



Full wwPDB EM Validation Report ⓘ

Jul 14, 2026 – 02:56 PM JST

PDB ID : 9XAK / pdb_00009xak
EMDB ID : EMD-66690
Title : Cryo-EM structure of the pre-40S ribosome (Enp1-Rrp12 Mut) 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 : 6G18

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:

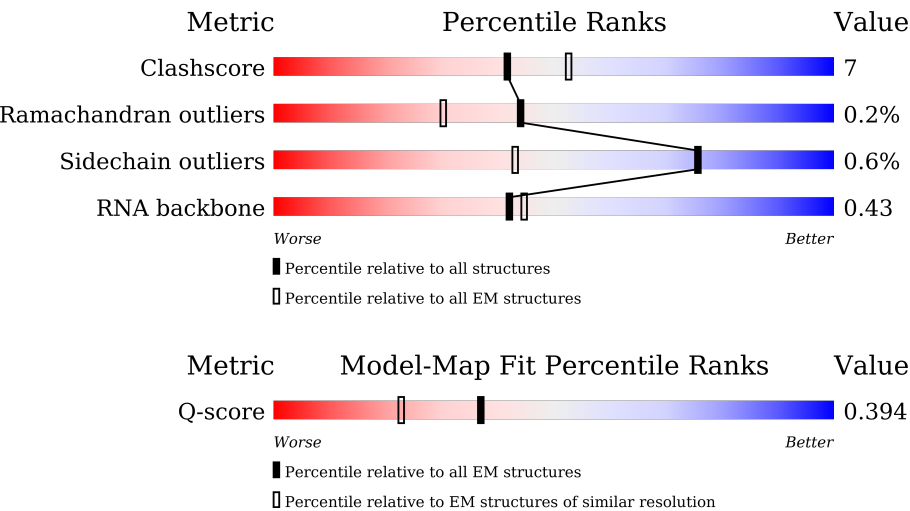
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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.



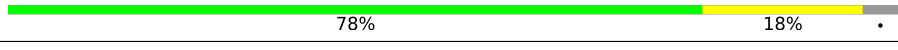
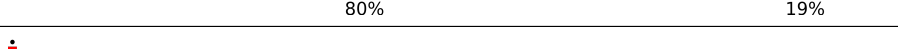
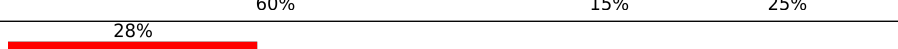
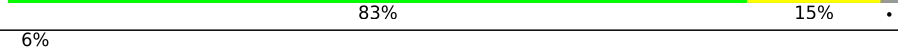
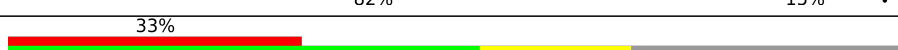
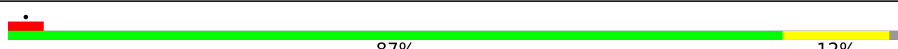
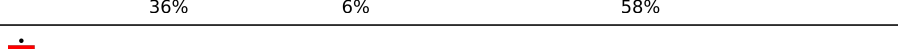
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	65%17%16%
2	H	264	92%7%
3	I	212	17%62%32%6%

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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	1797	
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	45%12%44%
30	5	445	13%5%82%
31	6	519	7%92%
32	7	1235	81%69%12%19%
33	8	938	5%93%

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 78493 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	132	Total	C	N	O	S	0	0
			1061	668	209	182	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 pre-18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	A	1464	Total	C	N	O	P	0	0
			31212	13948	5550	10250	1464		

- 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	699	Total	C	N	O	S	0	0
			5579	3506	997	1056	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	81	Total	C	N	O	S	0	0
			660	416	113	130	1		

- Molecule 31 is a protein called Serine/threonine-protein kinase RIO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6	43	Total	C	N	O	S	0	0
			352	222	74	54	2		

- Molecule 32 is a protein called Ribosomal RNA-processing protein 12-like conserved domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	7	1004	Total	C	N	O	S	0	0
			7841	5009	1353	1441	38		

- Molecule 33 is a protein called Utp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	8	62	Total	C	N	O	S	0	0
			537	335	112	89	1		

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

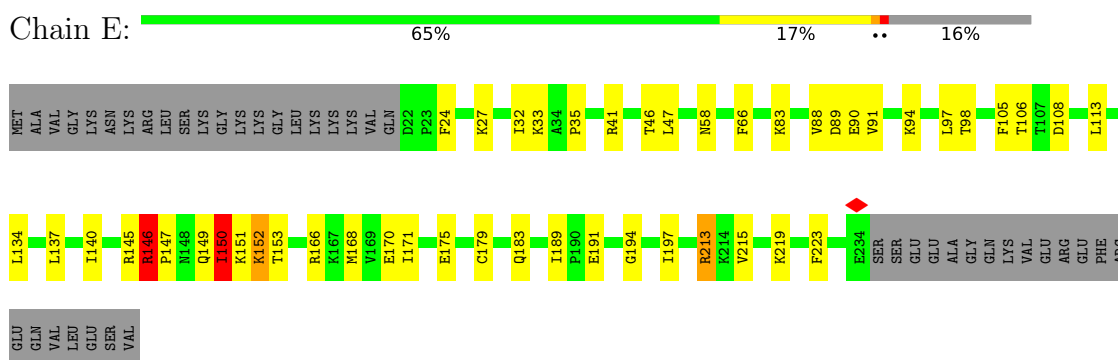
- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	A	4	Total	O	0
			4	4	

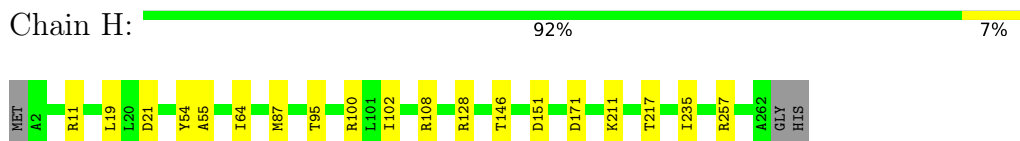
3 Residue-property plots

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.

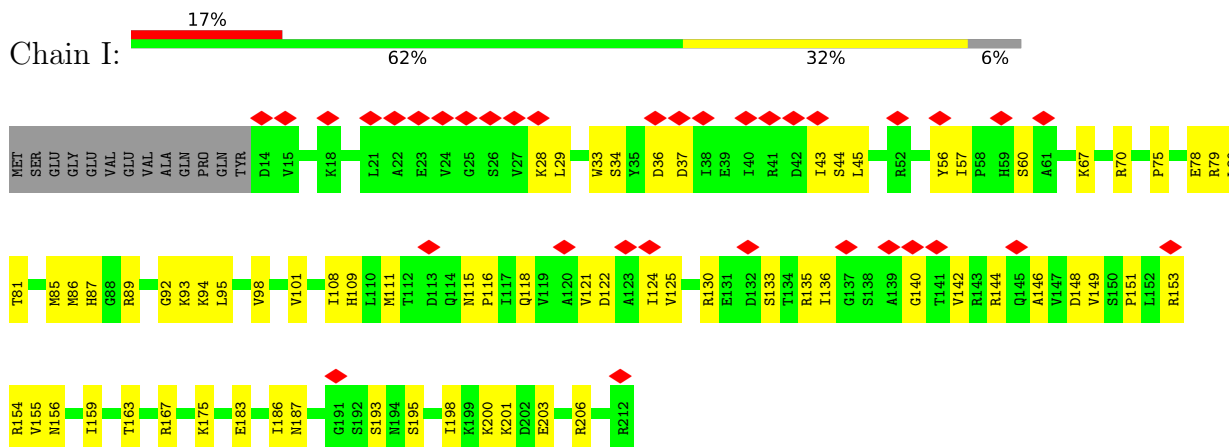
- Molecule 1: Small ribosomal subunit protein eS1



- Molecule 2: 40S ribosomal protein S4

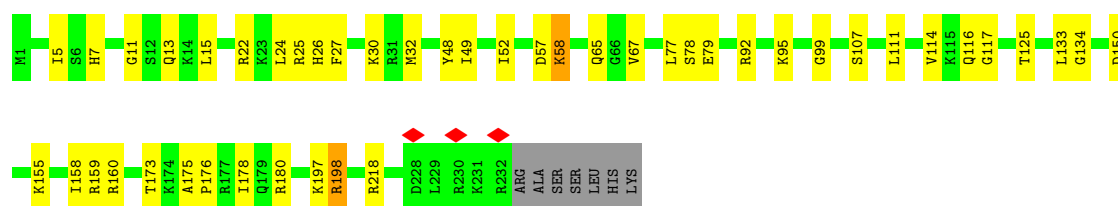


- Molecule 3: 40S ribosomal protein s5-like protein



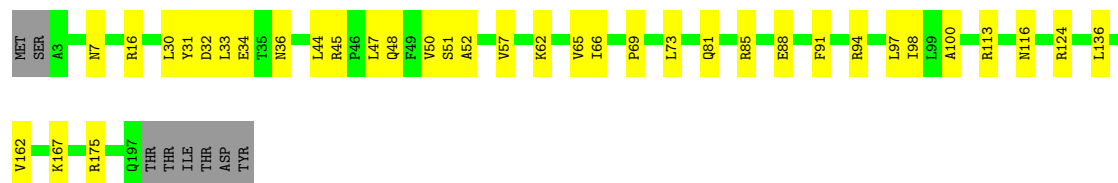
- Molecule 4: 40S ribosomal protein S6

Chain J:  78% 18%



- Molecule 5: 40S ribosomal protein S7

Chain K:  78% 18%



- Molecule 6: 40S ribosomal protein S8

Chain L:  80% 19%



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

Chain M:  82% 12% 6%



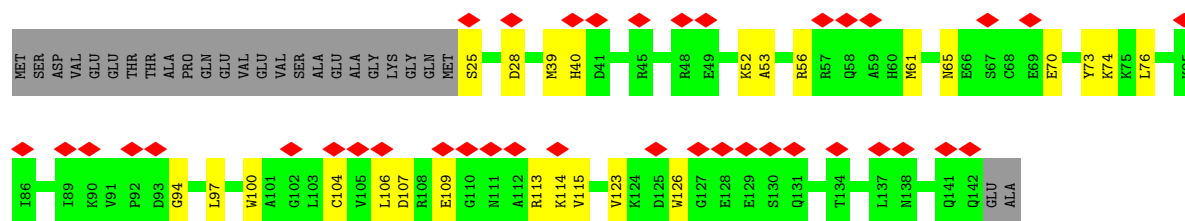
- Molecule 8: 40S ribosomal protein S11-like protein

Chain O:  84% 9% 7%

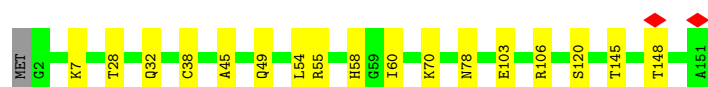
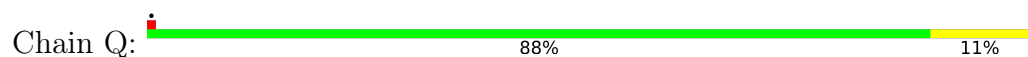


- Molecule 9: 40S ribosomal protein S12

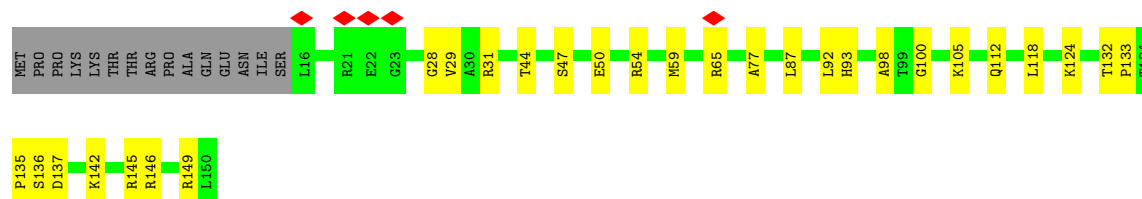
Chain P:  26% 65% 17% 18%



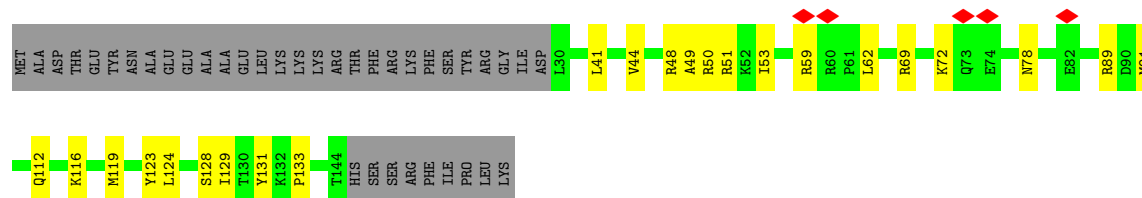
- Molecule 10: 40S ribosomal protein S13-like protein



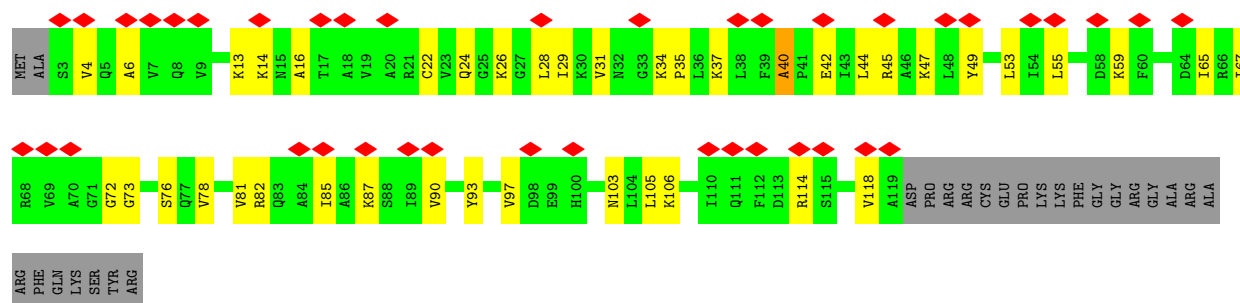
- Molecule 11: 40S ribosomal protein S14-like protein



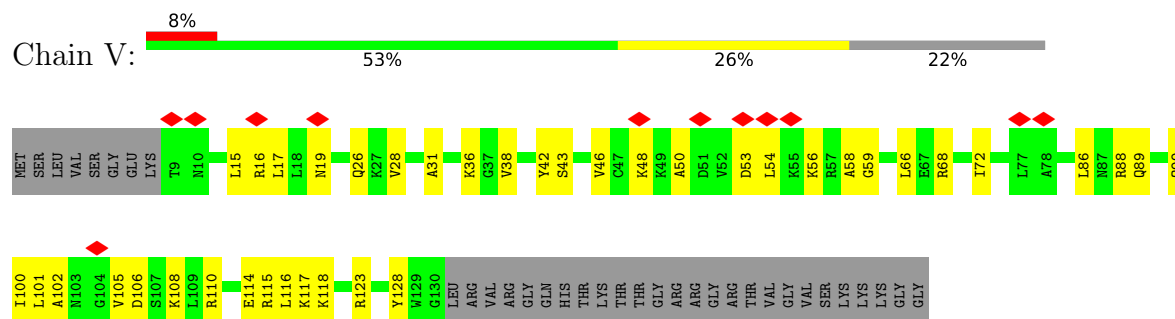
- Molecule 12: 40S ribosomal protein s15-like protein



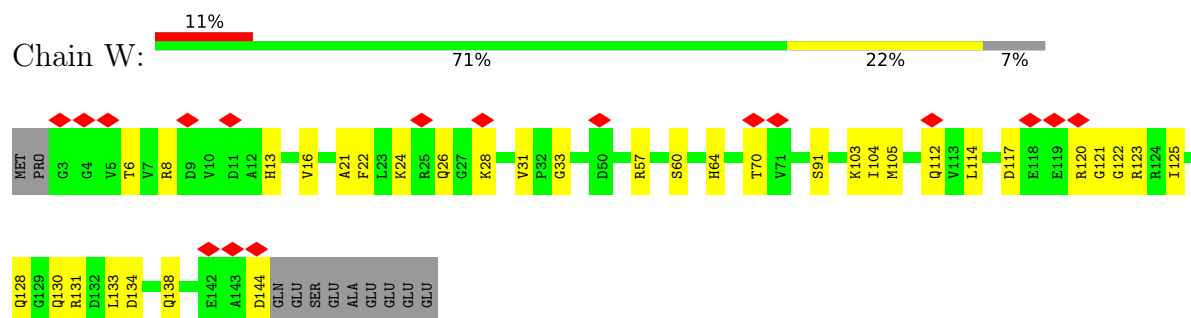
- Molecule 13: 40S ribosomal protein S16-like protein



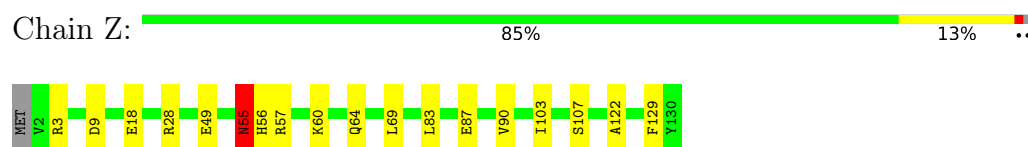
- Molecule 14: Putative ribosomal protein



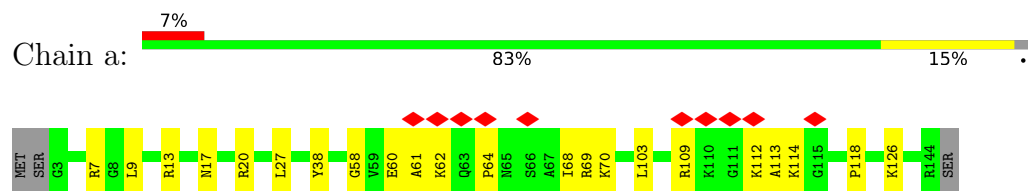
- Molecule 15: 40S ribosomal protein S19-like protein



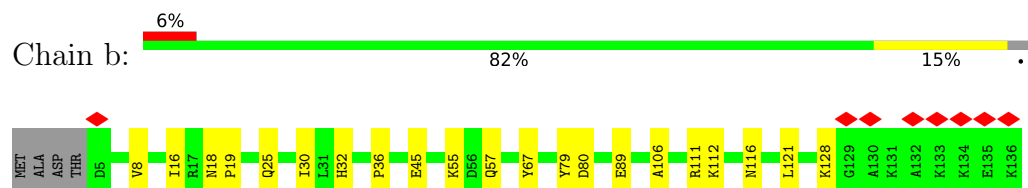
- Molecule 16: 40S ribosomal protein S22-like protein



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



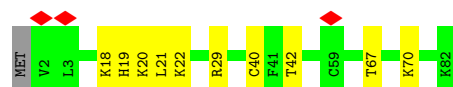
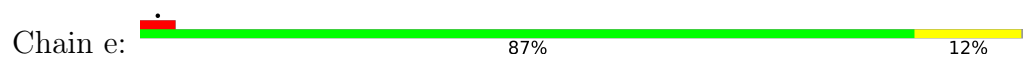
- Molecule 18: Small ribosomal subunit protein eS24



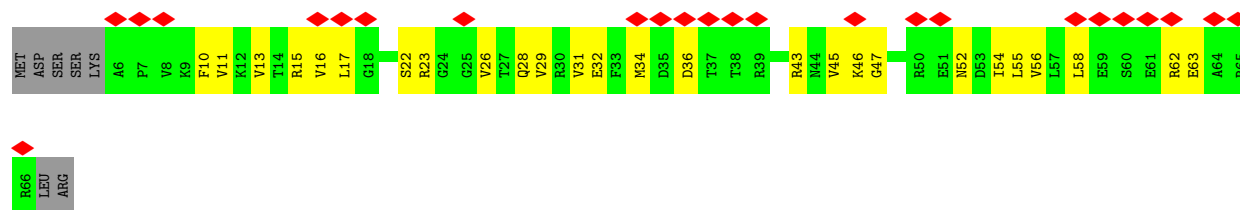
- Molecule 19: 40S ribosomal protein S25



- Molecule 20: Ribosomal protein s27-like protein



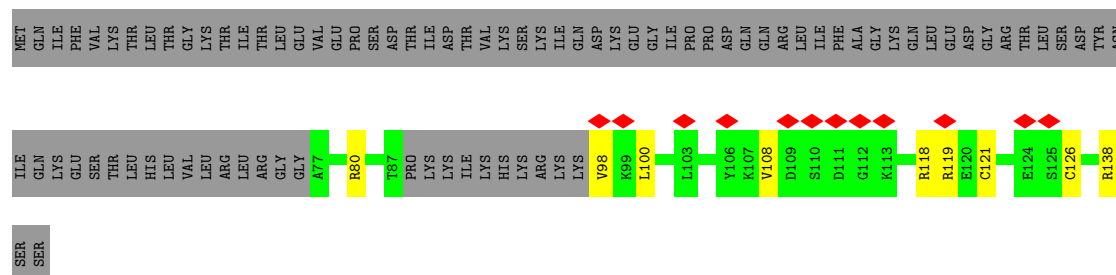
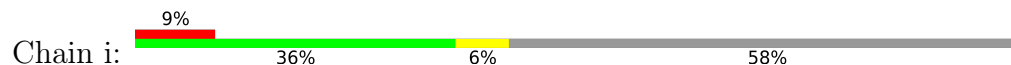
- Molecule 21: 40S ribosomal protein S28-like protein



- Molecule 22: 40S ribosomal protein S30



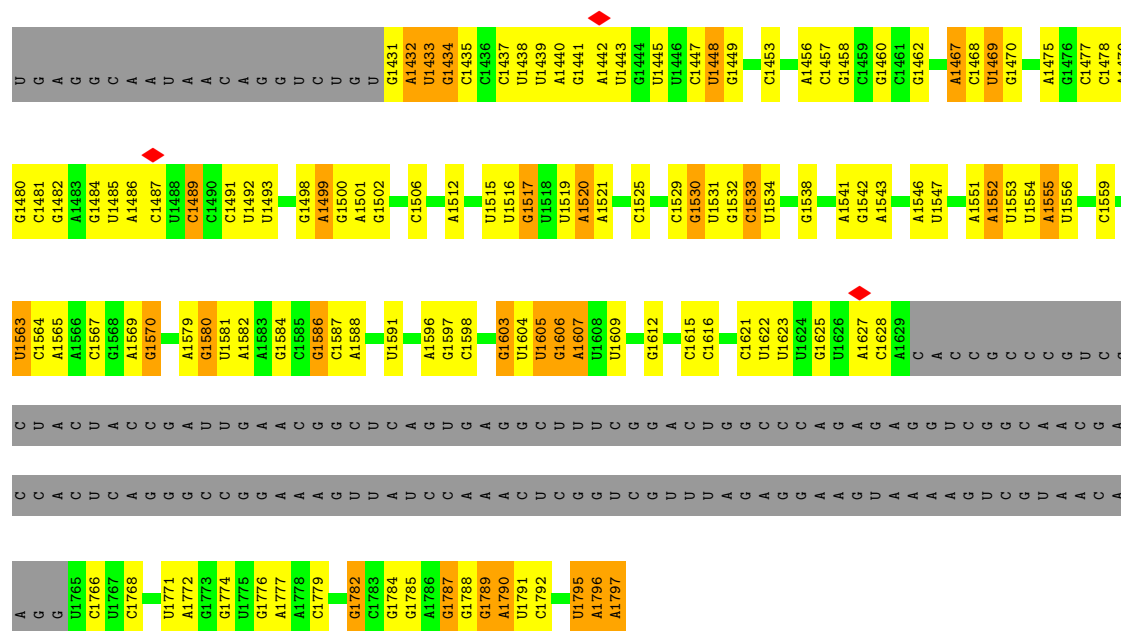
- Molecule 23: 40S ribosomal protein S27a-like protein



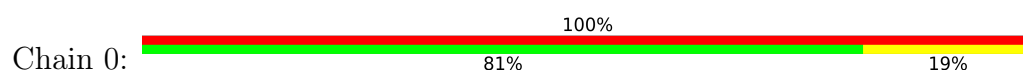
- Molecule 24: pre-18S



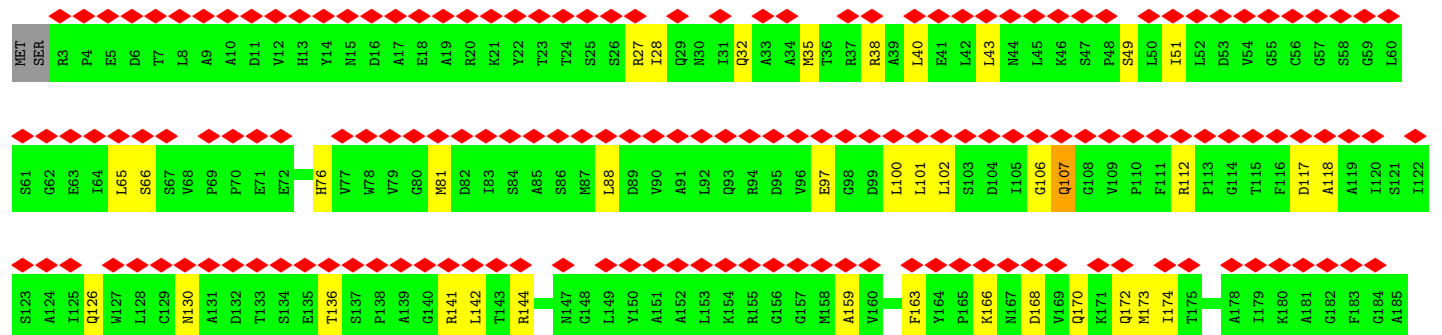
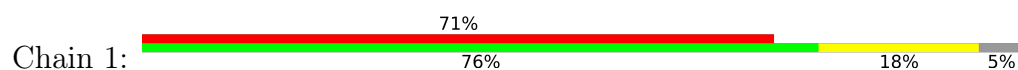


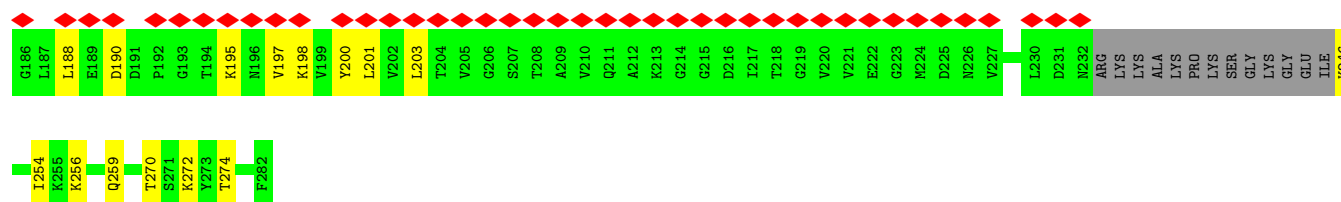


• Molecule 25: Trm112

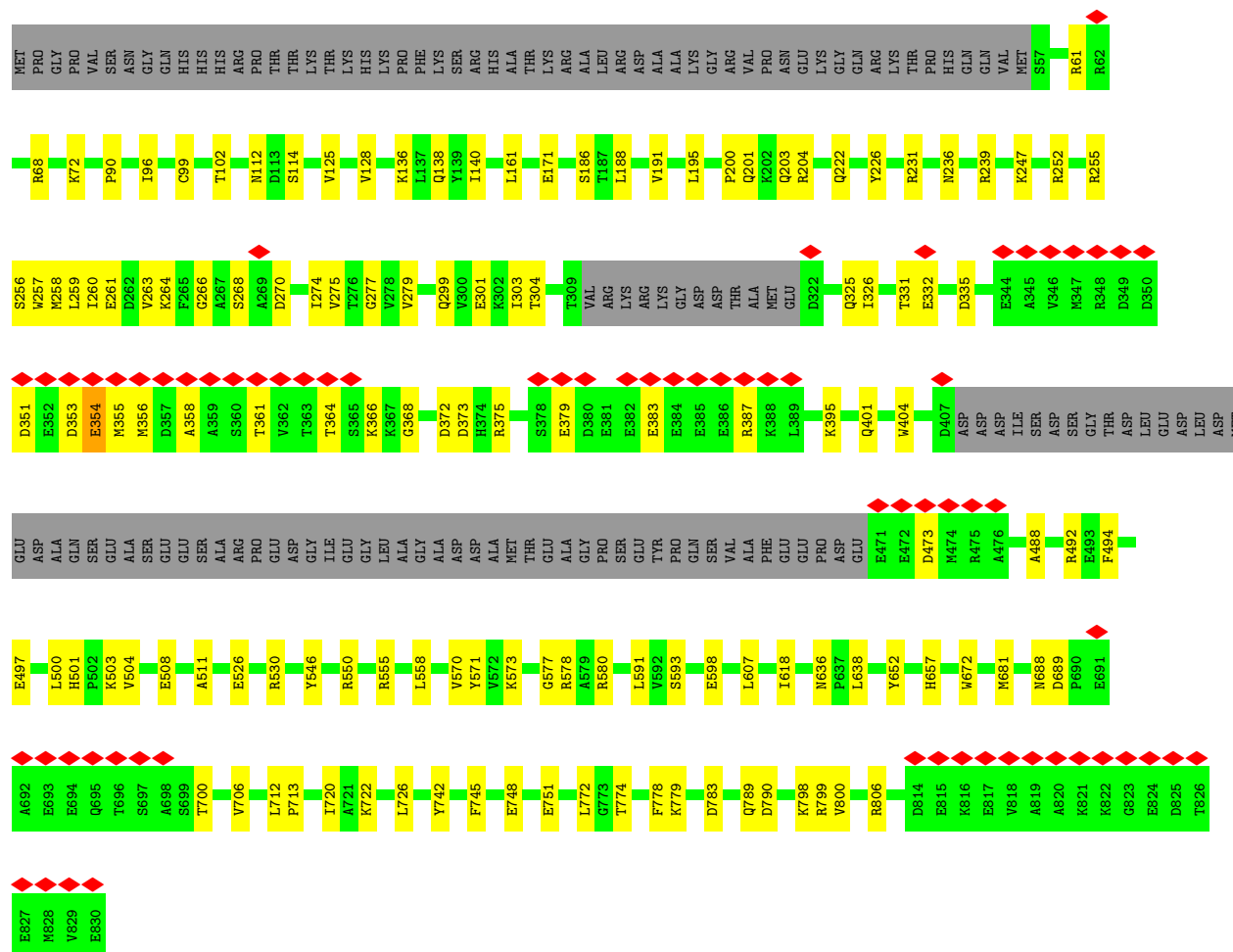


• Molecule 26: Methyltransferase-like protein

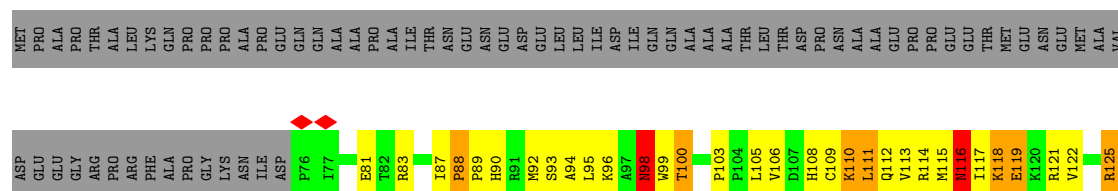




• Molecule 27: Bms1-type G domain-containing protein



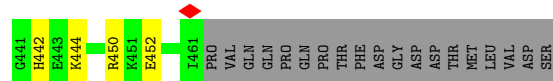
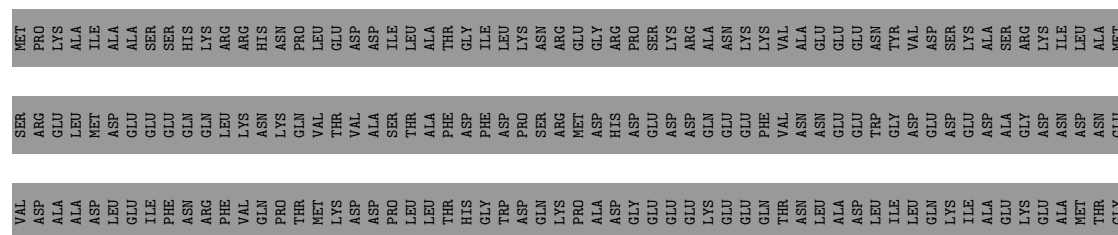
• Molecule 28: Pre-rRNA-processing protein PNO1





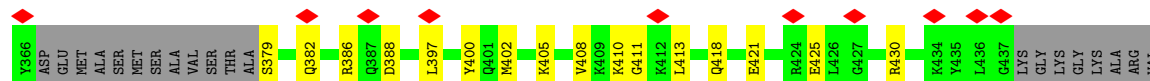
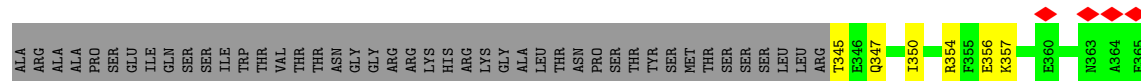
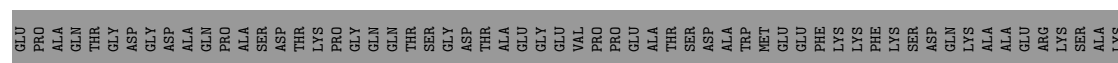
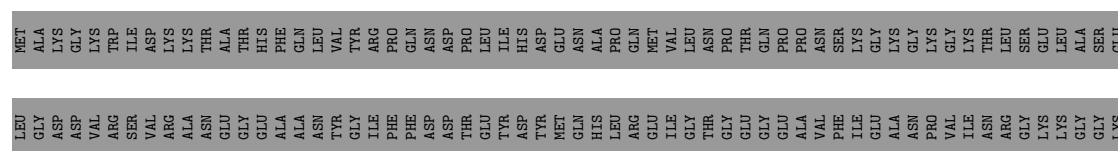
• Molecule 29: Bystin-like protein

Chain 4: 45% 12% 44%

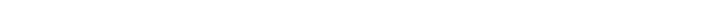


• Molecule 30: Putative low-temperature viability protein

Chain 5: 13% 5% 82%



• Molecule 31: Serine/threonine-protein kinase RIO1

- Chain 7:  81% 69% 12% 19%

E241	E242	L243	L244	G245	I246	A247	R248	H249	G250	N251	E252	H253	M254	S255	M256	A257	V258	F259	E260	I261	F262	E263	M264	I265	F266	E267	G268	M269	A270	D271	E272	V273	A274	S275	A276	K277	L278	P279	R280	L281	L282	E283	I284	I285	K286	E287	L288	R289	P290	A291	P292	N293	D294	V295	Q296	L297	L298	P299	R300
C181	A182	E183	T184	A185	M186	M187	S188	L189	R190	N191	V192	F193	D194	K195	A196	T197	K198	S199	E200	K201	E202	K203	K204	G205	S206	E207	S208	A209	H210	D211	P212	E213	L214	I215	H216	A217	L218	Q219	L220	V221	K222	T223	I224	A225	S226	G227	S228	G229	Q230	M231	P232	S233	K234	K235	I236	E237	P238	L239	C240
D121	A122	A123	G124	M125	E126	M127	S128	A129	A130	Q131	I132	G133	P134	R135	R136	V137	V138	G139	G140	L141	L142	S143	F144	A145	L146	D147	P148	R149	P150	L151	V152	R153	K154	R155	A156	D157	D158	A159	L160	R161	K162	I163	L164	R165	N166	P167	P168	P169	S170	P171	S172	L173	D174	H175	P176	V177	A178	P179	M180
I61	S62	H63	P64	V65	V66	V67	L68	L69	D70	V71	V72	T73	P74	F75	A76	P77	A78	P79	L80	L81	R82	K83	K84	F85	T86	O87	T88	R89	T90	L91	L92	A93	P94	V95	L96	S97	Q98	P99	E100	A101	D102	A103	P104	L105	I106	R107	S108	S109	I110	G111	C112	L113	E114	G115	L116	L117	L118	A119	C120
M1	A2	S3	L4	K5	E6	K7	L8	D9	K10	I11	R12	S13	P14	M15	L16	E17	M18	Q19	K20	Q21	T22	A23	A24	V25	L26	E27	A28	V29	E30	A31	A32	F33	K34	E35	R36	N37	T38	E39	P40	T41	P42	T43	A44	V45	F46	A47	A48	L49	L50	S51	L52	L53	M54	M55	D56	M57	G58	K59	L60

LEU	ASP	F901	D841	I781	P721	K661	A601	L541	Y481	T421	Q361	W301
LYS	ASN	L902	A842	P782	Q722	L662	Q602	T542	T482	I422	V362	I302
THR	GLU	I903	P843	M783	I723	A663	K603	E543	T483	G423	L363	A303
ALA	TYR	S904	K844	T784	Q724	Q664	M604	A544	M484	E424	V364	I304
ARG	GLN	M905	A845	S785	K725	A665	L605	F545	T485	I425	E365	L305
ARG	ALA	R906	T846	L786	K726	L666	E606	D546	M486	E426	P366	S306
GLY	LEU	R907	A847	H787	A727	Q667	Y607	T547	L487	T427	S367	R307
GLN	ASN	E908	S848	F788	Y728	E668	L608	A548	M488	E428	I368	A308
SER	SER	E909	L849	I789	K729	P669	G609	F549	H489	D429	I369	Y309
LYS	ASP	V910	E850	P790	L730	V670	E610	A550	F490	S430	D370	D310
LYS	SER	K911	E851	S791	I731	Q671	R611	E551	K491	F431	E371	V311
ASP	GLU	S912	Y852	I792	P732	K672	F612	M552	T492	G432	K372	A312
TRP	SER	Y913	M853	L793	R733	P673	A613	L553	E493	G433	V373	A313
ASP	GLU	H914	T854	S794	L734	K674	A614	T554	L494	K434	I374	Q314
ARG	SER	G915	M855	E795	A735	M675	D615	T555	V495	Q435	E375	I315
GLN	ASP	F916	V856	Y796	E736	P676	I616	V556	P496	E436	K376	S316
ASP	ASP	V917	S857	Y797	E737	M677	L617	L557	L497	A437	L377	P317
ASP	SER	K918	A858	I798	E738	Q678	A618	L558	S498	D438	V378	E318
ASP	ASP	C920	G859	G799	V739	E679	V619	E559	A499	V439	Q379	E319
GLY	ILE	R980	L860	C800	G740	Q680	L620	Q660	A500	V440	T380	T320
GLY	MET	K981	A861	K801	R741	V681	F621	P661	M501	L441	V381	F321
LYS	THR	I921	G862	E802	A742	P682	M622	E562	Y502	G442	Q382	Q322
THR	GLY	S923	S863	H803	A743	S683	V623	L563	Q503	K443	G383	E323
ILE	ARG	T924	T864	N804	L744	T684	Y624	R564	R504	A444	L384	I324
ARG	GLY	P925	P865	E805	E745	A685	S625	L565	V505	I445	L385	L325
GLU	GLN	T926	H866	K806	Q746	H686	T626	D566	L506	R446	E326	E326
ASP	LYS	D927	M867	A807	R747	T687	T627	V567	E507	A447	I387	P327
LYS	LYS	L928	T868	R808	H748	M688	T628	C568	H508	M448	K388	F328
ARG	ARG	N929	S869	T809	E749	M689	P629	R569	G509	G449	Y389	N329
GLU	GLU	K990	A870	T810	E750	D690	Q630	A570	N510	P450	L330	L330
GLY	THR	P931	T871	A811	V751	L691	K631	L571	A511	E451	Q390	V331
ALA	GLY	R932	L872	F812	Q752	V692	R632	R572	P512	A452	A392	A332
ALA	THR	L933	L873	D813	Q753	V693	G633	A573	K513	V453	W393	S333
LYS	TYR	K934	A874	L814	L754	T694	P634	L574	T514	L454	L394	Y334
GLY	ILE	T935	M875	L815	L755	M695	V635	V575	M515	N455	E395	L335
LEU	GLU	R936	T876	V816	L756	S696	L636	E576	E516	V456	T396	E336
ASP	ASP	I937	R877	L817	S757	I697	Q637	S577	V517	L457	F397	S337
ASP	ASP	P938	H878	M818	A758	V698	T638	N578	K518	E458	N398	E338
GLU	GLU	N939	L879	G819	A759	L699	I639	Q579	I519	L459	V399	A339
PRO	PRO	A1000	L879	H820	D760	P700	N640	A580	F520	N460	I400	K340
LEU	LEU	Y880	Y880	K821	K761	R701	S641	I581	E521	L461	G401	N341
LEU	LEU	E881	E881	M822	V762	E702	F642	V582	T522	I462	A402	I342
VAL	LEU	F882	F882	S823	S763	S703	L643	S583	V523	K463	M403	R343
ASP	ASP	R883	R883	E824	S764	F704	S644	A584	V524	P464	F404	I344
ARG	ARG	S944	E884	A825	P765	E705	T645	G585	Q525	A465	D405	S345
ASN	ASN	H945	A885	E826	A766	A706	I646	D586	Q526	R466	A406	A346
GLY	ALA	E946	L886	N826	R767	L707	P647	V587	I527	D467	L407	S347
LEU	SER	H947	K887	G827	R768	F708	K648	E588	W528	Q468	R408	E348
ASP	ASP	K948	K888	S828	R769	F709	T649	D589	I529	P469	W409	C349
ALA	ALA	G949	E889	L829	E769	K709	T649	D589	W529	G470	R410	L350
GLU	GLU	H950	T890	T830	R770	I710	R650	P590	I530	R471	S411	V351
VAL	VAL	F951	T891	D831	L771	A711	L651	V591	L531	A472	H412	S352
GLY	GLY	R952	L891	M832	A772	A712	M652	I592	P532	E473	P413	F353
LYS	LYS	A953	D893	S833	A773	L713	E653	L593	G533	M474	Y414	L354
ARG	ARG	K954	L894	K834	I774	V714	T654	C594	W534	L475	L415	A355
ARG	ARG	V955	V895	V835	A775	V715	F655	R595	C535	P476	L416	N356
PHE	PHE	K956	V896	V836	A776	F716	D656	V596	D536	L477	G417	C357
		H957	D897	P836	A777	F717	L657	S597	L537	L478	I418	V358
		T958	M898	H837	L777	D718	L657	K598	L538	L479	T419	P359
		F959	D899	P839	P779	D719	C659	Q599	L539	R479	K420	P360
		E960	L900	K840	I780	D720	E660	T600	D540	D480		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29832	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 ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.402	Depositor
Minimum map value	-0.199	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	376.19998, 376.19998, 376.19998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.045, 1.045, 1.045	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	0.41	0/1752	0.78	6/2361 (0.3%)
2	H	0.46	0/2112	0.59	0/2842
3	I	0.20	0/1578	0.55	0/2130
4	J	0.38	0/1906	0.60	0/2547
5	K	0.30	0/1587	0.63	0/2140
6	L	0.42	0/1654	0.65	0/2213
7	M	0.37	0/1489	0.52	0/1993
8	O	0.51	0/1249	0.62	0/1678
9	P	0.20	0/934	0.64	0/1255
10	Q	0.46	0/1205	0.62	0/1627
11	R	0.38	0/1014	0.71	1/1361 (0.1%)
12	S	0.24	0/932	0.63	0/1248
13	T	0.24	0/922	0.55	0/1241
14	V	0.20	0/1012	0.58	2/1360 (0.1%)
15	W	0.21	0/1137	0.61	0/1533
16	Z	0.43	0/1055	0.64	1/1416 (0.1%)
17	a	0.42	0/1116	0.58	0/1489
18	b	0.41	0/1075	0.58	0/1431
19	c	0.21	0/550	0.62	0/736
20	e	0.37	0/623	0.59	0/843
21	f	0.19	0/487	0.56	0/653
22	h	0.68	0/184	1.16	0/242
23	i	0.16	0/535	0.42	0/710
24	A	0.39	0/34903	0.49	3/54376 (0.0%)
25	0	0.15	0/1013	0.43	0/1378
26	1	0.20	0/2043	0.57	1/2753 (0.0%)
27	2	0.24	0/5694	0.48	2/7705 (0.0%)
28	3	0.53	0/1475	1.00	14/1982 (0.7%)
29	4	0.22	0/2205	0.62	2/2990 (0.1%)
30	5	0.25	0/670	0.73	1/896 (0.1%)
31	6	0.27	0/356	0.67	0/462
32	7	0.18	0/7995	0.43	2/10857 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	8	0.78	0/544	1.41	3/717 (0.4%)
All	All	0.36	0/83006	0.56	38/119165 (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
13	T	0	1
22	h	0	1
28	3	0	1
All	All	0	3

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	3	88	PRO	CB-CA-C	-8.18	100.94	110.92
28	3	121	ARG	O-C-N	-7.79	114.37	123.25
28	3	88	PRO	N-CA-CB	-7.65	95.66	103.08
28	3	132	SER	CA-C-N	-7.30	111.18	122.49
28	3	132	SER	C-N-CA	-7.30	111.18	122.49
16	Z	55	ASN	N-CA-C	-7.21	97.98	109.59
28	3	121	ARG	CA-C-N	-6.81	114.18	122.90
28	3	121	ARG	C-N-CA	-6.81	114.18	122.90
28	3	118	LYS	O-C-N	6.75	129.32	122.03
1	E	153	THR	CA-C-N	-6.66	112.44	123.37
1	E	153	THR	C-N-CA	-6.66	112.44	123.37
29	4	213	LYS	N-CA-C	-6.66	106.10	114.56
1	E	146	ARG	CB-CA-C	-6.38	99.45	109.09
1	E	113	LEU	O-C-N	-6.26	114.59	122.17
28	3	119	GLU	N-CA-C	-6.18	105.32	112.92
28	3	116	ASN	CA-CB-CG	6.09	118.69	112.60
28	3	89	PRO	N-CA-C	-6.05	105.64	113.57
1	E	151	LYS	CB-CA-C	5.87	120.57	109.37
28	3	93	SER	N-CA-C	-5.78	104.89	111.07
33	8	404	LYS	N-CA-C	-5.72	105.56	112.54
33	8	440	ARG	N-CA-C	-5.70	105.06	111.28
33	8	429	LYS	N-CA-C	-5.69	106.98	114.04
24	A	414	A	C2'-C3'-O3'	5.67	118.01	109.50
24	A	616	A	C4'-C3'-O3'	-5.65	104.53	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	152	LYS	N-CA-C	-5.54	105.78	112.54
32	7	186	MET	CA-C-N	-5.48	111.55	121.14
32	7	186	MET	C-N-CA	-5.48	111.55	121.14
30	5	356	GLU	N-CA-CB	5.30	119.18	110.39
26	1	102	LEU	CA-CB-CG	5.26	134.69	116.30
27	2	354	GLU	CA-C-N	-5.25	112.88	122.38
27	2	354	GLU	C-N-CA	-5.25	112.88	122.38
28	3	110	LYS	CA-C-O	-5.25	115.63	122.14
14	V	50	ALA	CA-C-N	5.11	131.29	121.54
14	V	50	ALA	C-N-CA	5.11	131.29	121.54
11	R	136	SER	N-CA-C	-5.10	107.56	112.97
24	A	929	C	P-O3'-C3'	5.06	127.79	120.20
28	3	100	THR	CB-CA-C	-5.05	100.37	110.42
29	4	267	GLU	N-CA-CB	5.02	117.59	110.16

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	3	108	HIS	Mainchain
13	T	40	ALA	Peptide
22	h	37	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1723	0	1804	28	0
2	H	2072	0	2155	16	0
3	I	1557	0	1608	54	0
4	J	1875	0	1983	32	0
5	K	1562	0	1641	24	0
6	L	1621	0	1645	30	0
7	M	1466	0	1582	17	0
8	O	1222	0	1289	13	0
9	P	923	0	946	19	0
10	Q	1182	0	1264	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	R	1002	0	1034	23	0
12	S	917	0	978	19	0
13	T	909	0	973	26	0
14	V	998	0	1042	24	0
15	W	1117	0	1133	24	0
16	Z	1037	0	1076	10	0
17	a	1099	0	1169	19	0
18	b	1061	0	1150	14	0
19	c	546	0	591	11	0
20	e	611	0	635	6	0
21	f	484	0	513	20	0
22	h	181	0	207	15	0
23	i	528	0	541	9	0
24	A	31212	0	15726	298	0
25	0	993	0	1018	16	0
26	1	2013	0	2043	34	0
27	2	5579	0	5570	87	0
28	3	1451	0	1524	39	0
29	4	2154	0	2242	34	0
30	5	660	0	648	19	0
31	6	352	0	402	6	0
32	7	7841	0	8114	86	0
33	8	537	0	573	16	0
34	A	1	0	0	0	0
34	Q	1	0	0	0	0
34	a	1	0	0	0	0
35	e	1	0	0	0	0
36	A	4	0	0	0	0
All	All	78493	0	64819	950	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (950) 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)
27:2:263:VAL:HA	27:2:274:ILE:O	1.30	1.27
24:A:1176:G:H21	24:A:1456:A:N6	1.56	1.03
24:A:1269:U:H3	24:A:1435:C:N4	1.60	0.99
24:A:1272:A:C2	24:A:1431:G:N1	2.34	0.94
24:A:1176:G:H21	24:A:1456:A:H61	0.93	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1265:G:H1	24:A:1438:U:H3	0.95	0.93
24:A:709:G:H1	24:A:722:U:H3	1.20	0.89
24:A:1272:A:H2	24:A:1431:G:H1	1.00	0.89
24:A:1176:G:N2	24:A:1456:A:H61	1.72	0.88
24:A:652:G:H1	24:A:673:U:H3	0.95	0.88
24:A:1272:A:H2	24:A:1431:G:N1	1.70	0.87
27:2:263:VAL:CA	27:2:274:ILE:O	2.22	0.85
33:8:431:ILE:HG23	33:8:439:TRP:HH2	1.45	0.82
24:A:1468:C:C2	24:A:1530:G:N2	2.48	0.82
26:1:190:ASP:O	26:1:197:VAL:HA	1.81	0.81
24:A:1584:G:H1	24:A:1604:U:H3	0.86	0.80
24:A:1467:A:H62	24:A:1534:U:H3	1.26	0.80
19:c:38:LYS:O	19:c:42:ASP:HB2	1.81	0.78
24:A:702:A:H62	24:A:731:G:N2	1.81	0.78
24:A:1467:A:N6	24:A:1534:U:H3	1.84	0.74
25:0:31:GLU:HG3	25:0:99:GLU:HB2	1.70	0.74
22:h:41:THR:HA	22:h:45:VAL:HG22	1.69	0.73
24:A:820:U:H3	24:A:848:G:H1	1.35	0.72
24:A:220:A:N1	24:A:835:G:C6	2.57	0.72
24:A:1200:A:C6	24:A:1551:A:C6	2.77	0.71
9:P:106:LEU:H	9:P:113:ARG:HH22	1.39	0.71
3:I:57:ILE:HD11	13:T:47:LYS:HG2	1.72	0.70
21:f:13:VAL:O	21:f:52:ASN:HA	1.91	0.70
24:A:702:A:N6	24:A:731:G:N2	2.40	0.70
28:3:116:ASN:C	28:3:118:LYS:H	1.99	0.70
24:A:1041:A:C2	33:8:421:HIS:CB	2.75	0.69
27:2:577:GLY:HA2	27:2:580:ARG:HD2	1.74	0.69
24:A:1269:U:C2	24:A:1434:G:O6	2.46	0.69
24:A:1480:G:N2	24:A:1587:C:O2	2.26	0.69
4:J:160:ARG:NH2	24:A:68:A:OP1	2.25	0.69
27:2:256:SER:HB3	27:2:593:SER:HB3	1.74	0.69
24:A:1468:C:O2	24:A:1530:G:N2	2.25	0.68
24:A:1198:G:O6	24:A:1591:U:C4	2.46	0.68
24:A:1236:U:O2	24:A:1240:G:C2	2.46	0.68
24:A:1269:U:N3	24:A:1435:C:N4	2.27	0.68
7:M:77:ARG:NH2	24:A:761:A:OP1	2.26	0.67
6:L:57:ALA:HB2	6:L:181:GLY:HA2	1.75	0.67
24:A:220:A:C6	24:A:835:G:C6	2.82	0.67
24:A:1796:A:H4'	24:A:1797:A:H5'	1.75	0.67
24:A:1480:G:H1	24:A:1587:C:H1'	1.58	0.67
22:h:26:LYS:HZ3	24:A:502:A:H61	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:476:U:H3	24:A:506:G:H1	1.43	0.67
24:A:1200:A:N6	24:A:1551:A:N6	2.43	0.67
28:3:110:LYS:O	28:3:130:THR:HG22	1.95	0.67
3:I:79:ARG:NH2	3:I:156:ASN:OD1	2.28	0.66
26:1:28:ILE:O	26:1:32:GLN:NE2	2.29	0.66
28:3:166:ILE:HA	28:3:218:ILE:O	1.95	0.66
24:A:1273:U:O2	24:A:1431:G:C6	2.49	0.65
11:R:29:VAL:HG12	11:R:93:HIS:HB2	1.79	0.65
24:A:1516:U:H4'	24:A:1517:G:H3'	1.78	0.65
8:O:107:LYS:O	17:a:13:ARG:NH2	2.30	0.65
24:A:483:G:H1	24:A:498:U:H3	1.42	0.65
3:I:130:ARG:HH12	21:f:58:LEU:HB3	1.62	0.65
3:I:135:ARG:HH12	3:I:142:VAL:HA	1.62	0.65
26:1:188:LEU:HB2	26:1:200:TYR:HB2	1.78	0.64
32:7:332:ALA:HA	32:7:335:LEU:HD12	1.79	0.64
3:I:79:ARG:HH22	3:I:155:VAL:HG13	1.62	0.64
1:E:89:ASP:HB3	1:E:223:PHE:HE1	1.62	0.64
15:W:120:ARG:NH1	15:W:121:GLY:O	2.30	0.64
4:J:58:LYS:HA	4:J:107:SER:HB3	1.78	0.64
14:V:101:LEU:O	14:V:105:VAL:N	2.30	0.64
24:A:1467:A:N6	24:A:1534:U:N3	2.40	0.64
11:R:142:LYS:HB3	24:A:988:C:H5'	1.81	0.63
12:S:116:LYS:H	12:S:119:MET:HE1	1.62	0.63
24:A:1272:A:N1	24:A:1431:G:O6	2.31	0.63
24:A:1432:A:H2	24:A:1434:G:H8	1.46	0.63
32:7:161:ARG:HD2	32:7:223:THR:HG23	1.79	0.63
9:P:109:GLU:OE1	30:5:345:THR:N	2.32	0.63
12:S:59:ARG:HH22	30:5:411:GLY:HA3	1.62	0.63
32:7:185:ALA:HB1	32:7:221:VAL:HG22	1.81	0.63
24:A:1220:G:H22	24:A:1259:U:H3	1.46	0.62
26:1:38:ARG:NH1	26:1:190:ASP:OD1	2.32	0.62
3:I:146:ALA:O	21:f:62:ARG:NH1	2.30	0.62
13:T:37:LYS:O	13:T:45:ARG:NH2	2.32	0.62
28:3:100:THR:O	28:3:103:PRO:HD2	1.99	0.62
24:A:688:U:C2	24:A:690:U:O4	2.53	0.62
1:E:35:PRO:O	1:E:41:ARG:NH1	2.32	0.62
33:8:445:LYS:HA	33:8:448:LEU:HB2	1.81	0.62
24:A:1218:A:H2	24:A:1261:G:H1	1.44	0.62
28:3:116:ASN:C	28:3:118:LYS:N	2.54	0.62
10:Q:38:CYS:SG	10:Q:78:ASN:ND2	2.73	0.61
27:2:550:ARG:HG3	27:2:672:TRP:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:S:72:LYS:O	30:5:430:ARG:NH2	2.33	0.61
1:E:150:ILE:HD11	33:8:414:LYS:HB2	1.81	0.61
13:T:34:LYS:HB2	15:W:8:ARG:HE	1.66	0.61
24:A:1200:A:C5	24:A:1551:A:N1	2.69	0.61
5:K:116:ASN:ND2	24:A:742:U:OP1	2.33	0.61
9:P:76:LEU:HD13	23:i:108:VAL:HG23	1.83	0.61
3:I:37:ASP:OD2	3:I:118:GLN:NE2	2.34	0.61
25:0:102:LEU:HB2	25:0:111:TYR:HB2	1.81	0.61
32:7:613:ALA:O	32:7:617:LEU:HB2	2.00	0.61
6:L:37:ARG:HH12	6:L:93:THR:HB	1.65	0.61
6:L:82:VAL:HG21	6:L:170:TYR:HE2	1.66	0.61
27:2:304:THR:HG22	27:2:326:ILE:HA	1.82	0.61
3:I:122:ASP:HA	3:I:125:VAL:HG12	1.82	0.60
15:W:60:SER:O	15:W:64:HIS:ND1	2.31	0.60
25:0:30:ALA:HA	25:0:99:GLU:O	2.01	0.60
27:2:270:ASP:O	27:2:573:LYS:NZ	2.33	0.60
24:A:1493:U:O4	24:A:1506:C:N3	2.34	0.60
25:0:123:PRO:HD2	25:0:126:LEU:HD12	1.82	0.60
31:6:495:LYS:HD3	31:6:499:ARG:HH21	1.65	0.60
24:A:487:U:N3	24:A:495:G:N1	2.50	0.60
28:3:96:LYS:HA	33:8:829:TRP:CH2	2.37	0.60
32:7:883:ARG:HH12	32:7:920:CYS:HA	1.67	0.60
2:H:87:MET:HE1	2:H:235:ILE:HD13	1.84	0.60
5:K:73:LEU:HD22	5:K:100:ALA:HB2	1.84	0.60
24:A:866:G:H1	24:A:958:U:H3	1.50	0.60
24:A:1236:U:C2	24:A:1240:G:N1	2.70	0.60
3:I:67:LYS:HB3	3:I:70:ARG:HG2	1.82	0.59
6:L:189:GLU:O	8:O:22:ASN:ND2	2.35	0.59
15:W:70:THR:HG23	15:W:122:GLY:HA3	1.83	0.59
5:K:7:ASN:O	5:K:48:GLN:NE2	2.34	0.59
7:M:131:HIS:ND1	7:M:160:SER:OG	2.29	0.59
3:I:193:SER:HA	3:I:198:ILE:HG21	1.84	0.59
13:T:29:ILE:HG23	13:T:65:ILE:HB	1.83	0.59
25:0:57:ARG:HG2	25:0:68:LEU:HB2	1.84	0.59
32:7:498:SER:HA	32:7:501:MET:HE2	1.83	0.59
2:H:257:ARG:NH2	24:A:784:U:O2'	2.35	0.59
3:I:81:THR:HG21	3:I:98:VAL:HG12	1.84	0.59
24:A:317:U:H3'	24:A:318:C:H2'	1.84	0.59
13:T:55:LEU:HD22	13:T:105:LEU:HD22	1.84	0.59
1:E:134:LEU:HB3	1:E:219:LYS:HB2	1.85	0.59
24:A:911:G:OP1	24:A:911:G:N2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1277:C:OP1	32:7:981:LYS:NZ	2.35	0.59
27:2:494:PHE:HB3	27:2:497:GLU:HG3	1.84	0.59
24:A:220:A:C6	24:A:835:G:N1	2.70	0.59
16:Z:3:ARG:NH1	16:Z:9:ASP:OD2	2.36	0.58
26:1:106:GLY:O	26:1:144:ARG:NH2	2.36	0.58
11:R:100:GLY:HA3	11:R:133:PRO:HG2	1.85	0.58
24:A:8:U:OP1	26:1:256:LYS:NZ	2.35	0.58
24:A:1041:A:C2	33:8:421:HIS:CG	2.91	0.58
11:R:28:GLY:O	11:R:92:LEU:HA	2.04	0.58
24:A:487:U:N3	24:A:495:G:C6	2.72	0.58
32:7:794:SER:O	32:7:797:VAL:HB	2.04	0.58
14:V:17:LEU:HD11	14:V:66:LEU:HD11	1.86	0.58
21:f:45:VAL:HG12	21:f:47:GLY:H	1.69	0.58
24:A:1541:A:H2'	24:A:1542:G:H8	1.69	0.58
27:2:368:GLY:O	27:2:375:ARG:NH1	2.36	0.58
28:3:116:ASN:O	28:3:118:LYS:N	2.36	0.58
8:O:60:ASP:HB3	8:O:63:CYS:HB2	1.86	0.58
26:1:49:SER:HB3	26:1:117:ASP:HB2	1.86	0.58
27:2:255:ARG:NH2	27:2:598:GLU:OE2	2.36	0.58
32:7:354:LEU:HD13	32:7:403:MET:HB2	1.85	0.57
32:7:397:PHE:HB3	32:7:440:VAL:HG21	1.86	0.57
16:Z:28:ARG:NH2	24:A:863:A:OP1	2.34	0.57
24:A:487:U:H3	24:A:494:G:H1	1.52	0.57
24:A:1437:C:O2	27:2:789:GLN:NE2	2.37	0.57
3:I:175:LYS:NZ	3:I:183:GLU:OE2	2.36	0.57
4:J:180:ARG:NH2	24:A:140:G:O6	2.36	0.57
4:J:198:ARG:HB2	24:A:175:G:H22	1.69	0.57
23:i:80:ARG:NH1	27:2:790:ASP:O	2.37	0.57
24:A:481:C:O3'	29:4:450:ARG:NH1	2.36	0.57
24:A:643:U:H2'	24:A:644:A:H8	1.70	0.57
28:3:112:GLN:HG3	28:3:125:ARG:HG2	1.85	0.57
1:E:32:ILE:HD11	1:E:46:THR:HB	1.86	0.57
4:J:13:GLN:NE2	24:A:148:G:N3	2.52	0.57
22:h:26:LYS:O	22:h:27:PRO:C	2.47	0.57
13:T:26:LYS:HE3	13:T:28:LEU:HD23	1.86	0.57
24:A:1269:U:O2	24:A:1435:C:N3	2.37	0.57
25:0:1:MET:N	25:0:97:ILE:O	2.36	0.57
2:H:11:ARG:NH1	2:H:21:ASP:O	2.32	0.57
12:S:112:GLN:NE2	27:2:395:LYS:O	2.37	0.57
13:T:34:LYS:NZ	13:T:35:PRO:O	2.37	0.57
15:W:112:GLN:O	15:W:128:GLN:NE2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:117:ASP:OD2	15:W:120:ARG:NH1	2.38	0.57
19:c:76:GLY:HA2	19:c:79:ARG:HH22	1.68	0.57
24:A:1269:U:O2	24:A:1434:G:O6	2.21	0.57
11:R:146:ARG:NH2	24:A:1782:G:OP2	2.37	0.57
24:A:974:G:N1	24:A:1021:A:O2'	2.35	0.57
6:L:163:GLN:HE22	6:L:170:TYR:HD1	1.52	0.56
3:I:86:MET:HE1	24:A:1162:G:H5''	1.88	0.56
9:P:39:MET:HB3	30:5:357:LYS:HZ2	1.70	0.56
24:A:1437:C:H1'	27:2:789:GLN:HE21	1.69	0.56
27:2:125:VAL:HG22	27:2:140:ILE:HG12	1.87	0.56
24:A:702:A:N6	24:A:731:G:C2	2.73	0.56
32:7:865:PRO:HB3	32:7:909:ILE:HD11	1.87	0.56
3:I:133:SER:HA	3:I:146:ALA:HA	1.88	0.56
19:c:48:LEU:HB3	19:c:53:THR:HG21	1.88	0.56
32:7:325:LEU:HD21	32:7:373:VAL:HG22	1.87	0.56
4:J:22:ARG:HG2	4:J:25:ARG:HH21	1.71	0.56
24:A:1795:U:H3	33:8:419:GLU:HB3	1.71	0.56
7:M:51:ARG:NH1	7:M:95:LEU:O	2.39	0.56
13:T:4:VAL:HG23	13:T:24:GLN:HE21	1.71	0.56
28:3:106:VAL:HG23	28:3:111:LEU:N	2.21	0.55
30:5:402:MET:HA	30:5:408:VAL:HG22	1.88	0.55
2:H:108:ARG:NH1	24:A:787:A:OP1	2.38	0.55
6:L:87:ASN:HB3	6:L:90:LEU:HG	1.87	0.55
29:4:422:ARG:NH1	29:4:452:GLU:OE2	2.39	0.55
24:A:1198:G:O6	24:A:1591:U:O4	2.24	0.55
24:A:1198:G:C6	24:A:1591:U:O4	2.59	0.55
32:7:82:ARG:NH1	32:7:120:GLN:OE1	2.38	0.55
10:Q:7:LYS:HE3	24:A:937:A:H4'	1.89	0.55
27:2:260:ILE:HD12	27:2:275:VAL:HB	1.88	0.55
32:7:161:ARG:NH1	32:7:223:THR:OG1	2.40	0.55
32:7:248:ARG:HG3	32:7:296:GLN:HE22	1.72	0.55
1:E:83:LYS:NZ	1:E:105:PHE:O	2.39	0.55
24:A:1157:A:O2'	24:A:1616:C:N3	2.39	0.55
24:A:1168:A:H2'	24:A:1169:G:C8	2.41	0.55
32:7:142:LEU:HG	32:7:220:LEU:HD11	1.89	0.55
32:7:394:LEU:O	32:7:397:PHE:HB2	2.05	0.55
32:7:605:LEU:HD22	32:7:645:ILE:HG21	1.87	0.55
2:H:128:ARG:HH11	24:A:292:A:H5''	1.72	0.55
2:H:151:ASP:OD2	4:J:218:ARG:NH1	2.37	0.55
15:W:105:MET:SD	15:W:123:ARG:NH1	2.79	0.55
24:A:184:G:C6	24:A:192:A:N6	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1041:A:H2	33:8:418:ARG:HA	1.72	0.55
27:2:266:GLY:O	27:2:580:ARG:NH1	2.36	0.55
32:7:325:LEU:HD22	32:7:376:LYS:HD2	1.88	0.55
13:T:114:ARG:O	13:T:114:ARG:NH1	2.40	0.55
21:f:16:VAL:HG12	21:f:29:VAL:HG12	1.89	0.55
24:A:1467:A:N6	24:A:1534:U:C2	2.75	0.55
9:P:65:ASN:O	9:P:74:LYS:NZ	2.38	0.54
12:S:69:ARG:NH1	30:5:425:GLU:O	2.32	0.54
24:A:1041:A:C2	33:8:421:HIS:HB2	2.41	0.54
24:A:1265:G:O6	24:A:1438:U:O4	2.25	0.54
27:2:364:THR:HB	27:2:366:LYS:HE3	1.89	0.54
29:4:230:TRP:HA	29:4:233:ILE:HD12	1.89	0.54
31:6:515:ASN:C	31:6:515:ASN:HD22	2.15	0.54
4:J:78:SER:OG	4:J:79:GLU:N	2.40	0.54
6:L:56:ARG:NH1	6:L:178:GLY:O	2.37	0.54
13:T:42:GLU:HA	13:T:45:ARG:HG2	1.89	0.54
28:3:158:LEU:HA	28:3:164:LEU:HD12	1.90	0.54
32:7:49:LEU:HD22	32:7:69:LEU:HD13	1.88	0.54
4:J:134:GLY:HA3	4:J:158:ILE:HD12	1.89	0.54
8:O:30:THR:O	8:O:37:ARG:NH2	2.40	0.54
27:2:201:GLN:HA	27:2:204:ARG:HE	1.72	0.54
7:M:27:LYS:HB2	22:h:44:PHE:HE1	1.72	0.54
24:A:565:G:H22	24:A:571:G:H1	1.55	0.54
24:A:1584:G:N2	24:A:1604:U:O2	2.30	0.54
28:3:106:VAL:HG23	28:3:110:LYS:HA	1.90	0.54
28:3:106:VAL:CG2	28:3:110:LYS:HA	2.37	0.54
3:I:34:SER:OG	3:I:36:ASP:OD1	2.23	0.54
3:I:111:MET:HA	19:c:47:ARG:HE	1.72	0.54
4:J:26:HIS:O	4:J:30:LYS:NZ	2.40	0.54
7:M:90:LYS:HB2	7:M:93:TYR:HD2	1.71	0.54
9:P:114:LYS:NZ	9:P:115:VAL:O	2.40	0.54
27:2:351:ASP:O	27:2:354:GLU:HB2	2.08	0.54
22:h:25:GLU:HG2	24:A:537:G:H21	1.71	0.54
24:A:355:U:O2'	24:A:357:A:OP1	2.26	0.54
27:2:652:TYR:HB2	27:2:720:ILE:HG22	1.88	0.54
12:S:72:LYS:HG3	30:5:430:ARG:HE	1.72	0.54
17:a:17:ASN:OD1	17:a:20:ARG:NH2	2.41	0.54
24:A:1245:C:H2'	24:A:1246:U:H5	1.73	0.54
15:W:22:PHE:O	15:W:26:GLN:HB2	2.08	0.54
22:h:28:LYS:O	22:h:29:THR:C	2.50	0.54
23:i:138:ARG:NH2	24:A:1247:U:O2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:225:PRO:HB3	29:4:261:VAL:HG11	1.88	0.54
11:R:50:GLU:HA	24:A:893:G:H1'	1.89	0.53
24:A:708:U:O2	24:A:723:G:O6	2.26	0.53
24:A:798:U:H2'	24:A:799:G:H8	1.72	0.53
27:2:236:ASN:OD1	27:2:239:ARG:NH2	2.36	0.53
28:3:106:VAL:HG23	28:3:111:LEU:H	1.73	0.53
29:4:234:ILE:HG21	29:4:269:ILE:HD11	1.90	0.53
13:T:103:ASN:HA	13:T:106:LYS:HG2	1.90	0.53
21:f:17:LEU:O	21:f:28:GLN:NE2	2.41	0.53
25:0:118:ALA:HB3	26:1:101:LEU:HG	1.89	0.53
27:2:264:LYS:HB2	27:2:274:ILE:HB	1.89	0.53
27:2:508:GLU:HA	27:2:511:ALA:HB2	1.89	0.53
27:2:636:ASN:OD1	27:2:806:ARG:NH2	2.42	0.53
5:K:7:ASN:HA	5:K:16:ARG:HH12	1.73	0.53
32:7:699:LEU:HD13	32:7:703:SER:HB3	1.89	0.53
4:J:7:HIS:O	4:J:11:GLY:N	2.41	0.53
4:J:155:LYS:NZ	24:A:77:A:OP2	2.38	0.53
9:P:94:GLY:HA2	9:P:97:LEU:HB3	1.90	0.53
24:A:1227:A:H2	24:A:1252:G:H21	1.56	0.53
28:3:109:CYS:SG	28:3:111:LEU:HB2	2.49	0.53
3:I:136:ILE:HD11	21:f:22:SER:H	1.74	0.53
10:Q:45:ALA:HB1	10:Q:49:GLN:HG3	1.90	0.53
14:V:16:ARG:HH22	14:V:19:ASN:HA	1.74	0.53
17:a:69:ARG:O	17:a:69:ARG:NE	2.41	0.53
24:A:213:A:H5''	24:A:828:U:H1'	1.91	0.53
27:2:325:GLN:NE2	27:2:326:ILE:O	2.42	0.53
32:7:888:LYS:NZ	32:7:892:THR:OG1	2.42	0.53
2:H:19:LEU:HD22	24:A:786:A:H2'	1.91	0.53
4:J:5:ILE:HD13	4:J:111:LEU:HB2	1.90	0.53
3:I:203:GLU:HA	3:I:206:ARG:HG2	1.91	0.53
12:S:131:TYR:O	27:2:404:TRP:NE1	2.31	0.53
24:A:443:A:N6	24:A:458:G:H21	2.07	0.53
24:A:1160:A:N3	24:A:1609:U:O2'	2.35	0.53
27:2:258:MET:HG2	27:2:279:VAL:HA	1.91	0.53
21:f:32:GLU:HG3	21:f:34:MET:H	1.74	0.53
24:A:1795:U:N3	33:8:419:GLU:HB3	2.24	0.53
3:I:33:TRP:HE1	3:I:109:HIS:CG	2.27	0.52
3:I:154:ARG:HH22	21:f:55:LEU:HB2	1.75	0.52
14:V:53:ASP:HB3	14:V:56:LYS:HE2	1.91	0.52
21:f:26:VAL:HG22	21:f:46:LYS:HB3	1.91	0.52
24:A:1148:A:O2'	28:3:249:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:57:VAL:HG22	5:K:62:LYS:HA	1.92	0.52
20:e:19:HIS:HB3	20:e:22:LYS:HG3	1.91	0.52
27:2:114:SER:HB2	27:2:231:ARG:HG3	1.91	0.52
32:7:363:LEU:HD12	32:7:410:ARG:HG2	1.90	0.52
32:7:557:LEU:O	32:7:564:ARG:NE	2.42	0.52
7:M:107:LEU:HB2	7:M:144:PHE:HB3	1.91	0.52
8:O:31:ARG:NH1	24:A:209:G:OP2	2.42	0.52
14:V:86:LEU:HD22	14:V:99:GLN:HB2	1.91	0.52
24:A:140:G:H2'	24:A:141:G:C8	2.45	0.52
5:K:136:LEU:HD21	5:K:162:VAL:HG21	1.92	0.52
9:P:40:HIS:ND1	9:P:126:TRP:O	2.42	0.52
12:S:51:ARG:HH12	24:A:1547:U:H3'	1.74	0.52
5:K:66:ILE:HD11	5:K:98:ILE:HG12	1.90	0.52
9:P:97:LEU:HA	9:P:100:TRP:HB2	1.92	0.52
10:Q:54:LEU:HD13	10:Q:60:ILE:HD11	1.92	0.52
24:A:1462:G:O2'	24:A:1598:C:OP1	2.26	0.52
24:A:844:G:H2'	24:A:845:A:H8	1.74	0.52
26:1:168:ASP:OD2	26:1:172:GLN:NE2	2.30	0.52
27:2:263:VAL:HG12	27:2:275:VAL:HG12	1.92	0.52
30:5:347:GLN:HA	30:5:350:ILE:HD12	1.92	0.52
3:I:44:SER:HA	21:f:54:ILE:HG23	1.90	0.52
3:I:108:ILE:HG13	3:I:116:PRO:HB3	1.91	0.52
3:I:149:VAL:O	3:I:154:ARG:NH1	2.43	0.52
4:J:150:ASP:OD1	4:J:150:ASP:N	2.43	0.52
24:A:1581:U:H2'	24:A:1582:A:H8	1.75	0.52
3:I:80:LEU:HD13	3:I:159:ILE:HG23	1.92	0.51
11:R:29:VAL:HG21	11:R:31:ARG:HH21	1.75	0.51
24:A:834:U:H2'	24:A:835:G:H8	1.75	0.51
24:A:1520:A:H2'	24:A:1521:A:C8	2.44	0.51
27:2:259:LEU:O	27:2:277:GLY:HA3	2.09	0.51
5:K:50:VAL:HG23	5:K:69:PRO:HD3	1.91	0.51
15:W:128:GLN:HA	15:W:131:ARG:HG2	1.92	0.51
23:i:119:ARG:NH1	23:i:121:CYS:SG	2.82	0.51
24:A:403:U:H2'	24:A:404:A:C8	2.45	0.51
24:A:1168:A:H2'	24:A:1169:G:H8	1.75	0.51
2:H:128:ARG:NH1	24:A:292:A:H5''	2.25	0.51
3:I:140:GLY:O	26:1:130:ASN:ND2	2.43	0.51
5:K:34:GLU:HB3	5:K:44:LEU:HD11	1.92	0.51
11:R:105:LYS:HD3	11:R:135:PRO:HD2	1.92	0.51
4:J:48:TYR:HE1	4:J:117:GLY:H	1.59	0.51
13:T:78:VAL:HA	13:T:81:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:f:26:VAL:HA	21:f:46:LYS:HA	1.91	0.51
24:A:824:U:O4	24:A:844:G:O6	2.27	0.51
24:A:1500:G:N3	24:A:1559:C:O2'	2.42	0.51
28:3:116:ASN:ND2	28:3:118:LYS:HB2	2.25	0.51
6:L:125:ARG:HE	6:L:132:VAL:HA	1.74	0.51
28:3:105:LEU:O	28:3:109:CYS:N	2.41	0.51
32:7:183:GLU:HA	32:7:186:MET:HE2	1.93	0.51
3:I:187:ASN:HB3	3:I:195:SER:HB2	1.92	0.51
13:T:6:ALA:HA	13:T:22:CYS:O	2.10	0.51
24:A:563:C:H2'	24:A:564:A:H8	1.75	0.51
24:A:697:G:H2'	24:A:698:G:H8	1.76	0.51
27:2:772:LEU:HD12	27:2:779:LYS:HD3	1.93	0.51
24:A:985:G:N7	31:6:484:LYS:NZ	2.59	0.51
25:0:26:HIS:ND1	25:0:62:GLU:OE2	2.43	0.51
27:2:798:LYS:NZ	27:2:799:ARG:O	2.44	0.51
22:h:27:PRO:HD2	24:A:502:A:C5	2.46	0.51
24:A:574:G:N7	24:A:575:U:O2'	2.42	0.51
26:1:65:LEU:HB3	26:1:76:HIS:HB2	1.92	0.51
27:2:188:LEU:O	27:2:222:GLN:NE2	2.44	0.51
12:S:89:ARG:NH2	12:S:128:SER:O	2.44	0.51
32:7:535:CYS:HB3	32:7:574:LEU:HG	1.92	0.51
6:L:142:VAL:O	6:L:146:GLN:HG3	2.11	0.50
9:P:39:MET:O	30:5:354:ARG:NH1	2.45	0.50
24:A:893:G:H1	24:A:915:U:H3	1.58	0.50
24:A:1272:A:N1	24:A:1431:G:C6	2.79	0.50
26:1:107:GLN:HA	26:1:144:ARG:HH12	1.77	0.50
33:8:427:ARG:C	33:8:429:LYS:H	2.19	0.50
24:A:363:G:OP1	24:A:757:U:O2'	2.29	0.50
24:A:487:U:C2	24:A:495:G:N1	2.79	0.50
3:I:85:MET:HE2	3:I:94:LYS:HD3	1.93	0.50
21:f:43:ARG:NH1	21:f:63:GLU:O	2.44	0.50
11:R:112:GLN:NE2	28:3:166:ILE:O	2.42	0.50
18:b:112:LYS:NZ	24:A:456:G:OP1	2.40	0.50
27:2:138:GLN:NE2	27:2:261:GLU:OE2	2.42	0.50
27:2:299:GLN:NE2	27:2:335:ASP:O	2.44	0.50
24:A:1198:G:C6	24:A:1591:U:C4	2.99	0.50
24:A:1482:G:H21	24:A:1588:A:H4'	1.77	0.50
32:7:883:ARG:NH1	32:7:923:SER:OG	2.44	0.50
24:A:482:A:H5''	29:4:438:LEU:HD21	1.94	0.50
28:3:116:ASN:HD21	28:3:119:GLU:HG2	1.76	0.50
31:6:495:LYS:HG2	31:6:499:ARG:HE	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:137:GLN:NE2	18:b:67:TYR:O	2.44	0.50
11:R:145:ARG:HD2	28:3:177:THR:HG21	1.93	0.50
19:c:64:LEU:HA	19:c:67:LYS:HZ3	1.76	0.50
32:7:525:GLN:NE2	32:7:562:GLU:OE1	2.42	0.50
20:e:67:THR:OG1	20:e:70:LYS:O	2.29	0.50
24:A:1041:A:C2	33:8:418:ARG:HA	2.47	0.50
6:L:89:GLU:OE1	6:L:92:ARG:NH1	2.45	0.49
7:M:23:ASP:HB2	22:h:44:PHE:HZ	1.77	0.49
15:W:134:ASP:O	15:W:138:GLN:NE2	2.45	0.49
25:0:61:THR:OG1	25:0:67:GLN:NE2	2.40	0.49
32:7:459:LEU:HB3	32:7:461:LEU:HG	1.94	0.49
4:J:22:ARG:HA	4:J:25:ARG:HG2	1.94	0.49
14:V:38:VAL:HG23	14:V:42:TYR:HB3	1.94	0.49
24:A:1157:A:H1'	24:A:1616:C:H42	1.76	0.49
5:K:88:GLU:OE2	5:K:175:ARG:NH1	2.41	0.49
15:W:21:ALA:HA	15:W:24:LYS:HG2	1.95	0.49
17:a:62:LYS:NZ	24:A:1134:A:OP1	2.45	0.49
9:P:25:SER:OG	9:P:28:ASP:OD2	2.30	0.49
24:A:1489:C:O5'	30:5:405:LYS:NZ	2.43	0.49
27:2:689:ASP:N	27:2:689:ASP:OD1	2.43	0.49
29:4:331:ILE:O	29:4:373:LYS:NZ	2.40	0.49
12:S:69:ARG:NH2	30:5:425:GLU:OE1	2.46	0.49
18:b:57:GLN:NE2	18:b:80:ASP:O	2.45	0.49
26:1:51:ILE:HG12	26:1:118:ALA:HB3	1.93	0.49
30:5:388:ASP:OD1	30:5:388:ASP:N	2.45	0.49
3:I:92:GLY:O	24:A:1605:U:O2'	2.26	0.49
12:S:59:ARG:HG3	12:S:62:LEU:HD21	1.93	0.49
16:Z:83:LEU:HG	16:Z:122:ALA:HB2	1.94	0.49
24:A:1233:A:N6	24:A:1247:U:H3	2.10	0.49
15:W:70:THR:OG1	15:W:120:ARG:NH2	2.44	0.49
26:1:40:LEU:HA	26:1:43:LEU:HD12	1.94	0.49
28:3:218:ILE:HG22	28:3:225:ILE:HG12	1.94	0.49
3:I:133:SER:HB2	3:I:144:ARG:HB3	1.94	0.49
24:A:1584:G:O6	24:A:1604:U:O4	2.31	0.49
26:1:163:PHE:HE1	26:1:201:LEU:HD23	1.77	0.49
3:I:133:SER:OG	3:I:144:ARG:NH1	2.40	0.49
18:b:106:ALA:O	18:b:111:ARG:NH1	2.45	0.49
22:h:31:LYS:HE2	24:A:542:A:H2'	1.95	0.49
24:A:1480:G:H2'	24:A:1481:C:C6	2.48	0.49
27:2:772:LEU:H	27:2:778:PHE:HA	1.77	0.49
29:4:290:ASN:HA	29:4:293:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:f:10:PHE:HB3	21:f:54:ILE:HD11	1.94	0.49
24:A:707:A:N1	24:A:724:U:O2'	2.45	0.49
24:A:937:A:H2'	24:A:938:A:C8	2.48	0.49
14:V:26:GLN:HE21	14:V:31:ALA:HA	1.78	0.48
32:7:114:GLU:HA	32:7:163:ILE:HD11	1.95	0.48
5:K:69:PRO:O	5:K:73:LEU:N	2.45	0.48
11:R:145:ARG:HH12	24:A:1784:G:H5''	1.78	0.48
24:A:1200:A:C5	24:A:1551:A:C6	3.02	0.48
2:H:19:LEU:HD11	2:H:108:ARG:HD2	1.94	0.48
3:I:167:ARG:NE	24:A:1469:U:O4	2.40	0.48
6:L:8:ARG:HA	6:L:8:ARG:HD3	1.51	0.48
13:T:93:TYR:HA	13:T:97:VAL:HG12	1.95	0.48
16:Z:55:ASN:HD21	16:Z:60:LYS:HG3	1.79	0.48
20:e:20:LYS:HG3	20:e:21:LEU:HD12	1.94	0.48
29:4:335:VAL:HG23	29:4:336:LEU:HD22	1.95	0.48
8:O:104:ARG:HB2	17:a:9:LEU:O	2.13	0.48
26:1:66:SER:OG	26:1:97:GLU:OE2	2.30	0.48
3:I:75:PRO:HB2	3:I:78:GLU:HG3	1.94	0.48
5:K:34:GLU:OE1	5:K:45:ARG:NH2	2.46	0.48
13:T:59:LYS:HD3	13:T:105:LEU:HD11	1.96	0.48
24:A:11:A:OP1	26:1:259:GLN:NE2	2.46	0.48
24:A:231:G:H2'	24:A:232:G:C8	2.48	0.48
24:A:1161:G:H2'	24:A:1162:G:C8	2.48	0.48
32:7:801:LYS:HD2	32:7:870:ALA:HB2	1.94	0.48
4:J:49:ILE:HG13	4:J:114:VAL:HB	1.96	0.48
14:V:68:ARG:O	14:V:72:ILE:HG12	2.13	0.48
19:c:84:HIS:NE2	24:A:1525:C:OP1	2.40	0.48
23:i:100:LEU:HD21	24:A:1225:G:H4'	1.95	0.48
24:A:561:G:N2	24:A:578:U:OP1	2.45	0.48
24:A:735:C:H2'	24:A:736:A:H8	1.78	0.48
24:A:1145:C:H2'	24:A:1147:G:C8	2.49	0.48
3:I:29:LEU:HB2	3:I:34:SER:HA	1.96	0.48
14:V:106:ASP:HB3	14:V:110:ARG:HH12	1.78	0.48
24:A:510:U:H2'	24:A:511:G:C8	2.48	0.48
24:A:1796:A:H61	28:3:96:LYS:HG2	1.79	0.48
27:2:681:MET:HG3	27:2:706:VAL:HG21	1.96	0.48
2:H:146:THR:HG21	24:A:122:G:H21	1.78	0.48
3:I:148:ASP:OD1	3:I:149:VAL:N	2.47	0.48
24:A:1498:G:N2	24:A:1501:A:OP2	2.45	0.48
1:E:24:PHE:HD2	11:R:87:LEU:HD11	1.78	0.47
10:Q:70:LYS:NZ	24:A:961:A:N7	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1517:G:O2'	24:A:1519:U:OP2	2.31	0.47
32:7:461:LEU:HD12	32:7:497:LEU:HD21	1.96	0.47
15:W:6:THR:HG23	15:W:8:ARG:H	1.78	0.47
24:A:768:A:H2'	24:A:769:A:C8	2.49	0.47
24:A:1261:G:H2'	24:A:1262:G:H8	1.79	0.47
26:1:159:ALA:HB3	26:1:203:LEU:HB2	1.96	0.47
5:K:65:VAL:HG12	5:K:97:LEU:HD12	1.97	0.47
9:P:107:ASP:OD1	9:P:107:ASP:N	2.47	0.47
14:V:36:LYS:HB2	14:V:102:ALA:HA	1.96	0.47
24:A:1216:A:H61	24:A:1263:U:H3	1.62	0.47
24:A:1468:C:C2	24:A:1530:G:C2	3.00	0.47
24:A:1580:G:O2'	24:A:1606:G:O6	2.27	0.47
29:4:383:ASP:HA	29:4:386:VAL:HG22	1.97	0.47
2:H:54:TYR:O	18:b:18:ASN:ND2	2.46	0.47
13:T:16:ALA:HB2	13:T:72:GLY:HA3	1.96	0.47
17:a:58:GLY:HA2	17:a:70:LYS:HA	1.96	0.47
26:1:32:GLN:HA	26:1:35:MET:SD	2.54	0.47
32:7:408:ARG:HH22	32:7:484:ASN:HB3	1.79	0.47
3:I:95:LEU:HA	3:I:98:VAL:HG22	1.96	0.47
3:I:198:ILE:HA	3:I:201:LYS:HZ3	1.80	0.47
22:h:27:PRO:O	22:h:28:LYS:C	2.57	0.47
24:A:884:U:H2'	24:A:885:A:C8	2.50	0.47
27:2:488:ALA:HB3	27:2:688:ASN:HB3	1.97	0.47
32:7:774:ILE:O	32:7:778:ILE:HG12	2.15	0.47
10:Q:145:THR:O	10:Q:148:THR:OG1	2.31	0.47
17:a:112:LYS:NZ	24:A:1134:A:N7	2.58	0.47
24:A:574:G:H21	24:A:577:A:H5''	1.79	0.47
24:A:1448:U:H2'	24:A:1449:G:C8	2.49	0.47
32:7:307:ARG:HA	32:7:310:ASP:HB2	1.96	0.47
6:L:125:ARG:HB2	6:L:131:GLN:HB2	1.97	0.47
14:V:15:LEU:HD21	14:V:59:GLY:HA2	1.97	0.47
14:V:114:GLU:HA	14:V:117:LYS:HG2	1.97	0.47
24:A:1054:U:H2'	24:A:1055:A:C8	2.50	0.47
29:4:428:ASP:N	29:4:428:ASP:OD1	2.48	0.47
1:E:33:LYS:HE2	1:E:41:ARG:HG3	1.96	0.47
6:L:182:ARG:NH1	24:A:255:C:O2	2.47	0.47
13:T:40:ALA:HB1	13:T:44:LEU:HB3	1.95	0.47
24:A:697:G:H2'	24:A:698:G:C8	2.50	0.47
6:L:37:ARG:HD2	6:L:59:ARG:HH12	1.79	0.47
8:O:130:VAL:HG12	8:O:144:VAL:HA	1.96	0.47
19:c:31:LEU:HD21	19:c:36:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:503:LYS:HA	27:2:503:LYS:HD3	1.77	0.47
32:7:69:LEU:O	32:7:73:THR:OG1	2.29	0.47
13:T:40:ALA:O	13:T:45:ARG:NH1	2.46	0.47
16:Z:107:SER:HB3	24:A:800:G:H21	1.79	0.47
24:A:184:G:N1	24:A:192:A:C5	2.83	0.47
24:A:904:A:H2'	24:A:905:A:C8	2.50	0.47
27:2:191:VAL:HG12	27:2:226:TYR:HB2	1.95	0.47
27:2:258:MET:HE3	27:2:591:LEU:HD13	1.96	0.47
29:4:296:LEU:HG	29:4:331:ILE:HG21	1.98	0.47
15:W:57:ARG:HH21	24:A:1475:A:P	2.38	0.46
24:A:1581:U:H2'	24:A:1582:A:C8	2.49	0.46
27:2:90:PRO:HA	27:2:136:LYS:O	2.15	0.46
1:E:137:LEU:HG	1:E:215:VAL:HG22	1.97	0.46
10:Q:54:LEU:HD23	10:Q:58:HIS:HE1	1.80	0.46
18:b:79:TYR:OH	18:b:89:GLU:OE1	2.32	0.46
32:7:527:ILE:HA	32:7:530:ILE:HD12	1.98	0.46
33:8:832:TRP:O	33:8:837:VAL:HG21	2.14	0.46
3:I:183:GLU:HA	3:I:186:ILE:HG12	1.96	0.46
4:J:176:PRO:HA	24:A:66:U:H5'	1.97	0.46
15:W:130:GLN:HA	15:W:133:LEU:HG	1.97	0.46
23:i:118:ARG:NH2	24:A:1249:C:OP2	2.48	0.46
3:I:98:VAL:HA	3:I:101:VAL:HG12	1.96	0.46
4:J:67:VAL:HG23	4:J:99:GLY:HA2	1.97	0.46
18:b:36:PRO:O	24:A:529:U:O2'	2.25	0.46
24:A:834:U:H2'	24:A:835:G:C8	2.50	0.46
24:A:922:A:H2'	24:A:923:G:C8	2.50	0.46
24:A:552:A:H2'	24:A:553:A:C8	2.51	0.46
24:A:844:G:H2'	24:A:845:A:C8	2.50	0.46
24:A:1172:U:H2'	24:A:1173:G:H8	1.80	0.46
24:A:1261:G:H2'	24:A:1262:G:C8	2.50	0.46
32:7:386:THR:O	32:7:393:TRP:NE1	2.44	0.46
8:O:104:ARG:NH1	17:a:7:ARG:O	2.48	0.46
15:W:13:HIS:HA	15:W:16:VAL:HG22	1.97	0.46
17:a:109:ARG:NH1	17:a:113:ALA:O	2.49	0.46
24:A:724:U:H3'	24:A:725:G:H5''	1.97	0.46
27:2:96:ILE:HD11	27:2:161:LEU:HD12	1.98	0.46
32:7:107:ARG:HD2	32:7:151:LYS:HB3	1.98	0.46
32:7:454:LEU:HD12	32:7:489:HIS:HE1	1.79	0.46
9:P:70:GLU:HB3	9:P:73:TYR:HB3	1.98	0.46
22:h:27:PRO:O	22:h:29:THR:N	2.48	0.46
27:2:200:PRO:HD2	27:2:203:GLN:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:98:ASN:O	28:3:99:TRP:C	2.59	0.46
29:4:442:HIS:HD2	29:4:444:LYS:H	1.62	0.46
30:5:400:TYR:HE1	30:5:410:LYS:HD3	1.80	0.46
1:E:168:MET:HG3	1:E:197:ILE:HD13	1.96	0.46
3:I:151:PRO:HA	3:I:154:ARG:HB2	1.98	0.46
4:J:15:LEU:HD22	24:A:150:G:H4'	1.96	0.46
4:J:159:ARG:HD2	4:J:175:ALA:HB2	1.98	0.46
24:A:1161:G:H2'	24:A:1162:G:H8	1.81	0.46
25:0:112:ALA:HB1	25:0:114:ARG:HH12	1.81	0.46
32:7:438:ASP:HB3	32:7:477:LEU:HD11	1.98	0.46
32:7:444:ALA:HB1	32:7:448:MET:HE1	1.98	0.46
3:I:163:THR:HB	3:I:167:ARG:HH22	1.81	0.46
4:J:24:LEU:O	4:J:27:PHE:N	2.48	0.46
6:L:123:ARG:HD3	6:L:125:ARG:HD3	1.98	0.46
14:V:116:LEU:HD21	14:V:123:ARG:HG3	1.98	0.46
24:A:1790:A:N3	28:3:193:LYS:HG2	2.31	0.46
26:1:141:ARG:HG2	26:1:144:ARG:HH21	1.79	0.46
2:H:211:LYS:HG3	2:H:217:THR:HG22	1.98	0.46
6:L:79:ILE:N	6:L:103:GLN:O	2.48	0.46
16:Z:18:GLU:HG2	16:Z:69:LEU:HB3	1.97	0.46
24:A:589:A:O2'	24:A:593:C:OP1	2.33	0.46
32:7:200:ARG:NH2	32:7:209:ALA:O	2.47	0.46
11:R:44:THR:OG1	11:R:50:GLU:O	2.23	0.45
12:S:41:LEU:HA	12:S:44:VAL:HG12	1.98	0.45
24:A:485:G:O6	24:A:496:U:O4	2.34	0.45
24:A:835:G:H2'	24:A:836:G:C8	2.51	0.45
24:A:1148:A:H2'	24:A:1149:A:C8	2.51	0.45
1:E:106:THR:OG1	1:E:108:ASP:OD1	2.32	0.45
4:J:197:LYS:HE2	4:J:197:LYS:HB2	1.82	0.45
5:K:81:GLN:HB3	5:K:85:ARG:HH22	1.82	0.45
9:P:106:LEU:HD23	9:P:106:LEU:HA	1.81	0.45
17:a:109:ARG:HH11	17:a:114:LYS:HA	1.80	0.45
25:0:2:LYS:HG2	25:0:96:GLN:HG2	1.97	0.45
26:1:81:MET:HG3	26:1:101:LEU:HB2	1.97	0.45
26:1:254:ILE:HD11	26:1:270:THR:HG21	1.98	0.45
27:2:748:GLU:HA	27:2:751:GLU:HG2	1.98	0.45
5:K:91:PHE:HB3	5:K:94:ARG:HG3	1.97	0.45
19:c:61:ASN:HB3	19:c:64:LEU:HD23	1.98	0.45
24:A:1210:G:O6	24:A:1447:C:N4	2.48	0.45
24:A:1229:U:H2'	24:A:1230:G:C8	2.52	0.45
27:2:618:ILE:HD11	27:2:681:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:226:THR:O	30:5:386:ARG:NH1	2.49	0.45
2:H:55:ALA:HB2	2:H:64:ILE:HD12	1.97	0.45
22:h:28:LYS:HE3	22:h:28:LYS:HB3	1.66	0.45
32:7:309:TYR:HD1	32:7:320:THR:HG23	1.81	0.45
32:7:387:ILE:O	32:7:390:GLN:HB2	2.15	0.45
32:7:802:GLU:O	32:7:808:ARG:NH1	2.43	0.45
4:J:92:ARG:O	24:A:402:C:O2'	2.26	0.45
10:Q:103:GLU:O	10:Q:106:ARG:NH1	2.48	0.45
24:A:1771:U:OP1	31:6:505:LYS:NZ	2.45	0.45
27:2:353:ASP:O	27:2:356:MET:HB3	2.17	0.45
27:2:366:LYS:NZ	27:2:379:GLU:OE2	2.49	0.45
33:8:431:ILE:HG23	33:8:439:TRP:CH2	2.36	0.45
15:W:26:GLN:HE22	15:W:28:LYS:HE3	1.82	0.45
26:1:136:THR:HB	26:1:141:ARG:HD2	1.99	0.45
28:3:165:TYR:O	28:3:219:LEU:HA	2.17	0.45
32:7:118:LEU:HD22	32:7:166:ASN:HD21	1.82	0.45
32:7:704:PHE:HE2	32:7:739:VAL:HG13	1.82	0.45
32:7:984:THR:HG22	32:7:988:LYS:HE3	1.98	0.45
2:H:100:ARG:HD2	2:H:102:ILE:HD11	1.99	0.45
3:I:92:GLY:HA2	3:I:94:LYS:HZ3	1.81	0.45
9:P:56:ARG:HH22	23:i:126:CYS:HA	1.82	0.45
13:T:49:TYR:HB3	13:T:53:LEU:HD13	1.97	0.45
21:f:15:ARG:HE	21:f:17:LEU:HD11	1.82	0.45
24:A:1005:C:H2'	24:A:1006:G:H8	1.82	0.45
24:A:1448:U:H2'	24:A:1449:G:H8	1.81	0.45
24:A:1479:A:N3	24:A:1603:G:O2'	2.36	0.45
27:2:783:ASP:OD1	27:2:783:ASP:N	2.49	0.45
24:A:29:U:H2'	24:A:30:G:C8	2.51	0.45
27:2:355:MET:O	27:2:358:ALA:HB3	2.16	0.45
28:3:175:ARG:HE	28:3:178:LEU:HD13	1.81	0.45
32:7:962:MET:HB3	32:7:971:VAL:HG21	1.98	0.45
6:L:76:THR:HG21	6:L:104:ILE:HD12	1.99	0.45
14:V:88:ARG:HH21	14:V:108:LYS:HD2	1.82	0.45
14:V:117:LYS:HD2	14:V:128:TYR:CE2	2.52	0.45
33:8:826:LEU:HD23	33:8:827:PRO:HD2	1.98	0.45
4:J:52:ILE:HA	4:J:111:LEU:HD23	1.99	0.45
15:W:31:VAL:HG12	15:W:33:GLY:H	1.80	0.45
17:a:61:ALA:HA	17:a:118:PRO:HD3	1.99	0.45
18:b:121:LEU:HD22	18:b:128:LYS:HE3	1.98	0.45
20:e:18:LYS:O	20:e:29:ARG:NH2	2.46	0.45
24:A:220:A:N6	24:A:835:G:O6	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1153:C:H2'	24:A:1154:A:H8	1.82	0.45
24:A:1621:C:H2'	24:A:1622:U:C6	2.52	0.45
32:7:719:ASP:OD1	32:7:719:ASP:N	2.50	0.45
6:L:16:ALA:HB2	24:A:351:C:H5''	1.99	0.44
19:c:43:VAL:O	19:c:92:ARG:NH1	2.50	0.44
27:2:68:ARG:CZ	27:2:72:LYS:HD2	2.48	0.44
27:2:268:SER:OG	27:2:270:ASP:OD1	2.28	0.44
27:2:303:ILE:HG12	27:2:570:VAL:HG22	1.98	0.44
29:4:404:LYS:HD3	29:4:440:HIS:HE1	1.81	0.44
32:7:561:PRO:HA	32:7:564:ARG:HB2	1.99	0.44
32:7:623:VAL:O	32:7:627:THR:OG1	2.25	0.44
32:7:900:LEU:O	32:7:903:THR:OG1	2.35	0.44
1:E:66:PHE:CE2	11:R:47:SER:HB3	2.52	0.44
27:2:259:LEU:O	27:2:277:GLY:CA	2.65	0.44
28:3:96:LYS:HA	33:8:829:TRP:HH2	1.82	0.44
32:7:572:ARG:O	32:7:576:GLU:HB2	2.17	0.44
6:L:37:ARG:NH1	6:L:93:THR:HB	2.31	0.44
14:V:123:ARG:H	14:V:123:ARG:HG2	1.57	0.44
24:A:824:U:H2'	24:A:825:C:C6	2.52	0.44
24:A:1245:C:H2'	24:A:1246:U:C5	2.53	0.44
24:A:1468:C:O2	24:A:1530:G:C2	2.69	0.44
1:E:58:ASN:HA	1:E:91:VAL:HG11	1.99	0.44
7:M:78:LEU:HD23	7:M:78:LEU:HA	1.85	0.44
7:M:128:ARG:HD2	7:M:128:ARG:HA	1.86	0.44
13:T:73:GLY:H	13:T:76:SER:HG	1.63	0.44
14:V:43:SER:HA	14:V:46:VAL:HG12	2.00	0.44
24:A:974:G:H1	24:A:1021:A:HO2'	1.57	0.44
28:3:83:ARG:NH1	28:3:137:GLN:OE1	2.51	0.44
32:7:117:LEU:HA	32:7:120:GLN:HG2	2.00	0.44
27:2:195:LEU:HG	27:2:204:ARG:HG2	2.00	0.44
29:4:232:ASP:OD1	29:4:232:ASP:N	2.50	0.44
32:7:264:MET:HA	32:7:267:GLU:HG3	1.99	0.44
3:I:200:LYS:HD3	3:I:200:LYS:HA	1.79	0.44
14:V:115:ARG:HA	14:V:118:LYS:HG2	1.99	0.44
27:2:264:LYS:HB2	27:2:274:ILE:HD12	2.00	0.44
1:E:145:ARG:HH22	1:E:152:LYS:HA	1.81	0.44
11:R:77:ALA:HB1	11:R:118:LEU:HD22	1.99	0.44
1:E:140:ILE:HB	1:E:213:ARG:HD3	1.99	0.44
6:L:110:ARG:O	6:L:114:GLU:HG2	2.18	0.44
24:A:709:G:O6	24:A:722:U:O4	2.36	0.44
24:A:1533:C:O2'	24:A:1567:C:N4	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:199:VAL:HG13	29:4:236:LEU:HD11	2.00	0.44
13:T:31:VAL:HG23	13:T:67:ILE:HB	1.98	0.44
24:A:992:G:H2'	24:A:993:A:C8	2.52	0.44
24:A:1787:G:O2'	24:A:1789:G:H5'	2.18	0.44
27:2:607:LEU:HB2	27:2:712:LEU:HD11	1.99	0.44
8:O:51:LYS:HE3	8:O:51:LYS:HB2	1.83	0.43
13:T:82:ARG:HA	13:T:85:ILE:HG12	2.00	0.43
17:a:62:LYS:HB3	17:a:64:PRO:HD2	1.98	0.43
24:A:390:C:H2'	24:A:391:C:C6	2.53	0.43
24:A:692:C:H4'	24:A:693:U:H5''	2.00	0.43
24:A:1570:G:O2'	26:1:27:ARG:NH1	2.33	0.43
28:3:116:ASN:HD22	28:3:118:LYS:HE2	1.83	0.43
32:7:629:PRO:HA	32:7:632:ARG:HD2	1.99	0.43
32:7:933:LEU:HD22	32:7:937:ILE:HD11	2.00	0.43
2:H:95:THR:HG22	18:b:19:PRO:HD2	2.00	0.43
24:A:219:C:H2'	24:A:220:A:C8	2.52	0.43
24:A:727:C:H2'	24:A:728:G:C8	2.54	0.43
24:A:1622:U:H2'	24:A:1623:U:C6	2.53	0.43
26:1:190:ASP:HB2	26:1:198:LYS:HB2	2.00	0.43
26:1:272:LYS:HB2	26:1:272:LYS:HE2	1.74	0.43
27:2:638:LEU:HD13	27:2:800:VAL:HG13	2.00	0.43
32:7:85:PHE:HD1	32:7:116:LEU:HD13	1.83	0.43
8:O:99:ILE:HD11	8:O:106:GLU:OE2	2.19	0.43
24:A:204:U:H2'	24:A:205:A:C8	2.52	0.43
24:A:1083:A:H2'	24:A:1084:A:C8	2.53	0.43
24:A:1482:G:N2	24:A:1588:A:H4'	2.33	0.43
27:2:274:ILE:HG12	27:2:571:TYR:CD1	2.53	0.43
29:4:292:LEU:HB3	29:4:327:VAL:HG11	2.00	0.43
30:5:379:SER:N	30:5:382:GLN:OE1	2.51	0.43
4:J:218:ARG:HA	4:J:218:ARG:HD3	1.84	0.43
6:L:37:ARG:HD2	6:L:59:ARG:NH1	2.33	0.43
12:S:123:TYR:OH	24:A:1552:A:OP1	2.34	0.43
22:h:40:TYR:O	22:h:41:THR:C	2.60	0.43
27:2:252:ARG:HG2	27:2:257:TRP:CD1	2.53	0.43
27:2:331:THR:HG22	27:2:332:GLU:H	1.83	0.43
6:L:83:TYR:HB2	6:L:200:LEU:HD21	2.01	0.43
7:M:124:ARG:HD2	22:h:33:ARG:HD3	2.01	0.43
24:A:1200:A:C6	24:A:1551:A:N6	2.86	0.43
14:V:15:LEU:HB3	14:V:17:LEU:HD13	2.01	0.43
24:A:487:U:C2	24:A:495:G:C2	3.07	0.43
24:A:1484:G:N1	24:A:1515:U:N3	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1484:G:O6	24:A:1515:U:O4	2.36	0.43
27:2:500:LEU:HD23	27:2:726:LEU:HD11	2.00	0.43
27:2:578:ARG:HE	27:2:578:ARG:HB3	1.58	0.43
1:E:171:ILE:O	1:E:175:GLU:HG2	2.19	0.43
11:R:149:ARG:HB2	28:3:233:VAL:HG11	2.01	0.43
12:S:48:ARG:HA	12:S:48:ARG:HD3	1.79	0.43
15:W:144:ASP:OD1	15:W:144:ASP:N	2.50	0.43
24:A:413:A:H3'	24:A:414:A:H8	1.84	0.43
24:A:1200:A:N6	24:A:1551:A:C6	2.84	0.43
32:7:572:ARG:NH2	32:7:576:GLU:OE2	2.52	0.43
3:I:28:LYS:HE2	3:I:56:TYR:CZ	2.54	0.43
3:I:60:SER:OG	3:I:78:GLU:OE2	2.32	0.43
6:L:23:LYS:HE2	24:A:383:G:H5''	2.00	0.43
24:A:1258:G:H2'	24:A:1259:U:C6	2.53	0.43
25:0:10:THR:HG23	26:1:112:ARG:HG2	1.99	0.43
27:2:492:ARG:HG2	27:2:657:HIS:CE1	2.54	0.43
32:7:184:THR:HA	32:7:187:MET:SD	2.59	0.43
3:I:153:ARG:NH2	21:f:46:LYS:HG3	2.34	0.43
7:M:171:ARG:NH1	24:A:508:A:OP1	2.49	0.43
8:O:42:ASP:O	24:A:244:A:O2'	2.33	0.43
11:R:145:ARG:NH1	24:A:1784:G:OP2	2.49	0.43
24:A:155:U:O2'	24:A:157:C:OP2	2.36	0.43
24:A:1542:G:OP2	24:A:1555:A:N6	2.52	0.43
27:2:501:HIS:HE1	27:2:503:LYS:HG2	1.84	0.43
32:7:693:VAL:HG22	32:7:730:LEU:HB2	2.00	0.43
4:J:32:MET:O	4:J:65:GLN:NE2	2.42	0.43
6:L:83:TYR:HB3	6:L:101:VAL:HB	2.01	0.43
11:R:105:LYS:HA	11:R:132:THR:HG21	2.01	0.43
14:V:88:ARG:NH1	14:V:89:GLN:O	2.51	0.43
23:i:138:ARG:HH22	24:A:1247:U:H1'	1.82	0.43
24:A:316:U:H4'	24:A:320:A:C8	2.54	0.43
24:A:563:C:H2'	24:A:564:A:C8	2.54	0.43
4:J:178:ILE:HG13	24:A:77:A:H1'	2.01	0.42
15:W:91:SER:OG	24:A:1586:G:OP1	2.36	0.42
21:f:36:ASP:OD1	21:f:36:ASP:N	2.51	0.42
24:A:1148:A:H2'	24:A:1149:A:H8	1.84	0.42
24:A:1460:G:OP2	26:1:195:LYS:NZ	2.52	0.42
26:1:142:LEU:HD13	26:1:174:ILE:HG22	2.00	0.42
3:I:43:ILE:HD12	3:I:43:ILE:HA	1.96	0.42
5:K:124:ARG:HD3	5:K:124:ARG:HA	1.77	0.42
6:L:139:SER:OG	24:A:186:C:N4	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:106:GLU:OE1	17:a:13:ARG:NH1	2.52	0.42
24:A:798:U:H2'	24:A:799:G:C8	2.51	0.42
24:A:1457:C:H2'	24:A:1458:G:C8	2.54	0.42
25:0:14:LYS:HA	25:0:14:LYS:HD2	1.92	0.42
27:2:99:CYS:O	27:2:102:THR:OG1	2.37	0.42
27:2:501:HIS:HB3	27:2:504:VAL:HG22	2.01	0.42
29:4:212:TYR:OH	29:4:215:GLY:O	2.32	0.42
12:S:133:PRO:HD3	27:2:404:TRP:CD1	2.54	0.42
24:A:1208:A:OP1	27:2:774:THR:OG1	2.33	0.42
1:E:166:ARG:O	1:E:170:GLU:HG3	2.19	0.42
11:R:124:LYS:NZ	28:3:81:GLU:HB3	2.34	0.42
12:S:49:ALA:O	12:S:53:ILE:HG12	2.19	0.42
13:T:13:LYS:HG3	13:T:14:LYS:H	1.84	0.42
24:A:414:A:H4'	24:A:415:G:O5'	2.19	0.42
27:2:171:GLU:OE1	27:2:700:THR:OG1	2.32	0.42
27:2:383:GLU:OE1	27:2:387:ARG:NH2	2.52	0.42
32:7:343:ARG:HD2	32:7:392:ALA:HB2	2.01	0.42
32:7:795:GLU:HA	32:7:798:ILE:HD12	2.02	0.42
1:E:88:VAL:HA	1:E:98:THR:HA	2.01	0.42
5:K:47:LEU:HD23	5:K:47:LEU:HA	1.87	0.42
11:R:54:ARG:NH2	24:A:894:U:O2	2.52	0.42
12:S:129:ILE:H	27:2:401:GLN:NE2	2.17	0.42
24:A:115:U:H2'	24:A:116:U:C6	2.55	0.42
25:0:2:LYS:HD3	25:0:93:MET:HA	2.02	0.42
27:2:373:ASP:OD1	27:2:373:ASP:N	2.52	0.42
3:I:135:ARG:HB3	21:f:23:ARG:HH22	1.84	0.42
13:T:114:ARG:HH22	13:T:118:VAL:HG11	1.84	0.42
24:A:992:G:H2'	24:A:993:A:H8	1.85	0.42
24:A:1546:A:H2'	24:A:1547:U:C6	2.54	0.42
27:2:742:TYR:HA	27:2:745:PHE:HE1	1.84	0.42
30:5:418:GLN:O	30:5:421:GLU:HG3	2.20	0.42
32:7:362:VAL:HG13	32:7:370:ASP:HB3	2.00	0.42
32:7:699:LEU:HD23	32:7:699:LEU:HA	1.93	0.42
6:L:82:VAL:HG21	6:L:170:TYR:CE2	2.50	0.42
14:V:100:ILE:HG23	14:V:105:VAL:HG12	2.02	0.42
25:0:44:LEU:HD21	25:0:93:MET:HE1	2.02	0.42
32:7:263:GLU:OE2	32:7:307:ARG:NE	2.49	0.42
5:K:113:ARG:NH1	24:A:692:C:O2	2.53	0.42
24:A:1541:A:H2'	24:A:1542:G:C8	2.50	0.42
27:2:652:TYR:HB3	27:2:722:LYS:HA	2.02	0.42
29:4:224:LEU:HD22	29:4:254:PHE:HZ	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:265:PHE:HD1	29:4:269:ILE:HD12	1.85	0.42
1:E:94:LYS:HA	1:E:94:LYS:HD3	1.92	0.42
6:L:159:ALA:O	6:L:163:GLN:HG2	2.19	0.42
11:R:65:ARG:NH1	24:A:903:A:H4'	2.34	0.42
11:R:98:ALA:H	11:R:132:THR:HG23	1.84	0.42
22:h:38:LEU:HD13	22:h:38:LEU:HA	1.81	0.42
24:A:187:U:O2	24:A:191:G:N2	2.53	0.42
24:A:702:A:H61	24:A:730:G:H1'	1.85	0.42
27:2:555:ARG:HA	27:2:558:LEU:HD12	2.01	0.42
29:4:340:ALA:O	29:4:344:THR:HG23	2.20	0.42
32:7:292:PRO:HA	32:7:298:LEU:HD22	2.02	0.42
3:I:89:ARG:O	3:I:93:LYS:NZ	2.44	0.42
4:J:57:ASP:OD1	4:J:58:LYS:N	2.50	0.42
4:J:133:LEU:O	24:A:163:C:O2'	2.38	0.42
10:Q:55:ARG:HA	10:Q:60:ILE:O	2.20	0.42
13:T:47:LYS:HA	13:T:47:LYS:HD2	1.85	0.42
18:b:16:ILE:HB	18:b:25:GLN:HG3	2.02	0.42
18:b:45:GLU:OE1	18:b:55:LYS:NZ	2.48	0.42
19:c:61:ASN:OD1	19:c:62:GLY:N	2.53	0.42
24:A:107:A:H2'	24:A:108:G:C8	2.54	0.42
24:A:1485:U:O2'	24:A:1489:C:O2	2.36	0.42
25:0:112:ALA:HB1	25:0:114:ARG:NH1	2.34	0.42
27:2:526:GLU:OE1	27:2:530:ARG:NH2	2.53	0.42
27:2:546:TYR:CG	27:2:713:PRO:HB3	2.55	0.42
28:3:128:LYS:HG3	28:3:129:TYR:H	1.85	0.42
29:4:377:LEU:HD12	29:4:378:PRO:HD2	2.01	0.42
32:7:394:LEU:HD11	32:7:433:GLY:HA3	2.02	0.42
32:7:690:ASP:OD2	32:7:726:LYS:NZ	2.52	0.42
3:I:45:LEU:HG	3:I:125:VAL:HG23	2.02	0.41
5:K:51:SER:OG	5:K:52:ALA:N	2.53	0.41
7:M:131:HIS:O	7:M:157:ALA:N	2.51	0.41
16:Z:103:ILE:HD11	16:Z:129:PHE:HE1	1.85	0.41
17:a:60:GLU:HG2	17:a:68:ILE:HG22	2.01	0.41
24:A:897:G:H2'	24:A:898:A:H8	1.85	0.41
24:A:1259:U:H2'	24:A:1260:G:H8	1.85	0.41
3:I:34:SER:O	3:I:115:ASN:ND2	2.42	0.41
6:L:193:LEU:O	6:L:197:GLN:HG3	2.20	0.41
7:M:61:ASP:OD1	7:M:62:GLU:N	2.53	0.41
9:P:52:LYS:HB2	9:P:52:LYS:HE3	1.88	0.41
9:P:104:CYS:SG	9:P:113:ARG:NH2	2.93	0.41
27:2:301:GLU:HG3	27:2:573:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:389:PHE:HA	29:4:392:TYR:HD2	1.84	0.41
24:A:561:G:O6	24:A:576:A:O2'	2.36	0.41
24:A:1789:G:C8	28:3:185:ARG:HD2	2.55	0.41
26:1:126:GLN:O	26:1:166:LYS:NZ	2.53	0.41
29:4:333:ILE:O	29:4:375:TYR:OH	2.33	0.41
4:J:116:GLN:HE22	4:J:125:THR:HB	1.85	0.41
18:b:8:VAL:HG23	18:b:32:HIS:HB3	2.03	0.41
24:A:29:U:H2'	24:A:30:G:H8	1.86	0.41
29:4:319:ARG:O	29:4:323:ILE:HG12	2.20	0.41
30:5:400:TYR:CE1	30:5:410:LYS:HD3	2.56	0.41
32:7:309:TYR:CZ	32:7:327:PRO:HG3	2.55	0.41
1:E:149:GLN:HE21	1:E:149:GLN:HB2	1.69	0.41
10:Q:28:THR:HG23	10:Q:32:GLN:HE21	1.85	0.41
20:e:40:CYS:SG	20:e:42:THR:OG1	2.69	0.41
24:A:17:C:O2'	24:A:1134:A:N1	2.49	0.41
28:3:87:ILE:HD11	28:3:122:VAL:HG23	2.01	0.41
31:6:503:MET:HB2	31:6:503:MET:HE3	1.83	0.41
8:O:28:LYS:HD2	8:O:28:LYS:HA	1.75	0.41
11:R:59:MET:HE1	24:A:897:G:H4'	2.03	0.41
12:S:50:ARG:HH21	24:A:1546:A:P	2.43	0.41
17:a:38:TYR:HE1	24:A:356:A:C5	2.39	0.41
26:1:270:THR:HG23	26:1:274:THR:HG21	2.03	0.41
32:7:560:GLN:HA	32:7:561:PRO:HD3	1.88	0.41
1:E:90:GLU:HB3	1:E:97:LEU:HB2	2.01	0.41
1:E:179:CYS:HB3	1:E:183:GLN:HB2	2.03	0.41
3:I:130:ARG:HH21	21:f:56:VAL:HG22	1.86	0.41
5:K:30:LEU:HA	5:K:33:LEU:HG	2.03	0.41
5:K:32:ASP:O	5:K:36:ASN:ND2	2.54	0.41
5:K:81:GLN:HB3	5:K:85:ARG:NH2	2.36	0.41
14:V:48:LYS:HB3	14:V:54:LEU:HD21	2.01	0.41
15:W:57:ARG:HG3	15:W:104:ILE:HD13	2.02	0.41
17:a:103:LEU:HB3	17:a:126:LYS:HB2	2.01	0.41
18:b:30:ILE:HG22	18:b:32:HIS:HD2	1.86	0.41
24:A:978:G:H4'	24:A:1772:A:H4'	2.02	0.41
27:2:90:PRO:HB2	27:2:138:GLN:HB2	2.01	0.41
27:2:112:ASN:HD21	27:2:128:VAL:HG21	1.86	0.41
27:2:186:SER:OG	27:2:247:LYS:O	2.29	0.41
30:5:411:GLY:O	30:5:413:LEU:N	2.52	0.41
32:7:63:HIS:HA	32:7:105:LEU:HD13	2.02	0.41
4:J:77:LEU:HD12	4:J:95:LYS:HB2	2.02	0.41
6:L:2:GLY:N	24:A:390:C:OP2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:V:28:VAL:HA	14:V:58:ALA:HB2	2.02	0.41
18:b:112:LYS:O	18:b:116:ASN:ND2	2.39	0.41
24:A:232:G:H2'	24:A:233:G:C8	2.56	0.41
24:A:1433:U:O2	29:4:412:GLN:NE2	2.48	0.41
24:A:1542:G:H2'	24:A:1543:A:H8	1.85	0.41
26:1:88:LEU:HD22	26:1:100:LEU:HD22	2.02	0.41
28:3:109:CYS:HB2	28:3:135:ALA:HB1	2.01	0.41
29:4:306:PHE:HD2	29:4:307:LEU:HD12	1.86	0.41
32:7:491:LYS:NZ	32:7:546:ASP:OD2	2.54	0.41
32:7:939:ASN:O	32:7:942:VAL:HB	2.21	0.41
1:E:146:ARG:HH11	1:E:147:PRO:HD3	1.86	0.41
1:E:146:ARG:H	1:E:149:GLN:NE2	2.19	0.41
1:E:189:ILE:HD13	1:E:189:ILE:HA	1.92	0.41
3:I:87:HIS:O	3:I:89:ARG:N	2.54	0.41
7:M:85:ASP:OD1	7:M:86:GLU:N	2.53	0.41
7:M:91:LEU:HD23	7:M:91:LEU:HA	1.92	0.41
14:V:36:LYS:HD2	24:A:1563:U:H4'	2.02	0.41
15:W:103:LYS:HD3	15:W:103:LYS:HA	1.79	0.41
17:a:64:PRO:HB3	26:1:246:LYS:HB2	2.03	0.41
24:A:187:U:O2	24:A:191:G:C2	2.74	0.41
24:A:1499:A:H3'	24:A:1500:G:H8	1.85	0.41
29:4:324:ILE:HD11	29:4:366:LEU:HD21	2.03	0.41
32:7:429:ASP:OD1	32:7:434:LYS:NZ	2.53	0.41
32:7:686:HIS:NE2	32:7:720:ASP:OD2	2.41	0.41
1:E:191:GLU:OE1	1:E:194:GLY:N	2.42	0.41
10:Q:120:SER:HB2	24:A:625:G:H5'	2.02	0.41
16:Z:49:GLU:HB3	16:Z:64:GLN:HG3	2.03	0.41
17:a:7:ARG:HD2	24:A:1099:G:OP2	2.21	0.41
24:A:588:A:H2'	24:A:589:A:C8	2.55	0.41
24:A:1236:U:C2	24:A:1240:G:C2	3.08	0.41
27:2:361:THR:O	27:2:364:THR:OG1	2.39	0.41
28:3:95:LEU:HD12	28:3:95:LEU:HA	1.76	0.41
32:7:720:ASP:HB3	32:7:723:ILE:HG22	2.03	0.41
32:7:911:LYS:HE3	32:7:954:LYS:HE3	2.03	0.41
1:E:149:GLN:HA	24:A:1064:C:H5'	2.02	0.40
3:I:121:VAL:HA	3:I:124:ILE:HG12	2.03	0.40
7:M:148:LEU:HD12	7:M:148:LEU:HA	1.86	0.40
13:T:87:LYS:HA	13:T:90:VAL:HG12	2.03	0.40
19:c:66:ARG:NH1	24:A:1529:C:OP2	2.40	0.40
24:A:6:G:H4'	24:A:550:G:H1'	2.03	0.40
24:A:227:U:O2	24:A:231:G:C6	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:572:C:H2'	24:A:573:G:C8	2.56	0.40
24:A:1596:A:O2'	24:A:1598:C:N4	2.53	0.40
32:7:359:PRO:HG2	32:7:362:VAL:HG23	2.03	0.40
32:7:853:MET:HE1	32:7:875:ILE:HG23	2.02	0.40
5:K:167:LYS:HE3	5:K:167:LYS:HB3	1.86	0.40
9:P:61:MET:HB3	9:P:123:VAL:HB	2.04	0.40
12:S:91:MET:HB3	12:S:124:LEU:HG	2.01	0.40
16:Z:87:GLU:HA	16:Z:90:VAL:HG22	2.03	0.40
24:A:893:G:H2'	24:A:894:U:C6	2.56	0.40
24:A:1542:G:H2'	24:A:1543:A:C8	2.56	0.40
24:A:1790:A:O2'	28:3:192:GLY:HA2	2.22	0.40
26:1:170:GLN:HA	26:1:173:MET:HG3	2.03	0.40
27:2:473:ASP:OD1	27:2:473:ASP:N	2.54	0.40
32:7:924:LEU:O	32:7:965:ARG:NH1	2.50	0.40
1:E:27:LYS:HB3	1:E:47:LEU:HD12	2.02	0.40
6:L:98:LYS:HB3	24:A:326:G:H5''	2.04	0.40
21:f:11:VAL:HG12	21:f:31:VAL:HB	2.04	0.40
24:A:651:C:H2'	24:A:652:G:H8	1.85	0.40
27:2:61:ARG:HE	27:2:61:ARG:HB3	1.73	0.40
29:4:197:LYS:HD2	30:5:397:LEU:HD11	2.02	0.40
29:4:201:VAL:O	29:4:205:ILE:HG12	2.21	0.40
3:I:94:LYS:HE3	24:A:1606:G:H4'	2.03	0.40
9:P:53:ALA:HA	9:P:56:ARG:HG3	2.04	0.40
15:W:22:PHE:O	15:W:26:GLN:CB	2.70	0.40
15:W:114:LEU:HB3	15:W:125:ILE:HD13	2.03	0.40
16:Z:55:ASN:C	16:Z:57:ARG:H	2.29	0.40
17:a:27:LEU:HD23	17:a:27:LEU:HA	1.93	0.40
20:e:18:LYS:HE2	20:e:18:LYS:HB3	1.92	0.40
24:A:1157:A:H2'	24:A:1158:C:C6	2.56	0.40
24:A:1479:A:H2'	24:A:1480:G:C8	2.56	0.40
24:A:1580:G:N2	24:A:1607:A:OP2	2.37	0.40
29:4:373:LYS:HA	29:4:373:LYS:HD3	1.83	0.40
32:7:278:LEU:HD21	32:7:311:VAL:HG13	2.04	0.40
2:H:19:LEU:HD13	24:A:786:A:C5	2.56	0.40
5:K:31:TYR:O	5:K:34:GLU:HG3	2.22	0.40
23:i:98:VAL:N	24:A:1227:A:OP1	2.55	0.40
24:A:966:U:H2'	24:A:967:C:O4'	2.21	0.40
28:3:94:ALA:O	28:3:95:LEU:C	2.64	0.40
28:3:247:ASN:O	28:3:251:ILE:HG12	2.22	0.40
29:4:364:ASN:C	29:4:364:ASN:HD22	2.28	0.40
29:4:373:LYS:HB3	29:4:375:TYR:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:7:101:ALA:HB3	32:7:106:ILE:HD11	2.04	0.40
32:7:303:ALA:HB1	32:7:307:ARG:NH1	2.36	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	E	211/255 (83%)	192 (91%)	18 (8%)	1 (0%)	24	55
2	H	259/264 (98%)	244 (94%)	14 (5%)	1 (0%)	30	60
3	I	197/212 (93%)	186 (94%)	11 (6%)	0	100	100
4	J	230/239 (96%)	223 (97%)	7 (3%)	0	100	100
5	K	193/203 (95%)	189 (98%)	4 (2%)	0	100	100
6	L	199/202 (98%)	188 (94%)	11 (6%)	0	100	100
7	M	177/190 (93%)	171 (97%)	6 (3%)	0	100	100
8	O	148/161 (92%)	139 (94%)	9 (6%)	0	100	100
9	P	116/144 (81%)	101 (87%)	15 (13%)	0	100	100
10	Q	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
11	R	133/150 (89%)	117 (88%)	15 (11%)	1 (1%)	16	45
12	S	113/153 (74%)	106 (94%)	7 (6%)	0	100	100
13	T	115/143 (80%)	107 (93%)	8 (7%)	0	100	100
14	V	120/156 (77%)	114 (95%)	6 (5%)	0	100	100
15	W	140/153 (92%)	130 (93%)	10 (7%)	0	100	100
16	Z	127/130 (98%)	115 (91%)	11 (9%)	1 (1%)	16	45
17	a	140/145 (97%)	129 (92%)	11 (8%)	0	100	100
18	b	130/136 (96%)	122 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	c	67/99 (68%)	64 (96%)	3 (4%)	0	100	100
20	e	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
21	f	59/68 (87%)	53 (90%)	6 (10%)	0	100	100
22	h	19/62 (31%)	14 (74%)	3 (16%)	2 (10%)	0	2
23	i	61/154 (40%)	56 (92%)	5 (8%)	0	100	100
25	0	125/127 (98%)	124 (99%)	1 (1%)	0	100	100
26	1	263/282 (93%)	252 (96%)	11 (4%)	0	100	100
27	2	693/830 (84%)	668 (96%)	24 (4%)	1 (0%)	48	75
28	3	182/259 (70%)	166 (91%)	13 (7%)	3 (2%)	7	31
29	4	268/480 (56%)	254 (95%)	14 (5%)	0	100	100
30	5	77/445 (17%)	72 (94%)	5 (6%)	0	100	100
31	6	41/519 (8%)	40 (98%)	1 (2%)	0	100	100
32	7	1002/1235 (81%)	983 (98%)	19 (2%)	0	100	100
33	8	58/938 (6%)	51 (88%)	7 (12%)	0	100	100
All	All	5890/8767 (67%)	5589 (95%)	291 (5%)	10 (0%)	44	71

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	R	137	ASP
28	3	98	ASN
28	3	117	ILE
22	h	27	PRO
22	h	28	LYS
27	2	372	ASP
28	3	90	HIS
2	H	171	ASP
16	Z	56	HIS
1	E	150	ILE

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%)	184 (98%)	3 (2%)	55	72
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%)	195 (98%)	3 (2%)	57	72
5	K	169/177 (96%)	169 (100%)	0	100	100
6	L	163/164 (99%)	162 (99%)	1 (1%)	78	81
7	M	154/162 (95%)	154 (100%)	0	100	100
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
12	S	99/132 (75%)	98 (99%)	1 (1%)	68	76
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%)	111 (99%)	1 (1%)	70	78
17	a	113/116 (97%)	113 (100%)	0	100	100
18	b	112/115 (97%)	112 (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%)	14 (74%)	5 (26%)	0	2
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%)	214 (100%)	1 (0%)	81	83
27	2	606/714 (85%)	606 (100%)	0	100	100
28	3	155/215 (72%)	145 (94%)	10 (6%)	15	43
29	4	229/411 (56%)	229 (100%)	0	100	100
30	5	70/373 (19%)	70 (100%)	0	100	100
31	6	36/447 (8%)	36 (100%)	0	100	100
32	7	864/1049 (82%)	864 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	8	57/765 (8%)	53 (93%)	4 (7%)	14	41
All	All	5080/7407 (69%)	5051 (99%)	29 (1%)	76	81

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	146	ARG
1	E	150	ILE
1	E	213	ARG
4	J	58	LYS
4	J	173	THR
4	J	198	ARG
6	L	8	ARG
12	S	78	ASN
16	Z	55	ASN
22	h	25	GLU
22	h	26	LYS
22	h	27	PRO
22	h	28	LYS
22	h	38	LEU
26	1	107	GLN
28	3	88	PRO
28	3	92	MET
28	3	98	ASN
28	3	111	LEU
28	3	113	VAL
28	3	114	ARG
28	3	115	MET
28	3	116	ASN
28	3	125	ARG
28	3	128	LYS
33	8	429	LYS
33	8	436	SER
33	8	443	HIS
33	8	826	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	58	ASN
1	E	149	GLN

Continued on next page...

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Mol	Chain	Res	Type
2	H	9	GLN
2	H	17	HIS
2	H	67	GLN
2	H	201	HIS
3	I	31	ASN
4	J	71	ASN
4	J	129	HIS
4	J	179	GLN
5	K	48	GLN
6	L	52	ASN
6	L	53	HIS
6	L	179	GLN
8	O	97	HIS
9	P	40	HIS
10	Q	62	GLN
12	S	54	ASN
13	T	24	GLN
14	V	10	ASN
16	Z	55	ASN
21	f	44	ASN
25	0	125	HIS
26	1	13	HIS
26	1	32	GLN
27	2	76	HIS
27	2	92	ASN
27	2	401	GLN
27	2	569	ASN
27	2	597	HIS
27	2	641	GLN
27	2	650	HIS
28	3	90	HIS
28	3	116	ASN
29	4	229	HIS
29	4	388	HIS
29	4	440	HIS
30	5	382	GLN
32	7	166	ASN
32	7	253	HIS
32	7	314	GLN
32	7	412	HIS
32	7	560	GLN
32	7	578	ASN

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Mol	Chain	Res	Type
33	8	421	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	A	1455/1797 (80%)	368 (25%)	21 (1%)

All (368) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
24	A	2	A
24	A	3	C
24	A	4	C
24	A	6	G
24	A	13	U
24	A	14	C
24	A	25	C
24	A	26	A
24	A	27	U
24	A	28	A
24	A	34	G
24	A	42	G
24	A	45	U
24	A	47	A
24	A	57	G
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	93	U
24	A	99	A
24	A	103	A
24	A	104	A
24	A	110	U
24	A	113	C

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Mol	Chain	Res	Type
24	A	114	G
24	A	115	U
24	A	127	U
24	A	136	A
24	A	137	C
24	A	142	A
24	A	150	G
24	A	155	U
24	A	156	U
24	A	165	A
24	A	176	A
24	A	188	U
24	A	189	C
24	A	191	G
24	A	192	A
24	A	195	G
24	A	212	U
24	A	213	A
24	A	214	A
24	A	215	A
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	254	A
24	A	257	U
24	A	258	C
24	A	262	A
24	A	264	U
24	A	268	A
24	A	269	C
24	A	270	G
24	A	271	G
24	A	274	U
24	A	275	U
24	A	277	C

Continued on next page...

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Mol	Chain	Res	Type
24	A	296	A
24	A	299	U
24	A	301	U
24	A	310	U
24	A	311	C
24	A	313	A
24	A	317	U
24	A	319	G
24	A	326	G
24	A	334	G
24	A	335	C
24	A	348	C
24	A	349	A
24	A	357	A
24	A	358	C
24	A	387	G
24	A	396	A
24	A	397	A
24	A	398	A
24	A	399	C
24	A	401	G
24	A	404	A
24	A	414	A
24	A	415	G
24	A	420	G
24	A	421	C
24	A	422	A
24	A	423	G
24	A	425	A
24	A	431	G
24	A	436	U
24	A	441	C
24	A	442	A
24	A	445	C
24	A	449	A
24	A	450	C
24	A	452	C
24	A	453	G
24	A	461	A
24	A	465	A
24	A	474	A
24	A	477	G

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Mol	Chain	Res	Type
24	A	480	A
24	A	481	C
24	A	490	U
24	A	492	C
24	A	493	G
24	A	495	G
24	A	502	A
24	A	505	U
24	A	511	G
24	A	512	A
24	A	516	C
24	A	522	A
24	A	523	A
24	A	524	A
24	A	531	A
24	A	535	A
24	A	536	G
24	A	538	A
24	A	539	A
24	A	549	G
24	A	551	C
24	A	552	A
24	A	553	A
24	A	554	G
24	A	556	C
24	A	563	C
24	A	574	G
24	A	575	U
24	A	576	A
24	A	577	A
24	A	578	U
24	A	579	U
24	A	580	C
24	A	583	G
24	A	591	A
24	A	592	G
24	A	604	G
24	A	607	G
24	A	608	U
24	A	611	A
24	A	612	G
24	A	616	A

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Mol	Chain	Res	Type
24	A	617	A
24	A	619	A
24	A	620	A
24	A	621	G
24	A	636	U
24	A	641	C
24	A	647	C
24	A	677	U
24	A	678	G
24	A	679	G
24	A	680	G
24	A	683	G
24	A	686	C
24	A	691	C
24	A	692	C
24	A	693	U
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
24	A	730	G
24	A	731	G
24	A	732	A
24	A	742	U
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	787	A
24	A	791	A
24	A	809	A
24	A	810	A
24	A	812	A

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Mol	Chain	Res	Type
24	A	813	G
24	A	818	U
24	A	819	G
24	A	822	G
24	A	823	U
24	A	828	U
24	A	830	U
24	A	832	G
24	A	844	G
24	A	858	U
24	A	859	U
24	A	861	A
24	A	862	U
24	A	871	U
24	A	874	G
24	A	879	G
24	A	896	A
24	A	897	G
24	A	901	U
24	A	911	G
24	A	912	G
24	A	930	A
24	A	931	A
24	A	933	U
24	A	940	G
24	A	957	U
24	A	958	U
24	A	964	A
24	A	968	A
24	A	990	A
24	A	991	A
24	A	994	C
24	A	996	A
24	A	998	C
24	A	999	A
24	A	1000	G
24	A	1001	A
24	A	1007	U
24	A	1019	C
24	A	1021	A
24	A	1023	A
24	A	1024	A

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Mol	Chain	Res	Type
24	A	1026	C
24	A	1030	G
24	A	1041	A
24	A	1042	U
24	A	1046	A
24	A	1052	U
24	A	1056	U
24	A	1057	U
24	A	1059	U
24	A	1060	U
24	A	1066	G
24	A	1073	A
24	A	1074	C
24	A	1077	U
24	A	1078	A
24	A	1080	G
24	A	1089	A
24	A	1093	G
24	A	1094	U
24	A	1095	U
24	A	1097	G
24	A	1135	A
24	A	1147	G
24	A	1148	A
24	A	1152	G
24	A	1155	C
24	A	1156	C
24	A	1157	A
24	A	1164	G
24	A	1182	U
24	A	1183	U
24	A	1198	G
24	A	1199	A
24	A	1204	C
24	A	1217	C
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	1228	U

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Mol	Chain	Res	Type
24	A	1235	A
24	A	1236	U
24	A	1239	A
24	A	1240	G
24	A	1241	A
24	A	1242	G
24	A	1243	C
24	A	1246	U
24	A	1248	U
24	A	1249	C
24	A	1253	A
24	A	1254	U
24	A	1266	U
24	A	1268	G
24	A	1270	G
24	A	1271	C
24	A	1272	A
24	A	1432	A
24	A	1433	U
24	A	1434	G
24	A	1439	U
24	A	1440	A
24	A	1441	G
24	A	1442	A
24	A	1443	U
24	A	1445	U
24	A	1448	U
24	A	1453	C
24	A	1467	A
24	A	1469	U
24	A	1470	G
24	A	1478	C
24	A	1486	A
24	A	1487	C
24	A	1489	C
24	A	1491	C
24	A	1492	U
24	A	1499	A
24	A	1502	G
24	A	1512	A
24	A	1517	G
24	A	1520	A

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Mol	Chain	Res	Type
24	A	1530	G
24	A	1532	G
24	A	1533	C
24	A	1538	G
24	A	1552	A
24	A	1553	U
24	A	1554	U
24	A	1555	A
24	A	1556	U
24	A	1563	U
24	A	1565	A
24	A	1569	A
24	A	1570	G
24	A	1579	A
24	A	1580	G
24	A	1586	G
24	A	1597	G
24	A	1603	G
24	A	1605	U
24	A	1606	G
24	A	1607	A
24	A	1612	G
24	A	1615	C
24	A	1625	G
24	A	1627	A
24	A	1628	C
24	A	1766	C
24	A	1768	C
24	A	1774	G
24	A	1776	G
24	A	1777	A
24	A	1779	C
24	A	1782	G
24	A	1785	G
24	A	1787	G
24	A	1788	G
24	A	1789	G
24	A	1790	A
24	A	1791	U
24	A	1792	C
24	A	1795	U
24	A	1796	A

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Mol	Chain	Res	Type
24	A	1797	A

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	A	113	C
24	A	175	G
24	A	211	U
24	A	231	G
24	A	233	G
24	A	269	C
24	A	414	A
24	A	449	A
24	A	522	A
24	A	552	A
24	A	611	A
24	A	678	G
24	A	1041	A
24	A	1094	U
24	A	1224	A
24	A	1252	G
24	A	1477	C
24	A	1531	U
24	A	1564	C
24	A	1569	A
24	A	1790	A

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

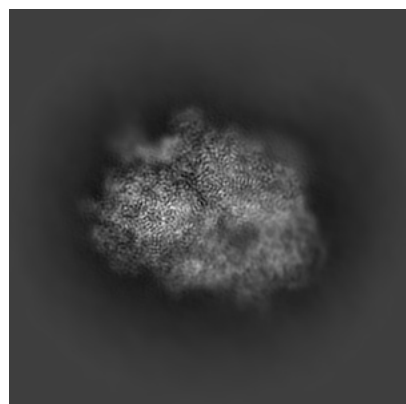
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66690. These allow visual inspection of the internal detail of the map and identification of artifacts.

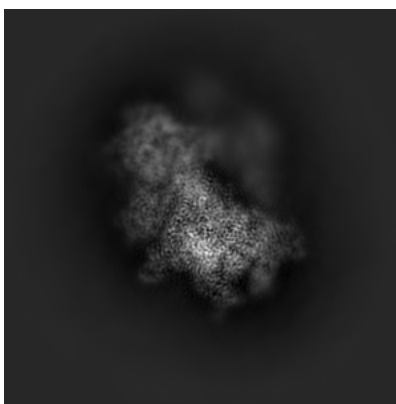
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

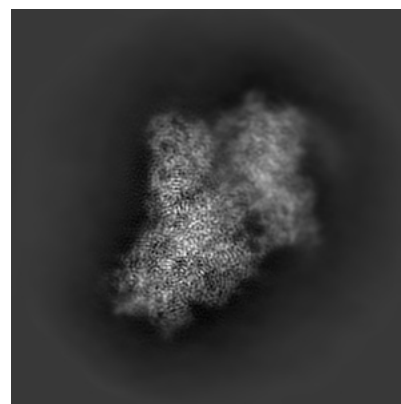
6.1.1 Primary map



X

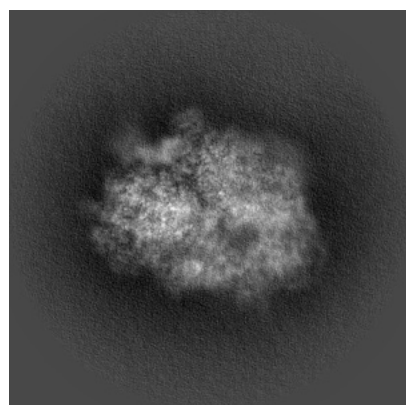


Y

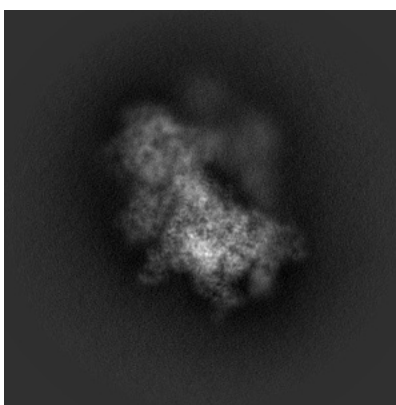


Z

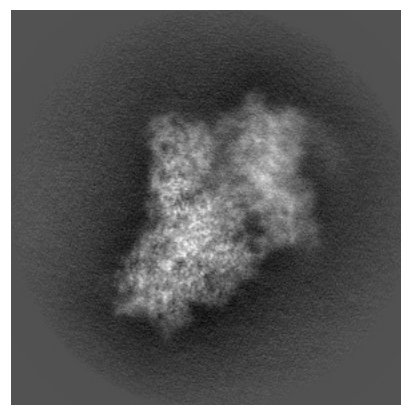
6.1.2 Raw map



X



Y

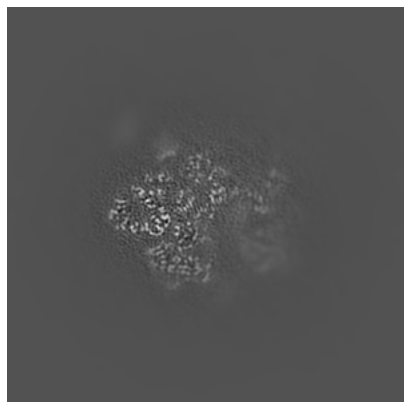


Z

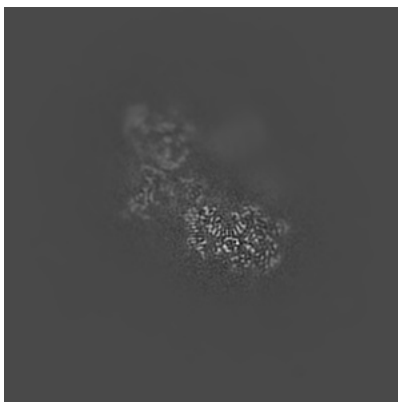
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

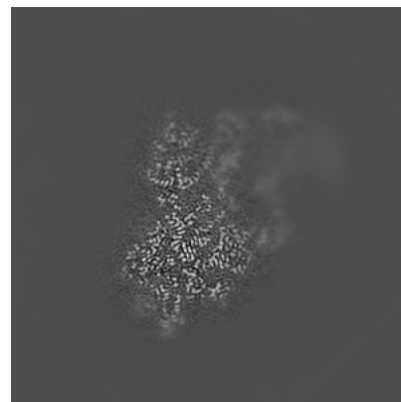
6.2.1 Primary map



X Index: 180

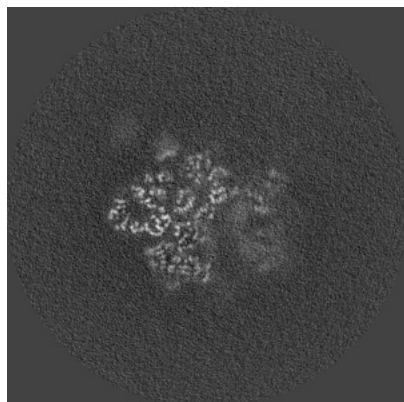


Y Index: 180

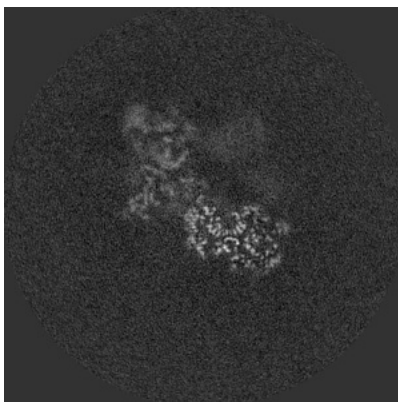


Z Index: 180

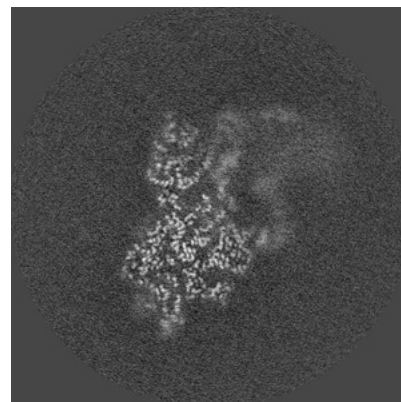
6.2.2 Raw map



X Index: 180



Y Index: 180

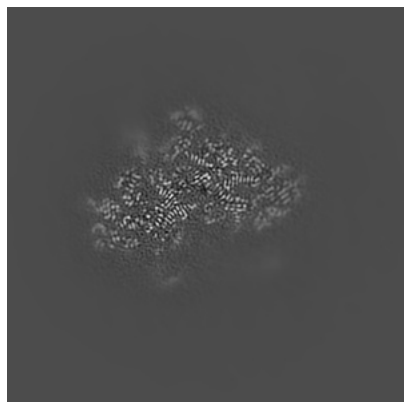


Z Index: 180

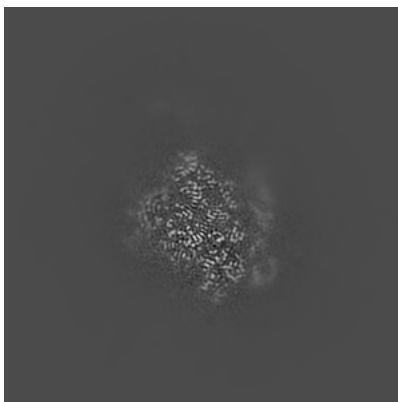
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

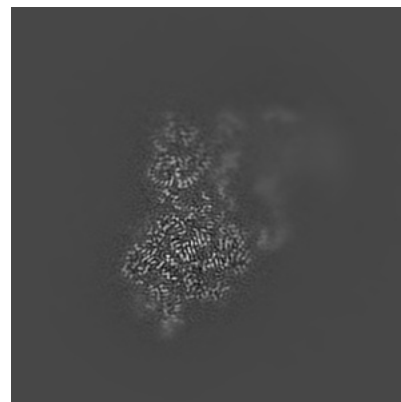
6.3.1 Primary map



X Index: 150

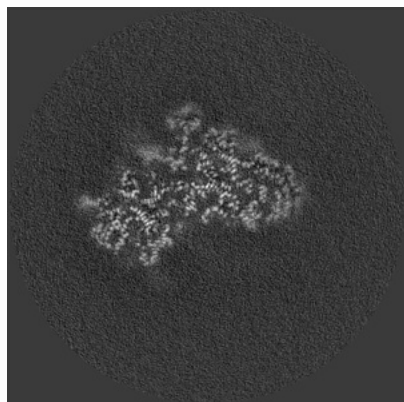


Y Index: 138

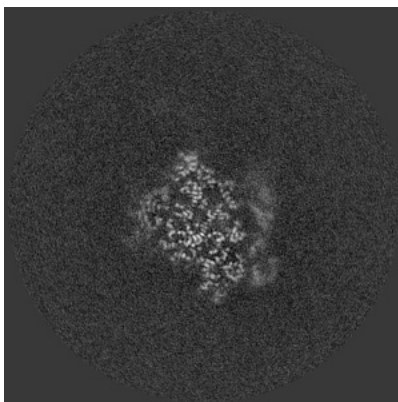


Z Index: 181

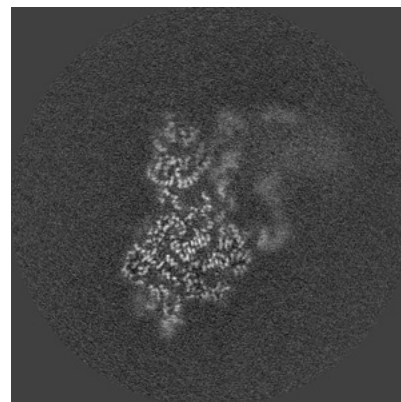
6.3.2 Raw map



X Index: 143



Y Index: 138

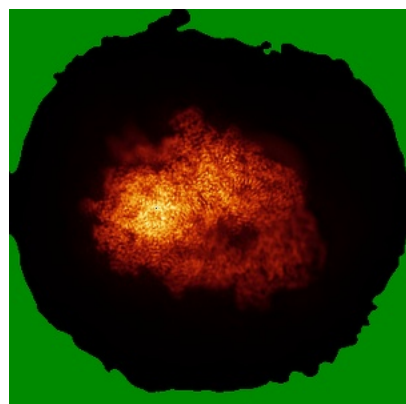


Z Index: 181

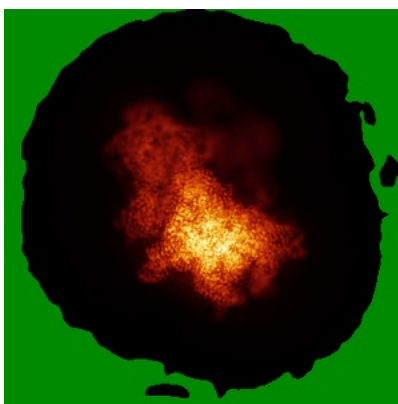
The images above show the largest variance slices of the map in three orthogonal directions.

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

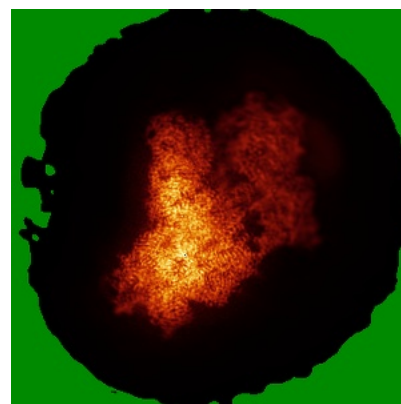
6.4.1 Primary map



X

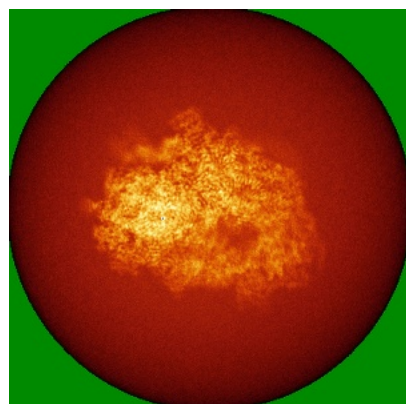


Y

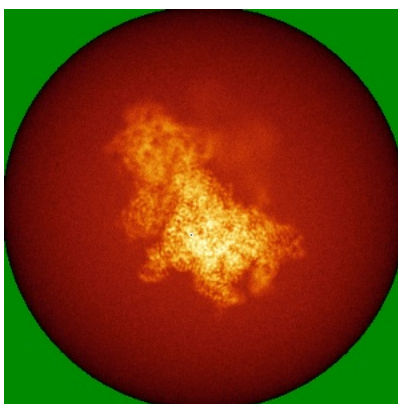


Z

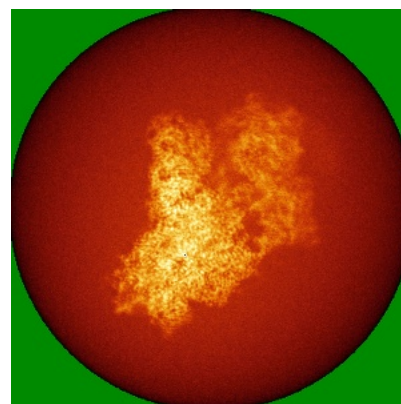
6.4.2 Raw map



X



Y



Z

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

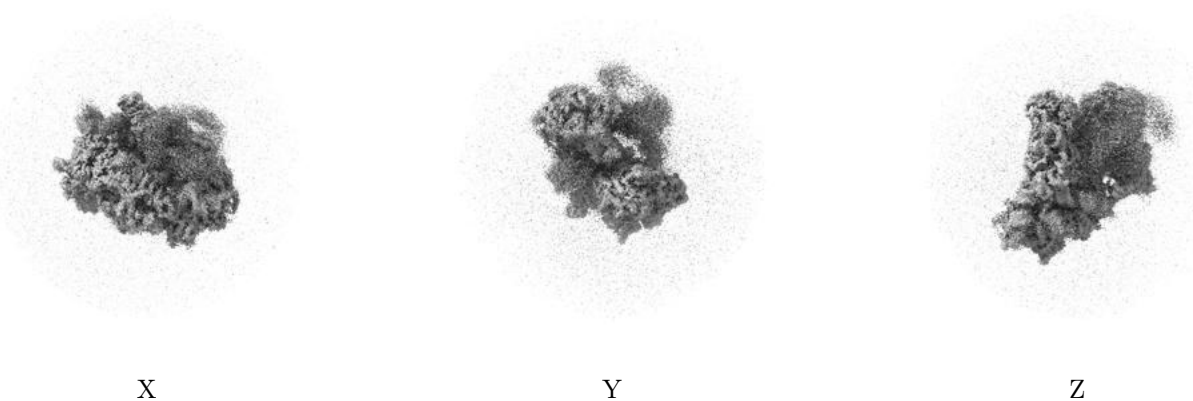
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

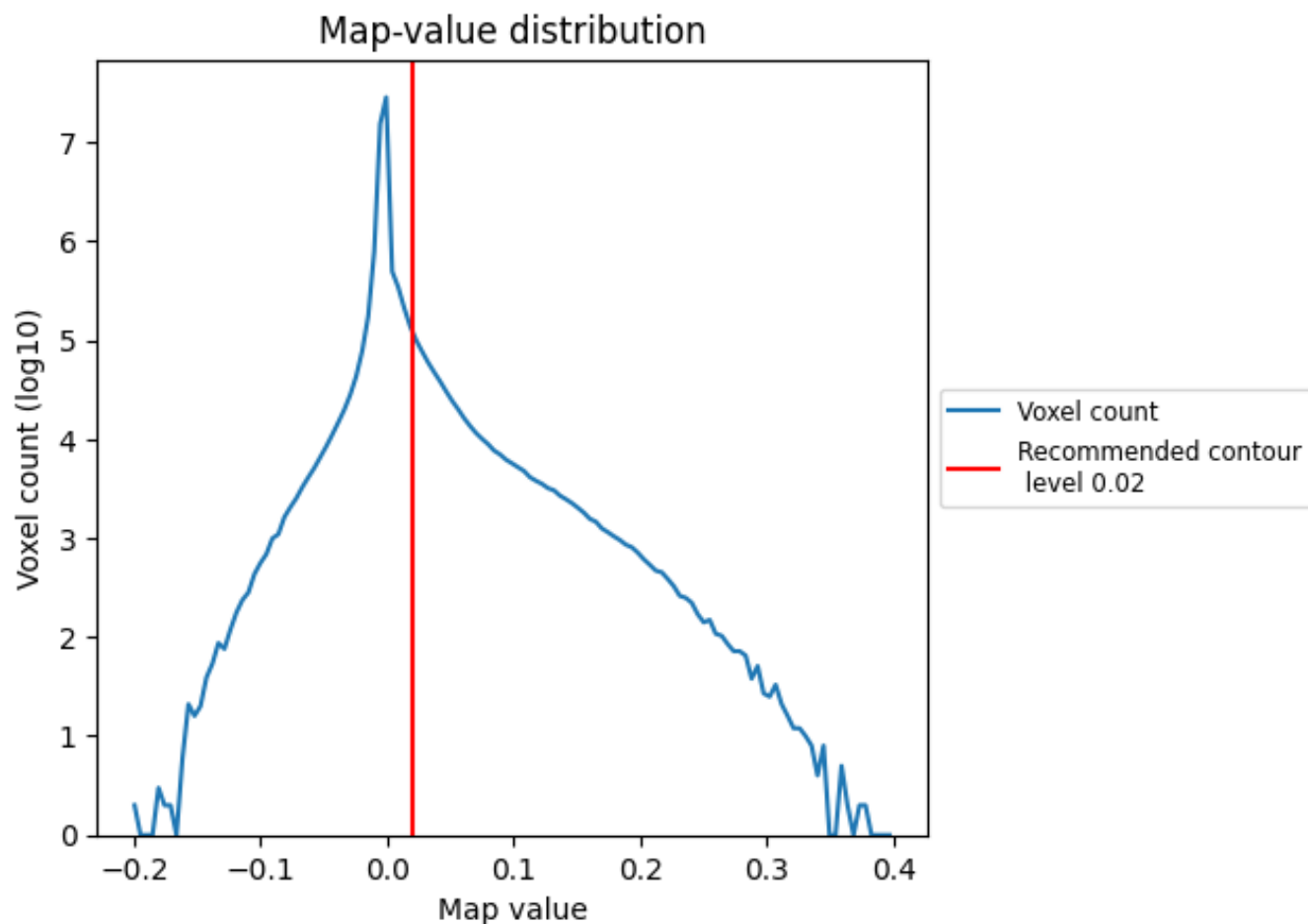
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

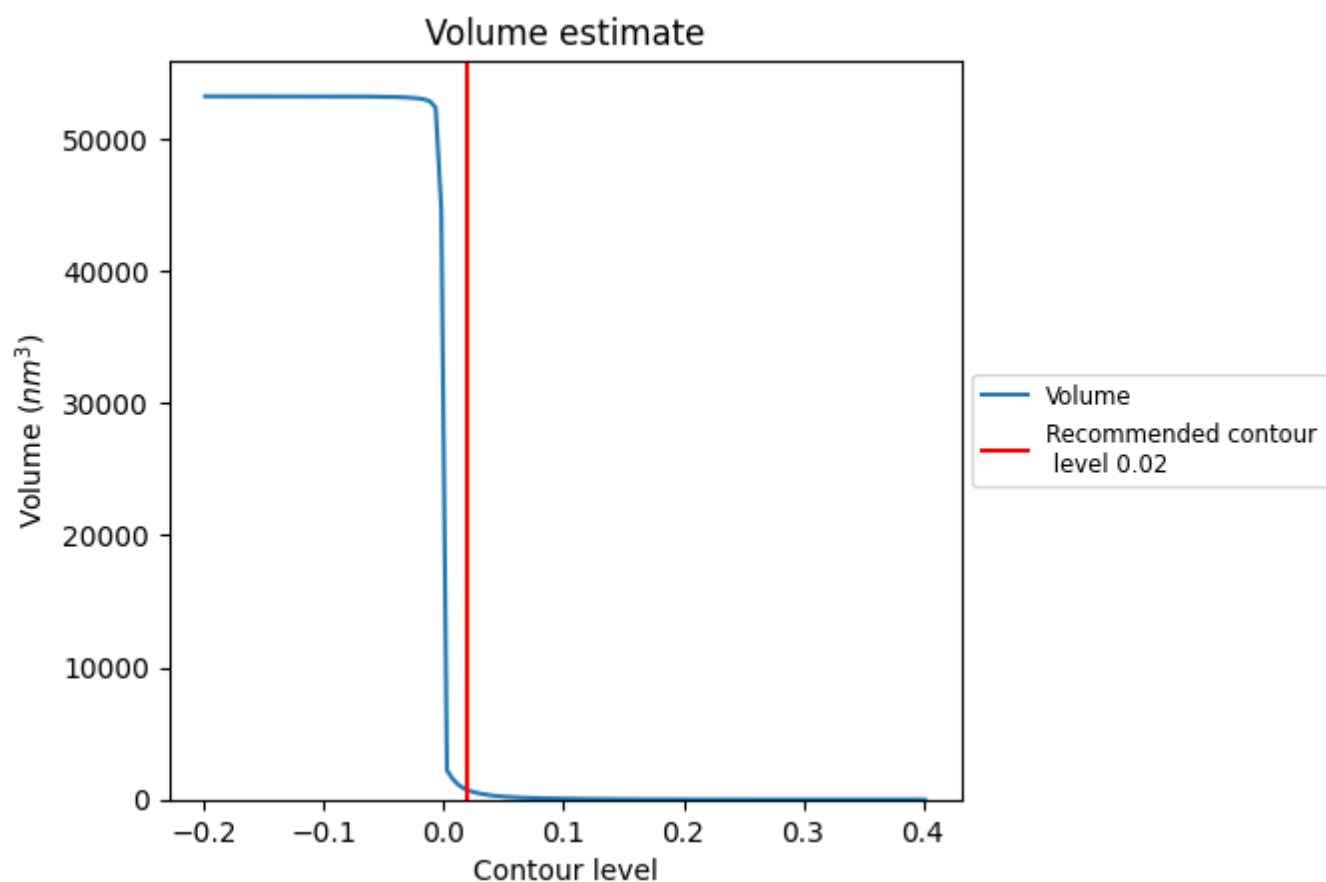
This section contains the results of statistical analysis of the map.

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.

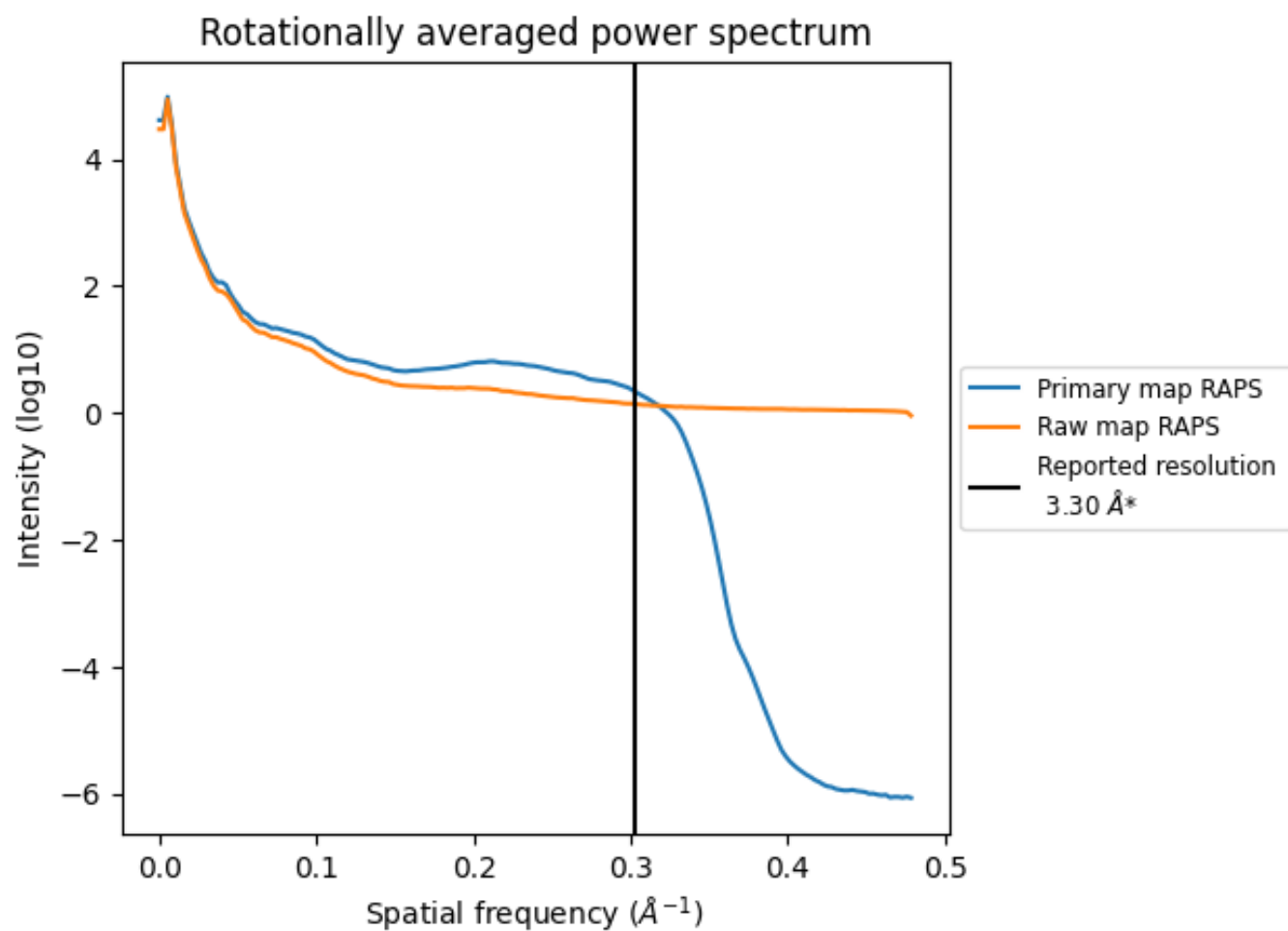
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 713 nm^3 ; this corresponds to an approximate mass of 644 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 ⓘ

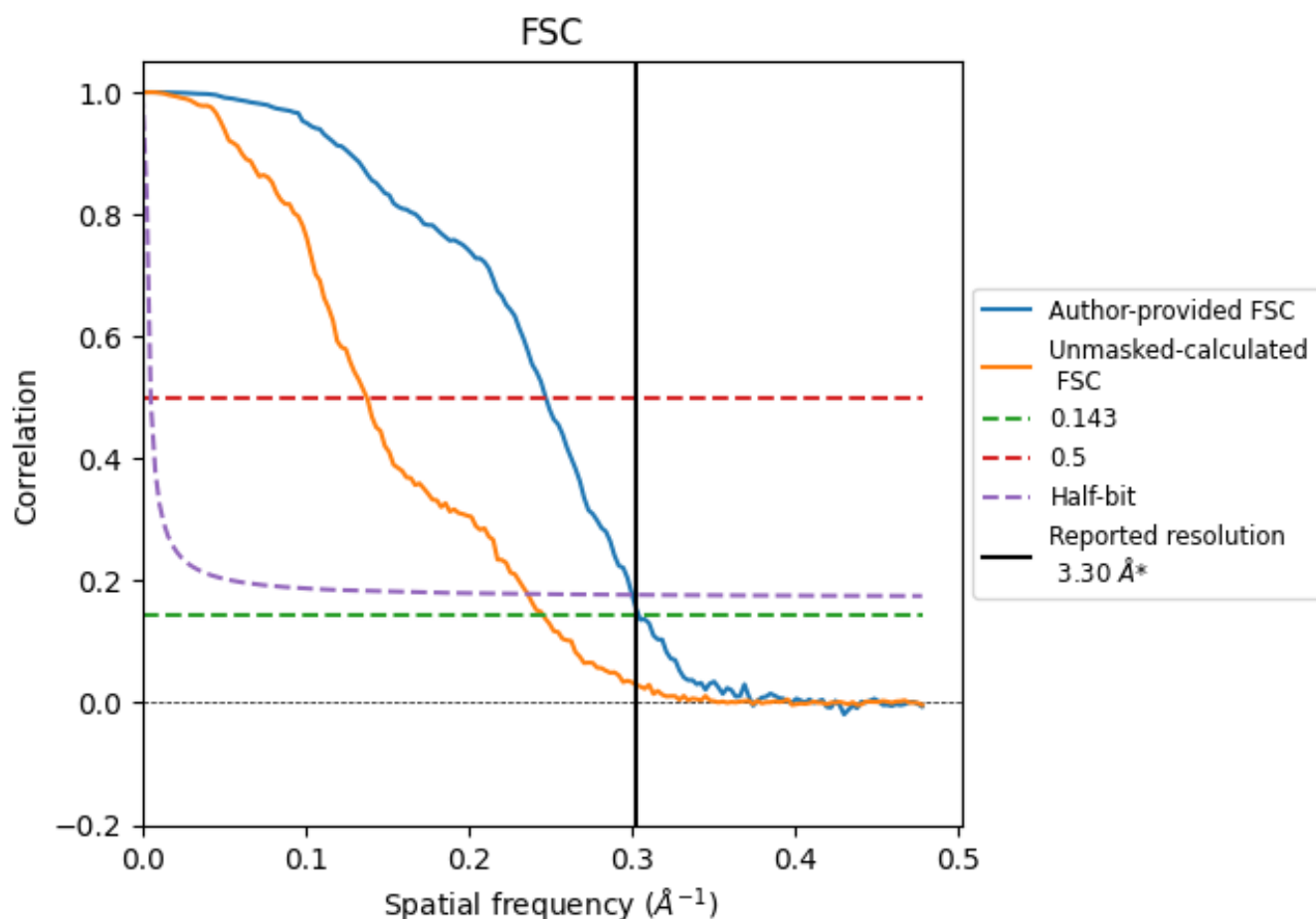


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

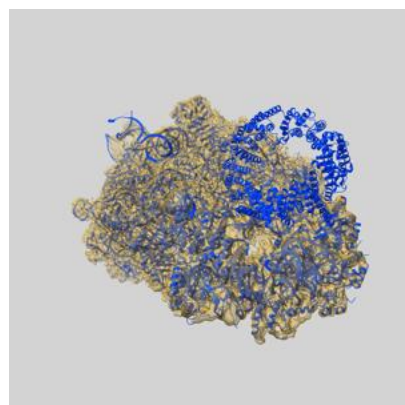
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.28	4.04	3.33
Unmasked-calculated*	4.07	7.26	4.23

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

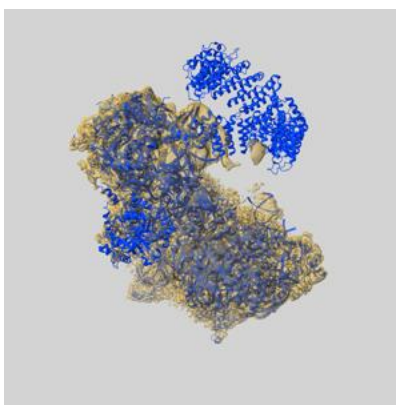
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66690 and PDB model 9XAK. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

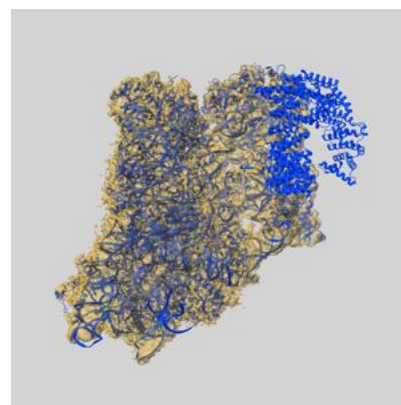
9.1 Map-model overlay [i](#)



X



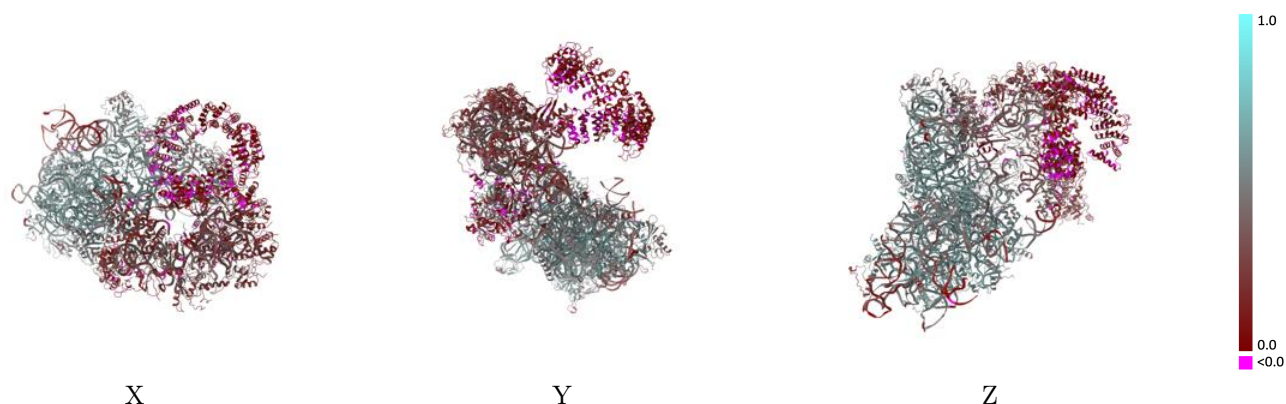
Y



Z

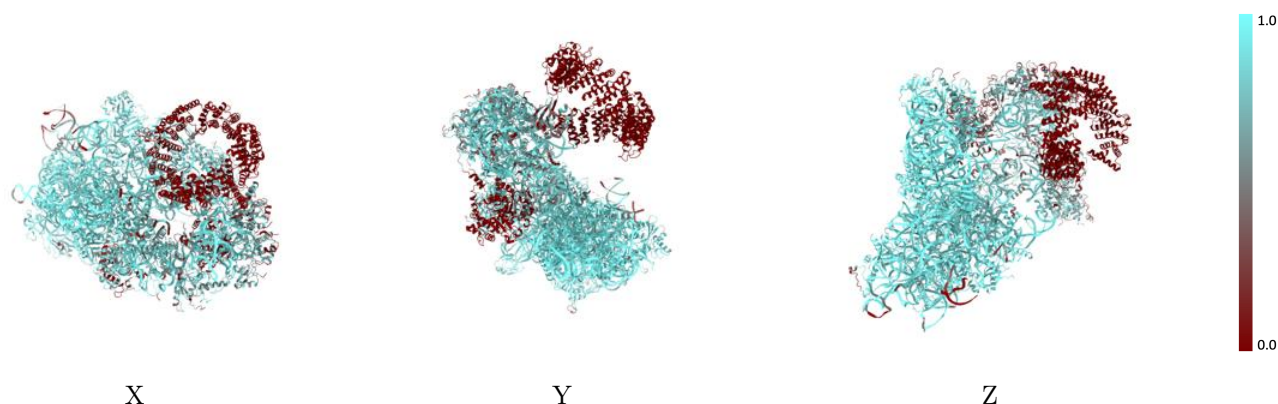
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



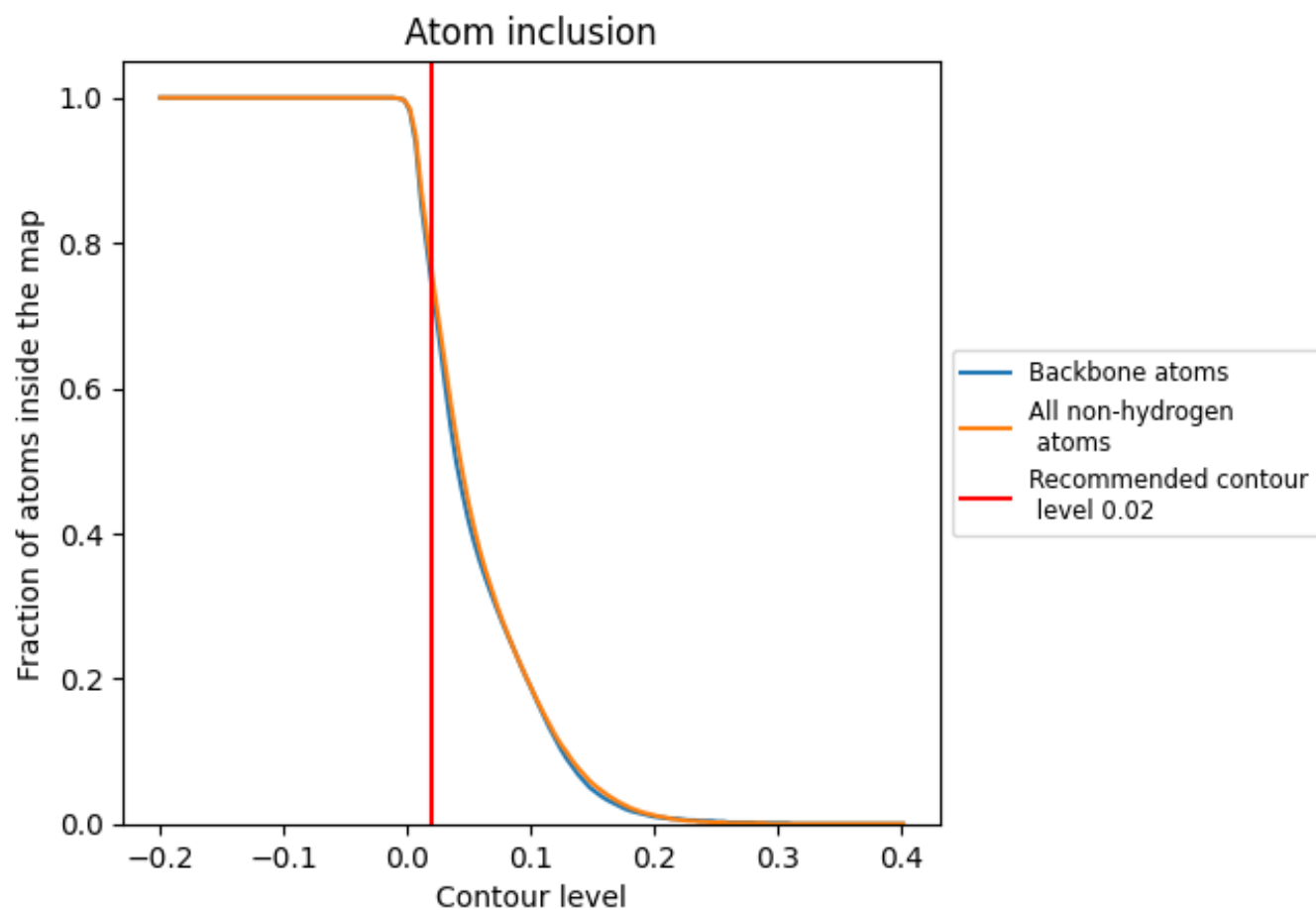
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 74% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7610	 0.3940
0	 0.0000	 0.1170
1	 0.2430	 0.1730
2	 0.8110	 0.4270
3	 0.8660	 0.4360
4	 0.7310	 0.3000
5	 0.6290	 0.2390
6	 0.8850	 0.4780
7	 0.0090	 0.0560
8	 0.6670	 0.3230
A	 0.9380	 0.4650
E	 0.9240	 0.5040
H	 0.9830	 0.5950
I	 0.6070	 0.2190
J	 0.9140	 0.5050
K	 0.9210	 0.4760
L	 0.9140	 0.5270
M	 0.9670	 0.5600
O	 0.9600	 0.5920
P	 0.5460	 0.1850
Q	 0.9620	 0.5670
R	 0.8860	 0.4650
S	 0.7630	 0.3250
T	 0.5130	 0.2070
V	 0.7110	 0.2940
W	 0.6630	 0.2580
Z	 0.9750	 0.5810
a	 0.8830	 0.5120
b	 0.9230	 0.5530
c	 0.4000	 0.1760
e	 0.9290	 0.5180
f	 0.4980	 0.2220
h	 0.9650	 0.5430
i	 0.6670	 0.2080

