



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 01:48 AM UTC

PDB ID : 9UJS / pdb_00009ujs
EMDB ID : EMD-64225
Title : RNA polymerase II elongation complex stalled at SHL(-4) of the H3-H4 octa-
some
Authors : Ho, C.-H.; Nozawa, K.; Nishimura, M.; Oi, M.; Kujirai, T.; Ogasawara, M.;
Ehara, H.; Sekine, S.; Takizawa, Y.; Kurumizaka, H.
Deposited on : 2025-04-17
Resolution : 3.62 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

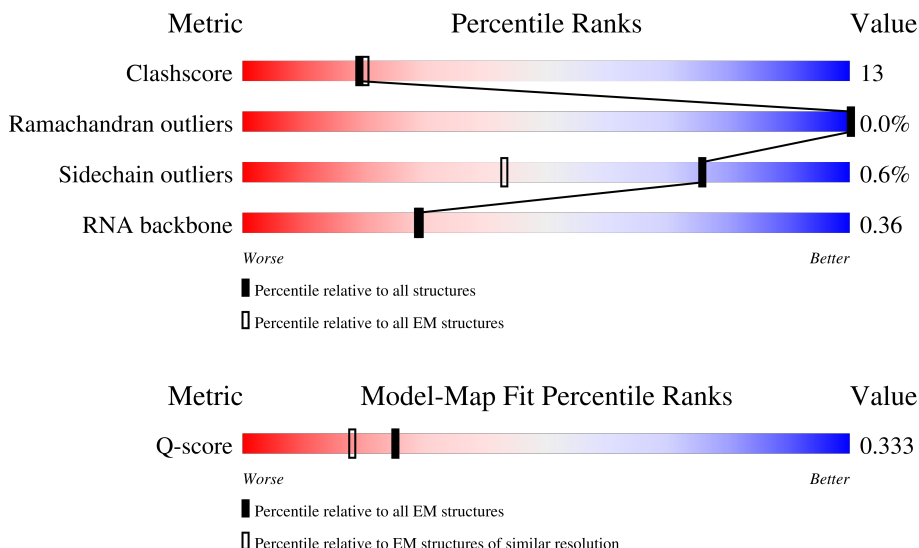
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.62 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11773 (3.12 - 4.12)

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

Mol	Chain	Length	Quality of chain
1	A	1743	
2	B	1227	
3	C	304	

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Mol	Chain	Length	Quality of chain
4	D	186	
5	E	214	
6	F	155	
7	G	171	
8	H	145	
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	P	11	
14	N	198	
15	T	198	
16	a	139	
16	c	139	
16	e	139	
16	g	139	
17	b	106	
17	d	106	
17	f	106	
17	h	106	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 42216 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1408	Total	C	N	O	S	0	0
			11095	6997	1935	2093	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1161	Total	C	N	O	S	0	0
			9261	5835	1636	1732	58		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	156	Total	C	N	O	S	0	0
			1210	753	210	245	2		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	11	Total	C	N	O	P	0	0
			232	103	36	82	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	141	Total	C	N	O	P	0	0
			2903	1379	511	872	141		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	150	Total	C	N	O	P	0	0
			3065	1450	596	869	150		

- Molecule 16 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	76	Total	C	N	O	S	0	0
			619	392	115	108	4		
16	c	77	Total	C	N	O	S	0	0
			625	395	116	110	4		
16	e	76	Total	C	N	O	S	0	0
			619	392	115	108	4		
16	g	77	Total	C	N	O	S	0	0
			625	395	116	110	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-3	GLY	-	expression tag	UNP P68431
a	-2	SER	-	expression tag	UNP P68431
a	-1	HIS	-	expression tag	UNP P68431
c	-3	GLY	-	expression tag	UNP P68431
c	-2	SER	-	expression tag	UNP P68431
c	-1	HIS	-	expression tag	UNP P68431
e	-3	GLY	-	expression tag	UNP P68431
e	-2	SER	-	expression tag	UNP P68431
e	-1	HIS	-	expression tag	UNP P68431
g	-3	GLY	-	expression tag	UNP P68431
g	-2	SER	-	expression tag	UNP P68431
g	-1	HIS	-	expression tag	UNP P68431

- Molecule 17 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	73	Total	C	N	O	S	0	0
			587	367	118	101	1		
17	d	71	Total	C	N	O	S	0	0
			568	357	113	97	1		
17	f	72	Total	C	N	O	S	0	0
			576	361	114	100	1		
17	h	73	Total	C	N	O	S	0	0
			587	367	118	101	1		

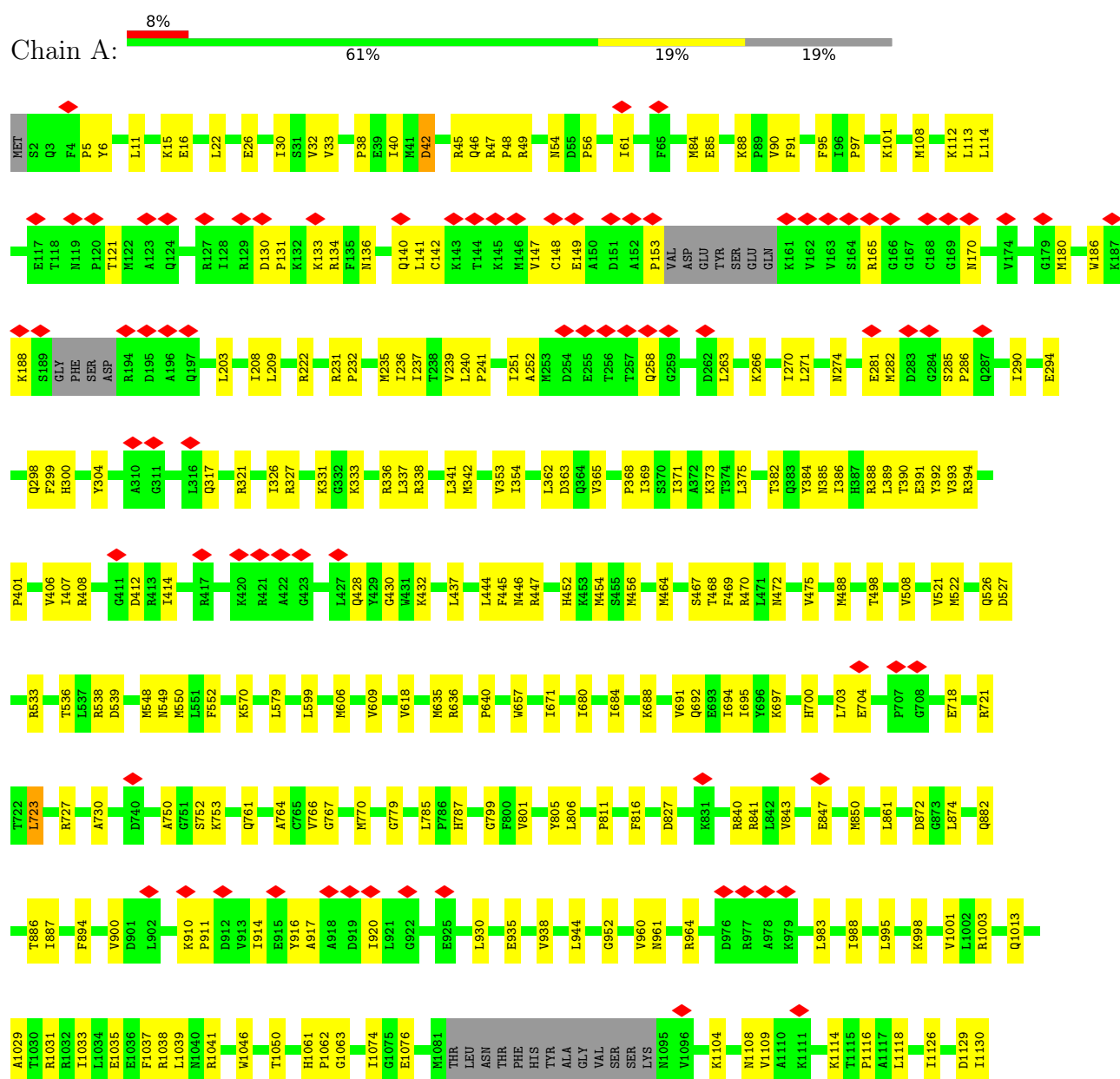
There are 12 discrepancies between the modelled and reference sequences:

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

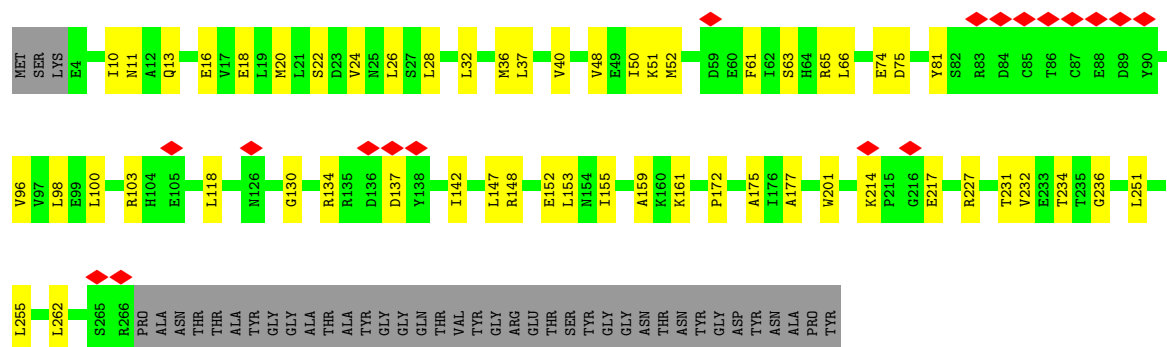
3 Residue-property plots

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

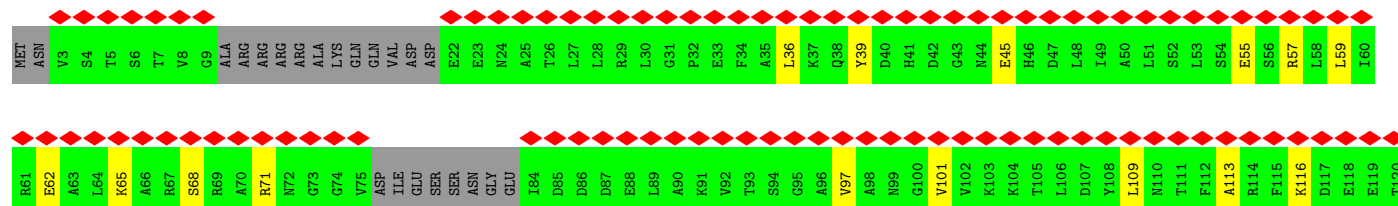
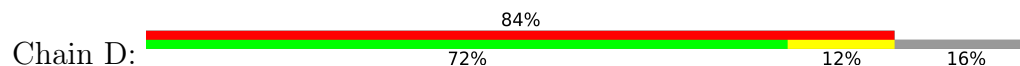
• Molecule 1: DNA-directed RNA polymerase subunit



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

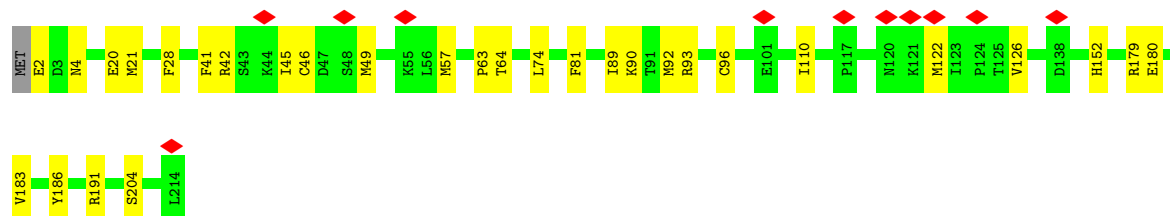
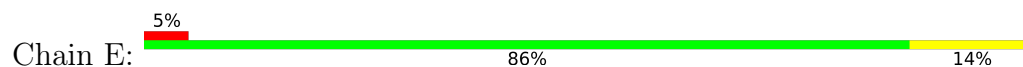


- Molecule 4: RNA polymerase II subunit B32

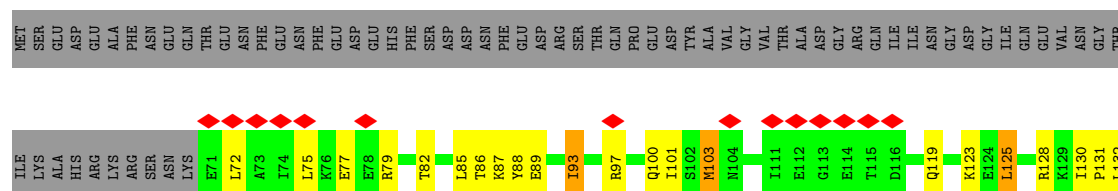
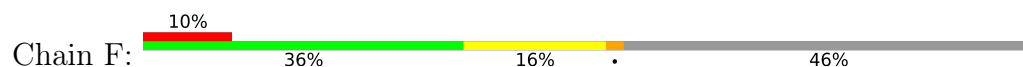




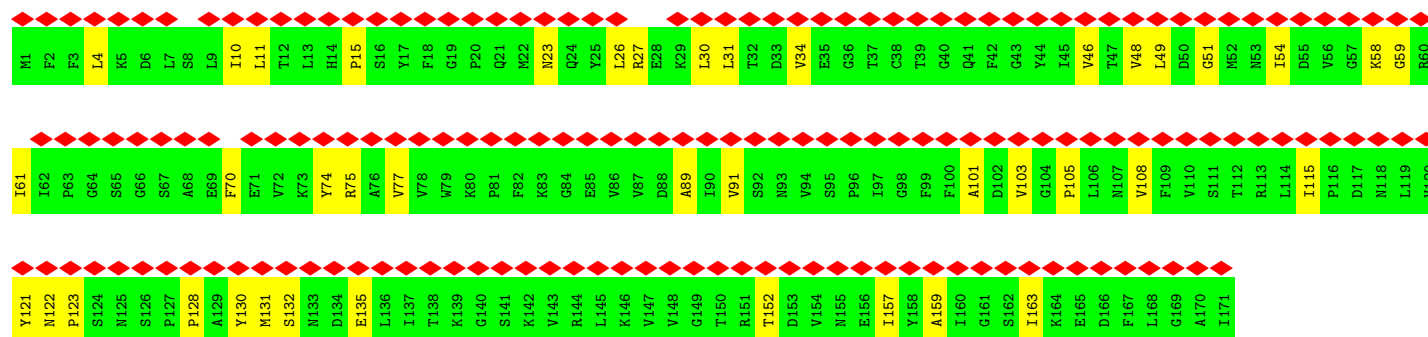
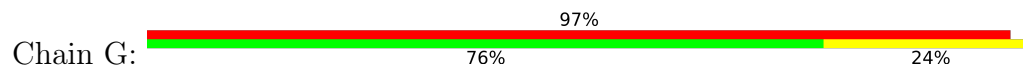
- Molecule 5: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III



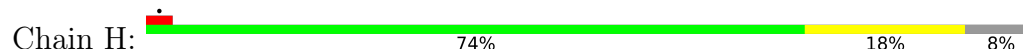
- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

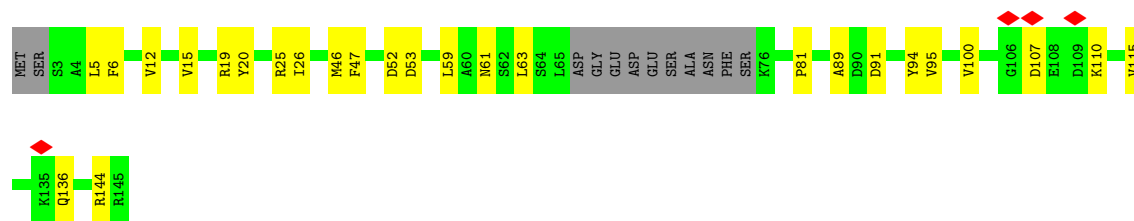


- Molecule 7: RNA polymerase II subunit

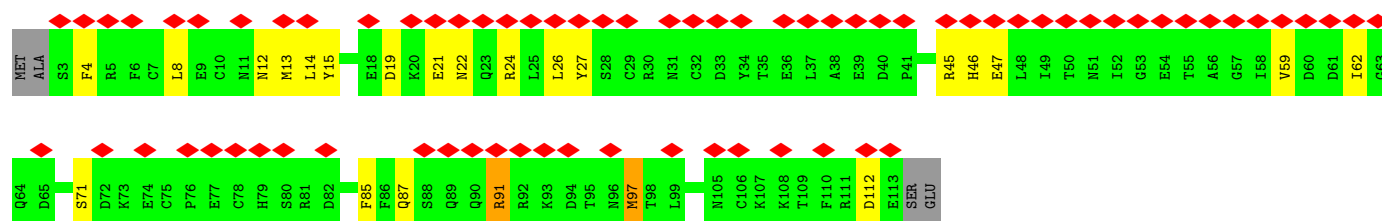
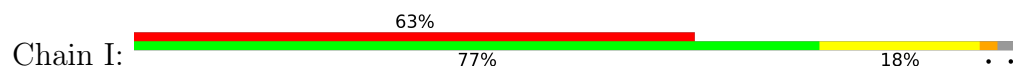


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3





- Molecule 9: DNA-directed RNA polymerase subunit



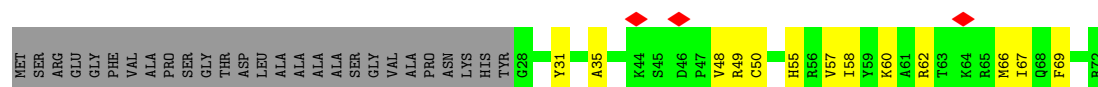
- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III



- Molecule 11: RNA polymerase II subunit B12.5



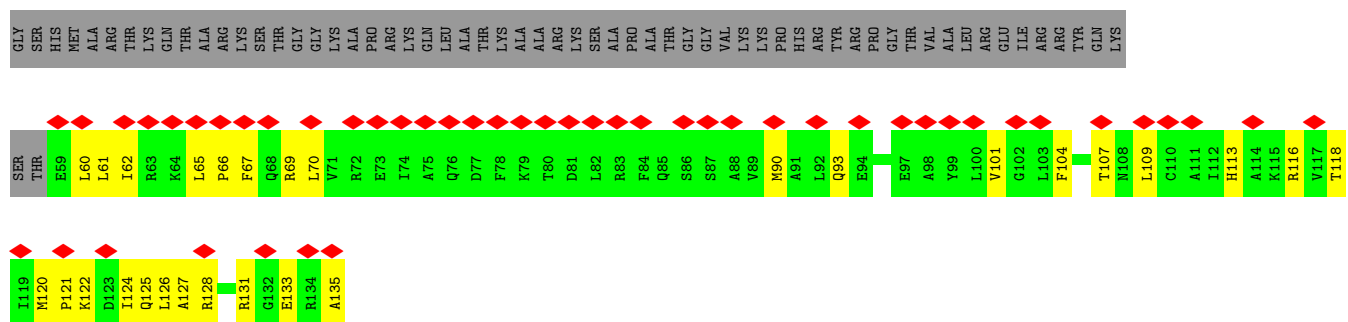
- Molecule 12: RNA polymerase subunit ABC10-alpha



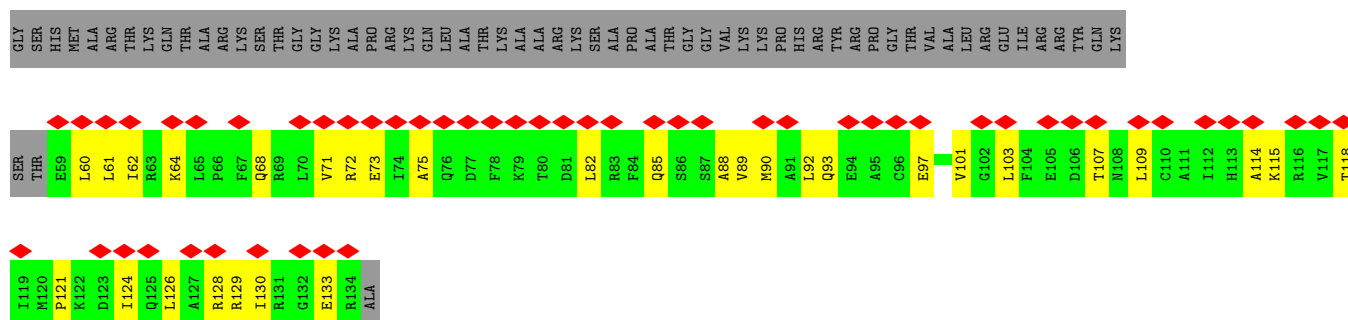
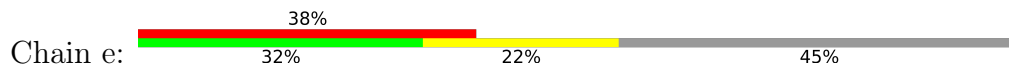
- Molecule 13: RNA (5'-R(P*GP*UP*GP*GP*CP*CP*GP*UP*UP*UP*U)-3')



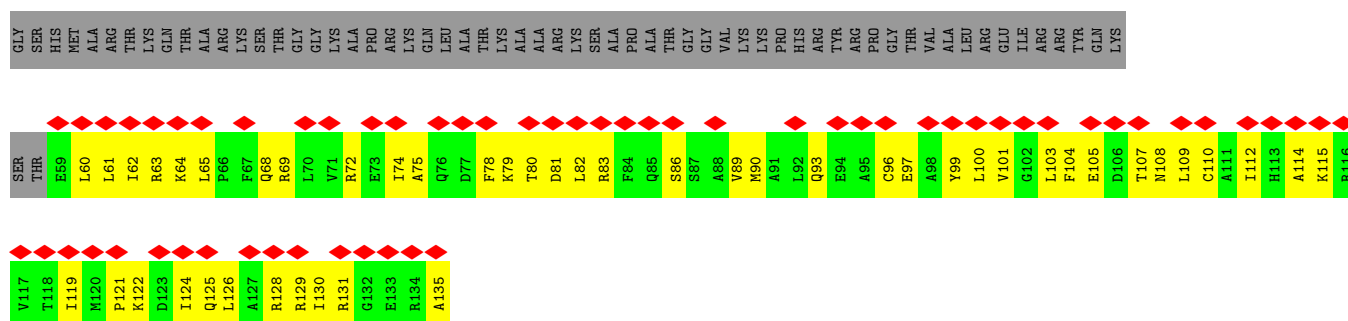
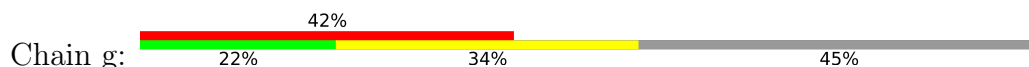




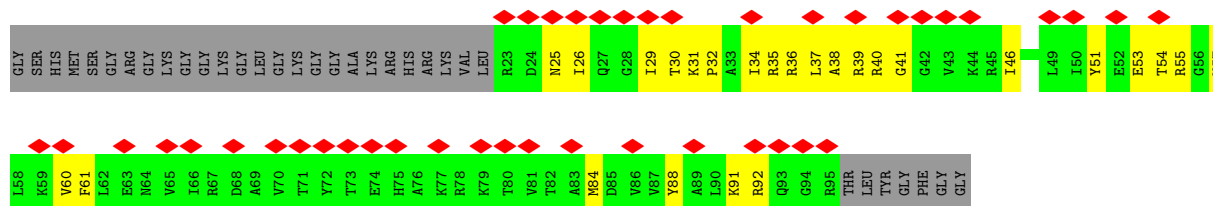
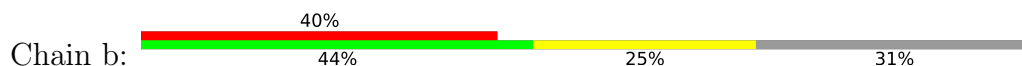
• Molecule 16: Histone H3.1



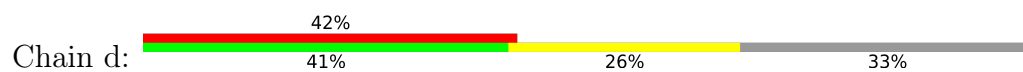
• Molecule 16: Histone H3.1



• Molecule 17: Histone H4



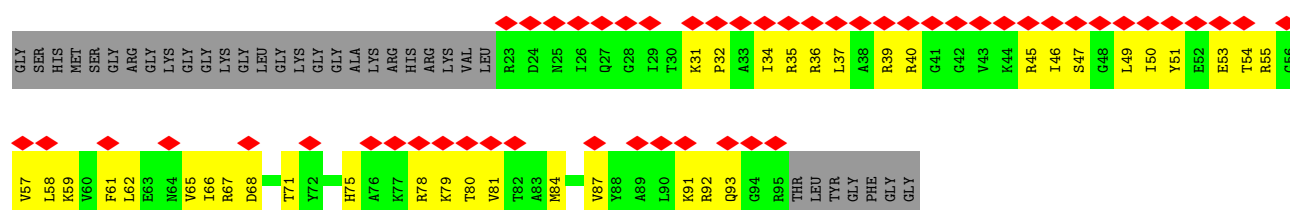
• Molecule 17: Histone H4



• Molecule 17: Histone H4



• Molecule 17: Histone H4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	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	0.043	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.007	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](#)

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	0.17	0/11299	0.40	0/15266
2	B	0.19	0/9441	0.41	1/12732 (0.0%)
3	C	0.16	0/2139	0.35	0/2895
4	D	0.09	0/1221	0.25	0/1648
5	E	0.15	0/1772	0.39	0/2385
6	F	0.18	0/687	0.43	0/931
7	G	0.19	0/1353	0.36	0/1837
8	H	0.16	0/1069	0.42	2/1444 (0.1%)
9	I	0.21	0/934	0.48	0/1257
10	J	0.20	0/554	0.46	0/742
11	K	0.19	0/953	0.42	0/1291
12	L	0.17	0/365	0.43	0/484
13	P	0.17	0/257	0.36	0/398
14	N	0.22	0/3249	0.47	0/5018
15	T	0.18	0/3446	0.34	0/5307
16	a	0.20	0/626	0.56	0/839
16	c	0.19	0/632	0.44	0/846
16	e	0.15	0/626	0.40	0/839
16	g	0.18	0/632	0.50	0/846
17	b	0.16	0/592	0.40	0/792
17	d	0.16	0/573	0.40	0/767
17	f	0.15	0/581	0.42	0/778
17	h	0.21	0/592	0.45	0/792
All	All	0.18	0/43593	0.41	3/60134 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	429	ILE	N-CA-C	-5.55	107.40	111.90
8	H	81	PRO	CA-C-N	5.08	127.70	120.49
8	H	81	PRO	C-N-CA	5.08	127.70	120.49

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11095	0	11137	266	0
2	B	9261	0	9269	233	0
3	C	2098	0	2061	42	0
4	D	1210	0	1205	14	0
5	E	1740	0	1754	22	0
6	F	677	0	693	30	0
7	G	1324	0	1342	27	0
8	H	1052	0	1050	18	0
9	I	917	0	872	27	0
10	J	545	0	564	19	0
11	K	932	0	944	39	0
12	L	359	0	362	16	0
13	P	232	0	117	6	0
14	N	2903	0	1597	60	0
15	T	3065	0	1669	78	0
16	a	619	0	649	29	0
16	c	625	0	654	24	0
16	e	619	0	649	30	0
16	g	625	0	654	57	0
17	b	587	0	631	28	0
17	d	568	0	614	29	0
17	f	576	0	618	27	0
17	h	587	0	631	42	0
All	All	42216	0	39736	1038	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 13.

All (1038) 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)
11:K:33:ILE:HD12	11:K:35:PHE:CE1	1.85	1.11
16:g:103:LEU:CD1	16:g:131:ARG:HH22	1.79	0.96
16:g:103:LEU:HD12	16:g:131:ARG:HH22	1.33	0.94
11:K:33:ILE:CD1	11:K:35:PHE:HE1	1.82	0.90
2:B:225:ILE:CD1	2:B:248:LYS:HD3	2.03	0.88
5:E:90:LYS:HA	5:E:93:ARG:HE	1.37	0.88
11:K:33:ILE:CD1	11:K:35:PHE:CE1	2.59	0.85
1:A:1148:VAL:HG21	1:A:1207:LYS:HE3	1.58	0.83
6:F:85:LEU:HD12	6:F:89:GLU:CD	2.04	0.83
1:A:1355:ILE:HG22	1:A:1371:MET:HE2	1.62	0.82
1:A:538:ARG:HB3	8:H:20:TYR:HE2	1.44	0.82
17:b:32:PRO:HA	17:b:35:ARG:HG2	1.62	0.81
2:B:550:PHE:HB3	2:B:593:MET:HE1	1.63	0.81
1:A:1439:MET:HE1	2:B:1142:GLY:HA2	1.63	0.81
17:h:47:SER:H	17:h:50:ILE:HD12	1.43	0.80
1:A:1448:ILE:HG22	7:G:59:GLY:H	1.47	0.79
16:g:72:ARG:HH22	16:g:83:ARG:HA	1.46	0.79
12:L:57:VAL:O	12:L:58:ILE:HD13	1.83	0.79
2:B:286:ASP:HB3	9:I:13:MET:HE3	1.64	0.78
11:K:21:ILE:HD11	11:K:31:ILE:HB	1.66	0.78
17:d:31:LYS:HG3	17:d:32:PRO:HD3	1.66	0.78
15:T:-31:DG:H2''	15:T:-30:DT:H71	1.64	0.77
2:B:883:LEU:HD21	2:B:932:HIS:HB3	1.67	0.77
17:d:36:ARG:HA	17:d:39:ARG:HE	1.50	0.77
16:e:64:LYS:HZ3	16:e:90:MET:HE3	1.49	0.77
16:a:97:GLU:HA	16:a:100:LEU:HD12	1.65	0.76
1:A:1430:ASN:HD22	1:A:1438:PRO:HD3	1.50	0.76
5:E:92:MET:HE1	5:E:122:MET:HB2	1.67	0.76
15:T:-4:DC:H4'	16:g:63:ARG:HE	1.51	0.75
2:B:918:ILE:HD11	2:B:935:ARG:HB2	1.67	0.74
1:A:811:PRO:HG2	2:B:702:MET:HE2	1.68	0.74
11:K:33:ILE:HD12	11:K:35:PHE:CZ	2.25	0.72
5:E:49:MET:HE3	5:E:49:MET:H	1.55	0.72
1:A:805:TYR:HE2	2:B:1021:MET:HE3	1.54	0.72
1:A:407:ILE:HB	1:A:432:LYS:HB2	1.71	0.72
2:B:910:ILE:HD13	2:B:938:SER:HB3	1.72	0.72
6:F:85:LEU:CD1	6:F:89:GLU:CD	2.62	0.72
6:F:146:TRP:HB3	6:F:151:LEU:HD11	1.72	0.72
1:A:22:LEU:HG	2:B:1213:ALA:HB2	1.71	0.72
1:A:1118:LEU:HD11	1:A:1314:ILE:HA	1.70	0.72
1:A:91:PHE:HB2	1:A:298:GLN:HE22	1.53	0.71
17:f:35:ARG:HG2	17:f:46:ILE:HD12	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:MET:HE1	1:A:640:PRO:HA	1.71	0.71
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.72	0.70
16:g:64:LYS:HG3	16:g:68:GLN:HE21	1.56	0.70
3:C:103:ARG:HG2	3:C:152:GLU:HG3	1.72	0.70
16:g:60:LEU:HB3	16:g:93:GLN:HE21	1.57	0.70
3:C:66:LEU:HD11	3:C:155:ILE:HD12	1.74	0.69
16:e:64:LYS:NZ	16:e:90:MET:CE	2.55	0.69
16:c:128:ARG:HG2	16:c:135:ALA:HB3	1.73	0.69
1:A:47:ARG:HD3	1:A:56:PRO:HD3	1.75	0.68
15:T:69:DA:H2''	15:T:70:DA:H5''	1.75	0.68
2:B:225:ILE:HD11	2:B:248:LYS:HD3	1.74	0.68
16:c:120:MET:HG3	16:c:122:LYS:HG2	1.76	0.68
17:f:26:ILE:HG13	17:f:55:ARG:HD3	1.75	0.68
2:B:221:ALA:HA	2:B:252:ARG:HE	1.58	0.68
15:T:-7:DA:H2''	15:T:-6:DC:C5	2.28	0.68
15:T:7:DT:H5'	17:h:80:THR:HB	1.77	0.67
15:T:28:DC:H5''	17:b:30:THR:HG21	1.77	0.67
16:e:64:LYS:NZ	16:e:90:MET:HE3	2.09	0.67
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.77	0.67
7:G:132:SER:HB2	7:G:135:GLU:HB2	1.76	0.67
1:A:447:ARG:HB2	1:A:488:MET:HE3	1.76	0.67
6:F:85:LEU:HD11	6:F:89:GLU:HG2	1.76	0.67
1:A:548:MET:HE3	11:K:59:VAL:H	1.60	0.66
17:d:36:ARG:HB3	17:d:39:ARG:HH21	1.60	0.66
15:T:6:DC:H2''	15:T:7:DT:H71	1.76	0.66
1:A:1266:ILE:HG22	1:A:1270:MET:HE2	1.76	0.66
3:C:11:ASN:HB3	3:C:13:GLN:HE22	1.60	0.66
11:K:26:ARG:HD2	11:K:27:VAL:HG23	1.76	0.66
3:C:40:VAL:HB	3:C:172:PRO:HG2	1.78	0.66
16:g:79:LYS:HG3	16:g:81:ASP:H	1.61	0.66
16:a:108:ASN:O	16:a:112:ILE:HG13	1.96	0.65
16:g:96:CYS:O	16:g:100:LEU:HG	1.96	0.65
14:N:37:DA:H2''	14:N:38:DT:H73	1.79	0.65
1:A:430:GLY:HA2	6:F:103:MET:HE1	1.79	0.65
11:K:9:LEU:HD23	11:K:69:ALA:HB2	1.78	0.65
17:d:69:ALA:O	17:d:73:THR:HG23	1.97	0.65
1:A:1338:ILE:HD13	1:A:1342:LEU:HD13	1.77	0.65
3:C:51:LYS:HA	12:L:66:MET:HE1	1.79	0.65
1:A:1262:MET:O	1:A:1266:ILE:HG12	1.97	0.65
2:B:1169:MET:HE1	2:B:1201:LYS:HG2	1.78	0.64
6:F:125:LEU:HA	6:F:130:ILE:HD11	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:48:VAL:CG1	12:L:58:ILE:HG13	2.27	0.64
16:a:104:PHE:HA	16:a:107:THR:HG22	1.80	0.64
16:a:126:LEU:HB2	16:c:109:LEU:HD11	1.79	0.64
2:B:24:PHE:HB2	2:B:678:TRP:CE3	2.32	0.64
8:H:107:ASP:HB2	8:H:110:LYS:HB2	1.80	0.64
16:c:61:LEU:HD21	17:d:36:ARG:HB2	1.79	0.64
1:A:231:ARG:HD2	1:A:232:PRO:HD2	1.79	0.64
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.79	0.64
7:G:152:THR:HA	7:G:157:ILE:HG22	1.79	0.64
16:g:129:ARG:HB2	16:g:135:ALA:HB3	1.78	0.64
1:A:389:LEU:O	1:A:393:VAL:HG23	1.98	0.64
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	1.80	0.64
6:F:89:GLU:OE2	6:F:134:ILE:HG13	1.97	0.64
1:A:270:ILE:HD13	1:A:300:HIS:HB3	1.80	0.63
1:A:983:LEU:HD13	1:A:988:ILE:HD11	1.80	0.63
17:f:26:ILE:HG12	17:f:59:LYS:HD2	1.78	0.63
6:F:130:ILE:HD12	6:F:130:ILE:H	1.61	0.63
16:c:118:THR:HB	17:d:45:ARG:HB3	1.80	0.63
1:A:671:ILE:HG12	1:A:806:LEU:HD21	1.80	0.63
15:T:63:DA:H2'	15:T:64:DG:C8	2.34	0.63
5:E:81:PHE:HE1	5:E:110:ILE:HD12	1.64	0.63
1:A:550:MET:HE3	1:A:657:TRP:HB2	1.81	0.62
9:I:59:VAL:H	9:I:62:ILE:HD11	1.64	0.62
1:A:134:ARG:HH12	1:A:222:ARG:HA	1.65	0.62
2:B:49:LEU:HD11	2:B:411:ARG:HG3	1.80	0.62
1:A:321:ARG:HG2	2:B:466:MET:HE2	1.82	0.62
1:A:910:LYS:HD2	1:A:911:PRO:HD2	1.81	0.62
1:A:263:LEU:HD11	1:A:326:ILE:HD11	1.82	0.62
8:H:5:LEU:HD11	8:H:61:ASN:HB2	1.82	0.62
8:H:15:VAL:HG23	8:H:26:ILE:HG22	1.82	0.62
16:e:92:LEU:HD22	17:f:86:VAL:HG21	1.81	0.62
14:N:0:DA:H2'	14:N:1:DC:C6	2.35	0.61
15:T:-48:DA:H2''	15:T:-47:DG:C8	2.35	0.61
2:B:342:ILE:HG22	2:B:346:LYS:HE2	1.82	0.61
16:e:64:LYS:HZ2	16:e:90:MET:CE	2.14	0.61
17:f:34:ILE:HA	17:f:37:LEU:HG	1.83	0.61
2:B:235:LEU:HD12	2:B:240:ARG:HE	1.65	0.61
14:N:-1:DT:H2'	14:N:0:DA:C8	2.34	0.61
16:g:61:LEU:HD23	17:h:37:LEU:HD23	1.82	0.61
16:c:62:ILE:HD11	17:d:37:LEU:HD11	1.81	0.61
16:g:64:LYS:HG3	16:g:68:GLN:NE2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:c:107:THR:HG21	16:c:124:ILE:HG13	1.82	0.61
16:g:126:LEU:O	16:g:130:ILE:HG12	2.00	0.61
1:A:237:ILE:HD13	2:B:1211:ASN:ND2	2.16	0.61
1:A:1037:PHE:HB3	1:A:1039:LEU:HD23	1.83	0.61
2:B:841:MET:HE3	2:B:1010:LEU:HD21	1.82	0.61
8:H:100:VAL:HG22	8:H:115:VAL:HG22	1.82	0.61
1:A:6:TYR:O	2:B:1175:LEU:HD11	2.00	0.61
16:e:68:GLN:O	16:e:72:ARG:HG2	2.01	0.61
1:A:341:LEU:HD12	1:A:1432:MET:HB2	1.81	0.60
2:B:609:ILE:HG12	2:B:694:GLU:HB2	1.82	0.60
9:I:22:ASN:HB3	9:I:24:ARG:HG2	1.83	0.60
16:e:129:ARG:HH22	16:g:110:CYS:HA	1.66	0.60
1:A:1062:PRO:HD2	6:F:86:THR:HG21	1.84	0.60
3:C:134:ARG:HH21	3:C:137:ASP:HA	1.67	0.60
2:B:883:LEU:HD23	2:B:935:ARG:HH21	1.64	0.60
5:E:90:LYS:HA	5:E:93:ARG:NE	2.12	0.60
17:d:73:THR:HG21	17:d:81:VAL:HG12	1.82	0.60
1:A:526:GLN:HA	1:A:752:SER:HB2	1.82	0.60
7:G:61:ILE:HD12	7:G:61:ILE:H	1.66	0.60
9:I:87:GLN:HG3	9:I:97:MET:HG2	1.84	0.60
16:e:60:LEU:HD11	16:e:93:GLN:HG2	1.84	0.60
2:B:883:LEU:HB2	2:B:935:ARG:HE	1.65	0.60
16:g:80:THR:HG22	16:g:80:THR:O	2.01	0.60
1:A:1003:ARG:HE	6:F:82:THR:HA	1.67	0.60
2:B:384:GLU:HG3	9:I:91:ARG:HE	1.66	0.60
15:T:48:DC:H2'	15:T:49:DA:C8	2.37	0.60
1:A:761:GLN:HG2	1:A:766:VAL:HA	1.84	0.60
13:P:5:C:H2'	13:P:6:G:C8	2.37	0.59
11:K:26:ARG:HH21	11:K:74:ARG:HH22	1.49	0.59
1:A:153:PRO:HD3	1:A:165:ARG:HD2	1.84	0.59
2:B:594:ARG:O	2:B:598:ARG:HG3	2.03	0.59
16:g:109:LEU:HA	16:g:112:ILE:HD12	1.82	0.59
1:A:408:ARG:HB2	1:A:412:ASP:HB2	1.83	0.59
2:B:1104:HIS:HD2	2:B:1122:ARG:HG2	1.67	0.59
17:f:54:THR:O	17:f:58:LEU:HG	2.01	0.59
16:g:86:SER:O	16:g:90:MET:HG2	2.01	0.59
1:A:47:ARG:HH11	1:A:56:PRO:HG3	1.67	0.59
1:A:337:LEU:HA	1:A:341:LEU:HB2	1.85	0.59
1:A:872:ASP:HB3	5:E:204:SER:HB3	1.85	0.59
17:b:92:ARG:HH12	17:h:67:ARG:HH21	1.49	0.59
2:B:262:LYS:HE2	2:B:273:PRO:HG3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1126:ILE:HD13	1:A:1136:ILE:HD11	1.84	0.58
2:B:417:LEU:HD13	2:B:445:THR:HG21	1.85	0.58
1:A:38:PRO:HG3	1:A:271:LEU:HG	1.85	0.58
17:h:51:TYR:O	17:h:55:ARG:HG3	2.03	0.58
1:A:1407:GLU:O	1:A:1411:ILE:HG22	2.02	0.58
4:D:169:VAL:HG12	4:D:171:LEU:H	1.69	0.58
1:A:371:ILE:HG23	1:A:375:LEU:HD12	1.84	0.58
10:J:7:CYS:HA	10:J:48:MET:HG3	1.86	0.58
16:a:65:LEU:HG	16:a:68:GLN:HE21	1.66	0.58
1:A:1126:ILE:HG23	1:A:1132:LYS:HB2	1.85	0.58
1:A:333:LYS:HA	1:A:338:ARG:HH11	1.68	0.58
1:A:456:MET:HE1	2:B:1134:GLU:HG3	1.86	0.58
2:B:24:PHE:HB2	2:B:678:TRP:CZ3	2.38	0.58
9:I:87:GLN:CG	9:I:97:MET:HG2	2.34	0.58
16:g:97:GLU:O	16:g:101:VAL:HG22	2.04	0.58
1:A:914:ILE:HG13	1:A:917:ALA:HB2	1.86	0.57
1:A:1157:ASP:H	1:A:1194:LEU:HD23	1.68	0.57
1:A:1356:LEU:HA	1:A:1371:MET:HE1	1.86	0.57
3:C:32:LEU:O	3:C:36:MET:HG3	2.03	0.57
16:g:65:LEU:HB3	16:g:69:ARG:HH12	1.69	0.57
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.70	0.57
16:c:70:LEU:HD21	17:d:26:ILE:HA	1.86	0.57
1:A:209:LEU:HD21	1:A:236:ILE:HB	1.87	0.57
17:d:36:ARG:O	17:d:40:ARG:HG2	2.05	0.57
3:C:234:THR:HG23	3:C:236:GLY:H	1.69	0.57
17:b:26:ILE:HG12	17:b:55:ARG:HD3	1.86	0.57
17:b:34:ILE:HD12	17:b:34:ILE:H	1.68	0.57
17:d:32:PRO:O	17:d:36:ARG:HG3	2.04	0.57
16:g:103:LEU:HD13	16:g:131:ARG:HH22	1.65	0.57
1:A:239:VAL:O	1:A:239:VAL:HG13	2.03	0.57
11:K:65:HIS:ND1	11:K:66:PRO:HD2	2.20	0.57
15:T:58:DG:H2'	15:T:59:DA:H4'	1.85	0.57
15:T:77:DA:H2'	15:T:78:DA:H8	1.70	0.57
2:B:792:MET:HE1	2:B:855:PHE:CE1	2.39	0.57
15:T:19:DT:H2'	15:T:20:DT:H71	1.87	0.57
16:e:107:THR:HG21	16:e:124:ILE:HG22	1.87	0.57
2:B:413:LEU:HD12	2:B:450:LEU:HD12	1.87	0.57
7:G:91:VAL:HA	7:G:101:ALA:HA	1.87	0.57
2:B:955:THR:HG22	12:L:57:VAL:HA	1.87	0.56
9:I:14:LEU:HD11	9:I:27:TYR:HB3	1.86	0.56
15:T:36:DA:H2''	15:T:37:DA:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:GLY:HA3	2:B:509:ASN:HB2	1.88	0.56
2:B:299:ASP:HB3	2:B:302:MET:HE2	1.87	0.56
15:T:43:DC:H2''	15:T:44:DA:C8	2.39	0.56
17:d:60:VAL:O	17:d:63:GLU:HG3	2.05	0.56
1:A:636:ARG:HB2	1:A:964:ARG:HH12	1.71	0.56
17:h:53:GLU:O	17:h:57:VAL:HG23	2.05	0.56
2:B:301:GLN:HG2	2:B:305:MET:HE1	1.87	0.56
8:H:63:LEU:HD13	8:H:89:ALA:HB2	1.87	0.56
1:A:84:MET:HE2	1:A:274:ASN:HD22	1.69	0.56
1:A:186:TRP:HB3	1:A:188:LYS:HG3	1.88	0.56
1:A:1136:ILE:O	1:A:1140:ILE:HG22	2.06	0.56
6:F:119:GLN:O	6:F:123:LYS:HE2	2.06	0.56
1:A:552:PHE:CE2	11:K:62:LYS:HG2	2.40	0.56
1:A:1398:GLY:O	1:A:1402:ARG:HG2	2.06	0.56
11:K:31:ILE:HG23	11:K:83:PRO:HG2	1.87	0.56
16:e:85:GLN:O	16:e:89:VAL:HG23	2.05	0.56
1:A:362:LEU:HA	1:A:472:ASN:HD22	1.70	0.56
1:A:900:VAL:HG12	1:A:1031:ARG:HE	1.71	0.56
2:B:645:LEU:HD22	2:B:707:LEU:HD12	1.86	0.56
2:B:653:ARG:HA	2:B:656:GLN:OE1	2.05	0.56
10:J:34:ALA:O	10:J:38:LEU:HD12	2.06	0.56
13:P:6:G:H2'	13:P:7:U:C6	2.41	0.56
1:A:1153:GLU:HG2	9:I:45:ARG:HE	1.71	0.56
17:b:61:PHE:O	17:b:61:PHE:HD1	1.89	0.56
2:B:343:GLN:HA	2:B:346:LYS:HG3	1.87	0.56
16:g:121:PRO:HA	16:g:124:ILE:HG12	1.88	0.56
16:a:113:HIS:CG	16:c:126:LEU:HD13	2.41	0.55
17:b:31:LYS:HG2	17:b:35:ARG:HH21	1.70	0.55
17:f:86:VAL:O	17:f:90:LEU:HG	2.05	0.55
2:B:17:CYS:O	2:B:21:ILE:HG13	2.05	0.55
17:f:31:LYS:HG3	17:f:35:ARG:HH21	1.70	0.55
1:A:688:LYS:HA	1:A:691:VAL:HG12	1.89	0.55
1:A:886:THR:HG1	1:A:894:PHE:HE1	1.49	0.55
1:A:1166:GLU:HA	1:A:1169:PHE:HB2	1.88	0.55
9:I:71:SER:HB2	9:I:85:PHE:HD2	1.71	0.55
16:e:126:LEU:HD11	16:e:129:ARG:HH21	1.70	0.55
16:g:103:LEU:HD12	16:g:131:ARG:NH2	2.12	0.55
2:B:66:ASN:HB3	2:B:69:ASP:H	1.70	0.55
2:B:842:ASN:HD22	2:B:999:MET:HG3	1.70	0.55
12:L:35:ALA:HB3	12:L:55:HIS:CE1	2.42	0.55
1:A:251:ILE:HG13	1:A:251:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:12:ASN:C	9:I:13:MET:HE2	2.32	0.55
1:A:1400:LEU:HB2	1:A:1429:GLU:HG3	1.88	0.55
17:b:36:ARG:HG3	17:b:40:ARG:HH21	1.70	0.55
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.89	0.55
2:B:87:PRO:HG3	2:B:111:TYR:CZ	2.42	0.54
15:T:23:DA:H2''	15:T:24:DC:C5	2.42	0.54
1:A:900:VAL:HG23	1:A:930:LEU:HD13	1.88	0.54
14:N:-73:DT:H3'	14:N:-72:DG:H21	1.71	0.54
16:g:122:LYS:O	16:g:125:GLN:HG3	2.07	0.54
1:A:1447:MET:HE3	1:A:1447:MET:HA	1.88	0.54
16:a:65:LEU:HA	16:a:68:GLN:HG3	1.87	0.54
1:A:42:ASP:HB3	1:A:49:ARG:HB3	1.89	0.54
1:A:841:ARG:HH22	1:A:1108:ASN:HD21	1.55	0.54
2:B:194:PHE:CE2	2:B:203:LEU:HD11	2.43	0.54
7:G:115:ILE:HG12	7:G:163:ILE:HD11	1.89	0.54
11:K:41:THR:HG23	11:K:42:LEU:N	2.21	0.54
16:g:61:LEU:HD11	17:h:36:ARG:HD2	1.88	0.54
2:B:437:LEU:HA	2:B:440:ALA:HB3	1.90	0.54
2:B:225:ILE:CG1	2:B:248:LYS:HD3	2.37	0.54
9:I:13:MET:HE2	9:I:13:MET:N	2.23	0.54
16:a:85:GLN:HG3	16:a:88:ALA:H	1.73	0.54
1:A:392:TYR:CE1	1:A:401:PRO:HB2	2.43	0.54
3:C:262:LEU:HD11	11:K:87:LEU:HD23	1.90	0.54
16:g:75:ALA:HB1	16:g:82:LEU:HD23	1.90	0.54
3:C:50:ILE:HG12	3:C:155:ILE:HG22	1.90	0.54
6:F:85:LEU:HD12	6:F:89:GLU:OE1	2.07	0.54
16:a:70:LEU:HD12	17:b:25:ASN:ND2	2.23	0.54
1:A:392:TYR:HE1	1:A:401:PRO:HB2	1.73	0.53
1:A:886:THR:OG1	1:A:894:PHE:HE1	1.91	0.53
2:B:442:LYS:O	2:B:445:THR:HG22	2.08	0.53
3:C:98:LEU:HD23	3:C:118:LEU:HD22	1.88	0.53
17:h:62:LEU:HA	17:h:65:VAL:HG12	1.90	0.53
1:A:84:MET:HE3	1:A:85:GLU:N	2.23	0.53
1:A:805:TYR:CE2	2:B:1021:MET:HE3	2.41	0.53
1:A:1001:VAL:H	1:A:1013:GLN:HE22	1.57	0.53
2:B:792:MET:HE1	2:B:855:PHE:HE1	1.73	0.53
5:E:2:GLU:HG3	5:E:4:ASN:H	1.72	0.53
12:L:48:VAL:HG12	12:L:58:ILE:HG13	1.89	0.53
15:T:70:DA:H2'	15:T:71:DA:C8	2.42	0.53
1:A:5:PRO:HG2	2:B:1159:ARG:HH22	1.73	0.53
1:A:446:ASN:HD22	1:A:447:ARG:H	1.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:ASN:HD22	2:B:963:PHE:HZ	1.56	0.53
4:D:68:SER:HA	4:D:71:ARG:HD3	1.91	0.53
1:A:354:ILE:HG22	1:A:469:PHE:HB2	1.90	0.53
1:A:887:ILE:HD11	1:A:944:LEU:HD23	1.91	0.53
2:B:349:LEU:HA	2:B:353:LEU:HD23	1.89	0.53
5:E:89:ILE:O	5:E:93:ARG:HG3	2.08	0.53
16:g:65:LEU:HD23	16:g:68:GLN:HE22	1.73	0.53
2:B:18:TRP:CE3	2:B:21:ILE:HD12	2.43	0.53
16:a:120:MET:HG2	16:a:121:PRO:HD2	1.90	0.53
1:A:180:MET:HE1	1:A:299:PHE:HA	1.91	0.53
2:B:856:PHE:HE1	2:B:969:ARG:HG3	1.73	0.53
3:C:100:LEU:HB2	3:C:118:LEU:HD23	1.88	0.53
10:J:44:CYS:O	10:J:47:ARG:HG2	2.08	0.53
16:g:86:SER:HA	16:g:89:VAL:HG12	1.91	0.53
2:B:90:THR:HA	2:B:96:THR:HG22	1.91	0.53
2:B:645:LEU:HB3	2:B:647:ILE:HG22	1.91	0.53
14:N:-12:DG:H2''	14:N:-11:DG:C8	2.43	0.53
16:g:100:LEU:HD22	17:h:58:LEU:HD22	1.91	0.53
1:A:914:ILE:CD1	1:A:917:ALA:HA	2.39	0.53
1:A:1428:SER:O	1:A:1432:MET:HG2	2.08	0.53
2:B:1159:ARG:HD3	2:B:1193:GLN:OE1	2.08	0.53
1:A:406:VAL:HB	1:A:414:ILE:HD12	1.90	0.53
2:B:590:VAL:HG11	2:B:610:ARG:HH11	1.73	0.53
15:T:-39:DA:H2''	15:T:-38:DA:C8	2.44	0.53
17:f:59:LYS:O	17:f:63:GLU:HG2	2.09	0.53
16:g:60:LEU:HB3	16:g:93:GLN:NE2	2.22	0.53
1:A:147:VAL:HG23	1:A:149:GLU:OE2	2.09	0.53
2:B:59:ASP:HB3	2:B:74:ARG:HD2	1.91	0.53
1:A:353:VAL:HG23	1:A:468:THR:HG22	1.91	0.52
1:A:843:VAL:O	1:A:847:GLU:HG3	2.08	0.52
2:B:1104:HIS:CD2	2:B:1122:ARG:HG2	2.44	0.52
5:E:81:PHE:CE1	5:E:110:ILE:HD12	2.44	0.52
1:A:753:LYS:HG3	2:B:1019:SER:HB3	1.91	0.52
1:A:1402:ARG:HG3	1:A:1411:ILE:HD11	1.92	0.52
10:J:3:ILE:HD12	10:J:4:PRO:HD2	1.89	0.52
14:N:-14:DG:H4'	14:N:-13:DG:OP1	2.09	0.52
14:N:0:DA:H2'	14:N:1:DC:H6	1.73	0.52
1:A:47:ARG:NH1	1:A:56:PRO:HG3	2.24	0.52
2:B:50:VAL:HG11	2:B:82:ILE:HD11	1.89	0.52
12:L:66:MET:HA	12:L:66:MET:HE2	1.91	0.52
16:c:122:LYS:O	16:c:125:GLN:HG3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:f:31:LYS:HG3	17:f:35:ARG:HE	1.74	0.52
1:A:382:THR:HG23	1:A:384:TYR:H	1.74	0.52
2:B:276:ILE:HB	2:B:316:ILE:HG21	1.91	0.52
3:C:81:TYR:HE2	3:C:161:LYS:HE2	1.74	0.52
16:g:121:PRO:HB3	17:h:53:GLU:HG3	1.91	0.52
17:h:54:THR:O	17:h:58:LEU:HG	2.09	0.52
1:A:1446:VAL:HG11	6:F:132:LEU:HD13	1.92	0.52
15:T:-44:DC:H2''	15:T:-43:DG:H8	1.75	0.52
1:A:32:VAL:HG23	1:A:33:VAL:HG13	1.92	0.52
1:A:1142:TYR:HA	1:A:1278:GLY:HA3	1.91	0.52
2:B:119:MET:HE1	2:B:121:LYS:HB2	1.91	0.52
2:B:1152:MET:HE1	2:B:1197:PRO:HD3	1.92	0.52
2:B:225:ILE:HD12	2:B:248:LYS:HB2	1.92	0.52
2:B:225:ILE:HG13	2:B:248:LYS:HD3	1.92	0.52
16:c:60:LEU:HD22	16:c:93:GLN:HG2	1.91	0.52
5:E:41:PHE:O	5:E:45:ILE:HG22	2.10	0.52
2:B:486:SER:HA	2:B:751:VAL:HG21	1.92	0.51
9:I:71:SER:HB2	9:I:85:PHE:CD2	2.44	0.51
15:T:7:DT:H2''	15:T:8:DG:H8	1.76	0.51
15:T:43:DC:H2''	15:T:44:DA:N7	2.25	0.51
17:f:91:LYS:HG2	17:f:92:ARG:HD2	1.92	0.51
2:B:30:LEU:HD13	2:B:485:LEU:HD22	1.93	0.51
2:B:883:LEU:HB2	2:B:935:ARG:NE	2.24	0.51
15:T:6:DC:H2''	15:T:7:DT:C7	2.40	0.51
1:A:113:LEU:HD12	1:A:114:LEU:H	1.76	0.51
2:B:55:ARG:HA	2:B:77:ILE:O	2.09	0.51
15:T:32:DG:H2''	15:T:33:DG:C8	2.46	0.51
16:g:82:LEU:HD12	16:g:83:ARG:H	1.76	0.51
2:B:446:ILE:O	2:B:450:LEU:HD13	2.09	0.51
7:G:26:LEU:HD11	7:G:70:PHE:CE1	2.46	0.51
16:e:64:LYS:HD3	16:e:90:MET:HE1	1.91	0.51
9:I:19:ASP:HB2	9:I:26:LEU:HD23	1.93	0.51
15:T:14:DC:H2''	15:T:15:DG:C8	2.46	0.51
17:h:49:LEU:O	17:h:53:GLU:HG2	2.11	0.51
14:N:-60:DC:H2''	14:N:-59:DT:C6	2.45	0.51
15:T:59:DA:H2''	15:T:60:DG:C8	2.46	0.51
15:T:77:DA:H2'	15:T:78:DA:C8	2.46	0.51
17:h:46:ILE:HD11	17:h:51:TYR:CZ	2.46	0.51
3:C:48:VAL:HG11	3:C:63:SER:HB2	1.92	0.51
16:e:103:LEU:O	16:e:107:THR:HG23	2.11	0.51
17:b:31:LYS:HE2	17:b:35:ARG:HH21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ILE:O	1:A:390:THR:HG23	2.11	0.51
11:K:59:VAL:HG13	11:K:59:VAL:O	2.10	0.51
1:A:983:LEU:HA	1:A:1041:ARG:HH11	1.76	0.51
11:K:31:ILE:O	11:K:32:ILE:HD13	2.11	0.51
16:e:114:ALA:O	16:e:115:LYS:HG2	2.11	0.51
1:A:391:GLU:HA	1:A:394:ARG:HE	1.76	0.50
2:B:252:ARG:HG3	2:B:253:GLU:H	1.77	0.50
3:C:96:VAL:HG11	3:C:130:GLY:HA3	1.92	0.50
6:F:103:MET:HE2	6:F:103:MET:HA	1.92	0.50
1:A:121:THR:OG1	1:A:141:LEU:HD21	2.11	0.50
1:A:240:LEU:HD23	1:A:241:PRO:O	2.10	0.50
2:B:303:LEU:HA	2:B:306:LEU:HB3	1.92	0.50
7:G:108:VAL:HG22	7:G:159:ALA:HB3	1.91	0.50
14:N:17:DG:H2''	14:N:18:DC:C5	2.47	0.50
15:T:59:DA:P	16:c:65:LEU:HD22	2.51	0.50
15:T:70:DA:H2'	15:T:71:DA:H8	1.77	0.50
6:F:97:ARG:O	6:F:101:ILE:HG22	2.10	0.50
14:N:-64:DC:H2''	14:N:-63:DT:C5	2.47	0.50
16:a:100:LEU:O	16:a:104:PHE:HB2	2.11	0.50
1:A:338:ARG:HH21	1:A:840:ARG:NE	2.09	0.50
1:A:533:ARG:HD3	1:A:750:ALA:HB2	1.94	0.50
2:B:245:MET:HE2	2:B:374:MET:HE3	1.93	0.50
2:B:300:TRP:CD1	2:B:300:TRP:N	2.79	0.50
16:c:116:ARG:CZ	16:c:120:MET:HE1	2.42	0.50
1:A:727:ARG:HD3	1:A:767:GLY:HA3	1.94	0.50
11:K:91:CYS:O	11:K:95:ILE:HG22	2.12	0.50
15:T:-8:DA:H2''	15:T:-7:DA:N7	2.27	0.50
16:g:101:VAL:O	16:g:105:GLU:HG2	2.11	0.50
14:N:-58:DC:H4'	14:N:-57:DG:OP1	2.12	0.50
14:N:15:DG:H2''	14:N:16:DT:H71	1.94	0.50
15:T:81:DC:H2'	15:T:82:DG:C8	2.47	0.50
2:B:837:ASP:O	2:B:988:GLY:HA3	2.11	0.50
2:B:46:ILE:O	2:B:50:VAL:HG22	2.12	0.49
2:B:678:TRP:HA	2:B:681:LEU:HB2	1.94	0.49
17:b:29:ILE:HD11	17:b:55:ARG:HG2	1.94	0.49
16:e:121:PRO:O	16:e:124:ILE:HG13	2.12	0.49
16:e:121:PRO:HG3	17:f:53:GLU:OE2	2.12	0.49
17:f:64:ASN:O	17:f:67:ARG:HG2	2.11	0.49
16:g:119:ILE:O	17:h:50:ILE:HD11	2.11	0.49
1:A:718:GLU:HG3	1:A:721:ARG:HH21	1.77	0.49
2:B:511:HIS:HB3	2:B:515:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-23:DT:C6	14:N:-22:DT:H72	2.47	0.49
1:A:108:MET:HE3	1:A:108:MET:HA	1.94	0.49
2:B:83:TYR:HB2	2:B:116:TYR:HB2	1.94	0.49
2:B:369:PHE:HD1	2:B:559:LEU:HD22	1.77	0.49
3:C:48:VAL:CG1	12:L:69:PHE:HB2	2.43	0.49
11:K:107:GLU:O	11:K:111:ILE:HG12	2.13	0.49
12:L:57:VAL:O	12:L:58:ILE:CD1	2.57	0.49
1:A:606:MET:HE1	1:A:618:VAL:HG22	1.93	0.49
6:F:125:LEU:HD22	6:F:130:ILE:HG12	1.92	0.49
14:N:1:DC:H2''	14:N:2:DG:H5'	1.93	0.49
5:E:63:PRO:HB3	5:E:74:LEU:HD23	1.94	0.49
11:K:26:ARG:HH21	11:K:74:ARG:NH2	2.11	0.49
14:N:-66:DT:H2'	14:N:-65:DT:H71	1.94	0.49
17:d:33:ALA:HA	17:d:36:ARG:NE	2.27	0.49
16:e:75:ALA:HB1	16:e:82:LEU:HD21	1.93	0.49
16:g:63:ARG:HH11	17:h:36:ARG:HH22	1.60	0.49
17:h:34:ILE:HA	17:h:37:LEU:HD12	1.95	0.49
1:A:48:PRO:HG2	1:A:54:ASN:HB3	1.94	0.49
1:A:570:LYS:HD3	8:H:46:MET:HE1	1.94	0.49
14:N:-1:DT:H2'	14:N:0:DA:H8	1.74	0.49
14:N:37:DA:H2''	14:N:38:DT:C7	2.42	0.49
2:B:377:ARG:HH21	2:B:386:LYS:HZ1	1.60	0.49
2:B:900:ALA:HA	12:L:60:LYS:HD2	1.94	0.49
11:K:6:ARG:HE	11:K:9:LEU:HD11	1.78	0.49
17:b:92:ARG:NH1	17:h:67:ARG:HH21	2.10	0.49
16:e:62:ILE:HG23	16:e:93:GLN:HE21	1.78	0.49
16:e:129:ARG:HD2	16:e:130:ILE:N	2.27	0.49
2:B:79:PHE:HB3	2:B:117:LEU:HD11	1.94	0.49
14:N:-3:DC:OP2	16:g:86:SER:HB3	2.12	0.49
17:f:61:PHE:O	17:f:65:VAL:HG22	2.13	0.49
2:B:261:ILE:HB	2:B:274:ILE:HD11	1.95	0.49
3:C:22:SER:HB2	3:C:227:ARG:HD2	1.94	0.49
16:g:101:VAL:HA	16:g:104:PHE:CD1	2.47	0.49
1:A:472:ASN:O	1:A:475:VAL:HG22	2.12	0.49
15:T:71:DA:H2'	15:T:72:DC:C6	2.48	0.49
1:A:391:GLU:HG2	1:A:394:ARG:HH21	1.78	0.48
14:N:3:DT:H2''	14:N:4:DG:C8	2.48	0.48
1:A:527:ASP:OD1	2:B:829:CYS:SG	2.72	0.48
1:A:1263:LEU:HD23	1:A:1264:LYS:HD2	1.96	0.48
7:G:122:ASN:HB3	7:G:131:MET:HE3	1.95	0.48
11:K:77:THR:HG21	11:K:83:PRO:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-95:DT:H3	15:T:94:DA:H61	1.61	0.48
15:T:37:DA:H2''	15:T:38:DA:C8	2.47	0.48
15:T:68:DA:H4'	15:T:69:DA:O5'	2.12	0.48
17:b:36:ARG:O	17:b:40:ARG:HG2	2.12	0.48
1:A:113:LEU:HD12	1:A:114:LEU:N	2.28	0.48
8:H:12:VAL:HG12	8:H:53:ASP:H	1.78	0.48
17:b:32:PRO:HA	17:b:35:ARG:CG	2.38	0.48
17:h:31:LYS:HB3	17:h:51:TYR:CD2	2.48	0.48
1:A:599:LEU:HG	8:H:25:ARG:HH12	1.77	0.48
1:A:882:GLN:OE1	1:A:961:ASN:HA	2.13	0.48
2:B:302:MET:HA	2:B:305:MET:SD	2.53	0.48
1:A:327:ARG:HG2	1:A:327:ARG:HH11	1.79	0.48
1:A:385:ASN:O	1:A:389:LEU:HD12	2.14	0.48
1:A:1216:ASP:O	1:A:1220:GLU:HG2	2.14	0.48
2:B:75:TYR:CD2	2:B:123:MET:HE1	2.48	0.48
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.49	0.48
6:F:128:ARG:HD2	6:F:149:ASP:O	2.13	0.48
14:N:41:DA:H4'	14:N:42:DG:OP1	2.13	0.48
15:T:16:DC:H2''	15:T:17:DG:C8	2.49	0.48
17:d:88:TYR:OH	17:h:59:LYS:NZ	2.47	0.48
16:g:125:GLN:HA	16:g:128:ARG:HG2	1.96	0.48
1:A:538:ARG:HB3	8:H:20:TYR:CE2	2.35	0.48
4:D:36:LEU:HD12	4:D:36:LEU:H	1.78	0.48
15:T:52:DA:H2''	15:T:53:DG:C8	2.48	0.48
17:d:90:LEU:HD12	17:d:91:LYS:N	2.28	0.48
16:g:104:PHE:HA	16:g:107:THR:HG22	1.96	0.48
1:A:237:ILE:HD13	2:B:1211:ASN:HD22	1.79	0.48
1:A:362:LEU:HD11	1:A:522:MET:SD	2.53	0.48
1:A:394:ARG:HB2	1:A:394:ARG:CZ	2.43	0.48
6:F:79:ARG:HD2	6:F:146:TRP:NE1	2.29	0.48
14:N:-24:DG:H2''	14:N:-23:DT:H73	1.94	0.48
1:A:394:ARG:HB2	1:A:394:ARG:NH1	2.28	0.48
8:H:91:ASP:HB2	8:H:144:ARG:HH22	1.79	0.48
10:J:8:PHE:HB2	10:J:47:ARG:HH22	1.79	0.48
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.96	0.48
16:e:109:LEU:HD22	16:g:129:ARG:HH12	1.79	0.48
1:A:97:PRO:O	1:A:101:LYS:HG2	2.12	0.48
1:A:1130:ILE:HD13	1:A:1307:TRP:CE2	2.49	0.48
1:A:1439:MET:SD	2:B:1144:ALA:HB2	2.53	0.48
2:B:291:GLN:NE2	2:B:564:PRO:HD2	2.28	0.48
2:B:586:PRO:O	2:B:590:VAL:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:-15:DC:H1'	14:N:-14:DG:O4'	2.13	0.48
16:c:90:MET:HA	16:c:90:MET:HE2	1.96	0.48
1:A:861:LEU:HD21	1:A:1397:THR:HA	1.95	0.47
1:A:1270:MET:SD	1:A:1274:ILE:HD11	2.54	0.47
2:B:348:ILE:HG23	2:B:349:LEU:HD12	1.96	0.47
2:B:568:THR:HG23	2:B:569:LYS:HD3	1.96	0.47
14:N:-26:DC:H2''	14:N:-25:DG:C8	2.48	0.47
17:d:33:ALA:HA	17:d:36:ARG:HE	1.78	0.47
16:e:128:ARG:HG3	16:e:133:GLU:HB2	1.96	0.47
1:A:203:LEU:HB3	1:A:208:ILE:HD11	1.95	0.47
1:A:281:GLU:HG3	1:A:282:MET:HE2	1.95	0.47
2:B:613:ARG:HA	2:B:613:ARG:NE	2.29	0.47
2:B:1201:LYS:HE3	2:B:1201:LYS:HB3	1.74	0.47
6:F:144:GLU:HG3	6:F:146:TRP:HD1	1.78	0.47
7:G:89:ALA:HB2	7:G:103:VAL:HG22	1.96	0.47
17:f:69:ALA:O	17:f:73:THR:HG23	2.14	0.47
1:A:45:ARG:HG2	1:A:46:GLN:OE1	2.14	0.47
2:B:911:ILE:HD11	2:B:941:LEU:HB2	1.95	0.47
17:h:47:SER:N	17:h:50:ILE:HD12	2.21	0.47
1:A:1190:GLN:HB2	1:A:1243:ARG:HH11	1.79	0.47
2:B:250:TYR:HB2	2:B:260:THR:O	2.13	0.47
9:I:97:MET:HE3	9:I:97:MET:HB3	1.64	0.47
15:T:13:DC:H1'	15:T:14:DC:C2	2.49	0.47
16:c:121:PRO:HD3	17:d:50:ILE:HG12	1.96	0.47
4:D:55:GLU:O	4:D:59:LEU:HG	2.13	0.47
14:N:-7:DA:H2''	14:N:-6:DG:C8	2.49	0.47
16:e:118:THR:HG22	17:f:45:ARG:HB3	1.96	0.47
17:f:38:ALA:HB3	17:f:46:ILE:HD13	1.96	0.47
1:A:1335:PHE:HA	1:A:1338:ILE:HB	1.94	0.47
5:E:28:PHE:HB2	5:E:64:THR:HG22	1.96	0.47
13:P:5:C:H2'	13:P:6:G:H8	1.78	0.47
15:T:64:DG:H2''	15:T:65:DA:C8	2.49	0.47
17:f:66:ILE:O	17:f:70:VAL:HG23	2.15	0.47
1:A:549:ASN:HD21	11:K:47:ARG:HH11	1.63	0.47
1:A:1029:ALA:O	1:A:1033:ILE:HG22	2.13	0.47
1:A:1046:TRP:O	1:A:1050:THR:HG23	2.15	0.47
2:B:202:VAL:HG21	2:B:488:LEU:HD23	1.96	0.47
2:B:225:ILE:HD12	2:B:248:LYS:HD3	1.93	0.47
2:B:563:ASP:HB3	2:B:566:GLN:HG2	1.96	0.47
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.96	0.47
3:C:251:LEU:HD22	11:K:98:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:255:LEU:HD21	11:K:94:ILE:HB	1.97	0.47
16:g:65:LEU:HD23	16:g:68:GLN:NE2	2.29	0.47
16:g:82:LEU:HD11	17:h:81:VAL:HG23	1.97	0.47
16:g:124:ILE:HD12	17:h:57:VAL:HG21	1.97	0.47
17:h:87:VAL:O	17:h:91:LYS:HG2	2.15	0.47
1:A:365:VAL:HG21	1:A:445:PHE:CE1	2.50	0.47
1:A:1222:PHE:HB3	1:A:1226:LEU:HB2	1.95	0.47
2:B:345:ALA:HA	2:B:348:ILE:HG22	1.97	0.47
3:C:11:ASN:HB3	3:C:13:GLN:NE2	2.29	0.47
7:G:121:TYR:HB2	7:G:130:TYR:CZ	2.49	0.47
16:g:119:ILE:HG13	17:h:50:ILE:HD13	1.97	0.47
17:h:84:MET:HA	17:h:87:VAL:HG22	1.97	0.47
5:E:96:CYS:SG	5:E:126:VAL:HG21	2.54	0.47
1:A:498:THR:HG22	2:B:1146:PHE:HA	1.96	0.47
1:A:766:VAL:HB	1:A:801:VAL:CG2	2.45	0.47
16:g:78:PHE:CZ	17:h:67:ARG:HG2	2.49	0.47
1:A:112:LYS:HB3	1:A:165:ARG:HH22	1.78	0.46
1:A:1061:HIS:ND1	6:F:87:LYS:HG2	2.31	0.46
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.98	0.46
8:H:89:ALA:HB1	8:H:95:VAL:HG21	1.97	0.46
13:P:6:G:H2'	13:P:7:U:H6	1.78	0.46
14:N:49:DC:H2''	14:N:50:DG:H8	1.79	0.46
17:d:63:GLU:O	17:d:67:ARG:HG3	2.14	0.46
1:A:40:ILE:HD12	1:A:40:ILE:H	1.79	0.46
1:A:342:MET:HE3	1:A:342:MET:HB3	1.84	0.46
1:A:452:HIS:HD2	1:A:1076:GLU:HG3	1.80	0.46
1:A:952:GLY:HA3	1:A:1301:TYR:CE1	2.50	0.46
1:A:1218:ILE:HD13	1:A:1274:ILE:HD13	1.97	0.46
3:C:96:VAL:HB	3:C:159:ALA:HB3	1.96	0.46
15:T:62:DC:H2''	15:T:63:DA:O4'	2.14	0.46
1:A:180:MET:CE	1:A:298:GLN:HG3	2.45	0.46
1:A:333:LYS:HA	1:A:338:ARG:NH1	2.31	0.46
1:A:700:HIS:HE1	9:I:112:ASP:HB3	1.80	0.46
10:J:1:MET:HA	10:J:55:LEU:HB2	1.96	0.46
14:N:-24:DG:H2''	14:N:-23:DT:C7	2.46	0.46
2:B:71:ILE:HG12	2:B:73:LYS:HG3	1.97	0.46
2:B:650:GLU:HA	2:B:653:ARG:HG2	1.96	0.46
3:C:18:GLU:HG3	3:C:231:THR:HG22	1.97	0.46
14:N:49:DC:H2''	14:N:50:DG:C8	2.49	0.46
17:b:51:TYR:O	17:b:54:THR:HG22	2.16	0.46
3:C:52:MET:HE1	3:C:152:GLU:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:128:LEU:HD13	4:D:142:ILE:HG23	1.96	0.46
15:T:35:DT:H2''	15:T:36:DA:C8	2.51	0.46
2:B:242:ILE:HG21	2:B:355:PRO:HG3	1.98	0.46
10:J:1:MET:HE3	10:J:59:PHE:HE2	1.81	0.46
13:P:1:U:H3'	13:P:2:G:H8	1.80	0.46
14:N:4:DG:H4'	14:N:5:DC:OP1	2.15	0.46
1:A:850:MET:HE3	1:A:1063:GLY:HA2	1.97	0.46
1:A:1131:GLU:HA	1:A:1134:LYS:HE2	1.98	0.46
2:B:275:VAL:HG21	2:B:310:ILE:HA	1.98	0.46
3:C:24:VAL:HG11	3:C:28:LEU:HD22	1.98	0.46
4:D:57:ARG:HA	4:D:109:LEU:HD13	1.98	0.46
8:H:91:ASP:HB2	8:H:144:ARG:NH2	2.30	0.46
15:T:67:DA:H2'	15:T:68:DA:C8	2.51	0.46
16:a:119:ILE:HD11	17:b:46:ILE:HG23	1.98	0.46
1:A:688:LYS:O	1:A:691:VAL:HG12	2.15	0.46
2:B:1010:LEU:HA	2:B:1010:LEU:HD23	1.71	0.46
14:N:-36:DT:H2''	14:N:-35:DA:C8	2.51	0.46
14:N:-24:DG:H3'	16:a:65:LEU:HB2	1.96	0.46
1:A:1193:TRP:HD1	1:A:1259:GLU:HB2	1.81	0.46
1:A:1203:ARG:CZ	1:A:1207:LYS:HD3	2.46	0.46
1:A:1204:MET:HA	1:A:1207:LYS:NZ	2.30	0.46
2:B:245:MET:SD	2:B:247:ILE:HG13	2.56	0.46
17:b:36:ARG:HA	17:b:39:ARG:HD2	1.98	0.46
1:A:11:LEU:CD1	2:B:1193:GLN:HE21	2.28	0.46
1:A:1203:ARG:HH11	1:A:1206:ASP:HB3	1.81	0.46
2:B:207:GLU:OE2	2:B:530:LYS:NZ	2.49	0.46
2:B:225:ILE:CD1	2:B:248:LYS:CD	2.87	0.46
2:B:345:ALA:O	2:B:349:LEU:HD13	2.16	0.46
2:B:841:MET:SD	2:B:846:ILE:HD11	2.56	0.46
3:C:142:ILE:HD12	3:C:142:ILE:N	2.31	0.46
10:J:1:MET:HA	10:J:55:LEU:H	1.81	0.46
14:N:-47:DT:H2''	14:N:-46:DC:C5	2.51	0.46
14:N:-46:DC:H2''	14:N:-45:DT:C5	2.50	0.46
14:N:52:DC:H2''	14:N:53:DA:C8	2.50	0.46
1:A:692:GLN:O	1:A:695:ILE:HG22	2.16	0.45
2:B:377:ARG:HG3	2:B:377:ARG:HH11	1.81	0.45
6:F:97:ARG:HA	6:F:100:GLN:HG2	1.98	0.45
7:G:23:ASN:HA	7:G:26:LEU:HD12	1.97	0.45
7:G:30:LEU:HD21	7:G:48:VAL:HG11	1.97	0.45
16:a:110:CYS:SG	16:a:126:LEU:HD21	2.56	0.45
17:h:68:ASP:OD2	17:h:92:ARG:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:h:78:ARG:NE	17:h:78:ARG:HA	2.31	0.45
1:A:452:HIS:CD2	1:A:1076:GLU:HG3	2.50	0.45
2:B:1164:GLY:HA3	2:B:1190:ASN:HB3	1.98	0.45
15:T:45:DA:H2''	15:T:46:DG:N7	2.31	0.45
1:A:16:GLU:OE2	2:B:1220:ARG:HA	2.16	0.45
1:A:391:GLU:HA	1:A:394:ARG:NE	2.31	0.45
1:A:1116:PRO:HB2	1:A:1314:ILE:HG23	1.98	0.45
2:B:608:ILE:HD12	2:B:619:ILE:HG12	1.97	0.45
7:G:4:LEU:HD23	7:G:4:LEU:HA	1.83	0.45
8:H:47:PHE:CD2	8:H:94:TYR:HB2	2.51	0.45
11:K:20:LYS:C	11:K:20:LYS:HD2	2.42	0.45
17:d:50:ILE:HG22	17:d:54:THR:HG23	1.96	0.45
1:A:237:ILE:HD11	1:A:239:VAL:O	2.16	0.45
1:A:317:GLN:OE1	1:A:321:ARG:HB2	2.15	0.45
2:B:225:ILE:HD11	2:B:248:LYS:CD	2.43	0.45
17:b:88:TYR:HA	17:b:91:LYS:HG2	1.98	0.45
17:f:50:ILE:HA	17:f:53:GLU:OE2	2.16	0.45
1:A:337:LEU:HD12	1:A:337:LEU:H	1.81	0.45
1:A:1126:ILE:CD1	1:A:1136:ILE:HD11	2.47	0.45
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	1.99	0.45
3:C:10:ILE:HD11	3:C:20:MET:HB2	1.97	0.45
3:C:148:ARG:NH2	10:J:64:PRO:HD3	2.31	0.45
11:K:33:ILE:HD11	11:K:35:PHE:HE1	1.76	0.45
17:b:53:GLU:O	17:b:57:VAL:HG22	2.16	0.45
17:d:91:LYS:HD2	17:d:91:LYS:HA	1.81	0.45
16:e:88:ALA:O	16:e:92:LEU:HD23	2.17	0.45
1:A:900:VAL:CG2	1:A:930:LEU:HD13	2.46	0.45
2:B:25:PHE:CZ	2:B:534:LEU:HD11	2.52	0.45
2:B:409:LEU:HD21	2:B:453:SER:HB2	1.99	0.45
2:B:844:SER:HB3	2:B:848:ARG:NH1	2.32	0.45
2:B:856:PHE:CE1	2:B:969:ARG:HG3	2.52	0.45
6:F:93:ILE:HD12	6:F:134:ILE:HD11	1.99	0.45
13:P:2:G:H2'	13:P:3:G:C8	2.51	0.45
1:A:730:ALA:HB1	1:A:764:ALA:HB1	1.98	0.45
2:B:358:THR:OG1	2:B:360:GLU:HG2	2.17	0.45
6:F:85:LEU:CD1	6:F:89:GLU:CG	2.95	0.45
11:K:21:ILE:HD13	11:K:33:ILE:HG22	1.98	0.45
1:A:454:MET:HE3	1:A:521:VAL:HG21	1.99	0.45
1:A:1038:ARG:HE	1:A:1038:ARG:HB2	1.58	0.45
2:B:120:GLU:OE1	2:B:122:SER:HB3	2.16	0.45
2:B:249:LEU:HA	2:B:261:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:HB2	2:B:1211:ASN:OD1	2.17	0.45
2:B:78:ARG:HB2	2:B:120:GLU:OE2	2.17	0.45
2:B:1072:MET:HE1	2:B:1087:PHE:CE1	2.52	0.45
6:F:85:LEU:HD13	6:F:151:LEU:HD22	1.98	0.45
8:H:61:ASN:OD1	8:H:136:GLN:HG2	2.17	0.45
12:L:67:ILE:N	12:L:67:ILE:HD12	2.32	0.45
15:T:-10:DT:H6	15:T:-10:DT:H2'	1.68	0.45
16:g:119:ILE:HG13	17:h:50:ILE:CD1	2.47	0.45
2:B:301:GLN:O	2:B:304:GLU:HB3	2.17	0.45
2:B:337:ARG:HA	2:B:337:ARG:CZ	2.47	0.45
2:B:974:PRO:HB3	2:B:980:PHE:HZ	1.82	0.45
15:T:-44:DC:H2''	15:T:-43:DG:C8	2.52	0.45
15:T:2:DC:H2''	15:T:3:DG:OP2	2.16	0.45
17:d:36:ARG:HA	17:d:39:ARG:NE	2.25	0.45
1:A:298:GLN:HA	1:A:298:GLN:OE1	2.17	0.44
1:A:1406:GLU:HG2	15:T:74:DA:H5''	1.99	0.44
2:B:280:ALA:HA	2:B:319:LYS:HG3	1.98	0.44
2:B:986:GLN:HE21	2:B:1022:THR:HG21	1.81	0.44
5:E:49:MET:H	5:E:49:MET:CE	2.27	0.44
6:F:85:LEU:HD11	6:F:89:GLU:CG	2.43	0.44
15:T:-19:DA:H2''	15:T:-18:DG:C8	2.52	0.44
17:d:32:PRO:HA	17:d:35:ARG:NH1	2.31	0.44
1:A:703:LEU:HD12	1:A:704:GLU:N	2.33	0.44
2:B:250:TYR:HE2	2:B:262:LYS:HB3	1.81	0.44
2:B:710:ARG:NH2	2:B:727:LYS:HB2	2.33	0.44
8:H:6:PHE:HB3	8:H:59:LEU:HB2	2.00	0.44
12:L:50:CYS:HB3	12:L:55:HIS:N	2.32	0.44
14:N:50:DG:H2''	14:N:51:DG:C8	2.53	0.44
1:A:799:GLY:HA2	1:A:816:PHE:CD2	2.52	0.44
1:A:1333:ASN:HB2	1:A:1354:GLU:OE2	2.17	0.44
1:A:1381:ARG:HE	1:A:1381:ARG:HB2	1.60	0.44
2:B:534:LEU:HD23	2:B:747:MET:SD	2.57	0.44
2:B:954:LEU:HD12	2:B:963:PHE:O	2.18	0.44
7:G:51:GLY:HA2	7:G:54:ILE:HD11	1.99	0.44
16:a:61:LEU:HD13	17:b:40:ARG:NH1	2.32	0.44
16:a:122:LYS:O	16:a:125:GLN:HG3	2.16	0.44
17:d:61:PHE:CD1	17:d:62:LEU:HD23	2.52	0.44
16:e:97:GLU:O	16:e:101:VAL:HG13	2.17	0.44
1:A:88:LYS:HD3	1:A:294:GLU:OE2	2.18	0.44
1:A:694:ILE:HA	1:A:697:LYS:HZ2	1.83	0.44
1:A:1227:PHE:CZ	1:A:1229:MET:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:384:GLU:HG3	9:I:91:ARG:NE	2.32	0.44
7:G:49:LEU:HD12	7:G:75:ARG:HG2	1.99	0.44
12:L:48:VAL:C	12:L:49:ARG:HD3	2.42	0.44
14:N:-74:DT:H6	14:N:-74:DT:H5'	1.82	0.44
14:N:-16:DG:H2''	14:N:-15:DC:C5	2.53	0.44
16:a:104:PHE:CD1	17:b:41:GLY:HA3	2.52	0.44
1:A:841:ARG:HH22	1:A:1108:ASN:ND2	2.15	0.44
2:B:276:ILE:HG13	2:B:316:ILE:HG12	2.00	0.44
5:E:152:HIS:CE1	5:E:183:VAL:HG11	2.52	0.44
1:A:113:LEU:HD11	1:A:142:CYS:SG	2.57	0.44
1:A:136:ASN:O	1:A:140:GLN:HG2	2.17	0.44
1:A:290:ILE:H	1:A:290:ILE:HG13	1.67	0.44
1:A:548:MET:CE	11:K:59:VAL:H	2.29	0.44
2:B:166:ARG:HH12	2:B:189:ASP:C	2.25	0.44
15:T:11:DC:H2''	15:T:12:DC:C5	2.53	0.44
17:h:67:ARG:O	17:h:71:THR:HG23	2.17	0.44
1:A:15:LYS:HB3	2:B:1220:ARG:NH1	2.33	0.44
1:A:131:PRO:HA	1:A:134:ARG:HD2	1.98	0.44
1:A:327:ARG:HH12	1:A:331:LYS:HZ2	1.65	0.44
2:B:38:PHE:HB2	2:B:164:MET:HE3	2.00	0.44
2:B:588:MET:HE3	2:B:588:MET:HB3	1.83	0.44
2:B:608:ILE:HG23	2:B:608:ILE:O	2.17	0.44
2:B:745:PRO:HB2	2:B:1047:PHE:CD2	2.52	0.44
2:B:953:LEU:HD21	2:B:955:THR:HG23	2.00	0.44
4:D:113:ALA:HB3	4:D:116:LYS:HZ3	1.82	0.44
17:h:84:MET:N	17:h:84:MET:HE2	2.32	0.44
1:A:1291:LYS:HG2	1:A:1305:GLU:HG2	2.00	0.44
2:B:64:HIS:H	2:B:66:ASN:ND2	2.15	0.44
15:T:-38:DA:H2''	15:T:-37:DT:C6	2.53	0.44
16:a:61:LEU:HB3	17:b:40:ARG:NH2	2.32	0.44
1:A:914:ILE:HG13	1:A:914:ILE:O	2.18	0.44
1:A:1193:TRP:CD1	1:A:1259:GLU:HB2	2.53	0.44
1:A:1386:ALA:O	1:A:1391:GLY:HA3	2.17	0.44
2:B:186:CYS:HB3	2:B:189:ASP:HB2	2.00	0.44
2:B:1036:SER:OG	10:J:43:TYR:HB2	2.18	0.44
4:D:101:VAL:HG13	7:G:105:PRO:HG3	1.99	0.44
12:L:31:TYR:HB3	12:L:58:ILE:CG2	2.48	0.44
15:T:-4:DC:H2'	16:g:65:LEU:HD12	1.99	0.44
2:B:231:ILE:HG22	2:B:245:MET:HE3	2.00	0.43
2:B:852:ARG:HH21	2:B:973:VAL:HG11	1.83	0.43
11:K:73:MET:HE3	11:K:73:MET:HB2	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:93:DA:H2"	15:T:94:DA:H8	1.83	0.43
16:e:73:GLU:OE1	17:f:25:ASN:HB2	2.18	0.43
17:f:51:TYR:CE1	17:f:52:GLU:HG2	2.53	0.43
16:g:80:THR:O	16:g:80:THR:CG2	2.66	0.43
1:A:90:VAL:HB	1:A:298:GLN:OE1	2.17	0.43
1:A:536:THR:HG21	1:A:579:LEU:HD22	2.00	0.43
1:A:843:VAL:HG11	2:B:1136:ASP:OD2	2.18	0.43
1:A:1074:ILE:HD13	1:A:1374:LEU:HD22	2.01	0.43
1:A:1132:LYS:HD3	1:A:1132:LYS:N	2.33	0.43
2:B:272:ILE:HG21	2:B:326:ILE:HG22	1.99	0.43
2:B:357:ILE:HG23	2:B:358:THR:N	2.33	0.43
16:e:61:LEU:HD22	17:f:40:ARG:HD3	1.98	0.43
3:C:61:PHE:HE1	3:C:65:ARG:HD2	1.84	0.43
3:C:100:LEU:HD22	3:C:155:ILE:HD11	2.00	0.43
17:f:53:GLU:O	17:f:57:VAL:HG23	2.19	0.43
1:A:252:ALA:HA	1:A:258:GLN:HA	2.00	0.43
1:A:336:ARG:O	1:A:341:LEU:HD23	2.18	0.43
2:B:508:HIS:ND1	2:B:510:THR:HG23	2.32	0.43
7:G:10:ILE:C	7:G:11:LEU:HD23	2.43	0.43
15:T:-38:DA:H2"	15:T:-37:DT:C5	2.53	0.43
16:c:70:LEU:HD23	16:c:70:LEU:HA	1.80	0.43
2:B:290:LEU:HD22	2:B:306:LEU:HD21	1.99	0.43
2:B:835:GLN:HA	2:B:1013:ASN:ND2	2.34	0.43
2:B:1082:MET:HE2	2:B:1082:MET:HB2	1.83	0.43
14:N:-91:DG:H2"	14:N:-90:DG:C8	2.53	0.43
15:T:4:DC:H2"	15:T:5:DG:N7	2.33	0.43
15:T:7:DT:C2	15:T:8:DG:N7	2.86	0.43
16:a:104:PHE:CZ	17:b:38:ALA:HA	2.53	0.43
17:b:37:LEU:HA	17:b:40:ARG:CZ	2.48	0.43
17:b:61:PHE:CD1	17:b:61:PHE:C	2.96	0.43
17:b:88:TYR:HE1	17:h:75:HIS:HA	1.83	0.43
16:c:66:PRO:HG3	16:c:69:ARG:HH21	1.84	0.43
1:A:1142:TYR:HB3	1:A:1282:ILE:O	2.19	0.43
2:B:79:PHE:HB3	2:B:117:LEU:HD21	2.00	0.43
2:B:500:LYS:H	2:B:500:LYS:HD2	1.83	0.43
9:I:59:VAL:N	9:I:62:ILE:HD11	2.30	0.43
14:N:-37:DT:H2"	14:N:-36:DT:C6	2.54	0.43
15:T:-9:DA:H2"	15:T:-8:DA:N7	2.33	0.43
17:f:50:ILE:HD12	17:f:53:GLU:OE2	2.18	0.43
16:g:74:ILE:HG21	17:h:66:ILE:HG21	2.00	0.43
1:A:15:LYS:HE2	2:B:1220:ARG:HH12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:LEU:HB3	1:A:787:HIS:HD2	1.83	0.43
2:B:42:MET:HE3	2:B:163:ILE:HD13	2.01	0.43
2:B:123:MET:HA	2:B:123:MET:HE2	2.00	0.43
2:B:320:GLU:H	2:B:320:GLU:CD	2.27	0.43
2:B:797:TYR:CD2	2:B:852:ARG:HB2	2.53	0.43
7:G:23:ASN:O	7:G:27:ARG:HD2	2.18	0.43
10:J:31:GLU:O	10:J:35:LEU:HD12	2.19	0.43
14:N:-71:DT:C6	14:N:-70:DT:H72	2.53	0.43
15:T:90:DC:H2''	15:T:91:DC:C5	2.53	0.43
16:g:78:PHE:HE2	17:h:66:ILE:HG23	1.84	0.43
1:A:446:ASN:HD22	1:A:447:ARG:N	2.16	0.43
4:D:97:VAL:O	4:D:101:VAL:HG23	2.19	0.43
15:T:17:DG:C8	15:T:17:DG:H5'	2.54	0.43
17:d:40:ARG:HG2	17:d:40:ARG:H	1.61	0.43
1:A:1389:ARG:HB3	1:A:1406:GLU:OE1	2.19	0.43
1:A:1447:MET:HE2	7:G:58:LYS:HB3	2.01	0.43
2:B:249:LEU:HA	2:B:261:ILE:CD1	2.48	0.43
2:B:530:LYS:HE3	2:B:530:LYS:HB2	1.77	0.43
2:B:904:ARG:NH2	2:B:948:ILE:HD11	2.34	0.43
2:B:1133:MET:HE3	2:B:1133:MET:HB2	1.84	0.43
8:H:12:VAL:HG13	8:H:52:ASP:H	1.84	0.43
16:c:101:VAL:HA	16:c:104:PHE:CD2	2.54	0.43
1:A:240:LEU:HD21	1:A:304:TYR:CE2	2.53	0.43
1:A:1428:SER:HA	1:A:1431:VAL:HG12	2.00	0.43
2:B:614:GLU:HA	2:B:614:GLU:OE2	2.19	0.43
2:B:1142:GLY:HA3	6:F:88:TYR:HE2	1.84	0.43
3:C:20:MET:SD	3:C:22:SER:HB3	2.58	0.43
3:C:142:ILE:HG23	10:J:15:GLY:HA3	2.01	0.43
9:I:4:PHE:CD1	9:I:4:PHE:N	2.86	0.43
9:I:14:LEU:HD12	9:I:15:TYR:H	1.84	0.43
15:T:-26:DC:H2''	15:T:-25:DA:C8	2.54	0.43
15:T:-14:DC:H2''	15:T:-13:DG:C8	2.54	0.43
16:g:62:ILE:HD11	17:h:37:LEU:HD11	2.00	0.43
1:A:1154:ILE:HD11	1:A:1193:TRP:HB3	2.01	0.42
9:I:45:ARG:HD2	9:I:47:GLU:HG3	2.01	0.42
11:K:41:THR:CG2	11:K:42:LEU:N	2.82	0.42
1:A:456:MET:HE2	1:A:456:MET:HB2	1.92	0.42
1:A:1130:ILE:HD12	1:A:1130:ILE:HA	1.91	0.42
1:A:1190:GLN:HB2	1:A:1243:ARG:HD2	2.01	0.42
1:A:1453:LEU:HD23	1:A:1456:LEU:HD12	1.99	0.42
2:B:910:ILE:HD11	2:B:912:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:-39:DA:H2''	15:T:-38:DA:N7	2.34	0.42
15:T:22:DA:H2''	15:T:23:DA:C8	2.54	0.42
16:e:126:LEU:HA	16:e:129:ARG:HG3	2.01	0.42
1:A:336:ARG:HD3	1:A:336:ARG:HA	1.87	0.42
1:A:548:MET:HG2	11:K:58:PHE:CE1	2.55	0.42
1:A:1031:ARG:HD2	1:A:1035:GLU:OE2	2.19	0.42
1:A:1104:LYS:O	1:A:1108:ASN:HB2	2.18	0.42
1:A:1109:VAL:HB	1:A:1386:ALA:HB2	2.00	0.42
1:A:1114:LYS:HD3	1:A:1114:LYS:HA	1.88	0.42
2:B:56:LEU:HD11	2:B:418:THR:HG23	2.01	0.42
2:B:797:TYR:HE1	2:B:854:LEU:HG	1.82	0.42
16:g:126:LEU:HD23	16:g:129:ARG:HH22	1.84	0.42
2:B:18:TRP:CZ2	2:B:807:GLN:HB3	2.55	0.42
2:B:112:SER:OG	2:B:160:LYS:HB3	2.18	0.42
3:C:142:ILE:HD12	3:C:142:ILE:H	1.84	0.42
15:T:59:DA:H2''	15:T:60:DG:N7	2.35	0.42
17:f:35:ARG:O	17:f:39:ARG:HG2	2.19	0.42
1:A:266:LYS:O	1:A:270:ILE:HG12	2.19	0.42
14:N:-50:DG:C8	14:N:-49:DT:H72	2.54	0.42
17:h:32:PRO:O	17:h:36:ARG:HG3	2.19	0.42
1:A:444:LEU:HD22	2:B:1146:PHE:CZ	2.54	0.42
1:A:464:MET:HG3	1:A:470:ARG:HD2	2.01	0.42
2:B:316:ILE:CD1	2:B:321:VAL:HG13	2.49	0.42
2:B:636:ASP:O	2:B:642:LYS:HB2	2.20	0.42
7:G:123:PRO:HA	7:G:128:PRO:HB3	2.01	0.42
11:K:46:LEU:HD23	11:K:46:LEU:HA	1.88	0.42
14:N:-26:DC:H2''	14:N:-25:DG:N7	2.35	0.42
14:N:-24:DG:OP2	16:a:65:LEU:HB3	2.19	0.42
15:T:-53:DT:H2''	15:T:-52:DG:C8	2.55	0.42
15:T:36:DA:H2''	15:T:37:DA:H8	1.84	0.42
17:d:30:THR:HG23	17:d:32:PRO:HD2	2.00	0.42
1:A:15:LYS:HB3	2:B:1220:ARG:HH11	1.85	0.42
2:B:371:LEU:O	2:B:375:VAL:HG12	2.20	0.42
4:D:148:LEU:HD13	4:D:159:LEU:HD22	2.02	0.42
5:E:42:ARG:O	5:E:46:CYS:HB2	2.20	0.42
9:I:14:LEU:HD21	9:I:27:TYR:HB3	2.00	0.42
15:T:52:DA:H2''	15:T:53:DG:H8	1.83	0.42
17:d:71:THR:O	17:d:74:GLU:HG3	2.19	0.42
1:A:368:PRO:HB3	1:A:467:SER:HA	2.00	0.42
1:A:1446:VAL:HG12	7:G:61:ILE:HD13	2.02	0.42
2:B:480:THR:HG23	2:B:483:SER:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:606:VAL:HG23	2:B:621:THR:HG22	2.01	0.42
3:C:74:GLU:HG3	3:C:75:ASP:OD1	2.20	0.42
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.54	0.42
11:K:96:ASN:O	11:K:99:LYS:HG2	2.20	0.42
14:N:-27:DG:H2''	14:N:-26:DC:C6	2.54	0.42
14:N:-5:DC:H1'	14:N:-4:DG:C4	2.55	0.42
16:a:61:LEU:HD22	17:b:40:ARG:NE	2.35	0.42
17:b:57:VAL:O	17:b:60:VAL:HG12	2.20	0.42
16:c:67:PHE:CE1	16:c:93:GLN:HB2	2.55	0.42
17:d:90:LEU:HD12	17:d:90:LEU:C	2.44	0.42
2:B:41:PHE:HA	2:B:45:SER:OG	2.19	0.42
2:B:575:VAL:HG12	2:B:576:ASN:ND2	2.34	0.42
4:D:62:GLU:HA	4:D:65:LYS:HG2	2.01	0.42
6:F:75:LEU:HG	6:F:77:GLU:HG2	2.02	0.42
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.85	0.42
12:L:48:VAL:HG12	12:L:58:ILE:CG1	2.49	0.42
15:T:-14:DC:O3'	17:h:45:ARG:HG3	2.20	0.42
1:A:1159:ASP:HA	1:A:1160:PRO:HD3	1.91	0.42
2:B:25:PHE:HZ	2:B:534:LEU:CD1	2.33	0.42
2:B:291:GLN:OE1	2:B:292:HIS:HD2	2.03	0.42
3:C:37:LEU:HA	3:C:37:LEU:HD23	1.86	0.42
11:K:37:ARG:C	11:K:38:GLU:HG3	2.45	0.42
14:N:17:DG:H2''	14:N:18:DC:H5	1.84	0.42
16:c:62:ILE:N	16:c:62:ILE:HD13	2.35	0.42
17:d:58:LEU:O	17:d:62:LEU:HG	2.20	0.42
1:A:428:GLN:N	1:A:428:GLN:OE1	2.53	0.41
2:B:592:THR:HA	2:B:595:ASP:OD2	2.20	0.41
2:B:995:ARG:HE	11:K:6:ARG:NH2	2.18	0.41
3:C:48:VAL:HG13	3:C:48:VAL:O	2.20	0.41
4:D:39:TYR:CE1	4:D:45:GLU:HG3	2.55	0.41
10:J:3:ILE:HD12	10:J:4:PRO:CD	2.50	0.41
15:T:68:DA:H1'	15:T:69:DA:O4'	2.20	0.41
16:c:127:ALA:O	16:c:131:ARG:HG2	2.19	0.41
2:B:707:LEU:HD23	2:B:707:LEU:HA	1.79	0.41
2:B:841:MET:HA	2:B:1010:LEU:HD23	2.02	0.41
3:C:177:ALA:HB3	3:C:231:THR:OG1	2.19	0.41
14:N:-57:DG:H2''	14:N:-56:DT:H72	2.03	0.41
15:T:-9:DA:H2''	15:T:-8:DA:C8	2.55	0.41
1:A:700:HIS:CE1	9:I:112:ASP:HB3	2.55	0.41
2:B:901:PRO:HG2	12:L:62:ARG:HA	2.02	0.41
2:B:1202:LEU:HG	2:B:1206:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:45:ILE:HD13	5:E:57:MET:HE2	2.01	0.41
16:a:96:CYS:O	16:a:100:LEU:HG	2.20	0.41
16:e:126:LEU:O	16:e:129:ARG:HG3	2.20	0.41
17:h:61:PHE:HE1	17:h:93:GLN:OE1	2.03	0.41
1:A:285:SER:HA	1:A:286:PRO:HD3	1.88	0.41
1:A:363:ASP:HB3	1:A:508:VAL:HB	2.02	0.41
1:A:723:LEU:HA	1:A:723:LEU:HD13	1.77	0.41
1:A:1259:GLU:HA	1:A:1262:MET:SD	2.61	0.41
2:B:519:GLU:OE2	2:B:752:ALA:HB3	2.20	0.41
10:J:41:LYS:HE3	10:J:41:LYS:HB3	1.90	0.41
14:N:-33:DC:H6	14:N:-33:DC:H2'	1.66	0.41
16:g:82:LEU:HD12	17:h:79:LYS:O	2.21	0.41
17:h:35:ARG:O	17:h:39:ARG:HG2	2.19	0.41
1:A:130:ASP:OD1	1:A:133:LYS:HG2	2.20	0.41
1:A:148:CYS:HB3	1:A:170:ASN:O	2.21	0.41
1:A:770:MET:HE3	1:A:770:MET:HA	2.02	0.41
1:A:935:GLU:HA	1:A:938:VAL:HG12	2.01	0.41
1:A:1449:ASP:HB2	6:F:133:VAL:HG23	2.02	0.41
2:B:363:PHE:HB3	2:B:366:ARG:HG3	2.01	0.41
3:C:147:LEU:HD21	3:C:153:LEU:HD12	2.01	0.41
7:G:46:VAL:HB	7:G:77:VAL:CG2	2.51	0.41
16:a:89:VAL:HG12	16:a:90:MET:HE2	2.02	0.41
16:e:129:ARG:HH22	16:g:110:CYS:CA	2.31	0.41
1:A:61:ILE:HD12	1:A:61:ILE:HA	1.84	0.41
1:A:437:LEU:HD12	1:A:437:LEU:HA	1.85	0.41
1:A:872:ASP:OD1	1:A:874:LEU:HB2	2.20	0.41
1:A:1278:GLY:C	1:A:1279:ILE:HD13	2.46	0.41
2:B:18:TRP:CE3	2:B:18:TRP:HA	2.56	0.41
2:B:377:ARG:HH21	2:B:386:LYS:NZ	2.18	0.41
2:B:784:ASN:HB3	10:J:62:TYR:OH	2.20	0.41
5:E:45:ILE:CD1	5:E:57:MET:HE2	2.50	0.41
9:I:8:LEU:HD12	9:I:8:LEU:C	2.45	0.41
10:J:29:LYS:HB3	10:J:29:LYS:HE3	1.80	0.41
11:K:35:PHE:HB3	11:K:38:GLU:OE1	2.20	0.41
14:N:-58:DC:H2''	14:N:-57:DG:C8	2.55	0.41
15:T:7:DT:H2''	15:T:8:DG:C8	2.55	0.41
15:T:64:DG:H2''	15:T:65:DA:H8	1.85	0.41
16:a:122:LYS:HG3	16:c:113:HIS:CE1	2.56	0.41
16:g:103:LEU:HD13	16:g:131:ARG:HH12	1.85	0.41
1:A:1372:ALA:O	1:A:1375:VAL:HG12	2.20	0.41
2:B:57:ILE:HD13	2:B:57:ILE:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:816:GLU:O	2:B:817:LEU:HD22	2.21	0.41
2:B:829:CYS:SG	2:B:1014:PRO:HD2	2.60	0.41
8:H:19:ARG:C	8:H:20:TYR:HD1	2.29	0.41
16:e:71:VAL:HG13	16:e:72:ARG:HE	1.86	0.41
1:A:467:SER:O	1:A:468:THR:HG23	2.20	0.41
2:B:106:LEU:HD23	2:B:106:LEU:HA	1.83	0.41
2:B:300:TRP:CD1	2:B:300:TRP:H	2.39	0.41
2:B:1106:ARG:CZ	2:B:1118:PRO:HB3	2.51	0.41
5:E:90:LYS:H	5:E:90:LYS:HG3	1.74	0.41
5:E:179:ARG:NH2	5:E:191:ARG:HB2	2.35	0.41
5:E:180:GLU:CD	5:E:180:GLU:H	2.29	0.41
14:N:-89:DT:H2''	14:N:-88:DG:C8	2.56	0.41
14:N:-13:DG:H1'	14:N:-12:DG:O4'	2.20	0.41
15:T:24:DC:H4'	15:T:25:DC:H5'	2.02	0.41
17:f:33:ALA:O	17:f:36:ARG:HG3	2.20	0.41
17:h:36:ARG:O	17:h:40:ARG:HG2	2.20	0.41
1:A:26:GLU:O	1:A:30:ILE:HG23	2.20	0.41
1:A:327:ARG:HD2	1:A:1409:VAL:HG11	2.02	0.41
1:A:369:ILE:HG22	1:A:373:LYS:HE2	2.01	0.41
1:A:1285:VAL:HG12	1:A:1311:THR:HG22	2.03	0.41
1:A:1378:MET:HE2	1:A:1378:MET:HB3	1.93	0.41
2:B:73:LYS:HB3	2:B:75:TYR:CE2	2.56	0.41
2:B:102:GLN:OE1	2:B:106:LEU:HG	2.21	0.41
2:B:216:VAL:HG21	2:B:381:CYS:HB2	2.02	0.41
2:B:218:LYS:HB2	2:B:388:GLN:OE1	2.21	0.41
2:B:323:LEU:HB2	2:B:342:ILE:CD1	2.50	0.41
2:B:425:MET:O	2:B:429:ILE:HG13	2.20	0.41
2:B:445:THR:HG23	2:B:446:ILE:H	1.86	0.41
2:B:801:LYS:HG2	10:J:51:THR:O	2.21	0.41
4:D:154:ASP:O	4:D:157:ILE:HG13	2.21	0.41
6:F:103:MET:HB3	7:G:15:PRO:HB2	2.02	0.41
9:I:91:ARG:HE	9:I:91:ARG:HB3	1.74	0.41
10:J:38:LEU:HB2	10:J:40:LEU:HD13	2.03	0.41
14:N:-85:DG:H4'	14:N:-84:DG:OP1	2.20	0.41
14:N:-23:DT:H6	14:N:-23:DT:H2''	1.64	0.41
14:N:27:DT:H2''	14:N:28:DC:C5	2.56	0.41
14:N:47:DC:H2''	14:N:48:DT:C6	2.56	0.41
15:T:-2:DC:H2''	15:T:-1:DG:C8	2.56	0.41
15:T:38:DA:H5''	16:a:118:THR:OG1	2.21	0.41
16:a:60:LEU:HD13	16:a:64:LYS:HD2	2.02	0.41
17:f:63:GLU:HB3	17:f:67:ARG:NH2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:g:99:TYR:HD2	16:g:100:LEU:HD23	1.85	0.41
16:g:104:PHE:O	16:g:108:ASN:HB2	2.21	0.41
1:A:539:ASP:OD1	1:A:539:ASP:C	2.64	0.41
2:B:377:ARG:HG3	2:B:377:ARG:NH1	2.36	0.41
2:B:629:PRO:O	2:B:630:LEU:HD23	2.20	0.41
2:B:719:LEU:HB3	2:B:720:ASN:H	1.60	0.41
7:G:27:ARG:O	7:G:31:LEU:HG	2.20	0.41
11:K:45:LEU:HD21	11:K:94:ILE:HG21	2.03	0.41
15:T:15:DG:H2''	15:T:16:DC:C6	2.56	0.41
16:a:101:VAL:O	16:a:105:GLU:HG2	2.21	0.41
1:A:1152:THR:OG1	9:I:46:HIS:HB3	2.21	0.40
2:B:617:PHE:CD1	2:B:617:PHE:C	2.99	0.40
14:N:-61:DT:H2''	14:N:-60:DC:C5	2.56	0.40
14:N:-58:DC:H2''	14:N:-57:DG:H8	1.85	0.40
15:T:-2:DC:H2''	15:T:-1:DG:H8	1.86	0.40
16:a:63:ARG:HB3	16:a:66:PRO:HD2	2.03	0.40
16:a:125:GLN:HE22	16:a:129:ARG:HH22	1.69	0.40
16:c:65:LEU:O	16:c:69:ARG:HG3	2.21	0.40
16:g:72:ARG:HA	16:g:72:ARG:HD3	1.81	0.40
16:g:114:ALA:O	16:g:115:LYS:HG2	2.20	0.40
17:h:47:SER:HB3	17:h:50:ILE:HG13	2.02	0.40
1:A:391:GLU:CG	1:A:394:ARG:HH21	2.35	0.40
1:A:1314:ILE:HD11	1:A:1337:GLU:HG2	2.03	0.40
1:A:1452:LEU:HD23	6:F:131:PRO:HA	2.04	0.40
2:B:320:GLU:HA	2:B:323:LEU:HD12	2.03	0.40
3:C:262:LEU:HD23	3:C:262:LEU:HA	1.92	0.40
14:N:48:DT:H2''	14:N:49:DC:C6	2.56	0.40
15:T:81:DC:H2'	15:T:82:DG:H8	1.84	0.40
1:A:388:ARG:HA	1:A:391:GLU:OE1	2.21	0.40
1:A:995:LEU:HA	1:A:998:LYS:HE2	2.02	0.40
3:C:214:LYS:HB2	3:C:217:GLU:HG3	2.02	0.40
5:E:21:MET:HB2	5:E:186:TYR:CE1	2.56	0.40
11:K:46:LEU:HD13	11:K:87:LEU:HD11	2.03	0.40
14:N:18:DC:H6	14:N:18:DC:H2'	1.73	0.40
15:T:-48:DA:H2''	15:T:-47:DG:N7	2.36	0.40
15:T:-20:DT:H2''	15:T:-19:DA:C8	2.56	0.40
16:c:104:PHE:CE2	17:d:37:LEU:HD23	2.56	0.40
1:A:609:VAL:O	1:A:609:VAL:HG13	2.21	0.40
1:A:680:ILE:O	1:A:684:ILE:HG23	2.22	0.40
1:A:827:ASP:OD2	1:A:827:ASP:C	2.65	0.40
2:B:214:VAL:O	2:B:214:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:ASP:OD2	2:B:271:ASP:C	2.65	0.40
2:B:575:VAL:O	2:B:578:VAL:HG22	2.22	0.40
3:C:16:GLU:HA	3:C:232:VAL:O	2.22	0.40
4:D:68:SER:O	4:D:71:ARG:HG2	2.21	0.40
1:A:95:PHE:HB3	1:A:235:MET:HG2	2.03	0.40
1:A:916:TYR:CD2	1:A:920:ILE:HD11	2.57	0.40
1:A:1129:ASP:OD2	1:A:1131:GLU:HG2	2.22	0.40
2:B:266:PRO:O	2:B:348:ILE:HD11	2.21	0.40
2:B:969:ARG:HG2	2:B:970:THR:N	2.36	0.40
9:I:19:ASP:HB2	9:I:26:LEU:CD2	2.52	0.40
9:I:21:GLU:OE1	9:I:21:GLU:N	2.55	0.40
14:N:39:DT:HI'	14:N:40:DG:C8	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1396/1743 (80%)	1338 (96%)	57 (4%)	1 (0%)	48	78
2	B	1151/1227 (94%)	1113 (97%)	38 (3%)	0	100	100
3	C	261/304 (86%)	253 (97%)	8 (3%)	0	100	100
4	D	148/186 (80%)	146 (99%)	2 (1%)	0	100	100
5	E	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
6	F	82/155 (53%)	77 (94%)	5 (6%)	0	100	100
7	G	169/171 (99%)	167 (99%)	2 (1%)	0	100	100
8	H	129/145 (89%)	123 (95%)	6 (5%)	0	100	100
9	I	109/115 (95%)	101 (93%)	8 (7%)	0	100	100
10	J	64/72 (89%)	61 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	111/118 (94%)	104 (94%)	7 (6%)	0	100	100
12	L	43/72 (60%)	40 (93%)	3 (7%)	0	100	100
16	a	74/139 (53%)	73 (99%)	1 (1%)	0	100	100
16	c	75/139 (54%)	73 (97%)	2 (3%)	0	100	100
16	e	74/139 (53%)	71 (96%)	3 (4%)	0	100	100
16	g	75/139 (54%)	72 (96%)	3 (4%)	0	100	100
17	b	71/106 (67%)	71 (100%)	0	0	100	100
17	d	69/106 (65%)	68 (99%)	1 (1%)	0	100	100
17	f	70/106 (66%)	70 (100%)	0	0	100	100
17	h	71/106 (67%)	71 (100%)	0	0	100	100
All	All	4453/5502 (81%)	4299 (96%)	153 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	960	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1223/1528 (80%)	1221 (100%)	2 (0%)	87	84
2	B	1016/1077 (94%)	1010 (99%)	6 (1%)	78	77
3	C	236/264 (89%)	235 (100%)	1 (0%)	84	79
4	D	133/160 (83%)	133 (100%)	0	100	100
5	E	196/197 (100%)	195 (100%)	1 (0%)	81	78
6	F	75/137 (55%)	71 (95%)	4 (5%)	20	45
7	G	148/148 (100%)	148 (100%)	0	100	100
8	H	120/130 (92%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	106/109 (97%)	104 (98%)	2 (2%)	50	64
10	J	60/66 (91%)	59 (98%)	1 (2%)	53	65
11	K	104/109 (95%)	103 (99%)	1 (1%)	68	72
12	L	38/56 (68%)	38 (100%)	0	100	100
16	a	66/113 (58%)	65 (98%)	1 (2%)	57	66
16	c	66/113 (58%)	65 (98%)	1 (2%)	57	66
16	e	66/113 (58%)	66 (100%)	0	100	100
16	g	66/113 (58%)	66 (100%)	0	100	100
17	b	61/81 (75%)	60 (98%)	1 (2%)	55	66
17	d	59/81 (73%)	58 (98%)	1 (2%)	53	65
17	f	60/81 (74%)	60 (100%)	0	100	100
17	h	61/81 (75%)	61 (100%)	0	100	100
All	All	3960/4757 (83%)	3938 (99%)	22 (1%)	76	77

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	723	LEU
2	B	47	GLN
2	B	249	LEU
2	B	303	LEU
2	B	815	ARG
2	B	836	GLU
2	B	1122	ARG
3	C	26	LEU
5	E	20	GLU
6	F	72	LEU
6	F	93	ILE
6	F	103	MET
6	F	125	LEU
9	I	91	ARG
9	I	97	MET
10	J	54	ASP
11	K	65	HIS
16	a	126	LEU
17	b	84	MET
16	c	133	GLU

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Mol	Chain	Res	Type
17	d	72	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	ASN
1	A	446	ASN
1	A	491	HIS
1	A	577	GLN
1	A	651	GLN
1	A	737	ASN
1	A	769	GLN
1	A	803	ASN
2	B	292	HIS
2	B	298	ASN
2	B	376	ASN
2	B	549	ASN
2	B	794	ASN
2	B	862	GLN
2	B	932	HIS
2	B	951	GLN
2	B	1015	HIS
2	B	1193	GLN
3	C	13	GLN
4	D	129	HIS
4	D	179	ASN
7	G	14	HIS
7	G	125	ASN
9	I	12	ASN
9	I	31	ASN
9	I	96	ASN
9	I	105	ASN
11	K	106	ASN
16	a	125	GLN
16	c	76	GLN
16	e	93	GLN
16	g	68	GLN
17	h	75	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	10/11 (90%)	1 (10%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	1	U

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

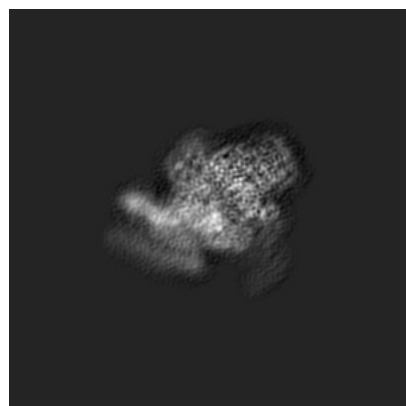
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64225. These allow visual inspection of the internal detail of the map and identification of artifacts.

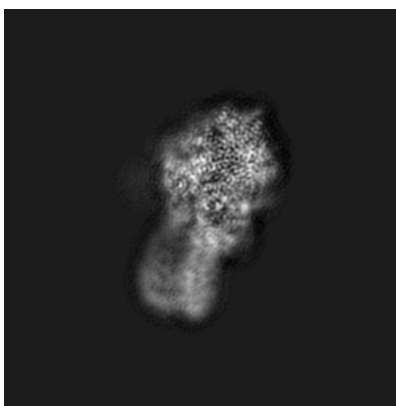
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

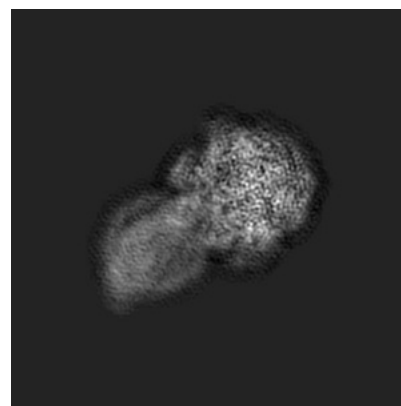
6.1.1 Primary map



X

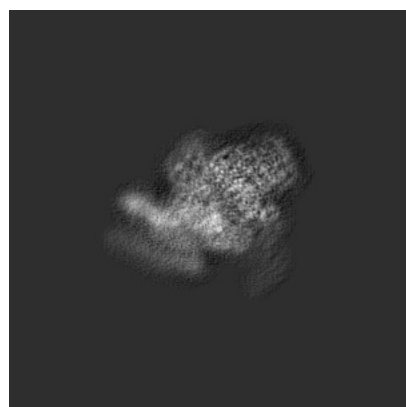


Y

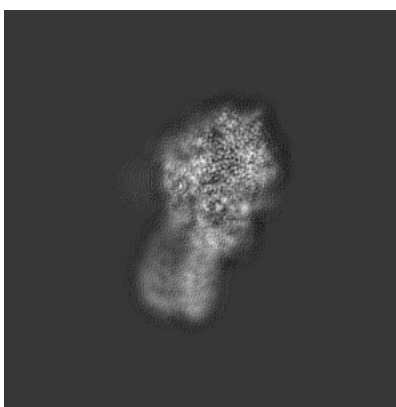


Z

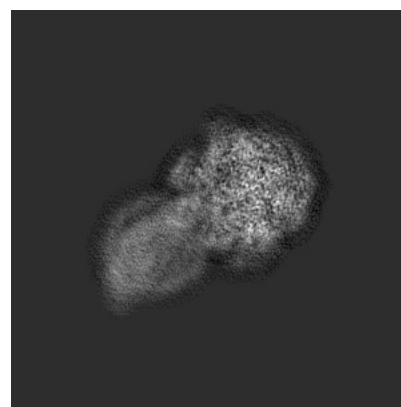
6.1.2 Raw map



X



Y

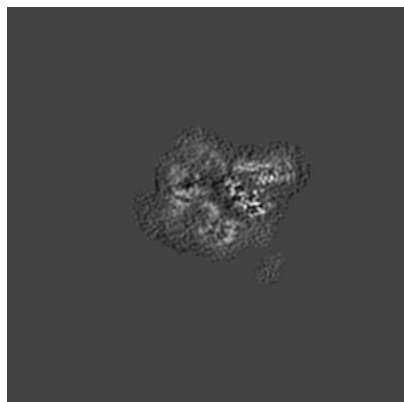


Z

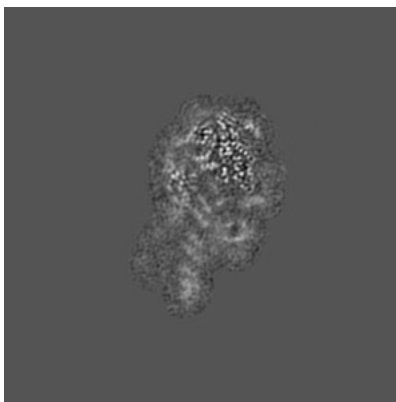
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

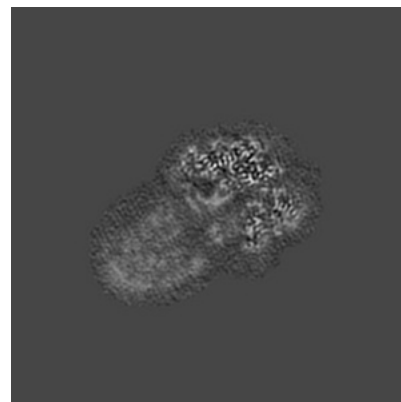
6.2.1 Primary map



X Index: 180

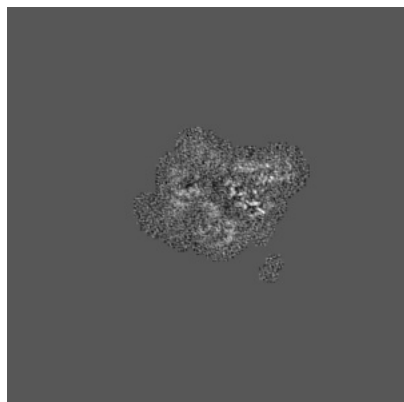


Y Index: 180

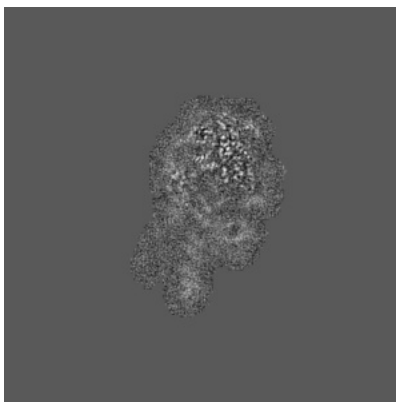


Z Index: 180

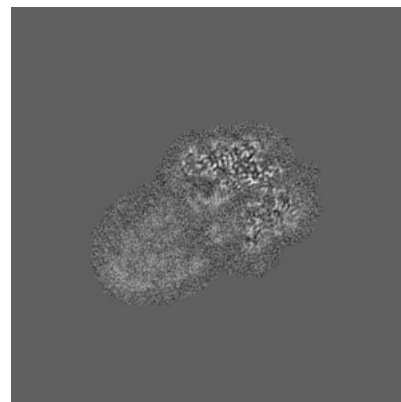
6.2.2 Raw map



X Index: 180



Y Index: 180

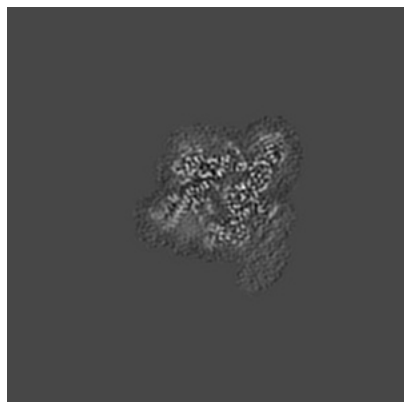


Z Index: 180

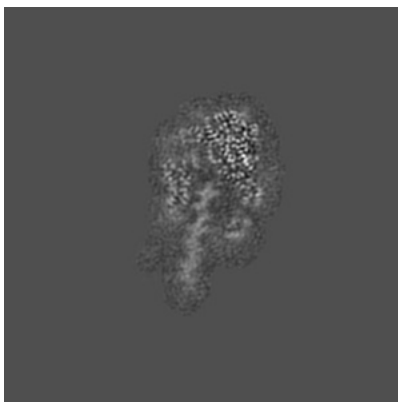
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

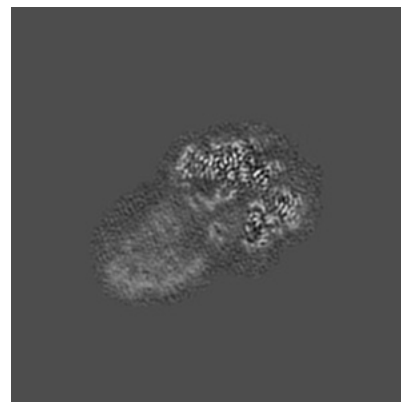
6.3.1 Primary map



X Index: 214

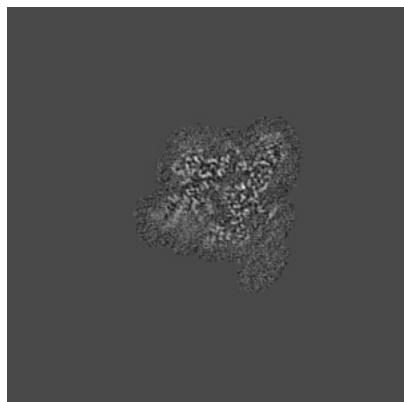


Y Index: 187

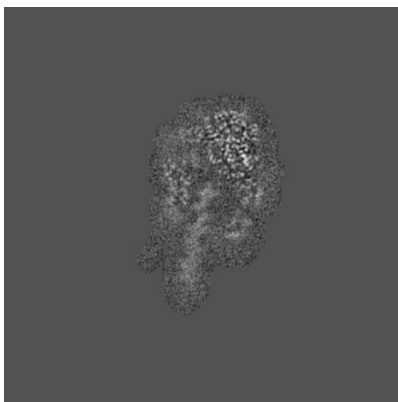


Z Index: 182

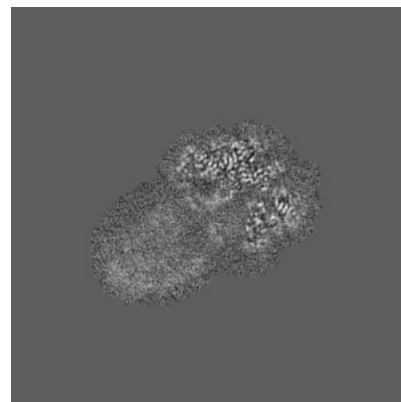
6.3.2 Raw map



X Index: 214



Y Index: 187

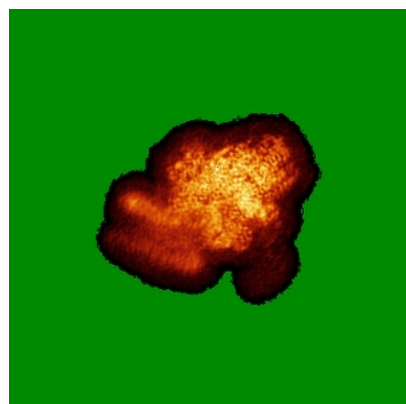


Z Index: 181

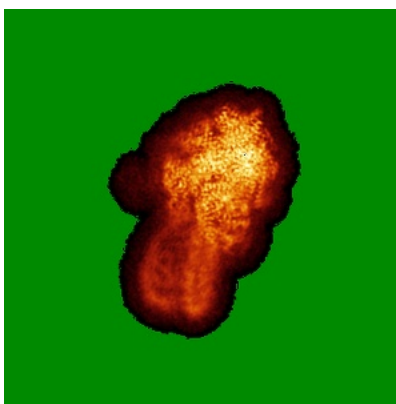
The images above show the largest variance slices of the map in three orthogonal directions.

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

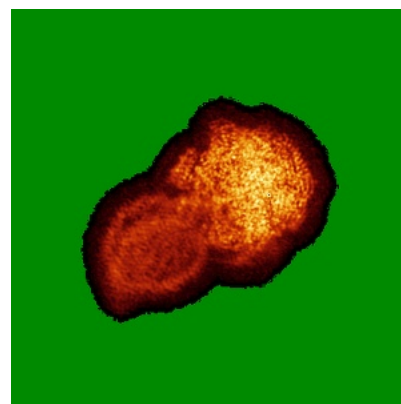
6.4.1 Primary map



X

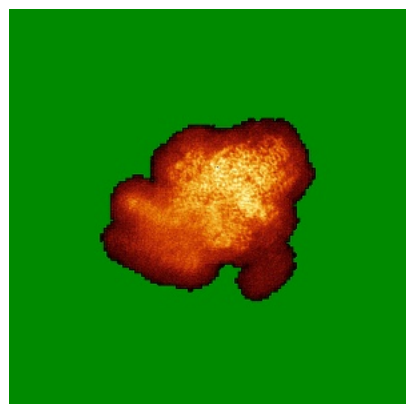


Y

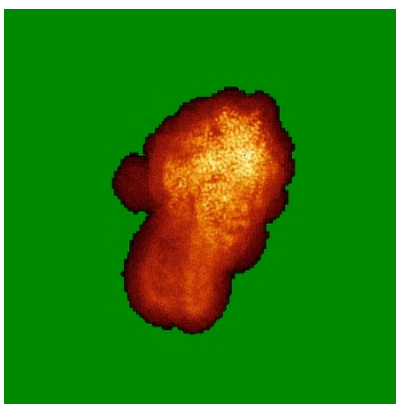


Z

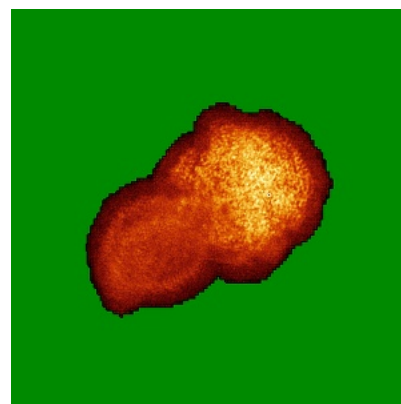
6.4.2 Raw map



X



Y



Z

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

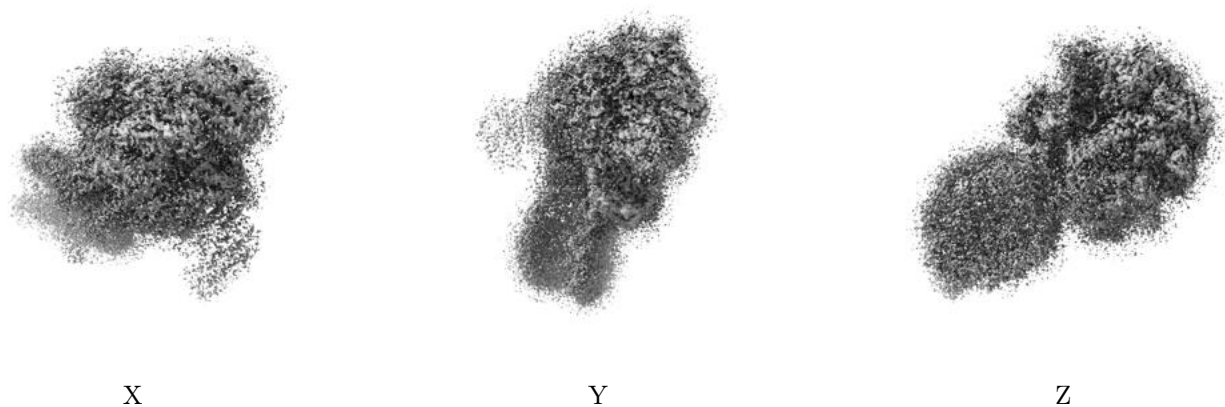
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

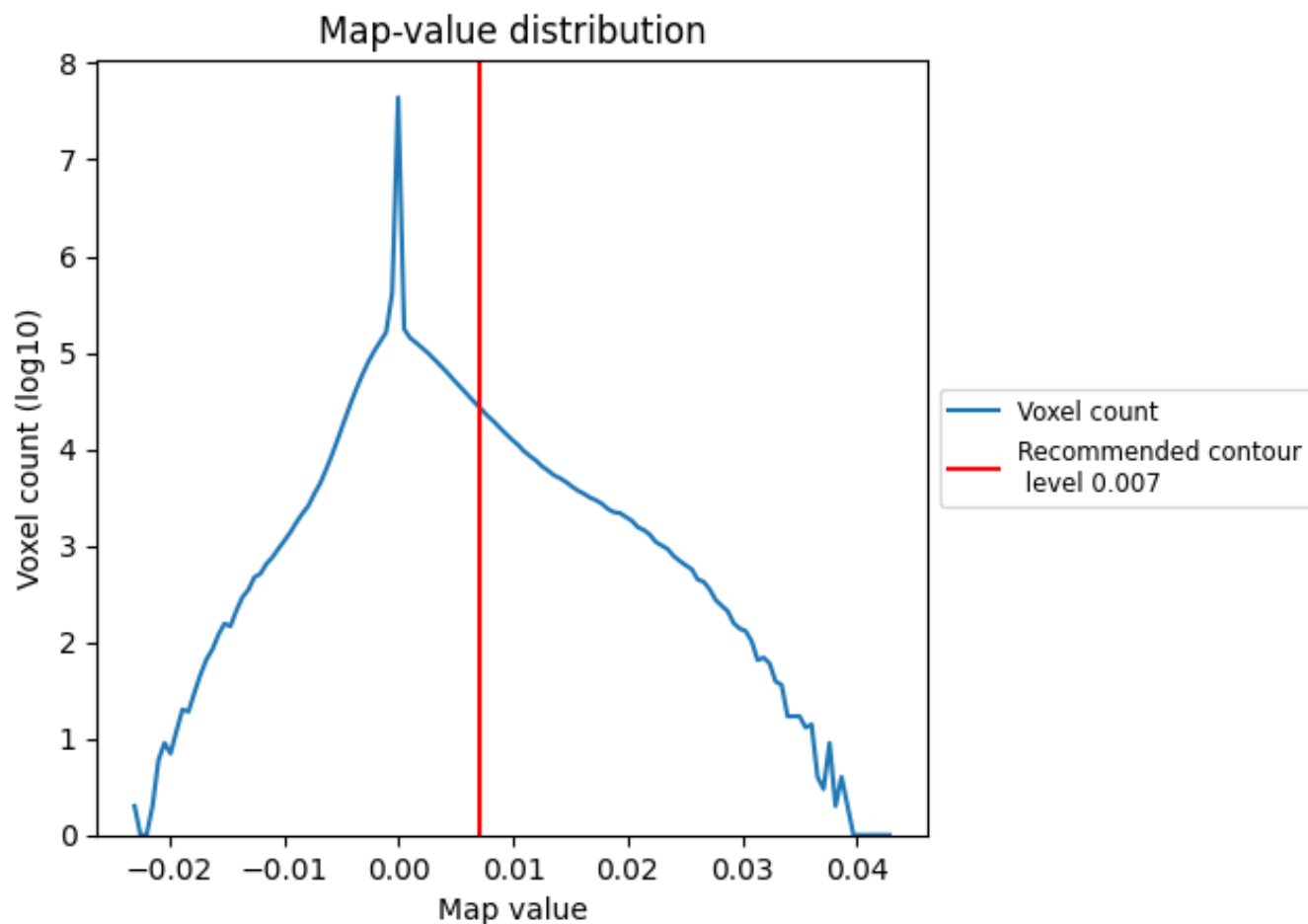
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

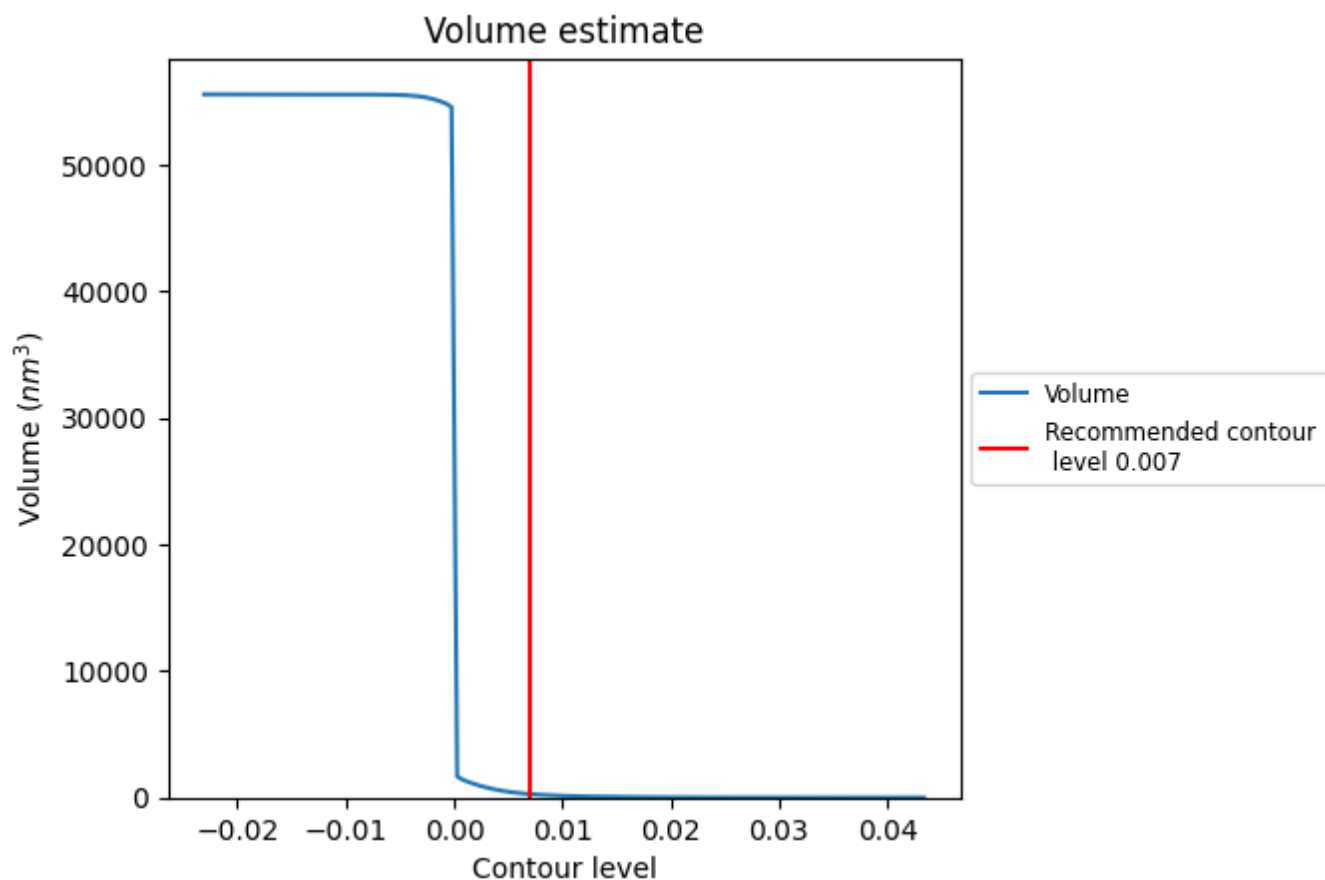
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

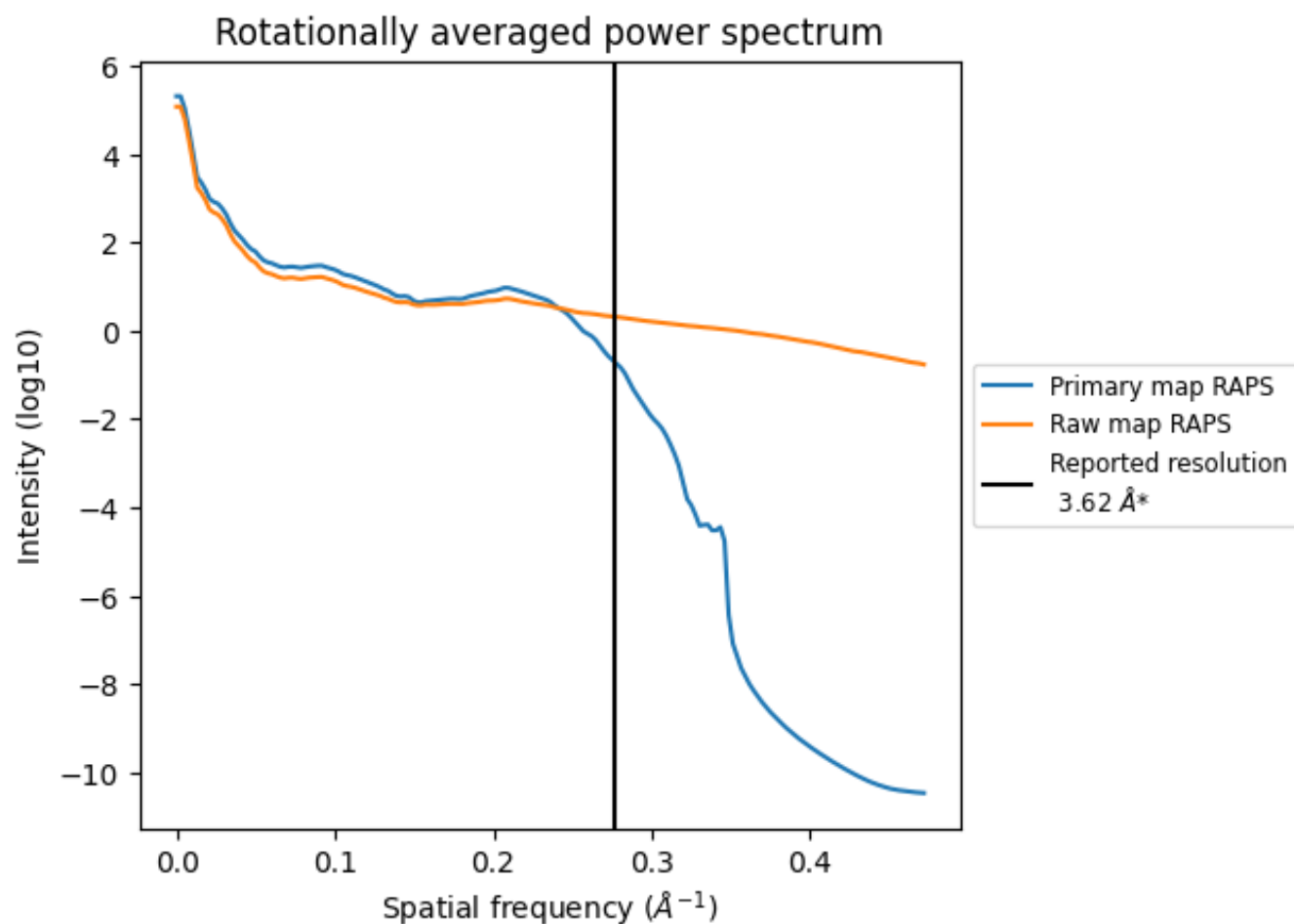
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 277 nm^3 ; this corresponds to an approximate mass of 250 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

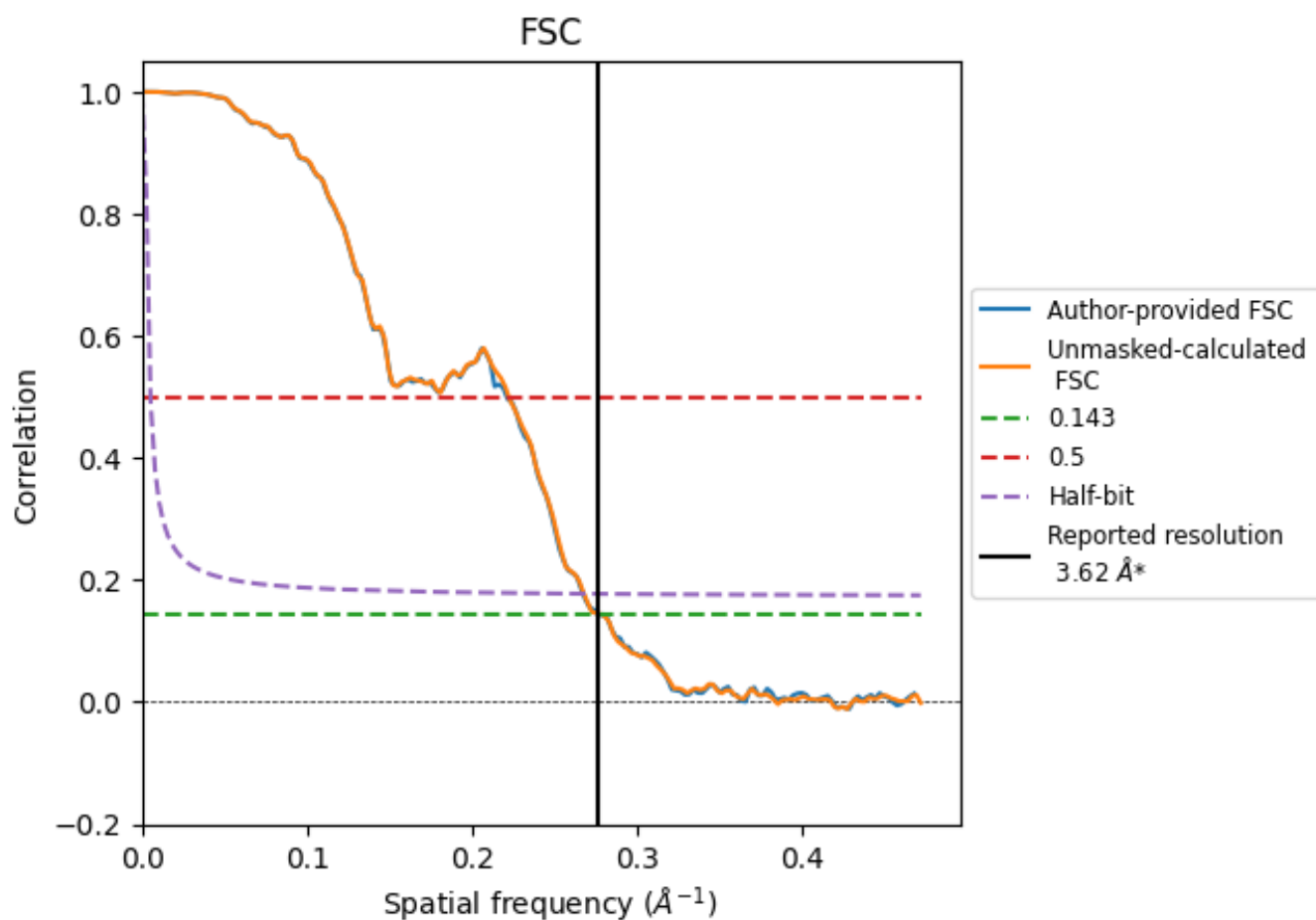


*Reported resolution corresponds to spatial frequency of 0.276 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.276 \AA^{-1}

8.2 Resolution estimates [i](#)

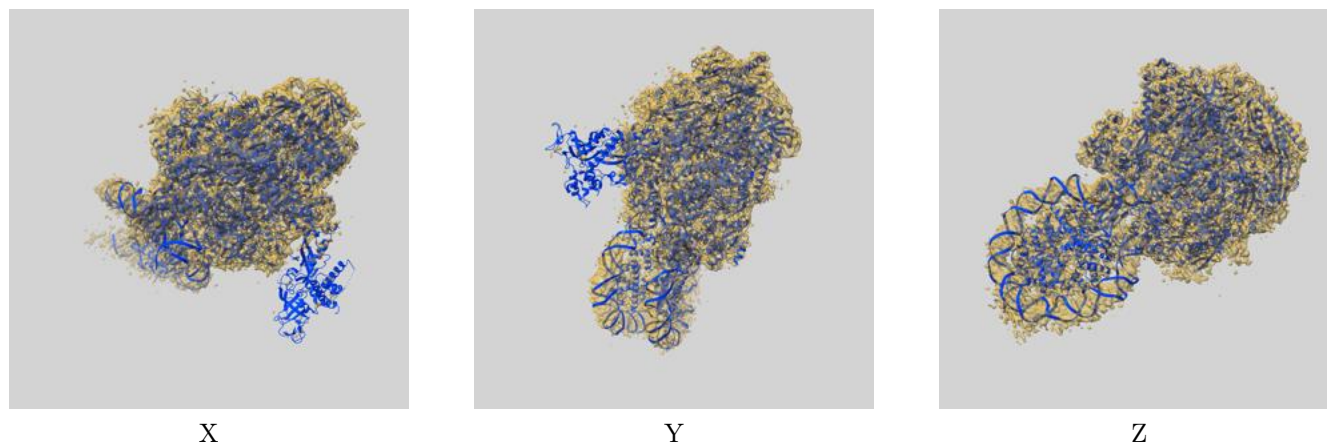
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	3.62	4.52	3.74
Unmasked-calculated*	3.59	4.50	3.74

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

9 Map-model fit [i](#)

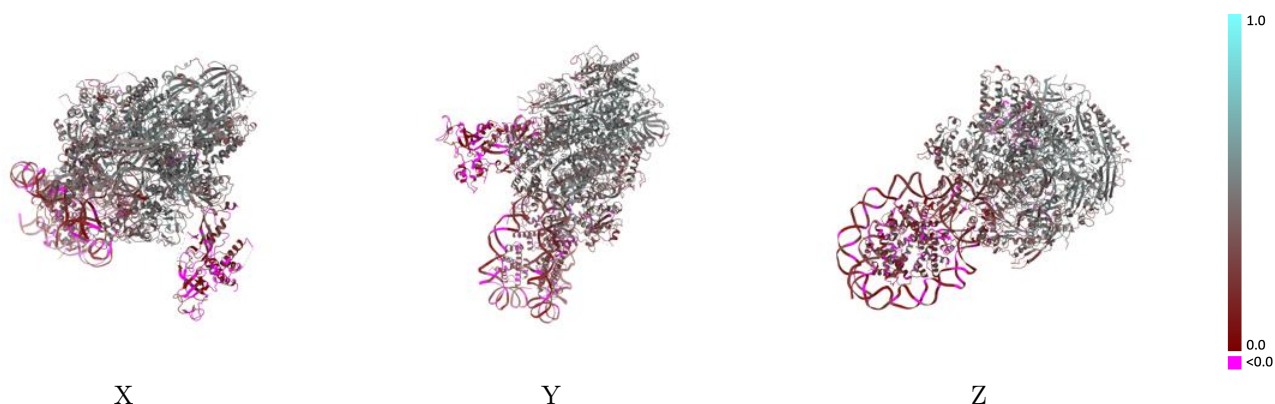
This section contains information regarding the fit between EMDB map EMD-64225 and PDB model 9UJS. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



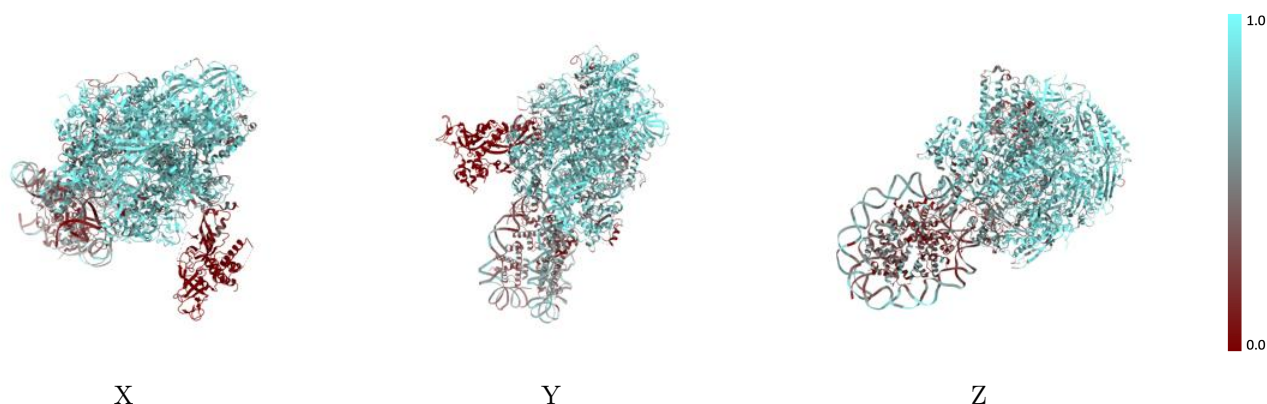
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



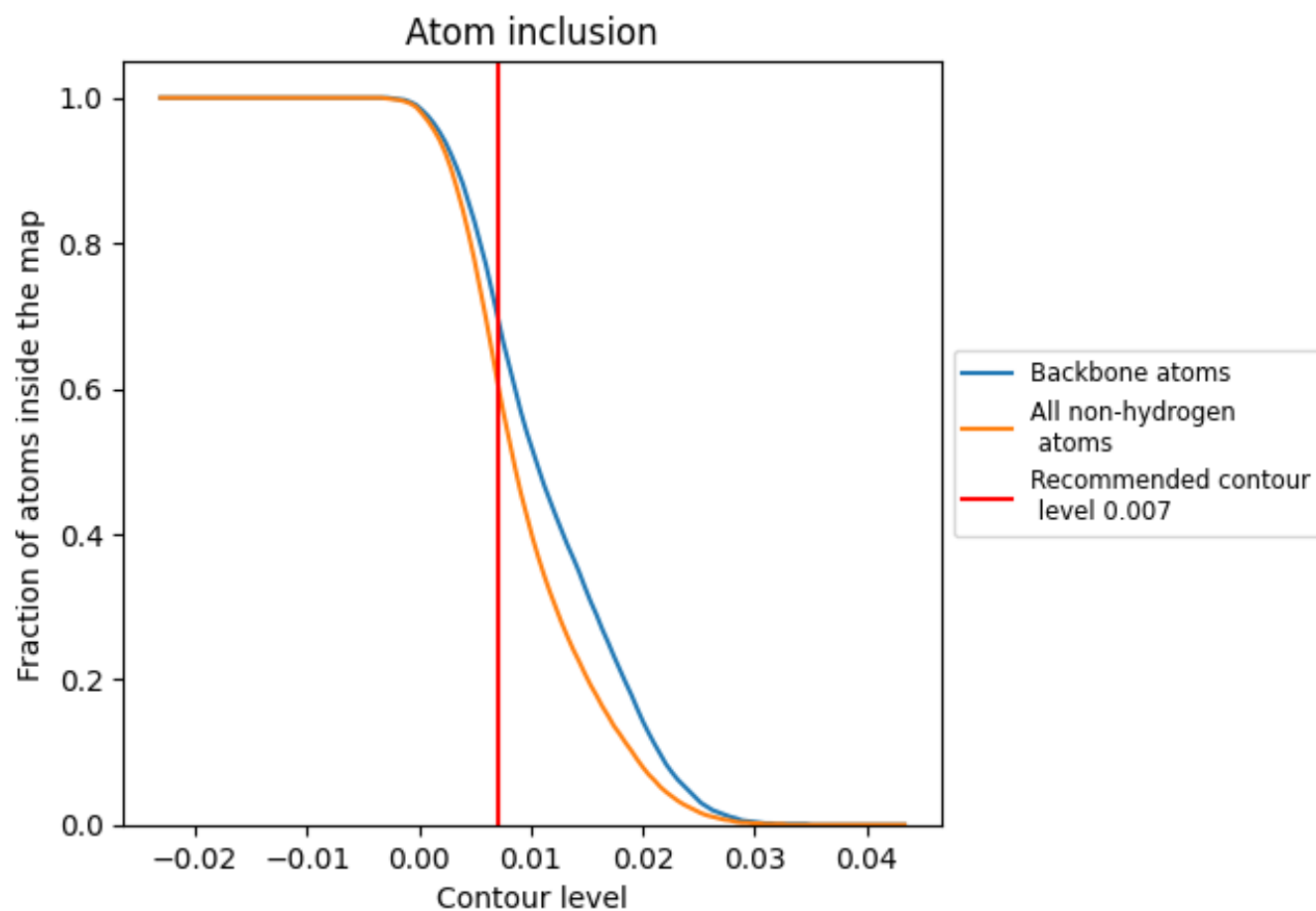
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

















































9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 61% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6110	 0.3330
A	 0.7330	 0.4210
B	 0.7410	 0.4320
C	 0.7880	 0.4570
D	 0.0060	 0.0740
E	 0.7800	 0.4220
F	 0.6750	 0.4240
G	 0.0450	 0.1150
H	 0.7890	 0.4590
I	 0.3020	 0.2020
J	 0.8510	 0.4770
K	 0.6970	 0.4120
L	 0.7640	 0.3680
N	 0.4830	 0.1120
P	 0.8190	 0.3820
T	 0.5350	 0.1530
a	 0.3830	 0.1820
b	 0.3830	 0.1860
c	 0.3630	 0.2010
d	 0.3080	 0.1930
e	 0.2770	 0.1520
f	 0.3290	 0.1760
g	 0.2540	 0.1730
h	 0.2790	 0.1620

