



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 06:02 AM UTC

PDB ID : 8CEE / pdb_00008cee
EMDB ID : EMD-16607
Title : Rnase R bound to a 30S degradation intermediate (State I - head-turning)
Authors : Paternoga, H.; Dimitrova-Paternoga, L.; Wilson, D.N.
Deposited on : 2023-02-01
Resolution : 3.70 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

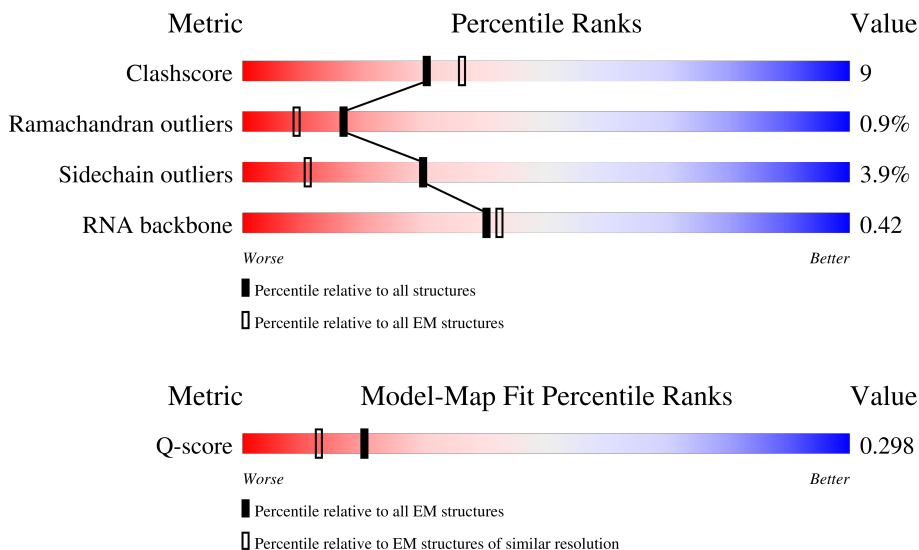
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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

Mol	Chain	Length	Quality of chain
1	A	1554	
2	B	7	
3	C	779	

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Mol	Chain	Length	Quality of chain
4	D	246	72% 76% 9% .. 11%
5	F	200	26% 70% 21% . 8%
6	G	166	15% 69% 24% . 5%
7	I	132	12% 73% 22% . ..
8	L	138	16% 68% 24% 7% .
9	O	89	13% 64% 30% ..
10	P	90	7% 56% 37% 6% .
11	Q	87	16% 67% 25% 5% .
12	S	88	26% 67% 23% 5% 6%
13	T	95	54% 86% 12% .
14	U	79	35% 67% 13% . 19%
15	V	131	73% 73% . 23%
16	E	218	94% 80% 13% 6%
17	H	156	95% 87% 7% ..
18	J	130	83% 72% 11% 17%
19	K	102	93% 82% 10% . 7%
20	M	121	89% 77% 11% . 11%
21	N	61	80% 72% 5% .. 20%
22	R	92	85% 66% 17% . 15%

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 51964 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1333	28597	12753	5245	9266	1333	0	0

- Molecule 2 is a RNA chain called RNA Substrate.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	7	154	70	35	42	7	0	0

- Molecule 3 is a protein called RNase R.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	708	5650	3559	962	1102	27	0	0

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	218	1757	1119	309	323	6	0	0

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	185	1490	942	276	270	2	0	0

- Molecule 6 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	158	1170	736	216	216	2	0	0

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	131	1036	655	191	187	3	0	0

- Molecule 8 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	136	1052	653	211	186	2	0	0

- Molecule 9 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	O	85	710	436	144	129	1	0	0

- Molecule 10 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	P	88	695	441	128	124	2	0	0

- Molecule 11 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	Q	84	691	435	128	126	2	0	0

- Molecule 12 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	S	83	637	390	130	116	1	0	0

- Molecule 13 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	T	95	784	492	138	152	2	0	0

- Molecule 14 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	64	Total	C	N	O	S	0	0
			518	332	96	88	2		

- Molecule 15 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	101	Total	C	N	O	S	0	0
			730	450	136	143	1		

- Molecule 16 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	205	Total	C	N	O	S	0	0
			1615	1009	303	300	3		

- Molecule 17 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	149	Total	C	N	O	S	0	0
			1181	740	220	215	6		

- Molecule 18 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	108	Total	C	N	O	S	0	0
			826	510	160	155	1		

- Molecule 19 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	95	Total	C	N	O	S	0	0
			761	479	139	141	2		

- Molecule 20 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	M	108	Total	C	N	O	0	0
			868	534	176	158		

- Molecule 21 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	N	49	409	263	79	63	4	0	0

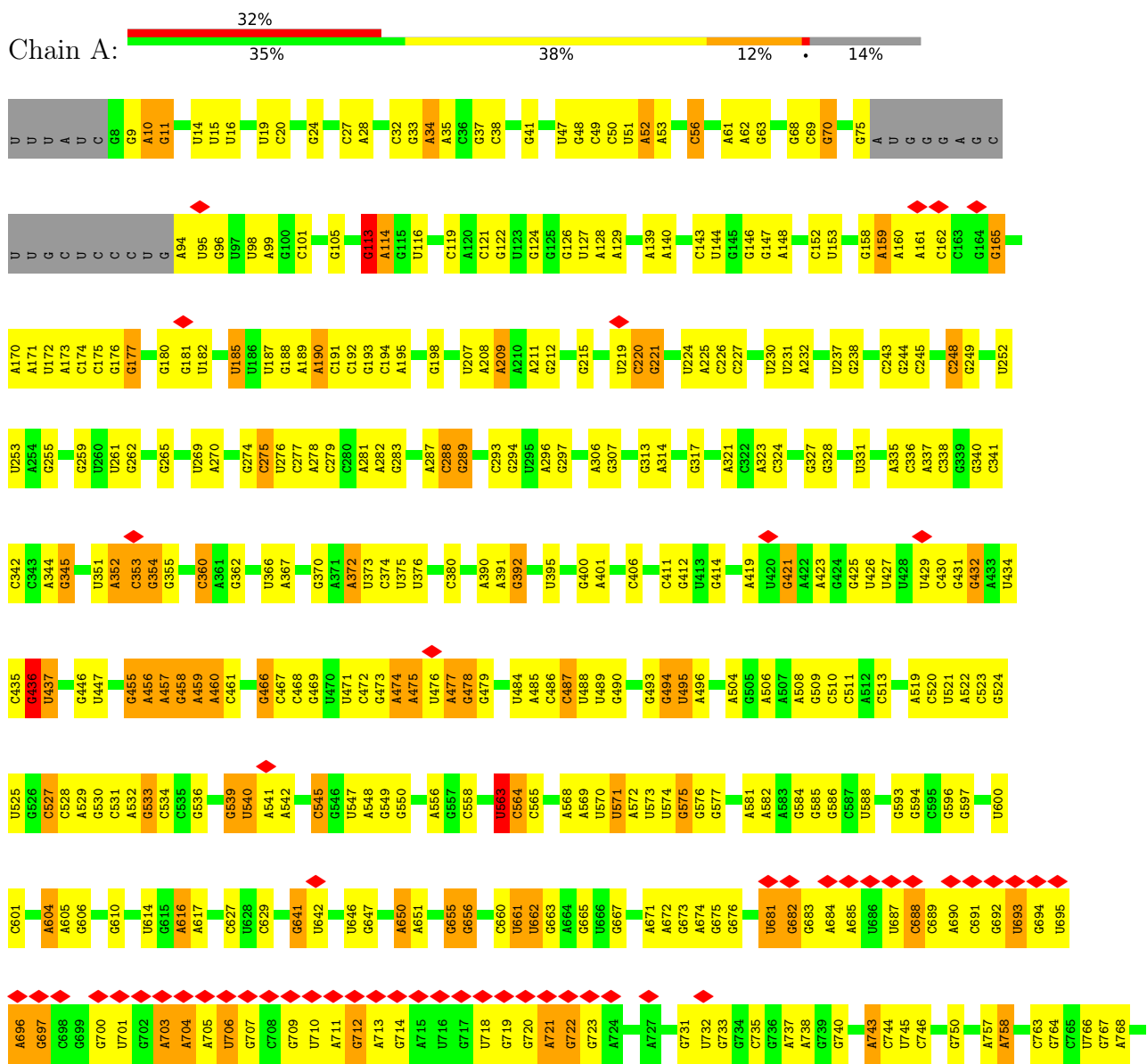
- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	R	78	633	409	112	110	2	0	0

3 Residue-property plots

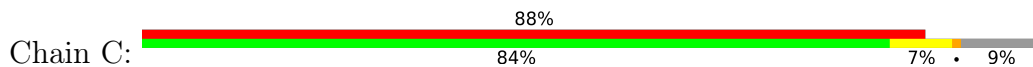
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S rRNA

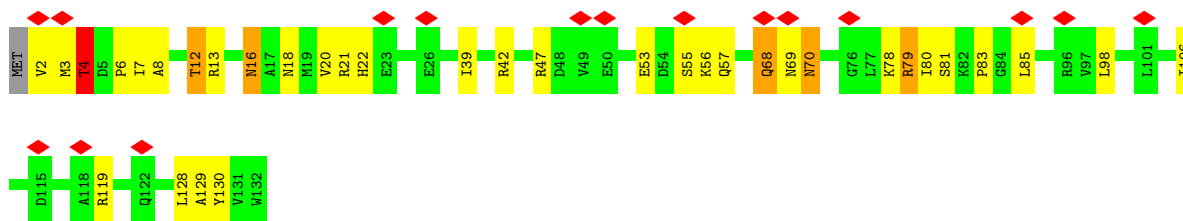


A9002
A9003
A9004
A9005
A9006
A9007
A9008

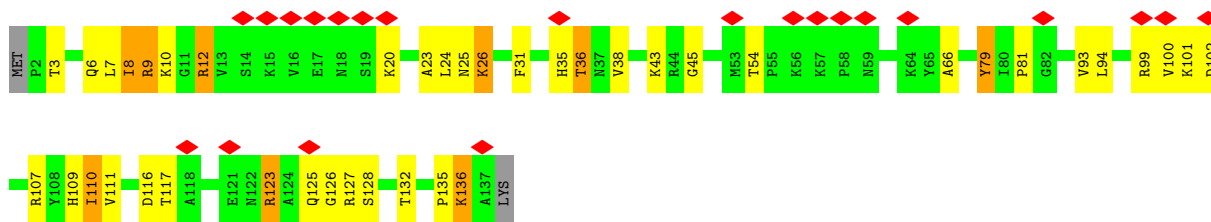
● Molecule 3: RNase R



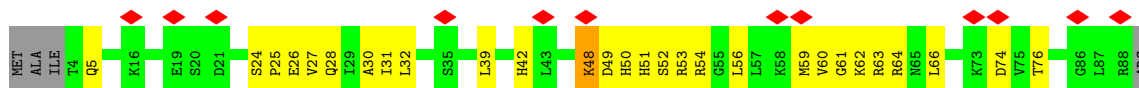
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D61	R62	Y63	G64	L65	P66	E67	K68	R69	N70	L71	I72	K73	G74	K75	I76	S77	A78	H79	A80	K81	L82	G82	F83	A84	F85	L86	L87	P88	E89	D90	T91	S92	L93	S94	D95	V96	F97	I98	P99	P100	M101	L102	L103	N104	T105	A106	M107	N108	M109	D110	I111	V112	M113	V114	R115	L116	M117	S118	Q119	S120	
S121	G122	S123	R124	Q125	E126	G127	T128	I129	I130	R131	I132	L133	E134	R135	A136	I137	Q138	H139	V140	V141	G142	T143	V144	T145	E146	T147	R148	M149	I150	G151	F152	V153	I154	P155	D156	D157	K158	K159	I160	T161	S162	D163	I164	F165	I166	P167	K168	M169	G170	K171	M172	G173	A174	A175	E176	G177	H178	K179	V180		
V181	V182	K183	L184	T185	S186	V187	P188	E189	G190	R191	M192	M193	A194	E195	G196	E197	V198	I199	T200	I201	L202	G203	H204	K205	N206	D207	P208	G209	I210	D211	L212	L213	S214	V215	I216	I217	K218	H219	G220	L221	P222	G223	E224	F225	P226	A227	D228	M229	M230	E231	D232	A233	S234	S235	T236	P237	D238	K239	I240		
D241	E242	K243	D244	L245	K246	D247	R248	R249	D250	L251	D252	D253	Q254	V255	I256	V257	T258	I259	D260	G261	A262	D263	A264	K265	D266	L267	D268	D269	A270	V271	T272	V273	T274	K275	L276	D277	D278	G279	S280	V281	K282	L283	G284	V285	H286	I287	A288	D289	V290	S291	H292	V293	V294	T295	E296	N297	S298	P299	I300		
D301	K302	E303	A304	L305	E306	R307	G308	D309	S310	V311	V312	L313	V314	D315	R316	V317	I318	P319	M320	I321	P322	H323	R324	L325	S326	N327	G328	I329	C330	S331	L332	N333	P334	K335	V336	D337	M338	L339	T340	L341	L342	A343	Q344	I405	L406	R407	D408	K409	R410	M411	D412	R413	G414	A415	V416	D417	F418	D419	F420	Q360	
S361	V362	I363	K364	T365	K366	E367	R368	M369	T370	G371	S372	D373	V374	N375	K376	I377	L378	V379	D380	D381	D382	E383	E384	L385	K386	Q387	K388	V389	E390	P391	L392	V393	P394	M395	F396	K397	D398	M399	E400	R401	L402	A403	Q404	I405	L406	R407	D408	K409	R410	M411	D412	R413	G414	A415	V416	D417	F418	D419	F420	Q360	
K421	F422	A423	K424	V425	L426	V427	D428	D429	F430	G431	A432	V433	K434	D435	V436	V437	I438	R439	T440	R441	S442	V443	A444	E445	P446	L447	I448	E449	E450	F451	M452	L453	V454	A455	A456	M457	T458	V459	A460	E461	H462	F463	H464	W465	S466	T467	M468	L469	R470	I471	V472	R473	I474	H475	E476	E477	N478	A480			
E481	K482	L483	Q484	K485	F486	L487	F488	V489	W490	T491	F492	F493	G494	Y495	V496	V497	K498	G499	T500	A501	G502	N503	I504	H505	P506	R507	L508	Q509	S510	I511	I512	L513	D514	A515	V516	R517	D518	R519	P520	E521	T522	T523	V524	I525	S526	S527	V528	M529	L530	R531	S532	M533	K534	Q535	G536	A537	K538	Y539	D540	P541	T600
Q541	S542	L543	G544	H545	F546	G547	L548	S549	T550	E551	F552	Y553	T554	H555	F556	T557	K558	P559	A560	R561	R562	Y563	P564	D565	P566	L567	V568	H569	I570	L571	D572	I573	R574	T575	Y576	L577	I578	N579	G580	V581	D582	E583	A584	T585	Q586	E587	K588	W589	I590	E591	R592	L593	P594	D595	I596	A597	D598	H599	T600		
S601	S602	M603	E604	R605	R606	A607	V608	D609	A610	E611	R612	E613	T614	D615	D616	L617	K618	K619	A620	E621	Y622	Y623	L624	R625	K626	I627	G628	I629	E630	F631	D632	G633	M634	I635	D636	S637	V638	T639	N640	F641	G642	M643	F644	V645	E646	L647	P648	N649	T650	I651	E652	G653	L654	P655	D656	V657	A658	F659	H660		
T661	D662	D663	Y664	Y665	R666	F667	D668	E669	Q670	H671	F672	A673	M674	I675	G676	E677	R678	T679	G680	N681	V682	F683	L684	I685	G686	D687	E688	I689	T690	V691	K692	G693	V694	D695	V696	N697	K698	D699	E700	R701	I702	I703	D704	F705	E706	I707	P708	G709	M710	LYS	GLY	THR	PRO	ARG	ARG	PRO	ARG	GLU	LEU		



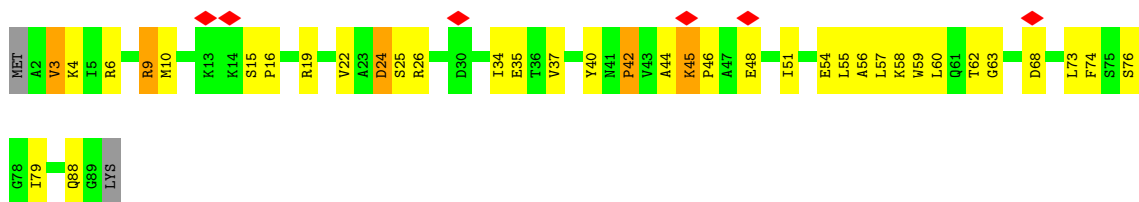
- Molecule 8: 30S ribosomal protein S12



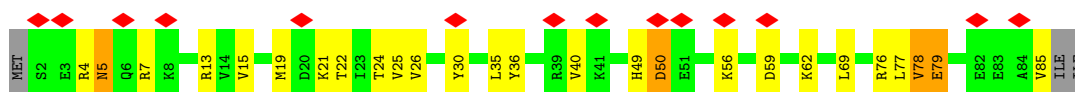
- Molecule 9: 30S ribosomal protein S15



- Molecule 10: 30S ribosomal protein S16

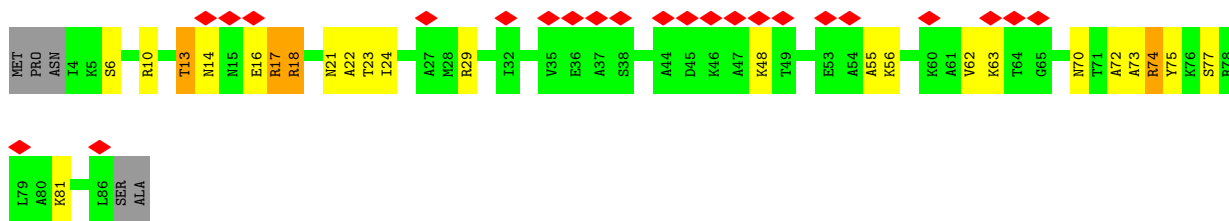


- Molecule 11: 30S ribosomal protein S17

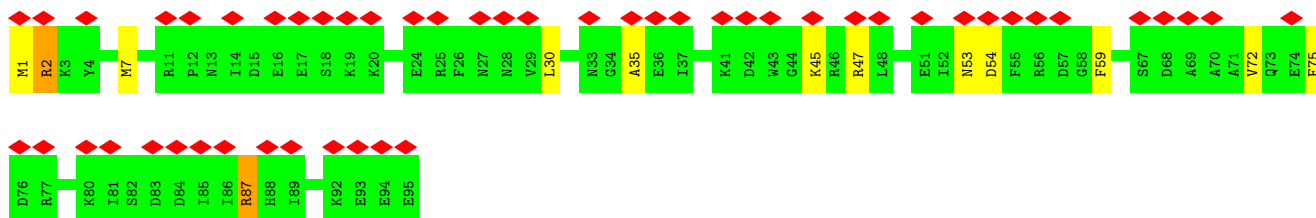
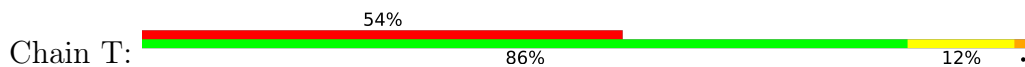


- Molecule 12: 30S ribosomal protein S20

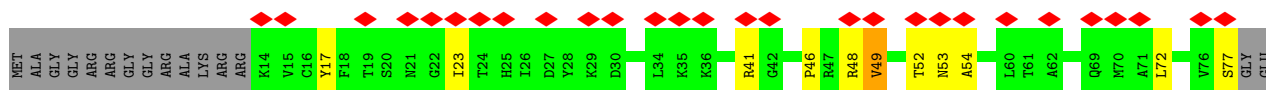




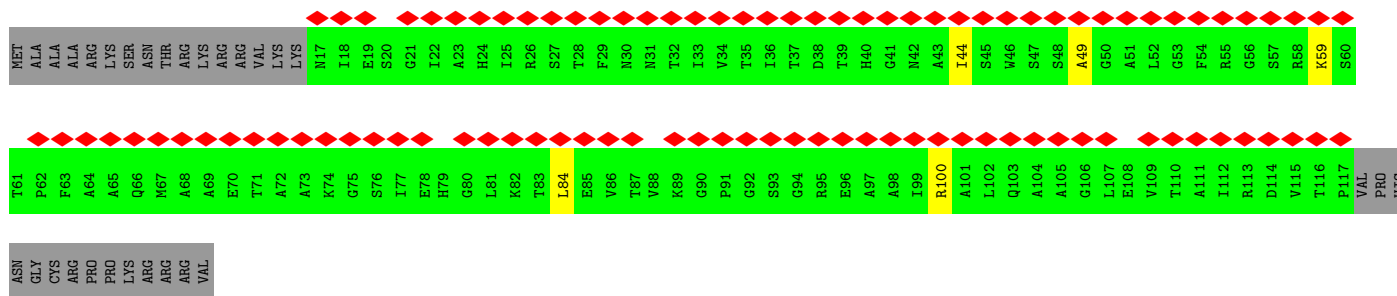
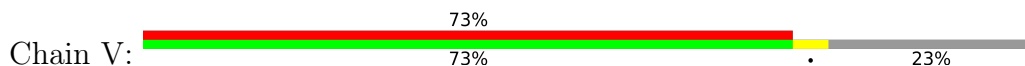
• Molecule 13: 30S ribosomal protein S6



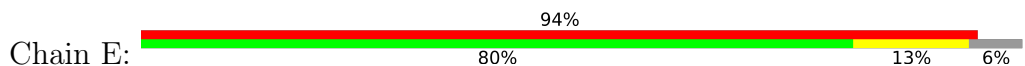
• Molecule 14: 30S ribosomal protein S18

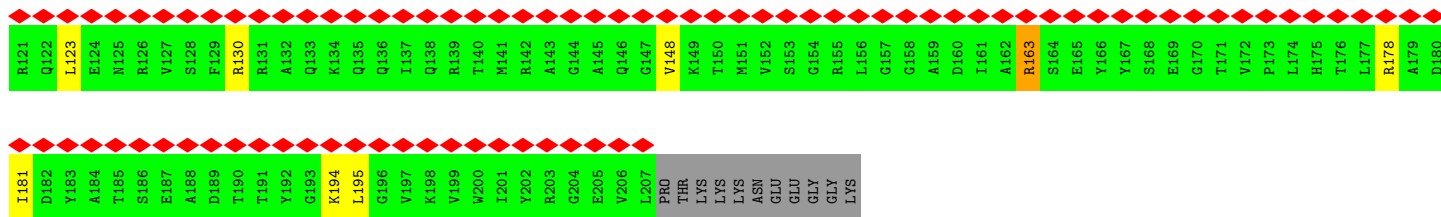


• Molecule 15: 30S ribosomal protein S11

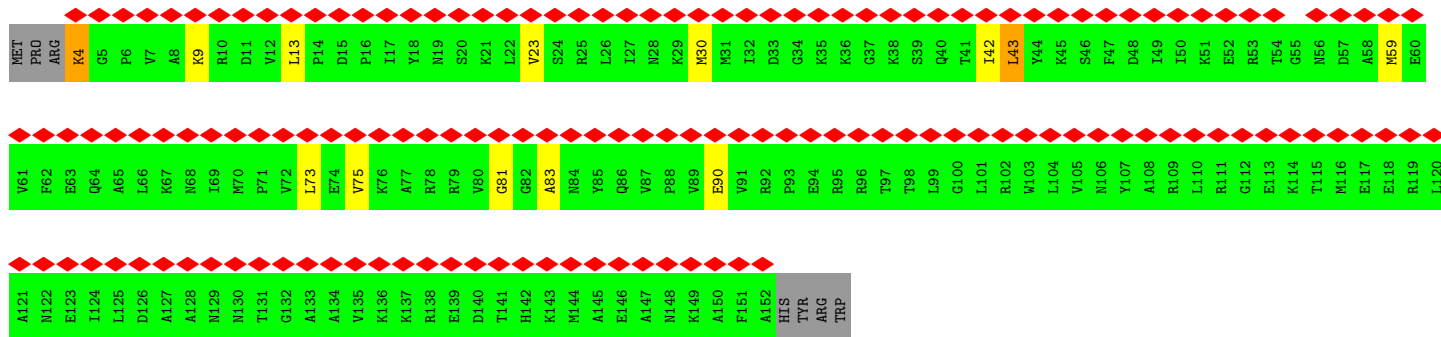
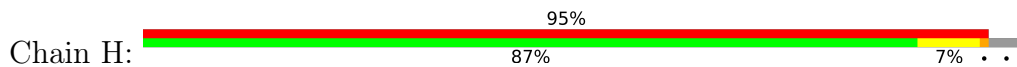


• Molecule 16: 30S ribosomal protein S3

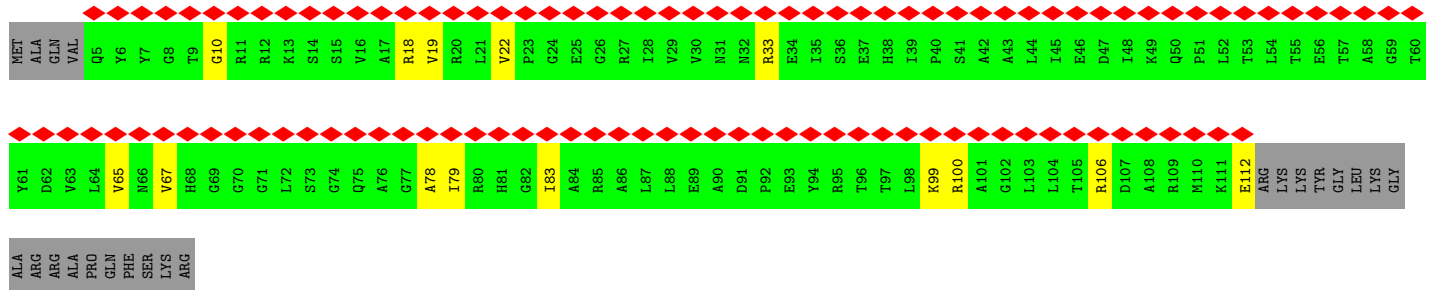
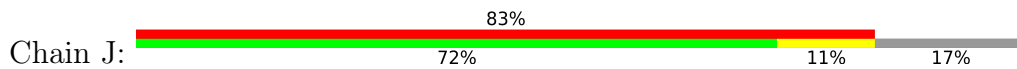




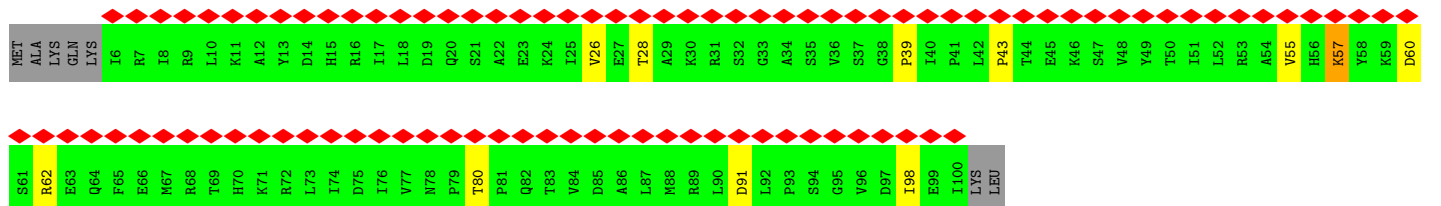
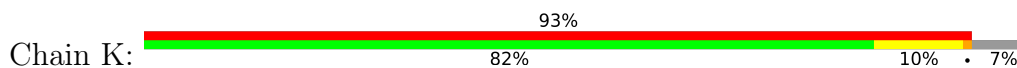
• Molecule 17: 30S ribosomal protein S7



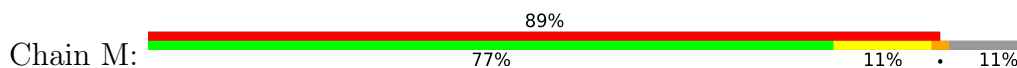
• Molecule 18: 30S ribosomal protein S9



• Molecule 19: 30S ribosomal protein S10

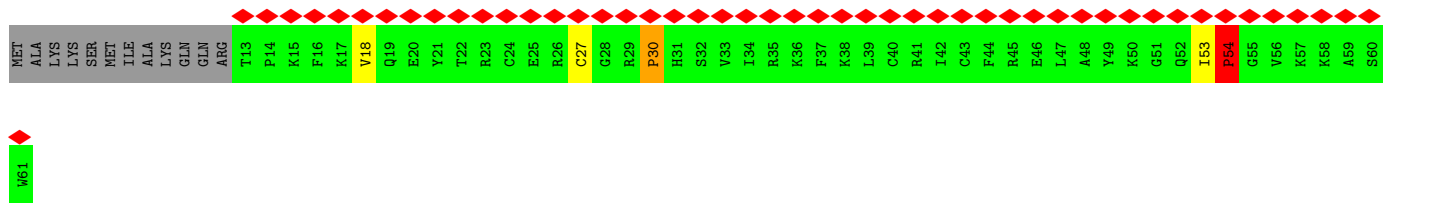
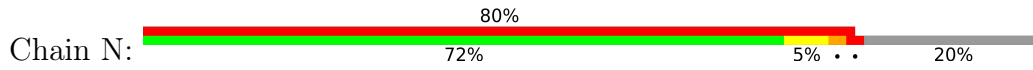


• Molecule 20: 30S ribosomal protein S13

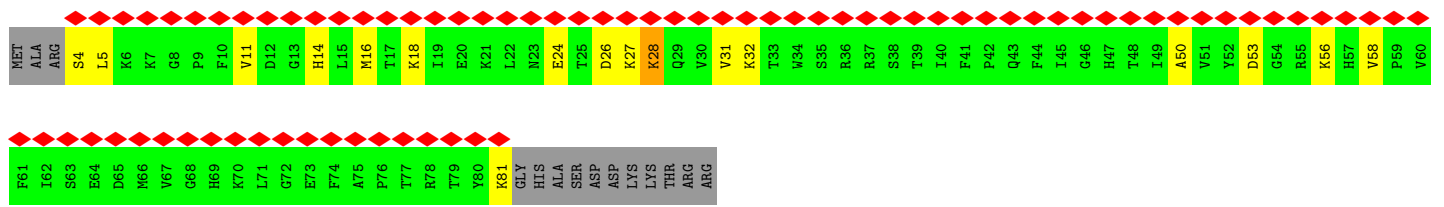
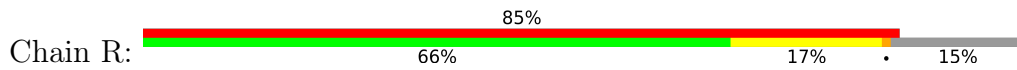




- Molecule 21: 30S ribosomal protein S14



- Molecule 22: 30S ribosomal protein S19



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13611	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0114	Depositor
Map size (Å)	307.2, 307.2, 307.2	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8, 0.8, 0.8	Depositor

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.60	0/32015	0.87	17/49936 (0.0%)
2	B	0.71	0/174	1.49	3/269 (1.1%)
3	C	0.53	0/5748	1.04	7/7760 (0.1%)
4	D	0.55	0/1782	1.22	8/2392 (0.3%)
5	F	0.61	0/1517	1.27	4/2036 (0.2%)
6	G	0.70	0/1182	1.38	7/1591 (0.4%)
7	I	0.73	0/1048	1.37	5/1407 (0.4%)
8	L	0.72	0/1069	1.33	8/1435 (0.6%)
9	O	0.70	0/718	1.37	1/960 (0.1%)
10	P	0.82	1/708 (0.1%)	1.47	4/950 (0.4%)
11	Q	0.71	0/699	1.31	3/933 (0.3%)
12	S	0.74	1/639 (0.2%)	1.42	1/852 (0.1%)
13	T	0.54	0/795	1.13	1/1067 (0.1%)
14	U	0.65	0/526	1.29	1/705 (0.1%)
15	V	0.56	0/740	1.04	1/1002 (0.1%)
16	E	0.57	0/1637	1.09	0/2203
17	H	0.55	0/1196	1.14	0/1604
18	J	0.59	0/836	1.07	0/1128
19	K	0.58	0/773	1.07	0/1044
20	M	0.58	0/873	1.15	0/1166
21	N	0.53	0/419	1.18	2/558 (0.4%)
22	R	0.56	0/649	1.08	0/872
All	All	0.61	2/55743 (0.0%)	1.01	73/81870 (0.1%)

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
3	C	0	4
4	D	0	4
5	F	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	G	0	2
7	I	0	4
8	L	0	3
10	P	0	5
11	Q	0	2
12	S	0	3
13	T	0	1
15	V	0	1
16	E	0	5
18	J	0	2
20	M	0	1
All	All	0	42

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	15	SER	CA-CB	-5.33	1.47	1.53
12	S	77	SER	CA-CB	-5.01	1.45	1.53

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	109	HIS	CA-CB-CG	-9.98	103.81	113.80
12	S	13	THR	CA-CB-OG1	-9.79	94.92	109.60
1	A	980	C	C2'-C3'-O3'	7.93	121.39	109.50
7	I	16	ASN	CA-CB-CG	-7.75	104.85	112.60
3	C	66	PRO	CB-CA-C	7.65	124.19	111.56
4	D	130	PRO	N-CA-C	7.10	127.10	112.47
2	B	9007	A	O3'-P-O5'	-7.01	93.48	104.00
1	A	1294	A	C2'-C3'-O3'	6.77	119.66	109.50
1	A	1113	C	C3'-C2'-C1'	-6.74	94.76	101.50
1	A	1075	U	C2'-C3'-O3'	6.72	119.57	109.50
2	B	9005	A	P-O3'-C3'	-6.68	110.18	120.20
1	A	946	C	C2'-C3'-O3'	6.62	119.44	109.50
3	C	418	PHE	CA-CB-CG	6.19	119.99	113.80
2	B	9002	A	O3'-P-O5'	-6.10	94.85	104.00
6	G	110	PRO	N-CD-CG	-6.06	94.11	103.20
5	F	7	PRO	CB-CA-C	-6.06	104.13	111.46
1	A	563	U	C4'-C3'-C2'	-6.03	96.57	102.60
3	C	69	MET	CA-C-N	6.00	132.99	121.54
3	C	69	MET	C-N-CA	6.00	132.99	121.54
1	A	1113	C	C2'-C3'-O3'	-5.99	100.51	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	102	ASP	CA-CB-CG	5.97	118.57	112.60
21	N	54	PRO	N-CA-C	5.97	124.76	112.47
13	T	87	ARG	CG-CD-NE	5.89	124.95	112.00
6	G	89	PHE	CB-CA-C	5.86	118.79	110.24
11	Q	5	ASN	CB-CA-C	-5.85	99.14	109.62
8	L	79	TYR	CB-CA-C	-5.84	100.22	109.80
4	D	15	HIS	CA-CB-CG	5.83	119.63	113.80
6	G	42	LYS	CB-CA-C	5.80	120.38	111.39
11	Q	24	THR	CA-CB-OG1	5.77	118.26	109.60
7	I	4	THR	N-CA-CB	5.77	120.24	110.49
7	I	69	ASN	CB-CA-C	5.75	121.86	110.42
8	L	54	THR	CB-CA-C	-5.74	104.48	110.17
1	A	487	C	C2'-C3'-O3'	5.73	122.29	113.70
3	C	66	PRO	N-CA-C	-5.72	100.68	112.47
1	A	190	A	C2'-C3'-O3'	5.71	118.07	109.50
7	I	12	THR	CB-CA-C	5.70	119.74	110.96
10	P	34	ILE	N-CA-C	-5.67	106.28	111.67
6	G	85	ILE	CA-C-N	-5.65	115.56	123.13
6	G	85	ILE	C-N-CA	-5.65	115.56	123.13
1	A	563	U	C2'-C3'-O3'	5.64	122.16	113.70
10	P	3	VAL	O-C-N	5.64	128.91	122.93
5	F	95	ASP	CA-CB-CG	5.63	118.23	112.60
8	L	35	HIS	CA-CB-CG	-5.59	108.20	113.80
14	U	52	THR	CB-CA-C	5.56	119.56	109.62
1	A	661	U	C2'-C3'-O3'	5.55	117.83	109.50
8	L	8	ILE	CA-CB-CG1	5.51	119.77	110.40
21	N	30	PRO	N-CA-CB	-5.50	97.48	103.25
15	V	44	ILE	N-CA-C	-5.49	105.74	110.74
1	A	1113	C	O3'-P-O5'	-5.49	95.77	104.00
6	G	140	THR	CA-CB-OG1	-5.47	101.39	109.60
4	D	129	LEU	CA-C-N	5.46	126.67	119.84
4	D	129	LEU	C-N-CA	5.46	126.67	119.84
4	D	123	ASN	CA-CB-CG	5.45	118.05	112.60
9	O	64	ARG	O-C-N	5.43	127.87	122.12
4	D	13	GLY	CA-C-N	5.42	127.59	120.60
4	D	13	GLY	C-N-CA	5.42	127.59	120.60
10	P	54	GLU	CB-CA-C	5.41	119.47	110.81
1	A	113	G	C2'-C3'-O3'	5.36	117.54	109.50
5	F	66	ARG	CG-CD-NE	5.33	123.72	112.00
10	P	42	PRO	CB-CA-C	-5.30	103.43	110.27
7	I	18	ASN	N-CA-C	-5.30	105.50	111.28
1	A	703	A	C2'-C3'-O3'	5.28	117.42	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	110	ILE	O-C-N	5.26	128.50	122.93
3	C	545	HIS	CA-CB-CG	-5.22	108.58	113.80
11	Q	69	LEU	N-CA-C	-5.21	107.47	113.88
1	A	1153	G	C3'-C2'-C1'	-5.18	96.32	101.50
6	G	106	ILE	N-CA-CB	-5.16	105.49	111.83
3	C	428	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	288	C	C2'-C3'-O3'	5.08	117.13	109.50
1	A	436	G	C4'-C3'-O3'	5.08	117.02	109.40
5	F	116	HIS	CA-CB-CG	-5.02	108.78	113.80
8	L	12	ARG	CG-CD-NE	-5.02	100.96	112.00
4	D	14	VAL	N-CA-C	5.01	115.62	110.36

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	441	ARG	Sidechain
3	C	573	ARG	Sidechain
3	C	69	MET	Peptide,Mainchain
4	D	10	LEU	Peptide
4	D	110	ARG	Sidechain
4	D	129	LEU	Peptide
4	D	130	PRO	Peptide
16	E	130	ARG	Sidechain
16	E	16	ARG	Sidechain
16	E	163	ARG	Sidechain
16	E	178	ARG	Sidechain
16	E	58	ARG	Sidechain
5	F	14	ARG	Sidechain
5	F	146	ARG	Sidechain
5	F	2	ALA	Peptide
5	F	3	ARG	Sidechain
5	F	58	ARG	Sidechain
6	G	14	ARG	Sidechain
6	G	32	ARG	Sidechain
7	I	119	ARG	Sidechain
7	I	47	ARG	Sidechain
7	I	68	GLN	Peptide
7	I	79	ARG	Sidechain
18	J	18	ARG	Sidechain
18	J	33	ARG	Sidechain
8	L	123	ARG	Sidechain

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Mol	Chain	Res	Type	Group
8	L	26	LYS	Peptide
8	L	9	ARG	Sidechain
20	M	46	ARG	Sidechain
10	P	44	ALA	Peptide
10	P	45	LYS	Peptide
10	P	6	ARG	Sidechain
10	P	63	GLY	Peptide
10	P	9	ARG	Sidechain
11	Q	4	ARG	Sidechain
11	Q	79	GLU	Peptide
12	S	17	ARG	Sidechain
12	S	29	ARG	Sidechain
12	S	74	ARG	Sidechain
13	T	47	ARG	Sidechain
15	V	84	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	28597	0	14401	546	0
2	B	154	0	78	20	0
3	C	5650	0	5619	53	0
4	D	1757	0	1830	28	0
5	F	1490	0	1518	23	0
6	G	1170	0	1245	22	0
7	I	1036	0	1095	20	0
8	L	1052	0	1112	25	0
9	O	710	0	735	22	0
10	P	695	0	721	15	0
11	Q	691	0	728	15	0
12	S	637	0	696	17	0
13	T	784	0	777	5	0
14	U	518	0	555	8	0
15	V	730	0	735	2	0
16	E	1615	0	1655	8	0
17	H	1181	0	1235	4	0
18	J	826	0	849	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	K	761	0	795	4	0
20	M	868	0	925	12	0
21	N	409	0	427	2	0
22	R	633	0	649	8	0
All	All	51964	0	38380	790	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 9.

All (790) 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)
1:A:344:A:C2'	1:A:345:G:H5''	1.64	1.25
1:A:344:A:H2'	1:A:345:G:C5'	1.73	1.17
1:A:344:A:O2'	1:A:345:G:H5''	1.53	1.08
1:A:344:A:C2'	1:A:345:G:C5'	2.34	1.00
1:A:344:A:H2'	1:A:345:G:H5''	1.36	0.97
1:A:344:A:H2'	1:A:345:G:H5'	1.46	0.96
1:A:955:G:H1	1:A:1245:A:H61	1.12	0.94
1:A:979:A:O2'	1:A:980:C:O2	1.88	0.92
1:A:985:A:H2'	1:A:1374:G:H1'	1.52	0.92
1:A:458:G:H5'	1:A:459:A:H3'	1.52	0.91
1:A:721:A:H3'	1:A:722:G:H5''	1.57	0.86
3:C:66:PRO:C	3:C:70:ASN:H	1.85	0.83
1:A:1251:G:H1	1:A:1304:U:H3	1.23	0.82
4:D:10:LEU:HD22	4:D:15:HIS:CG	2.15	0.81
6:G:83:HIS:ND1	6:G:84:GLU:O	2.14	0.80
1:A:824:A:H1'	1:A:826:C:H3'	1.63	0.79
2:B:9002:A:H62	3:C:531:ARG:HD3	1.47	0.79
4:D:10:LEU:HD11	4:D:14:VAL:HB	1.65	0.78
7:I:39:ILE:HG12	7:I:42:ARG:HH12	1.49	0.78
1:A:980:C:H2'	19:K:57:LYS:HG2	1.66	0.78
2:B:9002:A:N7	3:C:531:ARG:NE	2.34	0.76
1:A:673:G:H22	1:A:750:G:H1	1.32	0.75
1:A:1134:G:H1	1:A:1158:C:H42	1.32	0.75
3:C:66:PRO:O	3:C:69:MET:N	2.20	0.74
1:A:720:G:H2'	1:A:721:A:H8	1.52	0.73
2:B:9004:A:C2	3:C:418:PHE:HB2	2.23	0.73
1:A:948:A:H1'	1:A:1386:A:H5'	1.71	0.73
1:A:474:A:H2'	1:A:475:A:C8	2.24	0.71
3:C:66:PRO:O	3:C:70:ASN:N	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:10:LEU:HD11	4:D:14:VAL:N	2.04	0.71
4:D:10:LEU:HD21	4:D:13:GLY:C	2.14	0.71
4:D:10:LEU:HD22	4:D:15:HIS:ND1	2.05	0.71
1:A:1045:G:H3'	1:A:1046:G:H5''	1.74	0.70
3:C:420:PHE:CE2	3:C:530:LEU:HD11	2.26	0.70
1:A:1174:U:H3	1:A:1180:A:H62	1.40	0.69
1:A:1111:A:H4'	1:A:1112:A:H4'	1.73	0.69
6:G:15:LEU:HD11	6:G:17:THR:O	1.93	0.69
4:D:10:LEU:HD11	4:D:14:VAL:CA	2.23	0.69
1:A:421:G:H21	1:A:436:G:H1'	1.56	0.68
1:A:655:G:H3'	1:A:656:G:H5''	1.74	0.68
1:A:456:A:H2	1:A:495:U:H3	1.39	0.68
1:A:775:A:H2'	1:A:776:A:O4'	1.94	0.68
1:A:663:G:H1	1:A:763:C:H5	1.42	0.68
1:A:1057:G:H2'	1:A:1058:G:H8	1.59	0.68
1:A:1219:C:H1'	1:A:1223:U:H2'	1.77	0.67
1:A:1337:C:H2'	1:A:1338:G:C8	2.29	0.67
1:A:955:G:H1	1:A:1245:A:N6	1.88	0.67
4:D:10:LEU:HD11	4:D:14:VAL:CB	2.24	0.67
6:G:110:PRO:HG2	6:G:136:MET:HE3	1.77	0.67
1:A:989:C:H1'	1:A:1326:C:H42	1.61	0.66
1:A:1094:G:H1'	1:A:1113:C:H41	1.59	0.66
1:A:1245:A:H4'	1:A:1313:G:H4'	1.77	0.66
4:D:176:ALA:HB3	4:D:183:ILE:HD11	1.76	0.66
1:A:1183:G:H4'	3:C:148:ARG:HG2	1.77	0.65
1:A:713:A:H2'	1:A:714:G:H8	1.62	0.65
1:A:1150:U:H2'	1:A:1151:G:C8	2.32	0.65
1:A:1102:A:H2'	1:A:1103:A:C8	2.31	0.65
1:A:693:U:H3'	1:A:694:G:C8	2.32	0.65
1:A:1012:U:N3	1:A:1046:G:N7	2.45	0.65
1:A:1296:A:H2'	1:A:1297:A:C8	2.32	0.64
1:A:532:A:C2	8:L:101:LYS:HB3	2.32	0.64
1:A:713:A:H2'	1:A:714:G:C8	2.32	0.64
1:A:629:C:C2	5:F:128:ILE:HD13	2.32	0.64
3:C:58:THR:HG21	3:C:93:LEU:HD22	1.80	0.64
1:A:1314:G:H22	1:A:1340:G:H2'	1.61	0.63
3:C:567:ILE:HD13	3:C:596:ILE:HG21	1.80	0.63
4:D:10:LEU:CD1	4:D:14:VAL:HB	2.29	0.63
1:A:466:G:H1	1:A:484:U:H3	1.46	0.63
2:B:9004:A:C1'	3:C:530:LEU:HD22	2.28	0.63
1:A:224:U:H2'	1:A:225:A:C8	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:53:ARG:O	9:O:56:LEU:HB3	2.00	0.62
1:A:1385:U:H2'	1:A:1386:A:H8	1.64	0.62
1:A:720:G:H2'	1:A:721:A:C8	2.35	0.62
1:A:1385:U:H2'	1:A:1386:A:C8	2.34	0.62
1:A:1167:C:H4'	4:D:132:LYS:HE2	1.80	0.62
1:A:779:C:H2'	1:A:780:G:C8	2.35	0.62
1:A:1248:A:H62	1:A:1308:A:H62	1.47	0.62
1:A:974:A:H1'	1:A:980:C:H5'	1.81	0.62
18:J:65:VAL:HG11	18:J:79:ILE:HG12	1.82	0.62
1:A:27:C:H5'	1:A:533:G:H1'	1.82	0.61
8:L:79:TYR:HB2	8:L:100:VAL:HG21	1.82	0.61
1:A:269:U:OP2	12:S:74:ARG:NH2	2.34	0.61
1:A:277:C:H2'	1:A:278:A:C8	2.36	0.61
1:A:261:U:H2'	1:A:262:G:C8	2.36	0.61
1:A:1115:A:H2'	1:A:1116:G:C8	2.35	0.61
1:A:1020:C:H1'	1:A:1031:A:H1'	1.82	0.61
1:A:1097:G:N2	1:A:1109:G:H1'	2.16	0.61
1:A:931:U:H2'	1:A:932:G:C8	2.34	0.61
8:L:79:TYR:O	8:L:81:PRO:HD3	1.99	0.61
1:A:1265:C:H5''	1:A:1266:A:H5'	1.82	0.61
1:A:1250:G:H2'	1:A:1251:G:C8	2.35	0.61
2:B:9002:A:N7	3:C:531:ARG:CZ	2.64	0.61
1:A:331:U:O4'	12:S:14:ASN:ND2	2.34	0.60
10:P:73:LEU:O	10:P:76:SER:OG	2.15	0.60
1:A:681:U:H2'	1:A:682:G:H8	1.66	0.60
1:A:411:C:H5''	5:F:129:PRO:HD2	1.83	0.60
1:A:528:C:H2'	1:A:529:A:C8	2.37	0.60
1:A:700:G:H1'	1:A:706:U:H3	1.66	0.60
1:A:1014:A:H2'	1:A:1015:C:C6	2.37	0.60
1:A:1050:A:H2'	1:A:1051:G:C8	2.37	0.60
1:A:827:G:H1	1:A:829:U:H2'	1.67	0.60
1:A:1098:G:H1	1:A:1107:C:H42	1.50	0.60
1:A:1128:A:H1'	1:A:1188:A:C5	2.37	0.60
5:F:139:ILE:N	5:F:139:ILE:HD12	2.16	0.59
12:S:21:ASN:O	12:S:24:ILE:N	2.35	0.59
1:A:1166:A:N6	1:A:1187:G:H1'	2.17	0.59
1:A:819:C:H1'	1:A:909:C:H41	1.67	0.59
1:A:1364:G:H2'	1:A:1365:G:C8	2.37	0.59
1:A:75:G:H1'	1:A:94:A:N6	2.17	0.59
1:A:70:G:H1	1:A:99:A:H62	1.48	0.59
1:A:596:G:H4'	7:I:4:THR:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:491:THR:O	14:U:41:ARG:NH2	2.36	0.59
7:I:12:THR:O	7:I:13:ARG:C	2.43	0.58
1:A:1337:C:H2'	1:A:1338:G:H8	1.68	0.58
3:C:484:GLN:HE22	15:V:100:ARG:HG3	1.68	0.58
1:A:1026:A:H4'	1:A:1227:C:H4'	1.85	0.58
1:A:1375:C:H2'	1:A:1376:C:C6	2.38	0.58
1:A:513:C:H42	1:A:550:G:H1	1.50	0.58
1:A:1053:G:H2'	1:A:1054:A:C8	2.38	0.58
1:A:159:A:H1'	1:A:352:A:C5	2.39	0.58
1:A:1263:G:H2'	1:A:1264:G:H8	1.68	0.58
1:A:1060:G:H1	1:A:1217:C:H42	1.52	0.58
5:F:54:LYS:HG3	5:F:197:PHE:CD2	2.39	0.58
1:A:1154:C:H4'	1:A:1155:A:H8	1.69	0.57
9:O:27:VAL:O	9:O:30:ALA:HB3	2.04	0.57
20:M:9:ILE:HB	20:M:18:SER:HB3	1.86	0.57
1:A:70:G:H1	1:A:99:A:N6	2.02	0.57
3:C:71:LEU:HD23	3:C:115:ARG:HA	1.85	0.57
1:A:745:U:H2'	1:A:746:C:C6	2.39	0.57
1:A:1024:A:H2'	1:A:1025:G:C8	2.39	0.57
2:B:9002:A:N6	3:C:531:ARG:HD3	2.19	0.57
1:A:573:U:P	8:L:12:ARG:HH21	2.27	0.57
9:O:63:ARG:O	9:O:66:LEU:N	2.36	0.57
1:A:949:G:H1'	1:A:1385:U:H1'	1.86	0.57
2:B:9004:A:C2	3:C:418:PHE:CB	2.87	0.57
3:C:563:TYR:CE2	3:C:567:ILE:HD11	2.40	0.57
1:A:19:U:H2'	1:A:20:C:C6	2.39	0.57
1:A:1123:C:H42	1:A:1196:G:H1	1.53	0.57
1:A:1202:G:H2'	1:A:1203:U:C6	2.39	0.57
1:A:777:A:H3'	1:A:778:G:C8	2.39	0.56
1:A:1227:C:H2'	1:A:1228:U:C6	2.40	0.56
3:C:524:VAL:HG11	3:C:685:ILE:HG23	1.86	0.56
7:I:39:ILE:HG12	7:I:42:ARG:NH1	2.19	0.56
1:A:1017:A:H2'	1:A:1018:U:O4'	2.04	0.56
1:A:1034:U:H4'	1:A:1035:C:H5	1.70	0.56
10:P:9:ARG:CZ	10:P:16:PRO:HB3	2.36	0.56
10:P:57:LEU:O	10:P:58:LYS:C	2.48	0.56
1:A:1220:U:H5''	1:A:1221:U:H5''	1.87	0.56
1:A:1109:G:H5''	1:A:1110:C:H5	1.71	0.56
1:A:1387:C:C2	1:A:1388:G:H1'	2.41	0.56
1:A:1129:U:H3	1:A:1163:G:H1	1.54	0.56
5:F:75:ALA:HB2	5:F:89:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:A:H1'	1:A:283:G:C8	2.42	0.55
1:A:950:C:H2'	1:A:951:G:C8	2.42	0.55
1:A:1332:G:H2'	1:A:1333:A:C8	2.42	0.55
1:A:1187:G:N7	18:J:99:LYS:NZ	2.44	0.55
1:A:1315:A:H61	1:A:1340:G:H1'	1.70	0.55
11:Q:21:LYS:HA	11:Q:50:ASP:O	2.06	0.55
1:A:531:C:H1'	1:A:545:C:H5''	1.88	0.55
1:A:1024:A:H5''	22:R:14:HIS:CD2	2.42	0.55
1:A:1315:A:N6	1:A:1340:G:H1'	2.20	0.55
12:S:72:ALA:O	12:S:73:ALA:C	2.48	0.55
1:A:681:U:H2'	1:A:682:G:C8	2.41	0.55
1:A:1020:C:N4	1:A:1029:G:H1	2.05	0.55
1:A:1045:G:H3'	1:A:1046:G:C5'	2.36	0.55
1:A:1044:G:H2'	1:A:1045:G:C8	2.42	0.55
1:A:1131:U:H2'	1:A:1132:U:C6	2.41	0.55
8:L:66:ALA:HB3	8:L:110:ILE:HD11	1.87	0.55
1:A:1275:G:N2	1:A:1277:G:H3'	2.22	0.55
2:B:9004:A:C2	2:B:9005:A:C4	2.94	0.55
19:K:26:VAL:HG21	19:K:39:PRO:HD3	1.89	0.55
1:A:901:U:H2'	1:A:902:A:H8	1.72	0.54
1:A:951:G:H1	1:A:1351:C:H42	1.55	0.54
1:A:1073:C:H5'	1:A:1202:G:H22	1.72	0.54
4:D:133:GLU:OE1	4:D:134:VAL:HA	2.08	0.54
14:U:53:ASN:OD1	14:U:54:ALA:N	2.40	0.54
1:A:27:C:H2'	1:A:28:A:C8	2.43	0.54
1:A:527:C:H2'	1:A:539:G:C8	2.42	0.54
1:A:1016:A:H62	1:A:1033:G:H21	1.55	0.54
1:A:1079:C:H42	1:A:1116:G:H1	1.55	0.54
5:F:54:LYS:HG3	5:F:197:PHE:CE2	2.42	0.54
1:A:1016:A:H61	1:A:1033:G:H2'	1.72	0.54
1:A:1261:A:H2'	1:A:1262:G:H8	1.71	0.54
1:A:1314:G:N2	1:A:1340:G:H2'	2.21	0.54
1:A:548:A:H2'	1:A:549:G:C8	2.43	0.54
1:A:1357:U:H2'	1:A:1358:A:H8	1.73	0.54
7:I:20:VAL:O	7:I:21:ARG:C	2.50	0.54
7:I:80:ILE:HD11	7:I:130:TYR:CD2	2.42	0.54
1:A:477:A:H2'	1:A:478:G:H5'	1.90	0.54
1:A:1228:U:H2'	1:A:1229:G:C8	2.43	0.54
4:D:10:LEU:HG	4:D:13:GLY:H	1.73	0.54
6:G:135:ASN:O	6:G:136:MET:C	2.50	0.54
1:A:113:G:H4'	1:A:114:A:O5'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1185:A:H2'	1:A:1186:G:C8	2.43	0.54
7:I:78:LYS:O	7:I:129:ALA:HA	2.07	0.54
1:A:390:A:H2'	1:A:391:A:C8	2.43	0.54
1:A:903:C:H2'	1:A:904:G:C8	2.43	0.54
1:A:1052:U:H2'	1:A:1053:G:C4	2.43	0.54
1:A:778:G:H21	1:A:820:C:H1'	1.72	0.53
1:A:827:G:N1	1:A:829:U:H2'	2.23	0.53
1:A:1068:G:H1	1:A:1208:U:H3	1.56	0.53
1:A:1134:G:H3'	1:A:1153:G:H22	1.72	0.53
1:A:127:U:OP2	11:Q:5:ASN:ND2	2.41	0.53
3:C:56:VAL:HG11	3:C:116:LEU:HD13	1.89	0.53
1:A:276:U:H2'	1:A:277:C:C6	2.44	0.53
1:A:818:G:H2'	1:A:819:C:C6	2.43	0.53
1:A:896:G:H1	1:A:921:U:H3	1.57	0.53
1:A:960:U:H2'	1:A:961:G:H8	1.72	0.53
1:A:777:A:H3'	1:A:778:G:H8	1.73	0.53
1:A:979:A:O2'	1:A:980:C:C2	2.44	0.53
1:A:1341:A:H2'	1:A:1342:A:C8	2.44	0.53
1:A:1364:G:H2'	1:A:1365:G:H8	1.73	0.53
3:C:69:MET:O	3:C:71:LEU:HG	2.09	0.53
1:A:56:C:H2'	1:A:360:C:H41	1.72	0.53
1:A:956:A:H2'	1:A:957:G:C8	2.44	0.53
8:L:45:GLY:O	8:L:93:VAL:HG22	2.09	0.53
16:E:51:VAL:HG22	16:E:69:THR:HB	1.90	0.53
1:A:69:C:H2'	1:A:70:G:C8	2.43	0.53
1:A:1325:G:O6	22:R:4:SER:N	2.42	0.53
3:C:66:PRO:C	3:C:70:ASN:N	2.63	0.53
1:A:37:G:H2'	1:A:38:C:C6	2.44	0.52
3:C:116:LEU:HD22	3:C:125:GLN:HE21	1.74	0.52
1:A:1024:A:C2	1:A:1228:U:H1'	2.44	0.52
1:A:1150:U:H2'	1:A:1151:G:H8	1.72	0.52
9:O:50:HIS:O	9:O:53:ARG:N	2.42	0.52
1:A:1125:U:H3	1:A:1194:G:H1	1.58	0.52
1:A:1277:G:H2'	1:A:1278:A:C8	2.44	0.52
1:A:344:A:C3'	1:A:345:G:C5'	2.87	0.52
1:A:1174:U:H2'	1:A:1175:G:C8	2.45	0.52
8:L:127:ARG:HD2	8:L:132:THR:O	2.10	0.52
1:A:423:A:N6	1:A:436:G:H1	2.07	0.52
4:D:133:GLU:OE1	4:D:137:LEU:HD12	2.09	0.52
8:L:79:TYR:CB	8:L:100:VAL:HG21	2.39	0.52
1:A:909:C:H2'	1:A:910:A:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:PRO:HB2	3:C:93:LEU:HD21	1.90	0.52
1:A:160:A:H2'	1:A:161:A:C8	2.44	0.52
1:A:1018:U:H2'	1:A:1031:A:H61	1.75	0.52
1:A:1010:U:H2'	1:A:1011:C:C6	2.45	0.52
1:A:1181:C:H2'	1:A:1182:C:C6	2.45	0.52
3:C:69:MET:C	3:C:71:LEU:HG	2.35	0.52
5:F:75:ALA:HA	5:F:78:LEU:HD13	1.91	0.52
1:A:61:A:H5''	1:A:395:U:H5''	1.91	0.52
1:A:1037:C:H2'	1:A:1038:C:C6	2.45	0.52
1:A:1091:G:OP2	6:G:52:LYS:HE3	2.09	0.51
1:A:1030:G:H2'	1:A:1031:A:H8	1.75	0.51
1:A:1082:G:H2'	1:A:1083:U:C6	2.46	0.51
1:A:997:G:H1	1:A:1227:C:H42	1.56	0.51
1:A:1187:G:N2	1:A:1189:A:H3'	2.25	0.51
1:A:1274:C:H2'	1:A:1275:G:C8	2.46	0.51
3:C:567:ILE:CD1	3:C:596:ILE:HG21	2.40	0.51
1:A:144:U:H3	1:A:176:G:H1	1.57	0.51
1:A:224:U:H1'	1:A:475:A:H61	1.76	0.51
1:A:527:C:H6	1:A:539:G:H5'	1.75	0.51
1:A:1014:A:H3'	1:A:1034:U:C2	2.46	0.51
1:A:1047:C:H2'	1:A:1048:A:C8	2.45	0.51
1:A:11:G:H5'	6:G:108:GLY:HA3	1.92	0.51
1:A:851:U:O2'	1:A:854:C:N4	2.42	0.51
1:A:958:C:H42	1:A:1242:G:H1	1.57	0.51
1:A:1175:G:H1'	1:A:1179:A:H61	1.74	0.51
1:A:943:G:H2'	1:A:945:A:C8	2.45	0.51
6:G:49:GLY:N	6:G:67:ALA:HB2	2.26	0.51
1:A:95:U:H2'	1:A:96:G:C8	2.46	0.51
3:C:418:PHE:HB3	3:C:420:PHE:CE2	2.46	0.51
12:S:72:ALA:O	12:S:75:TYR:N	2.44	0.51
1:A:523:C:H2'	1:A:524:G:H8	1.74	0.51
1:A:1167:C:O2'	1:A:1169:G:H5'	2.11	0.51
1:A:1291:C:H2'	1:A:1292:C:C6	2.46	0.51
1:A:176:G:H3'	1:A:177:G:H8	1.75	0.51
1:A:523:C:H2'	1:A:524:G:C8	2.46	0.51
1:A:588:U:O3'	9:O:54:ARG:NH1	2.43	0.51
1:A:1265:C:H3'	1:A:1287:C:N4	2.25	0.51
6:G:131:ASN:O	6:G:136:MET:HE2	2.09	0.51
10:P:74:PHE:HB3	10:P:79:ILE:HB	1.93	0.51
1:A:779:C:H2'	1:A:780:G:H8	1.75	0.50
1:A:986:G:C2	1:A:1371:C:H2'	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:A:N6	1:A:355:G:H1'	2.27	0.50
1:A:495:U:H2'	1:A:496:A:H8	1.76	0.50
1:A:1235:C:H6	20:M:102:SER:HB2	1.77	0.50
1:A:1377:G:OP1	19:K:62:ARG:NH1	2.45	0.50
2:B:9003:A:H2'	3:C:531:ARG:HG2	1.93	0.50
3:C:66:PRO:HB2	3:C:70:ASN:HA	1.93	0.50
1:A:126:G:H5''	11:Q:5:ASN:HB3	1.93	0.50
1:A:1246:C:H4'	1:A:1309:G:H22	1.76	0.50
1:A:1347:G:H2'	1:A:1348:A:C8	2.45	0.50
5:F:191:GLU:O	5:F:194:ILE:HB	2.11	0.50
22:R:32:LYS:HA	22:R:50:ALA:HB3	1.92	0.50
1:A:980:C:H41	1:A:1240:G:H1'	1.77	0.50
1:A:400:G:H2'	1:A:401:A:C8	2.47	0.50
1:A:1005:C:H2'	1:A:1006:A:C8	2.47	0.50
1:A:1357:U:H2'	1:A:1358:A:C8	2.46	0.50
3:C:529:MET:O	3:C:532:SER:OG	2.27	0.50
10:P:59:TRP:O	10:P:60:LEU:C	2.52	0.50
1:A:243:C:H2'	1:A:244:G:H8	1.76	0.50
1:A:1154:C:H4'	1:A:1155:A:C8	2.46	0.50
18:J:10:GLY:HA3	18:J:78:ALA:O	2.12	0.49
1:A:146:G:H2'	1:A:147:G:C8	2.47	0.49
1:A:527:C:C6	1:A:539:G:H5'	2.47	0.49
1:A:870:A:H61	1:A:879:A:H1'	1.77	0.49
1:A:937:G:H4'	1:A:938:G:O5'	2.12	0.49
1:A:533:G:H2'	1:A:534:C:C6	2.47	0.49
1:A:563:U:H2'	1:A:564:C:C6	2.47	0.49
5:F:57:LEU:O	5:F:60:MET:HB3	2.13	0.49
1:A:1107:C:H2'	1:A:1108:C:C6	2.48	0.49
5:F:65:GLU:O	5:F:68:PHE:N	2.45	0.49
9:O:52:SER:O	9:O:53:ARG:C	2.55	0.49
2:B:9005:A:C6	2:B:9006:A:C5	3.01	0.49
9:O:50:HIS:O	9:O:51:HIS:C	2.52	0.49
1:A:614:U:H3	1:A:641:G:H1	1.61	0.49
1:A:823:A:H2'	1:A:825:A:H5'	1.94	0.49
1:A:1085:U:O3'	4:D:178:LYS:NZ	2.45	0.49
1:A:1261:A:H2'	1:A:1262:G:C8	2.47	0.49
2:B:9002:A:N7	3:C:531:ARG:CD	2.75	0.49
11:Q:25:VAL:HG12	11:Q:26:VAL:N	2.28	0.49
1:A:1054:A:C5	1:A:1055:C:H1'	2.48	0.49
4:D:10:LEU:HD11	4:D:14:VAL:H	1.75	0.49
1:A:468:C:H2'	1:A:469:G:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:G:N1	1:A:763:C:H5	2.10	0.49
1:A:1265:C:H5'	1:A:1267:G:H1'	1.94	0.49
5:F:29:ARG:O	5:F:31:TYR:N	2.46	0.49
1:A:215:G:H1	1:A:224:U:H3	1.60	0.49
1:A:1218:C:H2'	1:A:1219:C:H6	1.77	0.49
1:A:1228:U:H2'	1:A:1229:G:H8	1.76	0.49
1:A:1245:A:H2'	1:A:1246:C:O4'	2.12	0.49
1:A:352:A:H5'	1:A:353:C:C5	2.47	0.48
1:A:1273:C:H2'	1:A:1274:C:C6	2.48	0.48
3:C:495:TYR:CZ	3:C:516:VAL:HG12	2.47	0.48
10:P:10:MET:HE1	10:P:19:ARG:CZ	2.43	0.48
1:A:328:G:H1	1:A:341:C:H42	1.61	0.48
1:A:1025:G:H2'	1:A:1026:A:C8	2.47	0.48
1:A:1077:A:H5''	1:A:1104:G:N7	2.29	0.48
1:A:1167:C:H5''	1:A:1190:G:H22	1.77	0.48
1:A:1207:A:H2'	1:A:1208:U:C6	2.48	0.48
3:C:524:VAL:HG11	3:C:685:ILE:CG2	2.43	0.48
7:I:78:LYS:O	7:I:130:TYR:N	2.46	0.48
8:L:26:LYS:O	8:L:43:LYS:NZ	2.46	0.48
10:P:4:LYS:O	10:P:22:VAL:HA	2.12	0.48
10:P:24:ASP:OD2	10:P:26:ARG:HB2	2.12	0.48
1:A:1167:C:H5''	1:A:1190:G:N2	2.28	0.48
12:S:17:ARG:O	12:S:18:ARG:C	2.56	0.48
10:P:40:TYR:CZ	10:P:42:PRO:HB3	2.48	0.48
16:E:69:THR:O	16:E:104:GLU:HA	2.13	0.48
1:A:14:U:H3	1:A:24:G:H1	1.60	0.48
3:C:667:PHE:CZ	3:C:669:GLU:HA	2.49	0.48
14:U:41:ARG:HG2	14:U:41:ARG:HH11	1.78	0.48
1:A:192:C:H2'	1:A:193:G:H8	1.78	0.48
1:A:697:G:N2	1:A:713:A:O2'	2.47	0.48
1:A:1004:A:H61	1:A:1057:G:C1'	2.26	0.48
1:A:1178:A:H2'	1:A:1179:A:O4'	2.14	0.48
1:A:1250:G:H8	1:A:1250:G:H5''	1.78	0.48
1:A:1260:A:H2'	1:A:1261:A:C8	2.48	0.48
1:A:1396:G:H1'	1:A:1397:C:H1'	1.96	0.48
8:L:3:THR:O	8:L:6:GLN:HB2	2.13	0.48
16:E:50:SER:HB3	16:E:70:ALA:HB3	1.96	0.48
1:A:293:C:H2'	1:A:294:G:C8	2.48	0.48
4:D:10:LEU:CD2	4:D:15:HIS:H	2.26	0.48
10:P:3:VAL:CG1	10:P:22:VAL:HG13	2.43	0.48
10:P:74:PHE:CD2	10:P:79:ILE:HG21	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:86:TYR:O	20:M:90:ARG:HG2	2.14	0.48
1:A:1011:C:H42	1:A:1047:C:N4	2.12	0.48
11:Q:62:LYS:O	11:Q:78:VAL:HB	2.13	0.48
1:A:676:G:O2'	9:O:49:ASP:OD1	2.30	0.48
1:A:1032:C:H3'	1:A:1033:G:H8	1.79	0.48
1:A:1080:U:H2'	1:A:1081:C:C6	2.49	0.48
1:A:1265:C:H2'	1:A:1287:C:N3	2.29	0.48
1:A:988:A:C2	1:A:1327:A:H2'	2.49	0.47
1:A:1335:U:H2'	1:A:1336:G:H8	1.78	0.47
11:Q:15:VAL:HG12	11:Q:15:VAL:O	2.13	0.47
1:A:888:U:H5''	7:I:83:PRO:HB2	1.95	0.47
4:D:69:PHE:HB3	4:D:80:VAL:HG13	1.96	0.47
1:A:159:A:H2'	1:A:160:A:C8	2.50	0.47
1:A:1270:A:H1'	1:A:1284:A:C2	2.50	0.47
1:A:248:C:H2'	1:A:249:G:H8	1.80	0.47
1:A:610:G:H1	1:A:646:U:H3	1.62	0.47
1:A:1004:A:H61	1:A:1057:G:H1'	1.79	0.47
1:A:1246:C:O2'	1:A:1344:C:H5'	2.14	0.47
7:I:2:VAL:O	7:I:4:THR:N	2.47	0.47
11:Q:77:LEU:HD11	11:Q:79:GLU:O	2.15	0.47
1:A:1004:A:C4	1:A:1225:A:H4'	2.49	0.47
1:A:1262:G:H1'	1:A:1364:G:O2'	2.14	0.47
9:O:24:SER:OG	9:O:26:GLU:OE2	2.33	0.47
10:P:22:VAL:HG21	10:P:59:TRP:CG	2.50	0.47
1:A:660:C:H2'	1:A:661:U:C6	2.50	0.47
1:A:1057:G:H2'	1:A:1058:G:C8	2.44	0.47
1:A:1180:A:H2'	1:A:1181:C:C6	2.50	0.47
1:A:1267:G:H2'	1:A:1268:C:C6	2.50	0.47
1:A:1063:G:O6	1:A:1208:U:H2'	2.14	0.47
1:A:1287:C:H4'	1:A:1288:A:C4	2.49	0.47
1:A:1325:G:H4'	21:N:18:VAL:CG1	2.45	0.47
2:B:9005:A:C6	2:B:9006:A:C6	3.03	0.47
1:A:208:A:H2'	1:A:209:A:H5''	1.97	0.47
1:A:527:C:H5''	1:A:528:C:C6	2.50	0.47
1:A:1323:C:H2'	1:A:1324:U:C6	2.49	0.47
3:C:494:GLY:HA2	14:U:41:ARG:CZ	2.45	0.47
17:H:23:VAL:CG1	17:H:43:LEU:HD21	2.45	0.47
1:A:817:C:H2'	1:A:817:C:O2	2.13	0.47
1:A:1297:A:H2'	1:A:1298:A:C8	2.50	0.47
4:D:10:LEU:CD2	4:D:15:HIS:ND1	2.76	0.47
1:A:185:U:H5''	12:S:81:LYS:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:A:H2'	1:A:486:C:C6	2.50	0.46
1:A:995:C:H2'	1:A:996:A:C8	2.49	0.46
1:A:1043:G:H2'	1:A:1044:G:C8	2.50	0.46
1:A:1048:A:H2'	1:A:1049:G:C8	2.50	0.46
1:A:1296:A:H61	1:A:1380:G:H4'	1.79	0.46
10:P:25:SER:OG	10:P:26:ARG:N	2.47	0.46
1:A:209:A:H1'	1:A:230:U:O2'	2.15	0.46
1:A:704:A:H2'	1:A:705:A:C8	2.50	0.46
1:A:1111:A:H4'	1:A:1112:A:O5'	2.15	0.46
2:B:9004:A:N1	2:B:9005:A:C5	2.83	0.46
1:A:986:G:N2	1:A:1372:A:O4'	2.49	0.46
1:A:1028:A:H2'	1:A:1029:G:C8	2.50	0.46
1:A:1099:G:H1'	1:A:1176:A:H61	1.80	0.46
11:Q:13:ARG:O	11:Q:15:VAL:HG23	2.16	0.46
16:E:109:ASP:HA	16:E:115:VAL:CG2	2.45	0.46
22:R:11:VAL:HG11	22:R:16:MET:HE2	1.97	0.46
1:A:275:C:H2'	1:A:276:U:C6	2.49	0.46
1:A:955:G:C8	1:A:1346:G:H1'	2.50	0.46
1:A:1259:A:H61	1:A:1363:C:C4'	2.29	0.46
1:A:1286:C:H1'	1:A:1291:C:O2	2.16	0.46
2:B:9004:A:C2	2:B:9005:A:N9	2.84	0.46
11:Q:35:LEU:HD23	11:Q:36:TYR:CZ	2.50	0.46
1:A:116:U:H3'	1:A:296:A:H61	1.80	0.46
1:A:425:G:H2'	1:A:426:U:C6	2.50	0.46
1:A:1004:A:N6	1:A:1224:G:O2'	2.49	0.46
2:B:9002:A:H62	3:C:531:ARG:CD	2.25	0.46
14:U:46:PRO:O	14:U:49:VAL:HG12	2.15	0.46
1:A:230:U:H2'	1:A:231:U:C6	2.51	0.46
1:A:1070:U:H3'	1:A:1071:G:H8	1.81	0.46
1:A:1237:C:H2'	1:A:1238:A:H8	1.80	0.46
7:I:80:ILE:HD11	7:I:130:TYR:CG	2.49	0.46
12:S:62:VAL:CG2	12:S:72:ALA:HB2	2.45	0.46
1:A:691:C:H2'	1:A:692:G:C8	2.51	0.46
1:A:1319:C:OP1	20:M:79:ARG:NH2	2.49	0.46
1:A:1332:G:H2'	1:A:1333:A:H8	1.77	0.46
1:A:1351:C:H2'	1:A:1352:G:C8	2.50	0.46
2:B:9004:A:N9	3:C:530:LEU:HD22	2.30	0.46
2:B:9008:A:N7	3:C:561:ARG:NH1	2.64	0.46
5:F:131:TYR:CD1	5:F:131:TYR:C	2.94	0.46
1:A:961:G:H5''	1:A:985:A:P	2.56	0.46
13:T:7:MET:HE1	14:U:72:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:U:H2'	1:A:188:G:H8	1.81	0.46
1:A:940:C:N3	1:A:1397:C:H5	2.14	0.46
1:A:979:A:N3	1:A:979:A:H2'	2.31	0.46
4:D:14:VAL:HG13	4:D:202:ALA:HB1	1.97	0.46
5:F:193:LEU:O	5:F:197:PHE:N	2.40	0.46
9:O:60:VAL:O	9:O:63:ARG:HB3	2.16	0.46
14:U:41:ARG:O	14:U:77:SER:N	2.47	0.46
1:A:277:C:H2'	1:A:278:A:H8	1.80	0.46
8:L:99:ARG:HA	8:L:107:ARG:HA	1.97	0.46
1:A:471:U:H3	1:A:479:G:H1	1.63	0.45
1:A:513:C:N4	1:A:550:G:H1	2.14	0.45
1:A:547:U:H2'	1:A:548:A:H8	1.81	0.45
1:A:822:U:H5'	1:A:914:C:H5'	1.98	0.45
11:Q:19:MET:HB3	11:Q:22:THR:HB	1.98	0.45
1:A:1004:A:O5'	1:A:1004:A:H8	1.99	0.45
3:C:69:MET:HB2	3:C:71:LEU:H	1.82	0.45
1:A:220:C:H4'	1:A:221:G:C4	2.52	0.45
1:A:317:G:H1'	1:A:617:A:C2	2.51	0.45
1:A:391:A:C5	1:A:392:G:H1'	2.51	0.45
1:A:421:G:N2	1:A:436:G:H1'	2.29	0.45
1:A:456:A:H4'	1:A:456:A:OP1	2.16	0.45
1:A:958:C:C6	20:M:105:ASN:HB3	2.50	0.45
1:A:1023:G:N2	1:A:1025:G:H3'	2.32	0.45
1:A:1093:U:H5''	1:A:1096:U:H3	1.81	0.45
1:A:1247:A:N7	1:A:1308:A:N6	2.65	0.45
1:A:1270:A:H62	1:A:1283:A:H1'	1.81	0.45
3:C:296:GLU:OE1	3:C:592:ARG:NH1	2.49	0.45
6:G:89:PHE:CZ	6:G:138:ARG:HD3	2.52	0.45
13:T:2:ARG:HH11	13:T:2:ARG:HG3	1.82	0.45
22:R:26:ASP:O	22:R:28:LYS:N	2.50	0.45
1:A:457:A:H3'	1:A:458:G:H8	1.81	0.45
1:A:459:A:H4'	1:A:460:A:O5'	2.16	0.45
1:A:690:A:H2'	1:A:691:C:C6	2.51	0.45
1:A:1235:C:H2'	20:M:102:SER:HB3	1.98	0.45
1:A:1255:G:H2'	1:A:1256:A:O4'	2.16	0.45
1:A:1263:G:H2'	1:A:1264:G:C8	2.50	0.45
1:A:1355:A:N1	1:A:1383:A:H5''	2.32	0.45
1:A:1366:A:H2'	1:A:1367:U:C6	2.52	0.45
1:A:572:A:H4'	1:A:574:U:H5	1.81	0.45
1:A:743:A:C2	1:A:744:C:C2	3.04	0.45
1:A:981:G:H4'	1:A:982:C:OP2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1311:U:H5''	20:M:17:ILE:HD12	1.98	0.45
4:D:129:LEU:N	4:D:130:PRO:HD2	2.31	0.45
1:A:327:G:H1	1:A:342:C:H42	1.64	0.45
1:A:1032:C:H2'	1:A:1033:G:O4'	2.16	0.45
1:A:1307:C:H4'	1:A:1308:A:C5	2.52	0.45
22:R:18:LYS:HD2	22:R:31:VAL:HG13	1.98	0.45
1:A:47:U:H2'	1:A:48:G:C8	2.52	0.45
1:A:548:A:H2'	1:A:549:G:H8	1.80	0.45
1:A:864:U:H3'	1:A:881:U:H3	1.81	0.45
1:A:1014:A:H8	1:A:1034:U:O2'	2.00	0.45
1:A:1361:C:H2'	1:A:1362:G:H8	1.81	0.45
3:C:497:VAL:CG2	3:C:512:ILE:HD11	2.47	0.45
6:G:36:LEU:HD21	6:G:137:ILE:HD12	1.97	0.45
1:A:95:U:H2'	1:A:96:G:H8	1.82	0.45
1:A:248:C:H2'	1:A:249:G:C8	2.52	0.45
1:A:317:G:O2'	1:A:616:A:N1	2.46	0.45
1:A:351:U:O2'	1:A:354:G:O6	2.32	0.45
1:A:1041:C:H4'	1:A:1042:G:C2	2.51	0.45
1:A:1314:G:H1'	1:A:1341:A:N6	2.32	0.45
1:A:52:A:C4	8:L:31:PHE:CE2	3.05	0.45
10:P:51:ILE:HD12	10:P:77:GLN:HG3	1.99	0.45
1:A:600:U:H2'	1:A:601:C:C6	2.52	0.45
1:A:850:U:H3'	1:A:851:U:C6	2.52	0.45
1:A:1259:A:H2'	1:A:1260:A:C8	2.52	0.45
4:D:9:LEU:C	4:D:10:LEU:HD12	2.42	0.45
8:L:123:ARG:HD2	8:L:125:GLN:O	2.17	0.45
1:A:114:A:H61	1:A:321:A:H1'	1.82	0.44
1:A:960:U:H2'	1:A:961:G:C8	2.51	0.44
1:A:1080:U:H4'	6:G:30:ARG:HH22	1.82	0.44
1:A:62:A:H4'	1:A:63:G:O5'	2.17	0.44
1:A:105:G:N7	12:S:10:ARG:NH2	2.62	0.44
1:A:121:C:H2'	1:A:122:G:H8	1.82	0.44
1:A:161:A:C5	1:A:162:C:H1'	2.53	0.44
1:A:458:G:C5'	1:A:459:A:H3'	2.35	0.44
1:A:1116:G:H2'	1:A:1117:C:C6	2.53	0.44
1:A:1326:C:H5	21:N:18:VAL:HG21	1.81	0.44
3:C:420:PHE:CE2	3:C:530:LEU:HD21	2.52	0.44
9:O:74:ASP:OD1	9:O:76:THR:HB	2.17	0.44
1:A:999:U:H2'	1:A:1000:C:C6	2.51	0.44
1:A:1003:G:H2'	1:A:1003:G:N3	2.33	0.44
1:A:1018:U:C2'	1:A:1031:A:H61	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1034:U:H4'	1:A:1035:C:C5	2.52	0.44
1:A:1188:A:H2'	1:A:1189:A:C8	2.53	0.44
5:F:68:PHE:O	5:F:69:ARG:C	2.60	0.44
12:S:62:VAL:HG21	12:S:72:ALA:HB2	1.99	0.44
12:S:62:VAL:O	12:S:63:LYS:C	2.60	0.44
1:A:344:A:C3'	1:A:345:G:H5''	2.42	0.44
1:A:993:A:H1'	1:A:1059:U:O2	2.17	0.44
1:A:1125:U:H2'	1:A:1126:U:C6	2.53	0.44
1:A:1246:C:H4'	1:A:1309:G:N2	2.32	0.44
1:A:1339:U:H2'	1:A:1340:G:O4'	2.17	0.44
6:G:15:LEU:HD11	6:G:18:VAL:HG23	2.00	0.44
9:O:39:LEU:HD23	9:O:59:MET:HE1	1.99	0.44
1:A:472:C:H2'	1:A:473:G:O4'	2.17	0.44
1:A:1094:G:C8	1:A:1095:U:H2'	2.53	0.44
1:A:1249:U:O4'	17:H:42:ILE:HD11	2.17	0.44
1:A:1323:C:C5	22:R:4:SER:HA	2.52	0.44
1:A:158:G:N2	1:A:160:A:H3'	2.32	0.44
1:A:921:U:H2'	1:A:922:C:C6	2.53	0.44
1:A:980:C:N4	1:A:1240:G:H1'	2.32	0.44
1:A:1314:G:H1'	1:A:1341:A:H62	1.82	0.44
13:T:45:LYS:HB2	13:T:59:PHE:CE1	2.53	0.44
1:A:75:G:H1'	1:A:94:A:H61	1.82	0.44
1:A:427:U:H3	1:A:432:G:H1	1.64	0.44
1:A:511:C:OP1	8:L:128:SER:OG	2.29	0.44
1:A:671:A:H2'	1:A:672:A:C8	2.53	0.44
1:A:775:A:C6	1:A:823:A:H1'	2.53	0.44
1:A:1010:U:H1'	1:A:1051:G:H22	1.82	0.44
1:A:1094:G:H2'	1:A:1095:U:C6	2.52	0.44
6:G:110:PRO:O	6:G:113:ALA:HB3	2.17	0.44
1:A:34:A:H2'	1:A:35:A:C8	2.53	0.44
1:A:121:C:H2'	1:A:122:G:C8	2.53	0.44
1:A:180:G:H1	1:A:208:A:H2'	1.82	0.44
1:A:1003:G:H21	1:A:1005:C:H42	1.64	0.44
1:A:1166:A:H61	1:A:1187:G:H1'	1.82	0.44
1:A:1367:U:H3	1:A:1372:A:H62	1.65	0.44
6:G:91:ALA:O	6:G:92:GLY:C	2.59	0.44
6:G:111:VAL:HG12	6:G:115:LEU:HD12	2.00	0.44
1:A:10:A:N6	5:F:196:GLU:O	2.51	0.44
1:A:511:C:OP1	8:L:128:SER:CB	2.66	0.44
1:A:1024:A:H2	1:A:1228:U:H1'	1.83	0.44
1:A:1386:A:H4'	1:A:1387:C:H5	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:C:H2'	1:A:244:G:C8	2.52	0.43
1:A:425:G:H1	1:A:434:U:H3	1.65	0.43
1:A:437:U:H5'	5:F:9:TRP:CE3	2.53	0.43
1:A:563:U:OP1	8:L:25:ASN:ND2	2.42	0.43
1:A:604:A:H61	1:A:650:A:H2'	1.83	0.43
1:A:1077:A:H3'	1:A:1078:G:H4'	2.00	0.43
1:A:1105:U:H2'	1:A:1106:C:O4'	2.18	0.43
1:A:1109:G:N3	1:A:1109:G:H2'	2.33	0.43
1:A:1143:A:C6	1:A:1151:G:C6	3.05	0.43
1:A:1149:U:H2'	1:A:1150:U:C2	2.53	0.43
1:A:1339:U:H4'	20:M:23:PHE:CE2	2.53	0.43
3:C:527:THR:HG22	3:C:531:ARG:CZ	2.48	0.43
9:O:62:LYS:O	9:O:63:ARG:C	2.61	0.43
1:A:1111:A:C4'	1:A:1112:A:H4'	2.45	0.43
2:B:9007:A:P	3:C:562:ARG:HH12	2.41	0.43
18:J:19:VAL:HG11	18:J:83:ILE:HA	2.00	0.43
1:A:564:C:H2'	1:A:565:C:C6	2.53	0.43
1:A:1046:G:OP1	1:A:1046:G:H4'	2.18	0.43
7:I:7:ILE:O	7:I:8:ALA:C	2.59	0.43
17:H:73:LEU:HD23	17:H:90:GLU:HA	1.99	0.43
1:A:68:G:H1	1:A:101:C:H42	1.64	0.43
1:A:989:C:N4	1:A:1369:A:H62	2.16	0.43
1:A:1038:C:H2'	1:A:1039:U:O4'	2.18	0.43
7:I:79:ARG:HD2	7:I:128:LEU:O	2.18	0.43
8:L:23:ALA:O	8:L:24:LEU:C	2.60	0.43
11:Q:56:LYS:O	11:Q:59:ASP:CG	2.61	0.43
1:A:47:U:H2'	1:A:48:G:H8	1.83	0.43
1:A:525:U:O2'	1:A:528:C:N3	2.50	0.43
1:A:1015:C:H5'	1:A:1048:A:H1'	2.00	0.43
1:A:1051:G:H2'	1:A:1052:U:O4'	2.19	0.43
1:A:1128:A:H1'	1:A:1188:A:C4	2.54	0.43
1:A:1317:C:H42	1:A:1338:G:H1	1.66	0.43
4:D:23:TRP:CD1	4:D:23:TRP:C	2.97	0.43
5:F:146:ARG:HH21	5:F:146:ARG:HG2	1.82	0.43
1:A:696:A:O2'	1:A:709:G:N2	2.51	0.43
1:A:918:A:H2'	1:A:919:A:C8	2.54	0.43
1:A:1319:C:H2'	1:A:1320:A:H8	1.84	0.43
2:B:9008:A:OP2	3:C:561:ARG:NH2	2.48	0.43
3:C:71:LEU:HA	3:C:114:VAL:O	2.18	0.43
11:Q:19:MET:CB	11:Q:22:THR:HB	2.48	0.43
1:A:170:A:H2'	1:A:171:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:851:U:H2'	1:A:853:C:H5	1.84	0.43
1:A:907:C:H2'	1:A:908:G:C8	2.53	0.43
1:A:1004:A:N1	1:A:1057:G:H4'	2.34	0.43
9:O:25:PRO:O	9:O:26:GLU:C	2.62	0.43
1:A:224:U:H2'	1:A:225:A:H8	1.81	0.43
1:A:1023:G:H22	1:A:1025:G:H3'	1.82	0.43
5:F:69:ARG:O	5:F:72:PHE:N	2.52	0.43
1:A:821:G:H4'	1:A:822:U:C2	2.54	0.43
1:A:975:A:H1'	1:A:979:A:H5'	2.00	0.43
1:A:1224:G:H5'	1:A:1224:G:H8	1.84	0.43
1:A:1229:G:H2'	1:A:1230:G:O4'	2.19	0.43
9:O:50:HIS:O	9:O:53:ARG:HB3	2.19	0.43
10:P:55:LEU:O	10:P:56:ALA:C	2.62	0.43
12:S:16:GLU:O	12:S:17:ARG:C	2.61	0.43
12:S:55:ALA:O	12:S:56:LYS:C	2.61	0.43
1:A:344:A:C2'	1:A:345:G:H5'	2.25	0.43
1:A:539:G:OP1	1:A:540:U:H5'	2.19	0.43
1:A:1026:A:H1'	1:A:1227:C:H1'	2.01	0.43
1:A:1259:A:H61	1:A:1363:C:H4'	1.83	0.43
1:A:1299:U:H2'	1:A:1300:C:C6	2.54	0.43
3:C:248:ARG:NH2	3:C:339:LEU:HD13	2.34	0.43
4:D:10:LEU:HG	4:D:13:GLY:N	2.33	0.43
4:D:100:THR:HA	4:D:107:ILE:HG13	2.00	0.43
8:L:24:LEU:O	8:L:43:LYS:NZ	2.52	0.43
9:O:59:MET:O	9:O:60:VAL:C	2.62	0.43
1:A:995:C:H2'	1:A:996:A:H8	1.84	0.42
1:A:996:A:H2'	1:A:997:G:C8	2.54	0.42
1:A:1017:A:H3'	1:A:1018:U:C6	2.54	0.42
1:A:1094:G:H1'	1:A:1113:C:N4	2.30	0.42
1:A:1266:A:H4'	1:A:1267:G:O5'	2.19	0.42
1:A:98:U:H1'	1:A:99:A:C2	2.54	0.42
1:A:113:G:H1'	1:A:114:A:N7	2.33	0.42
1:A:510:C:H2'	1:A:511:C:C6	2.54	0.42
1:A:737:A:H2'	1:A:738:A:C8	2.54	0.42
1:A:861:U:H2'	1:A:862:A:C8	2.54	0.42
13:T:75:PHE:CD1	13:T:75:PHE:C	2.96	0.42
1:A:696:A:OP2	1:A:712:G:N2	2.52	0.42
5:F:69:ARG:O	5:F:72:PHE:HB3	2.19	0.42
6:G:112:ARG:O	6:G:116:GLU:N	2.42	0.42
8:L:8:ILE:O	8:L:9:ARG:C	2.62	0.42
9:O:24:SER:O	9:O:25:PRO:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:C:H4'	1:A:221:G:N3	2.34	0.42
1:A:244:G:H2'	1:A:245:C:O4'	2.19	0.42
1:A:721:A:H3'	1:A:722:G:C5'	2.39	0.42
1:A:942:C:H5''	17:H:4:LYS:HG2	2.00	0.42
1:A:1307:C:H4'	1:A:1308:A:C4	2.54	0.42
8:L:136:LYS:HE2	8:L:136:LYS:HA	2.01	0.42
13:T:30:LEU:C	13:T:35:ALA:HB3	2.44	0.42
1:A:174:C:H2'	1:A:175:C:C6	2.54	0.42
1:A:306:A:H2'	1:A:307:G:O4'	2.18	0.42
1:A:455:G:H3'	1:A:494:G:N1	2.35	0.42
1:A:665:G:O2'	9:O:28:GLN:OE1	2.37	0.42
1:A:1219:C:H1'	1:A:1223:U:C2'	2.45	0.42
1:A:1296:A:H61	1:A:1380:G:C4'	2.33	0.42
9:O:39:LEU:O	9:O:42:HIS:HB3	2.19	0.42
1:A:571:U:OP1	1:A:575:G:N2	2.53	0.42
1:A:835:C:H5'	7:I:13:ARG:NH2	2.34	0.42
1:A:1291:C:H2'	1:A:1292:C:H6	1.84	0.42
4:D:68:LEU:HD11	4:D:92:VAL:HG23	2.01	0.42
1:A:207:U:O3'	12:S:56:LYS:HG2	2.20	0.42
1:A:766:U:H2'	1:A:767:G:O4'	2.20	0.42
1:A:776:A:C4	1:A:777:A:H1'	2.55	0.42
1:A:989:C:H1'	1:A:1326:C:N4	2.31	0.42
1:A:1334:C:H2'	1:A:1335:U:C6	2.54	0.42
1:A:237:U:H2'	1:A:238:G:C8	2.55	0.42
1:A:870:A:N6	1:A:879:A:H1'	2.35	0.42
1:A:1010:U:H1'	1:A:1051:G:N2	2.35	0.42
1:A:1039:U:H3'	1:A:1041:C:O2	2.20	0.42
6:G:56:VAL:N	6:G:57:PRO:CD	2.82	0.42
6:G:96:LEU:HD22	6:G:123:ILE:HD11	2.02	0.42
8:L:126:GLY:O	8:L:127:ARG:C	2.63	0.42
1:A:226:C:H2'	1:A:227:C:C6	2.55	0.42
1:A:435:C:H2'	1:A:436:G:H21	1.83	0.42
1:A:593:G:H2'	1:A:594:G:C8	2.55	0.42
1:A:965:U:H2'	1:A:966:U:C6	2.55	0.42
1:A:1293:C:H3'	1:A:1294:A:H5''	2.01	0.42
7:I:20:VAL:HG23	7:I:22:HIS:CE1	2.55	0.42
9:O:31:ILE:O	9:O:32:LEU:C	2.62	0.42
1:A:1148:G:N3	1:A:1150:U:H5	2.17	0.42
3:C:76:ILE:HD11	3:C:112:VAL:HG21	2.01	0.42
1:A:1060:G:H2'	1:A:1060:G:N3	2.35	0.41
3:C:473:ARG:HD3	3:C:538:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:30:TYR:HA	11:Q:40:VAL:O	2.20	0.41
1:A:688:C:H2'	1:A:689:C:C6	2.55	0.41
1:A:696:A:H62	1:A:712:G:H1'	1.84	0.41
1:A:820:C:H4'	1:A:911:A:H61	1.84	0.41
1:A:1141:G:N1	1:A:1142:C:N4	2.67	0.41
1:A:1390:U:H2'	1:A:1391:C:O4'	2.20	0.41
6:G:90:GLY:O	6:G:91:ALA:HB3	2.20	0.41
8:L:116:ASP:O	8:L:117:THR:C	2.63	0.41
1:A:662:U:H3	7:I:57:GLN:HE21	1.66	0.41
1:A:971:U:O2'	1:A:1210:A:N6	2.53	0.41
1:A:988:A:H2	1:A:1327:A:H2'	1.83	0.41
1:A:1363:C:H2'	1:A:1364:G:C8	2.55	0.41
3:C:483:LEU:HD21	3:C:504:ILE:HG21	2.02	0.41
4:D:79:SER:O	4:D:83:GLU:HG2	2.20	0.41
7:I:16:ASN:OD1	7:I:16:ASN:N	2.50	0.41
9:O:61:GLY:O	9:O:62:LYS:C	2.62	0.41
1:A:98:U:H1'	1:A:99:A:H2	1.84	0.41
1:A:182:U:H4'	1:A:232:A:H5''	2.00	0.41
1:A:370:G:N2	1:A:372:A:H3'	2.35	0.41
1:A:576:G:H2'	1:A:577:G:O4'	2.20	0.41
1:A:1036:C:H2'	1:A:1037:C:C6	2.55	0.41
5:F:69:ARG:O	5:F:70:THR:C	2.62	0.41
6:G:82:PRO:HD2	6:G:147:LEU:HD22	2.02	0.41
8:L:7:LEU:HA	8:L:7:LEU:HD23	1.85	0.41
12:S:13:THR:O	12:S:14:ASN:C	2.62	0.41
1:A:510:C:H1'	1:A:558:C:H1'	2.02	0.41
1:A:1146:C:H2'	1:A:1147:A:C8	2.56	0.41
1:A:1237:C:H41	20:M:103:LYS:HA	1.85	0.41
1:A:1317:C:H5''	20:M:97:VAL:HG22	2.02	0.41
7:I:79:ARG:HG3	7:I:81:SER:O	2.21	0.41
1:A:270:A:O2'	12:S:70:ASN:ND2	2.54	0.41
1:A:675:G:H5'	1:A:735:C:H1'	2.03	0.41
1:A:691:C:H2'	1:A:692:G:H8	1.85	0.41
1:A:718:U:H2'	1:A:719:G:H8	1.86	0.41
1:A:974:A:H8	1:A:974:A:O5'	2.03	0.41
1:A:1250:G:H5''	1:A:1250:G:C8	2.55	0.41
1:A:1305:C:H5''	20:M:44:ARG:NH2	2.36	0.41
7:I:106:ILE:HD12	7:I:106:ILE:N	2.35	0.41
8:L:36:THR:HG22	8:L:38:VAL:HG23	2.03	0.41
11:Q:49:HIS:O	11:Q:76:ARG:HA	2.21	0.41
1:A:124:G:OP1	1:A:641:G:N2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:G:N3	1:A:165:G:H2'	2.36	0.41
1:A:521:U:H2'	1:A:522:A:C8	2.56	0.41
1:A:778:G:O2'	1:A:911:A:N3	2.50	0.41
1:A:827:G:H2'	1:A:827:G:N3	2.36	0.41
1:A:1140:A:H2'	1:A:1141:G:C8	2.56	0.41
1:A:1153:G:O2'	1:A:1154:C:H5''	2.21	0.41
1:A:1293:C:H3'	1:A:1294:A:C5'	2.51	0.41
4:D:129:LEU:HB2	4:D:133:GLU:OE2	2.21	0.41
5:F:191:GLU:OE2	5:F:191:GLU:N	2.53	0.41
12:S:22:ALA:O	12:S:23:THR:C	2.64	0.41
16:E:54:VAL:HG13	16:E:67:ILE:HG22	2.02	0.41
1:A:171:A:H2'	1:A:173:A:C8	2.56	0.41
1:A:293:C:H2'	1:A:294:G:H8	1.86	0.41
1:A:661:U:H1'	1:A:662:U:H6	1.86	0.41
1:A:780:G:N2	1:A:817:C:O2	2.52	0.41
1:A:890:C:H2'	1:A:891:G:H8	1.85	0.41
1:A:946:C:H4'	1:A:1392:C:C2	2.56	0.41
1:A:1004:A:H2'	1:A:1005:C:O4'	2.21	0.41
1:A:1019:C:H2'	1:A:1020:C:C6	2.56	0.41
1:A:1113:C:H1'	1:A:1114:G:P	2.61	0.41
1:A:1393:C:H2'	1:A:1394:G:C8	2.56	0.41
3:C:483:LEU:O	3:C:487:LEU:HG	2.21	0.41
1:A:757:A:H1'	1:A:758:A:N7	2.36	0.41
1:A:1219:C:H2'	1:A:1220:U:H5'	2.03	0.41
7:I:21:ARG:NH1	7:I:70:ASN:O	2.54	0.41
1:A:287:A:H5''	1:A:289:G:O4'	2.21	0.40
1:A:910:A:H2'	1:A:911:A:O4'	2.21	0.40
1:A:1336:G:N3	1:A:1336:G:H2'	2.36	0.40
1:A:1373:U:H4'	1:A:1374:G:OP1	2.21	0.40
6:G:139:ALA:O	6:G:140:THR:C	2.63	0.40
8:L:94:LEU:O	8:L:111:VAL:HG23	2.21	0.40
1:A:366:U:H2'	1:A:367:A:C8	2.56	0.40
1:A:985:A:N6	1:A:1241:U:O2	2.53	0.40
1:A:1246:C:O2'	1:A:1343:G:H2'	2.21	0.40
1:A:1294:A:H1'	1:A:1295:C:H5''	2.01	0.40
1:A:1303:U:H2'	1:A:1304:U:C6	2.56	0.40
9:O:48:LYS:O	9:O:50:HIS:N	2.54	0.40
11:Q:15:VAL:HG21	11:Q:26:VAL:HB	2.02	0.40
14:U:17:TYR:CE2	14:U:23:ILE:HD12	2.56	0.40
16:E:39:ARG:NH1	16:E:54:VAL:O	2.54	0.40
1:A:547:U:H2'	1:A:548:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:987:A:H1'	1:A:991:U:H3	1.86	0.40
1:A:1198:U:H5''	16:E:5:VAL:HG21	2.03	0.40
1:A:1215:G:H2'	1:A:1216:C:O4'	2.21	0.40
1:A:1318:G:N7	20:M:98:ARG:NH2	2.69	0.40
4:D:89:MET:HG3	4:D:221:ILE:HD13	2.02	0.40
5:F:15:LEU:HD13	5:F:56:LYS:HA	2.04	0.40
5:F:65:GLU:O	5:F:66:ARG:C	2.65	0.40
16:E:119:ILE:O	16:E:123:LEU:HG	2.21	0.40
1:A:278:A:H2'	1:A:279:C:C6	2.57	0.40
1:A:606:G:H2'	1:A:606:G:N3	2.36	0.40
1:A:841:G:H1	1:A:864:U:H3	1.69	0.40
1:A:937:G:H1'	1:A:938:G:N2	2.37	0.40
1:A:943:G:H1	1:A:1393:C:H42	1.69	0.40
1:A:1159:U:H4'	19:K:43:PRO:HG3	2.02	0.40
1:A:1279:G:H2'	1:A:1280:G:C8	2.57	0.40
1:A:1322:U:H5	22:R:5:LEU:HD22	1.86	0.40
3:C:448:ILE:O	3:C:449:GLU:C	2.64	0.40
15:V:49:ALA:HB1	15:V:59:LYS:HA	2.03	0.40
1:A:473:G:H8	1:A:473:G:O5'	2.04	0.40
1:A:970:U:H1'	1:A:1232:C:H5'	2.03	0.40
1:A:1004:A:C5	1:A:1225:A:H4'	2.57	0.40
2:B:9004:A:H1'	3:C:530:LEU:HD22	2.01	0.40
6:G:133:PRO:O	6:G:137:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	706/779 (91%)	691 (98%)	14 (2%)	1 (0%)	48 78
4	D	216/246 (88%)	201 (93%)	13 (6%)	2 (1%)	14 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	179/200 (90%)	164 (92%)	10 (6%)	5 (3%)	4	27
6	G	156/166 (94%)	143 (92%)	11 (7%)	2 (1%)	9	38
7	I	129/132 (98%)	118 (92%)	7 (5%)	4 (3%)	3	26
8	L	134/138 (97%)	123 (92%)	10 (8%)	1 (1%)	18	50
9	O	83/89 (93%)	76 (92%)	7 (8%)	0	100	100
10	P	86/90 (96%)	78 (91%)	5 (6%)	3 (4%)	3	24
11	Q	82/87 (94%)	75 (92%)	6 (7%)	1 (1%)	10	40
12	S	81/88 (92%)	72 (89%)	9 (11%)	0	100	100
13	T	93/95 (98%)	88 (95%)	5 (5%)	0	100	100
14	U	62/79 (78%)	56 (90%)	6 (10%)	0	100	100
15	V	99/131 (76%)	95 (96%)	4 (4%)	0	100	100
16	E	203/218 (93%)	169 (83%)	33 (16%)	1 (0%)	24	56
17	H	147/156 (94%)	138 (94%)	7 (5%)	2 (1%)	9	37
18	J	106/130 (82%)	100 (94%)	6 (6%)	0	100	100
19	K	93/102 (91%)	87 (94%)	6 (6%)	0	100	100
20	M	106/121 (88%)	101 (95%)	5 (5%)	0	100	100
21	N	47/61 (77%)	42 (89%)	4 (8%)	1 (2%)	5	31
22	R	76/92 (83%)	72 (95%)	2 (3%)	2 (3%)	4	28
All	All	2884/3200 (90%)	2689 (93%)	170 (6%)	25 (1%)	16	45

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	130	PRO
5	F	24	LYS
5	F	181	GLU
5	F	182	ARG
6	G	8	LYS
8	L	135	PRO
22	R	27	LYS
3	C	70	ASN
6	G	90	GLY
7	I	3	MET
7	I	4	THR
10	P	88	GLN
17	H	83	ALA

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Mol	Chain	Res	Type
7	I	56	LYS
7	I	85	LEU
16	E	60	ALA
21	N	54	PRO
10	P	46	PRO
22	R	28	LYS
5	F	180	PRO
17	H	81	GLY
4	D	71	GLY
5	F	62	GLY
10	P	45	LYS
11	Q	78	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	628/692 (91%)	621 (99%)	7 (1%)	65 73
4	D	189/212 (89%)	186 (98%)	3 (2%)	55 68
5	F	159/173 (92%)	150 (94%)	9 (6%)	18 45
6	G	123/130 (95%)	120 (98%)	3 (2%)	43 61
7	I	111/112 (99%)	105 (95%)	6 (5%)	20 46
8	L	114/116 (98%)	110 (96%)	4 (4%)	32 54
9	O	80/83 (96%)	78 (98%)	2 (2%)	42 61
10	P	74/76 (97%)	68 (92%)	6 (8%)	11 36
11	Q	77/80 (96%)	74 (96%)	3 (4%)	28 53
12	S	66/70 (94%)	63 (96%)	3 (4%)	24 49
13	T	84/84 (100%)	78 (93%)	6 (7%)	13 40
14	U	56/64 (88%)	54 (96%)	2 (4%)	31 54
15	V	74/100 (74%)	74 (100%)	0	100 100
16	E	168/178 (94%)	156 (93%)	12 (7%)	13 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	H	125/132 (95%)	118 (94%)	7 (6%)	19	46
18	J	85/102 (83%)	80 (94%)	5 (6%)	18	44
19	K	86/92 (94%)	79 (92%)	7 (8%)	11	36
20	M	94/104 (90%)	91 (97%)	3 (3%)	34	56
21	N	44/54 (82%)	40 (91%)	4 (9%)	9	33
22	R	70/81 (86%)	65 (93%)	5 (7%)	13	40
All	All	2507/2735 (92%)	2410 (96%)	97 (4%)	30	53

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	11	LEU
3	C	56	VAL
3	C	65	ILE
3	C	69	MET
3	C	147	THR
3	C	148	ARG
3	C	506	PRO
4	D	23	TRP
4	D	33	THR
4	D	123	ASN
5	F	66	ARG
5	F	71	LEU
5	F	132	LEU
5	F	141	VAL
5	F	146	ARG
5	F	149	SER
5	F	178	ARG
5	F	181	GLU
5	F	184	GLU
6	G	10	GLU
6	G	151	GLU
6	G	157	ARG
7	I	6	PRO
7	I	53	GLU
7	I	55	SER
7	I	68	GLN
7	I	70	ASN
7	I	98	LEU
8	L	10	LYS

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Mol	Chain	Res	Type
8	L	20	LYS
8	L	36	THR
8	L	136	LYS
9	O	5	GLN
9	O	48	LYS
10	P	24	ASP
10	P	35	GLU
10	P	37	VAL
10	P	48	GLU
10	P	62	THR
10	P	68	ASP
11	Q	7	ARG
11	Q	50	ASP
11	Q	85	VAL
12	S	6	SER
12	S	18	ARG
12	S	48	LYS
13	T	1	MET
13	T	2	ARG
13	T	53	ASN
13	T	54	ASP
13	T	72	VAL
13	T	87	ARG
14	U	48	ARG
14	U	49	VAL
16	E	10	LEU
16	E	12	ILE
16	E	30	ASP
16	E	35	ASP
16	E	48	ASP
16	E	75	VAL
16	E	100	ILE
16	E	148	VAL
16	E	163	ARG
16	E	181	ILE
16	E	194	LYS
16	E	195	LEU
17	H	4	LYS
17	H	9	LYS
17	H	13	LEU
17	H	30	MET
17	H	43	LEU

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Mol	Chain	Res	Type
17	H	59	MET
17	H	75	VAL
18	J	22	VAL
18	J	67	VAL
18	J	100	ARG
18	J	106	ARG
18	J	112	GLU
19	K	28	THR
19	K	55	VAL
19	K	57	LYS
19	K	60	ASP
19	K	80	THR
19	K	91	ASP
19	K	98	ILE
20	M	97	VAL
20	M	100	GLN
20	M	105	ASN
21	N	27	CYS
21	N	30	PRO
21	N	53	ILE
21	N	54	PRO
22	R	24	GLU
22	R	53	ASP
22	R	56	LYS
22	R	58	VAL
22	R	81	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	125	GLN
3	C	484	GLN
3	C	649	ASN
4	D	85	GLN
4	D	94	GLN
4	D	123	ASN
5	F	115	ASN
6	G	19	ASN
6	G	142	GLN
7	I	57	GLN
7	I	122	GLN
9	O	83	ASN

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Mol	Chain	Res	Type
11	Q	54	GLN
12	S	70	ASN
13	T	61	GLN
13	T	64	ASN
14	U	21	ASN
14	U	57	GLN
14	U	69	GLN
15	V	30	ASN
16	E	118	ASN
16	E	136	GLN
17	H	129	ASN
18	J	75	GLN
19	K	56	HIS
19	K	82	GLN
20	M	91	HIS
20	M	105	ASN
22	R	14	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1330/1554 (85%)	356 (26%)	101 (7%)
2	B	6/7 (85%)	3 (50%)	0
All	All	1336/1561 (85%)	359 (26%)	101 (7%)

All (359) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	10	A
1	A	11	G
1	A	15	U
1	A	16	U
1	A	32	C
1	A	33	G
1	A	34	A
1	A	41	G
1	A	49	C
1	A	50	C
1	A	51	U
1	A	52	A

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Mol	Chain	Res	Type
1	A	53	A
1	A	56	C
1	A	70	G
1	A	114	A
1	A	119	C
1	A	128	A
1	A	129	A
1	A	139	A
1	A	140	A
1	A	143	C
1	A	148	A
1	A	152	C
1	A	153	U
1	A	159	A
1	A	165	G
1	A	172	U
1	A	177	G
1	A	181	G
1	A	185	U
1	A	189	A
1	A	190	A
1	A	191	C
1	A	194	C
1	A	195	A
1	A	198	G
1	A	209	A
1	A	211	A
1	A	212	G
1	A	219	U
1	A	220	C
1	A	221	G
1	A	248	C
1	A	252	U
1	A	253	U
1	A	255	G
1	A	259	G
1	A	265	G
1	A	274	G
1	A	275	C
1	A	281	A
1	A	288	C
1	A	289	G

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Mol	Chain	Res	Type
1	A	297	G
1	A	313	G
1	A	314	A
1	A	324	C
1	A	335	A
1	A	336	C
1	A	337	A
1	A	338	C
1	A	340	G
1	A	345	G
1	A	352	A
1	A	353	C
1	A	354	G
1	A	360	C
1	A	362	G
1	A	373	U
1	A	374	C
1	A	375	U
1	A	376	U
1	A	380	C
1	A	392	G
1	A	406	C
1	A	412	G
1	A	414	G
1	A	419	A
1	A	421	G
1	A	429	U
1	A	430	C
1	A	431	G
1	A	432	G
1	A	436	G
1	A	437	U
1	A	446	G
1	A	447	U
1	A	456	A
1	A	458	G
1	A	459	A
1	A	460	A
1	A	461	C
1	A	466	G
1	A	467	C
1	A	474	A

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Mol	Chain	Res	Type
1	A	475	A
1	A	476	U
1	A	477	A
1	A	478	G
1	A	488	U
1	A	489	U
1	A	493	G
1	A	494	G
1	A	495	U
1	A	504	A
1	A	506	A
1	A	509	G
1	A	519	A
1	A	520	C
1	A	527	C
1	A	530	G
1	A	533	G
1	A	536	G
1	A	539	G
1	A	540	U
1	A	541	A
1	A	542	A
1	A	545	C
1	A	556	A
1	A	564	C
1	A	568	A
1	A	569	A
1	A	571	U
1	A	575	G
1	A	581	A
1	A	582	A
1	A	585	G
1	A	586	G
1	A	597	G
1	A	604	A
1	A	605	A
1	A	616	A
1	A	627	C
1	A	641	G
1	A	642	U
1	A	647	G
1	A	650	A

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Mol	Chain	Res	Type
1	A	651	A
1	A	655	G
1	A	656	G
1	A	662	U
1	A	667	G
1	A	674	A
1	A	682	G
1	A	683	G
1	A	684	A
1	A	685	A
1	A	687	U
1	A	688	C
1	A	693	U
1	A	695	U
1	A	696	A
1	A	697	G
1	A	701	U
1	A	703	A
1	A	704	A
1	A	706	U
1	A	707	G
1	A	710	U
1	A	711	A
1	A	712	G
1	A	721	A
1	A	722	G
1	A	723	G
1	A	731	G
1	A	732	U
1	A	733	G
1	A	740	G
1	A	743	A
1	A	758	A
1	A	764	G
1	A	768	A
1	A	775	A
1	A	777	A
1	A	779	C
1	A	818	G
1	A	819	C
1	A	822	U
1	A	824	A

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Mol	Chain	Res	Type
1	A	825	A
1	A	826	C
1	A	828	A
1	A	829	U
1	A	830	G
1	A	845	G
1	A	850	U
1	A	852	U
1	A	853	C
1	A	865	G
1	A	883	A
1	A	895	G
1	A	909	C
1	A	934	C
1	A	935	G
1	A	936	G
1	A	937	G
1	A	938	G
1	A	939	G
1	A	940	C
1	A	941	C
1	A	942	C
1	A	943	G
1	A	944	C
1	A	945	A
1	A	946	C
1	A	947	A
1	A	956	A
1	A	957	G
1	A	966	U
1	A	968	A
1	A	970	U
1	A	971	U
1	A	972	C
1	A	975	A
1	A	980	C
1	A	981	G
1	A	982	C
1	A	983	G
1	A	984	A
1	A	985	A
1	A	986	G

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Mol	Chain	Res	Type
1	A	987	A
1	A	988	A
1	A	989	C
1	A	992	U
1	A	1001	U
1	A	1002	U
1	A	1003	G
1	A	1004	A
1	A	1007	U
1	A	1008	C
1	A	1010	U
1	A	1012	U
1	A	1013	G
1	A	1014	A
1	A	1015	C
1	A	1017	A
1	A	1019	C
1	A	1023	G
1	A	1024	A
1	A	1028	A
1	A	1033	G
1	A	1035	C
1	A	1036	C
1	A	1037	C
1	A	1040	U
1	A	1041	C
1	A	1042	G
1	A	1046	G
1	A	1053	G
1	A	1054	A
1	A	1059	U
1	A	1060	G
1	A	1064	C
1	A	1065	A
1	A	1066	U
1	A	1071	G
1	A	1072	U
1	A	1073	C
1	A	1074	G
1	A	1075	U
1	A	1076	C
1	A	1077	A

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Mol	Chain	Res	Type
1	A	1078	G
1	A	1095	U
1	A	1096	U
1	A	1111	A
1	A	1112	A
1	A	1113	C
1	A	1114	G
1	A	1134	G
1	A	1135	U
1	A	1136	U
1	A	1139	C
1	A	1140	A
1	A	1145	U
1	A	1146	C
1	A	1147	A
1	A	1148	G
1	A	1149	U
1	A	1153	G
1	A	1154	C
1	A	1166	A
1	A	1167	C
1	A	1168	U
1	A	1169	G
1	A	1173	G
1	A	1177	C
1	A	1184	G
1	A	1185	A
1	A	1190	G
1	A	1193	G
1	A	1195	G
1	A	1199	G
1	A	1201	C
1	A	1202	G
1	A	1205	A
1	A	1209	C
1	A	1210	A
1	A	1211	U
1	A	1215	G
1	A	1222	A
1	A	1224	G
1	A	1225	A
1	A	1233	U

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Mol	Chain	Res	Type
1	A	1234	A
1	A	1235	C
1	A	1236	A
1	A	1247	A
1	A	1250	G
1	A	1254	A
1	A	1257	A
1	A	1259	A
1	A	1265	C
1	A	1266	A
1	A	1267	G
1	A	1269	G
1	A	1271	A
1	A	1282	U
1	A	1287	C
1	A	1288	A
1	A	1289	A
1	A	1294	A
1	A	1295	C
1	A	1296	A
1	A	1307	C
1	A	1308	A
1	A	1309	G
1	A	1310	U
1	A	1311	U
1	A	1314	G
1	A	1321	G
1	A	1325	G
1	A	1328	A
1	A	1329	C
1	A	1341	A
1	A	1344	C
1	A	1345	U
1	A	1347	G
1	A	1354	U
1	A	1355	A
1	A	1357	U
1	A	1369	A
1	A	1372	A
1	A	1373	U
1	A	1374	G
1	A	1387	C

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Mol	Chain	Res	Type
1	A	1388	G
1	A	1389	U
1	A	1390	U
1	A	1392	C
1	A	1395	G
1	A	1396	G
1	A	1397	C
2	B	9003	A
2	B	9004	A
2	B	9005	A

All (101) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	10	A
1	A	15	U
1	A	51	U
1	A	113	G
1	A	128	A
1	A	139	A
1	A	189	A
1	A	190	A
1	A	194	C
1	A	211	A
1	A	219	U
1	A	220	C
1	A	259	G
1	A	313	G
1	A	323	A
1	A	335	A
1	A	336	C
1	A	337	A
1	A	372	A
1	A	374	C
1	A	419	A
1	A	436	G
1	A	446	G
1	A	455	G
1	A	457	A
1	A	459	A
1	A	475	A

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Mol	Chain	Res	Type
1	A	487	C
1	A	490	G
1	A	508	A
1	A	520	C
1	A	527	C
1	A	540	U
1	A	542	A
1	A	563	U
1	A	570	U
1	A	584	G
1	A	604	A
1	A	641	G
1	A	650	A
1	A	655	G
1	A	662	U
1	A	681	U
1	A	684	A
1	A	707	G
1	A	710	U
1	A	712	G
1	A	721	A
1	A	722	G
1	A	731	G
1	A	817	C
1	A	824	A
1	A	894	U
1	A	935	G
1	A	937	G
1	A	938	G
1	A	942	C
1	A	944	C
1	A	956	A
1	A	965	U
1	A	970	U
1	A	980	C
1	A	981	G
1	A	984	A
1	A	986	G
1	A	988	A
1	A	1001	U
1	A	1003	G
1	A	1016	A

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Mol	Chain	Res	Type
1	A	1032	C
1	A	1036	C
1	A	1040	U
1	A	1041	C
1	A	1059	U
1	A	1072	U
1	A	1075	U
1	A	1076	C
1	A	1077	A
1	A	1095	U
1	A	1111	A
1	A	1113	C
1	A	1139	C
1	A	1146	C
1	A	1153	G
1	A	1166	A
1	A	1168	U
1	A	1176	A
1	A	1184	G
1	A	1233	U
1	A	1265	C
1	A	1266	A
1	A	1287	C
1	A	1294	A
1	A	1307	C
1	A	1308	A
1	A	1323	C
1	A	1344	C
1	A	1372	A
1	A	1373	U
1	A	1389	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

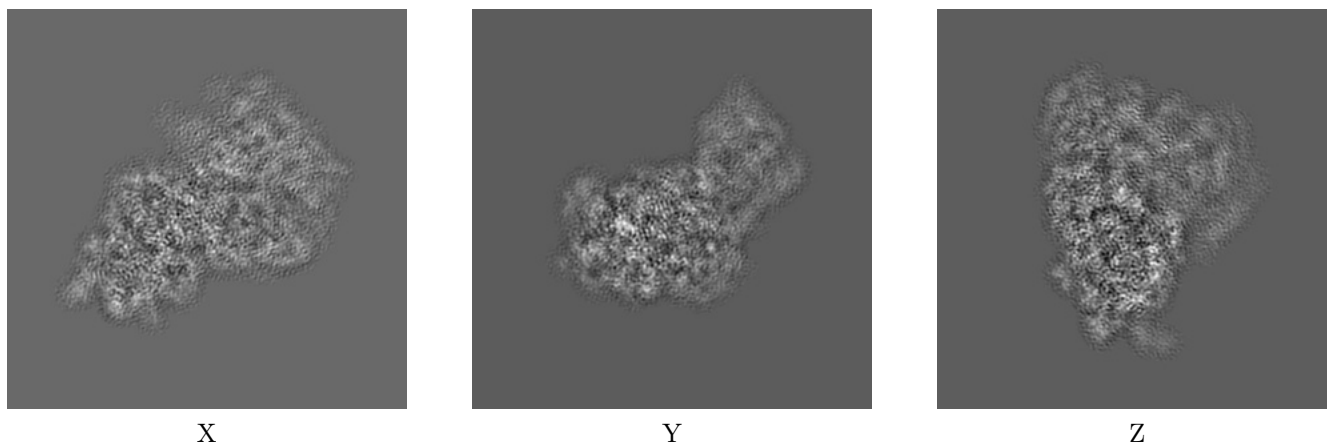
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16607. These allow visual inspection of the internal detail of the map and identification of artifacts.

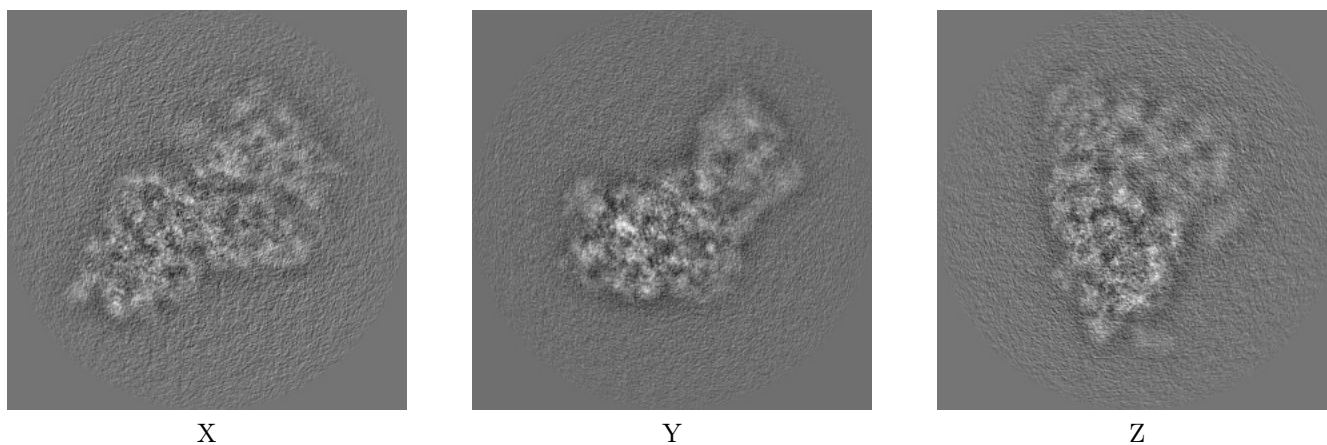
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



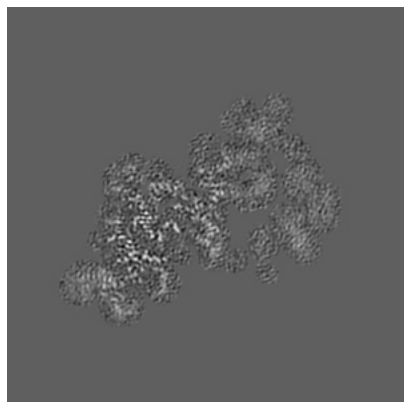
6.1.2 Raw map



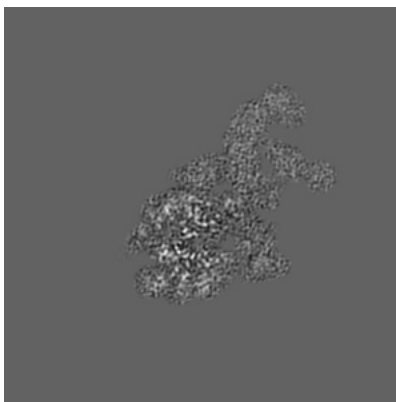
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

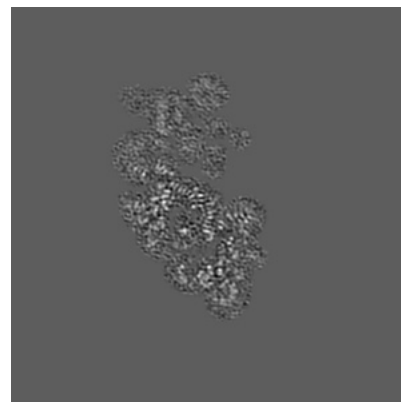
6.2.1 Primary map



X Index: 192

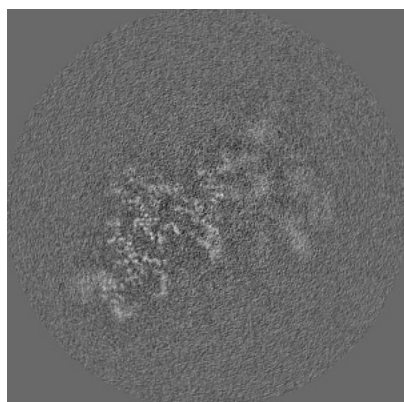


Y Index: 192

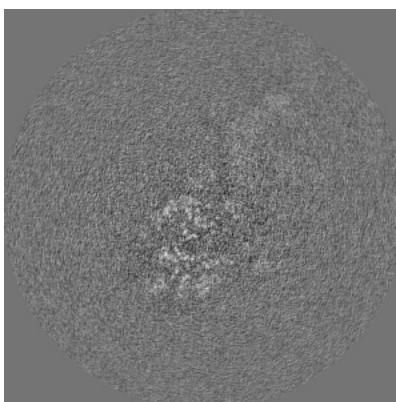


Z Index: 192

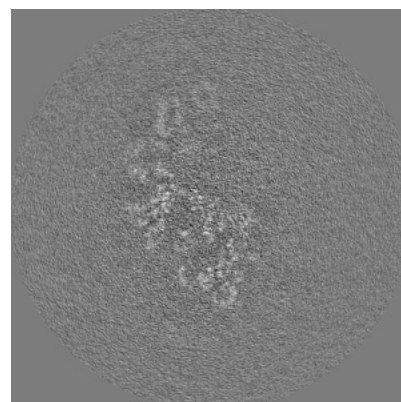
6.2.2 Raw map



X Index: 192



Y Index: 192

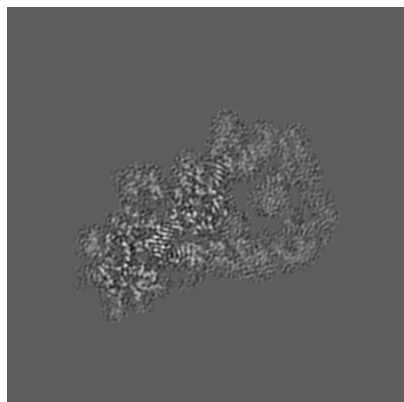


Z Index: 192

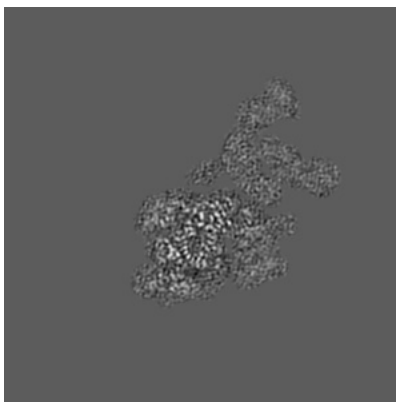
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

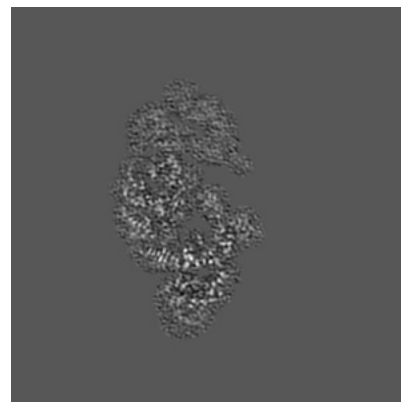
6.3.1 Primary map



X Index: 173

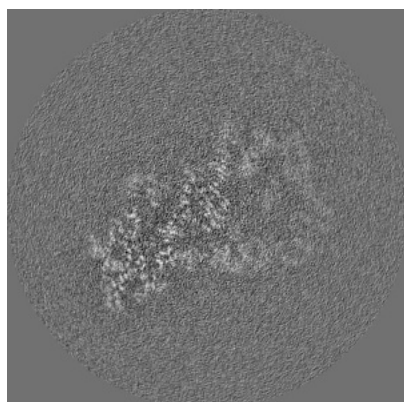


Y Index: 199

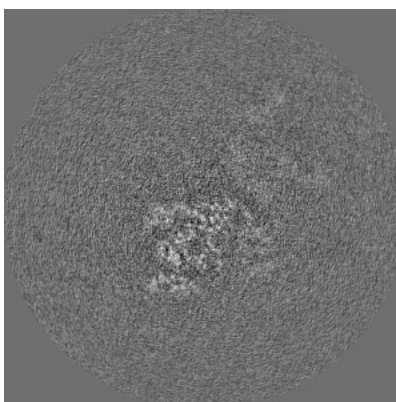


Z Index: 163

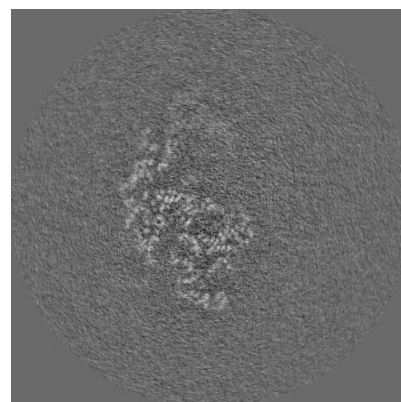
6.3.2 Raw map



X Index: 176



Y Index: 198

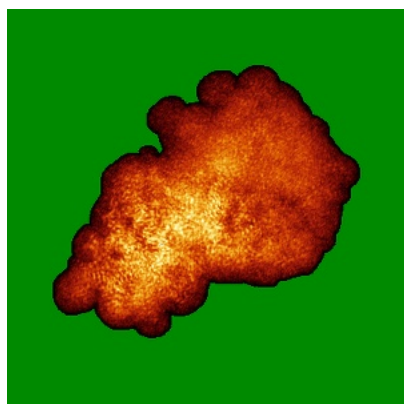


Z Index: 174

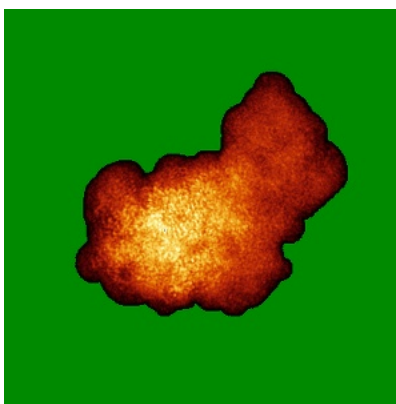
The images above show the largest variance slices of the map in three orthogonal directions.

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

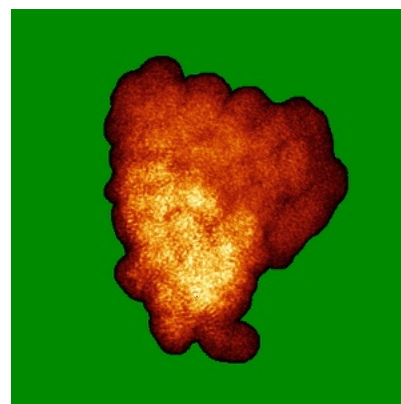
6.4.1 Primary map



X

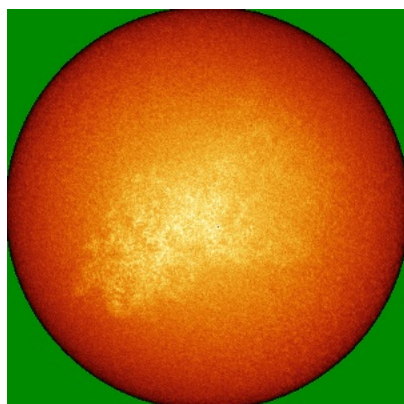


Y

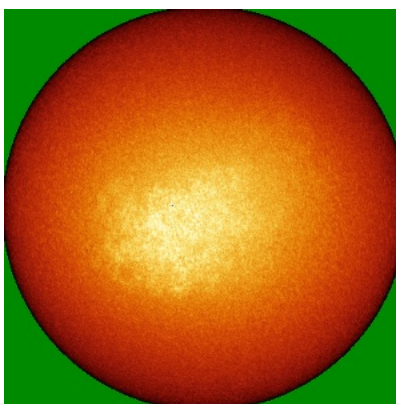


Z

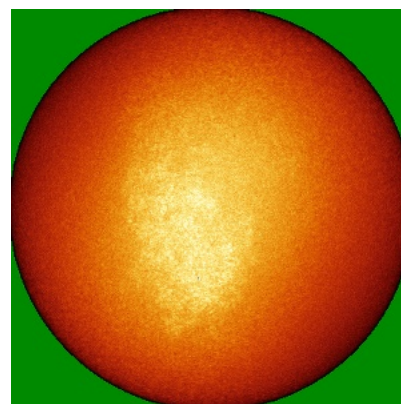
6.4.2 Raw map



X



Y

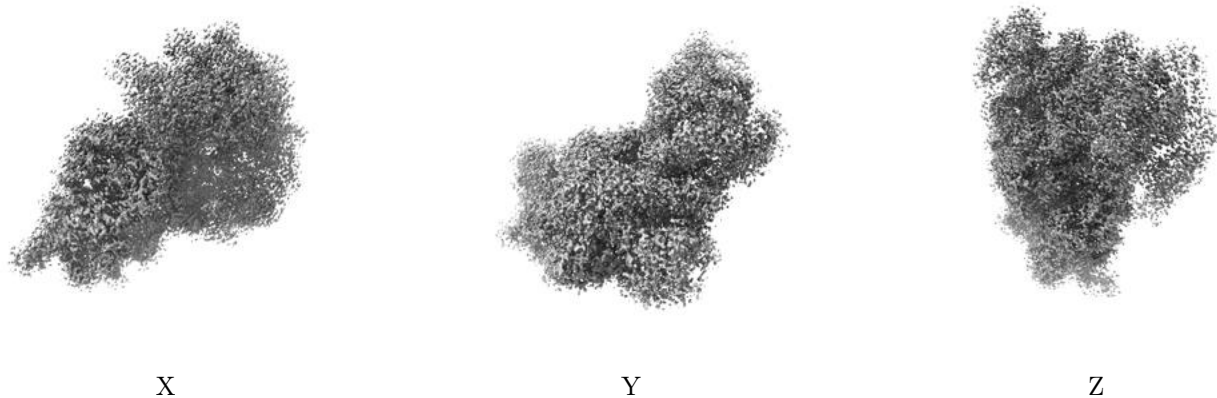


Z

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.

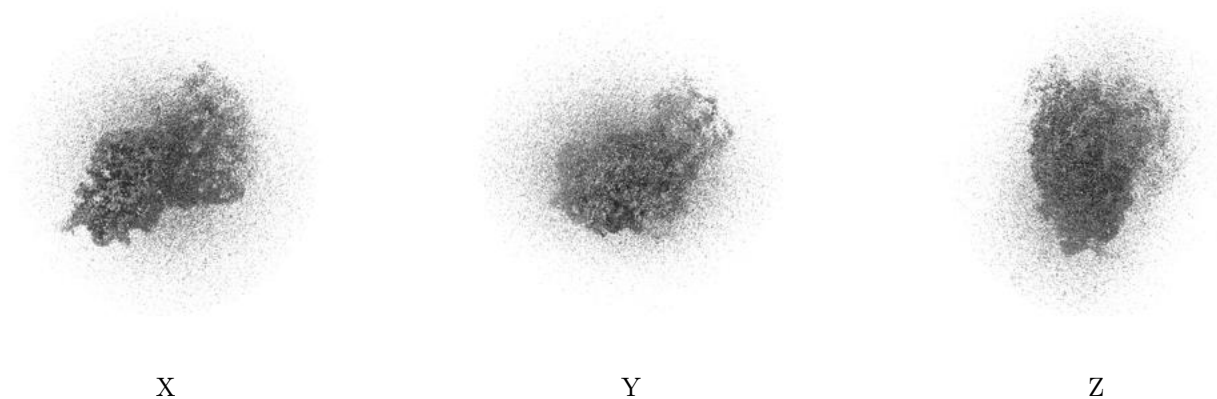
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0114. 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.

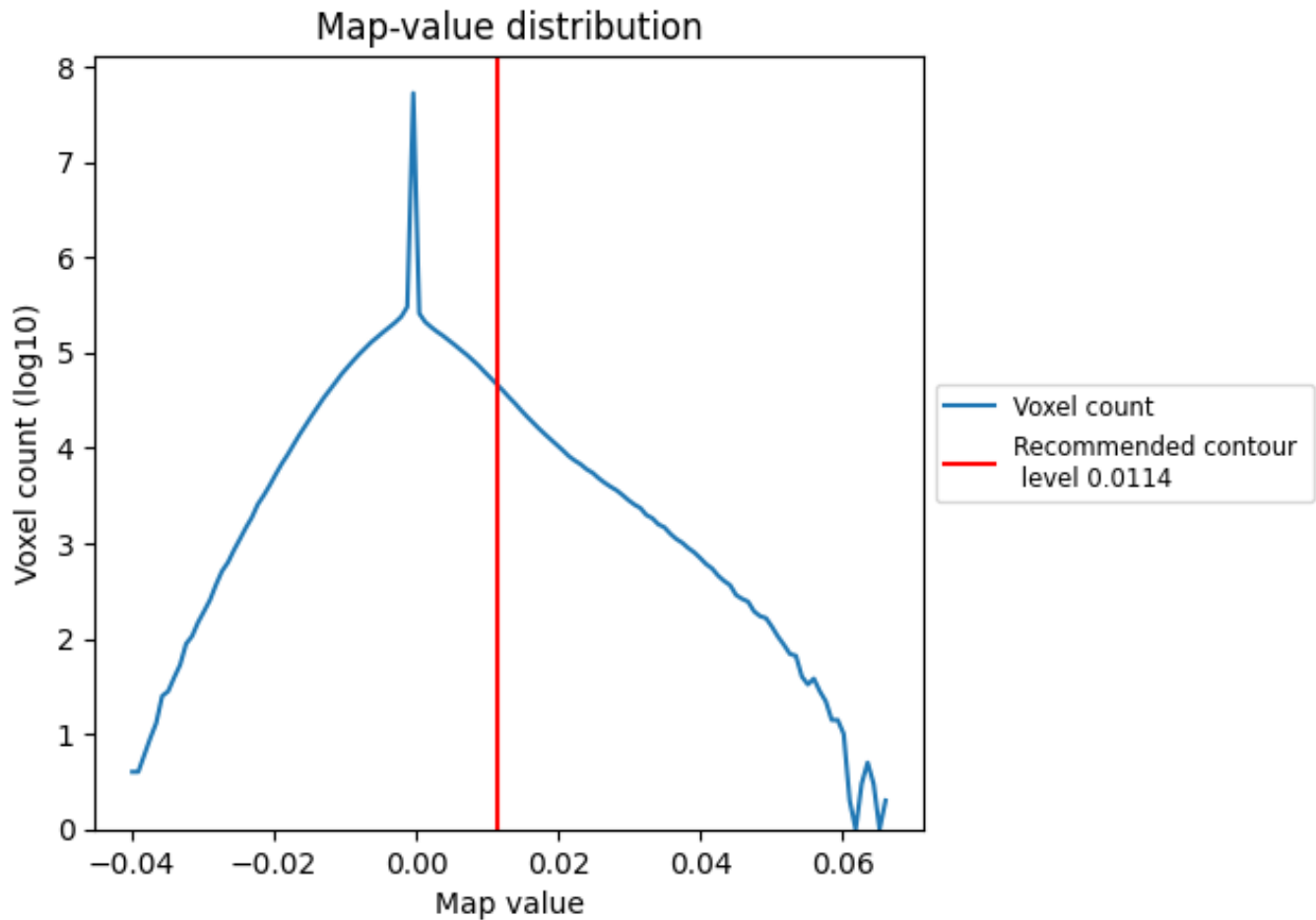
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

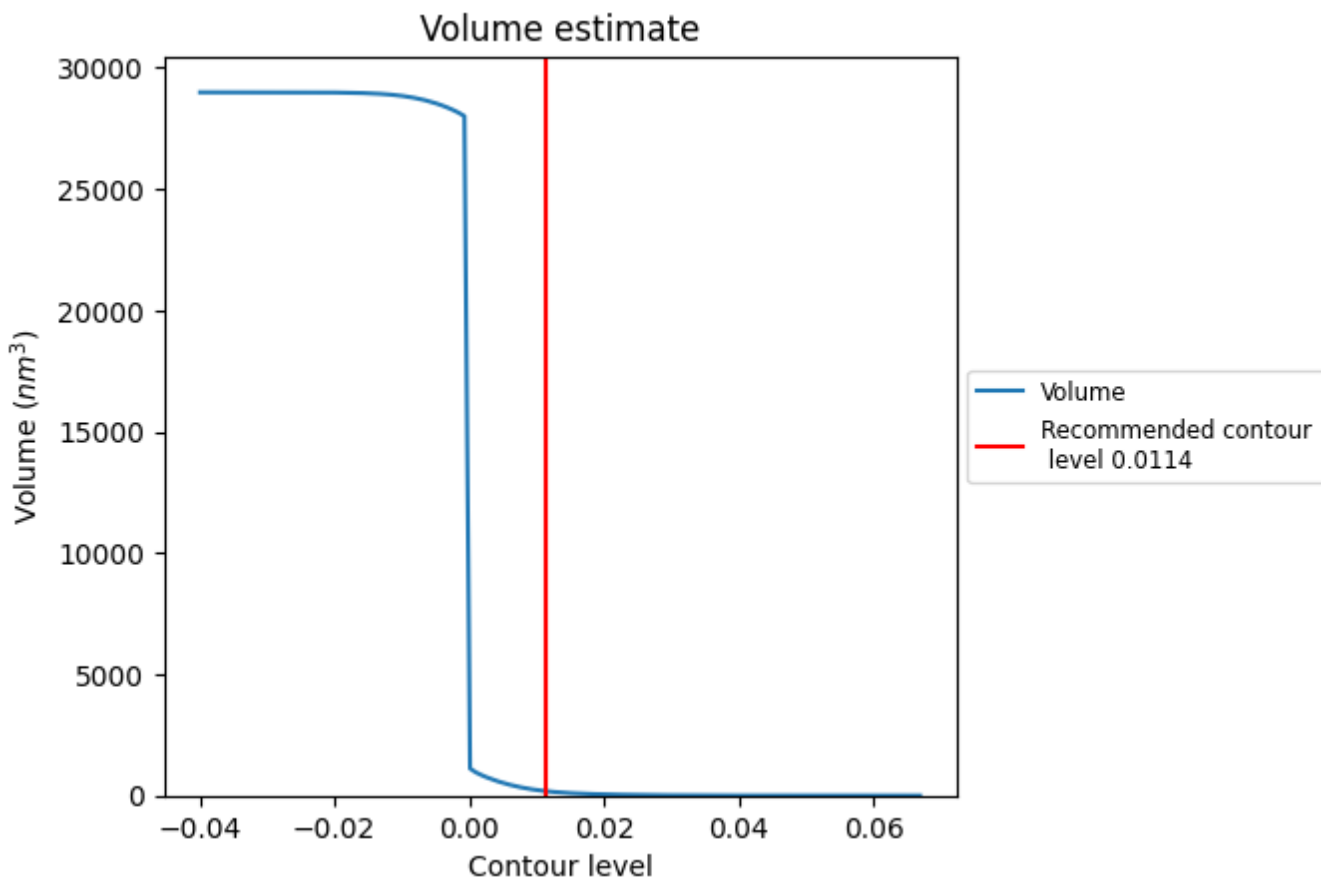
This section contains the results of statistical analysis of the map.

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.

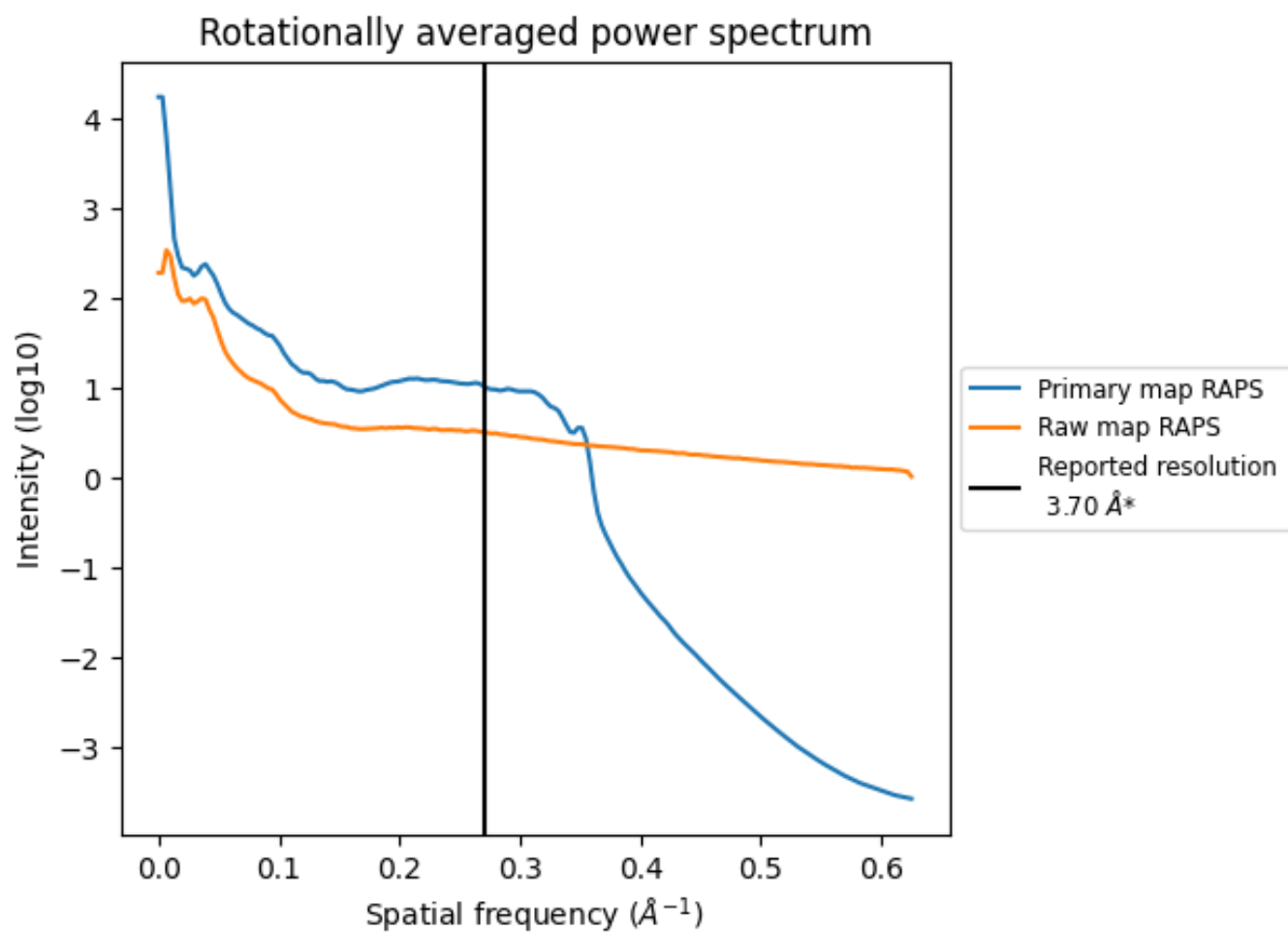
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 182 nm³; this corresponds to an approximate mass of 164 kDa.

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

7.3 Rotationally averaged power spectrum i

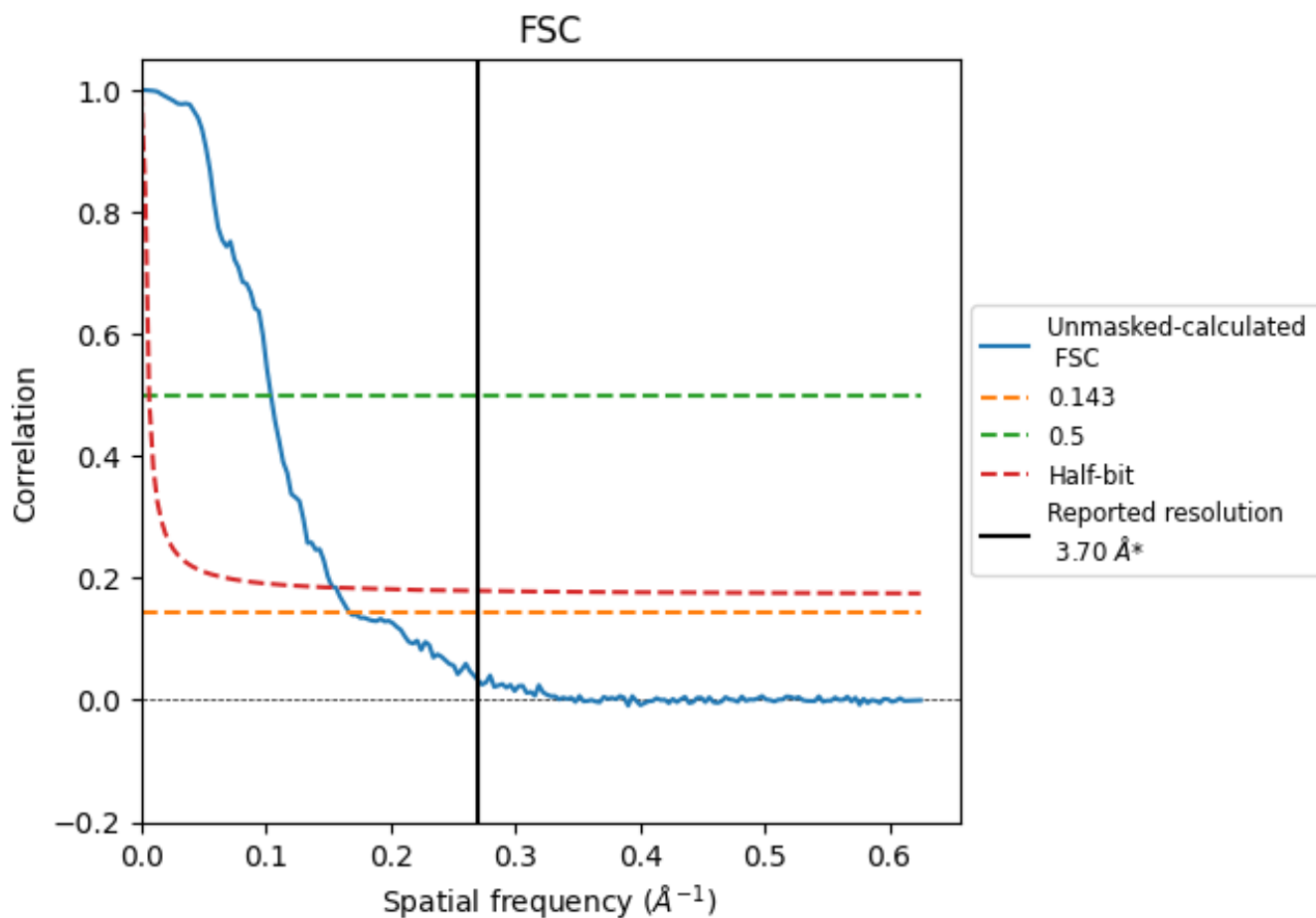


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

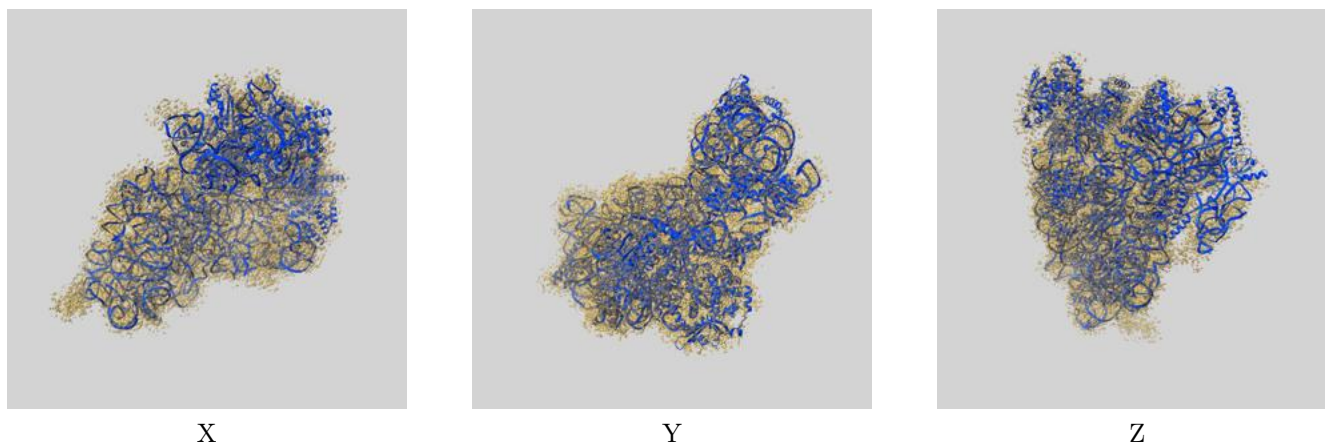
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.97	9.62	6.40

*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 5.97 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

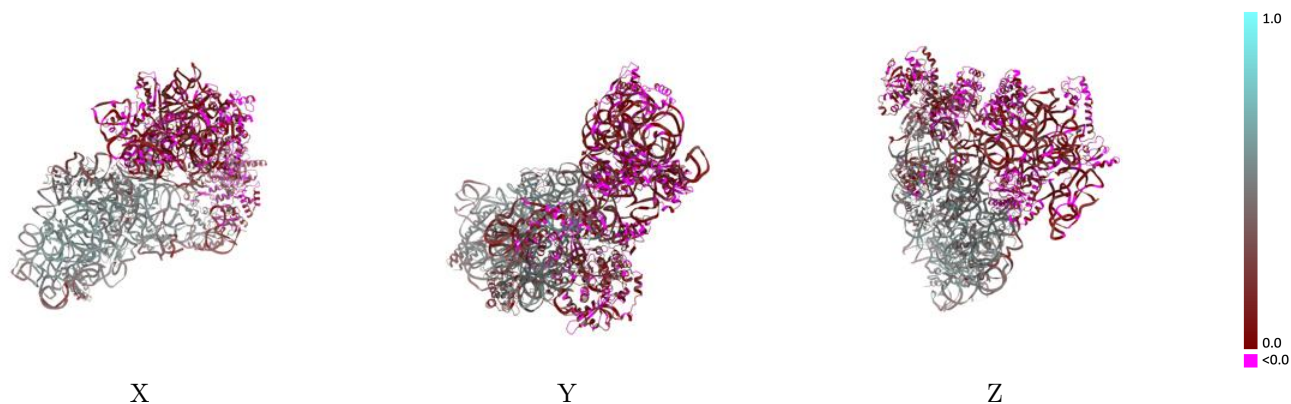
This section contains information regarding the fit between EMDB map EMD-16607 and PDB model 8CEE. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



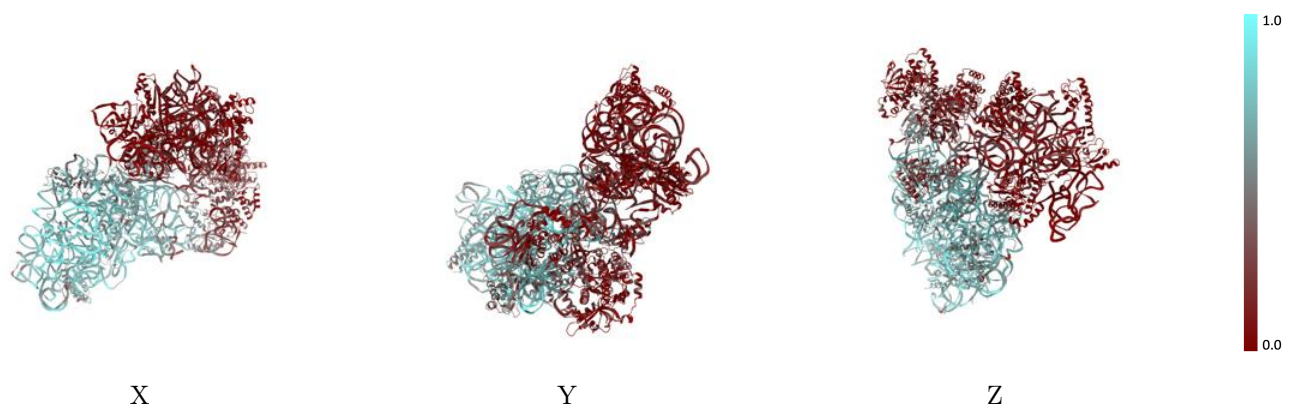
The images above show the 3D surface view of the map at the recommended contour level 0.0114 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



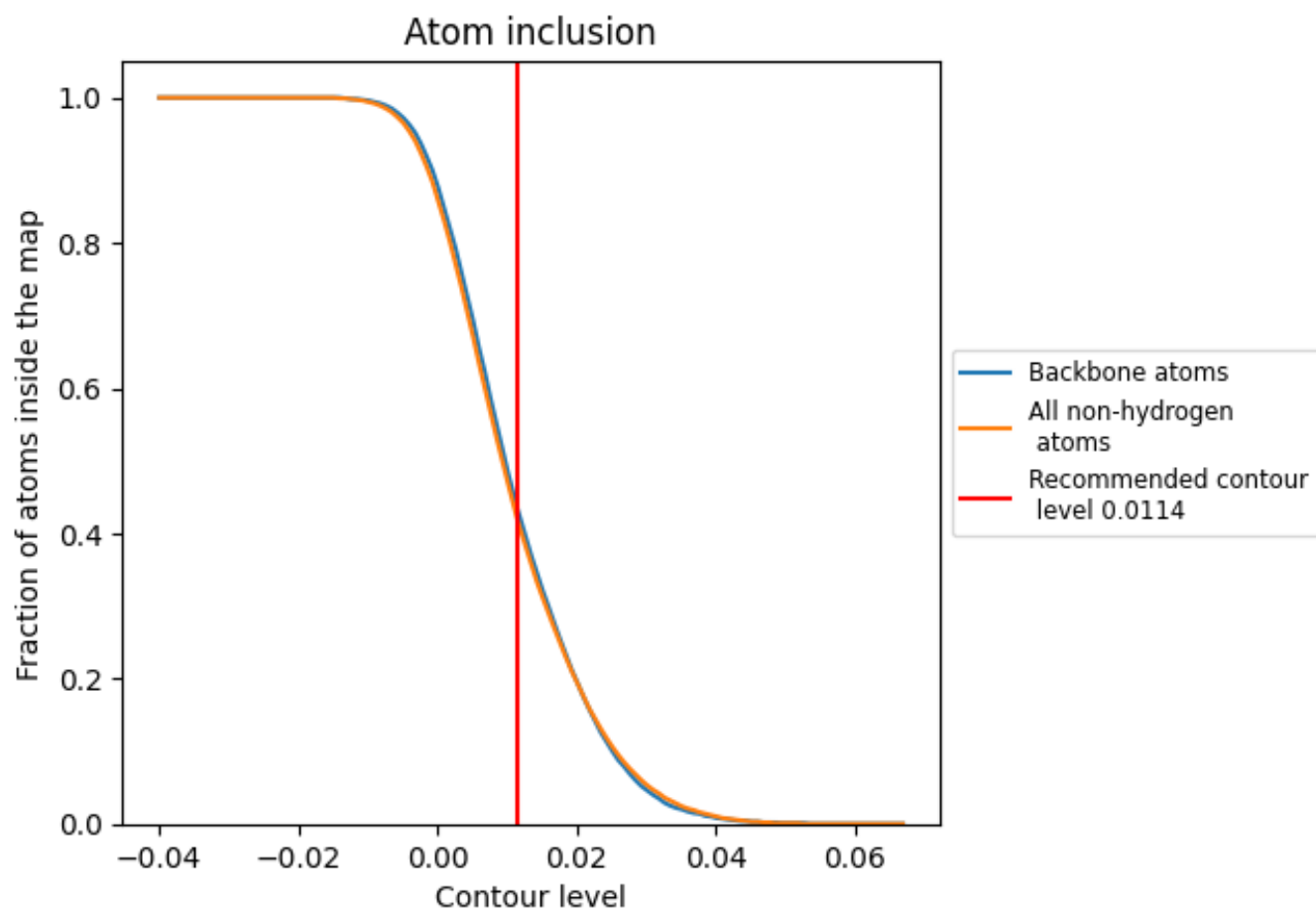
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0114).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 42% 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 (0.0114) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4230	 0.2980
A	 0.5420	 0.3640
B	 0.2270	 0.1760
C	 0.1120	 0.0950
D	 0.2430	 0.2360
E	 0.0490	 0.0250
F	 0.5080	 0.4070
G	 0.5920	 0.4350
H	 0.0550	 0.0370
I	 0.6480	 0.4810
J	 0.0430	 0.0550
K	 0.0500	 0.0600
L	 0.6050	 0.4530
M	 0.0230	 0.0240
N	 0.0280	 0.0570
O	 0.6180	 0.4370
P	 0.6800	 0.5090
Q	 0.6170	 0.4570
R	 0.0240	 0.0220
S	 0.5510	 0.4120
T	 0.3970	 0.2970
U	 0.4540	 0.3740
V	 0.1140	 0.1600

