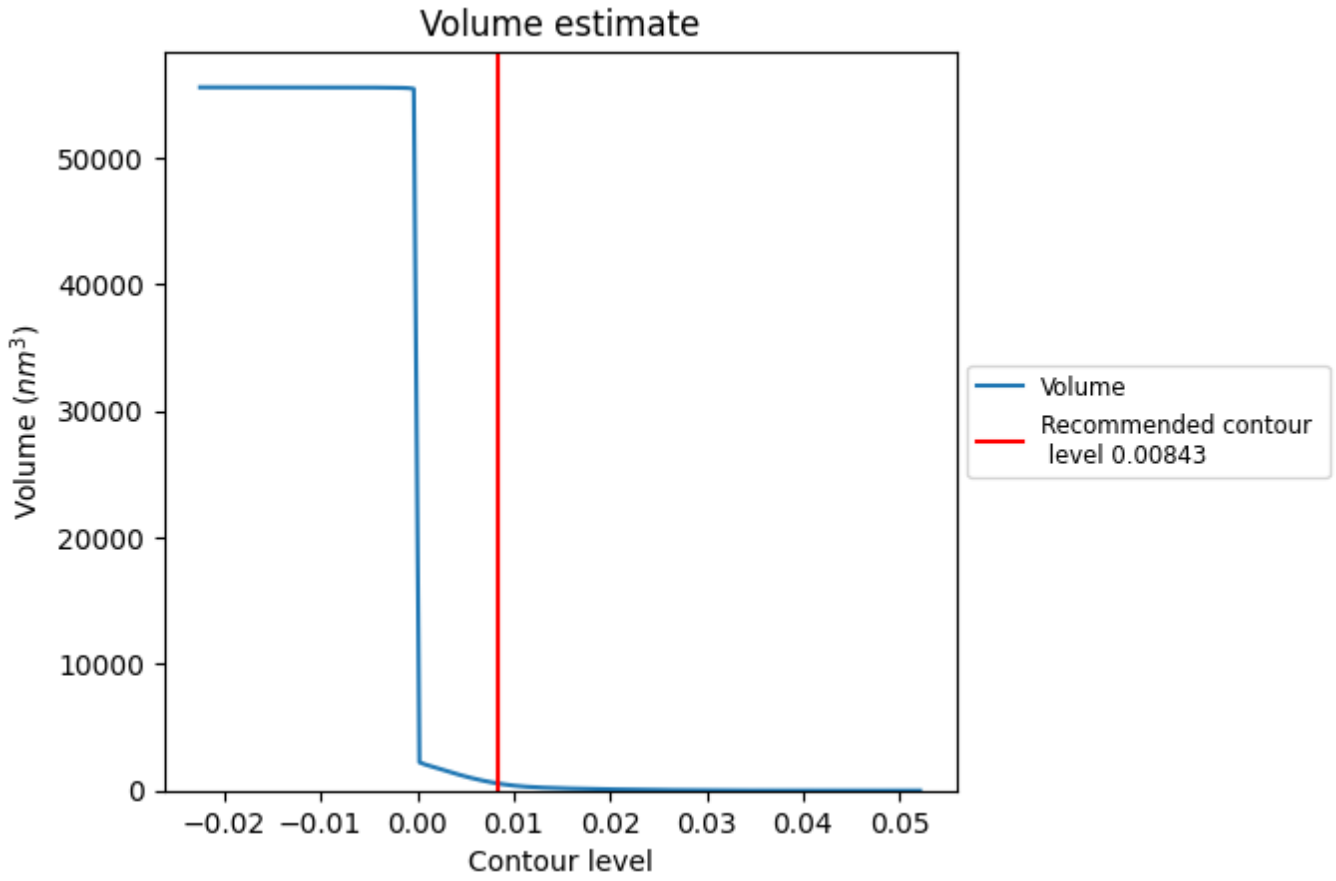
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

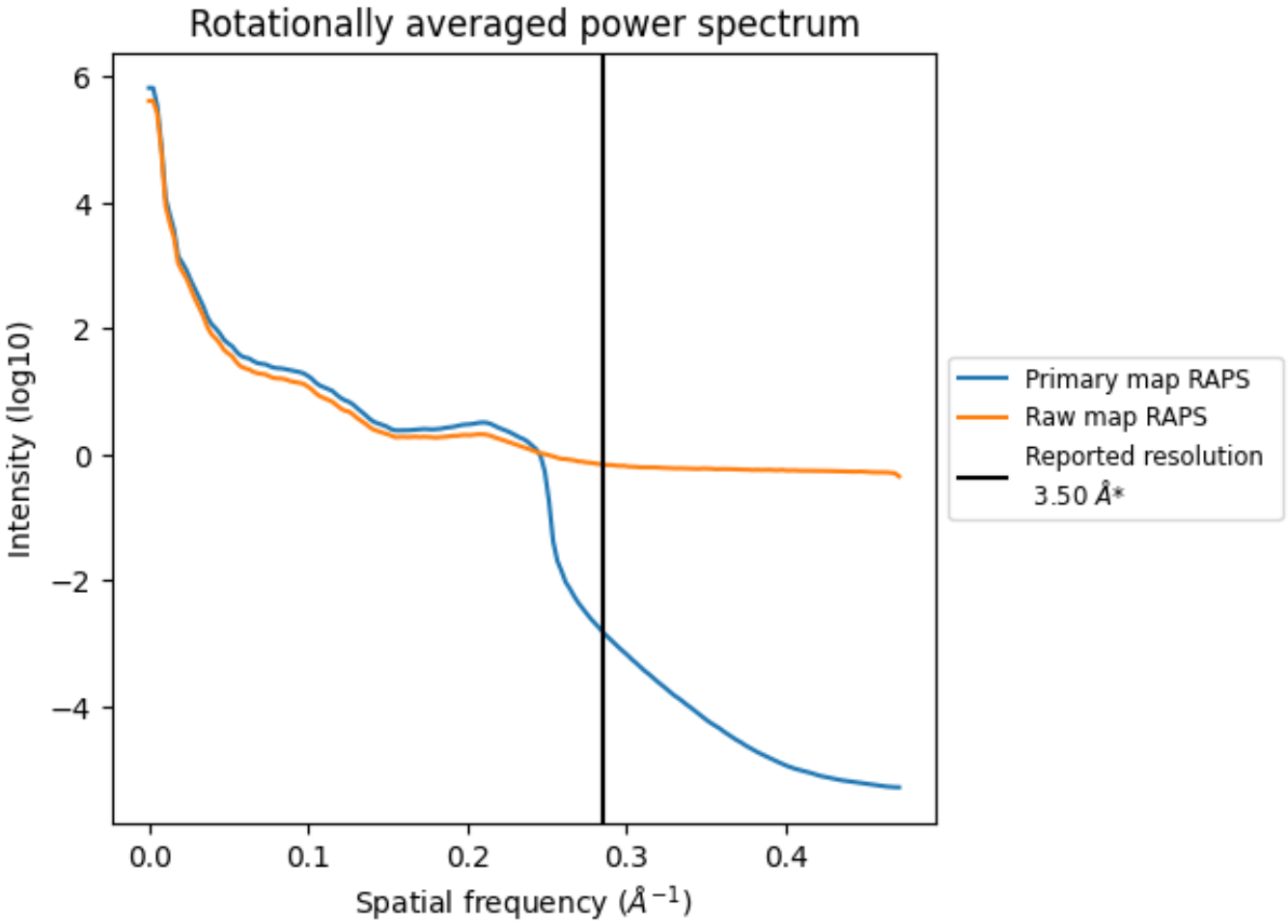
7.2 Volume estimate



The volume at the recommended contour level is 556 nm^3; this corresponds to an approximate mass of 502 kDa.

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

7.3 Rotationally averaged power spectrum (i)

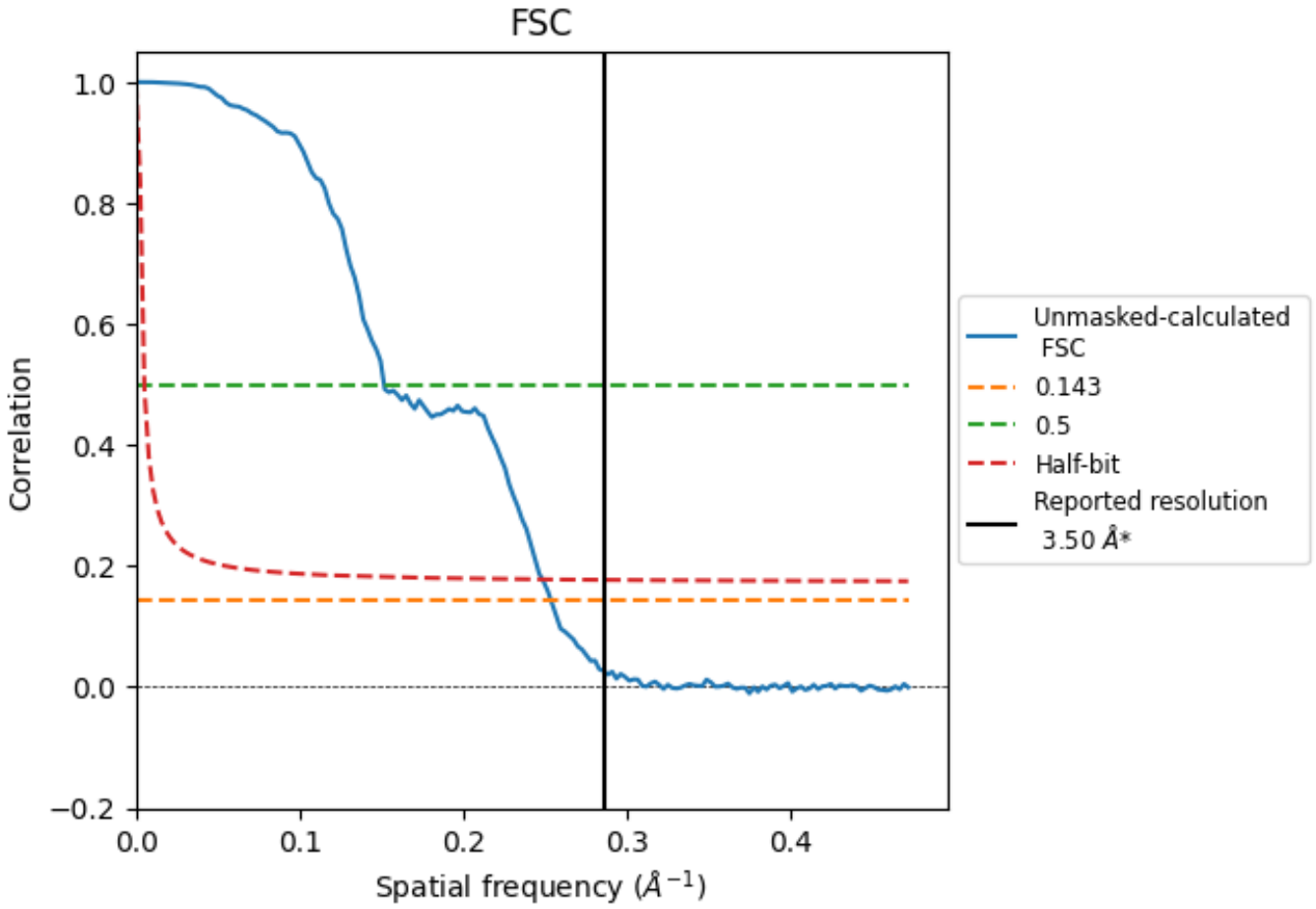


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

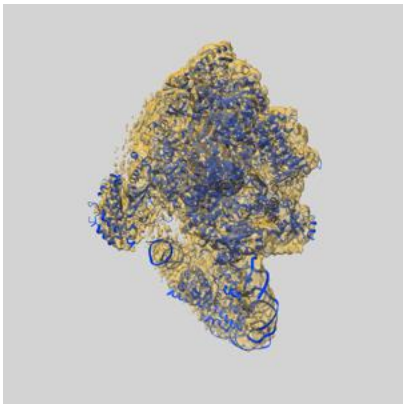
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.94	6.60	4.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 3.5 by more than 10 %

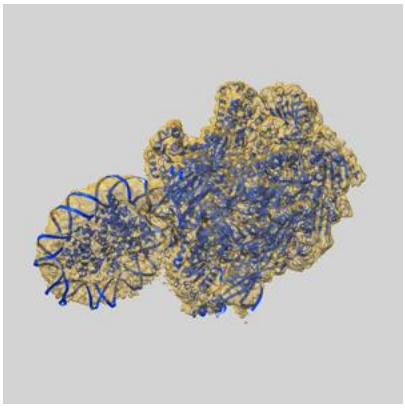
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60593 and PDB model 9II7. Per-residue inclusion information can be found in section 3 on page 9.

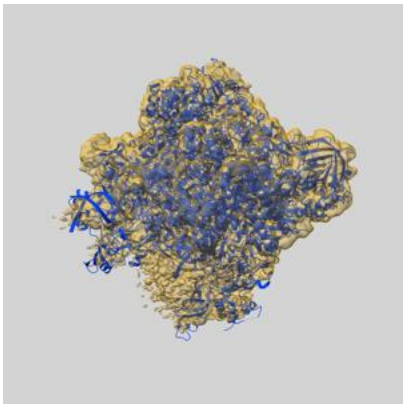
9.1 Map-model overlay



X



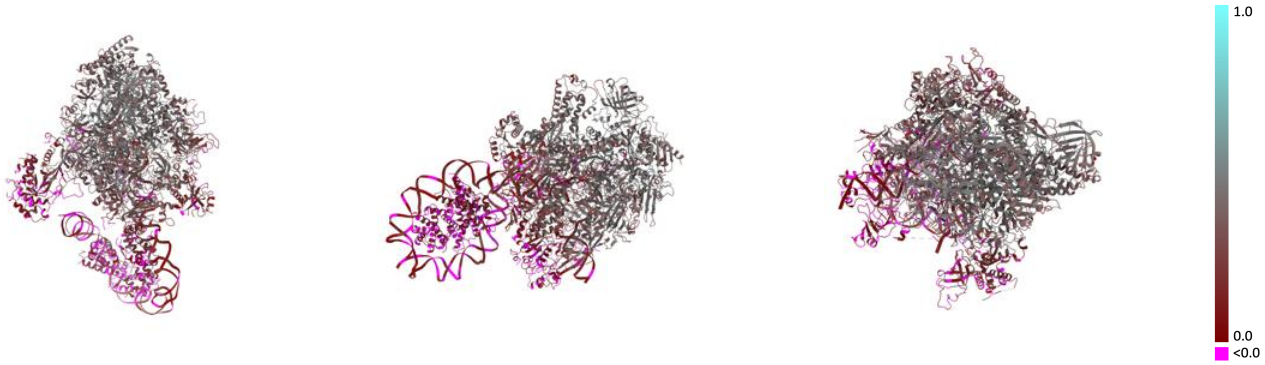
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00843 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.

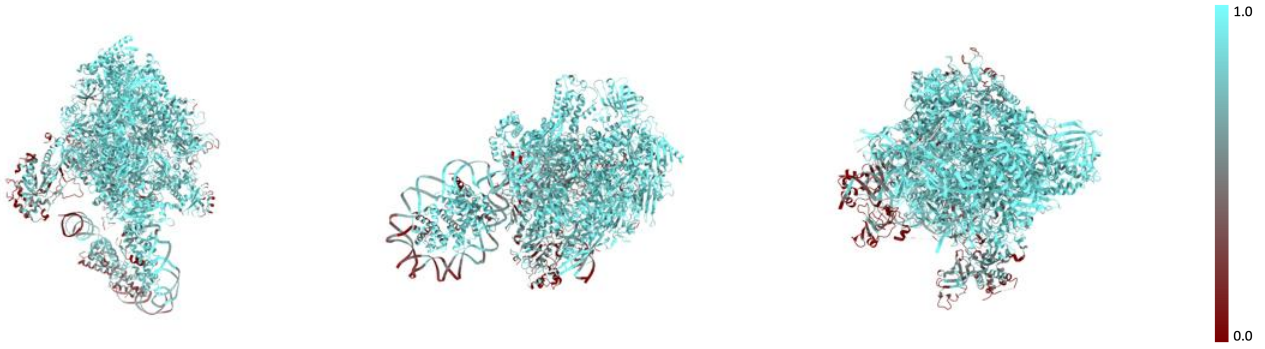
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

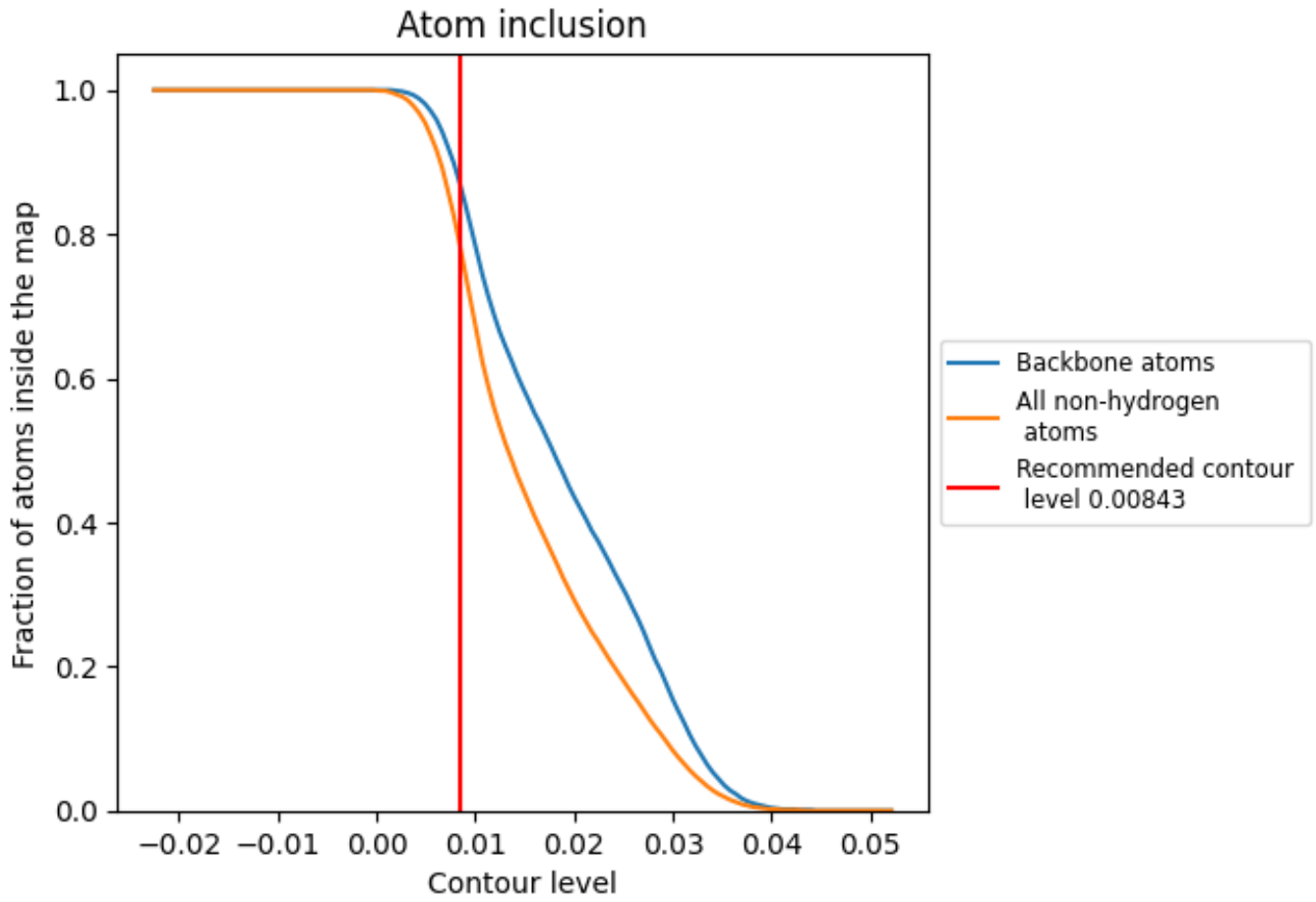
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.00843).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 79% 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 (0.00843) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7860	0.2850
A	0.8760	0.3760
B	0.8840	0.3930
C	0.9190	0.4140
D	0.4260	0.1040
E	0.9140	0.3690
F	0.9210	0.4150
G	0.5910	0.1980
H	0.9320	0.4150
I	0.6740	0.2150
J	0.9340	0.4320
K	0.9090	0.4020
L	0.9190	0.3550
M	0.5870	0.1240
N	0.6180	0.0870
P	0.9180	0.2810
T	0.6380	0.1160
V	0.3730	0.0240
W	0.4510	0.1110
a	0.7460	0.0280
b	0.7010	0.0460
c	0.7160	0.0400
d	0.7540	0.0340
e	0.7040	0.0680
f	0.8210	0.0870