



Full wwPDB EM Validation Report ⓘ

Jul 14, 2026 – 11:50 AM JST

PDB ID : 9XAC / pdb_00009xac
EMDB ID : EMD-66682
Title : Cryo-EM structure of the pre-40S ribosome (Enp1-Rrp12 WT) from *Chaetomium thermophilum*, state Rrp12-A1
Authors : Lau, B.; Li, Y.; Zhu, J.; Fischer, P.; Hong, X.; Yuan, R.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on : 2025-10-22
Resolution : 3.30 Å (reported)
Based on initial model : 6RXU

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.dev133
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) : 2.50

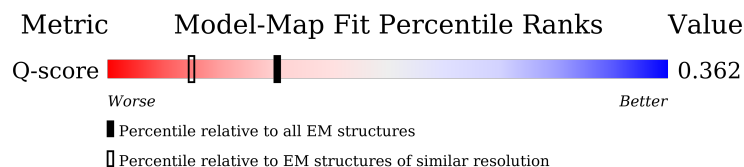
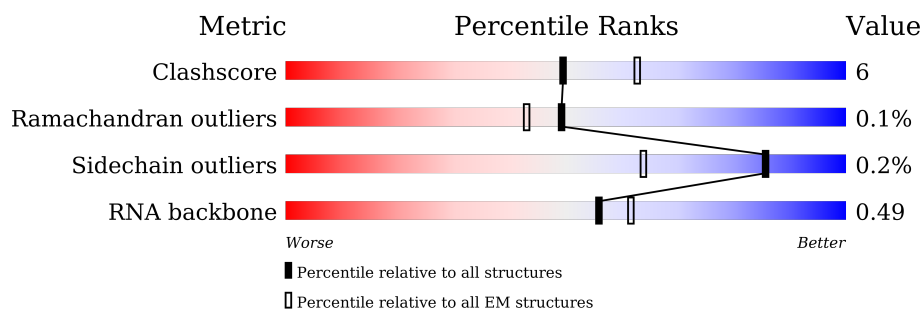
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.



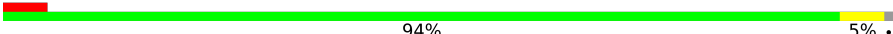
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	E	255	
2	H	264	
3	I	212	

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Mol	Chain	Length	Quality of chain
4	J	239	
5	K	203	
6	L	202	
7	M	190	
8	O	161	
9	P	144	
10	Q	151	
11	R	150	
12	S	153	
13	T	143	
14	V	156	
15	W	153	
16	Z	130	
17	a	145	
18	b	136	
19	c	99	
20	e	82	
21	f	68	
22	h	62	
23	i	154	
24	A	1796	
25	0	127	
26	1	282	
27	2	830	
28	3	259	

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Mol	Chain	Length	Quality of chain
29	4	480	33%48%9%44%
30	5	445	16%15%82%
31	7	1235	80%70%10%20%

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 80191 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 Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	213	Total	C	N	O	S	0	0
			1723	1096	319	303	5		

- Molecule 2 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	261	Total	C	N	O	S	0	0
			2072	1314	389	362	7		

- Molecule 3 is a protein called 40S ribosomal protein s5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	199	Total	C	N	O	S	0	0
			1557	971	294	285	7		

- Molecule 4 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	232	Total	C	N	O	S	0	0
			1875	1171	376	323	5		

- Molecule 5 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	195	Total	C	N	O	0	0
			1562	983	300	279		

- Molecule 6 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	201	Total	C	N	O	S	0	0
			1621	1009	330	281	1		

- Molecule 7 is a protein called 40S ribosomal protein s9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	179	Total	C	N	O	S	0	0
			1466	933	290	241	2		

- Molecule 8 is a protein called 40S ribosomal protein S11-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	150	Total	C	N	O	S	0	0
			1222	780	236	201	5		

- Molecule 9 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	118	Total	C	N	O	S	0	0
			923	577	167	171	8		

- Molecule 10 is a protein called 40S ribosomal protein S13-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	150	Total	C	N	O	S	0	0
			1182	756	220	205	1		

- Molecule 11 is a protein called 40S ribosomal protein S14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	135	Total	C	N	O	S	0	0
			1002	614	199	184	5		

- Molecule 12 is a protein called 40S ribosomal protein s15-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S	115	Total	C	N	O	S	0	0
			917	583	172	159	3		

- Molecule 13 is a protein called 40S ribosomal protein S16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	117	Total	C	N	O	S	0	0
			909	588	162	158	1		

- Molecule 14 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	122	Total	C	N	O	S	0	0
			998	629	191	177	1		

- Molecule 15 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	142	Total	C	N	O	S	0	0
			1117	694	221	201	1		

- Molecule 16 is a protein called 40S ribosomal protein S22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	129	Total	C	N	O	S	0	0
			1037	659	195	178	5		

- Molecule 17 is a protein called 40S ribosomal protein s23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	142	Total	C	N	O	S	0	0
			1099	694	215	188	2		

- Molecule 18 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	125	Total	C	N	O	S	0	0
			1006	633	198	173	2		

- Molecule 19 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	c	69	Total	C	N	O	S	0	0
			546	345	101	98	2		

- Molecule 20 is a protein called Ribosomal protein s27-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	e	81	Total	C	N	O	S	0	0
			611	386	111	107	7		

- Molecule 21 is a protein called 40S ribosomal protein S28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	f	61	Total	C	N	O	S	0	0
			484	298	97	88	1		

- Molecule 22 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	21	Total	C	N	O		0	0
			181	117	38	26			

- Molecule 23 is a protein called 40S ribosomal protein S27a-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	i	65	Total	C	N	O	S	0	0
			528	332	97	93	6		

- Molecule 24 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	A	1582	Total	C	N	O	P	0	0
			33747	15079	6022	11064	1582		

- Molecule 25 is a protein called Trm112.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	127	Total	C	N	O	S	0	0
			993	636	163	187	7		

- Molecule 26 is a protein called Methyltransferase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	267	Total	C	N	O	S	0	0
			2013	1260	355	388	10		

- Molecule 27 is a protein called Bms1-type G domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	728	Total	C	N	O	S	0	0
			5822	3656	1054	1092	20		

- Molecule 28 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	184	Total	C	N	O	S	0	0
			1451	921	267	256	7		

- Molecule 29 is a protein called Bystin-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	270	Total	C	N	O	S	0	0
			2154	1401	377	366	10		

- Molecule 30 is a protein called Putative low-temperature viability protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	80	Total	C	N	O	S	0	0
			656	414	112	129	1		

- Molecule 31 is a protein called Ribosomal RNA-processing protein 12-like conserved domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	7	987	Total	C	N	O	S	0	0
			7710	4932	1326	1414	38		

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	Q	1	Total	Mg	0
			1	1	
32	a	1	Total	Mg	0
			1	1	

- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
33	e	1	Total	Zn	0
			1	1	

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		AltConf
34	Q	1	Total	O	0
			1	1	

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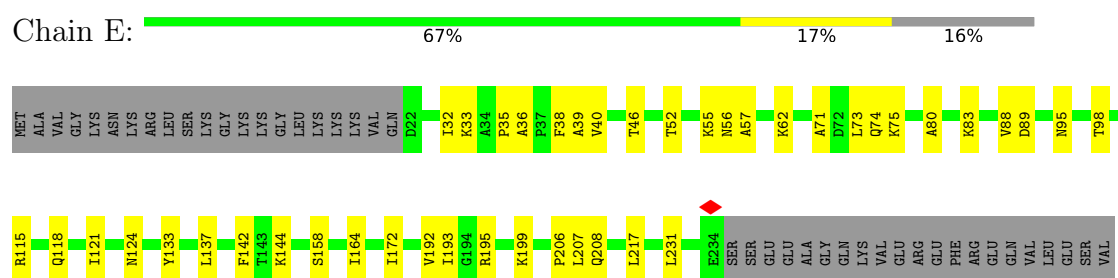
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Mol	Chain	Residues	Atoms		AltConf
34	A	3	Total	O	0
			3	3	

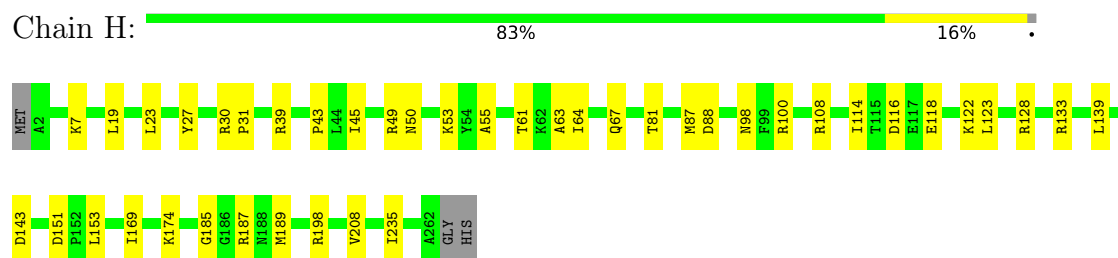
3 Residue-property plots [i](#)

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

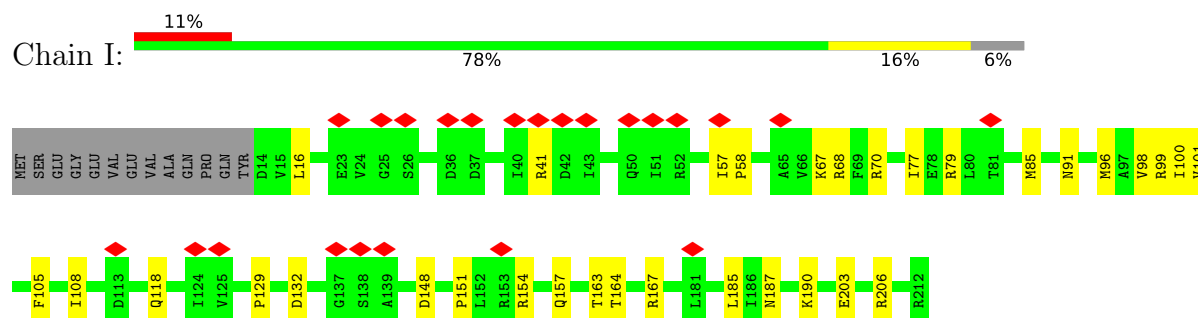
- Molecule 1: Small ribosomal subunit protein eS1



- Molecule 2: 40S ribosomal protein S4

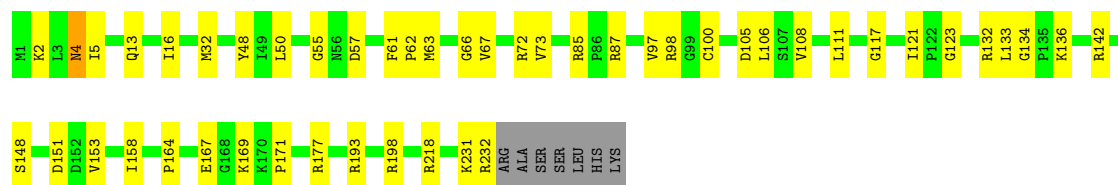


- Molecule 3: 40S ribosomal protein s5-like protein



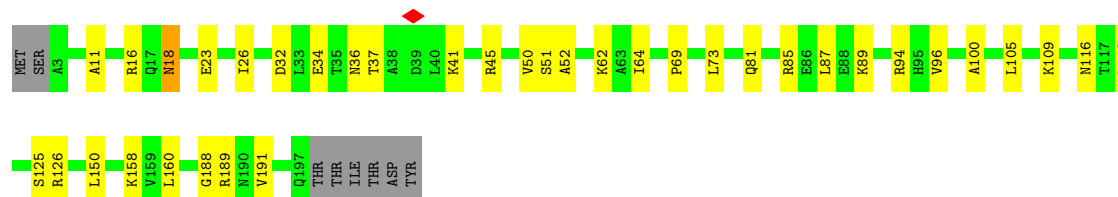
- Molecule 4: 40S ribosomal protein S6





- Molecule 5: 40S ribosomal protein S7

Chain K: 78% 18% .



- Molecule 6: 40S ribosomal protein S8

Chain L: 89% 11%



- Molecule 7: 40S ribosomal protein s9-like protein

Chain M: 81% 13% 6%



- Molecule 8: 40S ribosomal protein S11-like protein

Chain O: 83% 11% 7%



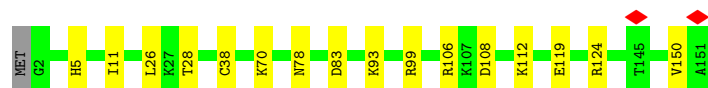
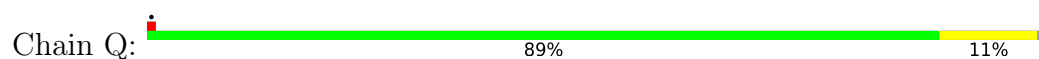
- Molecule 9: 40S ribosomal protein S12

Chain P: 76% 69% 13% 18%

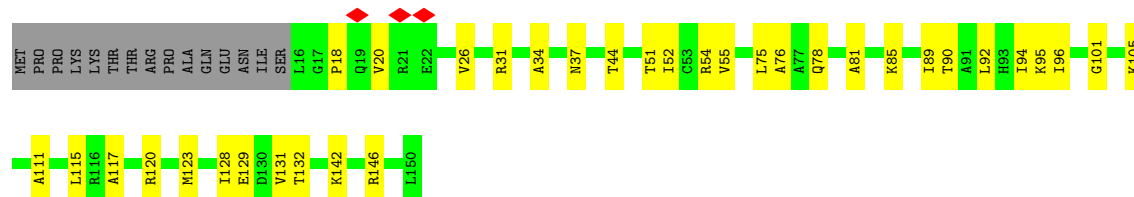




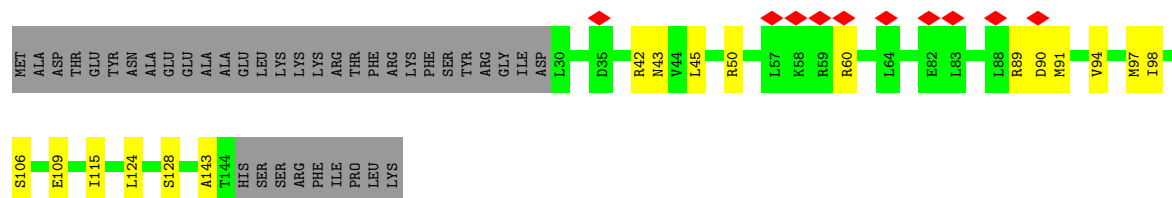
- Molecule 10: 40S ribosomal protein S13-like protein



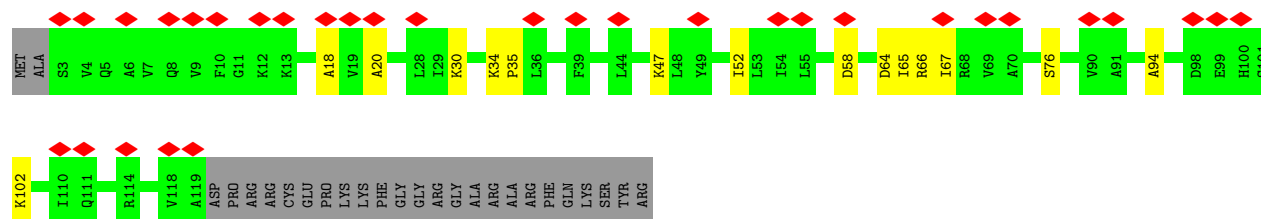
- Molecule 11: 40S ribosomal protein S14-like protein



- Molecule 12: 40S ribosomal protein s15-like protein

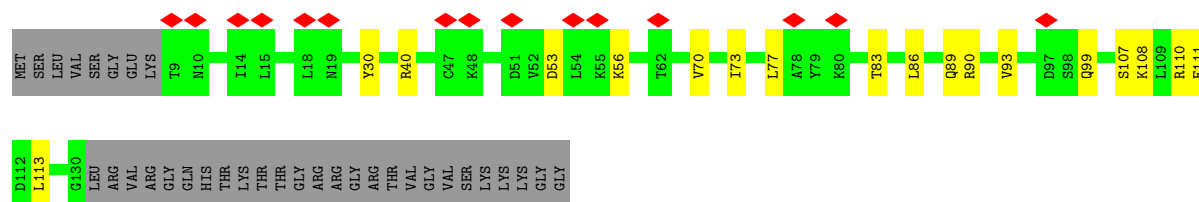


- Molecule 13: 40S ribosomal protein S16-like protein

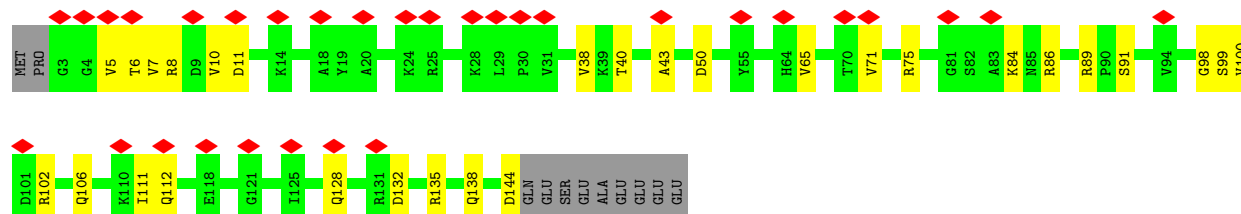
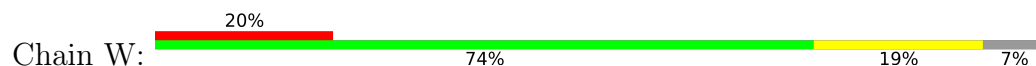


- Molecule 14: Putative ribosomal protein

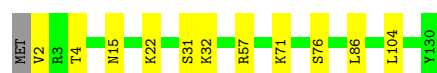
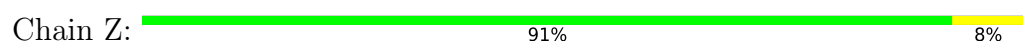




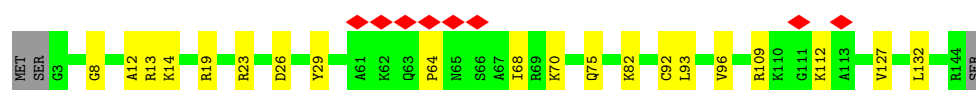
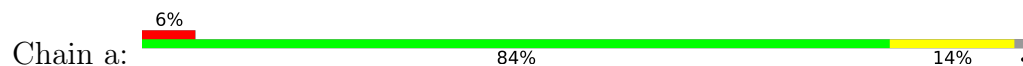
- Molecule 15: 40S ribosomal protein S19-like protein



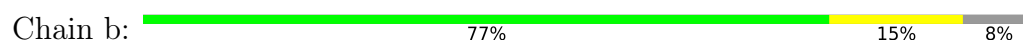
- Molecule 16: 40S ribosomal protein S22-like protein



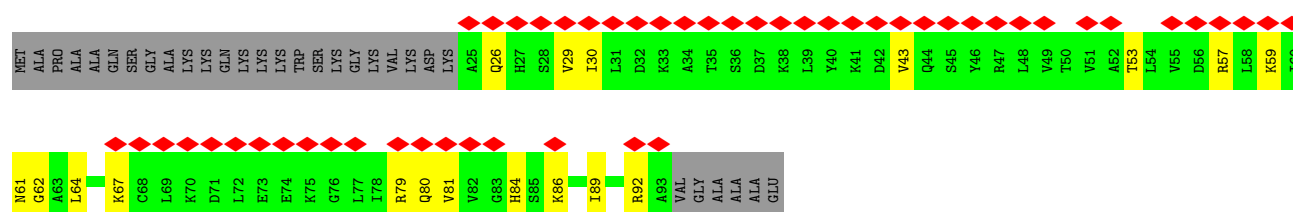
- Molecule 17: 40S ribosomal protein s23-like protein

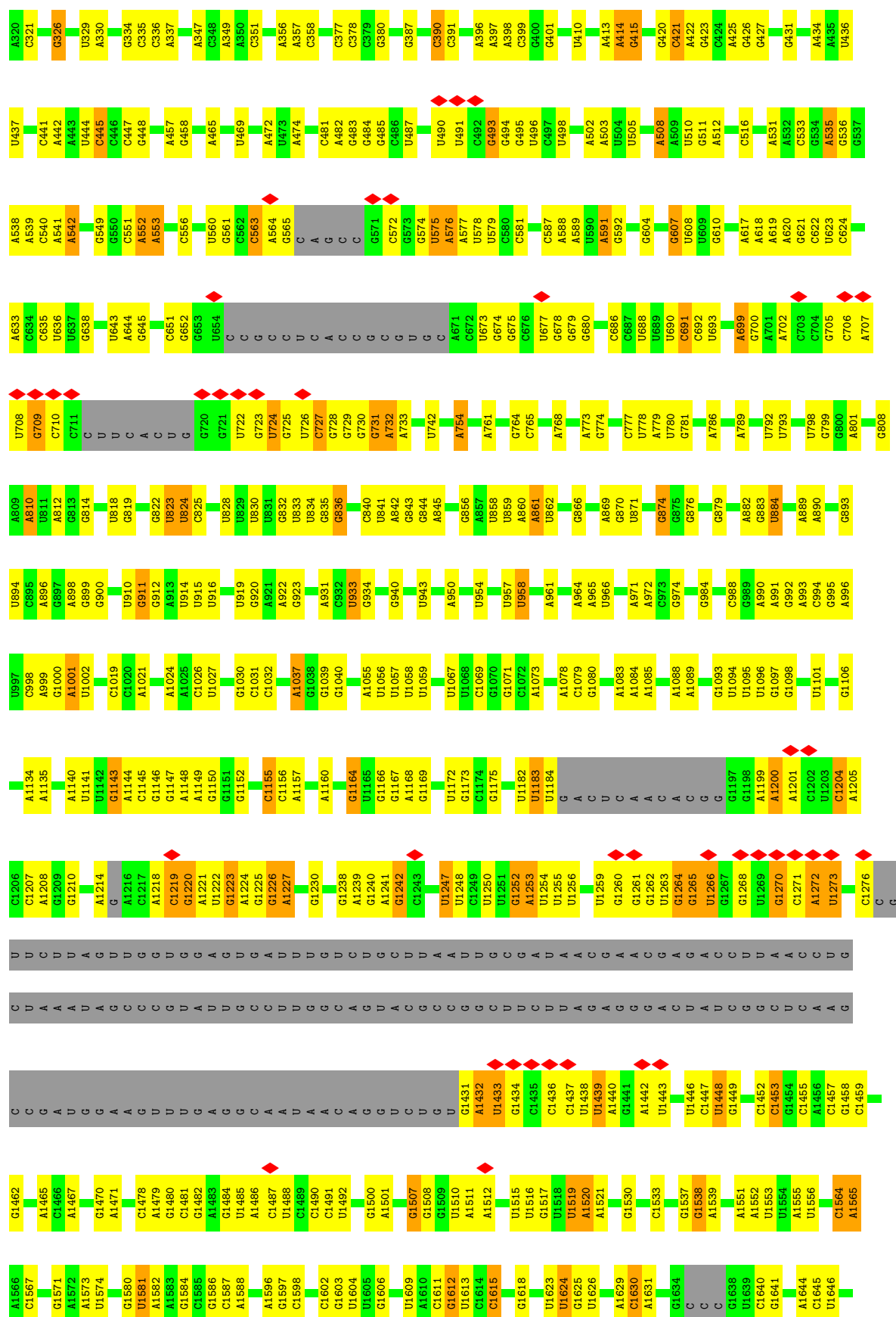


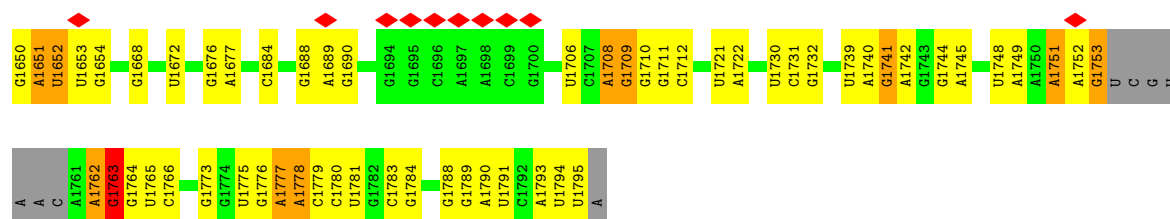
- Molecule 18: Small ribosomal subunit protein eS24



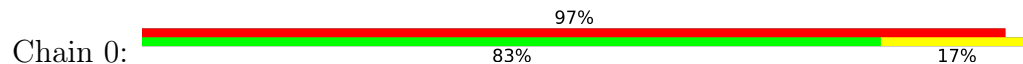
- Molecule 19: 40S ribosomal protein S25



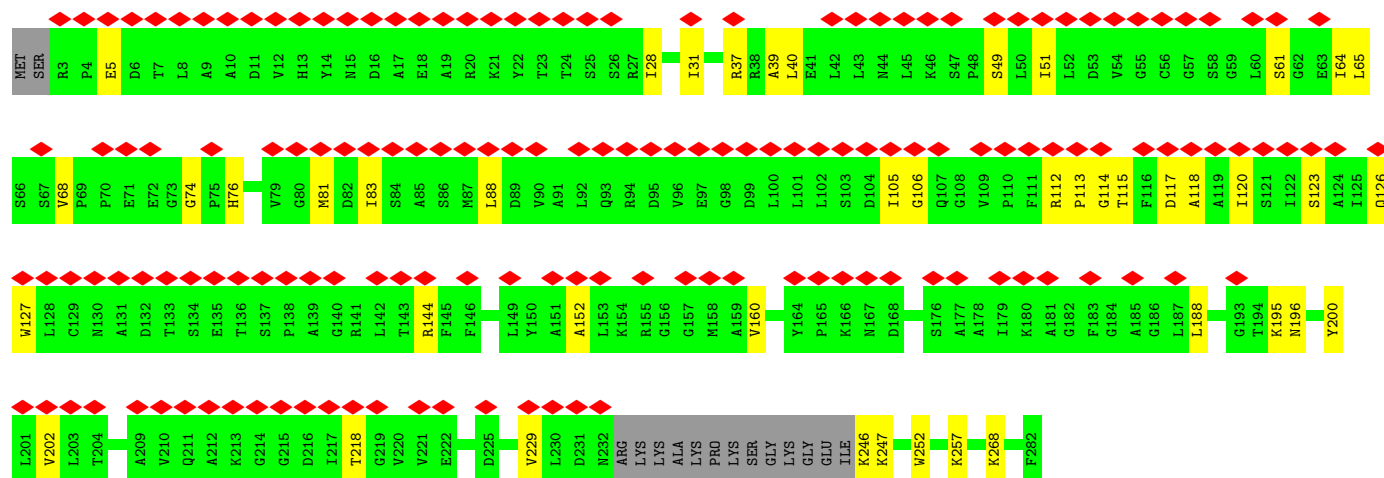
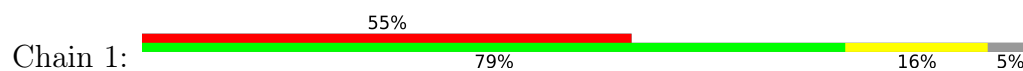




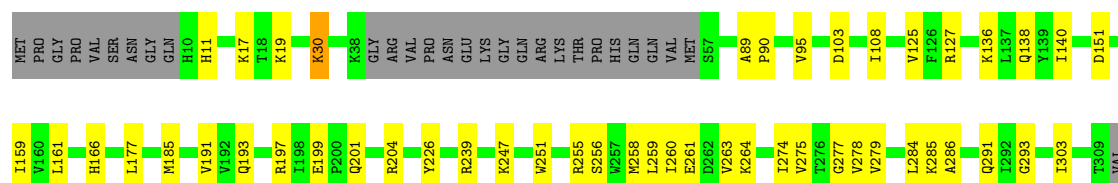
• Molecule 25: Trm112

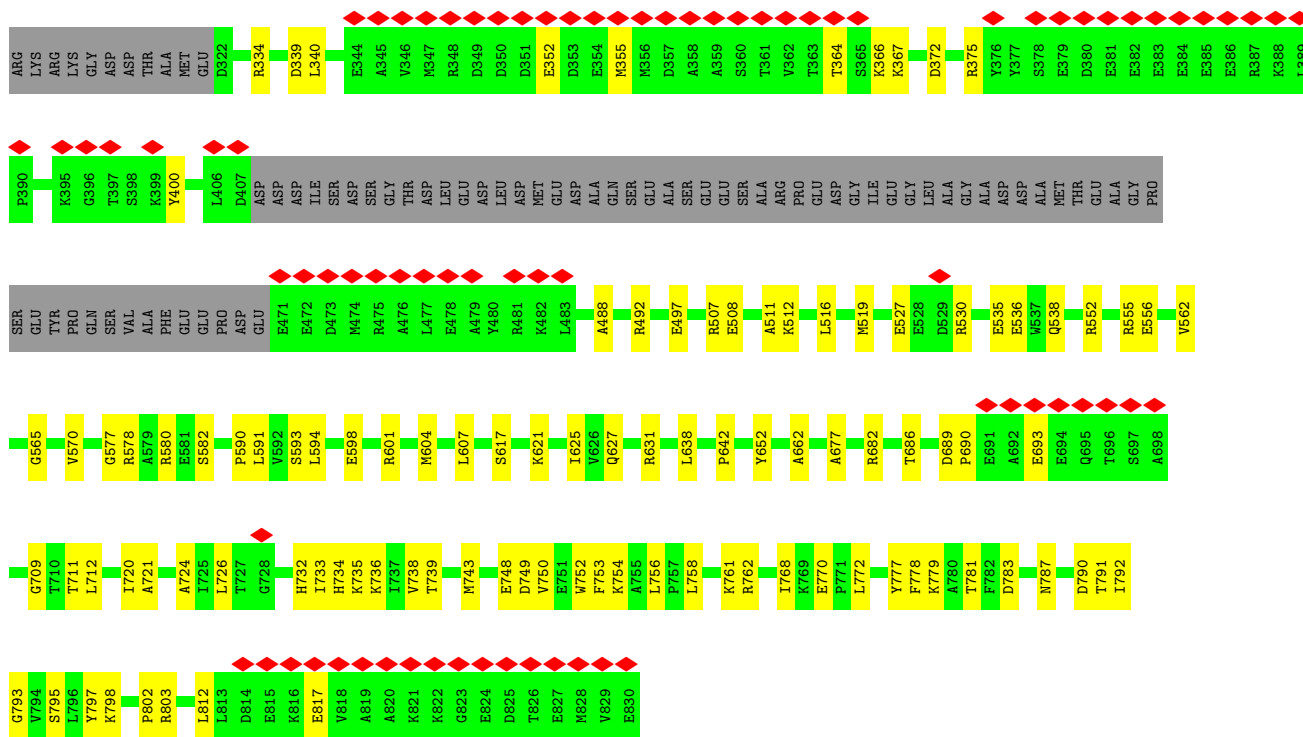


• Molecule 26: Methyltransferase-like protein

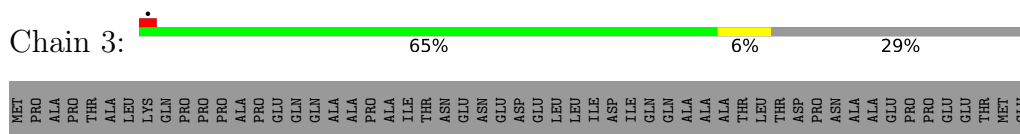


• Molecule 27: Bms1-type G domain-containing protein

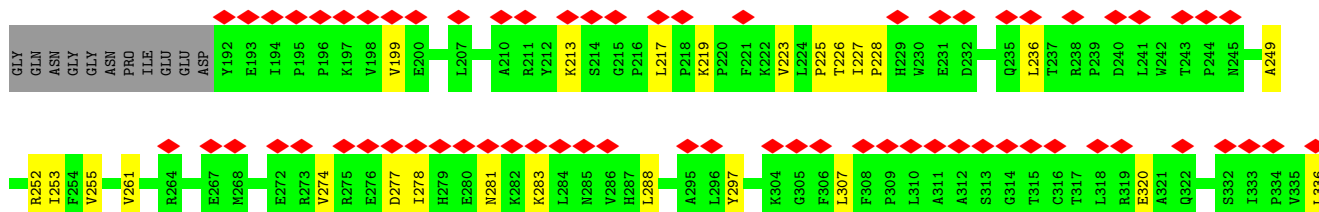
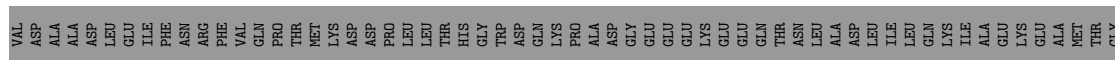




- Molecule 28: Pre-rRNA-processing protein PNO1



- Molecule 29: Bystin-like protein



D121	C181	E241	W301	Q361	T421	Y481	L541	A601	K661	P721	I781	D841	F901
A122	A182	L242	I302	V362	T422	T482	T542	Q602	L662	Q722	P782	A842	L902
A123	E183	L243	A303	L363	G423	T483	E543	K603	A663	I723	M783	P843	T903
G124	T184	L244	I304	V364	E424	M484	A544	M604	Q664	Q724	T784	K844	S904
M125	M185	L245	S305	E365	I425	T485	F545	L605	A665	K725	S785	A845	N905
M126	M186	L246	S306	P366	R426	M486	D546	E606	L666	K726	L786	T846	N906
M127	M187	A247	R307	S367	T427	L487	T547	Y607	Q667	A727	H787	A847	N907
S128	S188	R248	A308	I368	M428	M488	A548	L608	E668	Y728	F788	S848	F908
A129	R189	H249	Y309	Y369	D429	M489	F549	G609	P669	K729	I789	L849	I909
A130	R190	G250	D310	D370	S430	F490	A550	E610	V670	L730	P790	E849	V910
Q131	A191	N251	V311	E371	F431	K491	E551	R611	Q671	I731	S791	E851	K911
I132	V192	E252	A312	K372	T432	T492	M552	P612	K672	P732	I792	M852	S912
G133	F193	H253	A313	V373	G433	E493	L553	A613	P673	K733	L793	T853	V913
G134	D194	M254	Q314	I374	K434	L494	T554	D615	K674	L734	S794	M854	L914
R135	S255	S255	I315	E375	Q435	V495	T555	D615	M675	A735	E795	M855	G915
R136	ALA	M256	S316	K376	E436	P496	V556	L616	P676	E736	V796	V856	F916
V137	LYS	A257	F317	L377	A437	L497	L557	L617	M677	S737	V797	S857	V917
V138	THR	V258	E318	V378	D438	S498	Y558	A618	K678	E738	I798	A858	K918
G139	SER	F259	E319	Q379	V439	A499	E559	V619	E679	V739	G799	G859	V919
G140	GLU	E260	T320	T380	V440	A500	Q560	L620	Q680	G740	C800	L860	C920
L141	LYS	I261	F321	V381	L441	M501	P561	F621	M681	R741	R801	A861	I921
L142	GLY	F262	Q322	E382	G442	Y502	E562	N622	P682	A742	E802	C862	I922
S143	SER	E263	E323	G383	K443	Q503	L563	V623	S683	A743	H803	S863	S923
F144	GLU	M264	I324	L384	A444	R504	R564	Y624	T684	L744	M804	T864	L924
A145	SER	I265	Y325	L385	T445	V505	L565	S625	A685	E745	E805	P865	P925
L146	ALA	F266	E326	T386	R446	L506	D566	T626	H686	Q746	K806	H866	T926
D147	HIS	E267	P327	I387	A447	E507	V567	T627	T687	R747	A807	M867	D927
P148	ASP	G268	F328	K388	M448	H508	C568	T628	L688	H748	R808	S868	L928
R149	P212	M269	N329	Q389	G449	G509	R569	P629	M689	E749	T809	S869	M929
P150	E213	A270	L330	Y390	P450	N510	A570	Q630	D690	E750	T810	A870	L930
K151	L214	D271	V331	A391	E451	A511	L571	K631	L691	V751	A811	T871	P931
V152	H216	E272	A332	A392	A452	P512	R572	R632	V692	Q752	H812	L872	R932
R153	A217	V273	S333	W393	V453	K513	A573	G633	V693	Q753	D813	L873	L933
K154	L218	A274	Y334	L394	L454	T514	L574	P634	T694	L754	L814	A874	P934
R155	Q219	S275	L335	E395	M455	M515	V575	V635	M695	L755	L815	T875	T935
A156	Q219	A276	E336	T396	V456	E516	E576	L636	S696	L756	V816	T876	L936
Q157	K222	K277	E337	F397	L457	V517	S577	Q637	L697	S757	M818	R877	P937
D158	V221	K277	E338	N398	P458	K518	N578	T638	V698	A758	N818	V878	P938
A159	K223	P279	A339	V399	L459	I519	Q579	L639	L699	A759	G819	S879	N939
L160	I224	R280	K340	I400	M460	F520	A580	N640	P700	D760	H820	E881	V940
R161	A225	L281	N341	G401	L461	E521	I581	S641	R701	K761	K821	E881	L941
K162	S226	E283	R343	A402	L462	T522	V582	F642	E702	V762	M822	S883	V942
I163	G227	E283	I344	M403	K463	V523	S583	L643	S703	S763	W823	R883	W943
L164	S228	I284	I344	F404	P464	V524	A584	S644	F704	S764	E824	E884	S944
R165	G229	I285	S345	D405	A465	Q525	G585	T645	E705	P765	A825	A885	H945
N166	Q230	K286	A346	A406	R466	Q526	D586	T646	A706	A766	M826	L886	E946
P167	Q231	E287	S347	L407	D467	I527	V587	P647	L707	R767	G827	M887	H947
P168	P232	L288	E348	R408	Q468	M528	E588	K648	F708	R768	S828	K888	K948
P169	S233	R289	C349	W409	P469	S529	D589	T649	K709	E769	L829	E889	G949
S170	K234	P290	R350	M409	G470	H530	P590	R650	I710	R770	T830	T890	H950
P171	K235	A291	V351	S411	R471	L531	V591	L651	A711	L771	D831	L891	P951
S172	I236	P292	S352	H412	A472	P532	I592	M652	A712	A772	M832	T892	F952
L173	E237	N293	F353	P413	W473	G533	L593	E653	L713	A773	S833	D893	A953
D174	P238	D294	L354	Y414	M474	C534	C594	T654	V714	I774	K834	L894	K954
H175	L239	V295	A355	L415	L475	O535	R595	F655	V715	A775	W835	V895	V955
P176	V177	Q296	N356	L416	P476	D536	V596	D656	F716	A776	P836	Q896	K956
A177	C240	L297	C357	G417	L477	L537	S597	L657	K717	L777	H837	T897	H957
P179	P299	L298	V358	T418	L478	P538	K598	V658	D718	L778	M838	L898	P958
M180	P300	P299	P360	K420	D480	D540	T600	E660	D720	I780	K840	L900	E960

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52758	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Relion	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.479	Depositor
Minimum map value	-0.264	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	412.56, 412.56, 412.56	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.146, 1.146, 1.146	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	0.20	0/1752	0.54	0/2361
2	H	0.21	0/2112	0.46	0/2842
3	I	0.17	0/1578	0.49	0/2130
4	J	0.17	0/1906	0.48	1/2547 (0.0%)
5	K	0.22	0/1587	0.58	0/2140
6	L	0.20	0/1654	0.43	0/2213
7	M	0.22	0/1489	0.43	0/1993
8	O	0.20	0/1249	0.41	0/1678
9	P	0.17	0/934	0.51	0/1255
10	Q	0.19	0/1205	0.41	0/1627
11	R	0.23	0/1014	0.61	0/1361
12	S	0.18	0/932	0.46	0/1248
13	T	0.17	0/922	0.50	1/1241 (0.1%)
14	V	0.17	0/1012	0.51	0/1360
15	W	0.17	0/1137	0.50	1/1533 (0.1%)
16	Z	0.21	0/1055	0.51	0/1416
17	a	0.21	0/1116	0.46	0/1489
18	b	0.17	0/1020	0.41	0/1361
19	c	0.17	0/550	0.47	0/736
20	e	0.19	0/623	0.51	0/843
21	f	0.18	0/487	0.58	2/653 (0.3%)
22	h	0.42	0/184	0.75	0/242
23	i	0.13	0/535	0.37	0/710
24	A	0.21	0/37742	0.37	4/58803 (0.0%)
25	0	0.15	0/1013	0.39	0/1378
26	1	0.18	0/2043	0.43	0/2753
27	2	0.23	0/5944	0.47	0/8037
28	3	0.28	0/1475	0.53	0/1982
29	4	0.17	0/2205	0.46	0/2990
30	5	0.22	0/666	0.59	0/891
31	7	0.17	0/7862	0.40	0/10681
All	All	0.20	0/85003	0.42	9/122494 (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
27	2	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1763	G	C2'-C3'-O3'	-10.52	97.91	113.70
24	A	1763	G	C1'-O4'-C4'	-6.81	103.09	109.90
24	A	1763	G	C4'-C3'-O3'	6.09	122.14	113.00
15	W	111	ILE	N-CA-C	-5.61	107.02	112.29
13	T	76	SER	N-CA-C	-5.54	105.82	113.18
24	A	1763	G	C4'-C3'-C2'	-5.39	97.21	102.60
21	f	35	ASP	N-CA-C	-5.25	107.90	114.56
21	f	34	MET	CA-CB-CG	5.20	124.50	114.10
4	J	55	GLY	N-CA-C	5.05	117.85	110.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	2	199	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1723	0	1804	24	0
2	H	2072	0	2155	31	0
3	I	1557	0	1608	24	0
4	J	1875	0	1983	33	0
5	K	1562	0	1641	26	0
6	L	1621	0	1645	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	1466	0	1582	17	0
8	O	1222	0	1289	13	0
9	P	923	0	946	11	0
10	Q	1182	0	1264	11	0
11	R	1002	0	1034	22	0
12	S	917	0	978	13	0
13	T	909	0	973	10	0
14	V	998	0	1042	11	0
15	W	1117	0	1133	20	0
16	Z	1037	0	1076	10	0
17	a	1099	0	1169	14	0
18	b	1006	0	1082	13	0
19	c	546	0	591	10	0
20	e	611	0	633	3	0
21	f	484	0	513	13	0
22	h	181	0	207	6	0
23	i	528	0	541	9	0
24	A	33747	0	17006	313	0
25	0	993	0	1018	14	0
26	1	2013	0	2043	28	0
27	2	5822	0	5825	88	0
28	3	1451	0	1524	11	0
29	4	2154	0	2242	30	0
30	5	656	0	645	11	0
31	7	7710	0	7978	74	0
32	Q	1	0	0	0	0
32	a	1	0	0	0	0
33	e	1	0	0	0	0
34	A	3	0	0	0	0
34	Q	1	0	0	0	0
All	All	80191	0	65170	816	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 6.

All (816) 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)
24:A:700:G:N2	24:A:732:A:H2	1.41	1.17
24:A:700:G:N2	24:A:732:A:C2	2.14	1.15
24:A:1650:G:N2	24:A:1742:A:H62	1.60	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1265:G:H1	24:A:1438:U:H3	1.08	0.97
24:A:1584:G:H1	24:A:1604:U:H3	0.97	0.96
24:A:1762:A:H2'	24:A:1763:G:H1'	1.49	0.95
24:A:1164:G:H1	24:A:1574:U:H3	0.98	0.94
24:A:652:G:H1	24:A:673:U:H3	1.13	0.90
24:A:709:G:H1	24:A:722:U:H3	1.19	0.88
24:A:1650:G:H21	24:A:1742:A:H62	0.89	0.88
24:A:485:G:H1	24:A:496:U:H3	0.88	0.85
24:A:1650:G:H21	24:A:1742:A:N6	1.71	0.85
21:f:13:VAL:O	21:f:52:ASN:HA	1.77	0.84
24:A:1480:G:N2	24:A:1602:C:O2	2.12	0.82
24:A:1763:G:H2'	24:A:1764:G:C8	2.14	0.82
24:A:220:A:N1	24:A:835:G:C6	2.52	0.77
24:A:487:U:H3	24:A:494:G:H1	1.34	0.74
24:A:148:G:H22	24:A:160:G:H1	1.33	0.74
19:c:29:VAL:HG13	19:c:30:ILE:HD12	1.72	0.70
24:A:1226:G:H21	24:A:1253:A:H62	1.38	0.70
24:A:214:A:N6	24:A:840:C:H42	1.90	0.70
24:A:1651:A:N6	24:A:1741:G:N1	2.41	0.68
24:A:214:A:H61	24:A:840:C:N4	1.92	0.67
8:O:77:THR:HG22	8:O:129:VAL:HG22	1.77	0.66
5:K:73:LEU:HD22	5:K:100:ALA:HB2	1.77	0.66
4:J:231:LYS:HD2	4:J:232:ARG:HG2	1.78	0.66
24:A:214:A:N1	24:A:840:C:N3	2.43	0.66
24:A:898:A:H3'	24:A:899:G:H21	1.62	0.65
5:K:81:GLN:OE1	5:K:85:ARG:NH1	2.30	0.64
24:A:700:G:H21	24:A:732:A:H2	0.73	0.64
8:O:80:VAL:O	8:O:125:GLY:N	2.30	0.64
30:5:394:ASP:HA	30:5:397:LEU:HD23	1.80	0.64
11:R:142:LYS:HG2	24:A:988:C:H5'	1.80	0.63
24:A:158:U:H2'	24:A:159:A:H8	1.63	0.63
24:A:1155:C:H42	24:A:1160:A:H61	1.46	0.63
25:0:123:PRO:HD2	25:0:126:LEU:HD12	1.81	0.63
25:0:31:GLU:HB2	25:0:99:GLU:HB2	1.80	0.63
27:2:159:ILE:HD13	27:2:185:MET:HG3	1.80	0.63
31:7:650:ARG:NH1	31:7:654:THR:OG1	2.32	0.63
4:J:132:ARG:HB3	24:A:68:A:H61	1.64	0.63
6:L:34:ALA:HB2	6:L:56:ARG:HD2	1.81	0.63
8:O:107:LYS:O	17:a:13:ARG:NH2	2.32	0.63
13:T:94:ALA:HB2	13:T:102:LYS:HG3	1.81	0.62
27:2:367:LYS:O	27:2:375:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:19:LEU:HD11	2:H:108:ARG:HD2	1.82	0.62
24:A:699:A:H2	24:A:733:A:H61	1.48	0.62
2:H:151:ASP:OD1	4:J:218:ARG:NH1	2.31	0.62
23:i:126:CYS:SG	23:i:127:GLY:N	2.73	0.62
24:A:700:G:N3	24:A:732:A:N1	2.48	0.62
3:I:58:PRO:HB3	3:I:77:ILE:HG23	1.81	0.61
16:Z:15:ASN:HD21	16:Z:71:LYS:HD2	1.65	0.61
24:A:483:G:H1	24:A:498:U:H3	1.46	0.61
31:7:814:LEU:HG	31:7:818:MET:HE1	1.82	0.61
25:0:117:ILE:HD13	26:1:88:LEU:HD23	1.82	0.61
18:b:89:GLU:OE2	18:b:93:ARG:NH1	2.30	0.61
20:e:37:CYS:SG	20:e:61:ASN:ND2	2.74	0.61
25:0:57:ARG:HG2	25:0:68:LEU:HB2	1.80	0.61
14:V:86:LEU:HD22	14:V:99:GLN:HB2	1.83	0.61
27:2:256:SER:HB3	27:2:593:SER:HB3	1.82	0.61
24:A:1708:A:H2'	24:A:1709:G:H8	1.66	0.61
1:E:32:ILE:HD11	1:E:46:THR:HB	1.83	0.61
4:J:177:ARG:NH2	24:A:64:U:OP1	2.34	0.61
8:O:82:SER:HB3	8:O:90:ILE:HB	1.82	0.61
24:A:200:U:H2'	24:A:201:A:H8	1.65	0.60
24:A:866:G:H1	24:A:958:U:H3	1.48	0.60
31:7:445:ILE:HG12	31:7:453:VAL:HG21	1.83	0.60
11:R:54:ARG:HH22	24:A:914:U:H3	1.47	0.60
31:7:234:LYS:HD2	31:7:235:LYS:HG2	1.84	0.60
4:J:63:MET:HA	4:J:98:ARG:HB3	1.82	0.60
1:E:33:LYS:NZ	1:E:95:ASN:OD1	2.35	0.60
31:7:605:LEU:HD22	31:7:645:ILE:HG21	1.83	0.60
16:Z:2:VAL:N	24:A:1032:C:HO2'	1.98	0.60
24:A:565:G:N2	24:A:572:C:C2	2.70	0.60
4:J:4:ASN:C	4:J:4:ASN:HD22	2.10	0.60
27:2:512:LYS:HB3	27:2:798:LYS:HE2	1.83	0.59
2:H:185:GLY:HA2	2:H:189:MET:HE2	1.84	0.59
5:K:34:GLU:OE1	5:K:45:ARG:NH2	2.36	0.59
12:S:143:ALA:HB2	24:A:1175:G:H21	1.67	0.59
16:Z:32:LYS:NZ	24:A:635:C:OP2	2.35	0.59
24:A:1651:A:N6	24:A:1741:G:H1	1.99	0.59
23:i:143:ARG:NH1	24:A:1250:U:O2'	2.36	0.59
27:2:251:TRP:HB2	27:2:255:ARG:HH21	1.66	0.59
24:A:65:A:H2	24:A:83:A:H62	1.48	0.59
24:A:707:A:N1	24:A:724:U:O2'	2.34	0.59
29:4:278:ILE:HG21	29:4:320:GLU:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:7:450:PRO:HA	31:7:453:VAL:HG22	1.85	0.59
22:h:31:LYS:HE3	24:A:542:A:H2'	1.84	0.59
31:7:650:ARG:NH1	31:7:653:GLU:OE2	2.36	0.59
15:W:65:VAL:HG22	15:W:71:VAL:HG21	1.84	0.59
2:H:100:ARG:HB2	2:H:114:ILE:HD13	1.84	0.59
27:2:761:LYS:HD2	27:2:791:THR:HB	1.85	0.59
5:K:62:LYS:HE3	5:K:94:ARG:HE	1.66	0.59
23:i:81:LYS:NZ	27:2:497:GLU:OE2	2.36	0.59
3:I:129:PRO:HD2	3:I:157:GLN:HE21	1.68	0.58
27:2:125:VAL:HG22	27:2:140:ILE:HG12	1.85	0.58
22:h:31:LYS:NZ	24:A:541:A:O3'	2.36	0.58
31:7:113:LEU:HA	31:7:116:LEU:HD12	1.86	0.58
8:O:34:LYS:NZ	24:A:209:G:N7	2.46	0.58
25:0:50:ARG:HH21	26:1:114:GLY:HA3	1.67	0.58
31:7:663:ALA:O	31:7:667:GLN:NE2	2.37	0.58
4:J:2:LYS:HB2	4:J:108:VAL:HG22	1.86	0.58
4:J:177:ARG:HG3	24:A:77:A:H2	1.69	0.58
24:A:1273:U:O4'	24:A:1431:G:N2	2.36	0.58
24:A:1480:G:H21	24:A:1602:C:H1'	1.66	0.58
31:7:613:ALA:O	31:7:617:LEU:HB2	2.03	0.58
2:H:187:ARG:NH2	24:A:789:A:OP1	2.36	0.58
5:K:87:LEU:HB3	5:K:96:VAL:HG11	1.83	0.58
24:A:219:C:N4	24:A:220:A:N6	2.52	0.58
24:A:378:C:O2'	24:A:754:A:N1	2.36	0.58
26:1:113:PRO:HA	26:1:152:ALA:HA	1.86	0.58
7:M:35:ARG:NH1	24:A:591:A:OP1	2.37	0.58
15:W:38:VAL:HG12	15:W:40:THR:H	1.69	0.58
24:A:67:A:O2'	24:A:69:G:OP1	2.21	0.58
15:W:43:ALA:HA	15:W:84:LYS:HD3	1.85	0.58
24:A:869:A:H2'	24:A:870:G:C8	2.39	0.58
24:A:1227:A:H2	24:A:1252:G:H21	1.52	0.57
5:K:160:LEU:HB2	5:K:191:VAL:HG12	1.86	0.57
24:A:44:U:OP2	24:A:434:A:N6	2.35	0.57
24:A:220:A:C6	24:A:835:G:C6	2.92	0.57
16:Z:4:THR:HG1	24:A:1098:G:HO2'	1.50	0.57
3:I:79:ARG:NH2	24:A:1609:U:OP1	2.38	0.57
21:f:11:VAL:HB	21:f:31:VAL:HB	1.87	0.57
24:A:1265:G:N2	24:A:1438:U:O2	2.37	0.57
27:2:291:GLN:NE2	27:2:293:GLY:O	2.37	0.57
31:7:408:ARG:NH2	31:7:484:ASN:O	2.38	0.57
24:A:214:A:N6	24:A:840:C:N4	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:218:THR:HG23	26:1:229:VAL:HG11	1.87	0.57
27:2:258:MET:HG2	27:2:279:VAL:HA	1.87	0.57
3:I:105:PHE:HA	3:I:108:ILE:HD12	1.87	0.57
27:2:507:ARG:NH1	27:2:749:ASP:OD1	2.38	0.57
29:4:419:GLN:HG3	29:4:420:ARG:HE	1.70	0.57
31:7:185:ALA:HB1	31:7:221:VAL:HG22	1.85	0.57
24:A:688:U:OP2	24:A:691:C:N4	2.34	0.57
24:A:535:A:H5'	24:A:540:C:H41	1.70	0.56
25:0:1:MET:N	25:0:97:ILE:O	2.37	0.56
16:Z:71:LYS:NZ	24:A:1096:U:OP1	2.38	0.56
18:b:13:ARG:NH1	18:b:29:ASP:OD2	2.38	0.56
21:f:28:GLN:NE2	21:f:65:ARG:O	2.37	0.56
24:A:1448:U:H2'	24:A:1449:G:H8	1.71	0.56
27:2:787:ASN:HB3	27:2:790:ASP:HB2	1.86	0.56
29:4:336:LEU:HB3	30:5:358:LEU:HD13	1.87	0.56
1:E:83:LYS:NZ	11:R:129:GLU:OE2	2.38	0.56
10:Q:26:LEU:HG	10:Q:28:THR:HG22	1.86	0.56
24:A:574:G:H2'	24:A:576:A:H4'	1.88	0.56
27:2:95:VAL:HG21	27:2:108:ILE:HD11	1.87	0.56
18:b:6:SER:O	18:b:35:ARG:NH1	2.39	0.56
27:2:263:VAL:HG12	27:2:275:VAL:HG23	1.88	0.56
26:1:106:GLY:O	26:1:144:ARG:NH2	2.39	0.56
2:H:87:MET:HE1	2:H:235:ILE:HG21	1.88	0.56
5:K:69:PRO:O	5:K:73:LEU:N	2.39	0.56
27:2:366:LYS:HB3	27:2:375:ARG:HH12	1.70	0.56
28:3:207:THR:O	28:3:208:ARG:NH1	2.36	0.56
24:A:1263:U:O2'	24:A:1264:G:O4'	2.24	0.55
24:A:1459:C:OP1	26:1:196:ASN:ND2	2.39	0.55
27:2:625:ILE:HG21	27:2:812:LEU:HD11	1.87	0.55
5:K:41:LYS:O	5:K:45:ARG:NH1	2.39	0.55
27:2:90:PRO:HD2	27:2:278:VAL:HG11	1.88	0.55
4:J:57:ASP:HA	4:J:106:LEU:HA	1.88	0.55
18:b:115:LYS:NZ	24:A:55:A:OP1	2.39	0.55
27:2:598:GLU:O	27:2:631:ARG:NH1	2.38	0.55
11:R:101:GLY:O	11:R:105:LYS:NZ	2.39	0.55
24:A:798:U:H2'	24:A:799:G:H8	1.71	0.55
24:A:1210:G:O6	24:A:1447:C:N4	2.39	0.55
3:I:41:ARG:HH21	3:I:118:GLN:HE21	1.55	0.55
3:I:67:LYS:HB3	3:I:70:ARG:HG2	1.86	0.55
27:2:686:THR:HB	27:2:693:GLU:HG2	1.87	0.55
31:7:325:LEU:HD11	31:7:373:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:LYS:HG3	1:E:208:GLN:HB3	1.88	0.55
2:H:45:ILE:HG13	2:H:61:THR:HG21	1.89	0.55
3:I:163:THR:HG23	3:I:167:ARG:HH12	1.72	0.55
15:W:86:ARG:HB2	15:W:89:ARG:HB2	1.89	0.55
27:2:577:GLY:HA2	27:2:580:ARG:HD2	1.88	0.55
2:H:100:ARG:NH2	2:H:118:GLU:O	2.40	0.55
4:J:67:VAL:HG11	4:J:73:VAL:HG21	1.89	0.55
24:A:1150:G:OP1	28:3:256:LYS:NZ	2.39	0.55
24:A:1266:U:H1'	29:4:283:LYS:HD2	1.88	0.55
28:3:114:ARG:NH1	28:3:115:MET:O	2.39	0.55
24:A:1183:U:N3	24:A:1205:A:C6	2.74	0.55
1:E:199:LYS:HG2	24:A:1055:A:H4'	1.87	0.55
18:b:12:THR:HB	18:b:26:MET:HG3	1.88	0.55
18:b:91:ARG:NH2	18:b:101:ALA:O	2.40	0.55
24:A:1587:C:H2'	24:A:1588:A:H8	1.72	0.55
31:7:81:LEU:HG	31:7:116:LEU:HD23	1.88	0.55
3:I:132:ASP:OD1	21:f:46:LYS:NZ	2.40	0.54
7:M:155:ASP:OD1	7:M:156:PHE:N	2.40	0.54
24:A:844:G:H2'	24:A:845:A:H8	1.72	0.54
29:4:255:VAL:HG21	29:4:297:TYR:HB3	1.87	0.54
31:7:69:LEU:O	31:7:73:THR:OG1	2.25	0.54
24:A:213:A:N6	24:A:842:A:O4'	2.41	0.54
24:A:1651:A:N6	24:A:1741:G:C6	2.75	0.54
7:M:129:GLN:HB2	24:A:510:U:H4'	1.90	0.54
19:c:62:GLY:H	24:A:1530:G:H2'	1.73	0.54
24:A:702:A:H62	24:A:731:G:N2	2.06	0.54
31:7:921:ILE:O	31:7:965:ARG:NH1	2.41	0.54
23:i:82:LYS:NZ	24:A:1439:U:OP1	2.41	0.54
24:A:425:A:N3	24:A:437:U:O2'	2.36	0.54
7:M:171:ARG:NH1	24:A:508:A:OP1	2.41	0.54
23:i:139:GLN:HB2	23:i:148:TYR:HB2	1.90	0.54
4:J:133:LEU:O	24:A:163:C:O2'	2.24	0.54
10:Q:38:CYS:SG	10:Q:78:ASN:ND2	2.81	0.54
11:R:37:ASN:ND2	24:A:900:G:OP2	2.41	0.54
24:A:1484:G:C2	24:A:1515:U:O2	2.61	0.54
5:K:51:SER:OG	5:K:52:ALA:N	2.40	0.53
24:A:1167:G:N2	24:A:1567:C:O2'	2.41	0.53
24:A:1199:A:N6	24:A:1453:C:OP1	2.42	0.53
29:4:277:ASP:OD1	29:4:281:ASN:ND2	2.41	0.53
31:7:394:LEU:O	31:7:397:PHE:HB2	2.08	0.53
3:I:203:GLU:OE2	3:I:206:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:284:LEU:HB3	27:2:562:VAL:HB	1.90	0.53
27:2:339:ASP:HB3	27:2:601:ARG:HD2	1.90	0.53
24:A:1584:G:O6	24:A:1604:U:O4	2.26	0.53
7:M:77:ARG:NH2	24:A:761:A:OP1	2.37	0.53
24:A:643:U:H2'	24:A:644:A:H8	1.74	0.53
24:A:1172:U:H2'	24:A:1173:G:H8	1.73	0.53
24:A:1226:G:N2	24:A:1253:A:H62	2.06	0.53
24:A:1709:G:H2'	24:A:1710:G:H8	1.73	0.53
31:7:783:ASN:HA	31:7:786:LEU:HG	1.90	0.53
10:Q:11:ILE:HD11	24:A:862:U:H1'	1.90	0.53
11:R:117:ALA:HA	11:R:120:ARG:HD3	1.90	0.53
24:A:893:G:O6	24:A:915:U:O4	2.27	0.53
24:A:1184:U:O3'	27:2:735:LYS:NZ	2.42	0.53
31:7:879:LEU:HD12	31:7:916:PHE:HZ	1.74	0.53
31:7:165:ARG:HG3	31:7:227:GLY:HA2	1.89	0.53
9:P:108:ARG:O	30:5:347:GLN:NE2	2.42	0.53
14:V:86:LEU:O	14:V:89:GLN:NE2	2.39	0.53
27:2:364:THR:OG1	27:2:366:LYS:NZ	2.40	0.53
31:7:693:VAL:HG22	31:7:730:LEU:HD13	1.91	0.53
6:L:171:ALA:HB2	6:L:187:ILE:HD13	1.91	0.53
12:S:42:ARG:O	12:S:50:ARG:NH1	2.42	0.53
24:A:426:G:O2'	27:2:239:ARG:NH2	2.42	0.53
1:E:172:ILE:HG12	1:E:193:ILE:HD11	1.89	0.52
24:A:574:G:N7	24:A:575:U:O2'	2.41	0.52
27:2:161:LEU:HD21	27:2:177:LEU:HD13	1.90	0.52
1:E:62:LYS:NZ	1:E:89:ASP:O	2.32	0.52
14:V:107:SER:HA	14:V:110:ARG:HB2	1.91	0.52
24:A:1447:C:OP2	29:4:213:LYS:NZ	2.39	0.52
28:3:109:CYS:HB3	28:3:135:ALA:HB1	1.91	0.52
24:A:812:A:O2'	24:A:814:G:OP2	2.28	0.52
12:S:106:SER:HB3	12:S:128:SER:HB2	1.91	0.52
15:W:89:ARG:HH12	24:A:1596:A:H4'	1.75	0.52
5:K:188:GLY:HA3	24:A:638:G:H21	1.74	0.52
6:L:110:ARG:HD3	6:L:123:ARG:HH12	1.75	0.52
1:E:124:ASN:HA	1:E:137:LEU:O	2.09	0.52
1:E:192:VAL:HG23	1:E:195:ARG:HH21	1.74	0.52
3:I:68:ARG:NH1	24:A:1612:G:OP1	2.43	0.52
7:M:107:LEU:HB2	7:M:144:PHE:HB3	1.91	0.52
23:i:118:ARG:HE	23:i:131:PHE:HB3	1.73	0.52
26:1:112:ARG:NH2	26:1:114:GLY:O	2.43	0.52
2:H:49:ARG:NH2	24:A:445:C:OP1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:94:ILE:HD11	11:R:128:ILE:HG12	1.92	0.52
26:1:68:VAL:HG23	26:1:74:GLY:HA3	1.91	0.52
27:2:754:LYS:HG3	27:2:768:ILE:HD11	1.91	0.52
3:I:57:ILE:HD11	13:T:47:LYS:HG2	1.92	0.51
24:A:700:G:N2	24:A:731:G:O2'	2.41	0.51
27:2:733:ILE:HG22	27:2:738:VAL:HG22	1.92	0.51
31:7:963:ILE:HD12	31:7:990:LYS:HD2	1.92	0.51
4:J:136:LYS:NZ	4:J:177:ARG:O	2.36	0.51
24:A:954:U:OP1	24:A:1069:C:O2'	2.28	0.51
27:2:285:LYS:NZ	27:2:556:GLU:O	2.40	0.51
24:A:808:G:OP2	24:A:808:G:N2	2.39	0.51
7:M:133:ARG:NH1	7:M:156:PHE:O	2.40	0.51
19:c:43:VAL:O	19:c:92:ARG:NH1	2.44	0.51
26:1:123:SER:HB3	26:1:126:GLN:HE22	1.75	0.51
3:I:58:PRO:HG3	3:I:77:ILE:HG13	1.93	0.51
9:P:70:GLU:HB3	9:P:73:TYR:HB3	1.92	0.51
15:W:40:THR:HA	15:W:100:VAL:HG21	1.92	0.51
18:b:15:PHE:HZ	18:b:24:LYS:HD3	1.75	0.51
10:Q:108:ASP:OD1	24:A:876:G:O2'	2.28	0.51
24:A:563:C:H2'	24:A:564:A:H8	1.76	0.51
4:J:13:GLN:HE22	24:A:148:G:H21	1.59	0.51
15:W:6:THR:HG23	15:W:8:ARG:H	1.76	0.51
24:A:140:G:H2'	24:A:141:G:C8	2.46	0.51
24:A:155:U:O2'	24:A:157:C:OP2	2.25	0.51
27:2:508:GLU:HA	27:2:511:ALA:HB2	1.91	0.51
31:7:475:LEU:HA	31:7:478:LEU:HD12	1.93	0.51
12:S:42:ARG:HE	12:S:50:ARG:HA	1.76	0.51
4:J:142:ARG:HE	4:J:153:VAL:HG21	1.76	0.51
24:A:1641:G:O6	24:A:1751:A:N7	2.44	0.51
17:a:19:ARG:O	17:a:23:ARG:HB2	2.11	0.51
24:A:487:U:O4	24:A:494:G:O6	2.29	0.51
24:A:561:G:H1	24:A:576:A:HO2'	1.56	0.51
27:2:535:GLU:O	27:2:538:GLN:NE2	2.44	0.51
31:7:82:ARG:NH1	31:7:120:GLN:OE1	2.44	0.51
31:7:569:ARG:HH21	31:7:634:PRO:HB3	1.76	0.51
14:V:107:SER:OG	14:V:110:ARG:NH2	2.43	0.50
15:W:5:VAL:O	15:W:138:GLN:NE2	2.45	0.50
26:1:188:LEU:HB3	26:1:200:TYR:HB2	1.93	0.50
27:2:286:ALA:O	27:2:334:ARG:NH1	2.44	0.50
4:J:193:ARG:NH2	24:A:264:U:O4	2.44	0.50
11:R:34:ALA:HB2	11:R:111:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:14:LYS:NZ	24:A:1101:U:OP1	2.42	0.50
26:1:160:VAL:HG22	26:1:202:VAL:HG12	1.93	0.50
27:2:255:ARG:HG2	27:2:594:LEU:HA	1.93	0.50
5:K:116:ASN:ND2	24:A:742:U:OP1	2.40	0.50
22:h:36:LYS:HA	22:h:39:LEU:HD12	1.93	0.50
23:i:102:VAL:HG13	23:i:103:LEU:HD12	1.92	0.50
24:A:922:A:H2'	24:A:923:G:C8	2.47	0.50
24:A:966:U:OP1	24:A:1031:C:O2'	2.28	0.50
27:2:682:ARG:NH2	27:2:817:GLU:OE1	2.45	0.50
24:A:1230:G:OP1	29:4:252:ARG:NH1	2.44	0.50
14:V:110:ARG:O	14:V:113:LEU:HB3	2.11	0.50
15:W:144:ASP:N	15:W:144:ASP:OD1	2.44	0.50
21:f:19:ARG:HD2	21:f:27:THR:HB	1.93	0.50
24:A:1055:A:N6	24:A:1058:U:OP1	2.45	0.50
2:H:55:ALA:HB2	2:H:64:ILE:HD12	1.93	0.50
3:I:98:VAL:HA	3:I:101:VAL:HG22	1.93	0.50
3:I:164:THR:HA	3:I:167:ARG:HG2	1.94	0.50
15:W:99:SER:N	24:A:1500:G:OP1	2.44	0.50
24:A:220:A:N6	24:A:221:A:N1	2.60	0.50
24:A:1689:A:H2'	24:A:1690:G:H8	1.77	0.50
5:K:11:ALA:HA	5:K:16:ARG:HD2	1.94	0.50
24:A:919:U:H2'	24:A:920:G:H8	1.77	0.50
31:7:474:MET:HA	31:7:477:LEU:HD13	1.93	0.50
12:S:90:ASP:OD2	24:A:1551:A:O2'	2.30	0.50
18:b:11:ARG:HD2	24:A:778:U:H2'	1.93	0.50
22:h:39:LEU:HD23	22:h:42:ARG:NH2	2.26	0.50
27:2:259:LEU:O	27:2:277:GLY:HA3	2.12	0.50
2:H:30:ARG:NH2	24:A:295:C:O2'	2.45	0.50
7:M:140:ASN:ND2	18:b:67:TYR:OH	2.45	0.50
11:R:31:ARG:NH1	24:A:916:U:O2'	2.44	0.50
31:7:49:LEU:HD22	31:7:69:LEU:HD13	1.93	0.50
31:7:501:MET:HE1	31:7:523:VAL:HG12	1.93	0.50
11:R:92:LEU:HG	11:R:123:MET:HE2	1.93	0.49
24:A:1517:G:O2'	24:A:1519:U:OP2	2.26	0.49
27:2:201:GLN:HA	27:2:204:ARG:HD3	1.93	0.49
31:7:924:LEU:HD22	31:7:928:LEU:HD21	1.94	0.49
31:7:778:ILE:HD13	31:7:781:ILE:HD12	1.94	0.49
16:Z:76:SER:HB2	24:A:1098:G:H5''	1.95	0.49
27:2:621:LYS:HG2	27:2:803:ARG:HH21	1.78	0.49
2:H:143:ASP:OD1	2:H:143:ASP:N	2.45	0.49
3:I:16:LEU:HD21	13:T:52:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:70:LYS:NZ	24:A:961:A:N7	2.60	0.49
13:T:58:ASP:OD1	13:T:58:ASP:N	2.45	0.49
19:c:26:GLN:OE1	19:c:59:LYS:NZ	2.39	0.49
24:A:485:G:O6	24:A:496:U:O4	2.29	0.49
24:A:651:C:H2'	24:A:652:G:H8	1.77	0.49
27:2:340:LEU:HD21	27:2:536:GLU:HG2	1.94	0.49
27:2:758:LEU:HB3	27:2:792:ILE:HD11	1.93	0.49
26:1:257:LYS:NZ	26:1:268:LYS:O	2.36	0.49
31:7:689:MET:HE1	31:7:726:LYS:HB3	1.93	0.49
6:L:44:HIS:ND1	24:A:1672:U:OP1	2.39	0.49
10:Q:99:ARG:NH2	10:Q:119:GLU:OE2	2.39	0.49
24:A:1230:G:C2	24:A:1250:U:O2	2.66	0.49
6:L:2:GLY:N	24:A:390:C:OP2	2.46	0.49
6:L:114:GLU:OE2	6:L:123:ARG:NH1	2.46	0.49
7:M:85:ASP:HB2	7:M:88:ARG:HG2	1.94	0.49
29:4:227:ILE:HD12	29:4:228:PRO:HD2	1.94	0.49
24:A:1001:A:C4	28:3:251:ILE:HD11	2.48	0.49
27:2:488:ALA:HB1	27:2:617:SER:HB2	1.95	0.49
27:2:652:TYR:HB2	27:2:720:ILE:HG22	1.94	0.49
29:4:392:TYR:HA	29:4:395:MET:HE3	1.93	0.49
30:5:345:THR:OG1	30:5:346:GLU:OE1	2.30	0.49
31:7:183:GLU:HG2	31:7:187:MET:HE1	1.94	0.49
24:A:17:C:O2'	24:A:1134:A:N1	2.45	0.49
24:A:893:G:H2'	24:A:894:U:C6	2.48	0.49
24:A:1164:G:O6	24:A:1574:U:O4	2.30	0.49
24:A:1739:U:H2'	24:A:1740:A:C8	2.48	0.49
27:2:260:ILE:HD11	27:2:591:LEU:HB2	1.95	0.49
24:A:64:U:O2'	24:A:165:A:N3	2.41	0.49
26:1:28:ILE:HD13	26:1:31:ILE:HD11	1.95	0.49
27:2:492:ARG:NH2	27:2:617:SER:OG	2.45	0.49
4:J:66:GLY:HA2	24:A:1677:A:H1'	1.94	0.48
6:L:182:ARG:NH1	24:A:255:C:O2	2.46	0.48
19:c:64:LEU:HD13	19:c:67:LYS:HE3	1.94	0.48
21:f:15:ARG:NH1	21:f:16:VAL:O	2.46	0.48
24:A:893:G:H1	24:A:915:U:H3	1.57	0.48
24:A:1581:U:H2'	24:A:1582:A:H8	1.77	0.48
25:0:1:MET:HE1	25:0:6:LEU:HB2	1.95	0.48
10:Q:124:ARG:NH2	24:A:965:A:OP2	2.45	0.48
19:c:79:ARG:HE	19:c:80:GLN:H	1.60	0.48
24:A:700:G:C2	24:A:732:A:N1	2.81	0.48
24:A:1168:A:H2'	24:A:1169:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1448:U:H2'	24:A:1449:G:C8	2.47	0.48
29:4:336:LEU:HD22	30:5:355:PHE:HE1	1.78	0.48
27:2:726:LEU:O	27:2:793:GLY:HA2	2.12	0.48
29:4:274:VAL:HG12	29:4:288:LEU:HD13	1.94	0.48
30:5:395:GLU:O	30:5:399:ASN:ND2	2.46	0.48
31:7:81:LEU:HD22	31:7:119:ALA:HB3	1.94	0.48
24:A:1199:A:H62	24:A:1452:C:H3'	1.78	0.48
3:I:68:ARG:HD2	24:A:1611:C:H3'	1.95	0.48
5:K:125:SER:OG	5:K:126:ARG:NH1	2.46	0.48
6:L:98:LYS:HB3	24:A:326:G:H5''	1.94	0.48
12:S:109:GLU:HG2	27:2:400:TYR:HB3	1.96	0.48
21:f:12:LYS:O	21:f:31:VAL:HA	2.14	0.48
21:f:22:SER:HB2	24:A:1615:C:H5'	1.95	0.48
27:2:642:PRO:HD3	27:2:662:ALA:HA	1.94	0.48
24:A:469:U:O2'	24:A:768:A:N3	2.39	0.48
24:A:834:U:O4	24:A:835:G:O6	2.30	0.48
24:A:1709:G:H2'	24:A:1710:G:C8	2.48	0.48
24:A:1751:A:N7	24:A:1753:G:C6	2.82	0.48
27:2:762:ARG:HH11	27:2:787:ASN:HB2	1.78	0.48
29:4:225:PRO:HB3	29:4:261:VAL:HG11	1.94	0.48
2:H:7:LYS:HE2	24:A:93:U:H1'	1.94	0.48
4:J:136:LYS:NZ	24:A:65:A:OP1	2.40	0.48
17:a:92:CYS:HB3	17:a:132:LEU:HD22	1.95	0.48
24:A:510:U:H2'	24:A:511:G:C8	2.48	0.48
6:L:99:SER:HB3	24:A:326:G:H5'	1.95	0.48
27:2:352:GLU:O	27:2:355:MET:HB2	2.13	0.48
14:V:30:TYR:HE1	14:V:40:ARG:HD2	1.79	0.48
24:A:552:A:H2'	24:A:553:A:C8	2.49	0.48
31:7:456:VAL:HG12	31:7:457:LEU:HG	1.96	0.48
31:7:704:PHE:HE2	31:7:739:VAL:HG13	1.79	0.48
11:R:105:LYS:HA	11:R:132:THR:HG21	1.96	0.47
21:f:45:VAL:HG12	21:f:47:GLY:H	1.78	0.47
23:i:80:ARG:NH2	27:2:790:ASP:O	2.47	0.47
23:i:141:CYS:HB3	23:i:145:HIS:H	1.78	0.47
24:A:844:G:H2'	24:A:845:A:C8	2.48	0.47
27:2:753:PHE:HB3	27:2:756:LEU:HD13	1.95	0.47
10:Q:93:LYS:HG2	10:Q:150:VAL:HG13	1.96	0.47
24:A:843:G:H2'	24:A:844:G:C8	2.49	0.47
24:A:934:G:OP1	24:A:1071:G:N2	2.43	0.47
24:A:1207:C:H2'	24:A:1208:A:H8	1.79	0.47
1:E:115:ARG:HB3	1:E:118:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:95:LYS:HB3	11:R:131:VAL:HG11	1.96	0.47
13:T:20:ALA:HB1	13:T:65:ILE:HD11	1.95	0.47
24:A:1708:A:H2'	24:A:1709:G:C8	2.48	0.47
31:7:411:SER:HB3	31:7:448:MET:HE2	1.96	0.47
5:K:50:VAL:HG23	5:K:69:PRO:HD3	1.97	0.47
6:L:157:ASP:OD1	6:L:157:ASP:N	2.46	0.47
24:A:708:U:O2	24:A:723:G:O6	2.31	0.47
29:4:374:ARG:HH11	29:4:420:ARG:HD3	1.79	0.47
31:7:81:LEU:HD21	31:7:116:LEU:HA	1.96	0.47
31:7:918:LYS:HA	31:7:921:ILE:HD12	1.96	0.47
11:R:52:ILE:HD13	11:R:89:ILE:HD11	1.95	0.47
24:A:587:C:H2'	24:A:588:A:H8	1.79	0.47
24:A:607:G:O2'	24:A:610:G:O2'	2.30	0.47
27:2:604:MET:HE1	27:2:711:THR:HG23	1.96	0.47
27:2:689:ASP:N	27:2:689:ASP:OD1	2.45	0.47
5:K:109:LYS:NZ	24:A:692:C:O2	2.40	0.47
11:R:81:ALA:O	11:R:85:LYS:HG3	2.14	0.47
27:2:783:ASP:N	27:2:783:ASP:OD1	2.47	0.47
31:7:865:PRO:HB3	31:7:909:ILE:HD11	1.96	0.47
2:H:98:ASN:ND2	2:H:116:ASP:OD1	2.48	0.47
2:H:198:ARG:HG2	2:H:208:VAL:HG22	1.96	0.47
5:K:126:ARG:NH2	24:A:856:G:OP1	2.40	0.47
15:W:11:ASP:OD1	15:W:11:ASP:N	2.45	0.47
27:2:607:LEU:O	27:2:709:GLY:HA3	2.14	0.47
28:3:91:ARG:NH2	28:3:150:PHE:O	2.48	0.47
30:5:395:GLU:OE1	30:5:399:ASN:ND2	2.48	0.47
12:S:60:ARG:NH2	24:A:1239:A:OP1	2.47	0.47
24:A:1432:A:O2'	24:A:1433:U:O3'	2.32	0.47
26:1:37:ARG:HA	26:1:40:LEU:HG	1.96	0.47
26:1:83:ILE:HD11	26:1:105:ILE:HG12	1.96	0.47
27:2:736:LYS:NZ	27:2:781:THR:OG1	2.47	0.47
29:4:223:VAL:O	29:4:226:THR:OG1	2.32	0.47
2:H:139:LEU:HD11	2:H:169:ILE:HD11	1.97	0.47
16:Z:57:ARG:HG2	24:A:861:A:H4'	1.97	0.47
31:7:248:ARG:HB2	31:7:297:LEU:HD21	1.97	0.47
24:A:493:G:H2'	24:A:494:G:H8	1.80	0.47
27:2:527:GLU:HA	27:2:530:ARG:HH12	1.79	0.47
31:7:540:ASP:N	31:7:540:ASP:OD1	2.48	0.47
21:f:50:ARG:N	21:f:53:ASP:OD2	2.47	0.46
29:4:416:VAL:O	29:4:420:ARG:HB2	2.15	0.46
31:7:705:GLU:OE1	31:7:747:ARG:NE	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1538:G:N2	24:A:1565:A:OP2	2.47	0.46
17:a:93:LEU:HA	17:a:96:VAL:HG22	1.97	0.46
24:A:390:C:H2'	24:A:391:C:C6	2.49	0.46
24:A:487:U:N3	24:A:495:G:N1	2.64	0.46
27:2:627:GLN:O	27:2:677:ALA:HA	2.14	0.46
27:2:519:MET:SD	27:2:519:MET:N	2.88	0.46
27:2:638:LEU:HD13	27:2:802:PRO:HA	1.97	0.46
28:3:91:ARG:O	28:3:95:LEU:HB2	2.15	0.46
29:4:226:THR:HG21	30:5:386:ARG:HH21	1.80	0.46
13:T:30:LYS:HA	13:T:35:PRO:HA	1.97	0.46
24:A:276:G:H8	24:A:277:C:H4'	1.81	0.46
31:7:113:LEU:HD13	31:7:137:VAL:HG13	1.96	0.46
31:7:927:ASP:OD1	31:7:927:ASP:N	2.48	0.46
2:H:87:MET:HE3	2:H:87:MET:HB3	1.79	0.46
4:J:164:PRO:HD3	4:J:171:PRO:HA	1.98	0.46
7:M:50:ILE:HD13	7:M:78:LEU:HD21	1.96	0.46
9:P:116:VAL:HG11	24:A:1223:G:H2'	1.98	0.46
17:a:68:ILE:HD12	17:a:70:LYS:HE3	1.98	0.46
24:A:607:G:HO2'	24:A:610:G:HO2'	1.58	0.46
24:A:1644:A:H2'	24:A:1645:C:C6	2.51	0.46
26:1:81:MET:HG3	26:1:105:ILE:HG22	1.98	0.46
27:2:258:MET:HB3	27:2:591:LEU:HB3	1.97	0.46
1:E:88:VAL:HA	1:E:98:THR:HA	1.98	0.46
10:Q:106:ARG:O	10:Q:112:LYS:NZ	2.45	0.46
17:a:75:GLN:HA	17:a:82:LYS:HA	1.98	0.46
24:A:709:G:O6	24:A:722:U:O4	2.33	0.46
24:A:1462:G:O2'	24:A:1598:C:OP1	2.29	0.46
24:A:1688:G:N1	24:A:1706:U:N3	2.63	0.46
4:J:57:ASP:OD2	4:J:72:ARG:NH1	2.49	0.46
24:A:336:C:H2'	24:A:337:A:H8	1.81	0.46
24:A:1433:U:OP1	29:4:444:LYS:NZ	2.40	0.46
29:4:252:ARG:HH21	29:4:253:ILE:HD13	1.81	0.46
29:4:199:VAL:HG13	29:4:236:LEU:HD11	1.98	0.46
29:4:336:LEU:HD13	30:5:355:PHE:HD1	1.81	0.46
1:E:39:ALA:HB3	1:E:74:GLN:HA	1.99	0.45
3:I:108:ILE:HD11	3:I:185:LEU:HD21	1.98	0.45
5:K:81:GLN:HB3	5:K:85:ARG:HH22	1.80	0.45
8:O:104:ARG:HG3	17:a:12:ALA:HB2	1.98	0.45
22:h:31:LYS:HZ1	24:A:542:A:P	2.38	0.45
24:A:1230:G:N1	24:A:1250:U:C2	2.84	0.45
25:0:25:LEU:HB3	25:0:102:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:138:GLN:NE2	27:2:261:GLU:OE2	2.46	0.45
27:2:743:MET:HE3	27:2:792:ILE:HG23	1.98	0.45
31:7:387:ILE:O	31:7:390:GLN:HB2	2.15	0.45
4:J:85:ARG:O	4:J:87:ARG:NH1	2.49	0.45
6:L:56:ARG:HH22	24:A:329:U:P	2.40	0.45
6:L:125:ARG:HB2	6:L:131:GLN:HB2	1.98	0.45
7:M:133:ARG:HD3	7:M:157:ALA:HA	1.98	0.45
17:a:26:ASP:HB3	17:a:29:TYR:HB3	1.97	0.45
21:f:36:ASP:OD1	21:f:36:ASP:N	2.49	0.45
24:A:484:G:H2'	24:A:485:G:H8	1.81	0.45
27:2:151:ASP:HB3	27:2:590:PRO:HD3	1.98	0.45
30:5:386:ARG:H	30:5:389:PHE:HE1	1.65	0.45
22:h:26:LYS:O	22:h:27:PRO:C	2.60	0.45
1:E:133:TYR:HD2	1:E:217:LEU:HD11	1.81	0.45
11:R:44:THR:HG22	11:R:51:THR:HA	1.97	0.45
19:c:61:ASN:HB2	19:c:64:LEU:HD23	1.97	0.45
24:A:1629:A:H3'	24:A:1630:C:H6	1.81	0.45
25:0:30:ALA:HA	25:0:99:GLU:O	2.16	0.45
31:7:857:SER:HA	31:7:860:LEU:HD12	1.97	0.45
18:b:86:LYS:HB3	18:b:86:LYS:HE2	1.82	0.45
24:A:588:A:H2'	24:A:589:A:C8	2.52	0.45
24:A:1457:C:H2'	24:A:1458:G:H8	1.81	0.45
24:A:1480:G:N2	24:A:1602:C:C2	2.82	0.45
27:2:516:LEU:HD23	27:2:797:TYR:HB2	1.99	0.45
27:2:772:LEU:O	27:2:777:TYR:HB2	2.17	0.45
1:E:52:THR:HG22	1:E:55:LYS:HE3	1.99	0.45
24:A:706:C:H2'	24:A:707:A:C8	2.51	0.45
24:A:1168:A:H2'	24:A:1169:G:H8	1.80	0.45
31:7:454:LEU:HD22	31:7:458:PRO:HA	1.99	0.45
1:E:71:ALA:HB2	1:E:80:ALA:HA	1.98	0.45
24:A:1265:G:O6	24:A:1438:U:O4	2.35	0.45
24:A:1480:G:H2'	24:A:1481:C:C6	2.52	0.45
24:A:1623:U:H2'	24:A:1624:U:O4'	2.16	0.45
2:H:50:ASN:O	2:H:53:LYS:NZ	2.39	0.45
5:K:32:ASP:O	5:K:36:ASN:ND2	2.50	0.45
6:L:16:ALA:HB2	24:A:351:C:H5''	1.98	0.45
29:4:386:VAL:HG21	29:4:429:GLN:HB2	1.99	0.45
31:7:85:PHE:HD1	31:7:116:LEU:HD13	1.81	0.45
11:R:18:PRO:HB2	11:R:20:VAL:HG12	1.98	0.45
14:V:108:LYS:O	14:V:111:GLU:HG3	2.17	0.45
15:W:50:ASP:N	15:W:50:ASP:OD1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:132:ASP:OD1	15:W:135:ARG:NH2	2.43	0.45
31:7:535:CYS:HB3	31:7:574:LEU:HG	1.98	0.45
11:R:96:ILE:HD11	11:R:111:ALA:HB1	1.98	0.45
19:c:84:HIS:HE1	19:c:86:LYS:HE3	1.82	0.45
24:A:727:C:H2'	24:A:728:G:C8	2.51	0.45
1:E:40:VAL:HG21	1:E:75:LYS:HE2	1.98	0.44
8:O:29:SER:O	8:O:37:ARG:NH1	2.50	0.44
10:Q:83:ASP:OD1	10:Q:83:ASP:N	2.48	0.44
14:V:70:VAL:HA	14:V:73:ILE:HG12	1.99	0.44
19:c:81:VAL:HB	19:c:89:ILE:HG13	1.97	0.44
24:A:652:G:N2	24:A:673:U:O2	2.37	0.44
26:1:5:GLU:HG3	26:1:127:TRP:HD1	1.82	0.44
31:7:623:VAL:O	31:7:627:THR:OG1	2.28	0.44
2:H:23:LEU:HD11	7:M:4:ARG:HH12	1.82	0.44
15:W:98:GLY:N	24:A:1500:G:OP1	2.50	0.44
3:I:151:PRO:HA	3:I:154:ARG:HB2	2.00	0.44
9:P:97:LEU:HA	9:P:100:TRP:HB2	2.00	0.44
9:P:129:GLU:OE1	9:P:133:ARG:N	2.45	0.44
24:A:1167:G:H1	24:A:1465:A:H2	1.64	0.44
24:A:1480:G:H2'	24:A:1481:C:H6	1.82	0.44
24:A:1777:A:H2'	24:A:1778:A:C8	2.52	0.44
27:2:89:ALA:HB2	27:2:565:GLY:HA2	1.98	0.44
1:E:36:ALA:HB2	1:E:231:LEU:HB3	1.98	0.44
12:S:91:MET:HB3	12:S:124:LEU:HD12	1.98	0.44
27:2:264:LYS:HD2	27:2:274:ILE:HB	2.00	0.44
28:3:226:GLY:O	28:3:230:GLU:HG2	2.17	0.44
3:I:85:MET:HE1	24:A:1606:G:H4'	1.99	0.44
24:A:29:U:H2'	24:A:30:G:H8	1.81	0.44
28:3:181:ASP:N	28:3:181:ASP:OD1	2.48	0.44
12:S:89:ARG:NH2	12:S:128:SER:O	2.51	0.44
24:A:143:U:H2'	24:A:144:A:H8	1.82	0.44
4:J:48:TYR:HD1	4:J:117:GLY:H	1.64	0.44
24:A:874:G:O6	24:A:933:U:O4	2.36	0.44
28:3:96:LYS:HE2	28:3:115:MET:HE3	2.00	0.44
1:E:158:SER:OG	24:A:874:G:OP1	2.35	0.44
3:I:85:MET:HG3	3:I:91:ASN:HA	1.99	0.44
5:K:105:LEU:HD22	5:K:118:LEU:HD21	1.99	0.44
6:L:139:SER:OG	24:A:186:C:N4	2.42	0.44
11:R:26:VAL:HG12	11:R:90:THR:HG22	1.99	0.44
27:2:732:HIS:HB2	27:2:739:THR:HG22	1.99	0.44
29:4:307:LEU:HD23	29:4:345:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:97:VAL:HG23	4:J:98:ARG:H	1.82	0.43
4:J:121:ILE:HG22	4:J:123:GLY:H	1.83	0.43
9:P:77:VAL:O	9:P:81:CYS:HB2	2.18	0.43
24:A:1039:G:H2'	24:A:1040:G:C8	2.52	0.43
24:A:1739:U:H2'	24:A:1740:A:H8	1.83	0.43
24:A:1783:C:H2'	24:A:1784:G:C8	2.53	0.43
8:O:71:ILE:HG13	8:O:145:LEU:HD21	2.00	0.43
24:A:107:A:H2'	24:A:108:G:C8	2.53	0.43
24:A:270:G:H2'	24:A:271:G:H8	1.83	0.43
24:A:1084:A:H2'	24:A:1085:A:C8	2.54	0.43
26:1:51:ILE:HG12	26:1:118:ALA:HB3	2.01	0.43
26:1:112:ARG:HH21	26:1:115:THR:HA	1.83	0.43
31:7:407:LEU:HD13	31:7:410:ARG:HB2	1.99	0.43
3:I:148:ASP:N	3:I:148:ASP:OD1	2.46	0.43
24:A:974:G:N1	24:A:1021:A:O2'	2.39	0.43
24:A:1581:U:H2'	24:A:1582:A:C8	2.53	0.43
24:A:1730:U:H2'	24:A:1731:C:C6	2.53	0.43
29:4:387:PHE:HD1	29:4:390:LEU:HD21	1.83	0.43
2:H:133:ARG:HH11	24:A:290:U:H1'	1.83	0.43
5:K:64:ILE:HD11	5:K:96:VAL:HG12	1.99	0.43
6:L:113:TYR:CD2	6:L:121:LEU:HB2	2.53	0.43
15:W:75:ARG:HA	15:W:75:ARG:HD2	1.87	0.43
26:1:61:SER:HA	26:1:64:ILE:HG22	2.00	0.43
29:4:393:ALA:HB2	29:4:436:LEU:HD11	2.00	0.43
31:7:992:ARG:HA	31:7:995:ARG:HG2	2.00	0.43
4:J:148:SER:N	4:J:151:ASP:OD2	2.45	0.43
9:P:105:VAL:H	9:P:113:ARG:HH22	1.66	0.43
18:b:115:LYS:NZ	24:A:57:G:OP1	2.40	0.43
24:A:834:U:H2'	24:A:835:G:C8	2.53	0.43
24:A:1436:C:H2'	24:A:1437:C:C6	2.53	0.43
31:7:306:SER:OG	31:7:349:CYS:SG	2.64	0.43
12:S:98:ILE:HA	12:S:115:ILE:HG23	1.99	0.43
17:a:96:VAL:HG12	17:a:127:VAL:HG21	1.99	0.43
19:c:53:THR:HB	19:c:57:ARG:HE	1.84	0.43
24:A:139:U:H2'	24:A:140:G:H8	1.83	0.43
25:0:90:THR:HA	25:0:94:GLU:HB2	2.01	0.43
27:2:258:MET:HE1	27:2:260:ILE:HG13	2.01	0.43
31:7:498:SER:HA	31:7:501:MET:HE2	2.00	0.43
2:H:88:ASP:OD1	2:H:122:LYS:NZ	2.50	0.43
24:A:1167:G:O6	24:A:1465:A:N1	2.52	0.43
26:1:39:ALA:HB1	26:1:120:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:106:C:OP1	24:A:380:G:O2'	2.29	0.43
24:A:883:G:H2'	24:A:884:U:C6	2.54	0.43
27:2:748:GLU:O	27:2:752:TRP:HB2	2.19	0.43
31:7:883:ARG:HH21	31:7:919:VAL:HG12	1.83	0.43
2:H:87:MET:HE2	2:H:123:LEU:HB2	2.00	0.43
5:K:160:LEU:HD11	5:K:189:ARG:HH21	1.83	0.43
7:M:149:ASP:OD1	7:M:150:SER:N	2.52	0.43
9:P:97:LEU:O	9:P:101:ALA:N	2.51	0.43
12:S:42:ARG:HH22	12:S:45:LEU:HD12	1.83	0.43
14:V:53:ASP:HB2	14:V:56:LYS:HB2	2.00	0.43
24:A:824:U:O4	24:A:844:G:O6	2.36	0.43
24:A:1166:G:N1	24:A:1571:G:OP2	2.50	0.43
31:7:142:LEU:HD13	31:7:220:LEU:HD11	2.00	0.43
31:7:400:ILE:O	31:7:403:MET:HB3	2.19	0.43
6:L:119:GLN:HA	6:L:120:PRO:HD3	1.91	0.43
24:A:889:A:H2'	24:A:890:A:H8	1.84	0.43
24:A:1210:G:N2	24:A:1446:U:O2	2.49	0.43
29:4:219:LYS:HB3	30:5:392:LEU:HD11	2.01	0.43
31:7:271:ASP:O	31:7:275:SER:N	2.50	0.43
31:7:818:MET:HB3	31:7:822:MET:HE1	2.00	0.43
3:I:187:ASN:OD1	3:I:190:LYS:NZ	2.45	0.42
4:J:61:PHE:HA	4:J:62:PRO:HD3	1.90	0.42
24:A:622:C:H2'	24:A:623:U:C6	2.54	0.42
24:A:1155:C:N4	24:A:1160:A:H61	2.16	0.42
24:A:1270:G:H4'	24:A:1272:A:H61	1.83	0.42
26:1:247:LYS:H	26:1:252:TRP:CD1	2.37	0.42
1:E:121:ILE:HD13	1:E:164:ILE:HG21	2.01	0.42
2:H:87:MET:HE2	2:H:123:LEU:H	1.84	0.42
7:M:50:ILE:HG23	7:M:74:LEU:HD11	2.01	0.42
8:O:20:PHE:CG	24:A:206:U:H5''	2.54	0.42
27:2:303:ILE:HG13	27:2:570:VAL:HG22	2.00	0.42
29:4:383:ASP:HA	29:4:386:VAL:HG12	2.01	0.42
31:7:574:LEU:O	31:7:578:ASN:ND2	2.44	0.42
2:H:27:TYR:O	24:A:444:U:O2'	2.30	0.42
2:H:31:PRO:HA	2:H:81:THR:HB	2.01	0.42
16:Z:86:LEU:HD11	16:Z:104:LEU:HD11	2.00	0.42
18:b:106:ALA:O	18:b:111:ARG:NH1	2.52	0.42
24:A:231:G:H2'	24:A:232:G:C8	2.54	0.42
24:A:835:G:H2'	24:A:836:G:C8	2.53	0.42
31:7:412:HIS:HA	31:7:413:PRO:HA	1.83	0.42
1:E:144:LYS:HB3	1:E:206:PRO:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:125:ARG:HH21	6:L:132:VAL:HA	1.84	0.42
13:T:18:ALA:HB1	13:T:67:ILE:HD11	2.01	0.42
13:T:34:LYS:HE2	13:T:34:LYS:HB3	1.79	0.42
15:W:84:LYS:O	15:W:91:SER:HA	2.19	0.42
24:A:882:A:H2'	24:A:883:G:C8	2.55	0.42
24:A:971:A:H2'	24:A:972:A:C8	2.53	0.42
24:A:1507:G:H2'	24:A:1508:G:H8	1.85	0.42
24:A:1748:U:H2'	24:A:1749:A:H8	1.84	0.42
27:2:247:LYS:HB2	27:2:247:LYS:HE2	1.87	0.42
27:2:578:ARG:O	27:2:582:SER:OG	2.32	0.42
31:7:719:ASP:OD1	31:7:719:ASP:N	2.51	0.42
5:K:18:ASN:O	5:K:18:ASN:ND2	2.47	0.42
18:b:30:ILE:HD13	18:b:38:ILE:HG21	2.01	0.42
24:A:1731:C:H2'	24:A:1732:G:O4'	2.20	0.42
24:A:1744:G:H2'	24:A:1745:A:C8	2.53	0.42
31:7:386:THR:O	31:7:393:TRP:NE1	2.47	0.42
2:H:153:LEU:O	2:H:174:LYS:NZ	2.53	0.42
16:Z:22:LYS:NZ	20:e:3:LEU:H	2.18	0.42
24:A:52:U:H2'	24:A:53:G:C8	2.55	0.42
24:A:493:G:H2'	24:A:494:G:C8	2.54	0.42
24:A:1184:U:HO2'	27:2:734:HIS:CG	2.38	0.42
27:2:127:ARG:HH21	27:2:136:LYS:HD2	1.84	0.42
27:2:724:ALA:O	27:2:795:SER:HA	2.19	0.42
31:7:117:LEU:HA	31:7:120:GLN:HG2	2.01	0.42
8:O:130:VAL:HG12	8:O:144:VAL:HA	2.01	0.42
14:V:77:LEU:HD21	14:V:83:THR:HA	2.01	0.42
17:a:109:ARG:HB3	17:a:112:LYS:HB2	2.01	0.42
24:A:1465:A:H4'	24:A:1537:G:H4'	2.01	0.42
1:E:38:PHE:CG	1:E:73:LEU:HD23	2.55	0.42
3:I:96:MET:HG3	3:I:99:ARG:HH21	1.85	0.42
4:J:105:ASP:OD1	4:J:105:ASP:N	2.46	0.42
13:T:64:ASP:HB3	13:T:66:ARG:HH12	1.84	0.42
24:A:50:C:H2'	24:A:421:C:H41	1.84	0.42
24:A:51:A:C2	27:2:239:ARG:HD2	2.54	0.42
24:A:214:A:N6	24:A:841:U:O2	2.51	0.42
24:A:457:A:H3'	24:A:458:G:H8	1.84	0.42
31:7:39:GLU:HA	31:7:40:PRO:HD3	1.92	0.42
11:R:75:LEU:HA	11:R:78:GLN:HG2	2.01	0.42
24:A:992:G:H2'	24:A:993:A:H8	1.85	0.42
27:2:30:LYS:HE3	27:2:30:LYS:HB2	1.65	0.42
1:E:56:ASN:OD1	1:E:57:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:128:ARG:O	2:H:139:LEU:HA	2.19	0.42
5:K:23:GLU:HA	5:K:26:ILE:HG12	2.01	0.42
15:W:7:VAL:HA	15:W:10:VAL:HG12	2.02	0.42
15:W:112:GLN:O	15:W:128:GLN:NE2	2.33	0.42
24:A:426:G:H2'	24:A:427:G:H8	1.85	0.42
24:A:874:G:O6	24:A:933:U:C4	2.72	0.42
24:A:1470:G:H2'	24:A:1471:A:C8	2.55	0.42
31:7:124:GLY:HA2	31:7:127:MET:HE1	2.01	0.42
9:P:63:VAL:O	9:P:120:CYS:HA	2.20	0.41
24:A:1484:G:O2'	24:A:1491:C:O4'	2.30	0.41
24:A:1520:A:H2'	24:A:1521:A:C8	2.56	0.41
24:A:1645:C:H2'	24:A:1646:U:C6	2.55	0.41
28:3:91:ARG:HA	28:3:91:ARG:HD2	1.86	0.41
31:7:404:PHE:HB2	31:7:443:LYS:HB3	2.02	0.41
4:J:134:GLY:HA3	4:J:158:ILE:HG21	2.01	0.41
9:P:25:SER:OG	9:P:28:ASP:OD2	2.38	0.41
11:R:146:ARG:HH12	24:A:1781:U:H5''	1.86	0.41
24:A:252:U:H2'	24:A:253:A:H8	1.84	0.41
24:A:1640:C:H2'	24:A:1641:G:H8	1.85	0.41
25:0:26:HIS:ND1	25:0:62:GLU:OE2	2.50	0.41
26:1:65:LEU:HB3	26:1:76:HIS:HB2	2.02	0.41
29:4:377:LEU:HA	29:4:378:PRO:HD3	1.95	0.41
24:A:29:U:H2'	24:A:30:G:C8	2.55	0.41
24:A:148:G:N2	24:A:160:G:H22	2.18	0.41
24:A:810:A:H62	24:A:856:G:H2'	1.84	0.41
24:A:910:U:OP1	24:A:911:G:O2'	2.35	0.41
24:A:1207:C:H2'	24:A:1208:A:C8	2.56	0.41
24:A:1538:G:H22	24:A:1564:C:H1'	1.85	0.41
26:1:49:SER:HB3	26:1:117:ASP:HB2	2.02	0.41
7:M:15:ARG:HA	7:M:16:PRO:HD3	1.89	0.41
8:O:28:LYS:HA	8:O:28:LYS:HD2	1.91	0.41
8:O:71:ILE:HG21	8:O:145:LEU:HD11	2.01	0.41
24:A:227:U:O2	24:A:231:G:C6	2.74	0.41
24:A:560:U:H2'	24:A:561:G:H8	1.86	0.41
27:2:166:HIS:CE1	27:2:197:ARG:HB2	2.55	0.41
27:2:191:VAL:HG12	27:2:226:TYR:HB2	2.02	0.41
27:2:366:LYS:HB3	27:2:375:ARG:NH1	2.34	0.41
31:7:177:VAL:HA	31:7:180:MET:HE2	2.02	0.41
1:E:142:PHE:O	1:E:208:GLN:N	2.51	0.41
2:H:39:ARG:HA	2:H:39:ARG:HD2	1.80	0.41
24:A:220:A:N6	24:A:835:G:O6	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1219:C:H2'	24:A:1220:G:C8	2.56	0.41
2:H:19:LEU:HD13	24:A:786:A:C5	2.56	0.41
4:J:50:LEU:HD13	4:J:111:LEU:HD23	2.02	0.41
4:J:198:ARG:HA	4:J:198:ARG:HD3	1.71	0.41
16:Z:31:SER:HB2	24:A:633:A:H5''	2.02	0.41
24:A:1199:A:O2'	24:A:1204:C:N4	2.52	0.41
24:A:1641:G:C6	24:A:1751:A:N7	2.89	0.41
31:7:699:LEU:HD13	31:7:703:SER:HB3	2.03	0.41
3:I:96:MET:O	3:I:100:ILE:HG12	2.21	0.41
4:J:218:ARG:HA	4:J:218:ARG:HD3	1.90	0.41
13:T:34:LYS:HG2	15:W:8:ARG:HB3	2.01	0.41
24:A:971:A:H2'	24:A:972:A:H8	1.85	0.41
24:A:1143:G:H3'	24:A:1144:A:H8	1.86	0.41
24:A:1230:G:H5''	29:4:252:ARG:HH22	1.86	0.41
27:2:552:ARG:HA	27:2:555:ARG:HG2	2.03	0.41
2:H:31:PRO:HG3	2:H:43:PRO:HG3	2.02	0.41
7:M:64:ASP:HB3	7:M:67:ARG:HB3	2.02	0.41
15:W:102:ARG:O	15:W:106:GLN:N	2.48	0.41
24:A:1482:G:H21	24:A:1588:A:H4'	1.86	0.41
24:A:1652:U:O2	24:A:1741:G:N2	2.53	0.41
1:E:164:ILE:HD13	1:E:207:LEU:HD21	2.03	0.41
2:H:63:ALA:O	2:H:67:GLN:HG3	2.20	0.41
7:M:81:ILE:HA	7:M:147:ARG:HA	2.02	0.41
12:S:94:VAL:HB	12:S:97:MET:HE3	2.03	0.41
17:a:132:LEU:HD23	17:a:132:LEU:HA	1.84	0.41
21:f:59:GLU:HG2	21:f:62:ARG:HG3	2.02	0.41
24:A:414:A:H5'	24:A:415:G:C8	2.56	0.41
24:A:483:G:H2'	24:A:484:G:C8	2.56	0.41
24:A:644:A:H2'	24:A:645:G:C8	2.56	0.41
24:A:823:U:O2'	24:A:824:U:H5''	2.21	0.41
24:A:824:U:H2'	24:A:825:C:C6	2.56	0.41
24:A:1037:A:C5	24:A:1088:A:N6	2.88	0.41
24:A:1200:A:N7	24:A:1551:A:N6	2.69	0.41
24:A:1479:A:C2	24:A:1603:G:H1'	2.56	0.41
24:A:1721:U:O4	24:A:1722:A:N6	2.54	0.41
25:0:57:ARG:NH1	25:0:70:GLU:OE1	2.54	0.41
27:2:750:VAL:HG21	27:2:778:PHE:HB3	2.03	0.41
31:7:444:ALA:O	31:7:448:MET:HG2	2.21	0.41
24:A:482:A:H2'	24:A:483:G:H8	1.86	0.41
25:0:44:LEU:HD21	25:0:93:MET:HE1	2.03	0.41
27:2:712:LEU:HD23	27:2:712:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:770:GLU:HG2	27:2:779:LYS:HB3	2.03	0.41
31:7:280:ARG:HA	31:7:280:ARG:HD2	1.88	0.41
31:7:879:LEU:HD23	31:7:879:LEU:HA	1.88	0.41
4:J:32:MET:HG2	4:J:100:CYS:SG	2.62	0.40
5:K:150:LEU:HD21	5:K:158:LYS:HE3	2.03	0.40
8:O:104:ARG:HD3	17:a:8:GLY:O	2.21	0.40
11:R:55:VAL:HG13	11:R:76:ALA:HB1	2.03	0.40
21:f:19:ARG:HA	21:f:27:THR:HA	2.02	0.40
24:A:995:G:H2'	24:A:996:A:C8	2.56	0.40
27:2:103:ASP:O	27:2:193:GLN:NE2	2.54	0.40
29:4:217:LEU:HD11	29:4:249:ALA:HB1	2.01	0.40
4:J:5:ILE:HD13	4:J:16:ILE:HD13	2.03	0.40
4:J:167:GLU:HG2	4:J:169:LYS:HE2	2.03	0.40
5:K:36:ASN:OD1	5:K:37:THR:N	2.54	0.40
5:K:85:ARG:HB3	5:K:89:LYS:NZ	2.36	0.40
24:A:860:A:O2'	24:A:961:A:N6	2.51	0.40
24:A:1166:G:H1'	26:1:195:LYS:HE3	2.03	0.40
25:0:50:ARG:HG3	26:1:112:ARG:HH22	1.86	0.40
26:1:196:ASN:OD1	26:1:196:ASN:N	2.53	0.40
27:2:690:PRO:HA	27:2:693:GLU:HB2	2.03	0.40
27:2:721:ALA:HB1	27:2:797:TYR:HD2	1.86	0.40
31:7:445:ILE:HG21	31:7:478:LEU:HD23	2.03	0.40
9:P:137:LEU:HA	9:P:140:PHE:HD2	1.87	0.40
11:R:115:LEU:HD12	11:R:115:LEU:HA	1.79	0.40
12:S:43:ASN:O	14:V:90:ARG:NH2	2.55	0.40
24:A:447:C:H2'	24:A:448:G:C8	2.56	0.40
31:7:292:PRO:HA	31:7:298:LEU:HD22	2.03	0.40
10:Q:5:HIS:HD2	24:A:624:C:H5''	1.86	0.40
20:e:17:ARG:O	24:A:1067:U:O2'	2.38	0.40
24:A:674:G:H2'	24:A:675:G:C8	2.57	0.40
24:A:1490:C:H2'	24:A:1491:C:C6	2.56	0.40
24:A:1650:G:N2	24:A:1742:A:N6	2.44	0.40
17:a:64:PRO:HB3	26:1:246:LYS:HB2	2.03	0.40
24:A:1242:G:H1	24:A:1247:U:H3	1.69	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	E	211/255 (83%)	194 (92%)	16 (8%)	1 (0%)	24	55
2	H	259/264 (98%)	248 (96%)	11 (4%)	0	100	100
3	I	197/212 (93%)	187 (95%)	10 (5%)	0	100	100
4	J	230/239 (96%)	216 (94%)	14 (6%)	0	100	100
5	K	193/203 (95%)	186 (96%)	7 (4%)	0	100	100
6	L	199/202 (98%)	192 (96%)	7 (4%)	0	100	100
7	M	177/190 (93%)	170 (96%)	7 (4%)	0	100	100
8	O	148/161 (92%)	141 (95%)	7 (5%)	0	100	100
9	P	116/144 (81%)	105 (90%)	11 (10%)	0	100	100
10	Q	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
11	R	133/150 (89%)	123 (92%)	10 (8%)	0	100	100
12	S	113/153 (74%)	109 (96%)	4 (4%)	0	100	100
13	T	115/143 (80%)	108 (94%)	7 (6%)	0	100	100
14	V	120/156 (77%)	113 (94%)	6 (5%)	1 (1%)	16	45
15	W	140/153 (92%)	133 (95%)	7 (5%)	0	100	100
16	Z	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
17	a	140/145 (97%)	134 (96%)	6 (4%)	0	100	100
18	b	123/136 (90%)	121 (98%)	2 (2%)	0	100	100
19	c	67/99 (68%)	66 (98%)	1 (2%)	0	100	100
20	e	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
21	f	59/68 (87%)	54 (92%)	5 (8%)	0	100	100
22	h	19/62 (31%)	17 (90%)	1 (5%)	1 (5%)	1	10
23	i	61/154 (40%)	53 (87%)	8 (13%)	0	100	100
25	0	125/127 (98%)	125 (100%)	0	0	100	100
26	1	263/282 (93%)	254 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	2	720/830 (87%)	687 (95%)	32 (4%)	1 (0%)	48	75
28	3	182/259 (70%)	178 (98%)	4 (2%)	0	100	100
29	4	268/480 (56%)	262 (98%)	6 (2%)	0	100	100
30	5	76/445 (17%)	72 (95%)	4 (5%)	0	100	100
31	7	983/1235 (80%)	967 (98%)	16 (2%)	0	100	100
All	All	5791/7310 (79%)	5555 (96%)	232 (4%)	4 (0%)	49	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	35	PRO
14	V	93	VAL
27	2	372	ASP
22	h	27	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	187/223 (84%)	187 (100%)	0	100	100
2	H	219/221 (99%)	219 (100%)	0	100	100
3	I	167/178 (94%)	167 (100%)	0	100	100
4	J	198/204 (97%)	197 (100%)	1 (0%)	81	83
5	K	169/177 (96%)	168 (99%)	1 (1%)	78	81
6	L	163/164 (99%)	163 (100%)	0	100	100
7	M	154/162 (95%)	153 (99%)	1 (1%)	78	81
8	O	133/143 (93%)	133 (100%)	0	100	100
9	P	101/121 (84%)	101 (100%)	0	100	100
10	Q	129/130 (99%)	129 (100%)	0	100	100
11	R	102/117 (87%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	S	99/132 (75%)	99 (100%)	0	100	100
13	T	95/115 (83%)	95 (100%)	0	100	100
14	V	108/135 (80%)	108 (100%)	0	100	100
15	W	114/124 (92%)	114 (100%)	0	100	100
16	Z	112/113 (99%)	112 (100%)	0	100	100
17	a	113/116 (97%)	113 (100%)	0	100	100
18	b	107/115 (93%)	107 (100%)	0	100	100
19	c	60/80 (75%)	60 (100%)	0	100	100
20	e	70/71 (99%)	70 (100%)	0	100	100
21	f	54/61 (88%)	54 (100%)	0	100	100
22	h	19/52 (36%)	16 (84%)	3 (16%)	2	12
23	i	57/139 (41%)	57 (100%)	0	100	100
25	0	113/113 (100%)	113 (100%)	0	100	100
26	1	215/227 (95%)	215 (100%)	0	100	100
27	2	631/714 (88%)	627 (99%)	4 (1%)	78	81
28	3	155/215 (72%)	154 (99%)	1 (1%)	78	81
29	4	229/411 (56%)	229 (100%)	0	100	100
30	5	70/373 (19%)	70 (100%)	0	100	100
31	7	850/1049 (81%)	850 (100%)	0	100	100
All	All	4993/6195 (81%)	4982 (100%)	11 (0%)	85	88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	J	4	ASN
5	K	18	ASN
7	M	15	ARG
22	h	25	GLU
22	h	26	LYS
22	h	27	PRO
27	2	11	HIS
27	2	17	LYS
27	2	19	LYS
27	2	30	LYS
28	3	240	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	101	HIS
2	H	9	GLN
3	I	157	GLN
4	J	4	ASN
5	K	120	GLN
6	L	53	HIS
7	M	137	GLN
8	O	97	HIS
8	O	103	ASN
8	O	132	GLN
10	Q	69	ASN
10	Q	78	ASN
10	Q	105	ASN
12	S	122	HIS
13	T	8	GLN
15	W	26	GLN
15	W	92	HIS
16	Z	56	HIS
17	a	65	ASN
19	c	80	GLN
21	f	28	GLN
23	i	139	GLN
26	1	30	ASN
27	2	10	HIS
27	2	11	HIS
27	2	27	HIS
27	2	92	ASN
27	2	112	ASN
27	2	166	HIS
27	2	236	ASN
27	2	569	ASN
27	2	597	HIS
27	2	789	GLN
28	3	137	GLN
29	4	235	GLN
30	5	382	GLN
31	7	166	ASN
31	7	412	HIS
31	7	972	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	A	1572/1796 (87%)	367 (23%)	14 (0%)

All (367) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
24	A	2	A
24	A	3	C
24	A	4	C
24	A	5	U
24	A	25	C
24	A	26	A
24	A	27	U
24	A	34	G
24	A	42	G
24	A	43	A
24	A	45	U
24	A	47	A
24	A	50	C
24	A	57	G
24	A	60	U
24	A	63	G
24	A	66	U
24	A	68	A
24	A	69	G
24	A	71	A
24	A	72	A
24	A	73	U
24	A	74	U
24	A	75	A
24	A	76	U
24	A	77	A
24	A	93	U
24	A	103	A
24	A	110	U
24	A	113	C
24	A	127	U
24	A	138	A
24	A	150	G
24	A	153	A
24	A	155	U
24	A	158	U

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Mol	Chain	Res	Type
24	A	165	A
24	A	175	G
24	A	176	A
24	A	185	A
24	A	188	U
24	A	189	C
24	A	190	G
24	A	191	G
24	A	192	A
24	A	212	U
24	A	213	A
24	A	214	A
24	A	218	C
24	A	221	A
24	A	222	U
24	A	223	G
24	A	228	U
24	A	231	G
24	A	232	G
24	A	234	C
24	A	237	U
24	A	246	U
24	A	247	C
24	A	258	C
24	A	260	C
24	A	262	A
24	A	264	U
24	A	270	G
24	A	274	U
24	A	275	U
24	A	277	C
24	A	287	G
24	A	296	A
24	A	311	C
24	A	313	A
24	A	317	U
24	A	319	G
24	A	321	C
24	A	326	G
24	A	330	A
24	A	334	G
24	A	335	C

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Mol	Chain	Res	Type
24	A	347	A
24	A	349	A
24	A	356	A
24	A	357	A
24	A	358	C
24	A	377	C
24	A	387	G
24	A	390	C
24	A	396	A
24	A	397	A
24	A	398	A
24	A	399	C
24	A	401	G
24	A	410	U
24	A	413	A
24	A	415	G
24	A	420	G
24	A	421	C
24	A	422	A
24	A	423	G
24	A	431	G
24	A	436	U
24	A	441	C
24	A	442	A
24	A	445	C
24	A	465	A
24	A	472	A
24	A	474	A
24	A	481	C
24	A	490	U
24	A	491	U
24	A	493	G
24	A	502	A
24	A	503	A
24	A	505	U
24	A	508	A
24	A	512	A
24	A	516	C
24	A	531	A
24	A	533	C
24	A	535	A
24	A	536	G

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Mol	Chain	Res	Type
24	A	538	A
24	A	539	A
24	A	542	A
24	A	549	G
24	A	551	C
24	A	553	A
24	A	556	C
24	A	563	C
24	A	575	U
24	A	576	A
24	A	577	A
24	A	578	U
24	A	579	U
24	A	581	C
24	A	591	A
24	A	592	G
24	A	604	G
24	A	607	G
24	A	608	U
24	A	617	A
24	A	618	A
24	A	619	A
24	A	620	A
24	A	621	G
24	A	636	U
24	A	677	U
24	A	678	G
24	A	679	G
24	A	680	G
24	A	686	C
24	A	690	U
24	A	691	C
24	A	693	U
24	A	699	A
24	A	705	G
24	A	709	G
24	A	710	C
24	A	724	U
24	A	725	G
24	A	726	U
24	A	727	C
24	A	729	G

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Mol	Chain	Res	Type
24	A	730	G
24	A	731	G
24	A	732	A
24	A	754	A
24	A	764	G
24	A	765	C
24	A	773	A
24	A	774	G
24	A	777	C
24	A	779	A
24	A	780	U
24	A	781	G
24	A	792	U
24	A	793	U
24	A	801	A
24	A	810	A
24	A	818	U
24	A	819	G
24	A	822	G
24	A	823	U
24	A	824	U
24	A	828	U
24	A	830	U
24	A	832	G
24	A	833	U
24	A	836	G
24	A	858	U
24	A	859	U
24	A	861	A
24	A	871	U
24	A	874	G
24	A	879	G
24	A	884	U
24	A	896	A
24	A	912	G
24	A	931	A
24	A	933	U
24	A	940	G
24	A	943	U
24	A	950	A
24	A	957	U
24	A	958	U

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Mol	Chain	Res	Type
24	A	964	A
24	A	984	G
24	A	990	A
24	A	991	A
24	A	994	C
24	A	998	C
24	A	999	A
24	A	1000	G
24	A	1001	A
24	A	1002	U
24	A	1019	C
24	A	1024	A
24	A	1026	C
24	A	1027	U
24	A	1030	G
24	A	1037	A
24	A	1056	U
24	A	1057	U
24	A	1059	U
24	A	1073	A
24	A	1078	A
24	A	1079	C
24	A	1080	G
24	A	1083	A
24	A	1089	A
24	A	1093	G
24	A	1095	U
24	A	1097	G
24	A	1106	G
24	A	1135	A
24	A	1140	A
24	A	1141	U
24	A	1143	G
24	A	1145	C
24	A	1146	G
24	A	1147	G
24	A	1148	A
24	A	1149	A
24	A	1152	G
24	A	1155	C
24	A	1156	C
24	A	1157	A

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Mol	Chain	Res	Type
24	A	1164	G
24	A	1182	U
24	A	1183	U
24	A	1200	A
24	A	1201	A
24	A	1204	C
24	A	1214	A
24	A	1218	A
24	A	1219	C
24	A	1220	G
24	A	1221	A
24	A	1222	U
24	A	1223	G
24	A	1224	A
24	A	1225	G
24	A	1226	G
24	A	1227	A
24	A	1238	G
24	A	1240	G
24	A	1241	A
24	A	1242	G
24	A	1247	U
24	A	1248	U
24	A	1252	G
24	A	1254	U
24	A	1255	U
24	A	1256	U
24	A	1259	U
24	A	1260	G
24	A	1261	G
24	A	1262	G
24	A	1264	G
24	A	1265	G
24	A	1266	U
24	A	1268	G
24	A	1270	G
24	A	1271	C
24	A	1272	A
24	A	1273	U
24	A	1276	C
24	A	1432	A
24	A	1433	U

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Mol	Chain	Res	Type
24	A	1434	G
24	A	1439	U
24	A	1440	A
24	A	1442	A
24	A	1443	U
24	A	1448	U
24	A	1453	C
24	A	1455	C
24	A	1467	A
24	A	1478	C
24	A	1485	U
24	A	1486	A
24	A	1487	C
24	A	1488	U
24	A	1492	U
24	A	1501	A
24	A	1507	G
24	A	1510	U
24	A	1511	A
24	A	1512	A
24	A	1516	U
24	A	1519	U
24	A	1520	A
24	A	1533	C
24	A	1538	G
24	A	1539	A
24	A	1552	A
24	A	1553	U
24	A	1555	A
24	A	1556	U
24	A	1564	C
24	A	1565	A
24	A	1573	A
24	A	1580	G
24	A	1581	U
24	A	1586	G
24	A	1597	G
24	A	1612	G
24	A	1613	U
24	A	1615	C
24	A	1618	G
24	A	1624	U

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Mol	Chain	Res	Type
24	A	1625	G
24	A	1626	U
24	A	1630	C
24	A	1631	A
24	A	1651	A
24	A	1652	U
24	A	1653	U
24	A	1654	G
24	A	1668	G
24	A	1676	G
24	A	1684	C
24	A	1708	A
24	A	1709	G
24	A	1711	G
24	A	1712	C
24	A	1741	G
24	A	1751	A
24	A	1752	A
24	A	1753	G
24	A	1762	A
24	A	1763	G
24	A	1765	U
24	A	1766	C
24	A	1773	G
24	A	1775	U
24	A	1776	G
24	A	1777	A
24	A	1778	A
24	A	1779	C
24	A	1780	C
24	A	1788	G
24	A	1789	G
24	A	1790	A
24	A	1791	U
24	A	1793	A
24	A	1794	U
24	A	1795	U

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	A	222	U

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Mol	Chain	Res	Type
24	A	231	G
24	A	233	G
24	A	269	C
24	A	414	A
24	A	552	A
24	A	678	G
24	A	792	U
24	A	911	G
24	A	1094	U
24	A	1218	A
24	A	1253	A
24	A	1564	C
24	A	1776	G

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 3 ligands modelled in this entry, 3 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 ⓘ

There are no chain breaks in this entry.

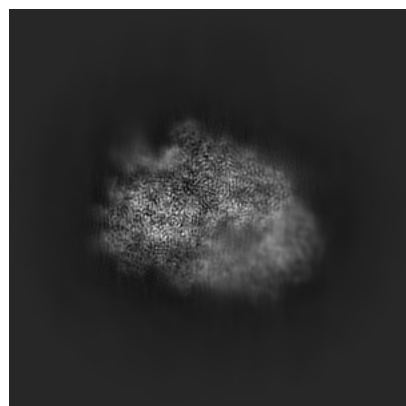
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66682. These allow visual inspection of the internal detail of the map and identification of artifacts.

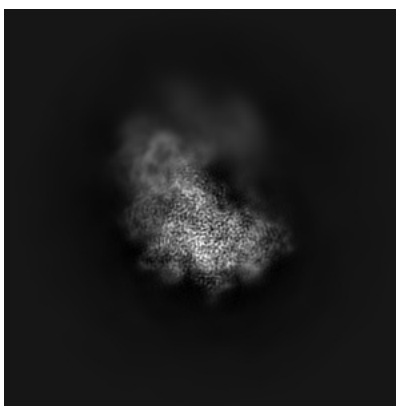
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

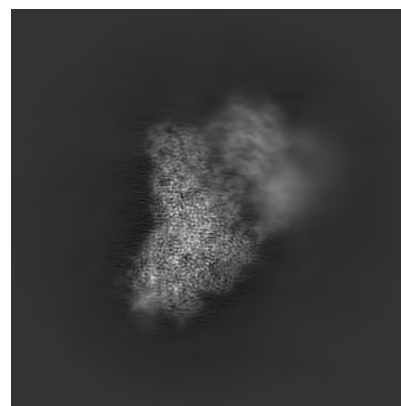
6.1.1 Primary map



X

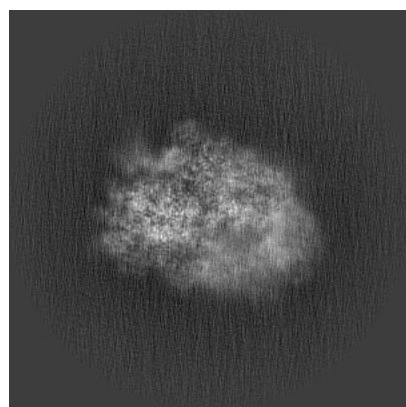


Y

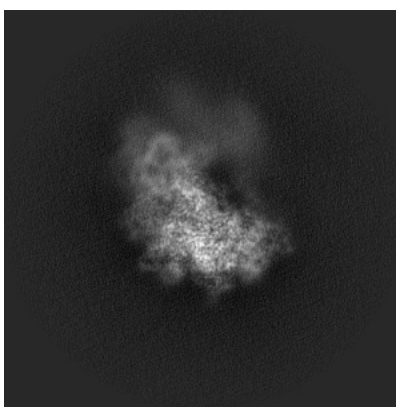


Z

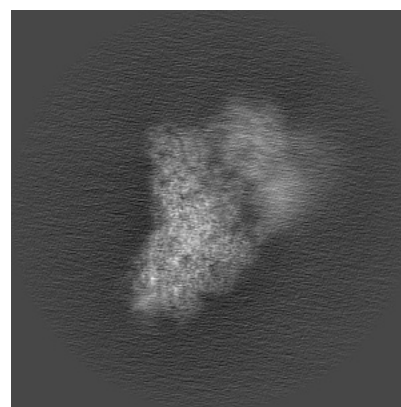
6.1.2 Raw map



X



Y

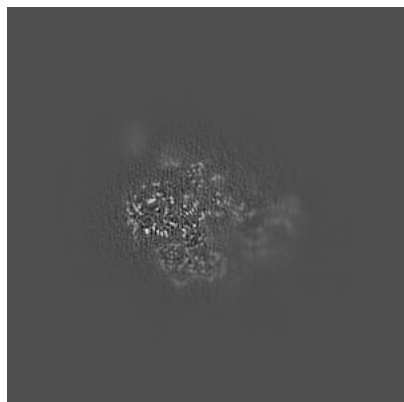


Z

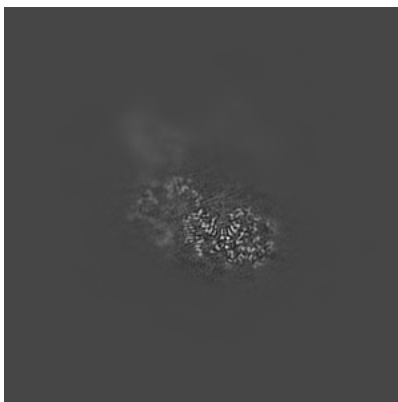
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

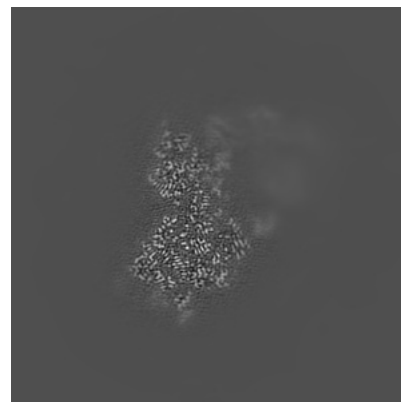
6.2.1 Primary map



X Index: 180

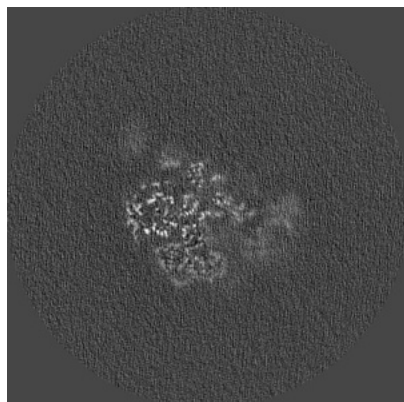


Y Index: 180

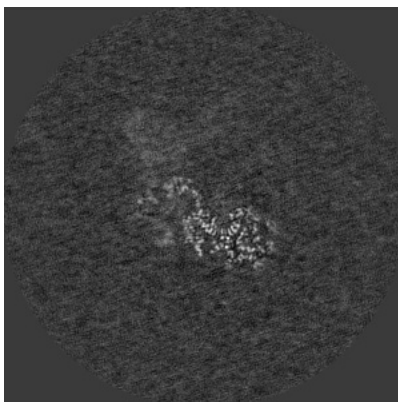


Z Index: 180

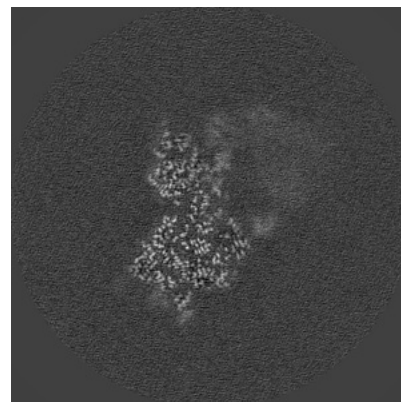
6.2.2 Raw map



X Index: 180



Y Index: 180

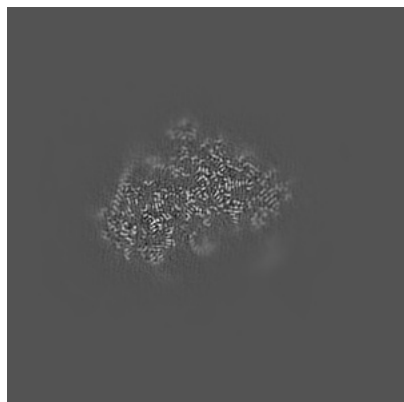


Z Index: 180

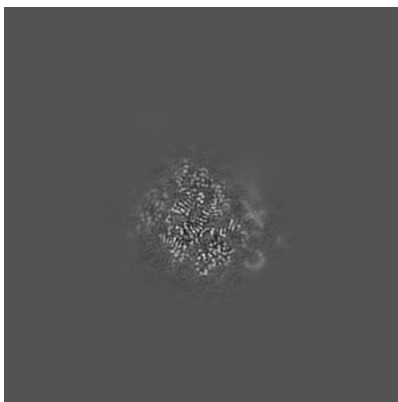
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

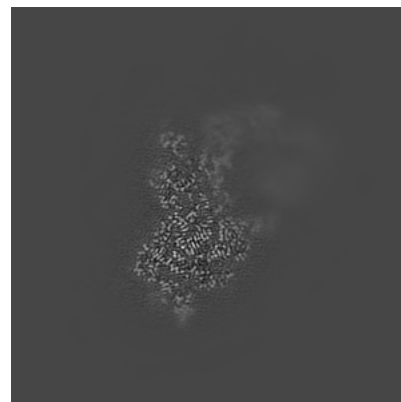
6.3.1 Primary map



X Index: 148

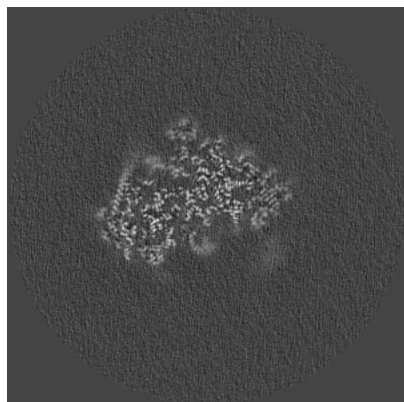


Y Index: 144

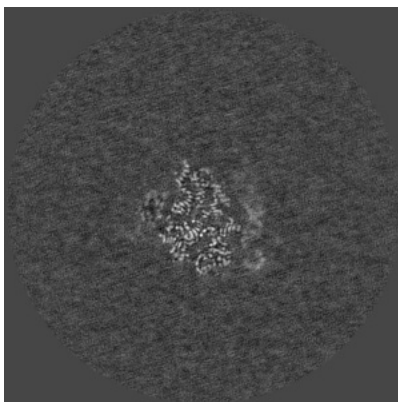


Z Index: 177

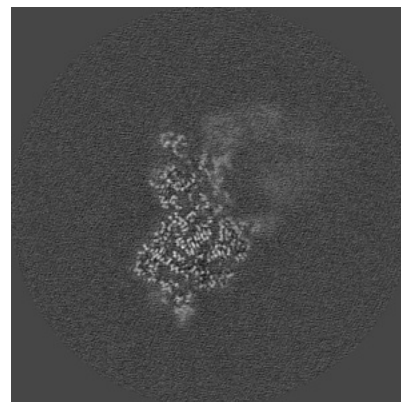
6.3.2 Raw map



X Index: 148



Y Index: 143

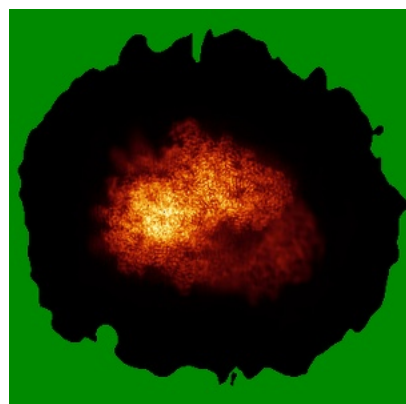


Z Index: 177

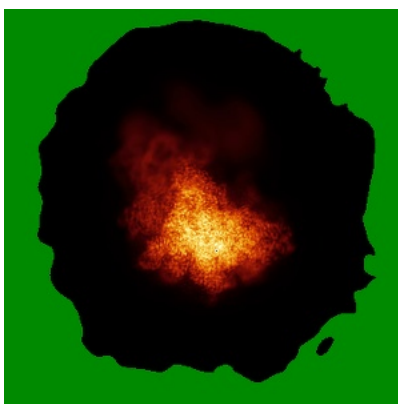
The images above show the largest variance slices of the map in three orthogonal directions.

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

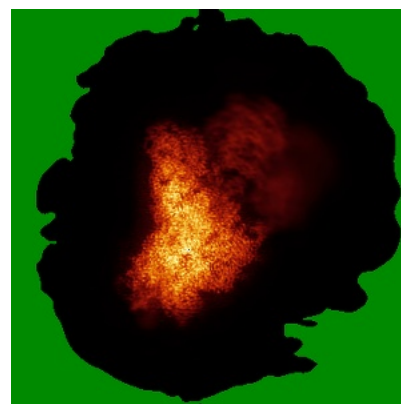
6.4.1 Primary map



X

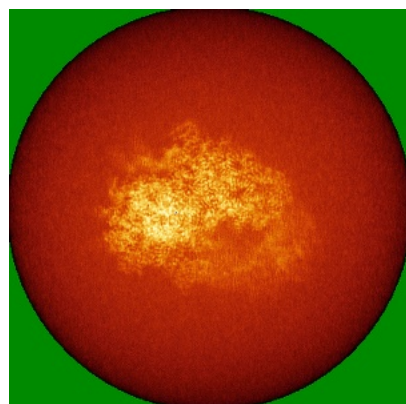


Y

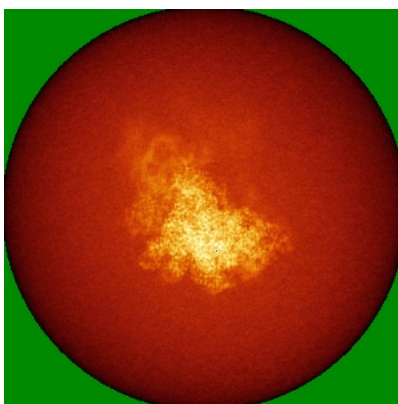


Z

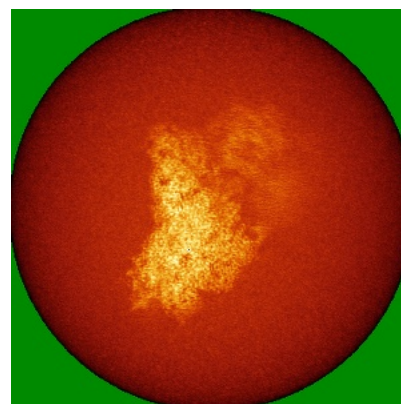
6.4.2 Raw map



X



Y

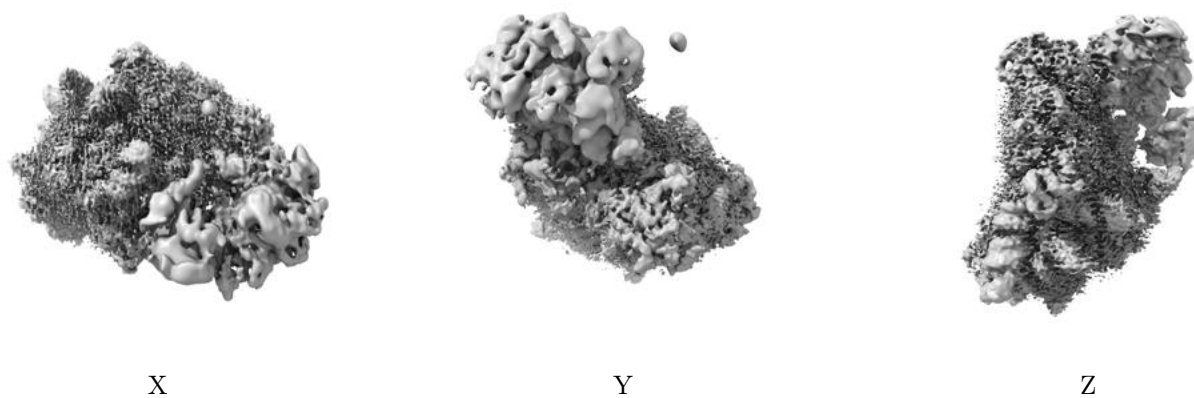


Z

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.

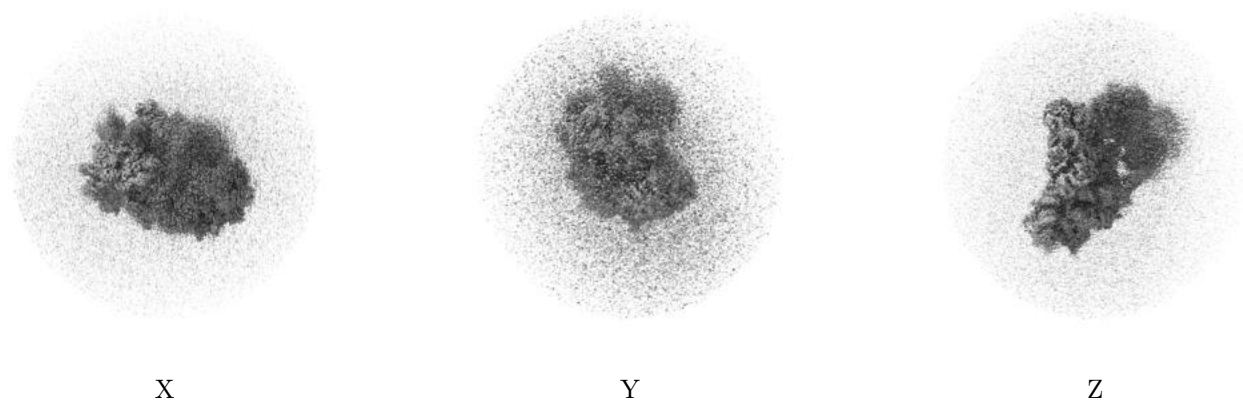
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

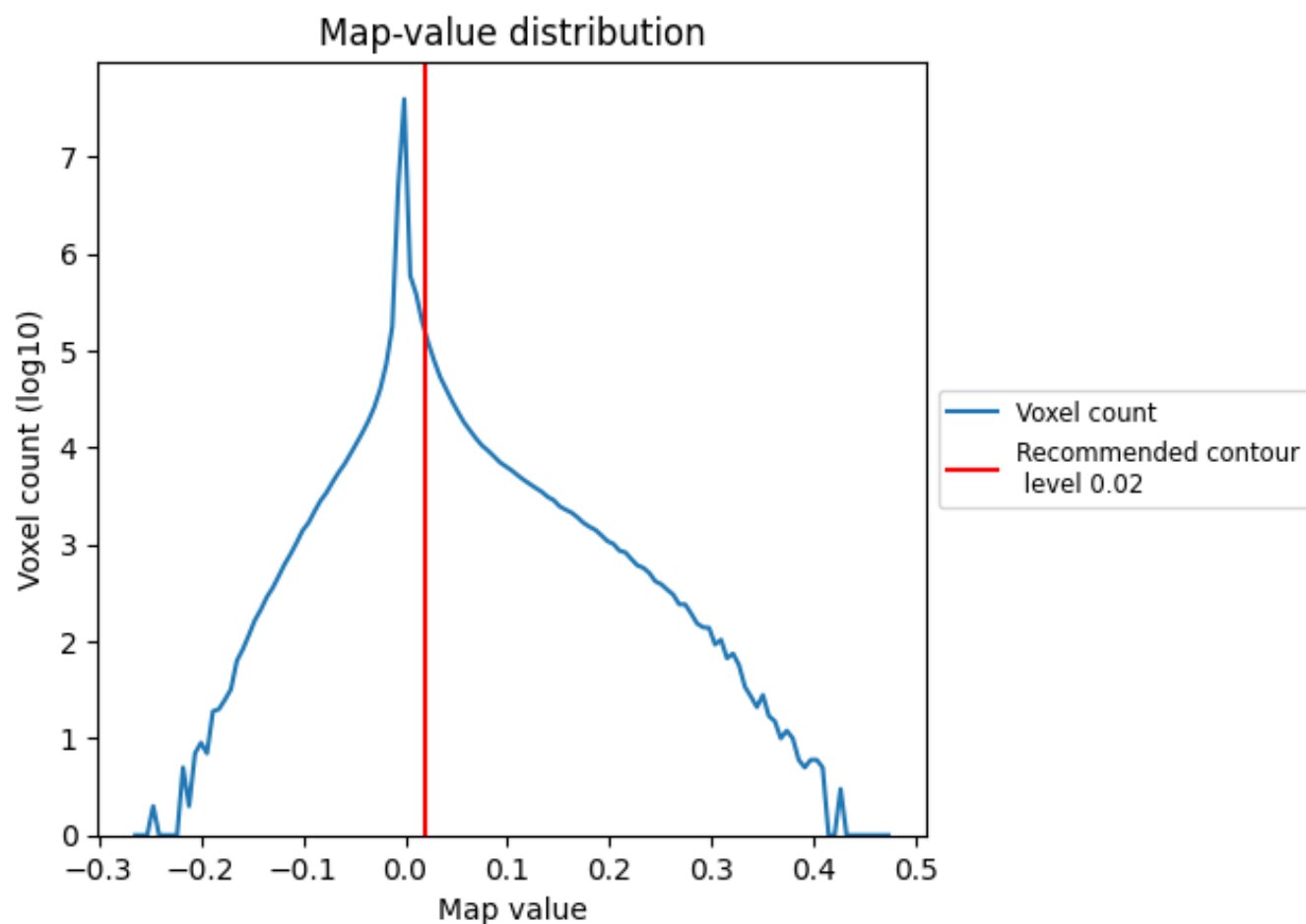
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

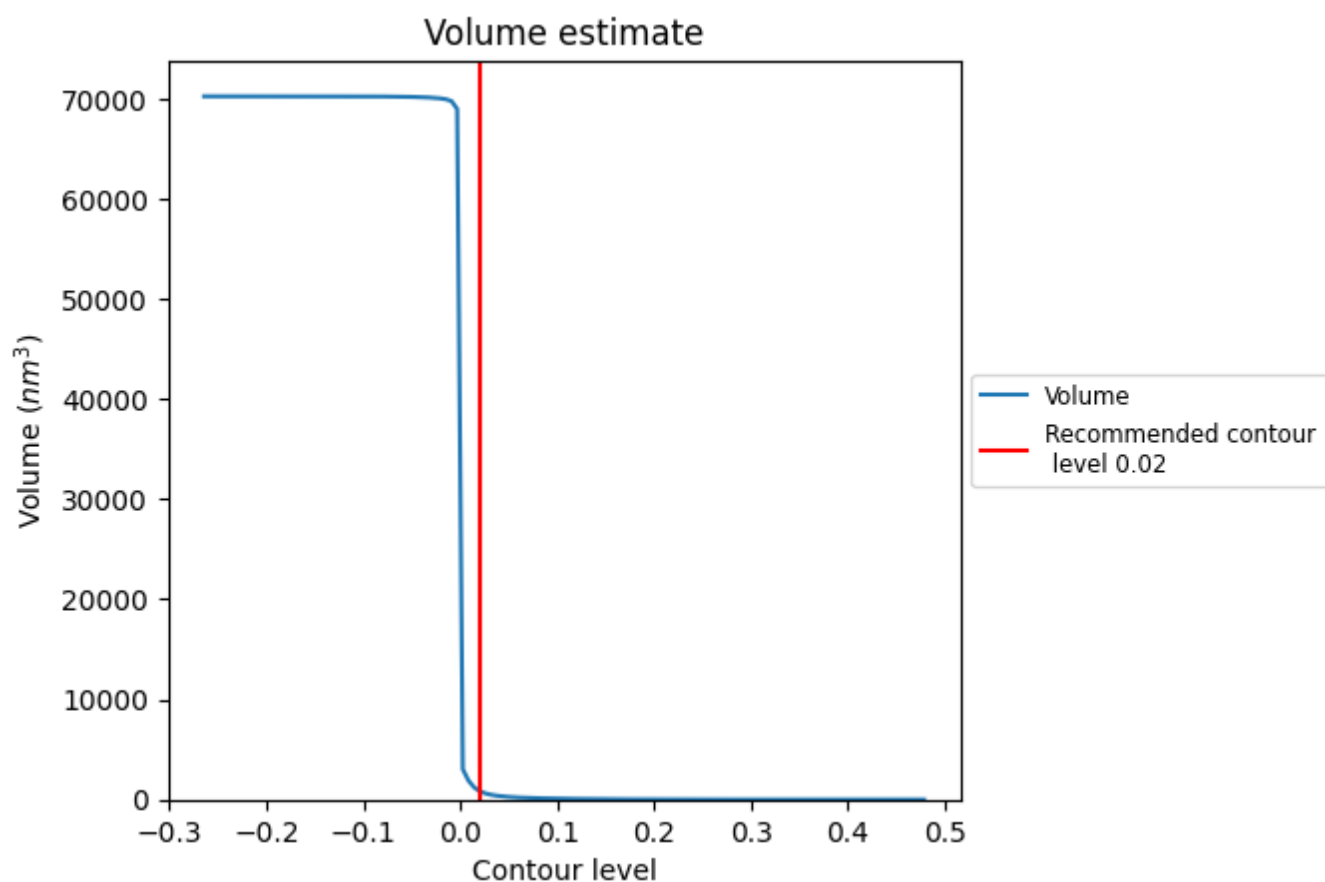
This section contains the results of statistical analysis of the map.

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.

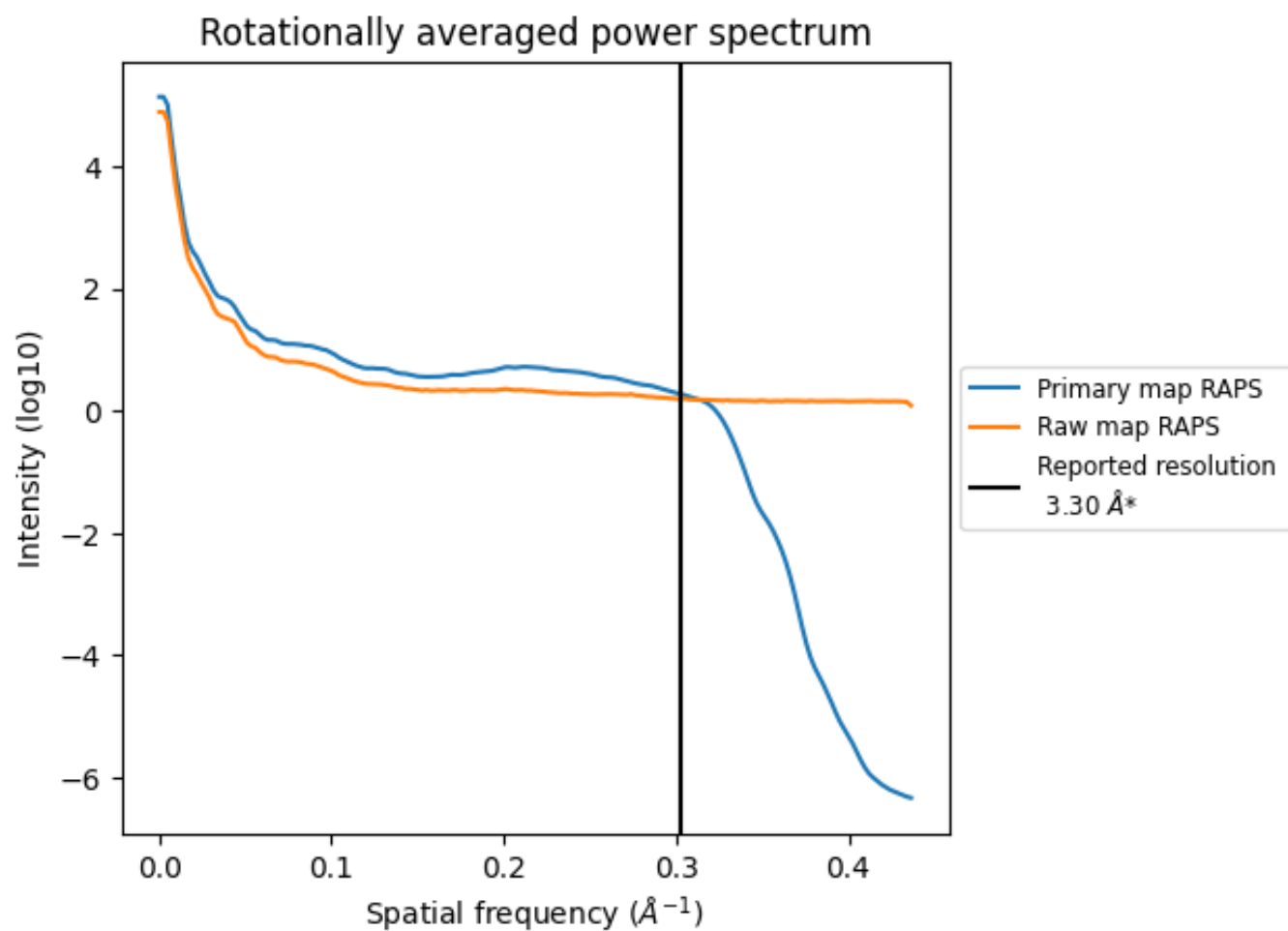
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 845 nm³; this corresponds to an approximate mass of 764 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 ⓘ

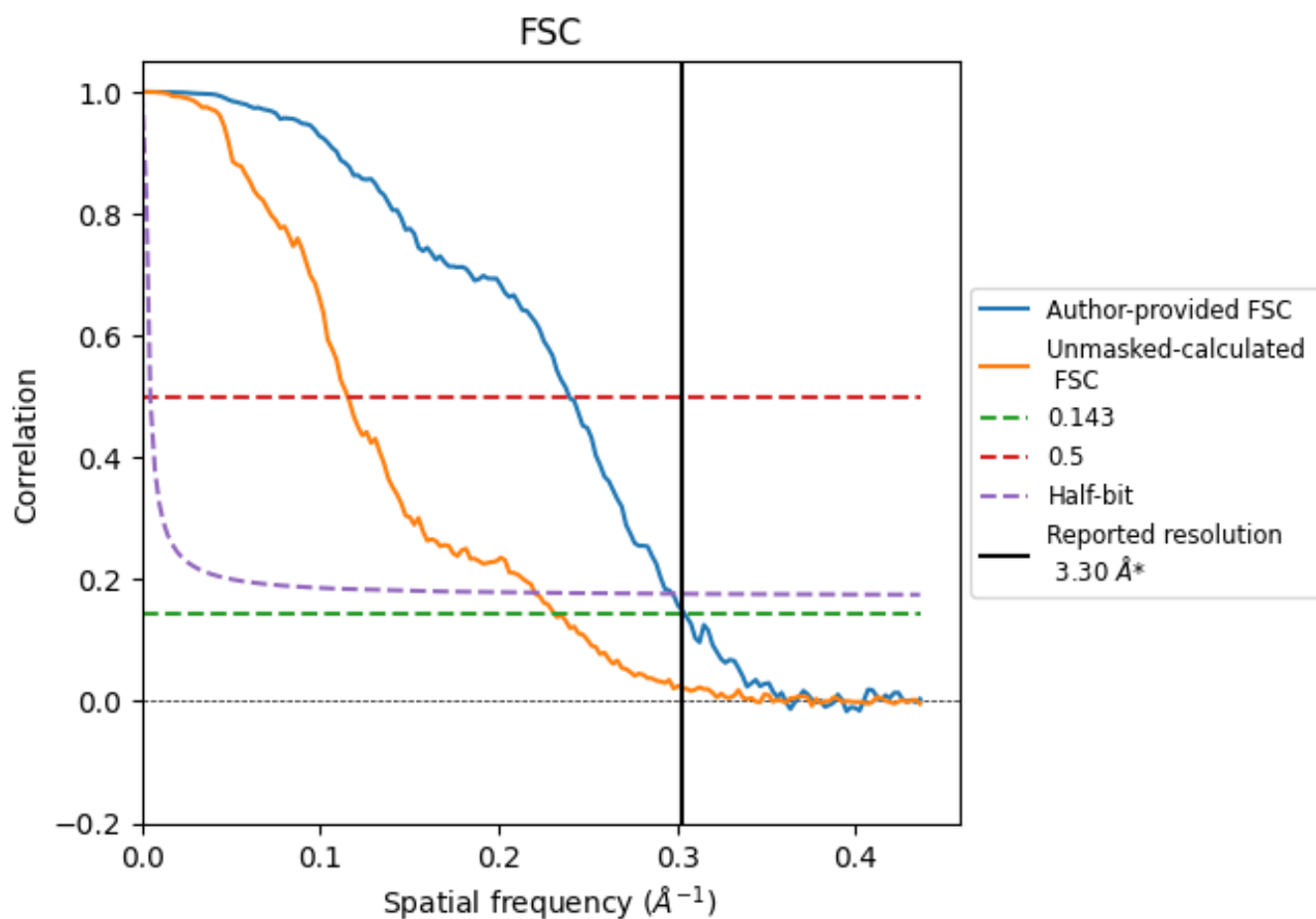


*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

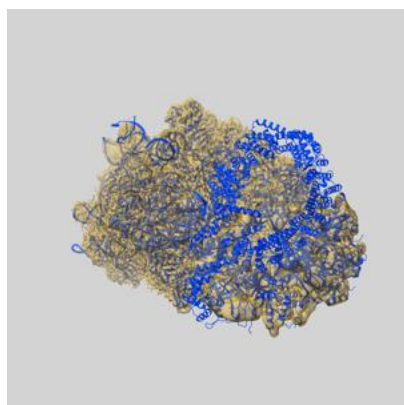
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	4.17	3.36
Unmasked-calculated*	4.32	8.67	4.54

*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 4.32 differs from the reported value 3.3 by more than 10 %

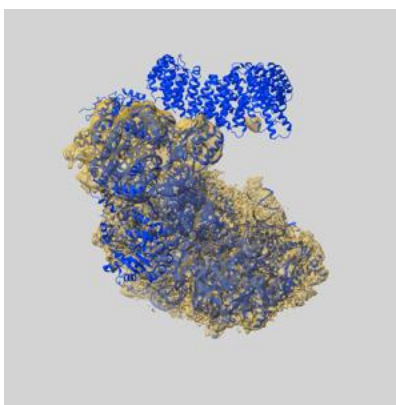
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66682 and PDB model 9XAC. Per-residue inclusion information can be found in section 3 on page 11.

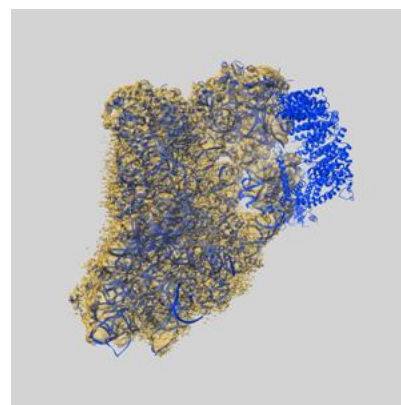
9.1 Map-model overlay [i](#)



X



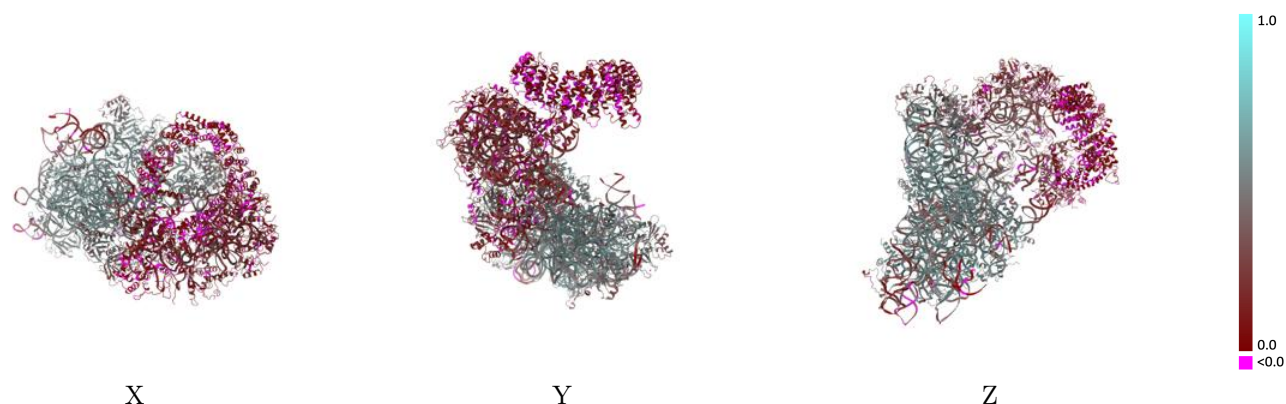
Y



Z

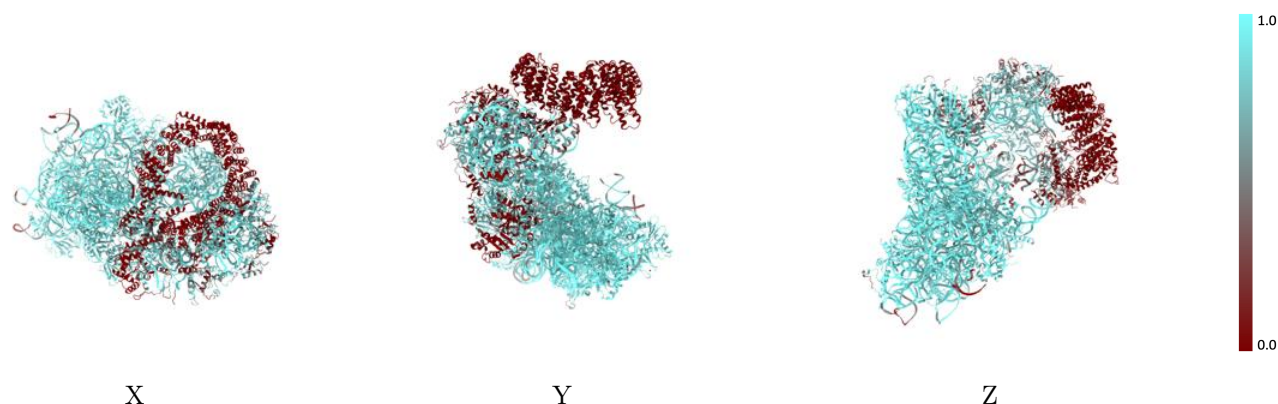
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



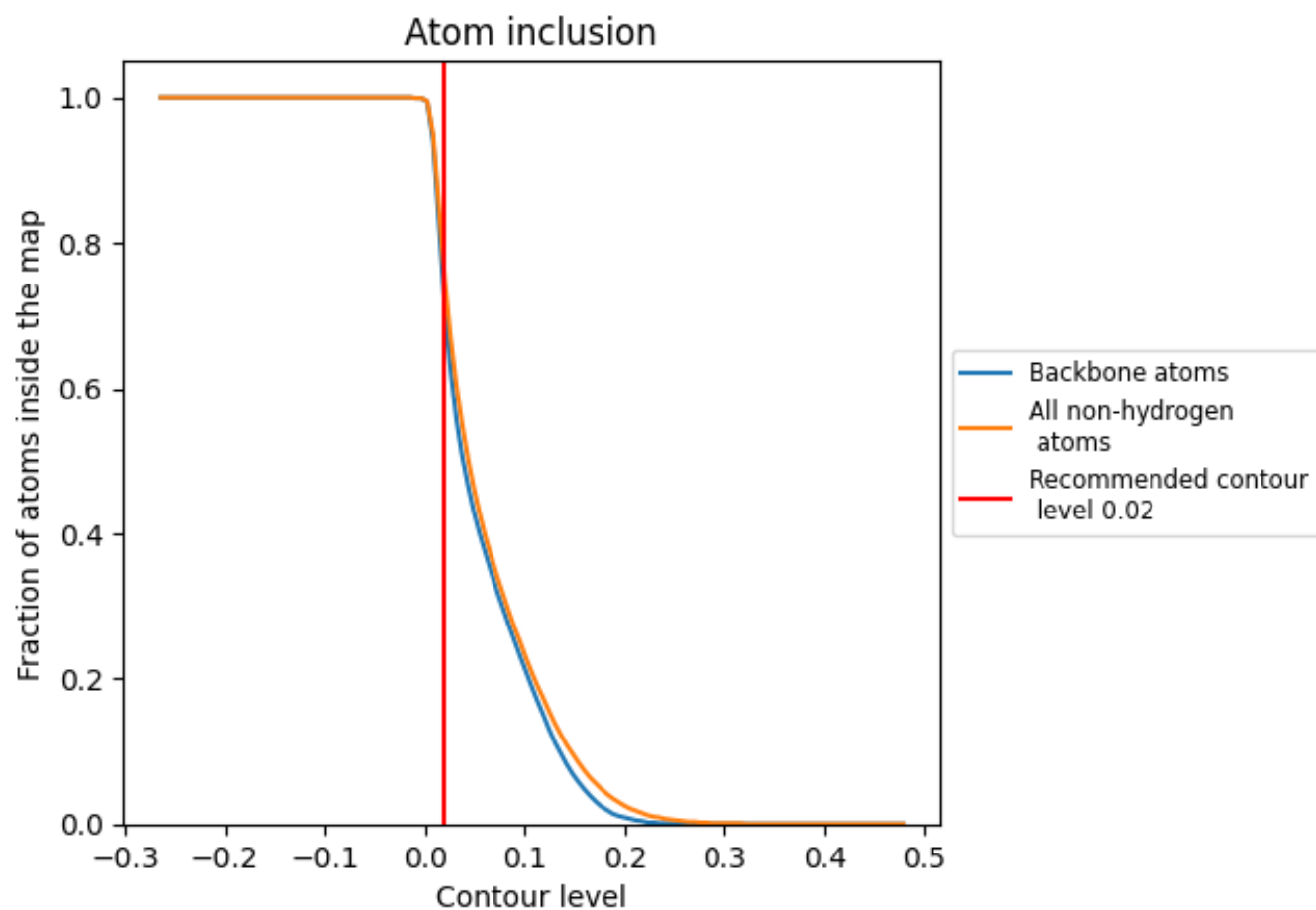
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 75% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7510	 0.3620
0	 0.0350	 0.1250
1	 0.3560	 0.1760
2	 0.7990	 0.3750
3	 0.9000	 0.4570
4	 0.3490	 0.1320
5	 0.1110	 0.0870
7	 0.0010	 0.0490
A	 0.9320	 0.4310
E	 0.9360	 0.4850
H	 0.9770	 0.5790
I	 0.7120	 0.1730
J	 0.9530	 0.4890
K	 0.9300	 0.4500
L	 0.9470	 0.5370
M	 0.9600	 0.5430
O	 0.9660	 0.5800
P	 0.0580	 0.0620
Q	 0.9580	 0.5470
R	 0.9080	 0.4650
S	 0.7240	 0.2110
T	 0.5930	 0.1300
V	 0.6830	 0.1770
W	 0.6600	 0.1710
Z	 0.9730	 0.5760
a	 0.9060	 0.5030
b	 0.9780	 0.5440
c	 0.2200	 0.1240
e	 0.9400	 0.5030
f	 0.6720	 0.1840
h	 0.9770	 0.5300
i	 0.4580	 0.0950

