



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:41 AM UTC

PDB ID : 8H0W / pdb_00008h0w
EMDB ID : EMD-34416
Title : RNA polymerase II transcribing a chromatosome (type II)
Authors : Hirano, R.; Ehara, H.; Tomoya, K.; Takizawa, Y.; Sekine, S.; Kurumizaka, H.
Deposited on : 2022-09-30
Resolution : 4.60 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

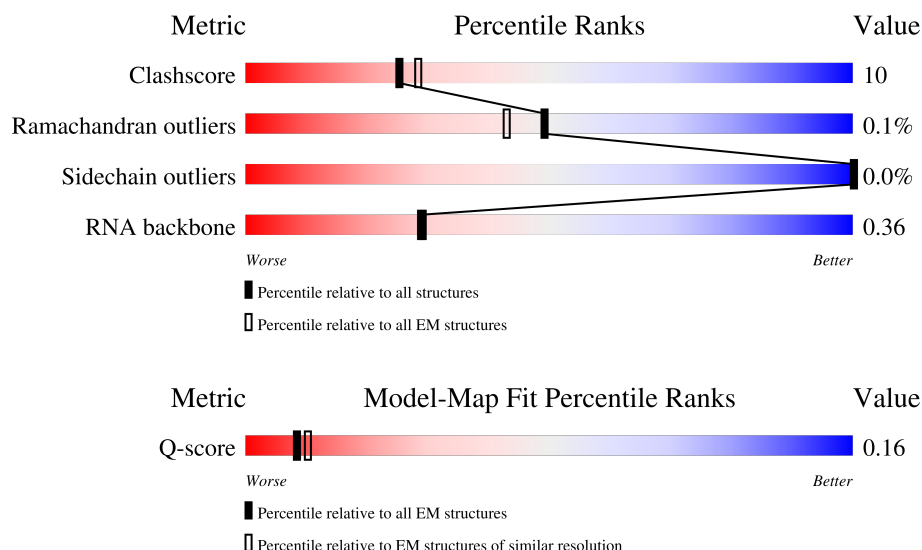
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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	2407 (4.10 - 5.10)

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	14	
14	T	261	
15	N	261	
16	a	139	
16	e	139	
17	b	106	
17	f	106	
18	c	133	
18	g	133	
19	d	129	
19	h	129	
20	u	219	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 46364 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	1412	Total	C	N	O	S	0	0
			11120	7015	1936	2099	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	168	Total	C	N	O	S	0	0
			1314	812	237	263	2		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	14	Total	C	N	O	P	0	0
			299	134	55	96	14		

- Molecule 14 is a DNA chain called DNA (261-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	205	Total	C	N	O	P	0	0
			4212	1997	790	1220	205		

- Molecule 15 is a DNA chain called DNA (261-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	196	Total	C	N	O	P	0	0
			4007	1906	719	1186	196		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	97	Total	C	N	O	S	0	0
			801	505	155	137	4		
16	e	97	Total	C	N	O	S	0	0
			800	503	155	138	4		

There are 8 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
a	0	MET	-	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
e	0	MET	-	expression tag	UNP P68431

- Molecule 17 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
17	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 18 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	c	105	Total	C	N	O	0	0
			810	511	158	141		
18	g	105	Total	C	N	O	0	0
			810	511	158	141		

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 19 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	d	95	Total	C	N	O	S	0	0
			746	468	136	140	2		
19	h	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

There are 6 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
h	-4	HIS	-	expression tag	UNP P06899

- Molecule 20 is a protein called Histone H1.2.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	u	73	Total	C	N	O	0	0
			525	331	95	99		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	214	LEU	-	expression tag	UNP P16403
u	215	GLU	-	expression tag	UNP P16403
u	216	VAL	-	expression tag	UNP P16403
u	217	LEU	-	expression tag	UNP P16403
u	218	PHE	-	expression tag	UNP P16403
u	219	GLN	-	expression tag	UNP P16403

- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

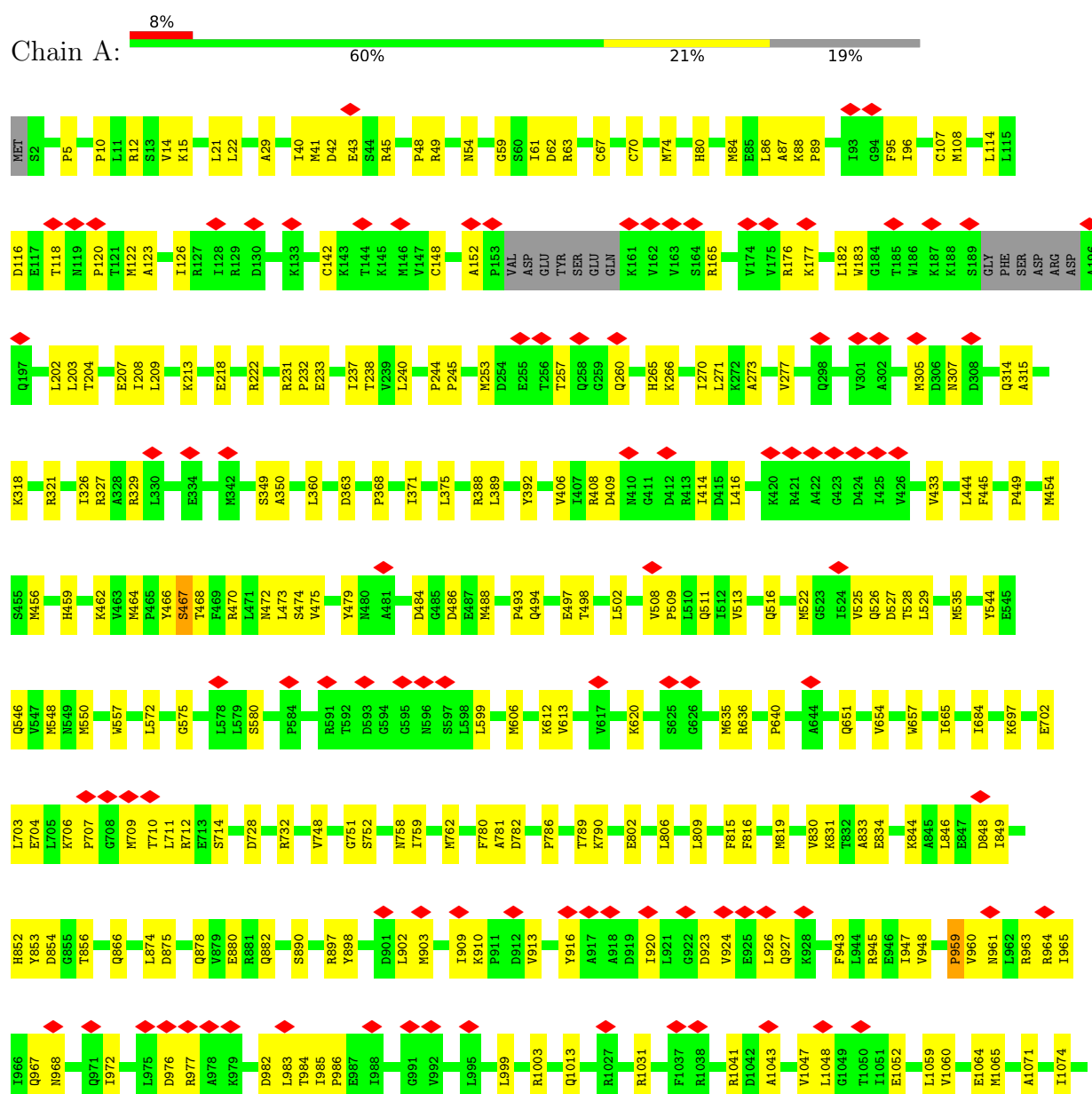
- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

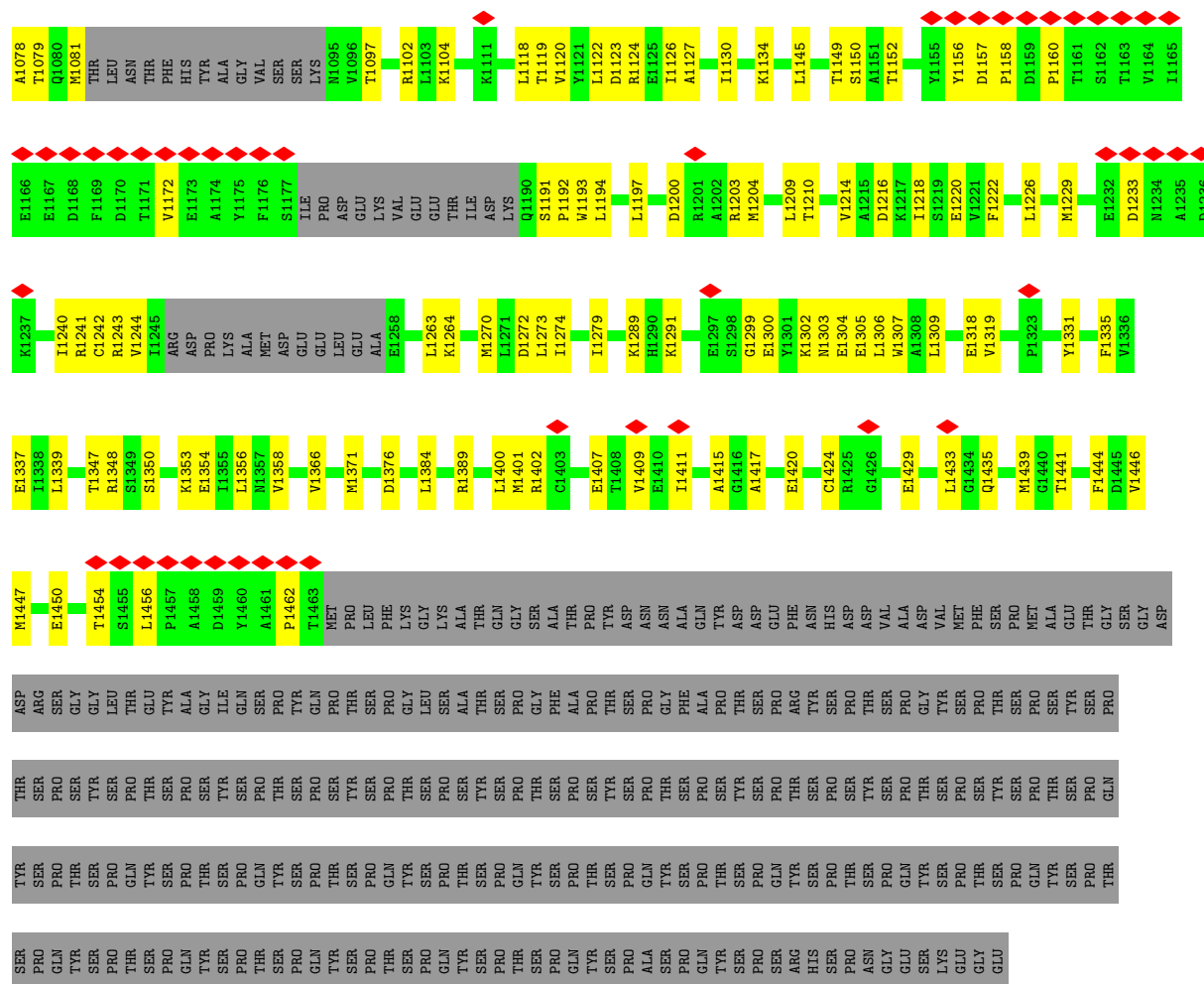
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	Mg	0
			1	1	

3 Residue-property plots

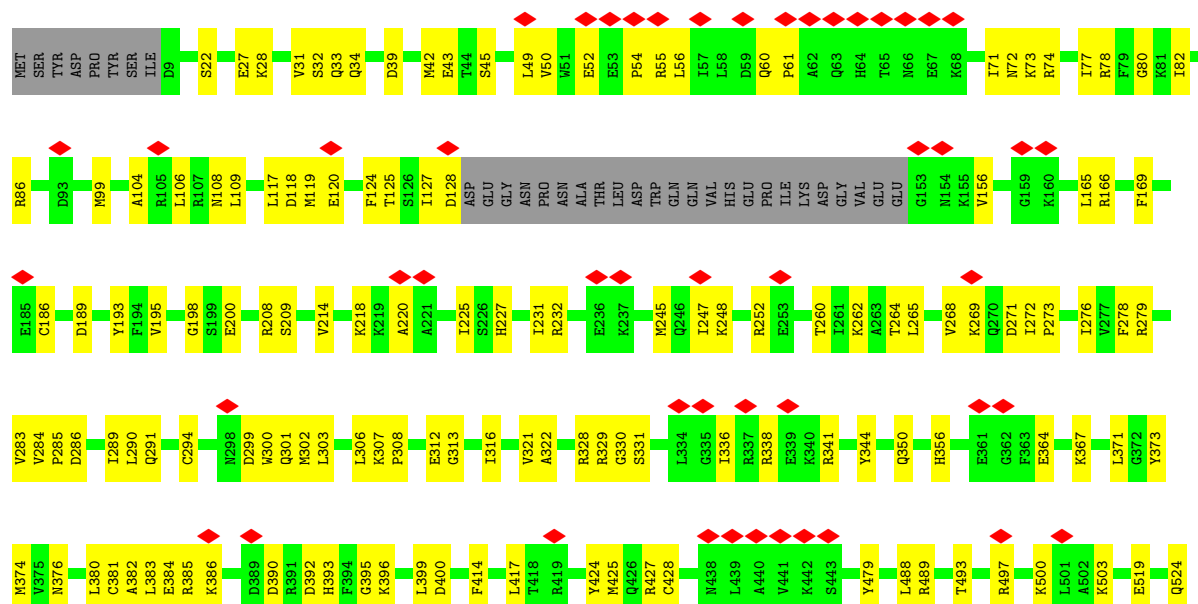
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

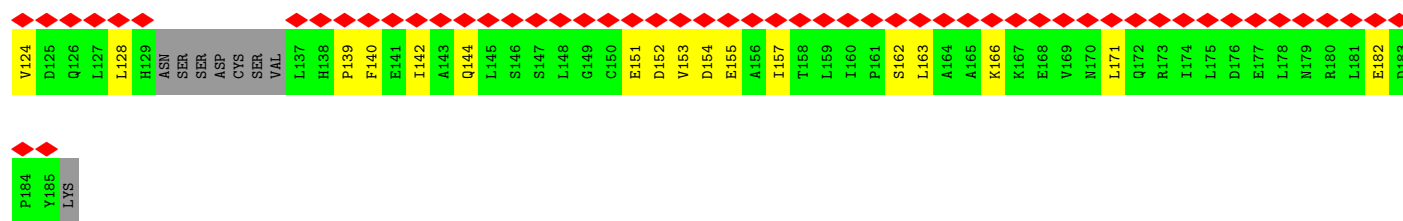
- Molecule 1: DNA-directed RNA polymerase subunit



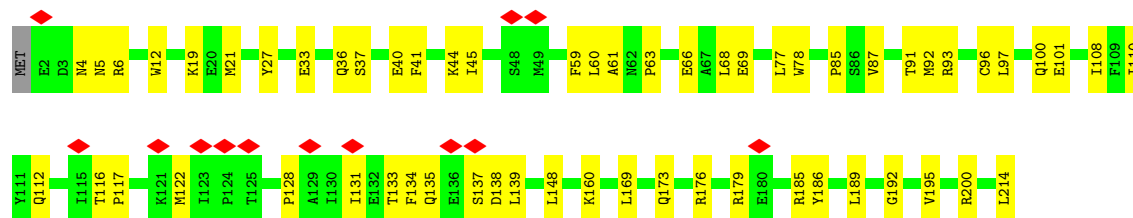


• Molecule 2: DNA-directed RNA polymerase subunit beta

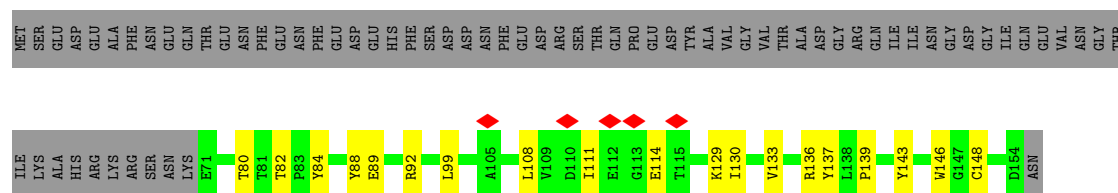




• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



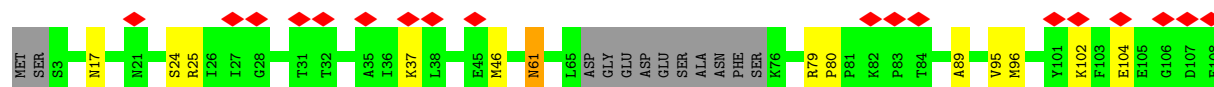
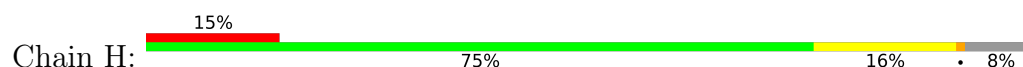
• Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III



• Molecule 7: RNA polymerase II subunit

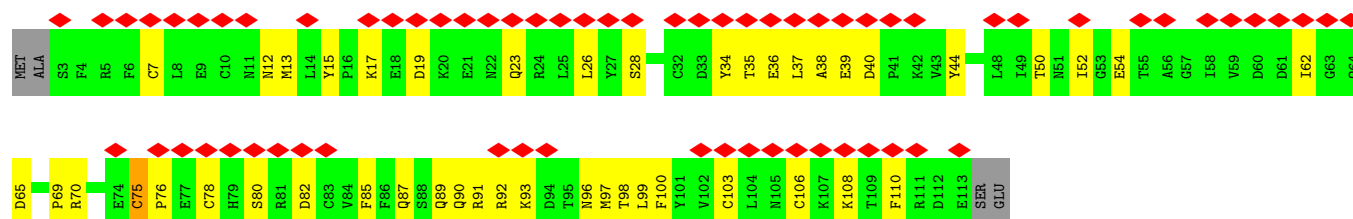


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

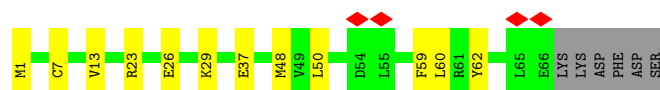
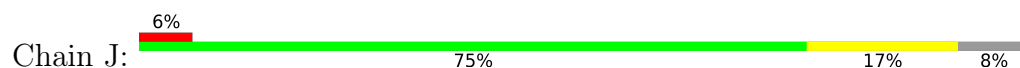




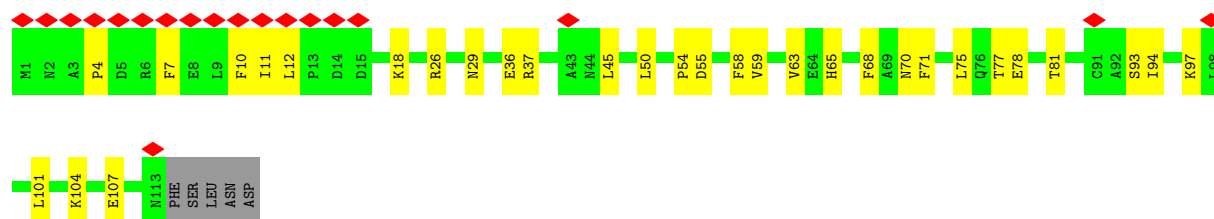
- Molecule 9: DNA-directed RNA polymerase subunit



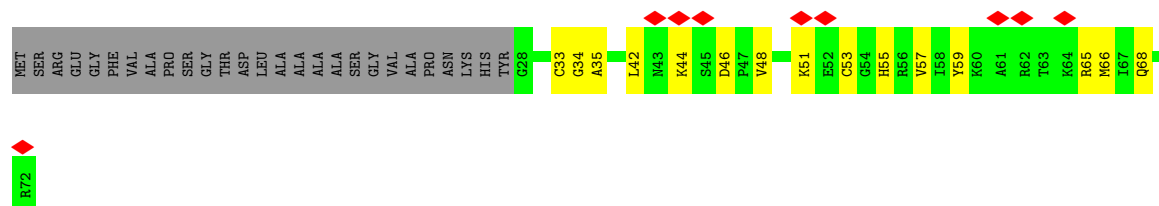
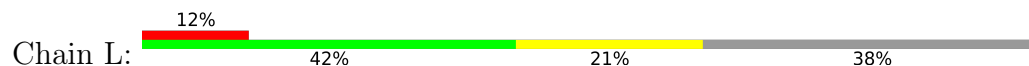
- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III



- Molecule 11: RNA polymerase II subunit B12.5



- Molecule 12: RNA polymerase subunit ABC10-alpha



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



M90		GLY	SER	HIS	MET	ALA	ARG	THR	LYS	GLN	THR	ALA	ARG	LYS	THR	GLY	GLY	LYS	ALA	PRO	ARG	LYS	SER	ALA	PRO	ALA	THR	GLY	GLY	VAL	LYS	LYS	PRO	R39		R42	P43		L61	L62	R63		R69		R72		Q76		L82	R83
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Chain b:

GLY	SER	HIS	MET	SER	GLY	ARG	GLY	LYS	GLY	LYS	GLY	LEU	GLY	LYS	GLY	GLY	ALA	LYS	ARG	HIS	ARG	K20	K21	L22	R23	D24	N25	R35	R39	R40	K59	E63	V70	E74	K77	R78	K79	T82	A83	M84	D85	Y88	K91	T96	G101	R102	K103	R104	K105	R106	K107	R108	K109	R110	K111	R112	K113	R114	K115	R116	K117	R118	K119	R120	K121	R122	K123	R124	K125	R126	K127	R128	K129	R130	K131	R132	K133	R134	K135	R136	K137	R138	K139	R140	K141	R142	K143	R144	K145	R146	K147	R148	K149	R150	K151	R152	K153	R154	K155	R156	K157	R158	K159	R160	K161	R162	K163	R164	K165	R166	K167	R168	K169	R170	K171	R172	K173	R174	K175	R176	K177	R178	K179	R180	K181	R182	K183	R184	K185	R186	K187	R188	K189	R190	K191	R192	K193	R194	K195	R196	K197	R198	K199	R200	K201	R202	K203	R204	K205	R206	K207	R208	K209	R210	K211	R212	K213	R214	K215	R216	K217	R218	K219	R220	K221	R222	K223	R224	K225	R226	K227	R228	K229	R230	K231	R232	K233	R234	K235	R236	K237	R238	K239	R240	K241	R242	K243	R244	K245	R246	K247	R248	K249	R250	K251	R252	K253	R254	K255	R256	K257	R258	K259	R260	K261	R262	K263	R264	K265	R266	K267	R268	K269	R270	K271	R272	K273	R274	K275	R276	K277	R278	K279	R280	K281	R282	K283	R284	K285	R286	K287	R288	K289	R290	K291	R292	K293	R294	K295	R296	K297	R298	K299	R300	K301	R302	K303	R304	K305	R306	K307	R308	K309	R310	K311	R312	K313	R314	K315	R316	K317	R318	K319	R320	K321	R322	K323	R324	K325	R326	K327	R328	K329	R330	K331	R332	K333	R334	K335	R336	K337	R338	K339	R340	K341	R342	K343	R344	K345	R346	K347	R348	K349	R350	K351	R352	K353	R354	K355	R356	K357	R358	K359	R360	K361	R362	K363	R364	K365	R366	K367	R368	K369	R370	K371	R372	K373	R374	K375	R376	K377	R378	K379	R380	K381	R382	K383	R384	K385	R386	K387	R388	K389	R390	K391	R392	K393	R394	K395	R396	K397	R398	K399	R400	K401	R402	K403	R404	K405	R406	K407	R408	K409	R410	K411	R412	K413	R414	K415	R416	K417	R418	K419	R420	K421	R422	K423	R424	K425	R426	K427	R428	K429	R430	K431	R432	K433	R434	K435	R436	K437	R438	K439	R440	K441	R442	K443	R444	K445	R446	K447	R448	K449	R450	K451	R452	K453	R454	K455	R456	K457	R458	K459	R460	K461	R462	K463	R464	K465	R466	K467	R468	K469	R470	K471	R472	K473	R474	K475	R476	K477	R478	K479	R480	K481	R482	K483	R484	K485	R486	K487	R488	K489	R490	K491	R492	K493	R494	K495	R496	K497	R498	K499	R500	K501	R502	K503	R504	K505	R506	K507	R508	K509	R510	K511	R512	K513	R514	K515	R516	K517	R518	K519	R520	K521	R522	K523	R524	K525	R526	K527	R528	K529	R530	K531	R532	K533	R534	K535	R536	K537	R538	K539	R540	K541	R542	K543	R544	K545	R546	K547	R548	K549	R550	K551	R552	K553	R554	K555	R556	K557	R558	K559	R560	K561	R562	K563	R564	K565	R566	K567	R568	K569	R570	K571	R572	K57
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Chain f:

[illegible]

Chain c: 68% 11% 21%

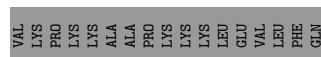
GLY	SER	HIS	MET	SER	GLY	ARG	GLY	GLN	GLY	LYS	ALA	ARG	ALA	LYS	LYS	R29	V30	R35	N38	L55	L63	R68	E91	K95	I102	L108	L115	K118	LVS	THR	GLU	SER	SER	HIS	HIS	LVS	ALA	LVS	GLY
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Chain g:

[illegible]

Chain d:

GLY	SER	HIS	MET	PRO	GLU	PRO	ALA	LYS	SER	ALA	PRO	ALA	LYS	GLY	SER	LYS	LYS	ALA	VAL	THR	LYS	ALA	GLN	LYS	LYS	ASP	GLY	LYS	LYS	ARG	LYS	R28	R29	R30	R31	R32	R33	Y37	L42	K43	Q44	S53	I58	M59	N60	V63	N64	F67	E68	Y69
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16916	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.2	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.076	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.016	Depositor
Map size ($\text{\AA}$)	357.6, 357.6, 357.6	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.49, 1.49, 1.49	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.21	0/11326	0.43	0/15306
2	B	0.22	0/9441	0.42	0/12732
3	C	0.21	0/2139	0.41	0/2895
4	D	0.13	0/1326	0.36	0/1788
5	E	0.19	0/1772	0.43	0/2385
6	F	0.20	0/687	0.46	0/931
7	G	0.16	0/1353	0.44	0/1837
8	H	0.18	0/1069	0.39	0/1444
9	I	0.24	0/934	0.71	6/1257 (0.5%)
10	J	0.25	0/554	0.49	0/742
11	K	0.20	0/953	0.41	0/1291
12	L	0.19	0/365	0.50	0/484
13	P	0.95	7/334 (2.1%)	0.33	0/518
14	T	0.39	0/4730	0.64	0/7299
15	N	0.38	0/4488	0.64	0/6921
16	a	0.22	0/813	0.39	0/1090
16	e	0.22	0/811	0.45	0/1086
17	b	0.21	0/669	0.39	0/894
17	f	0.24	0/626	0.45	0/837
18	c	0.21	0/820	0.38	0/1107
18	g	0.19	0/820	0.35	0/1107
19	d	0.21	0/757	0.38	0/1015
19	h	0.20	0/736	0.45	0/990
20	u	0.18	0/528	0.56	0/704
All	All	0.26	7/48051 (0.0%)	0.48	6/66660 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
3	C	0	1
14	T	0	1
15	N	0	3
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	4	G	C1'-N9	-6.67	1.38	1.48
13	P	3	G	C1'-N9	-6.27	1.38	1.48
13	P	1	U	C1'-N1	5.57	1.56	1.48
13	P	5	A	C1'-N9	-5.44	1.39	1.48
13	P	8	U	C1'-N1	5.29	1.56	1.48
13	P	-2	C	C1'-N1	5.20	1.56	1.48
13	P	0	A	C1'-N9	-5.09	1.40	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	78	CYS	N-CA-CB	-6.12	101.10	111.20
9	I	103	CYS	CA-CB-SG	5.88	127.92	114.40
9	I	78	CYS	CA-CB-SG	5.55	127.17	114.40
9	I	106	CYS	N-CA-CB	-5.53	102.29	110.53
9	I	106	CYS	CA-CB-SG	5.10	126.12	114.40
9	I	75	CYS	CA-CB-SG	5.08	126.08	114.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	525	VAL	Peptide
1	A	959	PRO	Peptide
3	C	89	ASP	Peptide
15	N	-77	DG	Sidechain
15	N	-80	DT	Sidechain
15	N	-81	DT	Sidechain
14	T	77	DC	Sidechain

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	11120	0	11150	279	0
2	B	9261	0	9265	238	0
3	C	2098	0	2057	34	0
4	D	1314	0	1314	32	0
5	E	1740	0	1754	42	0
6	F	677	0	693	17	0
7	G	1324	0	1342	50	0
8	H	1052	0	1050	23	0
9	I	917	0	865	41	0
10	J	545	0	560	10	0
11	K	932	0	944	30	0
12	L	359	0	358	12	0
13	P	299	0	152	4	0
14	T	4212	0	2299	76	0
15	N	4007	0	2209	55	0
16	a	801	0	839	18	0
16	e	800	0	836	18	0
17	b	662	0	709	14	0
17	f	619	0	659	10	0
18	c	810	0	866	13	0
18	g	810	0	866	25	0
19	d	746	0	771	16	0
19	h	725	0	745	25	0
20	u	525	0	581	12	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	C	1	0	0	0	0
21	I	2	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
22	A	1	0	0	0	0
All	All	46364	0	42884	926	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 10.

All (926) 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)
2:B:316:ILE:HG21	2:B:322:ALA:HB2	1.49	0.94
14:T:102:DC:C6	14:T:103:DT:H72	2.08	0.89
12:L:42:LEU:HD11	12:L:46:ASP:HB2	1.57	0.85
1:A:318:LYS:HE3	15:N:-105:DA:N6	1.92	0.84
1:A:548:MET:HE1	11:K:59:VAL:H	1.41	0.84
1:A:486:ASP:OD1	13:P:10:A:O2'	1.95	0.84
9:I:17:LYS:HD2	9:I:28:SER:HB2	1.59	0.84
1:A:203:LEU:HD23	1:A:208:ILE:HD11	1.58	0.84
1:A:709:MET:HE2	1:A:714:SER:HA	1.60	0.84
2:B:248:LYS:NZ	2:B:264:THR:OG1	2.12	0.82
1:A:999:LEU:O	1:A:1013:GLN:NE2	2.13	0.81
2:B:218:LYS:NZ	2:B:381:CYS:SG	2.54	0.81
8:H:112:LYS:NZ	8:H:125:GLU:OE2	2.15	0.79
2:B:887:HIS:NE2	13:P:-1:A:OP2	2.15	0.79
5:E:92:MET:HE1	5:E:131:ILE:HG21	1.66	0.78
1:A:1130:ILE:HG13	1:A:1134:LYS:HE2	1.66	0.78
2:B:291:GLN:HG3	2:B:564:PRO:HG2	1.66	0.78
4:D:86:ASP:OD2	4:D:110:ASN:ND2	2.16	0.78
1:A:977:ARG:H	8:H:135:LYS:HZ3	1.30	0.78
1:A:1347:THR:HG21	1:A:1384:LEU:HD11	1.67	0.77
2:B:265:LEU:HD13	2:B:272:ILE:HD13	1.66	0.77
1:A:89:PRO:HB3	1:A:238:THR:HG22	1.67	0.77
1:A:789:THR:HB	9:I:69:PRO:HD3	1.66	0.77
7:G:142:LYS:HG3	7:G:171:ILE:HG13	1.66	0.77
1:A:546:GLN:O	1:A:550:MET:HG3	1.84	0.76
14:T:89:DG:N2	15:N:-89:DC:O2	2.18	0.76
1:A:43:GLU:HB2	1:A:45:ARG:HE	1.50	0.76
2:B:301:GLN:NE2	9:I:50:THR:OG1	2.19	0.76
2:B:778:MET:HE1	2:B:1098:MET:HE3	1.68	0.76
2:B:612:ILE:HD11	9:I:62:ILE:HA	1.67	0.75
7:G:1:MET:N	7:G:80:LYS:O	2.20	0.75
4:D:114:ARG:HB3	4:D:182:GLU:HG3	1.68	0.74
17:f:29:ILE:HD13	17:f:58:LEU:HD23	1.70	0.74
11:K:10:PHE:C	11:K:37:ARG:HE	1.95	0.74
7:G:24:GLN:HE21	7:G:52:MET:HE1	1.51	0.74
18:g:63:LEU:HD13	19:h:42:LEU:HB2	1.69	0.74
1:A:445:PHE:CE2	1:A:488:MET:HE2	2.24	0.73
1:A:456:MET:HE3	2:B:1138:MET:HE3	1.68	0.73
19:h:29:SER:O	19:h:31:LYS:NZ	2.21	0.73
9:I:96:ASN:OD1	9:I:97:MET:N	2.22	0.73
2:B:612:ILE:HD13	9:I:65:ASP:HB2	1.70	0.73
1:A:1415:ALA:HA	1:A:1420:GLU:HG3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:MET:CE	11:K:59:VAL:H	2.03	0.72
1:A:1279:ILE:HD12	1:A:1318:GLU:HB3	1.72	0.71
2:B:941:LEU:HD21	2:B:968:MET:HE1	1.71	0.71
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.72	0.71
3:C:21:LEU:HD11	11:K:101:LEU:HD11	1.72	0.71
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.30	0.71
3:C:69:ILE:HD11	3:C:144:LEU:HD21	1.73	0.71
11:K:77:THR:HB	11:K:81:THR:HG23	1.71	0.71
1:A:968:ASN:O	1:A:972:ILE:HG13	1.89	0.70
20:u:87:LEU:HB3	20:u:93:LEU:HD23	1.73	0.70
15:N:-23:DC:OP1	16:a:72:ARG:NH1	2.23	0.70
1:A:1003:ARG:O	6:F:80:THR:OG1	2.10	0.70
5:E:100:GLN:HE22	5:E:128:PRO:HD2	1.56	0.70
2:B:72:ASN:ND2	2:B:128:ASP:OD1	2.25	0.69
15:N:71:DA:H2"	15:N:72:DG:C8	2.27	0.69
9:I:75:CYS:HB3	9:I:80:SER:H	1.57	0.69
1:A:1291:LYS:HE2	1:A:1303:ASN:HD22	1.58	0.69
1:A:10:PRO:HG2	1:A:12:ARG:NH2	2.08	0.69
1:A:1064:GLU:OE1	6:F:88:TYR:OH	2.11	0.69
2:B:611:ASP:HB3	2:B:616:GLU:HG2	1.74	0.69
1:A:406:VAL:HG23	1:A:416:LEU:HD11	1.74	0.69
1:A:1446:VAL:HG23	7:G:61:ILE:HB	1.74	0.68
1:A:445:PHE:HE2	1:A:488:MET:HE2	1.58	0.68
1:A:41:MET:HA	1:A:48:PRO:HB3	1.76	0.68
5:E:179:ARG:NH2	5:E:214:LEU:O	2.26	0.67
1:A:909:ILE:HD11	1:A:985:ILE:HD11	1.75	0.67
15:N:-27:DC:H2"	15:N:-26:DT:H71	1.76	0.67
16:a:107:THR:HG21	16:a:124:ILE:HG12	1.75	0.67
2:B:904:ARG:HD3	2:B:948:ILE:HG12	1.76	0.67
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.77	0.67
7:G:8:SER:HB3	7:G:73:LYS:HD2	1.76	0.67
18:g:20:ARG:HH11	19:h:118:TYR:HE1	1.43	0.67
5:E:134:PHE:HB3	5:E:139:LEU:HD21	1.77	0.67
2:B:54:PRO:HB2	2:B:78:ARG:HH12	1.60	0.67
1:A:557:TRP:O	11:K:26:ARG:NH1	2.28	0.66
1:A:1172:VAL:HG12	1:A:1229:MET:HE2	1.77	0.66
19:d:33:SER:HB2	19:d:60:ASN:HD21	1.58	0.66
8:H:79:ARG:NH2	11:K:54:PRO:O	2.29	0.66
1:A:782:ASP:HB2	1:A:790:LYS:HE3	1.78	0.66
6:F:130:ILE:HD11	6:F:148:CYS:SG	2.36	0.66
1:A:1400:LEU:HB2	1:A:1429:GLU:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:17:ASN:OD1	8:H:24:SER:OG	2.11	0.65
1:A:176:ARG:HG3	1:A:183:TRP:HB2	1.77	0.65
18:g:42:ARG:HB2	19:h:85:THR:HG22	1.77	0.65
1:A:349:SER:HB2	2:B:1128:LEU:HD12	1.79	0.65
14:T:-25:DC:H2"	14:T:-24:DT:H72	1.79	0.65
11:K:10:PHE:O	11:K:37:ARG:NH2	2.30	0.65
7:G:132:SER:HB2	7:G:135:GLU:HB2	1.79	0.65
17:b:84:MET:HG3	17:b:88:TYR:CE2	2.32	0.64
1:A:728:ASP:OD2	1:A:732:ARG:NH1	2.29	0.64
1:A:834:GLU:OE2	1:A:1104:LYS:NZ	2.24	0.64
2:B:883:LEU:HD12	2:B:884:ARG:H	1.61	0.64
9:I:87:GLN:O	9:I:89:GLN:NE2	2.29	0.64
14:T:15:DT:H2"	14:T:16:DA:C8	2.33	0.64
2:B:356:HIS:HD2	2:B:578:VAL:HG22	1.62	0.64
4:D:41:HIS:CE1	7:G:73:LYS:HE3	2.33	0.64
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.79	0.64
3:C:135:ARG:NE	3:C:136:ASP:OD2	2.22	0.64
1:A:497:GLU:OE2	6:F:99:LEU:HD22	1.98	0.64
2:B:593:MET:HB3	2:B:608:ILE:HD13	1.78	0.64
5:E:160:LYS:NZ	5:E:192:GLY:O	2.26	0.64
1:A:389:LEU:HD22	1:A:433:VAL:HG11	1.79	0.63
1:A:1197:LEU:HD11	1:A:1240:ILE:HD12	1.80	0.63
14:T:109:DT:H2"	14:T:110:DT:H71	1.79	0.63
9:I:26:LEU:HD12	9:I:35:THR:HG22	1.80	0.63
15:N:-72:DT:H2"	15:N:-71:DT:H71	1.79	0.63
18:g:30:VAL:HG13	19:h:67:PHE:HE2	1.62	0.63
8:H:37:LYS:HB3	8:H:125:GLU:OE1	1.98	0.63
2:B:71:ILE:HD11	2:B:125:THR:HB	1.80	0.63
1:A:1222:PHE:HB3	1:A:1226:LEU:HB3	1.81	0.63
2:B:316:ILE:HG23	2:B:321:VAL:HG13	1.80	0.63
7:G:115:ILE:HG12	7:G:163:ILE:HD11	1.81	0.63
4:D:162:SER:OG	4:D:166:LYS:NZ	2.32	0.62
5:E:27:TYR:CE2	5:E:77:LEU:HB2	2.35	0.62
1:A:253:MET:HG2	1:A:257:THR:HB	1.81	0.62
2:B:999:MET:HE3	2:B:1008:PRO:HG2	1.81	0.62
15:N:-26:DT:H2"	15:N:-25:DA:C8	2.34	0.62
1:A:1156:TYR:OH	9:I:23:GLN:OE1	2.18	0.62
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.32	0.62
2:B:396:LYS:HD2	2:B:693:GLU:OE2	1.99	0.62
16:e:42:ARG:HH11	16:e:43:PRO:HD2	1.64	0.62
7:G:13:LEU:HD22	7:G:26:LEU:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:u:45:THR:HG23	20:u:107:LEU:HD21	1.80	0.62
12:L:35:ALA:HB3	12:L:55:HIS:ND1	2.15	0.62
17:b:78:ARG:NH2	17:b:85:ASP:OD2	2.33	0.62
1:A:544:TYR:O	1:A:548:MET:HG3	2.00	0.62
2:B:957:ASN:ND2	2:B:959:GLU:OE2	2.33	0.61
1:A:305:MET:HG2	2:B:1210:MET:HG2	1.82	0.61
1:A:1123:ASP:OD1	1:A:1124:ARG:N	2.33	0.61
4:D:128:LEU:HD13	4:D:142:ILE:HG23	1.81	0.61
9:I:76:PRO:HD2	9:I:108:LYS:NZ	2.15	0.61
1:A:1291:LYS:HE2	1:A:1303:ASN:ND2	2.15	0.61
2:B:78:ARG:HB3	2:B:120:GLU:HG2	1.82	0.61
5:E:5:ASN:OD1	5:E:6:ARG:N	2.34	0.61
1:A:508:VAL:HG13	1:A:522:MET:HE1	1.83	0.61
1:A:550:MET:CE	1:A:657:TRP:HB2	2.31	0.61
2:B:268:VAL:HG11	2:B:272:ILE:HD11	1.82	0.61
2:B:568:THR:O	2:B:615:ARG:NH2	2.33	0.61
18:c:55:LEU:HD23	19:d:63:VAL:HG13	1.83	0.61
1:A:781:ALA:O	1:A:790:LYS:NZ	2.20	0.60
2:B:721:ASP:HB3	2:B:724:LYS:HG2	1.81	0.60
4:D:57:ARG:NH2	4:D:115:PHE:O	2.34	0.60
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.36	0.60
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.41	0.60
1:A:466:TYR:HB2	1:A:470:ARG:HH22	1.66	0.60
2:B:50:VAL:HG21	2:B:82:ILE:HD11	1.84	0.60
1:A:1229:MET:HB3	1:A:1241:ARG:HB2	1.83	0.60
6:F:111:ILE:HD11	6:F:114:GLU:O	2.00	0.60
2:B:875:GLU:OE2	2:B:934:LYS:NZ	2.35	0.60
1:A:697:LYS:HE3	1:A:703:LEU:HD12	1.82	0.60
11:K:65:HIS:HB3	11:K:68:PHE:HD2	1.67	0.60
14:T:104:DA:H5"	14:T:105:DT:H5"	1.83	0.60
1:A:903:MET:HE1	1:A:927:GLN:HG2	1.84	0.59
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.32	0.59
5:E:133:THR:O	5:E:185:ARG:NH2	2.36	0.59
19:d:33:SER:HB2	19:d:60:ASN:ND2	2.16	0.59
17:f:91:LYS:HE3	19:h:76:ARG:NH1	2.17	0.59
2:B:336:ILE:O	2:B:341:ARG:NH2	2.34	0.59
15:N:8:DC:H2"	15:N:9:DG:C8	2.36	0.59
7:G:5:LYS:HE2	7:G:78:VAL:HB	1.83	0.59
14:T:99:DC:H2'	14:T:100:DT:C6	2.38	0.59
2:B:759:PRO:HD2	2:B:1046:PRO:HB3	1.85	0.59
4:D:154:ASP:OD1	4:D:155:GLU:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1439:MET:SD	2:B:1139:ILE:HG23	2.42	0.59
2:B:55:ARG:CZ	2:B:78:ARG:HD2	2.31	0.59
2:B:587:SER:HA	2:B:610:ARG:HH21	1.66	0.59
3:C:55:SER:HA	3:C:151:GLN:HE21	1.68	0.59
14:T:-5:DG:OP1	16:e:42:ARG:NH2	2.35	0.59
17:f:84:MET:O	17:f:88:TYR:HD1	1.86	0.59
2:B:805:LYS:HE3	2:B:1041:GLU:HB2	1.85	0.59
1:A:1335:PHE:HD1	1:A:1384:LEU:HD21	1.67	0.59
1:A:1401:MET:HG3	1:A:1429:GLU:HG3	1.84	0.59
11:K:7:PHE:HB2	11:K:11:ILE:HD12	1.85	0.58
1:A:1130:ILE:HD13	1:A:1307:TRP:CE2	2.38	0.58
5:E:19:LYS:HD3	5:E:33:GLU:HG3	1.85	0.58
10:J:23:ARG:O	10:J:26:GLU:HG2	2.02	0.58
16:e:61:LEU:N	16:e:97:GLU:OE2	2.33	0.58
1:A:42:ASP:O	1:A:49:ARG:NH2	2.36	0.58
4:D:93:THR:HG21	4:D:102:VAL:HG21	1.85	0.58
20:u:96:THR:HG21	20:u:106:LYS:HE2	1.85	0.58
2:B:386:LYS:O	9:I:91:ARG:NH1	2.36	0.58
1:A:599:LEU:HD13	8:H:123:CYS:HB2	1.84	0.58
2:B:54:PRO:HB2	2:B:78:ARG:NH1	2.19	0.58
2:B:268:VAL:HG22	2:B:330:GLY:HA2	1.86	0.58
2:B:648:THR:OG1	2:B:650:GLU:OE2	2.20	0.58
2:B:290:LEU:O	2:B:294:CYS:N	2.31	0.58
8:H:112:LYS:HG2	8:H:125:GLU:HG3	1.85	0.58
5:E:189:LEU:HD21	5:E:195:VAL:HG13	1.86	0.58
7:G:80:LYS:HD2	7:G:81:PRO:HD2	1.86	0.58
1:A:408:ARG:HG3	1:A:414:ILE:HD11	1.85	0.58
2:B:373:TYR:HE1	2:B:572:ARG:CZ	2.16	0.58
15:N:-23:DC:OP2	16:a:72:ARG:NH2	2.36	0.58
5:E:135:GLN:NE2	5:E:137:SER:OG	2.27	0.57
14:T:111:DT:H3	15:N:-111:DA:H61	1.51	0.57
18:c:115:LEU:HD21	16:e:112:ILE:HD11	1.86	0.57
18:g:32:ARG:O	18:g:36:LYS:HG2	2.04	0.57
1:A:831:LYS:NZ	1:A:1079:THR:O	2.35	0.57
5:E:176:ARG:HD3	5:E:214:LEU:HD21	1.85	0.57
1:A:467:SER:HB3	2:B:1103:ILE:HD12	1.84	0.57
1:A:1097:THR:HG22	1:A:1102:ARG:HB2	1.87	0.57
1:A:1150:SER:N	1:A:1203:ARG:HH22	2.02	0.57
2:B:225:ILE:HD13	2:B:248:LYS:HD3	1.85	0.57
2:B:862:GLN:O	2:B:914:LYS:NZ	2.34	0.57
15:N:-47:DT:H2"	15:N:-46:DC:C5	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:HG21	1:A:152:ALA:HB1	1.87	0.57
1:A:307:ASN:HD21	1:A:315:ALA:HB3	1.69	0.57
1:A:1204:MET:HE3	1:A:1209:LEU:C	2.30	0.57
2:B:279:ARG:NH2	2:B:286:ASP:OD1	2.38	0.57
2:B:941:LEU:HD11	2:B:968:MET:SD	2.44	0.57
1:A:84:MET:HE2	1:A:271:LEU:HG	1.86	0.56
1:A:1350:SER:O	1:A:1354:GLU:HG2	2.04	0.56
2:B:225:ILE:O	2:B:252:ARG:NH2	2.37	0.56
1:A:572:LEU:HD11	8:H:46:MET:HE3	1.87	0.56
1:A:923:ASP:OD1	1:A:924:VAL:N	2.38	0.56
2:B:231:ILE:HG22	2:B:374:MET:HE1	1.87	0.56
7:G:86:VAL:HG22	7:G:146:LYS:HG2	1.86	0.56
11:K:55:ASP:HB2	11:K:81:THR:HG21	1.87	0.56
15:N:49:DC:H2''	15:N:50:DA:C8	2.41	0.56
1:A:1402:ARG:HB3	1:A:1411:ILE:HD13	1.87	0.56
4:D:139:PRO:HA	4:D:142:ILE:HB	1.88	0.56
14:T:39:DA:OP2	18:c:35:ARG:NH2	2.39	0.56
14:T:64:DA:H1'	14:T:65:DT:H5'	1.87	0.56
3:C:17:VAL:HG12	3:C:240:ALA:HB1	1.88	0.56
1:A:1078:ALA:HA	1:A:1081:MET:HG2	1.88	0.56
2:B:597:ARG:NH2	2:B:688:GLU:OE1	2.39	0.56
17:b:59:LYS:O	17:b:63:GLU:HG3	2.06	0.56
1:A:1304:GLU:HG2	1:A:1306:LEU:HD11	1.87	0.56
1:A:897:ARG:HD2	1:A:898:TYR:CZ	2.41	0.55
5:E:92:MET:HE3	5:E:96:CYS:SG	2.46	0.55
1:A:1150:SER:HA	1:A:1203:ARG:HH12	1.71	0.55
15:N:-71:DT:H2''	15:N:-70:DT:H71	1.86	0.55
9:I:96:ASN:HD21	9:I:98:THR:CG2	2.19	0.55
14:T:49:DC:O3'	19:d:30:ARG:NH2	2.40	0.55
1:A:231:ARG:HH11	1:A:232:PRO:HD2	1.71	0.55
2:B:550:PHE:HB3	2:B:593:MET:HE1	1.87	0.55
18:g:51:LEU:HD13	19:h:70:ILE:HG21	1.88	0.55
1:A:1462:PRO:HB3	7:G:17:TYR:HD1	1.72	0.55
2:B:73:LYS:HG2	2:B:125:THR:HG22	1.89	0.55
2:B:1017:ILE:HG21	2:B:1026:LEU:HD11	1.89	0.55
2:B:895:GLU:OE1	12:L:44:LYS:NZ	2.40	0.55
2:B:953:LEU:HD12	12:L:59:TYR:CE1	2.42	0.55
14:T:87:DG:O6	15:N:-88:DA:N6	2.40	0.55
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.86	0.55
2:B:789:MET:HE3	2:B:967:ARG:HB2	1.89	0.55
6:F:82:THR:HG22	6:F:84:TYR:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:e:42:ARG:HD2	16:e:43:PRO:HD2	1.88	0.55
2:B:71:ILE:HA	2:B:127:ILE:HA	1.88	0.55
14:T:-39:DT:H2"	14:T:-38:DA:C8	2.42	0.55
16:a:103:LEU:O	16:a:107:THR:HG23	2.07	0.55
16:e:72:ARG:O	16:e:76:GLN:HG3	2.07	0.55
1:A:22:LEU:HG	2:B:1213:ALA:HB2	1.89	0.55
2:B:649:LYS:HA	2:B:652:ILE:HG12	1.89	0.55
18:g:39:TYR:HB3	19:h:75:SER:HB2	1.88	0.55
5:E:93:ARG:HA	5:E:122:MET:HE1	1.89	0.54
2:B:1094:ARG:NH2	2:B:1098:MET:HE2	2.22	0.54
8:H:79:ARG:HD3	8:H:80:PRO:O	2.07	0.54
5:E:41:PHE:CE1	5:E:45:ILE:HG13	2.42	0.54
18:g:92:GLU:HG3	19:h:103:LEU:HG	1.88	0.54
1:A:1218:ILE:HD12	1:A:1270:MET:HE1	1.88	0.54
16:e:99:TYR:OH	16:e:133:GLU:OE1	2.25	0.54
2:B:86:ARG:HH21	2:B:169:PHE:HA	1.73	0.54
4:D:86:ASP:HB3	4:D:106:LEU:HB3	1.90	0.54
8:H:61:ASN:HD22	8:H:61:ASN:C	2.15	0.54
1:A:86:LEU:HD11	1:A:240:LEU:HB2	1.89	0.54
2:B:56:LEU:HD12	2:B:77:ILE:HD11	1.88	0.54
14:T:7:DC:H2"	14:T:8:DG:C8	2.43	0.54
1:A:484:ASP:HB2	2:B:987:LYS:HG3	1.89	0.54
2:B:49:LEU:O	2:B:52:GLU:HG3	2.08	0.54
4:D:106:LEU:HD23	4:D:109:LEU:HD12	1.90	0.54
2:B:214:VAL:HG21	2:B:374:MET:HG3	1.90	0.54
14:T:28:DA:OP1	17:b:79:LYS:N	2.41	0.54
18:g:102:ILE:HG23	19:h:58:ILE:HD13	1.90	0.54
2:B:660:ASP:OD1	2:B:661:ASP:N	2.40	0.54
5:E:4:ASN:OD1	5:E:5:ASN:N	2.41	0.54
18:c:24:GLN:NE2	19:d:44:GLN:HE22	2.06	0.54
1:A:1356:LEU:HD13	1:A:1371:MET:HE1	1.90	0.53
4:D:67:ARG:NH1	7:G:35:GLU:OE2	2.37	0.53
2:B:497:ARG:HD3	2:B:524:GLN:NE2	2.23	0.53
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.89	0.53
14:T:-30:DA:H1'	14:T:-29:DT:H5'	1.90	0.53
17:f:59:LYS:HE2	17:f:63:GLU:OE2	2.08	0.53
14:T:-43:DA:H5"	18:g:16:THR:HA	1.90	0.53
14:T:-27:DC:H2"	14:T:-26:DC:C5	2.43	0.53
18:g:49:VAL:HG21	19:h:118:TYR:CD2	2.43	0.53
1:A:1191:SER:HB3	1:A:1244:VAL:HB	1.91	0.53
20:u:85:LYS:HA	20:u:88:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:VAL:HG23	1:A:635:MET:HG2	1.90	0.53
18:g:39:TYR:O	19:h:75:SER:OG	2.15	0.53
2:B:214:VAL:HG11	2:B:373:TYR:HE2	1.74	0.53
2:B:885:LEU:HA	2:B:936:ASP:OD2	2.09	0.53
5:E:21:MET:HG3	5:E:186:TYR:CE1	2.44	0.53
1:A:852:HIS:ND1	6:F:139:PRO:HG3	2.24	0.53
3:C:91:CYS:SG	3:C:93:GLU:HG2	2.49	0.53
7:G:89:ALA:HB2	7:G:103:VAL:HG22	1.91	0.53
9:I:108:LYS:HD3	9:I:110:PHE:HB3	1.90	0.53
2:B:278:PHE:HB3	2:B:289:ILE:CD1	2.38	0.53
9:I:54:GLU:HG2	9:I:100:PHE:HZ	1.74	0.52
14:T:-17:DT:H4'	14:T:-16:DT:OP1	2.08	0.52
1:A:12:ARG:HH22	2:B:1192:TYR:HD1	1.57	0.52
2:B:644:GLU:N	2:B:644:GLU:OE1	2.43	0.52
14:T:-45:DG:H2''	14:T:-44:DG:C8	2.44	0.52
1:A:1194:LEU:HD11	1:A:1241:ARG:HB3	1.91	0.52
2:B:840:ILE:HG12	2:B:992:VAL:HG12	1.91	0.52
3:C:145:CYS:SG	3:C:146:LYS:N	2.83	0.52
1:A:218:GLU:O	1:A:222:ARG:HD2	2.10	0.52
1:A:1289:LYS:HD2	1:A:1305:GLU:HG2	1.91	0.52
1:A:697:LYS:HA	1:A:702:GLU:OE2	2.10	0.52
2:B:1149:GLU:HA	2:B:1153:GLU:OE1	2.10	0.52
3:C:13:GLN:HE21	3:C:16:GLU:HG2	1.75	0.52
6:F:137:TYR:HD1	6:F:143:TYR:HB3	1.74	0.52
3:C:47:LEU:HD11	12:L:68:GLN:HB3	1.92	0.52
2:B:80:GLY:N	2:B:118:ASP:O	2.41	0.52
14:T:43:DA:H1'	14:T:44:DT:H5'	1.91	0.52
1:A:548:MET:HE1	11:K:59:VAL:N	2.19	0.52
1:A:1331:TYR:HD1	5:E:148:LEU:HD11	1.75	0.52
1:A:1145:LEU:O	1:A:1149:THR:OG1	2.11	0.52
2:B:209:SER:OG	2:B:232:ARG:NH1	2.43	0.52
2:B:330:GLY:HA3	2:B:344:TYR:HE2	1.74	0.52
3:C:248:ILE:O	3:C:252:GLN:HG3	2.10	0.52
14:T:20:DG:H2''	14:T:21:DG:O5'	2.09	0.52
1:A:459:HIS:NE2	1:A:479:TYR:OH	2.37	0.51
1:A:853:TYR:OH	6:F:89:GLU:OE2	2.16	0.51
1:A:1270:MET:HA	1:A:1274:ILE:HG12	1.93	0.51
15:N:70:DC:H2''	15:N:71:DA:H5''	1.92	0.51
2:B:489:ARG:NH2	2:B:533:SER:O	2.44	0.51
9:I:70:ARG:NH1	9:I:82:ASP:OD1	2.43	0.51
14:T:69:DC:H2''	14:T:70:DA:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:PHE:HD1	1:A:819:MET:HE3	1.75	0.51
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.91	0.51
11:K:104:LYS:HA	11:K:107:GLU:HG2	1.91	0.51
18:g:16:THR:HG23	18:g:19:SER:H	1.75	0.51
1:A:388:ARG:HG2	1:A:392:TYR:CE2	2.46	0.51
1:A:1339:LEU:HD22	1:A:1384:LEU:HD13	1.92	0.51
7:G:37:THR:O	7:G:45:ILE:HG22	2.11	0.51
17:f:92:ARG:HH12	19:h:98:LEU:HD23	1.76	0.51
16:e:82:LEU:HD12	17:f:81:VAL:HG23	1.92	0.51
17:f:84:MET:HE3	17:f:88:TYR:HE1	1.75	0.51
1:A:61:ILE:HA	1:A:74:MET:SD	2.51	0.51
1:A:1214:VAL:O	1:A:1218:ILE:HG12	2.11	0.51
2:B:760:ASP:OD1	2:B:760:ASP:N	2.44	0.51
3:C:146:LYS:HB2	10:J:60:LEU:HD11	1.93	0.51
4:D:38:GLN:HG3	4:D:39:TYR:H	1.76	0.51
15:N:-35:DA:H5'	15:N:-35:DA:C8	2.45	0.51
2:B:299:ASP:OD2	2:B:385:ARG:NH2	2.43	0.51
2:B:776:GLN:HB3	2:B:1096:ARG:HG2	1.92	0.51
14:T:52:DC:H5'	14:T:52:DC:C6	2.45	0.51
5:E:97:LEU:O	5:E:101:GLU:HB2	2.10	0.51
2:B:268:VAL:HG13	2:B:329:ARG:HB3	1.92	0.51
18:g:63:LEU:HD22	19:h:42:LEU:HD12	1.93	0.51
1:A:982:ASP:O	1:A:1041:ARG:NH1	2.44	0.51
2:B:278:PHE:HB3	2:B:289:ILE:HD12	1.93	0.51
2:B:761:HIS:HB2	2:B:1024:ALA:HB2	1.92	0.51
9:I:87:GLN:HA	9:I:99:LEU:HA	1.91	0.51
15:N:17:DA:OP2	16:e:69:ARG:NH2	2.40	0.51
16:a:73:GLU:HB2	17:b:22:LEU:HB3	1.92	0.51
1:A:321:ARG:HH12	13:P:4:G:H4'	1.75	0.50
15:N:40:DG:H1'	15:N:41:DT:H5'	1.93	0.50
1:A:371:ILE:HD11	2:B:1103:ILE:HG13	1.93	0.50
1:A:948:VAL:O	5:E:200:ARG:HD2	2.10	0.50
15:N:-50:DC:H2''	15:N:-49:DG:C8	2.46	0.50
1:A:535:MET:O	1:A:575:GLY:HA3	2.09	0.50
1:A:976:ASP:HB3	8:H:135:LYS:HZ3	1.77	0.50
2:B:821:GLN:OE1	2:B:851:PHE:N	2.39	0.50
2:B:950:ASP:OD1	2:B:969:ARG:NH1	2.44	0.50
1:A:494:GLN:HB2	2:B:1149:GLU:OE2	2.10	0.50
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	1.93	0.50
2:B:1039:GLY:HA2	10:J:50:LEU:HD11	1.93	0.50
3:C:148:ARG:HG2	10:J:60:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:b:91:LYS:HB2	17:b:96:THR:HG22	1.93	0.50
16:e:90:MET:HE3	16:e:90:MET:HA	1.94	0.50
18:g:29:ARG:HD3	19:h:32:GLU:OE2	2.11	0.50
18:g:81:ARG:NH1	18:g:107:VAL:O	2.30	0.50
1:A:528:THR:HG23	1:A:654:VAL:HB	1.93	0.50
1:A:712:ARG:HH21	9:I:93:LYS:HA	1.76	0.50
5:E:44:LYS:HG3	5:E:45:ILE:HG12	1.93	0.50
9:I:90:GLN:HG3	9:I:92:ARG:HG3	1.93	0.50
15:N:-14:DA:H2''	15:N:-13:DA:C8	2.47	0.50
1:A:493:PRO:HG3	1:A:502:LEU:HD12	1.94	0.50
2:B:55:ARG:NH1	2:B:78:ARG:HD2	2.26	0.50
2:B:618:LYS:HE3	2:B:620:PHE:HE2	1.77	0.50
7:G:43:GLY:HA2	7:G:80:LYS:HD3	1.93	0.50
1:A:882:GLN:NE2	1:A:961:ASN:HA	2.27	0.50
17:b:82:THR:HG23	17:b:85:ASP:H	1.76	0.50
18:g:32:ARG:HH11	18:g:36:LYS:HD3	1.76	0.50
1:A:15:LYS:O	1:A:1424:CYS:HB2	2.12	0.50
2:B:866:PHE:HB2	2:B:870:ILE:HG22	1.93	0.50
5:E:135:GLN:HE21	5:E:137:SER:HG	1.52	0.50
9:I:7:CYS:N	9:I:12:ASN:O	2.43	0.50
10:J:1:MET:HE2	10:J:59:PHE:HE2	1.77	0.50
17:b:35:ARG:O	17:b:39:ARG:HG2	2.12	0.50
2:B:865:ARG:HA	2:B:871:VAL:HG12	1.93	0.49
7:G:153:ASP:HB3	7:G:156:GLU:O	2.12	0.49
18:c:26:PRO:HD3	19:d:37:TYR:CD2	2.47	0.49
1:A:636:ARG:NH2	1:A:878:GLN:OE1	2.46	0.49
1:A:1348:ARG:NE	1:A:1376:ASP:OD1	2.45	0.49
3:C:4:GLU:O	3:C:6:LYS:NZ	2.45	0.49
1:A:14:VAL:N	1:A:1435:GLN:OE1	2.45	0.49
8:H:25:ARG:HG3	8:H:25:ARG:HH11	1.77	0.49
15:N:68:DT:H2''	15:N:69:DC:C6	2.47	0.49
18:c:29:ARG:NH1	19:d:33:SER:O	2.45	0.49
1:A:926:LEU:HD11	1:A:986:PRO:HD3	1.93	0.49
1:A:1354:GLU:O	1:A:1358:VAL:HG23	2.12	0.49
2:B:109:LEU:O	2:B:198:GLY:N	2.44	0.49
2:B:1160:VAL:HG11	2:B:1201:LYS:HG3	1.94	0.49
15:N:30:DT:H2'	15:N:31:DT:H71	1.94	0.49
1:A:1200:ASP:H	1:A:1203:ARG:NH2	2.11	0.49
2:B:427:ARG:NH1	2:B:428:CYS:HB2	2.28	0.49
2:B:802:PRO:HG3	2:B:809:MET:HE1	1.95	0.49
5:E:36:GLN:OE1	5:E:40:GLU:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:g:74:LYS:HD3	18:g:74:LYS:N	2.28	0.49
2:B:384:GLU:HA	9:I:91:ARG:HH12	1.77	0.49
2:B:551:LEU:HB3	2:B:556:MET:HE2	1.95	0.49
2:B:655:ILE:HD11	2:B:681:LEU:HD11	1.94	0.49
5:E:77:LEU:HD11	5:E:108:ILE:HG13	1.94	0.49
15:N:5:DC:H2"	15:N:6:DC:C5	2.47	0.49
1:A:41:MET:HG3	1:A:45:ARG:H	1.78	0.49
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.53	0.49
1:A:806:LEU:HA	2:B:1023:VAL:HG11	1.95	0.49
1:A:875:ASP:HB2	1:A:1060:VAL:HA	1.95	0.49
1:A:1446:VAL:HA	6:F:133:VAL:O	2.12	0.49
2:B:27:GLU:OE1	2:B:678:TRP:HB3	2.13	0.49
2:B:883:LEU:HB2	2:B:932:HIS:HE1	1.78	0.49
3:C:51:LYS:HB2	3:C:154:ASN:HB3	1.95	0.49
1:A:84:MET:HE1	1:A:270:ILE:HG22	1.93	0.49
2:B:45:SER:O	2:B:49:LEU:HG	2.13	0.49
1:A:80:HIS:H	1:A:244:PRO:HB3	1.78	0.48
15:N:-54:DA:OP2	19:d:53:SER:HB3	2.13	0.48
1:A:890:SER:HB3	1:A:1300:GLU:HB2	1.95	0.48
2:B:165:LEU:HD11	2:B:195:VAL:HG23	1.95	0.48
5:E:21:MET:HG3	5:E:186:TYR:CD1	2.48	0.48
14:T:50:DG:H5'	19:d:30:ARG:HH22	1.76	0.48
2:B:376:ASN:O	2:B:380:LEU:HD23	2.13	0.48
2:B:269:LYS:HG3	2:B:331:SER:HB2	1.95	0.48
7:G:83:LYS:HG3	7:G:148:VAL:HA	1.94	0.48
9:I:13:MET:HE1	9:I:15:TYR:CE1	2.49	0.48
14:T:70:DA:P	16:e:42:ARG:HB2	2.53	0.48
14:T:87:DG:C6	15:N:-88:DA:N6	2.82	0.48
18:c:30:VAL:HG13	19:d:67:PHE:HE2	1.79	0.48
19:h:96:ARG:HE	19:h:108:VAL:HG21	1.78	0.48
1:A:1118:LEU:HD13	1:A:1319:VAL:HG11	1.94	0.48
2:B:99:MET:HE2	2:B:104:ALA:HB2	1.95	0.48
4:D:57:ARG:HD3	4:D:109:LEU:HB3	1.94	0.48
4:D:108:TYR:HE2	7:G:89:ALA:HA	1.78	0.48
9:I:15:TYR:O	9:I:28:SER:N	2.35	0.48
14:T:-14:DA:H5"	16:e:63:ARG:HH21	1.79	0.48
1:A:866:GLN:NE2	1:A:1376:ASP:OD2	2.42	0.48
2:B:573:ILE:HD11	2:B:583:HIS:HB2	1.94	0.48
2:B:649:LYS:HE3	2:B:652:ILE:HD11	1.94	0.48
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.48	0.48
2:B:837:ASP:OD1	2:B:1020:ARG:NH1	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:ASP:O	1:A:1127:ALA:N	2.47	0.48
2:B:301:GLN:HE22	9:I:50:THR:HG1	1.61	0.48
7:G:44:TYR:OH	7:G:106:LEU:HD21	2.14	0.48
2:B:916:THR:OG1	2:B:935:ARG:HG3	2.14	0.48
20:u:85:LYS:O	20:u:88:VAL:HG22	2.14	0.48
1:A:706:LYS:CG	1:A:707:PRO:HD2	2.44	0.48
1:A:1152:THR:HA	1:A:1197:LEU:HA	1.96	0.48
4:D:85:ASP:O	4:D:89:LEU:N	2.44	0.48
14:T:110:DT:H2''	14:T:111:DT:H72	1.95	0.48
15:N:-70:DT:H2''	15:N:-69:DG:N7	2.29	0.48
18:g:20:ARG:HD2	19:h:118:TYR:CE1	2.49	0.48
1:A:1065:MET:SD	1:A:1439:MET:HG3	2.54	0.48
1:A:1122:LEU:HD13	1:A:1126:ILE:HG22	1.96	0.48
2:B:479:TYR:CZ	2:B:1096:ARG:HB3	2.48	0.48
18:g:29:ARG:NH1	19:h:32:GLU:OE2	2.46	0.48
2:B:493:THR:HG22	2:B:528:LEU:O	2.14	0.47
9:I:19:ASP:O	9:I:23:GLN:N	2.36	0.47
7:G:56:VAL:HA	7:G:72:VAL:HG12	1.96	0.47
14:T:10:DG:H5''	16:a:40:ARG:HG3	1.96	0.47
19:h:76:ARG:O	19:h:80:TYR:HD2	1.96	0.47
1:A:526:GLN:HG2	2:B:836:GLU:HG3	1.96	0.47
3:C:98:LEU:HB3	3:C:118:LEU:HD22	1.96	0.47
4:D:140:PHE:O	4:D:144:GLN:HG2	2.13	0.47
4:D:153:VAL:O	4:D:157:ILE:HG12	2.14	0.47
7:G:151:ARG:O	7:G:157:ILE:HG23	2.14	0.47
8:H:102:LYS:HE2	8:H:104:GLU:HG2	1.96	0.47
15:N:-57:DC:H2''	15:N:-56:DC:C5	2.49	0.47
19:h:33:SER:HA	19:h:60:ASN:HD21	1.79	0.47
4:D:100:GLY:HA2	4:D:103:LYS:HG2	1.95	0.47
8:H:96:MET:HE2	8:H:117:PHE:HB3	1.96	0.47
18:c:38:ASN:ND2	18:g:41:GLU:OE2	2.48	0.47
1:A:237:ILE:HG12	2:B:1211:ASN:ND2	2.30	0.47
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.79	0.47
10:J:7:CYS:HA	10:J:48:MET:HG3	1.96	0.47
18:g:63:LEU:HD11	19:h:38:VAL:HG13	1.96	0.47
2:B:273:PRO:HD2	2:B:276:ILE:HD12	1.96	0.47
4:D:54:SER:O	4:D:58:LEU:HG	2.15	0.47
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.50	0.47
11:K:50:LEU:HD13	11:K:75:LEU:HD13	1.97	0.47
1:A:1289:LYS:HD3	1:A:1306:LEU:O	2.15	0.47
2:B:39:ASP:O	2:B:43:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:865:ARG:NE	2:B:867:GLY:O	2.46	0.47
3:C:195:VAL:HG22	3:C:200:GLU:OE2	2.15	0.47
4:D:108:TYR:OH	7:G:102:ASP:O	2.24	0.47
7:G:100:PHE:CD2	7:G:109:PHE:HB3	2.48	0.47
16:a:134:ARG:HH12	18:c:95:LYS:HA	1.80	0.47
1:A:1331:TYR:CZ	1:A:1353:LYS:HD3	2.49	0.47
8:H:111:ILE:HG13	8:H:128:TYR:HA	1.97	0.47
11:K:29:ASN:ND2	11:K:78:GLU:O	2.48	0.47
1:A:183:TRP:CZ3	1:A:202:LEU:HG	2.50	0.47
1:A:456:MET:HE2	2:B:1137:CYS:HB2	1.96	0.47
1:A:910:LYS:O	1:A:913:VAL:HG22	2.15	0.47
1:A:1048:LEU:O	1:A:1052:GLU:OE1	2.33	0.47
2:B:74:ARG:HD2	2:B:124:PHE:HB2	1.96	0.47
2:B:532:LEU:HB3	2:B:536:SER:OG	2.14	0.47
3:C:61:PHE:CE1	3:C:65:ARG:HD2	2.50	0.47
17:b:88:TYR:CZ	19:d:80:TYR:HE1	2.32	0.47
20:u:95:GLN:NE2	20:u:105:PHE:HE1	2.13	0.47
1:A:318:LYS:HE3	15:N:-105:DA:C6	2.48	0.47
1:A:706:LYS:HD2	1:A:709:MET:SD	2.55	0.47
2:B:773:MET:HE1	2:B:987:LYS:HB3	1.97	0.47
4:D:67:ARG:NH2	7:G:48:VAL:O	2.48	0.47
5:E:169:LEU:HD22	5:E:173:GLN:HB2	1.97	0.47
14:T:70:DA:H2''	14:T:71:DA:O5'	2.14	0.47
15:N:16:DA:H1'	15:N:17:DA:N7	2.30	0.47
1:A:108:MET:O	1:A:108:MET:HG2	2.15	0.46
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.14	0.46
1:A:350:ALA:HB2	1:A:375:LEU:HD11	1.96	0.46
1:A:529:LEU:HB3	1:A:752:SER:HB3	1.97	0.46
1:A:976:ASP:HB3	8:H:135:LYS:NZ	2.29	0.46
1:A:948:VAL:HA	5:E:200:ARG:HG3	1.98	0.46
3:C:53:ASN:ND2	3:C:59:ASP:OD1	2.28	0.46
7:G:2:PHE:HA	7:G:79:TRP:HA	1.97	0.46
7:G:116:PRO:HG2	7:G:119:LEU:HD12	1.97	0.46
14:T:-28:DC:H2''	14:T:-27:DC:C6	2.50	0.46
14:T:62:DG:H2''	14:T:63:DG:C8	2.51	0.46
14:T:109:DT:H2''	14:T:110:DT:C7	2.46	0.46
1:A:580:SER:HB3	1:A:612:LYS:HA	1.98	0.46
2:B:245:MET:SD	2:B:247:ILE:HD11	2.55	0.46
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.50	0.46
15:N:45:DC:H2''	15:N:46:DA:N7	2.31	0.46
1:A:368:PRO:HB3	1:A:467:SER:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:ARG:NH1	2:B:78:ARG:HB2	2.30	0.46
7:G:2:PHE:HB3	7:G:79:TRP:HD1	1.81	0.46
8:H:89:ALA:HB1	8:H:95:VAL:HG21	1.98	0.46
1:A:449:PRO:HG3	14:T:94:DG:H21	1.81	0.46
1:A:706:LYS:HG2	1:A:707:PRO:HD2	1.97	0.46
1:A:1204:MET:HE3	1:A:1209:LEU:HB3	1.98	0.46
2:B:301:GLN:CD	9:I:52:ILE:HD12	2.41	0.46
2:B:328:ARG:HH21	2:B:338:ARG:NH2	2.14	0.46
12:L:33:CYS:SG	12:L:34:GLY:N	2.88	0.46
14:T:62:DG:H2"	14:T:63:DG:H8	1.81	0.46
18:g:54:VAL:HG21	19:h:95:VAL:HG21	1.98	0.46
1:A:636:ARG:HG3	1:A:880:GLU:OE2	2.15	0.46
2:B:574:PHE:CE2	2:B:579:TRP:HB2	2.50	0.46
2:B:586:PRO:O	2:B:590:VAL:HG23	2.15	0.46
6:F:108:LEU:HD12	6:F:129:LYS:O	2.15	0.46
7:G:95:SER:OG	7:G:98:GLY:O	2.22	0.46
7:G:102:ASP:HA	7:G:107:ASN:HA	1.98	0.46
17:b:77:LYS:HE3	19:d:89:ARG:NH2	2.31	0.46
16:e:103:LEU:HD11	16:e:128:ARG:HG2	1.97	0.46
1:A:758:ASN:O	1:A:762:MET:HG3	2.15	0.46
3:C:80:LYS:HG3	3:C:94:CYS:HB3	1.97	0.46
1:A:70:CYS:HB2	2:B:1173:ALA:O	2.16	0.46
1:A:209:LEU:O	1:A:213:LYS:HG3	2.15	0.46
1:A:363:ASP:HB3	1:A:509:PRO:HD3	1.98	0.46
1:A:620:LYS:HD2	1:A:751:GLY:O	2.16	0.46
1:A:710:THR:HG22	1:A:711:LEU:N	2.31	0.46
1:A:874:LEU:HD23	1:A:1059:LEU:HD23	1.97	0.46
1:A:1193:TRP:HB3	1:A:1263:LEU:HD22	1.97	0.46
9:I:96:ASN:ND2	9:I:98:THR:OG1	2.49	0.46
17:f:92:ARG:HH12	19:h:98:LEU:CD2	2.28	0.46
1:A:1120:VAL:HB	1:A:1309:LEU:HB2	1.96	0.46
5:E:116:THR:HG23	5:E:117:PRO:HD2	1.97	0.46
8:H:133:SER:O	8:H:136:GLN:NE2	2.47	0.46
14:T:-23:DT:H5"	16:e:83:ARG:HG2	1.98	0.46
1:A:307:ASN:ND2	1:A:315:ALA:HB3	2.31	0.45
1:A:462:LYS:HD3	1:A:464:MET:HE3	1.98	0.45
2:B:776:GLN:OE1	2:B:1097:HIS:NE2	2.45	0.45
1:A:62:ASP:OD1	1:A:63:ARG:N	2.48	0.45
1:A:260:GLN:HB2	1:A:265:HIS:CD2	2.51	0.45
2:B:497:ARG:HB3	2:B:524:GLN:HE21	1.81	0.45
2:B:797:TYR:CE1	2:B:854:LEU:HG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:29:LYS:HE2	10:J:37:GLU:OE2	2.16	0.45
11:K:77:THR:HB	11:K:81:THR:CG2	2.41	0.45
14:T:-54:DC:H2''	14:T:-53:DA:C8	2.51	0.45
14:T:-5:DG:H8	14:T:-5:DG:OP2	1.99	0.45
14:T:108:DC:H2''	14:T:109:DT:H72	1.97	0.45
1:A:122:MET:O	1:A:126:ILE:HG12	2.16	0.45
2:B:956:THR:HG23	12:L:48:VAL:HG21	1.99	0.45
15:N:-42:DT:H1'	15:N:-41:DG:H5'	1.99	0.45
15:N:26:DG:H2''	15:N:27:DG:C8	2.51	0.45
1:A:266:LYS:HD2	1:A:266:LYS:HA	1.82	0.45
1:A:464:MET:SD	1:A:470:ARG:HG3	2.56	0.45
2:B:587:SER:HA	2:B:610:ARG:NH2	2.31	0.45
2:B:1039:GLY:HA2	10:J:50:LEU:CD1	2.47	0.45
9:I:96:ASN:HD21	9:I:98:THR:HG23	1.80	0.45
11:K:7:PHE:HA	11:K:10:PHE:CE1	2.51	0.45
1:A:454:MET:HG2	1:A:511:GLN:HB3	1.97	0.45
1:A:1447:MET:HB2	6:F:133:VAL:HB	1.97	0.45
1:A:1462:PRO:HB3	7:G:17:TYR:CD1	2.52	0.45
14:T:101:DC:H2''	14:T:102:DC:C6	2.52	0.45
1:A:473:LEU:HD23	2:B:836:GLU:OE2	2.17	0.45
1:A:635:MET:HE1	1:A:640:PRO:HB3	1.98	0.45
2:B:756:ILE:HG12	2:B:770:GLN:HG2	1.99	0.45
1:A:1389:ARG:HD2	1:A:1407:GLU:OE2	2.17	0.45
4:D:163:LEU:HD22	4:D:171:LEU:HD21	1.99	0.45
5:E:37:SER:OG	5:E:40:GLU:HG2	2.16	0.45
14:T:67:DC:H2''	14:T:68:DC:C5	2.52	0.45
14:T:89:DG:H2''	14:T:90:DG:OP1	2.17	0.45
14:T:111:DT:H3	15:N:-111:DA:N6	2.13	0.45
1:A:327:ARG:HD2	1:A:1409:VAL:HG11	1.97	0.45
1:A:550:MET:HE1	1:A:657:TRP:HB2	1.98	0.45
1:A:1450:GLU:O	1:A:1454:THR:HG23	2.17	0.45
7:G:45:ILE:HD12	7:G:77:VAL:O	2.17	0.45
16:a:113:HIS:NE2	16:e:123:ASP:OD1	2.49	0.45
17:b:70:VAL:O	17:b:74:GLU:HG3	2.17	0.45
9:I:23:GLN:OE1	9:I:23:GLN:HA	2.17	0.45
14:T:-42:DG:C6	14:T:-41:DA:N6	2.84	0.45
2:B:119:MET:HE3	2:B:156:VAL:HB	1.99	0.45
2:B:373:TYR:HE1	2:B:572:ARG:NH2	2.15	0.45
2:B:884:ARG:HD3	13:P:-1:A:C5	2.51	0.45
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.50	0.45
8:H:25:ARG:HG3	8:H:25:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:-25:DA:H1'	15:N:-24:DG:C8	2.52	0.45
1:A:414:ILE:O	1:A:416:LEU:HD12	2.16	0.44
1:A:1194:LEU:HD12	1:A:1242:CYS:O	2.17	0.44
2:B:307:LYS:HG3	2:B:308:PRO:HD3	1.99	0.44
4:D:151:GLU:HG2	4:D:152:ASP:N	2.33	0.44
16:a:61:LEU:HD11	17:b:40:ARG:HE	1.82	0.44
1:A:120:PRO:HA	1:A:123:ALA:HB3	1.99	0.44
1:A:527:ASP:OD2	2:B:835:GLN:HG2	2.16	0.44
1:A:916:TYR:CZ	1:A:984:THR:HA	2.52	0.44
2:B:186:CYS:HA	10:J:62:TYR:OH	2.16	0.44
2:B:208:ARG:HE	2:B:400:ASP:CG	2.26	0.44
2:B:383:LEU:O	2:B:383:LEU:HD23	2.16	0.44
2:B:652:ILE:HG13	2:B:653:ARG:N	2.31	0.44
3:C:4:GLU:HB3	3:C:5:PRO:HD3	1.99	0.44
5:E:59:PHE:HE2	5:E:61:ALA:HB2	1.81	0.44
5:E:63:PRO:CB	5:E:68:LEU:HD21	2.47	0.44
7:G:108:VAL:HG22	7:G:159:ALA:HB3	1.98	0.44
15:N:-59:DT:H2''	15:N:-58:DG:C8	2.52	0.44
15:N:35:DC:H2''	15:N:36:DC:C5	2.53	0.44
1:A:87:ALA:O	1:A:88:LYS:HD2	2.17	0.44
1:A:204:THR:OG1	1:A:207:GLU:OE1	2.25	0.44
2:B:399:LEU:HD23	2:B:399:LEU:HA	1.72	0.44
3:C:148:ARG:HB2	3:C:151:GLN:OE1	2.18	0.44
3:C:251:LEU:O	3:C:255:LEU:HD23	2.16	0.44
17:f:89:ALA:O	17:f:92:ARG:HB2	2.17	0.44
1:A:846:LEU:HA	1:A:849:ILE:HD12	1.99	0.44
1:A:852:HIS:CG	6:F:139:PRO:HG3	2.52	0.44
1:A:1456:LEU:HD21	6:F:108:LEU:HD22	2.00	0.44
11:K:63:VAL:HG23	11:K:63:VAL:O	2.18	0.44
15:N:-30:DG:H2''	15:N:-29:DC:OP2	2.18	0.44
15:N:70:DC:OP1	16:a:42:ARG:HG3	2.18	0.44
1:A:1122:LEU:HD21	1:A:1309:LEU:HD13	1.98	0.44
2:B:165:LEU:HD22	2:B:193:TYR:CE2	2.53	0.44
2:B:302:MET:HE1	2:B:380:LEU:HD22	1.99	0.44
5:E:60:LEU:HB2	5:E:78:TRP:HZ3	1.83	0.44
12:L:65:ARG:HG3	12:L:66:MET:H	1.82	0.44
14:T:-63:DT:C2	14:T:-62:DA:N7	2.86	0.44
1:A:116:ASP:CG	1:A:165:ARG:HH21	2.25	0.44
1:A:498:THR:HG22	2:B:1146:PHE:HA	1.99	0.44
1:A:1200:ASP:H	1:A:1203:ARG:HH21	1.66	0.44
2:B:367:LYS:O	2:B:371:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:ASP:HB3	2:B:393:HIS:HB2	1.98	0.44
5:E:12:TRP:HB2	5:E:41:PHE:CD2	2.53	0.44
5:E:135:GLN:O	5:E:139:LEU:HD23	2.16	0.44
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.53	0.44
19:d:112:THR:HA	19:d:115:VAL:HG12	1.99	0.44
1:A:231:ARG:HD2	1:A:232:PRO:HD2	1.99	0.44
1:A:445:PHE:CD2	1:A:488:MET:HE2	2.52	0.44
1:A:748:VAL:HG21	1:A:759:ILE:HD11	2.00	0.44
2:B:860:MET:SD	2:B:861:ASP:N	2.90	0.44
2:B:946:ASN:O	2:B:968:MET:HE2	2.18	0.44
9:I:13:MET:HE1	9:I:15:TYR:CZ	2.52	0.44
9:I:70:ARG:NH2	9:I:82:ASP:OD2	2.51	0.44
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.99	0.44
11:K:63:VAL:HG12	11:K:71:PHE:HB3	1.99	0.44
12:L:53:CYS:SG	12:L:55:HIS:CG	3.11	0.44
14:T:90:DG:H2''	14:T:91:DA:C8	2.53	0.44
1:A:21:LEU:HD11	1:A:95:PHE:CE2	2.53	0.44
1:A:273:ALA:O	1:A:277:VAL:HG23	2.17	0.44
2:B:260:THR:HG21	2:B:312:GLU:OE1	2.18	0.44
3:C:47:LEU:HD23	3:C:158:ILE:HG13	2.00	0.44
4:D:120:THR:O	4:D:124:VAL:HG23	2.18	0.44
8:H:117:PHE:HE2	8:H:122:MET:HB2	1.83	0.44
14:T:-34:DA:OP1	19:h:83:ARG:HD3	2.17	0.44
16:a:107:THR:HG22	16:a:124:ILE:HA	2.00	0.44
1:A:844:LYS:HA	1:A:844:LYS:HD2	1.76	0.44
1:A:1074:ILE:HD11	1:A:1371:MET:HG2	1.99	0.44
5:E:110:ILE:HD12	5:E:134:PHE:HB2	2.00	0.44
7:G:46:VAL:HG13	7:G:47:THR:H	1.83	0.44
14:T:-14:DA:H5''	16:e:63:ARG:NH2	2.33	0.44
14:T:49:DC:H2''	14:T:50:DG:C8	2.53	0.44
15:N:70:DC:H1'	15:N:71:DA:O4'	2.18	0.44
1:A:466:TYR:CZ	11:K:4:PRO:HD2	2.53	0.43
1:A:880:GLU:OE1	1:A:964:ARG:NH2	2.39	0.43
2:B:279:ARG:NH1	2:B:313:GLY:O	2.51	0.43
2:B:778:MET:HE1	2:B:1098:MET:CE	2.44	0.43
5:E:63:PRO:HB2	5:E:68:LEU:HD21	1.99	0.43
8:H:145:ARG:HE	8:H:145:ARG:HB2	1.69	0.43
15:N:47:DG:H2''	15:N:48:DG:C8	2.53	0.43
18:c:63:LEU:HD13	19:d:42:LEU:HB2	1.99	0.43
1:A:830:VAL:O	2:B:500:LYS:NZ	2.51	0.43
2:B:60:GLN:O	2:B:60:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:66:GLU:O	5:E:69:GLU:HG3	2.19	0.43
5:E:85:PRO:HA	5:E:112:GLN:HB2	2.00	0.43
15:N:-67:DG:H2''	15:N:-66:DA:C8	2.53	0.43
18:g:79:ILE:HG12	18:g:82:HIS:CE1	2.53	0.43
1:A:326:ILE:O	1:A:329:ARG:HB2	2.18	0.43
1:A:529:LEU:HD23	1:A:752:SER:HA	1.99	0.43
1:A:704:GLU:O	1:A:704:GLU:HG2	2.18	0.43
1:A:984:THR:HB	1:A:986:PRO:HD2	2.00	0.43
3:C:173:CYS:SG	3:C:243:VAL:HG11	2.58	0.43
9:I:96:ASN:CG	9:I:98:THR:H	2.26	0.43
14:T:-17:DT:H6	14:T:-17:DT:H2'	1.71	0.43
16:a:73:GLU:OE1	17:b:25:ASN:ND2	2.33	0.43
1:A:307:ASN:OD1	1:A:314:GLN:HB3	2.18	0.43
1:A:1043:ALA:O	1:A:1047:VAL:HG23	2.19	0.43
4:D:57:ARG:HE	4:D:113:ALA:HB2	1.83	0.43
7:G:44:TYR:CZ	7:G:106:LEU:HD21	2.53	0.43
11:K:12:LEU:HD13	11:K:37:ARG:NH1	2.34	0.43
11:K:18:LYS:HE2	11:K:37:ARG:HH12	1.84	0.43
12:L:33:CYS:SG	12:L:35:ALA:N	2.88	0.43
15:N:-91:DT:H2'	15:N:-90:DC:C6	2.54	0.43
1:A:983:LEU:HD13	1:A:1041:ARG:HA	2.01	0.43
2:B:395:GLY:HA3	2:B:693:GLU:HG2	2.00	0.43
2:B:834:ASN:OD1	2:B:834:ASN:N	2.51	0.43
4:D:98:ALA:O	4:D:102:VAL:HG23	2.18	0.43
5:E:87:VAL:HG23	5:E:91:THR:HB	2.00	0.43
14:T:1:DC:H2''	14:T:2:DG:C8	2.54	0.43
15:N:-24:DG:OP1	16:a:85:GLN:HG2	2.19	0.43
16:a:65:LEU:HD12	16:a:65:LEU:HA	1.89	0.43
1:A:96:ILE:HG22	1:A:177:LYS:HD2	2.01	0.43
1:A:203:LEU:HA	1:A:207:GLU:OE2	2.18	0.43
1:A:516:GLN:NE2	1:A:1366:VAL:HG22	2.34	0.43
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.54	0.43
19:d:64:ASN:O	19:d:68:GLU:HG2	2.19	0.43
1:A:456:MET:HE3	2:B:1138:MET:CE	2.43	0.43
2:B:31:VAL:HG11	2:B:488:LEU:HD13	2.01	0.43
2:B:1171:VAL:HG22	2:B:1191:ILE:HD12	2.00	0.43
15:N:-69:DG:H1'	15:N:-68:DG:H5'	2.00	0.43
1:A:10:PRO:HB3	7:G:10:ILE:HD11	2.00	0.43
1:A:848:ASP:OD1	1:A:848:ASP:N	2.51	0.43
1:A:1429:GLU:O	1:A:1433:LEU:HD13	2.18	0.43
2:B:106:LEU:HD22	2:B:953:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:46:VAL:HG13	7:G:47:THR:N	2.33	0.43
1:A:40:ILE:HG23	1:A:54:ASN:OD1	2.19	0.43
1:A:466:TYR:O	1:A:468:THR:N	2.52	0.43
1:A:684:ILE:HG21	1:A:802:GLU:HG3	2.00	0.43
1:A:943:PHE:HD1	1:A:947:ILE:HD12	1.84	0.43
1:A:1218:ILE:HG23	1:A:1270:MET:HE1	2.01	0.43
18:c:102:ILE:HG23	19:d:58:ILE:HD13	2.01	0.43
1:A:12:ARG:NH2	2:B:1192:TYR:CD1	2.82	0.43
1:A:95:PHE:CE1	1:A:1417:ALA:HB2	2.53	0.43
1:A:182:LEU:O	1:A:203:LEU:HB2	2.18	0.43
2:B:86:ARG:NH2	2:B:169:PHE:HA	2.33	0.43
11:K:36:GLU:OE1	11:K:70:ASN:HB3	2.19	0.43
14:T:-48:DC:H2''	14:T:-47:DC:C5	2.54	0.43
1:A:1441:THR:O	6:F:92:ARG:HD3	2.19	0.42
2:B:571:THR:HG21	2:B:586:PRO:HB3	2.01	0.42
7:G:129:ALA:HB1	7:G:137:ILE:O	2.19	0.42
8:H:61:ASN:O	8:H:61:ASN:ND2	2.27	0.42
1:A:833:ALA:HB3	2:B:500:LYS:HZ1	1.84	0.42
1:A:1216:ASP:O	1:A:1220:GLU:HG2	2.19	0.42
2:B:227:HIS:NE2	2:B:382:ALA:HA	2.34	0.42
2:B:392:ASP:OD2	2:B:503:LYS:HG3	2.18	0.42
3:C:98:LEU:HD22	3:C:118:LEU:HD13	2.01	0.42
8:H:79:ARG:HH11	8:H:80:PRO:HD2	1.83	0.42
11:K:93:SER:O	11:K:97:LYS:HG3	2.19	0.42
1:A:472:ASN:O	1:A:475:VAL:HG22	2.19	0.42
2:B:108:ASN:ND2	2:B:860:MET:HE2	2.34	0.42
2:B:303:LEU:HA	2:B:306:LEU:HD12	2.01	0.42
2:B:364:GLU:H	2:B:364:GLU:CD	2.26	0.42
4:D:59:LEU:HD13	7:G:49:LEU:HD11	2.00	0.42
7:G:11:LEU:O	7:G:69:GLU:HA	2.19	0.42
20:u:44:ILE:O	20:u:48:VAL:HG23	2.19	0.42
1:A:780:PHE:CZ	1:A:786:PRO:HD3	2.55	0.42
1:A:1119:THR:CG2	1:A:1331:TYR:HB3	2.50	0.42
3:C:55:SER:HA	3:C:151:GLN:NE2	2.34	0.42
14:T:20:DG:H4'	14:T:21:DG:OP1	2.19	0.42
15:N:-43:DT:C2'	15:N:-42:DT:H71	2.49	0.42
16:a:109:LEU:HD23	16:a:109:LEU:HA	1.70	0.42
1:A:12:ARG:NH1	2:B:1192:TYR:CD1	2.83	0.42
1:A:606:MET:HE1	1:A:613:VAL:HG13	2.01	0.42
1:A:854:ASP:OD1	1:A:856:THR:OG1	2.33	0.42
1:A:1210:THR:OG1	1:A:1233:ASP:OD2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:MET:HB2	2:B:169:PHE:CE1	2.54	0.42
2:B:82:ILE:CD1	2:B:117:LEU:HD13	2.50	0.42
2:B:393:HIS:HE2	2:B:696:GLU:CD	2.27	0.42
4:D:66:ALA:HA	4:D:69:ARG:HG2	2.02	0.42
15:N:-27:DC:H2''	15:N:-26:DT:C7	2.48	0.42
1:A:209:LEU:HD12	1:A:233:GLU:HB2	2.00	0.42
1:A:548:MET:CE	11:K:58:PHE:HA	2.49	0.42
1:A:697:LYS:HA	1:A:702:GLU:CD	2.44	0.42
1:A:963:ARG:O	1:A:967:GLN:HG3	2.20	0.42
2:B:262:LYS:HD3	2:B:271:ASP:O	2.20	0.42
2:B:613:ARG:NH2	9:I:89:GLN:HB3	2.34	0.42
4:D:59:LEU:HD23	4:D:59:LEU:HA	1.84	0.42
5:E:116:THR:CG2	5:E:117:PRO:HD2	2.48	0.42
14:T:16:DA:H1'	14:T:17:DA:C8	2.55	0.42
14:T:30:DC:H2'	14:T:31:DT:H71	2.00	0.42
14:T:34:DC:H2''	14:T:35:DT:OP2	2.19	0.42
20:u:52:LYS:HB3	20:u:52:LYS:HE3	1.80	0.42
20:u:88:VAL:HG11	20:u:95:GLN:HE21	1.85	0.42
1:A:5:PRO:HD2	2:B:1159:ARG:NH2	2.35	0.42
1:A:815:PHE:CE2	1:A:819:MET:HE2	2.54	0.42
2:B:384:GLU:HA	9:I:91:ARG:NH1	2.34	0.42
2:B:905:VAL:HG23	2:B:968:MET:HE3	2.01	0.42
9:I:37:LEU:HD12	9:I:38:ALA:H	1.84	0.42
14:T:17:DA:OP2	16:a:69:ARG:NH2	2.51	0.42
14:T:55:DC:H2''	14:T:56:DG:N7	2.35	0.42
15:N:-4:DC:H2''	15:N:-3:DG:C8	2.54	0.42
1:A:897:ARG:O	1:A:1031:ARG:HD2	2.19	0.42
1:A:1337:GLU:HA	1:A:1337:GLU:OE1	2.20	0.42
2:B:350:GLN:O	2:B:367:LYS:NZ	2.53	0.42
9:I:69:PRO:HB2	9:I:85:PHE:CE1	2.55	0.42
1:A:5:PRO:HD2	2:B:1159:ARG:HH22	1.85	0.42
1:A:809:LEU:O	2:B:725:ARG:NH1	2.53	0.42
2:B:42:MET:HE3	2:B:42:MET:HB3	1.91	0.42
5:E:135:GLN:HB3	5:E:138:ASP:OD2	2.19	0.42
14:T:61:DC:H2''	14:T:62:DG:C8	2.55	0.42
14:T:89:DG:O6	15:N:-90:DC:N4	2.53	0.42
15:N:16:DA:H1'	15:N:17:DA:C8	2.55	0.42
1:A:961:ASN:O	1:A:965:ILE:HG12	2.20	0.42
2:B:284:VAL:HG23	2:B:285:PRO:HD3	2.02	0.42
14:T:7:DC:H2''	14:T:8:DG:H8	1.85	0.42
18:c:88:ARG:HB3	18:c:108:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:u:84:LEU:HD21	20:u:105:PHE:CZ	2.54	0.42
1:A:444:LEU:HD22	2:B:1146:PHE:CE2	2.54	0.41
2:B:278:PHE:CE1	2:B:371:LEU:HB3	2.55	0.41
2:B:283:VAL:HG23	2:B:283:VAL:O	2.20	0.41
2:B:572:ARG:O	2:B:616:GLU:HA	2.20	0.41
2:B:953:LEU:HD21	2:B:955:THR:HG23	2.02	0.41
14:T:-69:DG:C6	14:T:-68:DA:C6	3.08	0.41
14:T:70:DA:O5'	16:e:42:ARG:HB2	2.20	0.41
14:T:95:DT:H2'	14:T:96:DA:C8	2.55	0.41
15:N:55:DT:H2''	15:N:56:DC:C5	2.54	0.41
18:g:83:LEU:HD22	19:h:59:MET:HE1	2.01	0.41
1:A:466:TYR:HB2	1:A:470:ARG:NH2	2.33	0.41
2:B:746:SER:HB2	2:B:1046:PRO:HG2	2.02	0.41
1:A:945:ARG:NH1	1:A:1299:GLY:O	2.50	0.41
1:A:985:ILE:N	1:A:986:PRO:HD2	2.34	0.41
1:A:1304:GLU:HG2	1:A:1306:LEU:CD1	2.50	0.41
1:A:1348:ARG:HE	1:A:1376:ASP:CG	2.28	0.41
2:B:33:GLN:HG2	2:B:34:GLN:N	2.35	0.41
2:B:757:PRO:HG2	2:B:984:HIS:HE1	1.85	0.41
3:C:104:HIS:HB3	3:C:148:ARG:O	2.20	0.41
5:E:100:GLN:OE1	5:E:100:GLN:HA	2.20	0.41
14:T:56:DG:H2''	14:T:57:DG:N7	2.35	0.41
17:b:82:THR:HG22	17:b:85:ASP:OD2	2.19	0.41
1:A:360:LEU:HA	1:A:360:LEU:HD23	1.77	0.41
1:A:780:PHE:CE1	1:A:786:PRO:HD3	2.55	0.41
1:A:1289:LYS:HE3	1:A:1307:TRP:CZ3	2.56	0.41
2:B:870:ILE:HG23	2:B:917:PRO:HG2	2.03	0.41
14:T:18:DG:H1'	14:T:19:DC:H5'	2.03	0.41
14:T:58:DC:H2''	14:T:59:DA:C8	2.56	0.41
15:N:56:DC:C2	15:N:57:DA:C6	3.08	0.41
1:A:1160:PRO:HA	1:A:1243:ARG:NH2	2.34	0.41
2:B:519:GLU:HG3	2:B:771:SER:HB3	2.03	0.41
2:B:882:THR:OG1	2:B:885:LEU:HD11	2.20	0.41
7:G:6:ASP:OD1	7:G:75:ARG:HB3	2.20	0.41
1:A:61:ILE:HD13	1:A:245:PRO:HB2	2.03	0.41
1:A:409:ASP:OD1	1:A:409:ASP:N	2.54	0.41
1:A:1157:ASP:CG	1:A:1243:ARG:HH22	2.28	0.41
1:A:1272:ASP:O	1:A:1273:LEU:HD12	2.20	0.41
16:a:133:GLU:C	16:a:134:ARG:HD2	2.45	0.41
18:c:91:GLU:O	18:c:95:LYS:HG3	2.19	0.41
1:A:1158:PRO:HA	1:A:1192:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1289:LYS:HD2	1:A:1305:GLU:CG	2.50	0.41
2:B:424:TYR:HD1	2:B:425:MET:HE2	1.86	0.41
3:C:97:VAL:HG22	3:C:158:ILE:HD12	2.02	0.41
3:C:187:LYS:HG3	3:C:219:PHE:CE1	2.56	0.41
4:D:102:VAL:HG22	7:G:46:VAL:HG22	2.02	0.41
16:a:126:LEU:HD22	16:e:113:HIS:CG	2.56	0.41
17:f:35:ARG:O	17:f:39:ARG:HG2	2.21	0.41
2:B:82:ILE:HD13	2:B:117:LEU:HD13	2.02	0.41
2:B:955:THR:HG21	12:L:57:VAL:HG12	2.03	0.41
2:B:1028:GLU:OE1	2:B:1090:THR:HG23	2.20	0.41
2:B:1097:HIS:HB3	2:B:1102:LYS:HE3	2.03	0.41
3:C:166:GLU:HB3	11:K:10:PHE:CE1	2.55	0.41
4:D:108:TYR:CE2	7:G:89:ALA:HA	2.56	0.41
7:G:2:PHE:HA	7:G:78:VAL:O	2.21	0.41
1:A:474:SER:OG	1:A:651:GLN:NE2	2.54	0.41
1:A:854:ASP:CG	1:A:856:THR:HG1	2.25	0.41
1:A:1302:LYS:NZ	1:A:1304:GLU:OE2	2.50	0.41
2:B:22:SER:OG	2:B:811:TYR:OH	2.36	0.41
2:B:300:TRP:NE1	9:I:52:ILE:HD11	2.35	0.41
2:B:1152:MET:O	2:B:1157:ALA:HB2	2.21	0.41
3:C:189:THR:HG22	3:C:190:ASP:N	2.36	0.41
7:G:127:PRO:HA	7:G:128:PRO:HD3	1.93	0.41
12:L:51:LYS:HB3	12:L:51:LYS:HE3	1.91	0.41
14:T:44:DT:H6	14:T:44:DT:H2'	1.71	0.41
14:T:68:DC:H2''	14:T:69:DC:C6	2.56	0.41
15:N:25:DG:H2''	15:N:26:DG:N7	2.36	0.41
20:u:40:VAL:O	20:u:44:ILE:HG13	2.21	0.41
1:A:1264:LYS:HE2	9:I:44:TYR:CD1	2.56	0.41
15:N:-70:DT:H2''	15:N:-69:DG:C8	2.56	0.41
15:N:-14:DA:H2''	15:N:-13:DA:H8	1.84	0.41
2:B:678:TRP:CH2	2:B:687:ILE:HG21	2.56	0.40
7:G:119:LEU:HA	7:G:132:SER:OG	2.21	0.40
11:K:10:PHE:O	11:K:37:ARG:NE	2.53	0.40
14:T:-43:DA:C2	14:T:-42:DG:C5	3.10	0.40
14:T:35:DT:OP2	14:T:35:DT:H2'	2.21	0.40
15:N:4:DC:H2''	15:N:5:DC:OP2	2.20	0.40
1:A:253:MET:HB2	14:T:104:DA:C2	2.56	0.40
1:A:833:ALA:HB3	2:B:500:LYS:NZ	2.36	0.40
1:A:846:LEU:HD12	1:A:1071:ALA:HB2	2.03	0.40
2:B:166:ARG:NH1	2:B:189:ASP:O	2.55	0.40
2:B:193:TYR:CE2	2:B:200:GLU:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:533:SER:OG	2:B:747:MET:O	2.38	0.40
3:C:70:PRO:HG3	10:J:13:VAL:HG21	2.03	0.40
7:G:133:ASN:O	7:G:134:ASP:HB2	2.21	0.40
9:I:39:GLU:HG2	9:I:40:ASP:N	2.37	0.40
1:A:665:ILE:HG22	2:B:1014:PRO:HB3	2.02	0.40
1:A:1444:PHE:HZ	6:F:92:ARG:HB3	1.86	0.40
2:B:214:VAL:HG11	2:B:373:TYR:CE2	2.53	0.40
2:B:220:ALA:O	2:B:252:ARG:NH2	2.55	0.40
11:K:18:LYS:CE	11:K:37:ARG:HH12	2.35	0.40
1:A:29:ALA:HB1	2:B:1184:SER:HA	2.04	0.40
1:A:80:HIS:N	1:A:244:PRO:HB3	2.36	0.40
2:B:283:VAL:O	2:B:289:ILE:HD11	2.22	0.40
2:B:414:PHE:CE1	2:B:417:LEU:HD23	2.57	0.40
9:I:97:MET:HE2	9:I:97:MET:HB3	1.91	0.40
11:K:12:LEU:HD13	11:K:37:ARG:HH11	1.87	0.40
14:T:37:DC:H2''	14:T:38:DG:C8	2.56	0.40
1:A:114:LEU:HB2	1:A:142:CYS:SG	2.62	0.40
1:A:902:LEU:HD22	1:A:920:ILE:CG2	2.51	0.40
2:B:28:LYS:O	2:B:32:SER:HB3	2.21	0.40
2:B:954:LEU:HD12	2:B:963:PHE:O	2.21	0.40
7:G:31:LEU:HD23	7:G:31:LEU:HA	1.94	0.40
14:T:8:DG:C2'	14:T:9:DT:H71	2.52	0.40
20:u:84:LEU:HD21	20:u:105:PHE:CE2	2.57	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%)	1337 (96%)	60 (4%)	3 (0%)	43 77
2	B	1151/1227 (94%)	1103 (96%)	47 (4%)	1 (0%)	48 83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	261/304 (86%)	253 (97%)	8 (3%)	0	100	100
4	D	162/186 (87%)	154 (95%)	8 (5%)	0	100	100
5	E	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
6	F	82/155 (53%)	80 (98%)	2 (2%)	0	100	100
7	G	169/171 (99%)	162 (96%)	7 (4%)	0	100	100
8	H	129/145 (89%)	123 (95%)	6 (5%)	0	100	100
9	I	109/115 (95%)	106 (97%)	3 (3%)	0	100	100
10	J	64/72 (89%)	62 (97%)	2 (3%)	0	100	100
11	K	111/118 (94%)	109 (98%)	2 (2%)	0	100	100
12	L	43/72 (60%)	40 (93%)	3 (7%)	0	100	100
16	a	95/139 (68%)	94 (99%)	1 (1%)	0	100	100
16	e	95/139 (68%)	92 (97%)	3 (3%)	0	100	100
17	b	81/106 (76%)	79 (98%)	2 (2%)	0	100	100
17	f	76/106 (72%)	74 (97%)	2 (3%)	0	100	100
18	c	103/133 (77%)	99 (96%)	4 (4%)	0	100	100
18	g	103/133 (77%)	99 (96%)	4 (4%)	0	100	100
19	d	93/129 (72%)	91 (98%)	2 (2%)	0	100	100
19	h	91/129 (70%)	90 (99%)	1 (1%)	0	100	100
20	u	71/219 (32%)	65 (92%)	6 (8%)	0	100	100
All	All	4700/5755 (82%)	4516 (96%)	180 (4%)	4 (0%)	49	83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	467	SER
1	A	959	PRO
2	B	61	PRO
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	1225/1528 (80%)	1225 (100%)	0	100	100
2	B	1016/1077 (94%)	1016 (100%)	0	100	100
3	C	236/264 (89%)	236 (100%)	0	100	100
4	D	143/160 (89%)	143 (100%)	0	100	100
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%)	73	77
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
16	a	85/113 (75%)	85 (100%)	0	100	100
16	e	84/113 (74%)	84 (100%)	0	100	100
17	b	68/81 (84%)	68 (100%)	0	100	100
17	f	63/81 (78%)	63 (100%)	0	100	100
18	c	83/102 (81%)	83 (100%)	0	100	100
18	g	83/102 (81%)	83 (100%)	0	100	100
19	d	81/107 (76%)	81 (100%)	0	100	100
19	h	79/107 (74%)	79 (100%)	0	100	100
20	u	56/155 (36%)	56 (100%)	0	100	100
All	All	4149/4942 (84%)	4148 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	61	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	307	ASN

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Mol	Chain	Res	Type
1	A	359	ASN
1	A	385	ASN
1	A	428	GLN
1	A	446	ASN
1	A	737	ASN
1	A	955	ASN
1	A	1072	GLN
2	B	301	GLN
2	B	343	GLN
2	B	376	ASN
2	B	388	GLN
2	B	524	GLN
2	B	736	HIS
2	B	984	HIS
2	B	1074	ASN
3	C	150	HIS
3	C	151	GLN
3	C	252	GLN
5	E	53	GLN
5	E	135	GLN
5	E	165	GLN
5	E	173	GLN
7	G	24	GLN
9	I	90	GLN
9	I	105	ASN
11	K	85	GLN
12	L	43	ASN
19	d	44	GLN
19	d	60	ASN
19	d	79	HIS
18	g	110	ASN
19	h	64	ASN
19	h	79	HIS
20	u	95	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	13/14 (92%)	2 (15%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	0	A
13	P	11	C

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 9 ligands modelled in this entry, 9 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.

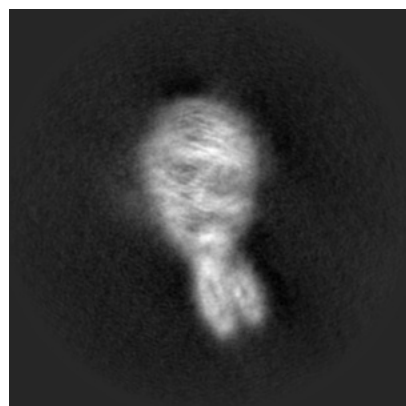
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34416. These allow visual inspection of the internal detail of the map and identification of artifacts.

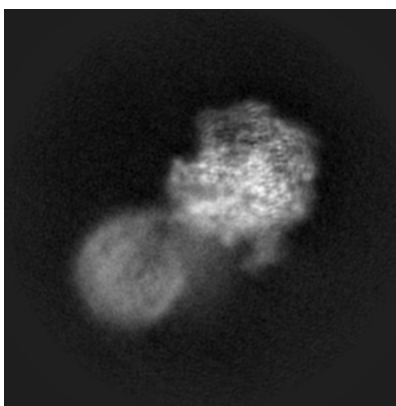
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

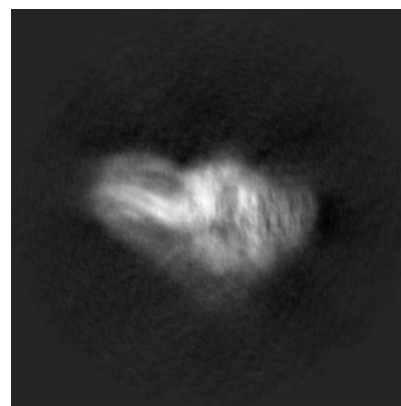
6.1.1 Primary map



X

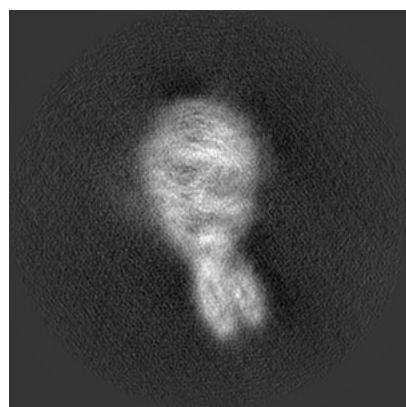


Y

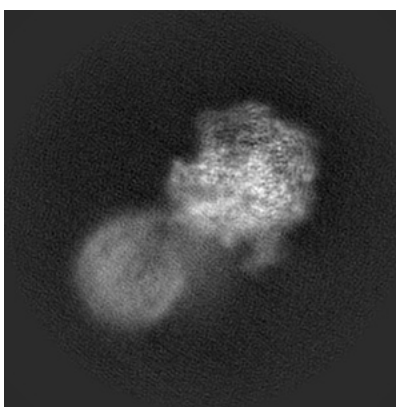


Z

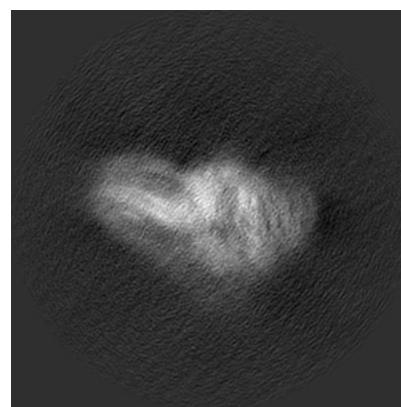
6.1.2 Raw map



X



Y

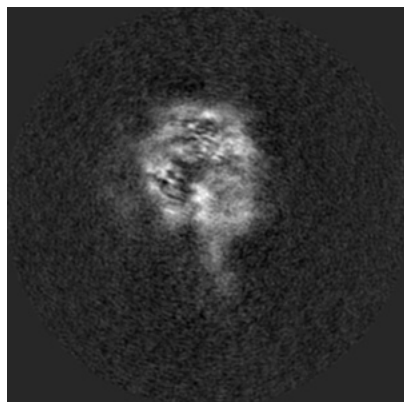


Z

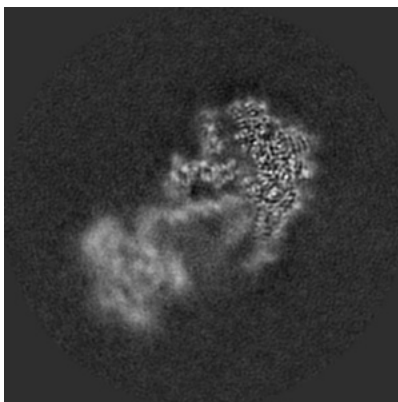
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

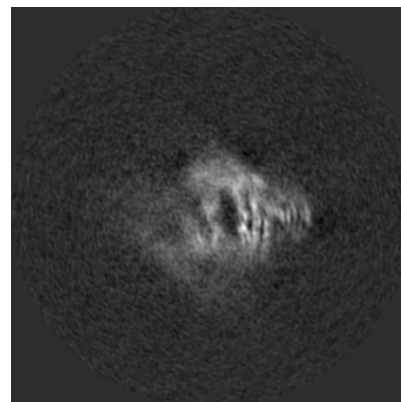
6.2.1 Primary map



X Index: 120

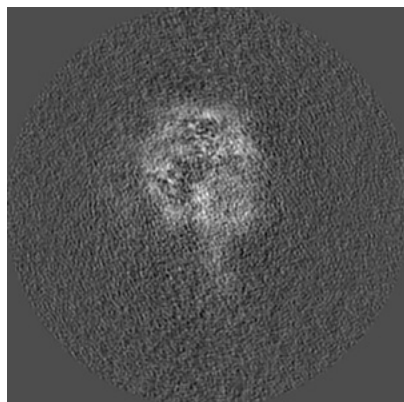


Y Index: 120

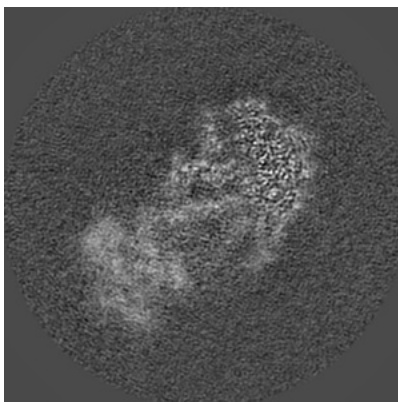


Z Index: 120

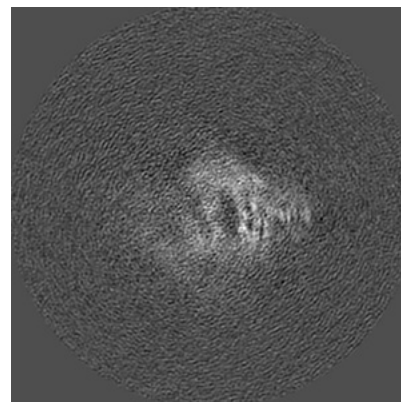
6.2.2 Raw map



X Index: 120



Y Index: 120

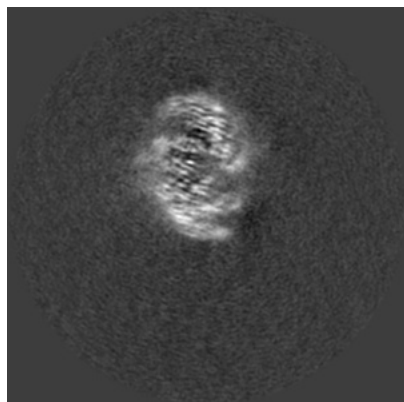


Z Index: 120

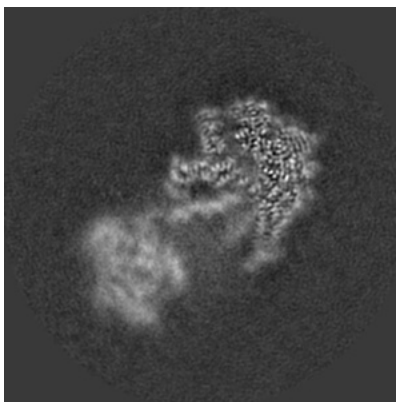
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

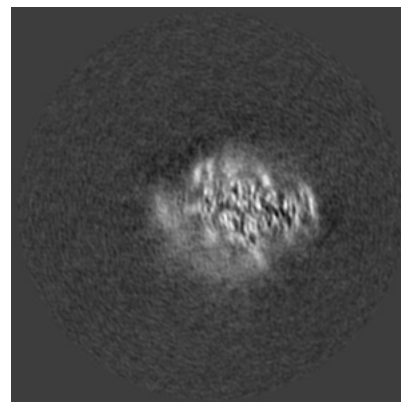
6.3.1 Primary map



X Index: 145

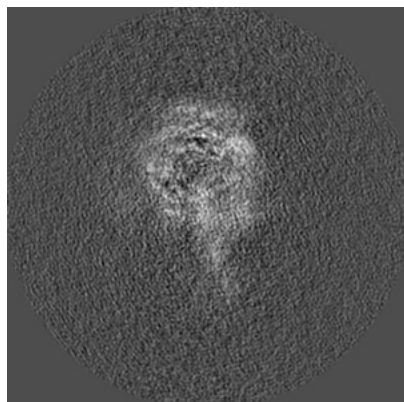


Y Index: 118

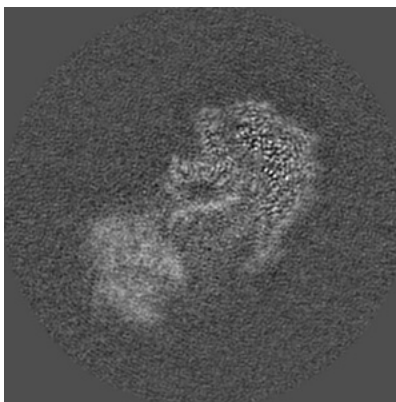


Z Index: 154

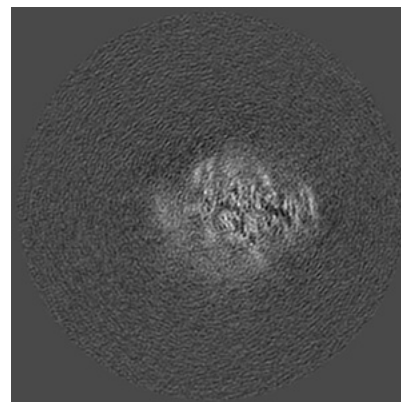
6.3.2 Raw map



X Index: 119



Y Index: 117

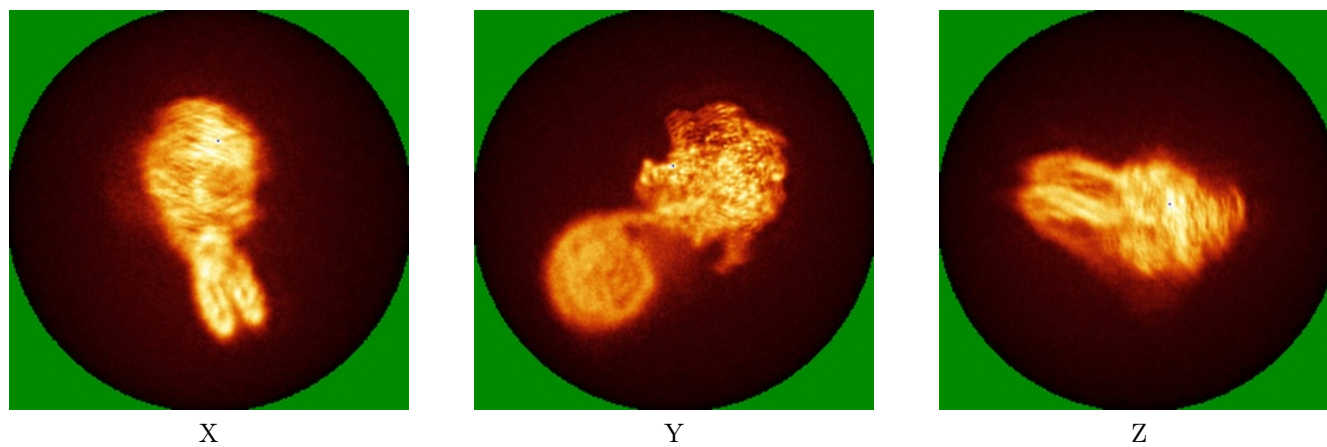


Z Index: 154

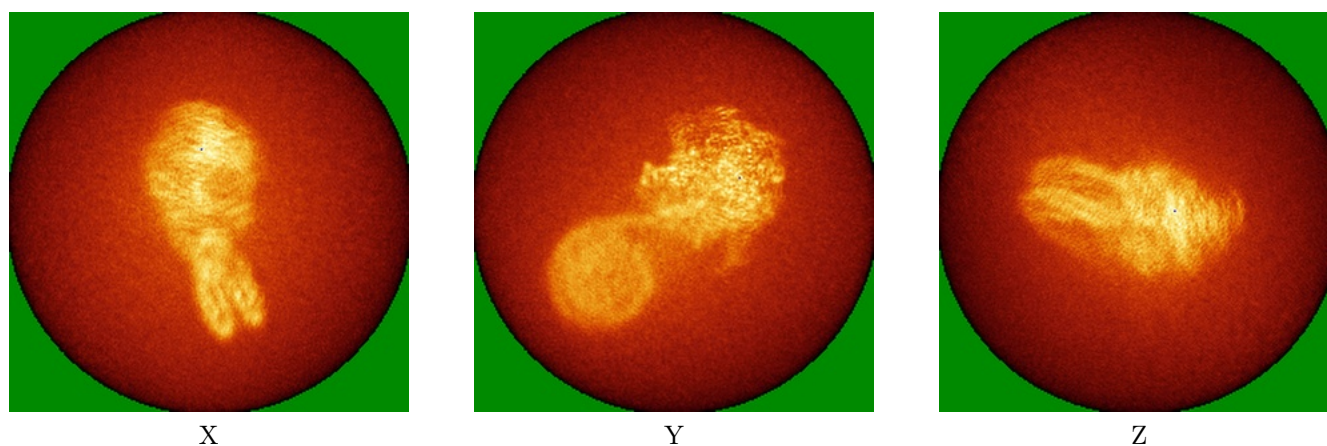
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

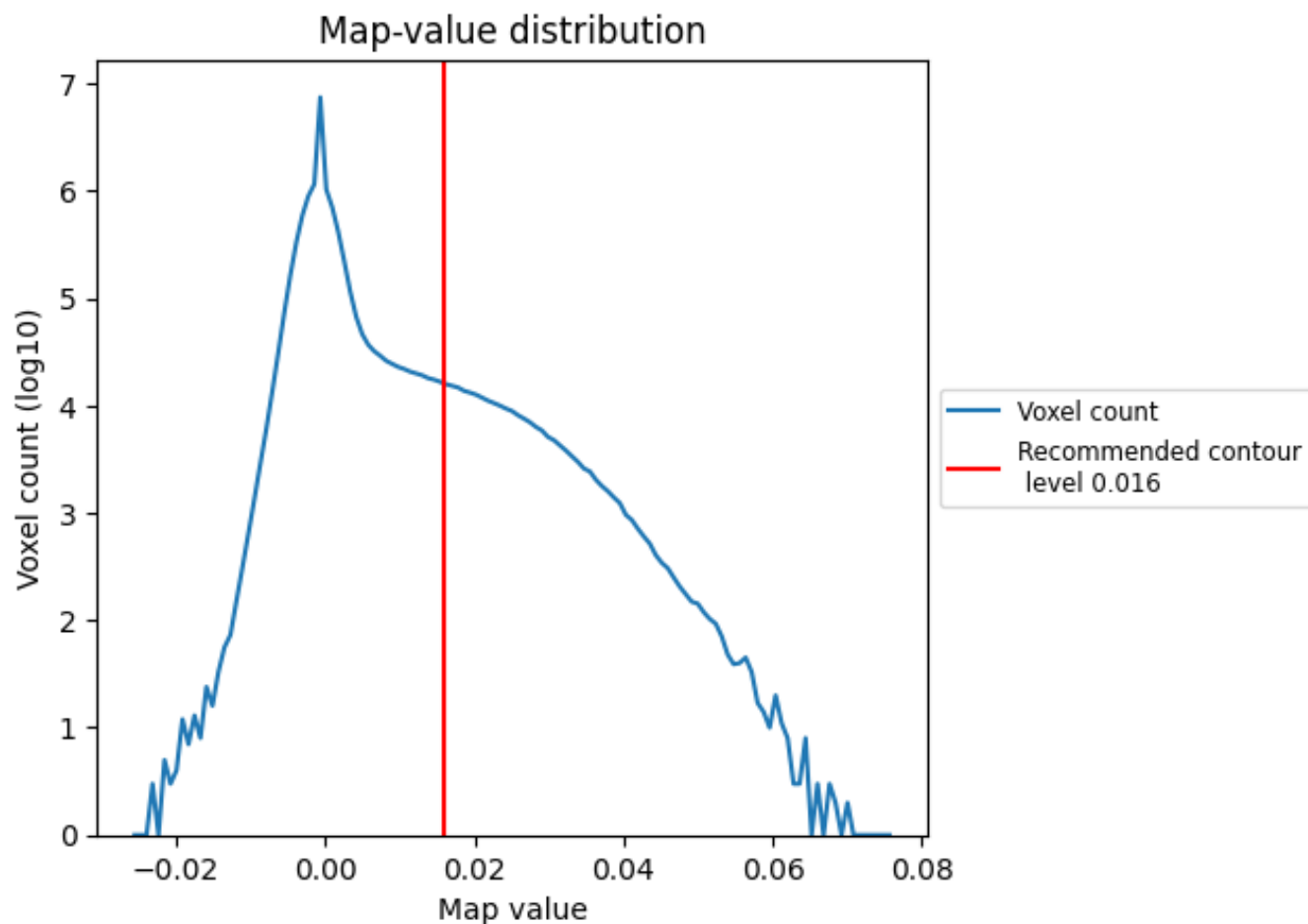
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

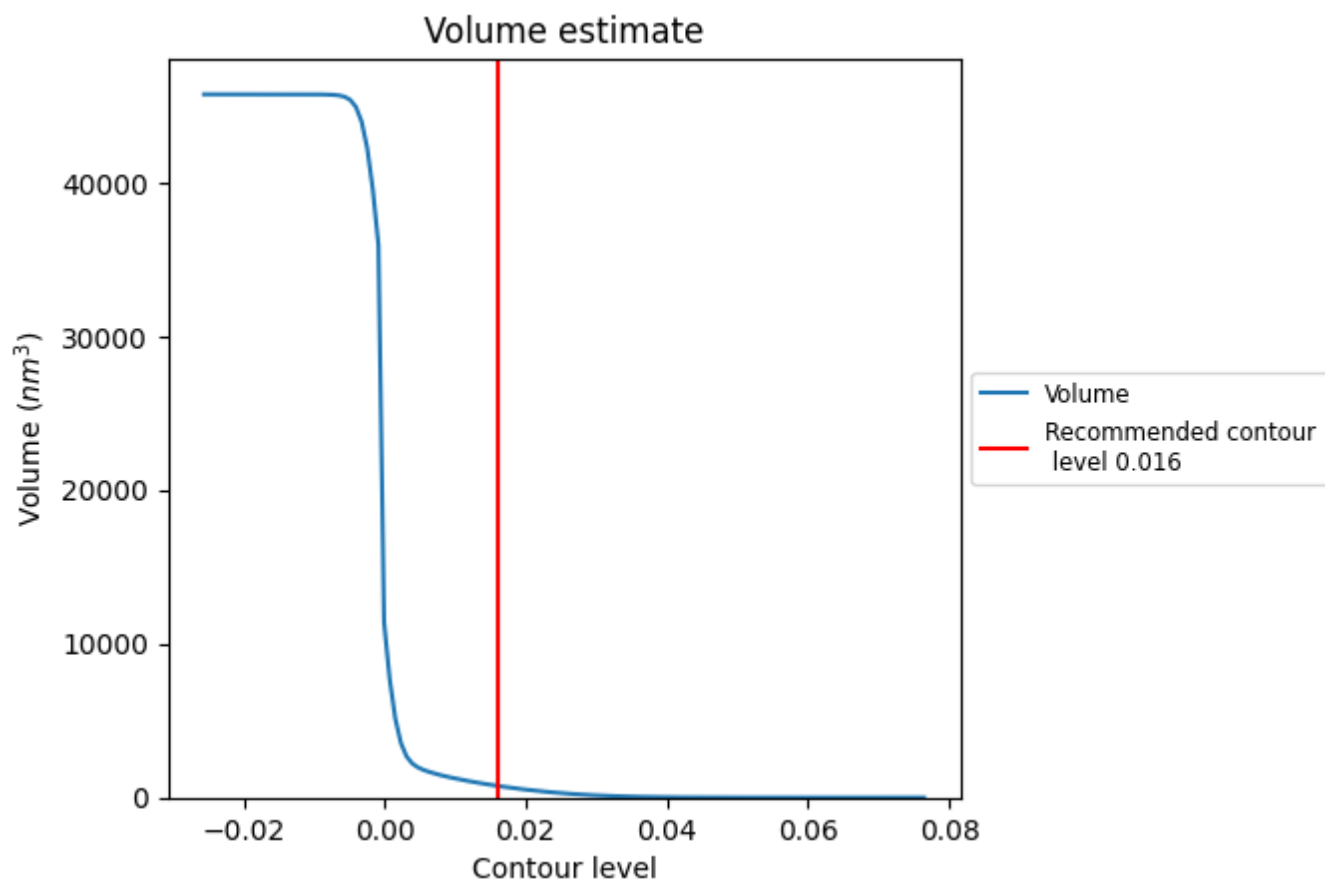
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

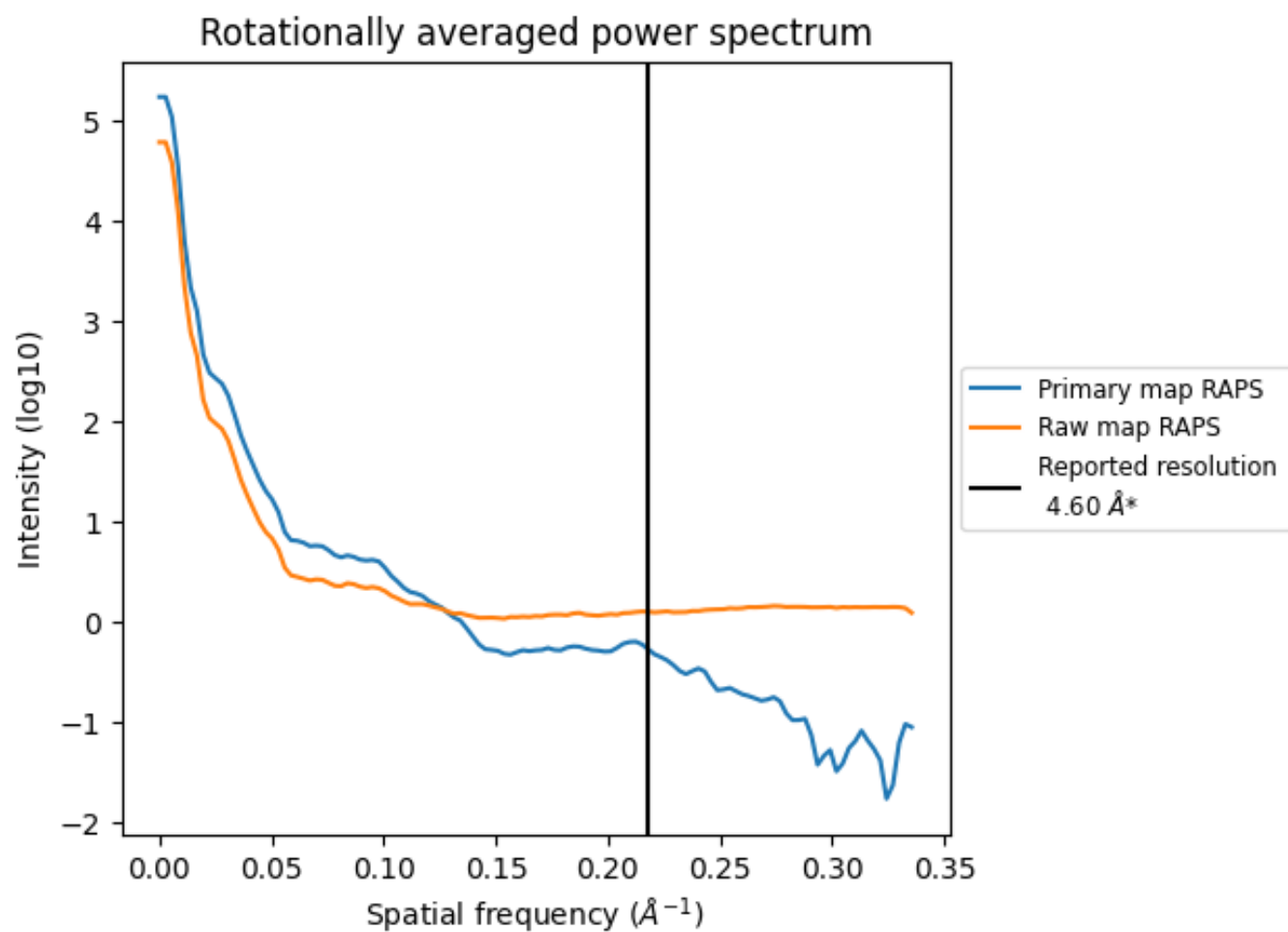
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 760 nm³; this corresponds to an approximate mass of 687 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 ⓘ

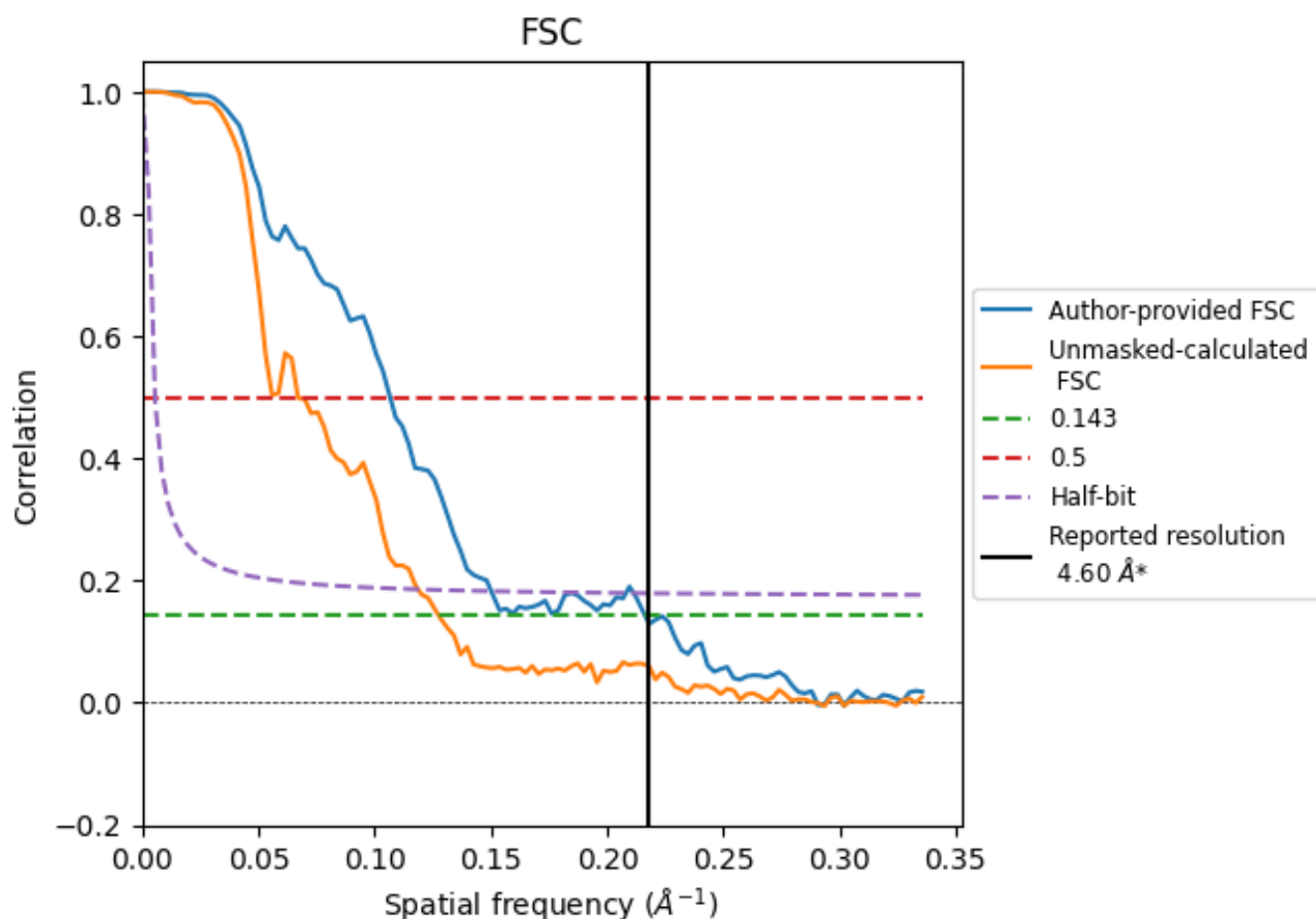


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 $0.217 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

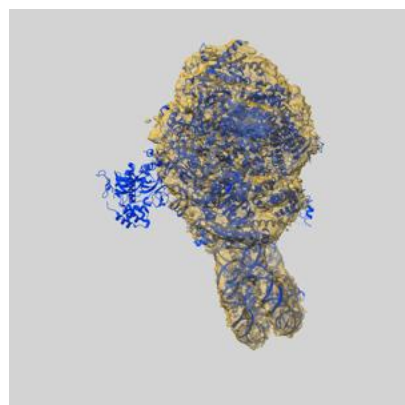
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.62	9.38	6.66
Unmasked-calculated*	7.84	14.93	8.42

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.84 differs from the reported value 4.6 by more than 10 %

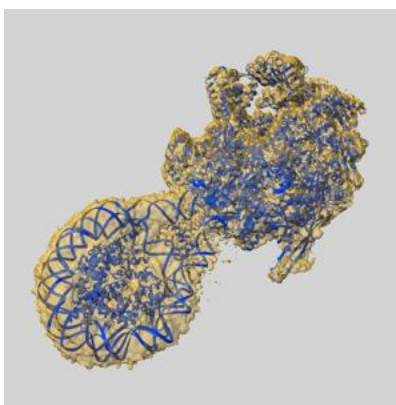
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34416 and PDB model 8H0W. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

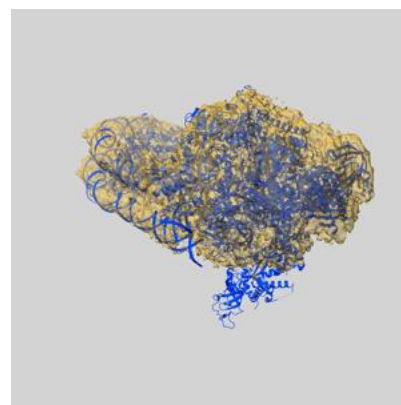
9.1 Map-model overlay [i](#)



X



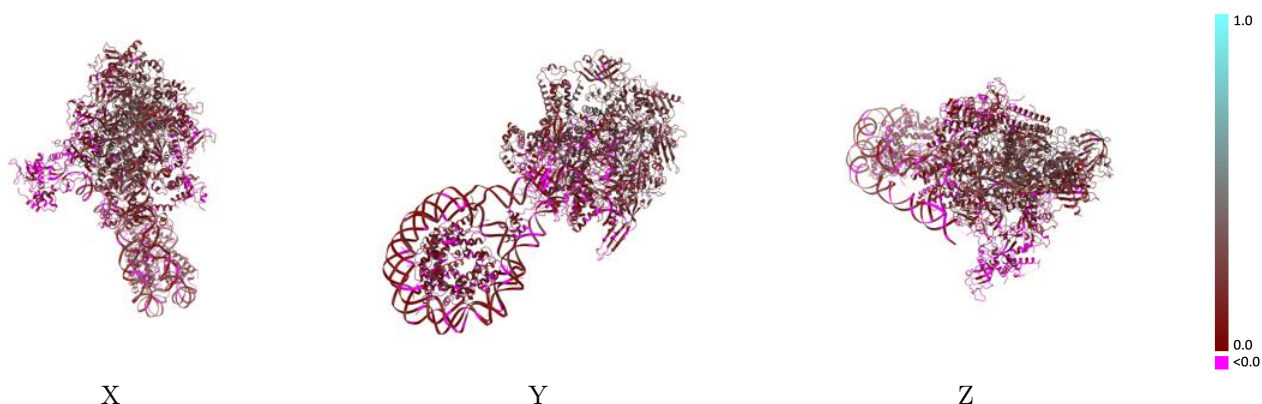
Y



Z

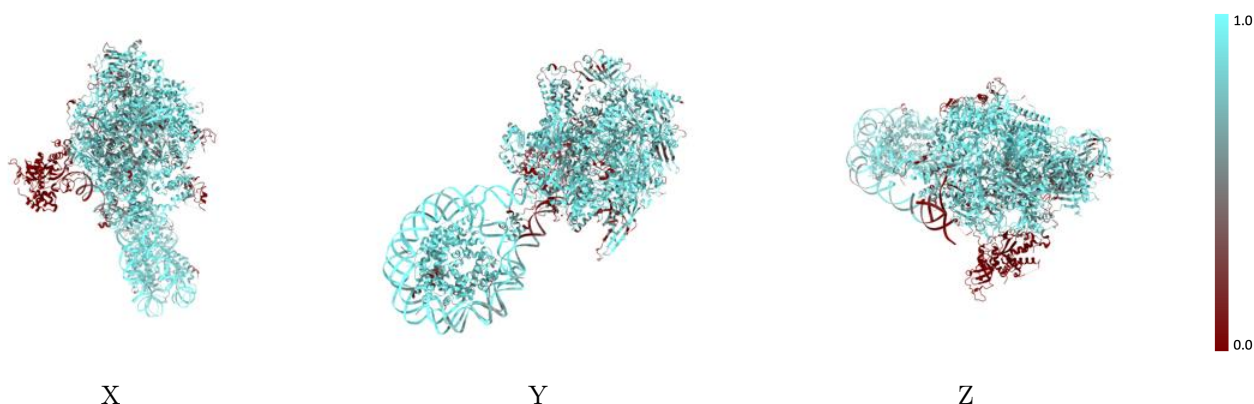
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



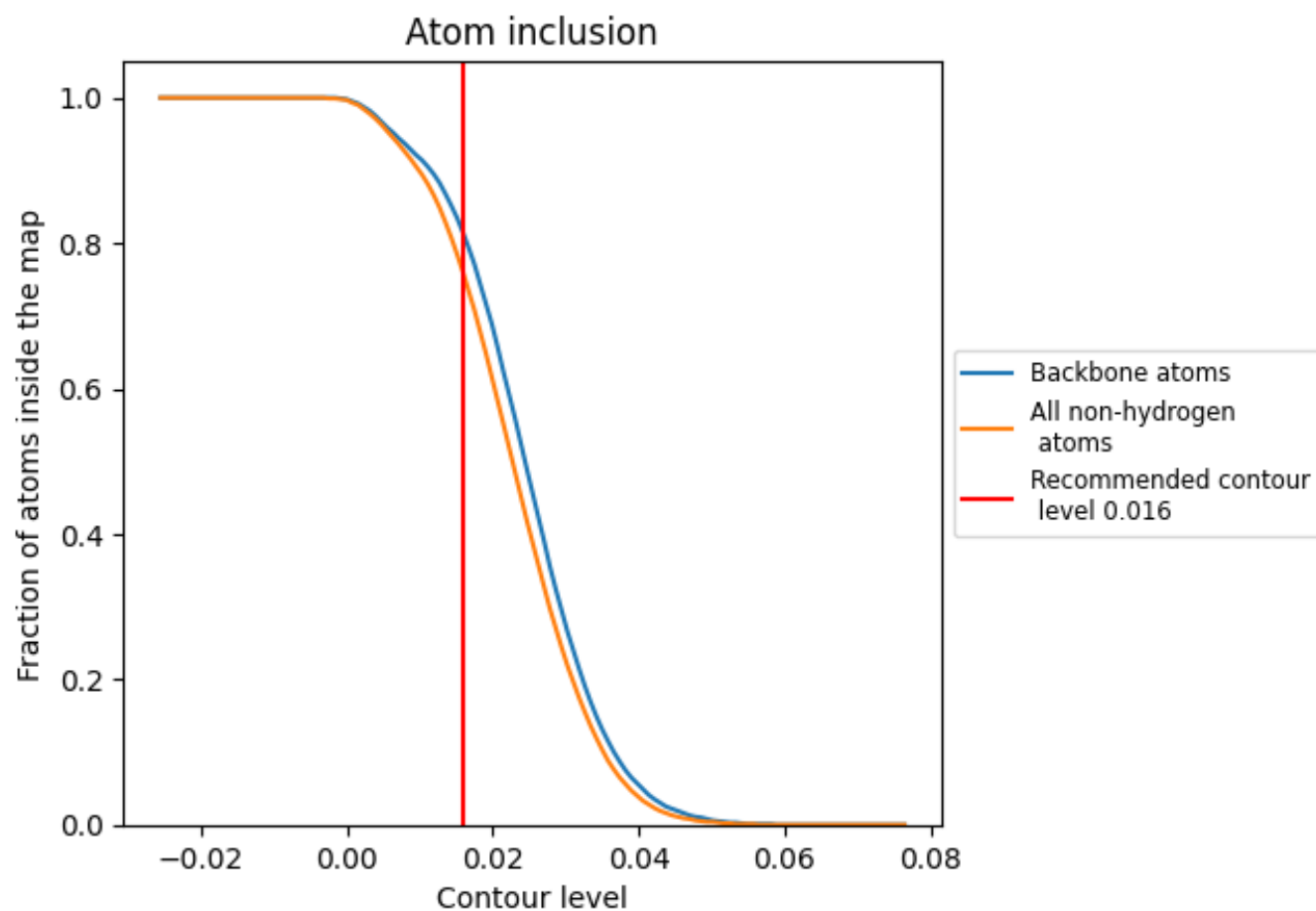
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7570	 0.1600
A	 0.7900	 0.2130
B	 0.8260	 0.2030
C	 0.7620	 0.2350
D	 0.0190	 -0.0060
E	 0.8360	 0.2090
F	 0.8160	 0.1480
G	 0.0740	 0.0050
H	 0.6970	 0.2530
I	 0.4080	 0.0280
J	 0.8210	 0.2520
K	 0.6960	 0.1510
L	 0.6720	 0.1830
N	 0.7780	 0.0830
P	 0.8190	 0.2500
T	 0.8290	 0.1200
a	 0.8750	 0.0850
b	 0.8260	 0.1060
c	 0.9250	 0.0960
d	 0.7950	 0.1330
e	 0.9830	 0.1240
f	 0.9480	 0.0760
g	 0.8990	 0.0950
h	 0.8830	 0.1070
u	 0.5420	 0.0570

