



## Full wwPDB EM Validation Report ⓘ

Dec 8, 2025 – 01:16 PM JST

PDB ID : 9KRP / pdb\_00009krp  
EMDB ID : EMD-62535  
Title : Structure of the HCV IRES-dependent 48S translation initiation complex with eIF5B and eIF3  
Authors : Iwasaki, W.; Kashiwagi, K.; Sakamoto, A.; Nishimoto, M.; Takahashi, M.; Machida, K.; Imataka, H.; Matsumoto, A.; Shichino, Y.; Iwasaki, S.; Imami, K.; Ito, T.  
Deposited on : 2024-11-28  
Resolution : 3.20 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.47

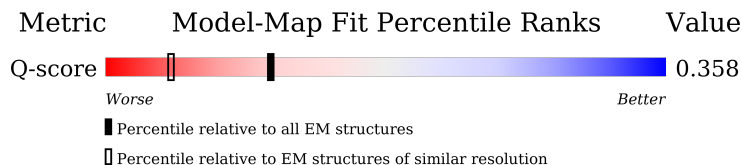
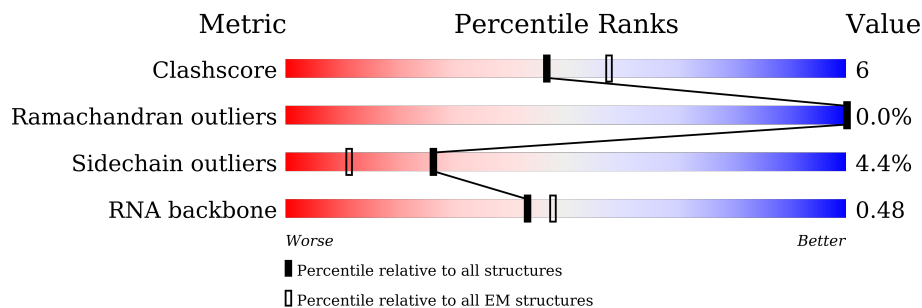
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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.











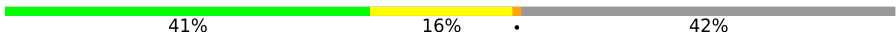
















Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	15020 ( 2.70 - 3.70 )

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  $\geq 3$ , 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	SA	295	
2	SB	264	







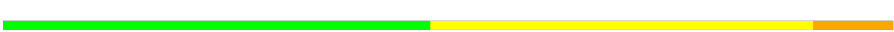





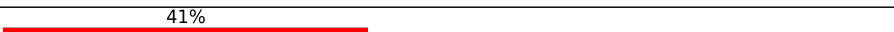



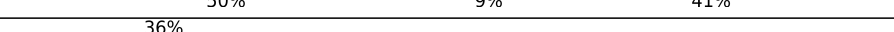

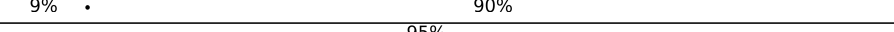

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Mol	Chain	Length	Quality of chain
3	SC	293	
4	SD	243	
5	SE	263	
6	SF	204	
7	SG	249	
8	SH	194	
9	SI	208	
10	SJ	194	
11	SK	165	
12	SL	158	
13	Sf	132	
14	SN	151	
15	SO	151	
16	SP	145	
17	SQ	146	
18	SR	135	
19	SS	152	
20	ST	145	
21	SU	119	
22	SV	83	
23	SW	130	
24	SX	143	
25	SY	133	
26	SZ	125	
27	Sa	115	

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Mol	Chain	Length	Quality of chain
28	Sb	84	
29	Sc	69	
30	Sd	56	
31	Se	59	
32	sh	156	
33	Sg	317	
34	zy	75	
35	Ln	25	
36	S2	1869	
37	zz	332	
38	5B	621	
39	3m	374	
40	3f	357	
41	3a	1382	
42	3e	445	
43	3c	913	
44	3h	352	
45	3d	548	
46	3k	218	
47	3l	564	

## 2 Entry composition [i](#)

There are 50 unique types of molecules in this entry. The entry contains 114768 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 uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	SA	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 2 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SB	212	Total	C	N	O	S	0	0
			1722	1093	308	307	14		

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SC	220	Total	C	N	O	S	0	0
			1709	1106	294	299	10		

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SD	226	Total	C	N	O	S	0	0
			1756	1119	316	314	7		

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SE	260	Total	C	N	O	S	0	0
			2065	1319	384	354	8		

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SF	192	Total	C	N	O	S	0	0
			1518	948	287	276	7		

- Molecule 7 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SH	187	Total	C	N	O	S	0	0
			1506	961	277	267	1		

- Molecule 9 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SI	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 10 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SJ	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 11 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SK	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 12 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SL	150	Total	C	N	O	S	0	0
			1220	776	228	210	6		

- Molecule 13 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Sf	121	Total	C	N	O	S	0	0
			935	586	165	175	9		

- Molecule 14 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SN	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 15 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SO	135	Total	C	N	O	S	0	0
			1007	617	198	186	6		

- Molecule 16 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SP	119	Total	C	N	O	S	0	0
			984	625	187	165	7		

- Molecule 17 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SQ	140	Total	C	N	O	S	0	0
			1116	710	211	192	3		

- Molecule 18 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SR	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 19 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SS	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 20 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	ST	142	Total	C	N	O	S	0	0
			1103	691	212	197	3		

- Molecule 21 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SU	101	Total	C	N	O	S	0	0
			803	504	153	142	4		

- Molecule 22 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 23 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 24 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 25 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SY	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 26 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SZ	75	Total	C	N	O	S	0	0
			601	385	111	104	1		

- Molecule 27 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Sa	100	Total	C	N	O	S	0	0
			803	501	166	131	5		

- Molecule 28 is a protein called 40S ribosomal protein S27.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 29 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Sc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 30 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Sd	52	Total	C	N	O	S	0	0
			436	273	88	70	5		

- Molecule 31 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Se	52	Total	C	N	O	S	0	0
			417	259	92	65	1		

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	sh	64	Total	C	N	O	S	0	0
			522	329	99	87	7		

- Molecule 33 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 34 is a RNA chain called Initiator Met-tRNA-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	zy	75	Total	C	N	O	P	0	0
			1607	717	298	517	75		

- Molecule 35 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 36 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	S2	1759	Total	C	N	O	P	5	0
			37646	16804	6762	12317	1763		

- Molecule 37 is a RNA chain called HCV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	zz	313	Total	C	N	O	P	0	0
			6675	2975	1189	2198	313		

- Molecule 38 is a protein called Eukaryotic translation initiation factor 5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	5B	621	Total	C	N	O	S	0	0
			4917	3135	847	913	22		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	3m	363	Total	C	N	O	S	0	0
			2638	1666	450	510	12		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	3f	269	Total	C	N	O	S	0	0
			2057	1300	351	394	12		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3a	592	Total	C	N	O	S	0	0
			4497	2849	805	822	21		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	3e	430	Total	C	N	O	S	0	0
			3220	2051	561	592	16		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	3c	543	Total	C	N	O	S	0	0
			3924	2463	721	716	24		

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	3h	317	Total	C	N	O	S	0	0
			2512	1595	429	473	15		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3d	55	Total	C	N	O	S	0	0
			347	222	65	59	1		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3k	215	Total	C	N	O	S	0	0
			1471	930	250	281	10		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3l	520	Total	C	N	O	S	0	0
			4331	2806	714	792	19		

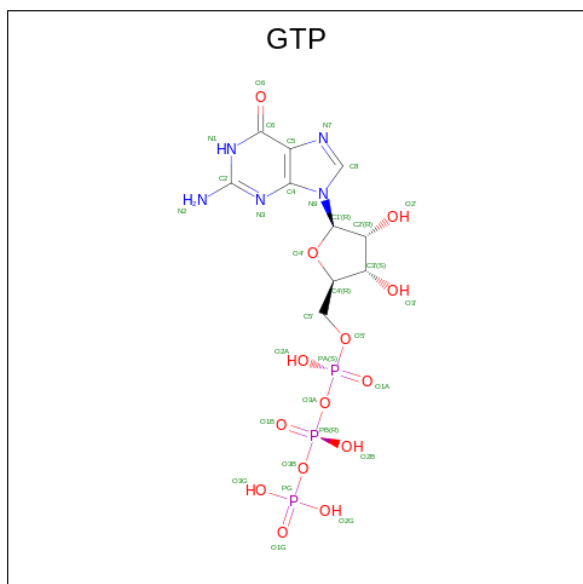
- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
48	Sa	1	Total	Zn	0
			1	1	
48	sh	1	Total	Zn	0
			1	1	

- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

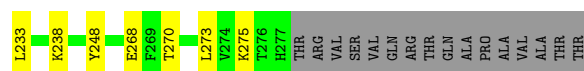
Mol	Chain	Residues	Atoms		AltConf
49	S2	8	Total	Mg	0
			8	8	
49	5B	1	Total	Mg	0
			1	1	

- Molecule 50 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



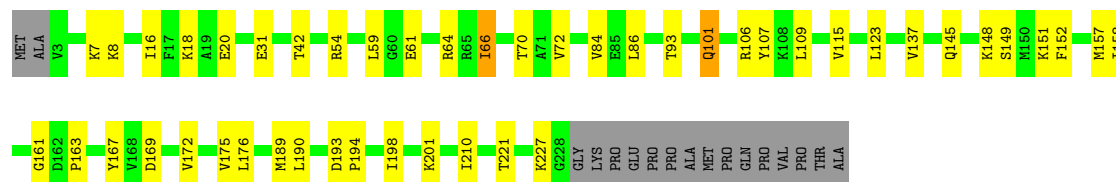
Mol	Chain	Residues	Atoms					AltConf
50	5B	1	Total	C	N	O	P	0
			32	10	5	14	3	





• Molecule 4: 40S ribosomal protein S3

Chain SD: 74% 19% 7%



• Molecule 5: 40S ribosomal protein S4, X isoform

Chain SE: 84% 15% 1%



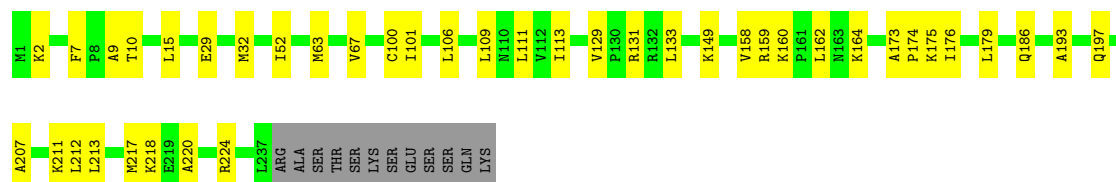
• Molecule 6: 40S ribosomal protein S5

Chain SF: 84% 10% 6%



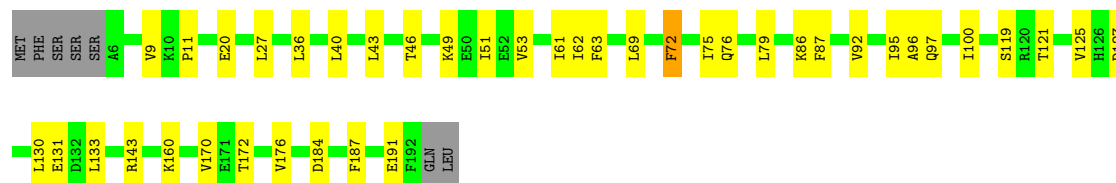
• Molecule 7: 40S ribosomal protein S6

Chain SG: 79% 16% 5%

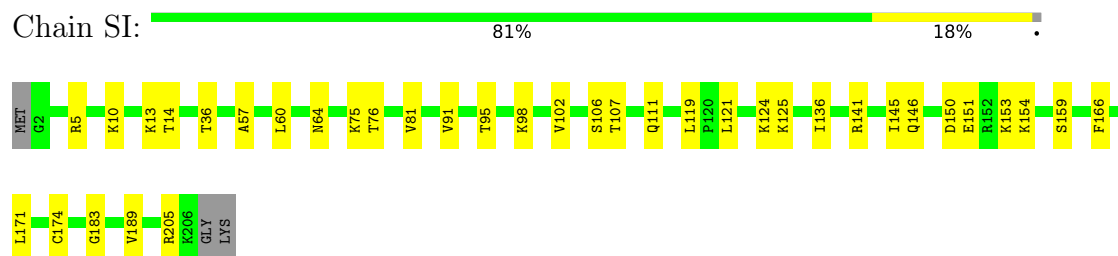


• Molecule 8: 40S ribosomal protein S7

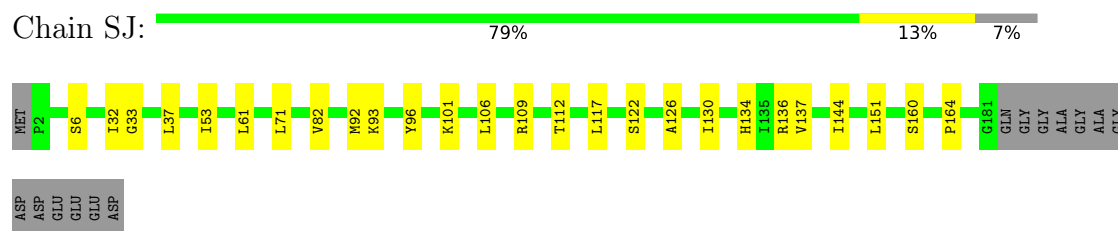
Chain SH: 75% 21% 4%



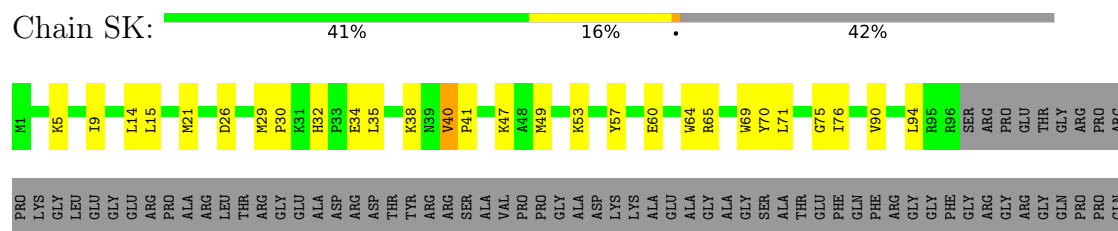
- Molecule 9: 40S ribosomal protein S8



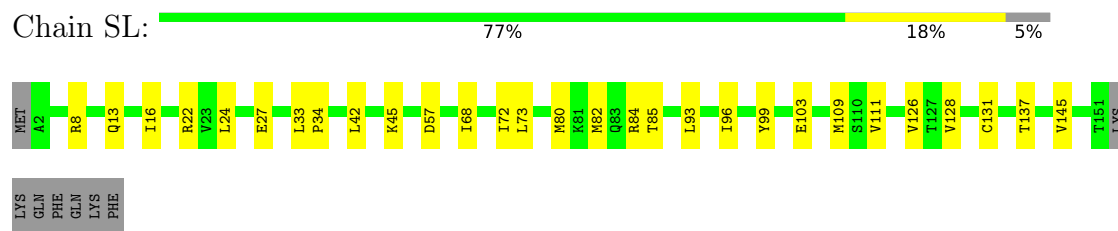
- Molecule 10: 40S ribosomal protein S9



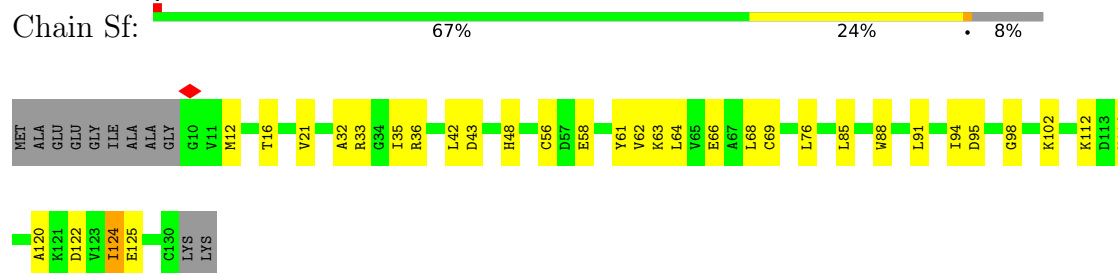
- Molecule 11: 40S ribosomal protein S10



- Molecule 12: 40S ribosomal protein S11



- Molecule 13: 40S ribosomal protein S12



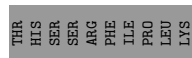
- Molecule 14: 40S ribosomal protein S13



- Molecule 15: 40S ribosomal protein S14



- Molecule 16: 40S ribosomal protein S15



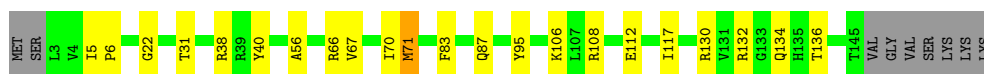
- Molecule 17: 40S ribosomal protein S16



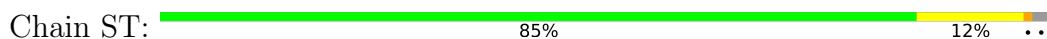
- Molecule 18: 40S ribosomal protein S17



- Molecule 19: 40S ribosomal protein S18



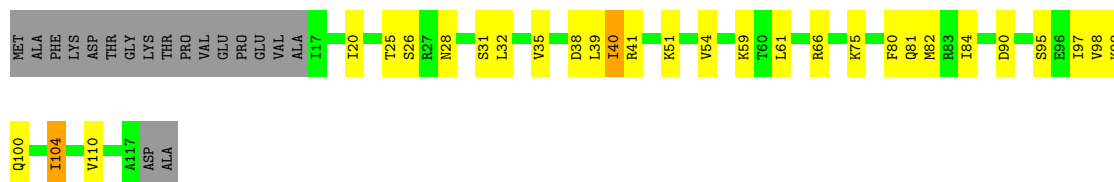
- Molecule 20: 40S ribosomal protein S19



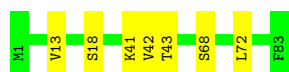




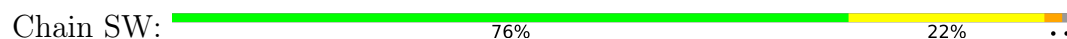
- Molecule 21: 40S ribosomal protein S20



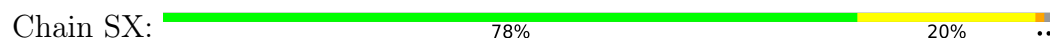
- Molecule 22: 40S ribosomal protein S21



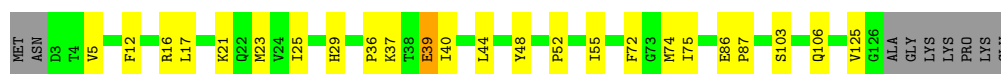
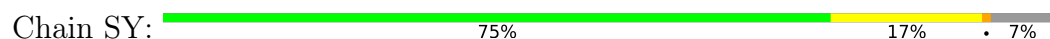
- Molecule 23: 40S ribosomal protein S15a



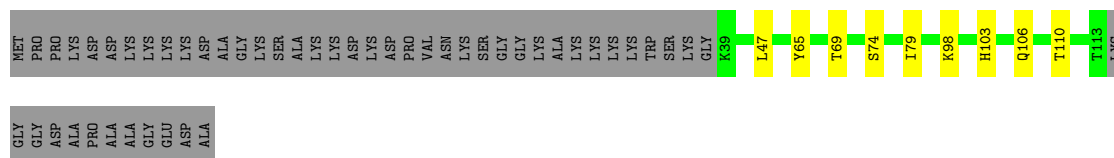
- Molecule 24: 40S ribosomal protein S23




- Molecule 25: 40S ribosomal protein S24



- Molecule 26: 40S ribosomal protein S25



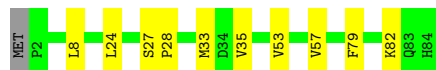
- Molecule 27: 40S ribosomal protein S26

Chain Sa:  73% 13% 13%



- Molecule 28: 40S ribosomal protein S27

Chain Sb:  87% 12%




- Molecule 29: 40S ribosomal protein S28

Chain Sc:  70% 19% 10%



- Molecule 30: 40S ribosomal protein S29

Chain Sd:  77% 14% 7%



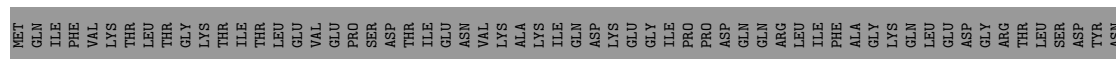
- Molecule 31: 40S ribosomal protein S30

Chain Se:  73% 15% 12%




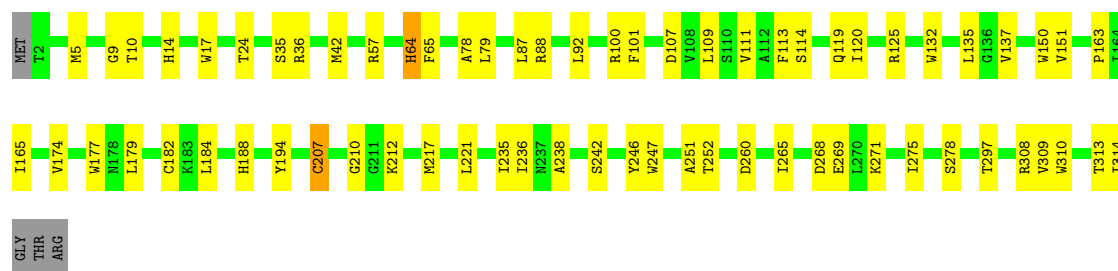
- Molecule 32: Ubiquitin-40S ribosomal protein S27a

Chain sh:  31% 9% 59%



- Molecule 33: Receptor of activated protein C kinase 1

Chain Sg:  78% 21% ..



- Molecule 34: Initiator Met-tRNA-i

Chain zy:  48% 43% 9%



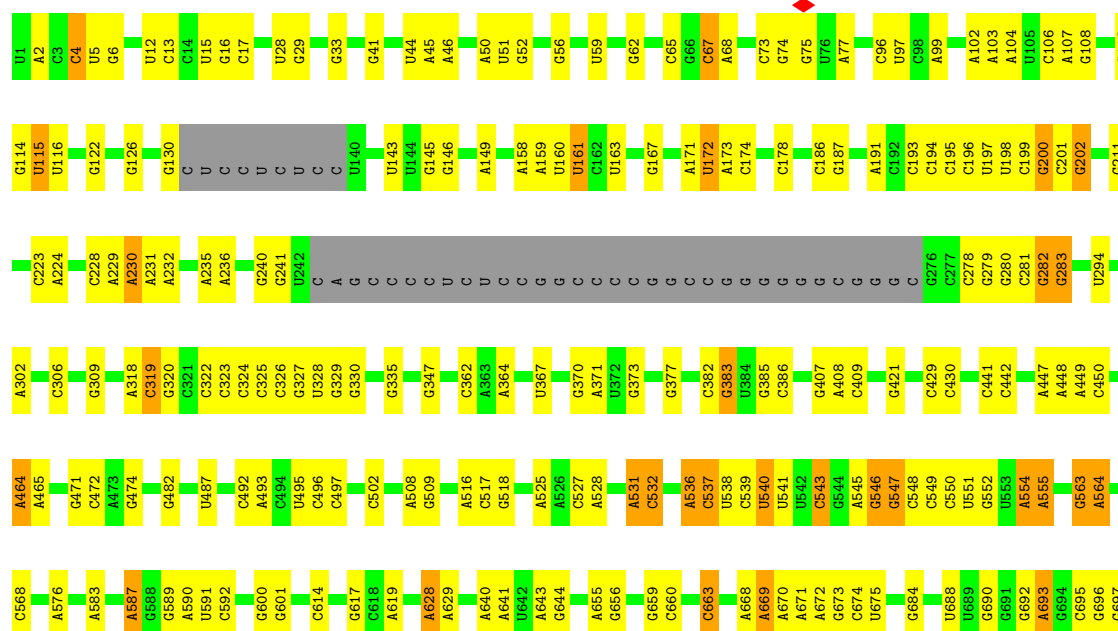
- Molecule 35: 60S ribosomal protein L41

Chain Ln:  68% 28% .



- Molecule 36: 18S rRNA

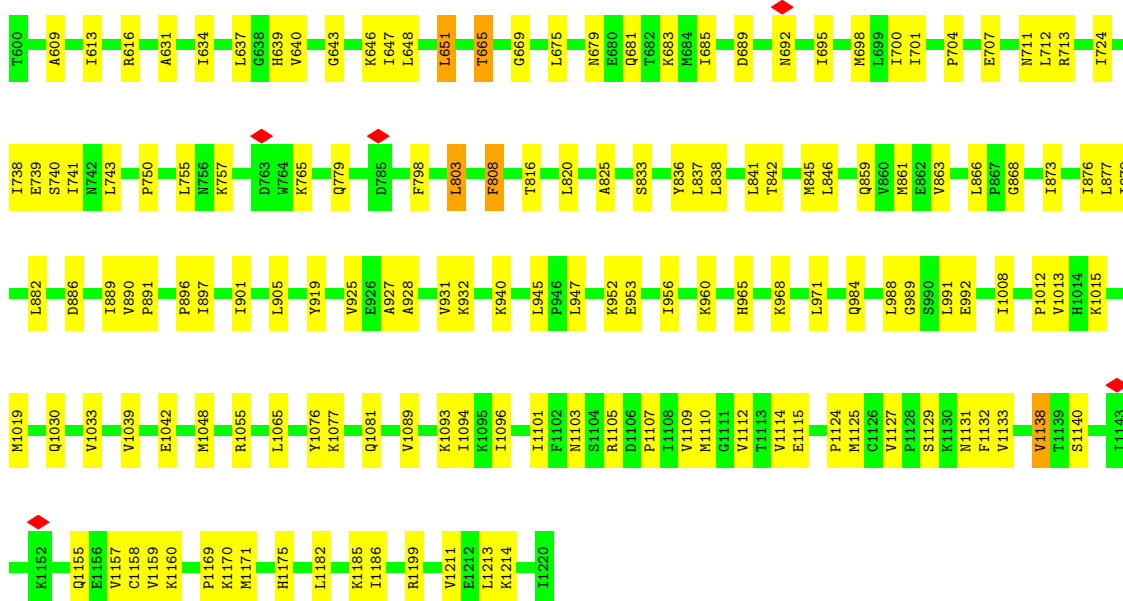
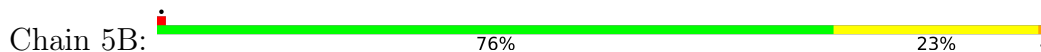
Chain S2:  63% 27% . 6%



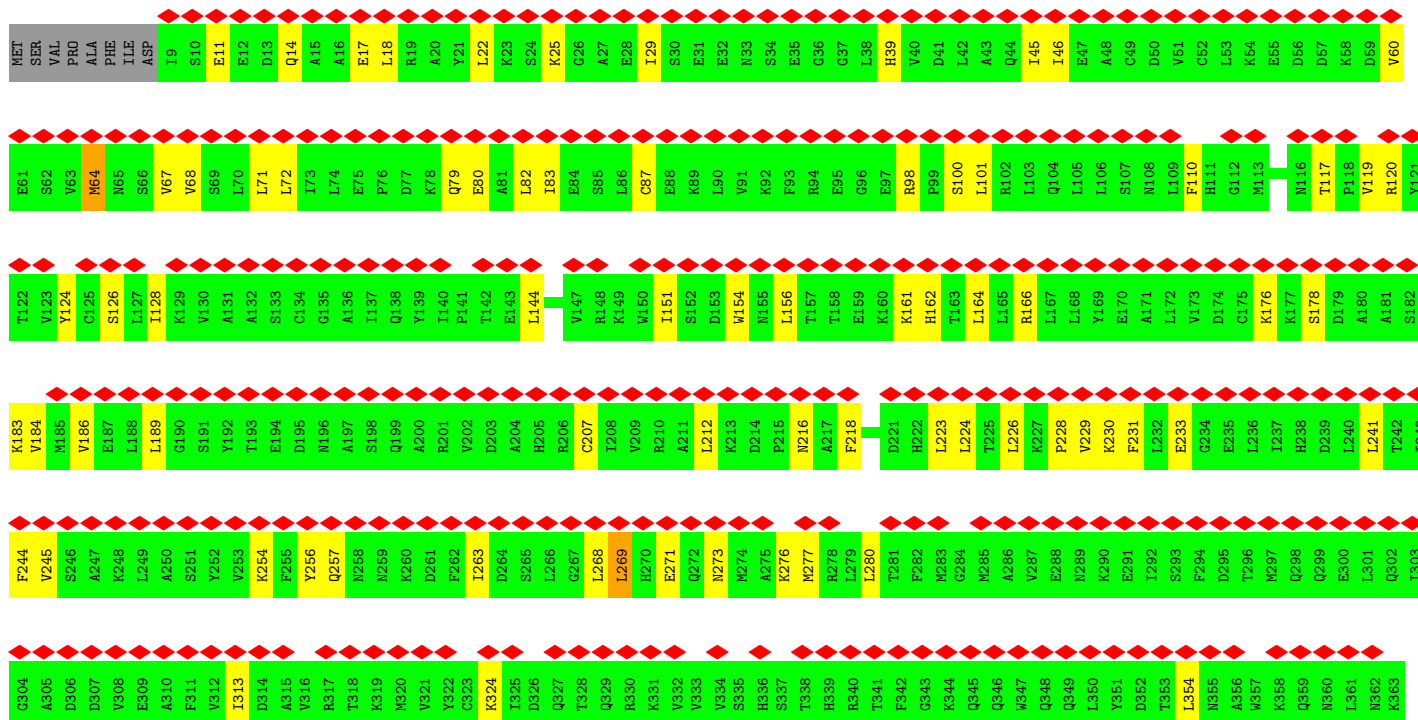
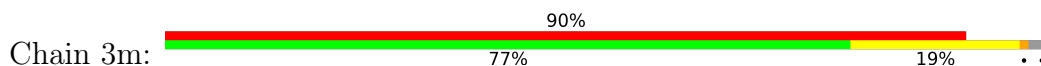




• Molecule 38: Eukaryotic translation initiation factor 5B

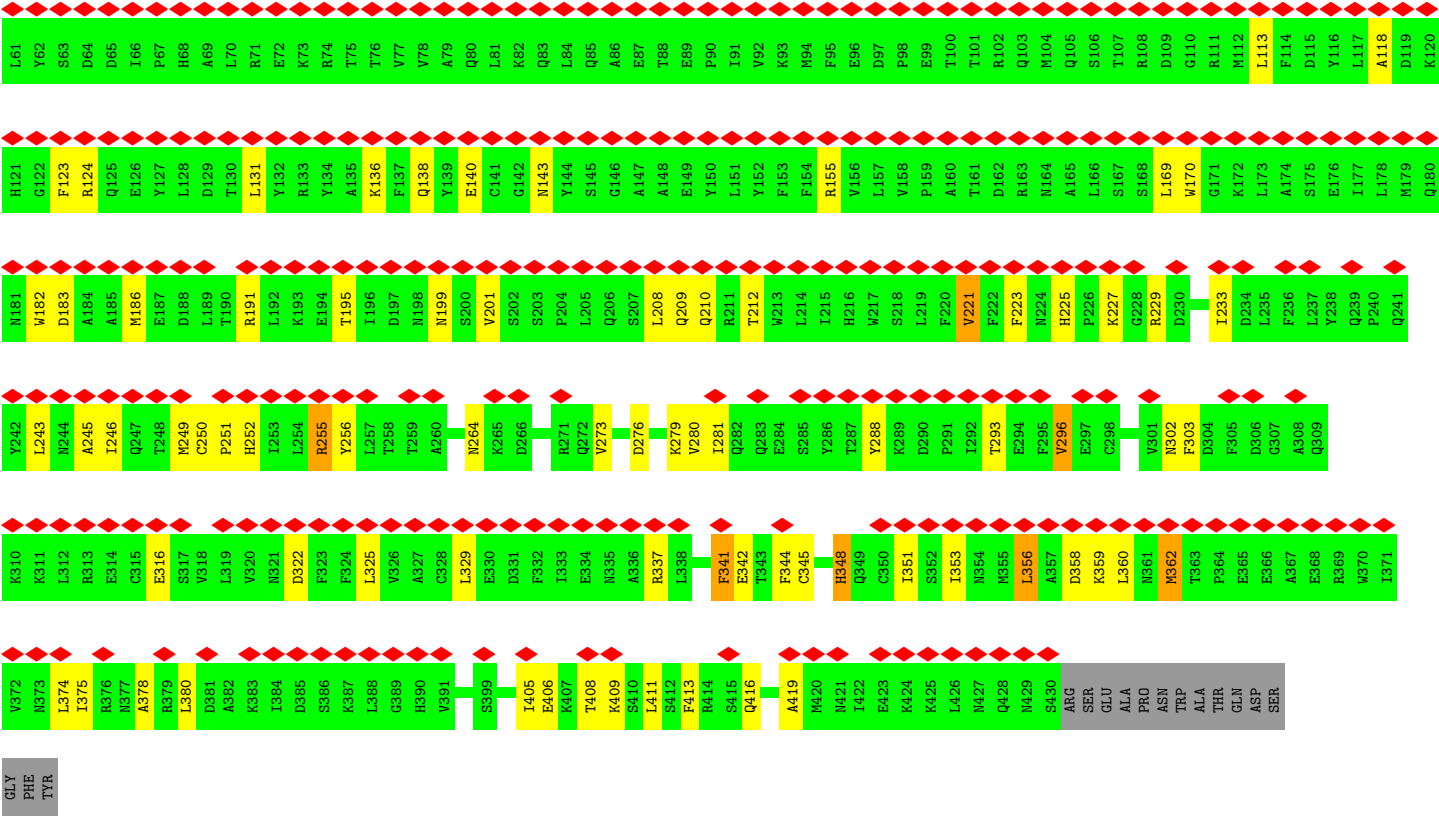


• Molecule 39: Eukaryotic translation initiation factor 3 subunit M

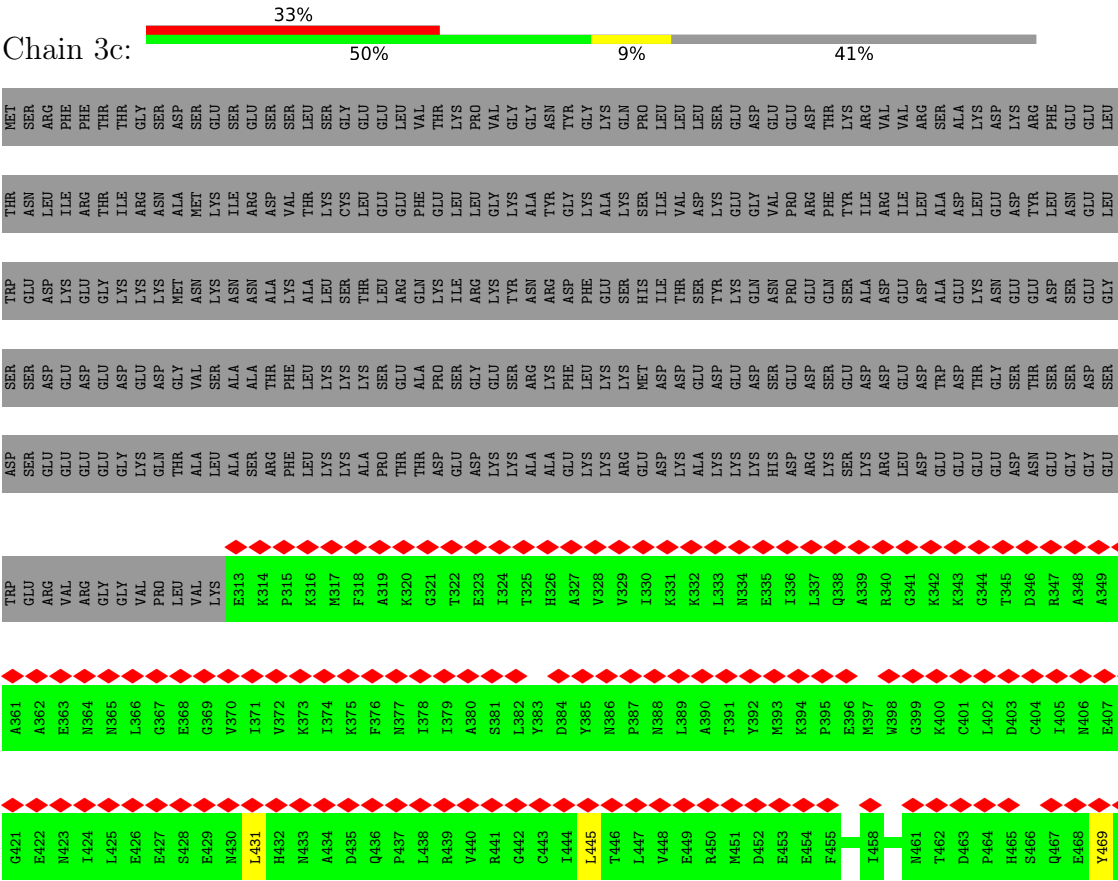








• Molecule 43: Eukaryotic translation initiation factor 3 subunit C

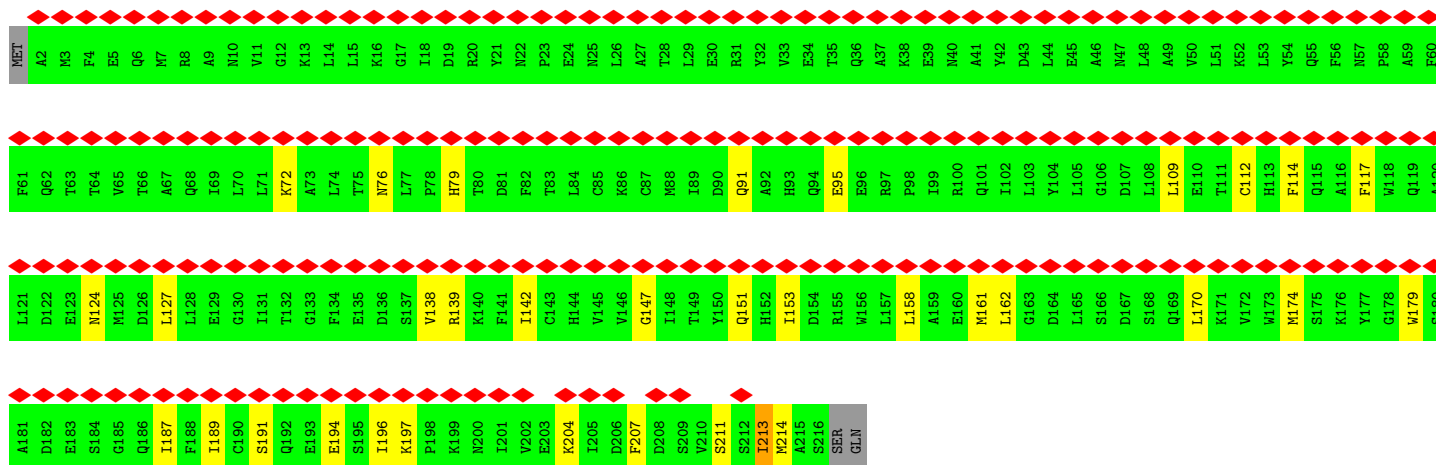
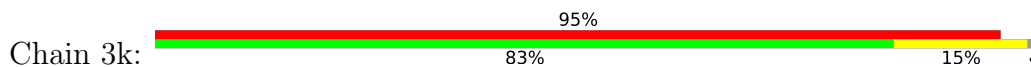




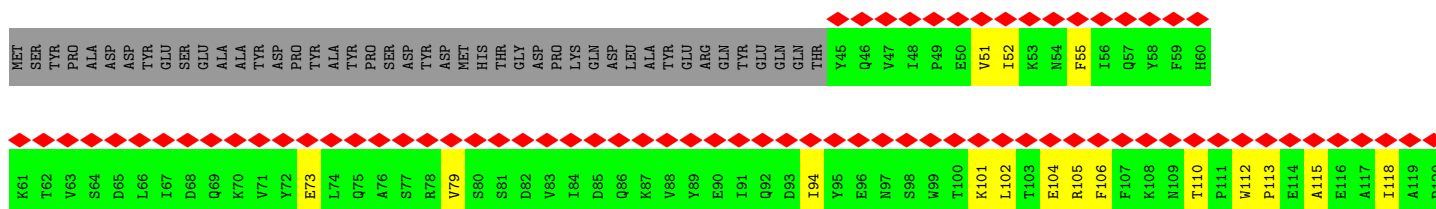
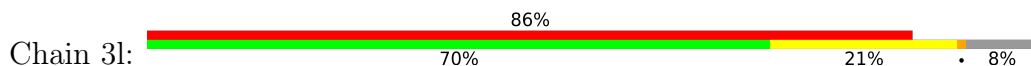


[illegible]

- Molecule 46: Eukaryotic translation initiation factor 3 subunit K



- Molecule 47: Eukaryotic translation initiation factor 3 subunit L



Q121	Q181	N241	K301	N361	V425	E485	R545
V122	V182	R242	K302	K362	P426	F486	E552
G123	L183	Q243	S303	Q363	M427	R487	L553
N124	V184	L244	M304	N364	Y428	T488	R554
D125	D185	E245	S305	E365	D429	Q489	R555
A126	I186	V246	S306	Q366	M430	L490	T556
V127	I187	Y247	R307	M367	V431	L491	L557
F128	D188	T248	V308	L370	H432	V492	K558
L129	E189	S249	F309	L371	P433	F493	K559
I130	F190	G250	E310	A372	M434	K494	R560
L131	I191	G251	C311	I373	Y435	H495	R561
Y132	Y192	D252	Q312	A374	H436	K496	Q562
K133	Q193	P253	V313	L375	K437	M497	R563
E134	F194	E254	T314	T376	E438	K498	P564
L135	Q195	S255	T315	M377	P439	L500	
Y136	S196	V256	Y316	Y378	F440	V501	
Y137	F197	A257	Y317	P379	L441	W502	
R138	S198	G258	Y318	M380	Q442	T503	
H139	Q199	E259	V319	R381	Q443	S504	
I140	Y200	Y260	G320	I382	L444	G505	
Y141	R201	G261	F321	D383	K445	I506	
A142	C202	R262	A322	I386	V446	S507	
K143	K203	H263	Y323	H387	F447	L508	
V144	T204	S264	L324	L388	S448	L509	
S145	A205	L265	M325	Q389	D449	D510	
G146	K206	Y266	M326	L390	E450	G511	
G147	K207	K267	R327		V451	E512	
P148	S208	M268	R328	Y394	Q452	F513	
S149	E209	L269	Y329	G395	Q453	Q514	
L150	E210	G270	Q330	D396	Q454	S515	
E151	E211	Y271	D331	K397	A455	A516	
Q152	I212	F272	A332	M398	Q456	S517	
R153	D213	S273	I333	L399	L457	E518	
F154	F214	L274	R334	R400	S458	V519	
E155	L215	V275	V335	M401	T459	D520	
S156	R216	G276	F336	Q402	I460	F521	
Y157	S217	L277	A337	K403	R461	V522	
Y158	N218	N217	N338	G404	F463	I523	
N159	P219	R279	I339	D405	L464	D524	
Y160	K220	L280	L340	P406	K465	K525	
C161	I221	H281	L341	Q407	L466	D526	
N162	W222	S282	Y342	V408	Y467	W527	
L163	N223	L283	I343	Y409	T468	I528	
F164	V224	L284	Q344	E410	M470	R529	
N165	H225	G285	R345	E411	P471	A531	
M166	S226	D286	T346	L412	M470	D532	
L167	V227	Y287	K347	F413	P471	T533	
L168	L228	Y288	S348	S414	V472	K534	
N169	N229	Q289	M349	Y415	A473	V535	
A170	V230	A290	F350	S416	K474	A536	
D171	L231	I291	Q351	C417	L475	R537	
G172	H232	K292	R352	P418	G477	R538	
P173	S233	V293	T353	K419	F478	Y539	
A174	L234	L294	Y354	F420	L479	G540	
P175	V235	E295	K355	L421	D480	D541	
L176	D236	N296	Y357	S422	L481	F542	
E177	K237	I297	E358	P423	T482	P543	
L178	S238	E298	M359	V424	E483	I544	
P179	N239	L299	I360		Q484		
N180	I240	N300					

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24895	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	56.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.105	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size ( $\text{\AA}$ )	636.0, 636.0, 636.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.272, 1.272, 1.272	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, GTP

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	SA	0.24	0/1742	0.39	0/2367
2	SB	0.20	0/1749	0.38	0/2340
3	SC	0.24	0/1746	0.41	0/2358
4	SD	0.20	0/1784	0.35	0/2402
5	SE	0.24	0/2107	0.40	0/2836
6	SF	0.21	0/1540	0.37	0/2071
7	SG	0.18	0/1946	0.36	0/2590
8	SH	0.18	0/1529	0.37	0/2048
9	SI	0.20	0/1711	0.34	0/2282
10	SJ	0.20	0/1524	0.35	0/2035
11	SK	0.23	0/834	0.49	0/1125
12	SL	0.23	0/1241	0.38	0/1662
13	Sf	0.20	0/945	0.54	0/1269
14	SN	0.24	0/1226	0.36	0/1649
15	SO	0.22	0/1020	0.41	0/1368
16	SP	0.22	0/1003	0.46	0/1340
17	SQ	0.24	0/1133	0.43	0/1517
18	SR	0.26	0/1082	0.62	0/1452
19	SS	0.20	0/1202	0.40	0/1610
20	ST	0.20	0/1122	0.42	0/1504
21	SU	0.22	0/813	0.48	0/1092
22	SV	0.22	0/643	0.44	0/860
23	SW	0.27	0/1051	0.40	0/1406
24	SX	0.24	0/1116	0.44	0/1490
25	SY	0.21	0/1031	0.45	0/1370
26	SZ	0.24	0/607	0.55	0/815
27	Sa	0.24	0/817	0.40	0/1095
28	Sb	0.23	0/665	0.39	0/891
29	Sc	0.21	0/490	0.45	0/656
30	Sd	0.25	0/446	0.41	0/591
31	Se	0.17	0/422	0.36	0/555
32	sh	0.15	0/533	0.35	0/706

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Sg	0.20	0/2493	0.42	0/3394
34	zy	0.17	0/1798	0.31	0/2802
35	Ln	0.21	0/231	0.38	0/294
36	S2	0.23	0/42095	0.32	2/65610 (0.0%)
37	zz	0.14	0/7458	0.30	0/11626
38	5B	0.21	0/4999	0.49	0/6740
39	3m	0.16	0/2675	0.41	0/3634
40	3f	0.12	0/2093	0.34	0/2849
41	3a	0.14	0/4583	0.37	0/6237
42	3e	0.14	0/3284	0.34	0/4470
43	3c	0.14	0/3990	0.35	0/5424
44	3h	0.14	0/2563	0.34	0/3473
45	3d	0.09	0/358	0.26	0/493
46	3k	0.12	0/1498	0.34	0/2047
47	3l	0.14	0/4442	0.34	0/6008
All	All	0.20	0/121380	0.36	2/174453 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	S2	1662	U	OP1-P-O3'	-9.05	80.84	108.00
36	S2	1662	U	OP2-P-O3'	-8.03	83.92	108.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	SA	1705	0	1706	24	0
2	SB	1722	0	1794	20	0
3	SC	1709	0	1797	19	0
4	SD	1756	0	1851	29	0
5	SE	2065	0	2169	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	SF	1518	0	1569	13	0
7	SG	1923	0	2089	23	0
8	SH	1506	0	1603	19	0
9	SI	1682	0	1769	18	0
10	SJ	1499	0	1618	13	0
11	SK	810	0	836	18	0
12	SL	1220	0	1289	20	0
13	Sf	935	0	964	20	0
14	SN	1202	0	1289	18	0
15	SO	1007	0	1032	21	0
16	SP	984	0	1033	13	0
17	SQ	1116	0	1185	10	0
18	SR	1068	0	1121	17	0
19	SS	1184	0	1244	10	0
20	ST	1103	0	1133	9	0
21	SU	803	0	873	20	0
22	SV	636	0	637	4	0
23	SW	1034	0	1080	14	0
24	SX	1098	0	1167	18	0
25	SY	1014	0	1082	13	0
26	SZ	601	0	662	5	0
27	Sa	803	0	850	10	0
28	Sb	651	0	672	7	0
29	Sc	488	0	514	7	0
30	Sd	436	0	434	10	0
31	Se	417	0	463	6	0
32	sh	522	0	530	11	0
33	Sg	2436	0	2393	37	0
34	zy	1607	0	815	12	0
35	Ln	230	0	276	1	0
36	S2	37646	0	19026	240	0
37	zz	6675	0	3378	61	0
38	5B	4917	0	5099	94	0
39	3m	2638	0	2439	45	0
40	3f	2057	0	2043	42	0
41	3a	4497	0	4224	65	0
42	3e	3220	0	2921	48	0
43	3c	3924	0	3512	44	0
44	3h	2512	0	2436	53	0
45	3d	347	0	259	2	0
46	3k	1471	0	1233	20	0
47	3l	4331	0	4266	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	Sa	1	0	0	0	0
48	sh	1	0	0	0	0
49	5B	1	0	0	0	0
49	S2	8	0	0	0	0
50	5B	32	0	11	1	0
All	All	114768	0	92386	1220	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1220) 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)
34:zy:12:G:H1	34:zy:21:G:H22	1.15	0.94
36:S2:197:U:H3	36:S2:202:G:H1	1.11	0.92
36:S2:885:U:H3	36:S2:901:G:H1	0.91	0.89
23:SW:8:ALA:HA	23:SW:74:VAL:HG11	1.65	0.77
39:3m:14:GLN:HA	39:3m:17:GLU:HG2	1.66	0.77
33:Sg:87:LEU:HD21	33:Sg:111:VAL:HG11	1.67	0.76
17:SQ:40:GLU:HA	17:SQ:48:GLN:HE22	1.51	0.75
33:Sg:109:LEU:HD11	33:Sg:125:ARG:HG3	1.68	0.75
30:Sd:17:GLY:HA2	30:Sd:27:ARG:HD3	1.67	0.75
36:S2:1824:A:H2'	36:S2:1825:A:H2'	1.68	0.74
36:S2:1723:G:H2'	36:S2:1724:A:H8	1.52	0.74
12:SL:57:ASP:HB2	12:SL:84:ARG:HH21	1.53	0.73
38:5B:905:LEU:HB2	38:5B:932:LYS:HB3	1.69	0.73
1:SA:184:ARG:HD3	1:SA:191:ARG:HG2	1.70	0.72
6:SF:204:ARG:HD2	29:Sc:60:GLU:HG2	1.71	0.72
30:Sd:5:GLN:HE21	30:Sd:5:GLN:N	1.87	0.72
40:3f:95:HIS:HB2	40:3f:98:ILE:HD13	1.71	0.72
36:S2:851:C:H5''	36:S2:852:G:H5'	1.72	0.72
15:SO:30:VAL:HG23	15:SO:94:HIS:HB2	1.70	0.72
6:SF:133:THR:HG23	6:SF:135:ARG:H	1.54	0.71
4:SD:59:LEU:HD23	4:SD:66:ILE:HG13	1.70	0.71
36:S2:1751:C:H42	36:S2:1782:G:H21	1.38	0.71
15:SO:34:PHE:HB3	15:SO:41:PHE:HB2	1.73	0.71
4:SD:106:ARG:HG3	4:SD:175:VAL:HG22	1.71	0.71
3:SC:190:SER:HB3	36:S2:1143:A:H5'	1.72	0.71
44:3h:244:GLN:HA	44:3h:247:MET:HE2	1.73	0.71
47:3l:535:VAL:HG12	47:3l:538:ARG:H	1.56	0.71
15:SO:45:THR:HG22	15:SO:52:THR:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:zz:248:U:H2'	37:zz:249:G:H8	1.54	0.70
41:3a:202:ARG:HH22	41:3a:205:LEU:HD22	1.56	0.70
7:SG:32:MET:HB2	7:SG:100:CYS:HB2	1.73	0.70
36:S2:231:A:H2	36:S2:898:U:H3	1.37	0.69
37:zz:175:U:H3'	37:zz:176:G:H8	1.57	0.69
47:3l:487:ARG:HH12	47:3l:523:ILE:HG21	1.58	0.69
38:5B:863:VAL:HG12	38:5B:873:ILE:HG22	1.75	0.69
36:S2:172:U:H3	36:S2:174:C:N4	1.91	0.68
36:S2:1764:G:O6	36:S2:1768:A:N7	2.26	0.68
47:3l:195:GLN:HG2	47:3l:421:LEU:HD11	1.74	0.68
10:SJ:82:VAL:HG21	10:SJ:92:MET:HE1	1.76	0.68
40:3f:97:VAL:HG13	40:3f:98:ILE:HD12	1.76	0.68
8:SH:36:LEU:O	8:SH:40:LEU:HB2	1.94	0.68
40:3f:171:GLY:HA3	40:3f:198:ILE:HG22	1.75	0.67
21:SU:59:LYS:HG3	21:SU:84:ILE:HB	1.76	0.67
36:S2:669:A:H8	36:S2:1164:G:HO2'	1.43	0.67
36:S2:1723:G:H2'	36:S2:1724:A:C8	2.30	0.67
38:5B:1094:ILE:HG12	38:5B:1114:VAL:HG12	1.77	0.67
19:SS:22:GLY:HA2	19:SS:56:ALA:HB3	1.76	0.67
38:5B:798:PHE:CZ	38:5B:803:LEU:HB2	2.30	0.67
46:3k:153:ILE:HD12	46:3k:158:LEU:HD13	1.76	0.66
44:3h:129:VAL:HB	44:3h:322:GLN:HG3	1.76	0.66
39:3m:212:LEU:HD21	39:3m:268:LEU:HD11	1.75	0.66
13:Sf:35:ILE:HD12	13:Sf:35:ILE:H	1.61	0.66
46:3k:147:GLY:HA2	46:3k:189:ILE:HG21	1.78	0.66
21:SU:66:ARG:HH21	21:SU:75:LYS:HA	1.61	0.66
36:S2:1756:C:H2'	36:S2:1757:G:H8	1.59	0.66
47:3l:198:SER:HA	47:3l:201:ARG:HD3	1.77	0.66
12:SL:126:VAL:HG12	12:SL:145:VAL:HG22	1.78	0.66
36:S2:282:G:H2'	36:S2:283:G:H8	1.61	0.66
44:3h:131:ARG:HH21	44:3h:315:ASP:HB2	1.60	0.66
46:3k:207:PHE:O	46:3k:211:SER:HB2	1.96	0.65
41:3a:7:ARG:HG3	41:3a:10:ASN:HB3	1.78	0.65
41:3a:251:LYS:HA	41:3a:254:GLU:HB2	1.79	0.65
41:3a:290:LEU:HA	41:3a:329:ILE:HG12	1.79	0.65
44:3h:176:VAL:HG21	44:3h:192:ILE:HD11	1.78	0.65
47:3l:308:VAL:HG12	47:3l:311:CYS:H	1.62	0.65
14:SN:71:ILE:HD13	36:S2:1018:U:H5''	1.79	0.64
16:SP:111:MET:HA	19:SS:117:ILE:HD11	1.78	0.64
36:S2:587:A:H5'	36:S2:592:C:H41	1.62	0.64
41:3a:241:ILE:HB	41:3a:278:LYS:HE2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:S2:1757:G:H1	36:S2:1775:U:H3	1.44	0.64
42:3e:245:ALA:O	42:3e:249:MET:HB3	1.97	0.64
38:5B:1125:MET:HG3	38:5B:1182:LEU:HD22	1.80	0.64
43:3c:859:LEU:HD12	43:3c:862:LYS:HD3	1.80	0.64
21:SU:61:LEU:HD13	21:SU:82:MET:HE3	1.80	0.64
39:3m:223:LEU:HD12	39:3m:226:LEU:HD12	1.80	0.64
42:3e:223:PHE:HZ	42:3e:256:TYR:HB3	1.63	0.64
23:SW:6:VAL:HG12	23:SW:34:ILE:HD11	1.79	0.64
36:S2:1536:G:H2'	36:S2:1537:A:H8	1.61	0.64
33:Sg:107:ASP:HB2	33:Sg:125:ARG:HD2	1.80	0.63
38:5B:877:LEU:HD11	38:5B:882:LEU:HG	1.80	0.63
42:3e:251:PRO:HB2	42:3e:288:TYR:HB2	1.81	0.63
33:Sg:163:PRO:HB2	33:Sg:179:LEU:HB2	1.81	0.63
36:S2:870:A:H4'	36:S2:871:U:H3'	1.80	0.63
32:sh:100:LEU:HB3	32:sh:103:LEU:HD23	1.81	0.63
38:5B:1012:PRO:HA	38:5B:1039:VAL:HG13	1.80	0.63
16:SP:86:LEU:H	16:SP:89:MET:HE2	1.63	0.63
9:SI:150:ASP:HA	9:SI:153:LYS:HG3	1.80	0.63
41:3a:321:ARG:HH21	41:3a:324:LEU:HD22	1.62	0.63
47:3l:521:PHE:HB3	47:3l:530:ILE:HG13	1.80	0.62
8:SH:100:ILE:HG12	8:SH:125:VAL:HG21	1.81	0.62
38:5B:1094:ILE:HB	38:5B:1182:LEU:HB2	1.80	0.62
39:3m:324:LYS:H	41:3a:448:GLN:HB2	1.64	0.62
37:zz:305:U:O4	37:zz:313:G:O6	2.18	0.62
39:3m:128:ILE:HD11	39:3m:164:LEU:HD22	1.80	0.62
36:S2:536:A:H3'	36:S2:537:C:H5''	1.82	0.62
40:3f:103:VAL:HG12	44:3h:210:LEU:HD21	1.82	0.62
7:SG:7:PHE:HE1	7:SG:9:ALA:HB3	1.65	0.61
38:5B:886:ASP:HB2	38:5B:901:ILE:HD12	1.82	0.61
40:3f:211:MET:HE3	40:3f:213:ILE:HD11	1.82	0.61
39:3m:230:LYS:HA	39:3m:233:GLU:HB3	1.81	0.61
40:3f:97:VAL:HG23	44:3h:47:LEU:HB3	1.81	0.61
36:S2:1776:G:H2'	36:S2:1777:G:H4'	1.83	0.61
42:3e:413:PHE:HB2	47:3l:388:LEU:HD21	1.83	0.61
38:5B:1096:ILE:HA	38:5B:1112:VAL:HG12	1.82	0.61
7:SG:10:THR:HA	7:SG:129:VAL:HG12	1.83	0.61
47:3l:461:ARG:HB2	47:3l:519:VAL:HG21	1.81	0.60
36:S2:172:U:H3	36:S2:174:C:H41	1.48	0.60
5:SE:45:ILE:HA	5:SE:61:VAL:HG21	1.83	0.60
12:SL:68:ILE:HD13	12:SL:131:CYS:HB3	1.83	0.60
40:3f:202:VAL:HG22	40:3f:213:ILE:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:3a:331:ILE:H	41:3a:331:ILE:HD12	1.67	0.60
42:3e:406:GLU:HA	42:3e:409:LYS:HE3	1.84	0.60
38:5B:648:LEU:HD21	38:5B:700:ILE:HG21	1.84	0.59
41:3a:71:LEU:HD21	41:3a:90:VAL:HG12	1.82	0.59
3:SC:108:LYS:HD3	3:SC:110:MET:HB3	1.82	0.59
14:SN:88:LEU:O	14:SN:92:ILE:HG13	2.02	0.59
37:zz:252:A:H4'	37:zz:253:G:H5'	1.82	0.59
16:SP:28:MET:HE3	16:SP:29:SER:N	2.18	0.59
21:SU:26:SER:HB2	21:SU:110:VAL:HG12	1.85	0.59
36:S2:981:A:H2'	36:S2:982:G:C8	2.36	0.59
39:3m:183:LYS:HA	39:3m:186:VAL:HG22	1.84	0.59
47:3l:102:LEU:HD22	47:3l:106:PHE:HE1	1.67	0.59
2:SB:189:ILE:HG13	2:SB:190:PRO:HD3	1.85	0.59
37:zz:294:U:H2'	37:zz:295:G:H2'	1.84	0.59
38:5B:750:PRO:HG2	38:5B:846:LEU:HD11	1.85	0.59
41:3a:223:PRO:HA	41:3a:226:GLN:HB2	1.84	0.59
44:3h:141:GLN:HE21	44:3h:174:MET:HG3	1.67	0.59
1:SA:34:MET:HE1	1:SA:148:CYS:HB2	1.85	0.59
30:Sd:8:TRP:HZ3	36:S2:1512:C:H5''	1.68	0.59
13:Sf:85:LEU:HA	13:Sf:88:TRP:HB2	1.85	0.58
37:zz:153:G:H5'	41:3a:7:ARG:HH12	1.67	0.58
37:zz:180:G:H2'	37:zz:181:G:H8	1.68	0.58
40:3f:92:VAL:HB	40:3f:237:VAL:HG13	1.84	0.58
8:SH:170:VAL:HG23	8:SH:187:PHE:HB2	1.85	0.58
32:sh:132:MET:HE2	32:sh:139:HIS:HB3	1.84	0.58
38:5B:956:ILE:HD12	38:5B:956:ILE:H	1.67	0.58
8:SH:9:VAL:HG21	8:SH:20:GLU:HB3	1.84	0.58
24:SX:28:LYS:HZ2	24:SX:32:LEU:HD13	1.67	0.58
32:sh:107:LYS:HB2	32:sh:117:LEU:HD21	1.86	0.58
42:3e:233:ILE:HD13	42:3e:273:VAL:HG11	1.85	0.58
47:3l:180:ASN:HB3	47:3l:268:MET:HE1	1.86	0.58
1:SA:145:ILE:HG12	1:SA:159:ILE:HB	1.84	0.58
36:S2:1228:A:H2'	36:S2:1229:G:H8	1.68	0.58
37:zz:72:A:H5''	37:zz:93:A:H61	1.67	0.58
2:SB:129:THR:HG23	2:SB:131:ASP:H	1.68	0.58
13:Sf:66:GLU:HB3	13:Sf:76:LEU:HD22	1.86	0.58
23:SW:69:LEU:HD11	23:SW:72:CYS:HB3	1.85	0.58
4:SD:158:ILE:HG23	4:SD:189:MET:HE1	1.85	0.58
17:SQ:97:GLN:HB2	17:SQ:105:LYS:HD2	1.85	0.58
33:Sg:87:LEU:HB2	33:Sg:101:PHE:HB2	1.86	0.57
36:S2:1228:A:H2'	36:S2:1229:G:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:S2:1536:G:H2'	36:S2:1537:A:C8	2.38	0.57
25:SY:52:PRO:HA	25:SY:55:ILE:HD12	1.86	0.57
47:3l:471:PRO:HG2	47:3l:474:LYS:HB2	1.85	0.57
40:3f:350:LEU:HD11	42:3e:419:ALA:HB2	1.86	0.57
16:SP:30:TYR:HA	16:SP:33:LEU:HB2	1.86	0.57
24:SX:53:GLU:HG3	24:SX:71:ARG:HB3	1.85	0.57
41:3a:448:GLN:HA	41:3a:493:PHE:HB2	1.86	0.57
47:3l:345:ARG:HG2	47:3l:553:LEU:HD21	1.86	0.57
35:Ln:2:ARG:HH21	35:Ln:4:LYS:HE3	1.69	0.57
3:SC:179:THR:HG22	3:SC:221:ASP:HB2	1.86	0.57
3:SC:183:LYS:HG2	3:SC:196:ILE:HG23	1.86	0.57
24:SX:68:LYS:HB3	24:SX:91:LEU:HD22	1.87	0.57
16:SP:75:VAL:HG12	16:SP:93:MET:HB3	1.87	0.57
37:zz:262:U:O2	37:zz:271:G:O6	2.23	0.57
18:SR:100:PRO:HG3	18:SR:122:PRO:HD3	1.86	0.57
20:ST:41:LYS:HE3	20:ST:93:SER:HB2	1.87	0.57
46:3k:158:LEU:HG	46:3k:170:LEU:HD11	1.87	0.57
38:5B:968:LYS:HA	38:5B:971:LEU:HG	1.86	0.57
11:SK:60:GLU:HG3	11:SK:69:TRP:NE1	2.20	0.56
25:SY:25:ILE:HG21	25:SY:40:ILE:HD11	1.86	0.56
36:S2:1183:A:H2'	36:S2:1184:G:H8	1.70	0.56
41:3a:74:TYR:HD2	41:3a:86:LEU:HD13	1.71	0.56
37:zz:134:A:H3'	37:zz:135:G:H8	1.69	0.56
38:5B:859:GLN:HG2	38:5B:878:ILE:HD11	1.88	0.56
41:3a:529:VAL:HA	41:3a:532:LYS:HE3	1.86	0.56
42:3e:405:ILE:HA	42:3e:408:THR:HG22	1.87	0.56
38:5B:1013:VAL:HG23	38:5B:1039:VAL:HG11	1.86	0.56
6:SF:136:ARG:HB2	6:SF:203:ASN:ND2	2.21	0.56
40:3f:98:ILE:HG23	40:3f:134:CYS:HB3	1.86	0.56
42:3e:303:PHE:HB2	43:3c:823:SER:HB3	1.86	0.56
37:zz:137:G:O6	37:zz:287:U:O2	2.24	0.56
12:SL:111:VAL:HG11	12:SL:128:VAL:HG11	1.88	0.56
14:SN:4:MET:HE2	14:SN:121:ARG:HG2	1.88	0.56
32:sh:126:CYS:HB3	32:sh:130:VAL:HG21	1.87	0.56
38:5B:738:ILE:HA	38:5B:741:ILE:HD12	1.87	0.56
46:3k:138:VAL:O	46:3k:142:ILE:HG12	2.06	0.56
47:3l:523:ILE:HG12	47:3l:528:ILE:HG12	1.87	0.56
36:S2:1277:C:H2'	36:S2:1278:A:H8	1.71	0.56
37:zz:181:G:H2'	37:zz:182:A:C8	2.41	0.56
38:5B:1103:ASN:HB2	38:5B:1109:VAL:HG22	1.88	0.56
47:3l:101:LYS:O	47:3l:105:ARG:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:zz:180:G:H2'	37:zz:181:G:C8	2.41	0.56
22:SV:68:SER:O	22:SV:72:LEU:HD12	2.06	0.56
24:SX:67:ARG:HG3	24:SX:115:ILE:HB	1.87	0.56
41:3a:24:LYS:HG3	41:3a:61:LEU:HD11	1.87	0.56
1:SA:128:ARG:HH21	1:SA:153:PRO:HD3	1.71	0.55
36:S2:240:G:H2'	36:S2:241:G:C8	2.41	0.55
36:S2:1217:A:H2'	36:S2:1218:C:C6	2.40	0.55
43:3c:775:VAL:HA	43:3c:778:MET:HG2	1.86	0.55
47:3l:274:LEU:O	47:3l:278:LEU:HG	2.06	0.55
23:SW:51:GLU:HG3	28:Sb:8:LEU:HD11	1.88	0.55
20:ST:65:TYR:HE1	20:ST:128:GLN:HG3	1.71	0.55
24:SX:114:ASP:HB2	36:S2:619:A:N1	2.22	0.55
37:zz:178:C:H2'	37:zz:179:A:H8	1.71	0.55
40:3f:124:VAL:HB	40:3f:170:LEU:HD21	1.89	0.55
43:3c:672:PRO:HD2	43:3c:675:LEU:HD21	1.88	0.55
43:3c:764:LYS:HG3	43:3c:765:VAL:HG23	1.88	0.55
44:3h:338:LEU:HD22	46:3k:214:MET:HE1	1.87	0.55
11:SK:32:HIS:HB3	11:SK:35:LEU:HB2	1.89	0.55
21:SU:97:ILE:HD12	21:SU:97:ILE:H	1.71	0.55
5:SE:18:TRP:HH2	5:SE:31:PRO:HD3	1.71	0.55
43:3c:582:TRP:HZ2	43:3c:625:LEU:HD12	1.70	0.55
44:3h:45:VAL:HG13	44:3h:81:CYS:HB2	1.89	0.55
25:SY:55:ILE:HG12	25:SY:75:ILE:HD12	1.89	0.55
36:S2:5:U:H2'	36:S2:6:G:H8	1.71	0.55
44:3h:208:SER:H	44:3h:211:ILE:HD12	1.71	0.55
10:SJ:126:ALA:O	10:SJ:130:ILE:HG13	2.07	0.55
36:S2:1813:A:H3'	36:S2:1814:G:H8	1.72	0.55
41:3a:165:ARG:HE	41:3a:166:ASN:HB2	1.72	0.55
8:SH:75:ILE:HG13	8:SH:79:LEU:HD11	1.88	0.55
34:zy:47:C:H2'	34:zy:57:A:H1'	1.89	0.55
42:3e:118:ALA:HA	42:3e:123:PHE:H	1.72	0.55
36:S2:792:C:H2'	36:S2:793:G:C8	2.42	0.54
40:3f:100:ALA:HA	44:3h:214:LEU:HD11	1.89	0.54
16:SP:43:ARG:HE	16:SP:47:ARG:HD2	1.72	0.54
38:5B:1127:VAL:HB	38:5B:1133:VAL:HG23	1.90	0.54
39:3m:218:PHE:HD1	39:3m:276:LYS:HE3	1.73	0.54
42:3e:353:ILE:HA	42:3e:356:LEU:HD23	1.89	0.54
7:SG:52:ILE:HA	7:SG:111:LEU:HD23	1.87	0.54
33:Sg:10:THR:HG22	33:Sg:308:ARG:HG2	1.88	0.54
36:S2:28:U:H2'	36:S2:29:G:H8	1.73	0.54
40:3f:96:PRO:HA	40:3f:99:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:3e:252:HIS:HA	42:3e:288:TYR:CZ	2.43	0.54
29:Sc:9:ILE:HG22	29:Sc:59:LEU:HA	1.88	0.54
38:5B:952:LYS:HD3	38:5B:953:GLU:N	2.23	0.54
21:SU:26:SER:HB3	21:SU:32:LEU:HD22	1.89	0.54
5:SE:31:PRO:HG3	5:SE:43:PRO:HG3	1.88	0.54
16:SP:20:VAL:HG12	16:SP:25:LEU:HD12	1.90	0.54
25:SY:5:VAL:HG12	25:SY:29:HIS:HB3	1.88	0.54
36:S2:235:A:H2'	36:S2:236:A:C8	2.43	0.54
38:5B:863:VAL:HG22	38:5B:988:LEU:HB2	1.89	0.54
44:3h:255:GLN:HA	44:3h:258:VAL:HG22	1.89	0.54
47:3l:400:ARG:HG2	47:3l:408:VAL:HG21	1.90	0.54
36:S2:874:G:H2'	36:S2:875:A:H8	1.72	0.54
37:zz:178:C:H2'	37:zz:179:A:C8	2.42	0.54
47:3l:191:ILE:HD12	47:3l:280:LEU:HD11	1.90	0.54
19:SS:5:ILE:HD12	19:SS:6:PRO:HD2	1.91	0.53
40:3f:121:LEU:HD13	40:3f:133:ASN:HB3	1.88	0.53
41:3a:296:LEU:HB3	41:3a:322:VAL:HG23	1.90	0.53
25:SY:40:ILE:O	25:SY:44:LEU:HD12	2.08	0.53
36:S2:1217:A:H2'	36:S2:1218:C:H6	1.73	0.53
37:zz:130:C:H2'	37:zz:131:G:H8	1.72	0.53
6:SF:174:ALA:O	6:SF:178:ILE:HG13	2.09	0.53
12:SL:99:TYR:HD1	24:SX:13:LEU:HD23	1.73	0.53
16:SP:28:MET:HE2	16:SP:32:GLN:HG2	1.90	0.53
4:SD:7:LYS:HD2	21:SU:25:THR:HG21	1.88	0.53
30:Sd:27:ARG:HD2	36:S2:1263:U:H4'	1.90	0.53
36:S2:1769:C:H2'	36:S2:1770:G:H8	1.73	0.53
41:3a:55:LEU:HD13	41:3a:96:MET:HE2	1.90	0.53
20:ST:40:ALA:HB3	20:ST:43:LYS:HG2	1.90	0.53
30:Sd:5:GLN:N	30:Sd:5:GLN:NE2	2.55	0.53
36:S2:669:A:H8	36:S2:1164:G:O2'	1.91	0.53
47:3l:231:LEU:HD13	47:3l:277:LEU:HB2	1.91	0.53
37:zz:216:U:C4	41:3a:69:GLU:HB3	2.44	0.53
42:3e:191:ARG:O	42:3e:195:THR:HG23	2.08	0.53
43:3c:614:VAL:HG13	43:3c:682:LEU:HD13	1.90	0.53
4:SD:8:LYS:HB3	21:SU:61:LEU:HD21	1.89	0.53
38:5B:1125:MET:SD	38:5B:1182:LEU:HB3	2.49	0.53
9:SI:81:VAL:HG22	9:SI:102:VAL:HG12	1.91	0.53
39:3m:110:PHE:HE1	39:3m:120:ARG:HH21	1.57	0.53
4:SD:64:ARG:HD2	11:SK:94:LEU:HD13	1.90	0.53
12:SL:85:THR:HG21	36:S2:373:G:H4'	1.90	0.53
41:3a:147:THR:HA	41:3a:150:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:3c:594:LEU:HG	43:3c:598:ILE:HG12	1.91	0.53
3:SC:65:LYS:HD2	3:SC:273:LEU:HD13	1.91	0.53
7:SG:186:GLN:HE22	36:S2:318:A:H61	1.57	0.53
36:S2:885:U:O4	36:S2:901:G:O6	2.27	0.53
36:S2:1413:G:H2'	36:S2:1414:A:H8	1.74	0.53
40:3f:129:VAL:HG23	40:3f:170:LEU:HD13	1.91	0.53
23:SW:3:ARG:HH22	23:SW:28:ARG:HH21	1.57	0.52
36:S2:201:C:H3'	36:S2:202:G:H8	1.74	0.52
4:SD:161:GLY:HA3	36:S2:1388:A:H61	1.73	0.52
36:S2:1653:U:H2'	36:S2:1654:G:C8	2.44	0.52
37:zz:73:A:H2'	37:zz:74:A:H8	1.73	0.52
37:zz:87:G:H2'	37:zz:88:G:H8	1.72	0.52
38:5B:724:ILE:HD11	38:5B:838:LEU:HD21	1.91	0.52
38:5B:808:PHE:HB2	38:5B:837:LEU:HD21	1.91	0.52
38:5B:1089:VAL:HG11	38:5B:1124:PRO:HD2	1.90	0.52
42:3e:316:GLU:HG3	42:3e:329:LEU:HD11	1.92	0.52
47:3l:560:MET:HA	47:3l:563:ARG:HG2	1.90	0.52
6:SF:49:LEU:HD12	17:SQ:50:LYS:HG2	1.91	0.52
36:S2:197:U:O4	36:S2:202:G:O6	2.27	0.52
47:3l:540:GLY:HA2	47:3l:543:PHE:CZ	2.45	0.52
37:zz:133:G:C2	37:zz:134:A:H1'	2.45	0.52
38:5B:845:MET:HG3	38:5B:846:LEU:HD22	1.89	0.52
47:3l:115:ALA:H	47:3l:133:LYS:HE3	1.74	0.52
9:SI:205:ARG:HH22	12:SL:8:ARG:HH21	1.58	0.52
38:5B:952:LYS:HD3	38:5B:953:GLU:H	1.73	0.52
44:3h:277:TYR:HB3	44:3h:281:ARG:HH21	1.74	0.52
5:SE:100:ARG:HB2	5:SE:114:ILE:HD13	1.92	0.52
31:Se:11:LYS:O	31:Se:15:GLN:HG2	2.09	0.52
37:zz:312:U:H2'	37:zz:313:G:H8	1.75	0.52
39:3m:269:LEU:HD12	39:3m:271:GLU:HB2	1.91	0.52
42:3e:246:ILE:HA	42:3e:249:MET:HE2	1.91	0.52
43:3c:565:ARG:HH21	43:3c:566:THR:HG22	1.73	0.52
2:SB:124:HIS:HA	2:SB:137:LEU:O	2.09	0.52
4:SD:137:VAL:HG22	4:SD:151:LYS:HG2	1.92	0.52
36:S2:1756:C:H2'	36:S2:1757:G:C8	2.44	0.52
14:SN:92:ILE:HG23	14:SN:141:TYR:HE1	1.74	0.52
33:Sg:238:ALA:H	33:Sg:251:ALA:HB3	1.74	0.52
36:S2:367:U:H4'	36:S2:371:A:C8	2.45	0.52
36:S2:791:C:H2'	36:S2:792:C:C6	2.45	0.52
38:5B:956:ILE:HG22	38:5B:960:LYS:HD3	1.92	0.52
39:3m:354:LEU:HD21	40:3f:286:VAL:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:3h:88:THR:HG23	44:3h:90:ASP:H	1.74	0.52
14:SN:20:ARG:HG3	14:SN:65:PHE:CZ	2.45	0.51
33:Sg:125:ARG:HG2	33:Sg:150:TRP:CG	2.45	0.51
36:S2:223:C:H2'	36:S2:224:A:C8	2.45	0.51
36:S2:282:G:H2'	36:S2:283:G:C8	2.42	0.51
36:S2:845:G:H2'	36:S2:846:G:C8	2.46	0.51
9:SI:98:LYS:HB3	36:S2:377:G:H5'	1.91	0.51
36:S2:1035:A:N6	36:S2:1081:U:H3	2.09	0.51
36:S2:1545:A:H2'	36:S2:1546:G:C8	2.44	0.51
37:zz:240:C:H2'	37:zz:241:G:C8	2.45	0.51
44:3h:258:VAL:O	44:3h:262:THR:HG23	2.09	0.51
36:S2:1768:A:H2'	36:S2:1769:C:C6	2.45	0.51
38:5B:646:LYS:HG3	38:5B:825:ALA:HB1	1.91	0.51
40:3f:343:LEU:HD21	42:3e:411:LEU:HD11	1.92	0.51
44:3h:288:ARG:HD3	44:3h:293:GLU:HG3	1.93	0.51
9:SI:64:ASN:HA	9:SI:75:LYS:HA	1.93	0.51
12:SL:73:LEU:HD12	12:SL:109:MET:HE1	1.93	0.51
33:Sg:275:ILE:HG22	33:Sg:278:SER:H	1.75	0.51
38:5B:984:GLN:HG3	38:5B:1013:VAL:HG22	1.92	0.51
4:SD:145:GLN:HG2	36:S2:628:A:H62	1.76	0.51
5:SE:44:LEU:HD21	5:SE:72:ILE:HD11	1.93	0.51
33:Sg:5:MET:CE	33:Sg:310:TRP:HB3	2.40	0.51
2:SB:133:TYR:HD2	2:SB:181:LEU:HD13	1.76	0.51
38:5B:1105:ARG:HH21	38:5B:1169:PRO:HG2	1.75	0.51
41:3a:393:TRP:CE2	41:3a:406:ARG:HD3	2.45	0.51
2:SB:133:TYR:HE2	2:SB:181:LEU:HD22	1.76	0.51
4:SD:163:PRO:O	4:SD:167:TYR:HB2	2.11	0.51
21:SU:35:VAL:HG21	21:SU:110:VAL:HG21	1.92	0.51
40:3f:137:VAL:HG13	40:3f:152:PHE:HD2	1.76	0.51
41:3a:355:LEU:HA	41:3a:358:LEU:HD12	1.92	0.51
42:3e:345:CYS:HA	42:3e:351:ILE:HD11	1.93	0.51
3:SC:207:ALA:HB2	36:S2:4:C:H4'	1.93	0.51
1:SA:99:ILE:HD11	1:SA:117:ARG:HE	1.76	0.51
34:zy:68:U:H2'	34:zy:69:G:C8	2.46	0.51
36:S2:1232:U:H2'	36:S2:1233:G:H8	1.76	0.51
38:5B:1186:ILE:HB	38:5B:1213:LEU:HD11	1.93	0.51
39:3m:313:ILE:HA	41:3a:446:ILE:HD11	1.93	0.51
20:ST:27:LYS:HB2	20:ST:110:LEU:HD11	1.93	0.51
41:3a:258:GLY:O	41:3a:262:LEU:HD23	2.11	0.51
39:3m:156:LEU:HB2	39:3m:161:LYS:HG3	1.92	0.50
36:S2:878:G:H22	36:S2:908:A:H2	1.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:3m:22:LEU:HD11	39:3m:45:ILE:HG13	1.92	0.50
47:3l:448:SER:HA	47:3l:451:VAL:HB	1.92	0.50
39:3m:189:LEU:HB2	39:3m:226:LEU:HD13	1.93	0.50
30:Sd:40:ARG:HD3	36:S2:1256:G:C4	2.47	0.50
36:S2:1337:C:H2'	36:S2:1338:G:H8	1.77	0.50
37:zz:312:U:H2'	37:zz:313:G:C8	2.45	0.50
38:5B:651:LEU:HD13	38:5B:681:GLN:HG3	1.92	0.50
47:3l:280:LEU:O	47:3l:284:LEU:HG	2.11	0.50
10:SJ:32:ILE:HD13	10:SJ:37:LEU:HB2	1.93	0.50
24:SX:55:VAL:HG13	24:SX:69:CYS:HB2	1.92	0.50
38:5B:675:LEU:HD23	38:5B:675:LEU:H	1.76	0.50
38:5B:712:LEU:HD21	38:5B:989:GLY:HA3	1.94	0.50
7:SG:159:ARG:HG2	7:SG:173:ALA:HB2	1.94	0.50
36:S2:942:G:H2'	36:S2:943:U:C6	2.47	0.50
39:3m:79:GLN:HG2	39:3m:119:VAL:HG21	1.93	0.50
41:3a:421:GLU:HG2	41:3a:423:GLU:HG2	1.94	0.50
2:SB:133:TYR:CE2	2:SB:181:LEU:HD22	2.47	0.50
36:S2:5:U:H2'	36:S2:6:G:C8	2.47	0.50
10:SJ:134:HIS:HE1	10:SJ:164:PRO:HD2	1.77	0.50
13:Sf:64:LEU:HD21	32:sh:106:TYR:HD2	1.76	0.50
36:S2:730:C:H2'	36:S2:731:G:H4'	1.94	0.50
36:S2:793:G:H2'	36:S2:794:A:O4'	2.12	0.50
1:SA:77:ILE:HG21	1:SA:133:PRO:HG2	1.94	0.50
7:SG:63:MET:HE3	7:SG:106:LEU:HD11	1.94	0.50
21:SU:80:PHE:HB3	30:Sd:52:PHE:HB3	1.94	0.50
43:3c:608:LEU:HD12	43:3c:611:ARG:HD2	1.94	0.50
44:3h:288:ARG:HB2	44:3h:295:PRO:HA	1.93	0.50
13:Sf:48:HIS:HB3	13:Sf:114:TYR:CZ	2.47	0.49
15:SO:31:CYS:HA	15:SO:43:HIS:O	2.12	0.49
21:SU:66:ARG:NH2	21:SU:75:LYS:HA	2.27	0.49
21:SU:97:ILE:HA	21:SU:100:GLN:HG2	1.93	0.49
36:S2:928:G:H2'	36:S2:929:G:C8	2.46	0.49
38:5B:679:ASN:O	38:5B:683:LYS:HG2	2.12	0.49
42:3e:182:TRP:HB3	42:3e:221:VAL:HG23	1.94	0.49
42:3e:243:LEU:HD11	42:3e:280:VAL:HG21	1.93	0.49
22:SV:18:SER:HB3	22:SV:72:LEU:HD21	1.94	0.49
34:zy:4:A:H2'	34:zy:5:G:C8	2.47	0.49
36:S2:640:A:H2'	36:S2:641:A:C8	2.46	0.49
37:zz:95:U:H2'	37:zz:96:A:C8	2.47	0.49
41:3a:205:LEU:HD12	41:3a:229:HIS:HE2	1.77	0.49
1:SA:163:CYS:HB2	1:SA:174:MET:HE3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:SB:33:VAL:HG23	2:SB:44:ILE:HB	1.94	0.49
5:SE:23:LEU:HD11	10:SJ:6:SER:HB3	1.93	0.49
20:ST:5:THR:HG22	20:ST:6:VAL:H	1.77	0.49
36:S2:1432:U:H5''	36:S2:1433:C:H5''	1.94	0.49
39:3m:162:HIS:O	39:3m:166:ARG:HG2	2.11	0.49
24:SX:75:ILE:HD13	38:5B:1019:MET:HE3	1.93	0.49
36:S2:1628:C:H2'	36:S2:1629:C:H6	1.77	0.49
37:zz:158:G:H2'	37:zz:159:G:H8	1.78	0.49
39:3m:80:GLU:HA	39:3m:119:VAL:HG23	1.93	0.49
3:SC:121:ARG:HH12	3:SC:123:ARG:HD2	1.77	0.49
11:SK:64:TRP:CD2	30:Sd:23:VAL:HG22	2.47	0.49
12:SL:103:GLU:HB3	24:SX:10:ALA:HB3	1.95	0.49
15:SO:136:PRO:HB2	15:SO:139:SER:HB3	1.93	0.49
33:Sg:174:VAL:HB	33:Sg:188:HIS:HB2	1.94	0.49
36:S2:1010:G:H2'	36:S2:1011:A:C8	2.48	0.49
36:S2:1758:G:H2'	36:S2:1759:G:H8	1.77	0.49
37:zz:134:A:H3'	37:zz:135:G:C8	2.47	0.49
37:zz:141:U:H2'	37:zz:142:A:H8	1.76	0.49
40:3f:250:ASP:HA	40:3f:253:MET:HB2	1.94	0.49
5:SE:48:LEU:HD12	5:SE:61:VAL:HG23	1.94	0.49
7:SG:193:ALA:O	7:SG:197:GLN:HG2	2.13	0.49
8:SH:9:VAL:HG12	8:SH:11:PRO:HD3	1.93	0.49
12:SL:33:LEU:HD12	12:SL:34:PRO:HD2	1.93	0.49
38:5B:842:THR:HA	38:5B:846:LEU:HB2	1.94	0.49
39:3m:144:LEU:HD11	39:3m:184:VAL:HG22	1.93	0.49
42:3e:322:ASP:HB3	42:3e:325:LEU:HB2	1.94	0.49
47:3l:373:ILE:HD11	47:3l:412:LEU:HB3	1.95	0.49
47:3l:533:THR:HG23	47:3l:534:LYS:H	1.78	0.49
4:SD:31:GLU:HA	4:SD:107:TYR:CE2	2.48	0.49
4:SD:123:LEU:HD22	4:SD:152:PHE:HB3	1.94	0.49
15:SO:66:ARG:HB2	36:S2:962:A:H5''	1.95	0.49
25:SY:86:GLU:OE1	25:SY:87:PRO:HD2	2.13	0.49
37:zz:115:C:H2'	37:zz:116:A:C8	2.47	0.49
36:S2:1010:G:H2'	36:S2:1011:A:H8	1.77	0.49
41:3a:442:GLN:O	41:3a:446:ILE:HG22	2.13	0.49
47:3l:52:ILE:HG13	47:3l:102:LEU:HD13	1.95	0.49
33:Sg:207:CYS:HB3	33:Sg:221:LEU:HD21	1.94	0.49
37:zz:87:G:H2'	37:zz:88:G:C8	2.48	0.49
5:SE:146:THR:HG21	36:S2:122:G:H21	1.77	0.49
33:Sg:5:MET:HE1	33:Sg:310:TRP:HB3	1.95	0.49
36:S2:794:A:H2'	36:S2:795:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:3a:21:VAL:HG23	41:3a:23:LYS:HG2	1.94	0.49
47:3l:55:PHE:HE1	47:3l:94:ILE:HG23	1.78	0.49
47:3l:112:TRP:HB2	47:3l:136:TYR:HD1	1.78	0.49
47:3l:153:ARG:HD2	47:3l:197:PHE:HD1	1.77	0.49
13:Sf:42:LEU:HD13	13:Sf:68:LEU:HB3	1.95	0.48
36:S2:322:C:H2'	36:S2:323:C:C6	2.48	0.48
36:S2:1562:C:H2'	36:S2:1563:G:H8	1.77	0.48
41:3a:442:GLN:HE21	41:3a:509:PRO:HG3	1.78	0.48
46:3k:194:GLU:HA	46:3k:197:LYS:HB2	1.95	0.48
21:SU:20:ILE:HG21	21:SU:98:VAL:HG11	1.95	0.48
36:S2:804:U:H2'	36:S2:805:U:C6	2.48	0.48
36:S2:1351:G:H1	36:S2:1360:U:H3	1.60	0.48
36:S2:1588:A:H2'	36:S2:1589:A:C8	2.49	0.48
36:S2:1755:C:H2'	36:S2:1756:C:H6	1.78	0.48
38:5B:1155:GLN:HG3	38:5B:1157:VAL:HG13	1.95	0.48
45:3d:21:VAL:HG13	45:3d:26:ARG:HD3	1.95	0.48
36:S2:1365:G:H2'	36:S2:1366:G:H8	1.77	0.48
36:S2:1759:G:H2'	36:S2:1760:G:C8	2.49	0.48
37:zz:98:G:H2'	37:zz:99:A:C8	2.48	0.48
39:3m:11:GLU:HA	39:3m:14:GLN:HG3	1.96	0.48
46:3k:139:ARG:HD3	46:3k:162:LEU:HD22	1.95	0.48
47:3l:298:GLU:HG3	47:3l:301:LYS:HB2	1.94	0.48
4:SD:101:GLN:HA	4:SD:101:GLN:NE2	2.28	0.48
12:SL:93:LEU:HD11	24:SX:8:ARG:HD3	1.95	0.48
21:SU:28:ASN:OD1	21:SU:31:SER:HB3	2.12	0.48
28:Sb:35:VAL:HG12	28:Sb:79:PHE:HB2	1.94	0.48
36:S2:1453:C:H2'	36:S2:1454:A:H4'	1.94	0.48
38:5B:925:VAL:HG21	38:5B:931:VAL:HG21	1.96	0.48
40:3f:156:MET:HE1	40:3f:160:HIS:CE1	2.48	0.48
41:3a:424:LEU:HD12	41:3a:425:GLN:HG2	1.95	0.48
44:3h:149:VAL:HG23	44:3h:167:TYR:HB2	1.95	0.48
47:3l:112:TRP:HD1	47:3l:139:HIS:CD2	2.31	0.48
15:SO:135:ILE:HD12	15:SO:136:PRO:HD2	1.95	0.48
38:5B:890:VAL:HG23	38:5B:897:ILE:HB	1.96	0.48
39:3m:60:VAL:HG11	39:3m:101:LEU:HD11	1.96	0.48
39:3m:244:PHE:HA	39:3m:277:MET:HE2	1.94	0.48
47:3l:268:MET:HE2	47:3l:272:PHE:CZ	2.48	0.48
5:SE:182:MET:HG3	5:SE:192:ILE:HG22	1.96	0.48
41:3a:87:GLU:HA	41:3a:90:VAL:HG22	1.94	0.48
12:SL:42:LEU:HD13	12:SL:72:ILE:HD11	1.96	0.48
18:SR:36:GLU:HB3	18:SR:47:ARG:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Sg:114:SER:HB3	33:Sg:119:GLN:HB2	1.95	0.48
36:S2:186:C:H2'	36:S2:187:G:H8	1.78	0.48
37:zz:80:U:H2'	37:zz:81:A:H8	1.77	0.48
38:5B:896:PRO:HB2	38:5B:960:LYS:HG2	1.96	0.48
40:3f:118:GLY:HA3	40:3f:173:TYR:CZ	2.48	0.48
41:3a:170:VAL:HG22	41:3a:173:LEU:HB3	1.95	0.48
41:3a:189:THR:HG23	41:3a:243:MET:HG3	1.95	0.48
1:SA:97:THR:HG21	1:SA:117:ARG:HD3	1.96	0.48
4:SD:31:GLU:HA	4:SD:107:TYR:HE2	1.78	0.48
14:SN:17:PRO:HG3	28:Sb:28:PRO:HG3	1.95	0.48
18:SR:71:ILE:HD11	18:SR:74:GLN:HG3	1.95	0.48
36:S2:1533:A:H2	36:S2:1536:G:N3	2.12	0.48
37:zz:205:A:H2'	37:zz:206:A:C8	2.49	0.48
40:3f:283:LEU:HA	40:3f:286:VAL:HG12	1.95	0.48
41:3a:238:ASP:HA	41:3a:241:ILE:HG22	1.95	0.48
47:3l:398:MET:O	47:3l:402:GLN:HG2	2.13	0.48
4:SD:148:LYS:HZ2	37:zz:350:G:H1	1.60	0.48
36:S2:107:A:H2'	36:S2:108:G:C8	2.48	0.48
36:S2:1405:A:H2'	36:S2:1406:G:O4'	2.14	0.48
40:3f:348:ILE:HG23	44:3h:253:MET:HE1	1.96	0.48
46:3k:112:CYS:HB2	47:3l:491:LEU:HD21	1.96	0.48
2:SB:137:LEU:HG	2:SB:215:VAL:HG22	1.96	0.47
36:S2:527:C:H2'	36:S2:528:A:H8	1.79	0.47
28:Sb:33:MET:HE2	28:Sb:79:PHE:CD1	2.50	0.47
33:Sg:242:SER:HB2	33:Sg:247:TRP:HB2	1.96	0.47
40:3f:115:ARG:HD3	40:3f:117:ILE:HG12	1.95	0.47
47:3l:457:LEU:HD23	47:3l:461:ARG:HD3	1.95	0.47
8:SH:43:LEU:HD12	8:SH:72:PHE:CD2	2.49	0.47
27:Sa:26:CYS:HB3	27:Sa:77:CYS:SG	2.53	0.47
33:Sg:42:MET:HB2	33:Sg:57:ARG:HB3	1.95	0.47
36:S2:441:C:H2'	36:S2:442:C:C6	2.50	0.47
36:S2:736:C:H2'	36:S2:737:G:C8	2.49	0.47
38:5B:866:LEU:HB2	38:5B:868:GLY:O	2.14	0.47
42:3e:223:PHE:CZ	42:3e:256:TYR:HB3	2.45	0.47
47:3l:383:ASP:HB3	47:3l:386:ILE:HG22	1.96	0.47
23:SW:5:ASN:HB3	23:SW:8:ALA:HB3	1.95	0.47
36:S2:656:G:N2	36:S2:663:C:H5''	2.29	0.47
36:S2:1755:C:H2'	36:S2:1756:C:C6	2.49	0.47
43:3c:431:LEU:H	43:3c:431:LEU:HD23	1.80	0.47
44:3h:41:ILE:HD13	44:3h:164:LEU:HD21	1.96	0.47
2:SB:122:GLU:HG2	2:SB:140:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Sg:125:ARG:HG2	33:Sg:150:TRP:CD2	2.49	0.47
36:S2:495:U:H2'	36:S2:496:C:O4'	2.14	0.47
36:S2:958:G:H2'	36:S2:959:G:C8	2.49	0.47
36:S2:1714:U:H2'	36:S2:1715:A:C8	2.50	0.47
38:5B:889:ILE:HD12	38:5B:956:ILE:HG23	1.96	0.47
38:5B:1171:MET:HB2	38:5B:1175:HIS:ND1	2.29	0.47
39:3m:228:PRO:HA	39:3m:231:PHE:HB3	1.95	0.47
3:SC:163:VAL:HG22	3:SC:164:PRO:HD2	1.97	0.47
4:SD:169:ASP:HB2	4:SD:190:LEU:HD11	1.97	0.47
41:3a:248:GLU:HA	41:3a:251:LYS:NZ	2.30	0.47
42:3e:249:MET:HG2	42:3e:250:CYS:HB2	1.96	0.47
44:3h:228:HIS:CD2	44:3h:230:LEU:HB2	2.50	0.47
44:3h:262:THR:HG22	44:3h:265:ARG:HH21	1.79	0.47
47:3l:113:PRO:HB2	47:3l:118:ILE:HD11	1.97	0.47
2:SB:105:LEU:HG	2:SB:213:ARG:HA	1.97	0.47
4:SD:210:ILE:HD12	18:SR:16:ILE:HD11	1.96	0.47
9:SI:119:LEU:HD11	9:SI:153:LYS:HD3	1.97	0.47
19:SS:130:ARG:HD2	19:SS:134:GLN:HE21	1.78	0.47
31:Se:52:LYS:HD2	31:Se:52:LYS:HA	1.63	0.47
36:S2:232:A:H5''	36:S2:890:U:H3	1.79	0.47
36:S2:668:A:H2'	36:S2:669:A:H2	1.80	0.47
36:S2:963:A:H2'	36:S2:964:A:C8	2.50	0.47
36:S2:1769:C:H2'	36:S2:1770:G:C8	2.49	0.47
37:zz:152:G:H2'	37:zz:153:G:C8	2.50	0.47
38:5B:1103:ASN:O	38:5B:1107:PRO:HD2	2.15	0.47
42:3e:302:ASN:HB2	43:3c:820:SER:HB2	1.96	0.47
42:3e:337:ARG:HH12	42:3e:362:MET:HG2	1.78	0.47
43:3c:781:ARG:HH12	43:3c:782:LYS:HE2	1.80	0.47
12:SL:13:GLN:HB2	12:SL:16:ILE:HG12	1.96	0.47
36:S2:28:U:H2'	36:S2:29:G:C8	2.50	0.47
36:S2:1763:G:H2'	36:S2:1764:G:H8	1.80	0.47
38:5B:1170:LYS:HZ3	38:5B:1175:HIS:HB3	1.78	0.47
39:3m:256:TYR:HA	39:3m:263:ILE:HD12	1.96	0.47
41:3a:385:PRO:HA	41:3a:388:LYS:HD2	1.97	0.47
43:3c:850:THR:HG22	43:3c:853:GLN:HG2	1.97	0.47
44:3h:130:THR:HA	44:3h:318:LEU:HD11	1.96	0.47
47:3l:187:ILE:O	47:3l:191:ILE:HG12	2.15	0.47
3:SC:203:GLY:O	3:SC:221:ASP:HA	2.14	0.47
13:Sf:35:ILE:HG12	13:Sf:61:TYR:CE1	2.50	0.47
13:Sf:122:ASP:HA	13:Sf:125:GLU:HG3	1.96	0.47
23:SW:93:LEU:HD12	23:SW:102:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Sc:46:VAL:HG11	29:Sc:56:LEU:HD21	1.97	0.47
36:S2:907:G:H2'	36:S2:908:A:C8	2.49	0.47
37:zz:308:C:H2'	37:zz:309:G:H8	1.80	0.47
41:3a:433:ASN:HA	41:3a:436:ILE:HG12	1.97	0.47
44:3h:67:LEU:HD11	44:3h:120:TYR:HB3	1.97	0.47
4:SD:227:LYS:HD2	33:Sg:184:LEU:HD22	1.96	0.47
16:SP:22:LEU:HD21	16:SP:109:PRO:HB3	1.96	0.47
36:S2:546:G:H1'	36:S2:547:G:C8	2.50	0.47
40:3f:120:LEU:HD22	40:3f:131:VAL:HG11	1.97	0.47
25:SY:12:PHE:HZ	25:SY:21:LYS:HD3	1.80	0.46
36:S2:1759:G:H2'	36:S2:1760:G:H8	1.80	0.46
36:S2:1797:U:H2'	36:S2:1798:C:C6	2.50	0.46
42:3e:195:THR:O	42:3e:199:ASN:HB2	2.14	0.46
42:3e:416:GLN:HG3	47:3l:344:GLN:HE22	1.80	0.46
43:3c:638:SER:HB2	43:3c:712:LYS:HB3	1.96	0.46
4:SD:157:MET:HA	4:SD:157:MET:HE2	1.97	0.46
15:SO:95:ILE:HD11	15:SO:126:ILE:HD12	1.96	0.46
21:SU:51:LYS:HB2	21:SU:90:ASP:HB2	1.96	0.46
47:3l:359:MET:HA	47:3l:362:LYS:HD2	1.97	0.46
27:Sa:79:ILE:HD13	36:S2:1863:A:H1'	1.95	0.46
36:S2:554:A:H4'	36:S2:555:A:H8	1.80	0.46
42:3e:155:ARG:HH22	42:3e:169:LEU:HD22	1.79	0.46
44:3h:160:GLY:HA2	44:3h:230:LEU:HG	1.96	0.46
2:SB:87:ILE:HG22	2:SB:101:HIS:HB2	1.98	0.46
8:SH:53:VAL:HG11	8:SH:172:THR:HA	1.97	0.46
9:SI:13:LYS:HB2	12:SL:137:THR:HG21	1.98	0.46
13:Sf:102:LYS:HD3	13:Sf:102:LYS:HA	1.80	0.46
15:SO:57:THR:H	15:SO:60:MET:HE2	1.79	0.46
18:SR:72:LYS:HA	18:SR:75:GLU:OE2	2.16	0.46
24:SX:60:LYS:HE3	24:SX:116:PRO:HB3	1.97	0.46
36:S2:171:A:H3'	36:S2:172:U:C6	2.50	0.46
36:S2:201:C:H3'	36:S2:202:G:C8	2.51	0.46
36:S2:1856:C:H2'	36:S2:1857:G:H8	1.80	0.46
38:5B:861:MET:SD	38:5B:876:ILE:HD11	2.56	0.46
38:5B:1140:SER:HB3	38:5B:1160:LYS:HB3	1.97	0.46
8:SH:160:LYS:HZ2	8:SH:191:GLU:HB3	1.80	0.46
36:S2:674:C:H2'	36:S2:675:U:C6	2.50	0.46
42:3e:281:ILE:HD13	42:3e:296:VAL:HG21	1.98	0.46
43:3c:610:ASN:HB3	43:3c:636:ILE:HD11	1.98	0.46
47:3l:474:LYS:HG3	47:3l:478:PHE:CZ	2.51	0.46
47:3l:497:MET:HE1	47:3l:521:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SH:143:ARG:HD2	23:SW:53:ILE:HG12	1.97	0.46
33:Sg:78:ALA:HB2	33:Sg:92:LEU:HD11	1.98	0.46
36:S2:115:U:H2'	36:S2:116:U:C6	2.50	0.46
36:S2:1768:A:H2'	36:S2:1769:C:H6	1.80	0.46
43:3c:507:ILE:O	43:3c:511:TYR:HB3	2.15	0.46
44:3h:193:THR:HG22	44:3h:195:GLU:H	1.80	0.46
44:3h:271:GLN:HA	44:3h:274:LYS:HD2	1.96	0.46
11:SK:14:LEU:HD12	11:SK:21:MET:HE1	1.98	0.46
36:S2:1417:C:H42	36:S2:1422:G:H1	1.64	0.46
38:5B:646:LYS:HA	38:5B:646:LYS:HD2	1.84	0.46
41:3a:64:SER:HB3	41:3a:152:PHE:HD1	1.81	0.46
46:3k:76:ASN:HB3	46:3k:79:HIS:CE1	2.51	0.46
47:3l:179:PRO:HB2	47:3l:182:TRP:HB2	1.97	0.46
7:SG:176:ILE:HD12	7:SG:176:ILE:H	1.81	0.46
10:SJ:93:LYS:HD2	10:SJ:96:TYR:HE2	1.81	0.46
11:SK:53:LYS:HB3	11:SK:53:LYS:HE3	1.72	0.46
34:zy:66:U:H2'	34:zy:67:C:C6	2.51	0.46
36:S2:907:G:H2'	36:S2:908:A:H8	1.81	0.46
39:3m:87:CYS:HB3	39:3m:126:SER:OG	2.16	0.46
41:3a:400:PRO:HG3	41:3a:442:GLN:HB3	1.98	0.46
5:SE:48:LEU:HD11	5:SE:70:ILE:HD11	1.97	0.46
6:SF:40:ALA:HB3	6:SF:67:PRO:HA	1.98	0.46
8:SH:61:ILE:HD11	8:SH:176:VAL:HG22	1.98	0.46
37:zz:173:A:H2'	37:zz:174:U:C6	2.51	0.46
5:SE:31:PRO:HD2	5:SE:38:LEU:HD21	1.98	0.46
13:Sf:21:VAL:HG22	13:Sf:120:ALA:HB1	1.98	0.46
33:Sg:5:MET:HB2	33:Sg:268:ASP:OD2	2.15	0.46
36:S2:1764:G:C6	36:S2:1768:A:N7	2.84	0.46
39:3m:64:MET:HE3	39:3m:64:MET:HB3	1.88	0.46
39:3m:68:VAL:HA	39:3m:71:LEU:HD12	1.97	0.46
44:3h:215:MET:HA	44:3h:218:LEU:HD22	1.98	0.46
1:SA:203:PHE:HZ	18:SR:91:LEU:HD21	1.81	0.45
4:SD:109:LEU:HD21	4:SD:115:VAL:HG22	1.98	0.45
11:SK:5:LYS:O	11:SK:9:ILE:HG12	2.16	0.45
38:5B:613:ILE:HA	38:5B:616:ARG:HG2	1.97	0.45
38:5B:634:ILE:HD11	38:5B:698:MET:HE2	1.98	0.45
38:5B:837:LEU:O	38:5B:841:LEU:HG	2.16	0.45
39:3m:223:LEU:HG	39:3m:229:VAL:HG21	1.96	0.45
47:3l:383:ASP:HB2	47:3l:545:ARG:HH21	1.80	0.45
7:SG:176:ILE:HB	7:SG:179:LEU:HD23	1.98	0.45
8:SH:86:LYS:HG2	8:SH:87:PHE:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:SV:41:LYS:HB2	22:SV:41:LYS:HE2	1.83	0.45
32:sh:95:ARG:HE	32:sh:95:ARG:HB3	1.51	0.45
36:S2:102:A:H4'	36:S2:104:A:C8	2.52	0.45
36:S2:1798:C:H2'	36:S2:1799:G:O4'	2.16	0.45
38:5B:711:ASN:ND2	38:5B:992:GLU:HB2	2.31	0.45
39:3m:67:VAL:O	39:3m:71:LEU:HG	2.17	0.45
40:3f:102:ILE:HG12	40:3f:173:TYR:CZ	2.51	0.45
43:3c:714:PHE:O	43:3c:717:GLN:HG3	2.15	0.45
43:3c:822:ILE:HG13	43:3c:825:MET:HE2	1.98	0.45
47:3l:541:ASP:HA	47:3l:544:ILE:HB	1.96	0.45
1:SA:90:PHE:HD1	1:SA:179:ALA:HB2	1.82	0.45
4:SD:7:LYS:HB2	4:SD:7:LYS:HE2	1.71	0.45
6:SF:100:ILE:HG13	6:SF:174:ALA:HB1	1.98	0.45
20:ST:51:ASN:HB3	20:ST:54:TYR:HD2	1.79	0.45
36:S2:172:U:H2'	36:S2:173:A:H8	1.81	0.45
37:zz:244:A:H2'	37:zz:245:G:C8	2.51	0.45
38:5B:609:ALA:O	38:5B:613:ILE:HG23	2.16	0.45
44:3h:327:CYS:HA	44:3h:330:ILE:HG22	1.98	0.45
47:3l:321:PHE:HD1	47:3l:370:LEU:HD11	1.80	0.45
8:SH:63:PHE:HD2	8:SH:97:GLN:HG2	1.80	0.45
17:SQ:19:ALA:HB2	17:SQ:75:GLY:HA3	1.99	0.45
36:S2:145:G:H2'	36:S2:146:G:C8	2.51	0.45
36:S2:1533:A:C8	36:S2:1604:G:H1'	2.52	0.45
37:zz:151:C:H2'	37:zz:152:G:C8	2.52	0.45
39:3m:276:LYS:HE2	39:3m:280:LEU:HG	1.98	0.45
42:3e:208:LEU:O	42:3e:212:THR:HG23	2.17	0.45
43:3c:445:LEU:HA	43:3c:502:ILE:HD11	1.97	0.45
5:SE:36:HIS:CG	5:SE:85:GLY:HA3	2.51	0.45
5:SE:100:ARG:HG2	5:SE:102:ILE:HG12	1.98	0.45
7:SG:2:LYS:HB3	7:SG:15:LEU:HD11	1.98	0.45
17:SQ:103:ALA:O	17:SQ:107:GLU:HG3	2.16	0.45
18:SR:8:THR:HG21	36:S2:1387:G:N2	2.32	0.45
20:ST:134:ILE:O	20:ST:138:VAL:HG23	2.16	0.45
31:Se:25:LYS:HA	31:Se:25:LYS:HD3	1.62	0.45
33:Sg:313:THR:HG22	33:Sg:314:ILE:HD12	1.99	0.45
36:S2:1808:U:H2'	36:S2:1809:A:H8	1.81	0.45
38:5B:1077:LYS:O	38:5B:1081:GLN:HG3	2.17	0.45
39:3m:39:HIS:HA	39:3m:82:LEU:HD21	1.98	0.45
40:3f:335:LEU:HD23	40:3f:335:LEU:HA	1.82	0.45
43:3c:634:LEU:HD21	43:3c:711:SER:HA	1.98	0.45
44:3h:169:LEU:HG	44:3h:173:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:zy:67:C:H2'	34:zy:68:U:C6	2.52	0.45
36:S2:198:U:H2'	36:S2:200:G:OP2	2.17	0.45
38:5B:891:PRO:HG2	38:5B:945:LEU:HB3	1.97	0.45
41:3a:552:LEU:HA	41:3a:555:THR:HG22	1.98	0.45
47:3l:371:LEU:HD23	47:3l:390:LEU:HD21	1.98	0.45
2:SB:129:THR:HG22	2:SB:133:TYR:HB2	1.98	0.45
20:ST:71:GLY:O	20:ST:75:MET:HG2	2.17	0.45
21:SU:38:ASP:HA	21:SU:41:ARG:HG2	1.99	0.45
25:SY:23:MET:HE1	25:SY:48:TYR:CE2	2.50	0.45
33:Sg:14:HIS:CE1	33:Sg:35:SER:HB2	2.51	0.45
41:3a:392:ASN:O	41:3a:396:VAL:HB	2.16	0.45
3:SC:200:ARG:HA	3:SC:221:ASP:OD2	2.17	0.45
14:SN:20:ARG:HA	14:SN:65:PHE:CE2	2.52	0.45
15:SO:61:LYS:HD3	15:SO:76:LEU:HB3	1.99	0.45
38:5B:631:ALA:HB3	38:5B:928:ALA:HB1	1.99	0.45
40:3f:120:LEU:HG	40:3f:173:TYR:HD2	1.82	0.45
41:3a:481:GLN:HE21	41:3a:494:GLY:H	1.65	0.45
44:3h:270:GLN:HE22	44:3h:308:PRO:HD2	1.82	0.45
47:3l:184:TRP:HH2	47:3l:314:THR:HG21	1.82	0.45
7:SG:131:ARG:HH21	7:SG:160:LYS:HG3	1.82	0.45
8:SH:69:LEU:HD22	8:SH:96:ALA:HB2	1.97	0.45
11:SK:35:LEU:HD13	11:SK:40:VAL:HG11	1.99	0.45
11:SK:38:LYS:HB2	11:SK:40:VAL:HG12	1.99	0.45
36:S2:12:U:H2'	36:S2:13:C:C6	2.52	0.45
36:S2:508:A:H3'	36:S2:509:G:H8	1.81	0.45
36:S2:1344:A:H4'	36:S2:1345:G:H5'	1.99	0.45
41:3a:378:ASN:HB2	41:3a:380:LEU:HD12	1.99	0.45
42:3e:255:ARG:HG2	42:3e:293:THR:HG23	1.99	0.45
43:3c:846:ARG:HE	43:3c:846:ARG:HB3	1.61	0.45
47:3l:51:VAL:HG23	47:3l:52:ILE:HD12	1.99	0.45
47:3l:263:HIS:HB2	47:3l:266:TYR:CD2	2.52	0.45
36:S2:496:C:H2'	36:S2:497:C:H6	1.82	0.45
36:S2:531:A:H2'	36:S2:532:C:C6	2.52	0.45
37:zz:130:C:H2'	37:zz:131:G:C8	2.52	0.45
38:5B:669:GLY:O	38:5B:701:ILE:HA	2.17	0.45
1:SA:207:PRO:O	1:SA:211:GLU:HG2	2.17	0.44
15:SO:56:VAL:HA	15:SO:60:MET:HE2	1.97	0.44
36:S2:106:C:H2'	36:S2:107:A:H8	1.82	0.44
36:S2:527:C:H2'	36:S2:528:A:C8	2.52	0.44
36:S2:698:G:H5'	36:S2:733:C:H42	1.82	0.44
36:S2:1767:C:H1'	36:S2:1768:A:C2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:S2:1845:A:H2'	36:S2:1846:G:C8	2.52	0.44
38:5B:1015:LYS:HB2	38:5B:1048:MET:HE3	1.98	0.44
44:3h:141:GLN:HE22	44:3h:169:LEU:HD23	1.83	0.44
44:3h:239:LEU:HD12	44:3h:239:LEU:HA	1.85	0.44
8:SH:62:ILE:HD13	8:SH:92:VAL:HG13	1.98	0.44
14:SN:32:ASP:HA	14:SN:35:GLU:HG3	1.99	0.44
36:S2:756:C:H2'	36:S2:757:C:H6	1.82	0.44
39:3m:224:LEU:HD11	39:3m:245:VAL:HG11	1.98	0.44
40:3f:93:ARG:HB3	40:3f:240:ALA:HB2	1.99	0.44
40:3f:141:GLU:HA	40:3f:146:VAL:HG12	1.99	0.44
41:3a:175:HIS:ND1	41:3a:228:MET:HB3	2.32	0.44
1:SA:76:VAL:HG23	1:SA:98:PRO:HA	1.99	0.44
10:SJ:106:LEU:HD23	10:SJ:109:ARG:HD2	1.99	0.44
11:SK:15:LEU:HD22	11:SK:49:MET:HE1	1.99	0.44
11:SK:57:TYR:HB3	11:SK:75:GLY:HA2	1.99	0.44
36:S2:186:C:H2'	36:S2:187:G:C8	2.52	0.44
36:S2:693:A:H2	36:S2:737:G:H2'	1.83	0.44
36:S2:1101:U:H2'	36:S2:1102:G:C8	2.52	0.44
39:3m:241:LEU:O	39:3m:245:VAL:HG12	2.18	0.44
47:3l:134:GLU:HA	47:3l:137:TYR:CD2	2.52	0.44
15:SO:131:ASP:OD1	15:SO:133:THR:HG22	2.17	0.44
16:SP:33:LEU:HD23	16:SP:33:LEU:HA	1.87	0.44
19:SS:108:ARG:HG2	19:SS:112:GLU:OE2	2.17	0.44
26:SZ:74:SER:HA	26:SZ:79:ILE:HG13	1.99	0.44
33:Sg:9:GLY:H	33:Sg:309:VAL:HG23	1.81	0.44
33:Sg:88:ARG:HE	33:Sg:100:ARG:HH11	1.63	0.44
36:S2:1736:G:H2'	36:S2:1737:G:C8	2.52	0.44
37:zz:125:C:H2'	37:zz:126:C:C6	2.51	0.44
38:5B:940:LYS:O	38:5B:940:LYS:HG3	2.17	0.44
2:SB:125:VAL:HG11	2:SB:172:MET:HB3	1.99	0.44
3:SC:170:TRP:CE2	3:SC:199:PRO:HG3	2.53	0.44
23:SW:78:ARG:HD3	23:SW:126:LEU:HD23	2.00	0.44
37:zz:72:A:H3'	37:zz:73:A:H8	1.83	0.44
37:zz:95:U:H2'	37:zz:96:A:H8	1.83	0.44
37:zz:139:C:H2'	37:zz:140:A:C8	2.53	0.44
37:zz:147:U:H2'	37:zz:148:C:C6	2.52	0.44
37:zz:248:U:H2'	37:zz:249:G:C8	2.44	0.44
38:5B:1033:VAL:HG12	38:5B:1055:ARG:HB2	1.99	0.44
38:5B:1211:VAL:HG13	38:5B:1214:LYS:HE2	1.99	0.44
43:3c:852:GLN:H	43:3c:852:GLN:HG3	1.61	0.44
10:SJ:134:HIS:CE1	10:SJ:164:PRO:HD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:SR:41:ILE:HA	18:SR:42:PRO:HD3	1.81	0.44
30:Sd:22:ARG:HH21	36:S2:1553:C:H41	1.65	0.44
36:S2:196:C:H2'	36:S2:197:U:H6	1.82	0.44
36:S2:278:C:H2'	36:S2:279:G:C8	2.53	0.44
36:S2:1593:C:H2'	36:S2:1594:A:H8	1.82	0.44
38:5B:639:HIS:CD2	38:5B:640:VAL:HG12	2.52	0.44
4:SD:61:GLU:H	4:SD:61:GLU:HG3	1.56	0.44
9:SI:141:ARG:HB2	9:SI:146:GLN:HG2	1.99	0.44
36:S2:804:U:H2'	36:S2:805:U:H6	1.83	0.44
36:S2:1365:G:H2'	36:S2:1366:G:C8	2.52	0.44
3:SC:238:LYS:HB2	3:SC:238:LYS:HE2	1.63	0.44
11:SK:47:LYS:HE2	36:S2:1274:G:H4'	2.00	0.44
13:Sf:12:MET:HB2	13:Sf:16:THR:HB	1.99	0.44
32:sh:123:SER:HB3	32:sh:126:CYS:HB2	1.99	0.44
36:S2:746:C:H1'	36:S2:747:U:H5	1.83	0.44
41:3a:331:ILE:HG23	41:3a:367:ARG:HG2	1.98	0.44
42:3e:344:PHE:O	42:3e:348:HIS:HB2	2.18	0.44
1:SA:24:HIS:HB3	1:SA:51:LEU:HD21	2.00	0.44
6:SF:136:ARG:C	6:SF:203:ASN:HD21	2.26	0.44
19:SS:132:ARG:HD3	36:S2:1623[B]:A:C6	2.53	0.44
33:Sg:269:GLU:HB3	33:Sg:271:LYS:NZ	2.33	0.44
36:S2:158:A:H2'	36:S2:159:A:O4'	2.18	0.44
36:S2:753:C:H2'	36:S2:754:G:H8	1.82	0.44
36:S2:1751:C:H3'	36:S2:1752:C:H4'	1.99	0.44
36:S2:1808:U:H2'	36:S2:1809:A:C8	2.53	0.44
37:zz:161:G:H2'	37:zz:162:A:C8	2.53	0.44
40:3f:284:SER:O	40:3f:287:LEU:HG	2.17	0.44
41:3a:25:GLN:HB2	41:3a:26:PRO:HD3	2.00	0.44
41:3a:74:TYR:CD2	41:3a:86:LEU:HD13	2.53	0.44
42:3e:124:ARG:HA	42:3e:124:ARG:HD3	1.82	0.44
43:3c:574:TYR:HD2	43:3c:612:THR:HG22	1.82	0.44
47:3l:104:GLU:HB3	47:3l:143:LYS:HZ3	1.83	0.44
47:3l:115:ALA:HB2	47:3l:133:LYS:HD3	1.99	0.44
47:3l:240:ILE:HD11	47:3l:267:LYS:HA	2.00	0.44
5:SE:95:THR:HG22	25:SY:16:ARG:HB2	1.99	0.43
5:SE:240:ARG:HH22	36:S2:844:U:P	2.41	0.43
14:SN:54:LEU:HB3	14:SN:60:VAL:HG12	2.00	0.43
38:5B:665:THR:HG23	38:5B:704:PRO:HA	1.99	0.43
39:3m:178:SER:HB3	39:3m:216:ASN:HD21	1.83	0.43
41:3a:408:THR:HA	41:3a:411:LEU:HB2	1.99	0.43
12:SL:24:LEU:HA	12:SL:27:GLU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:SO:142:ARG:HH21	27:Sa:27:ALA:HB2	1.82	0.43
15:SO:149:ARG:HH12	15:SO:151:LEU:HD11	1.83	0.43
36:S2:540:U:H3	36:S2:543:C:H41	1.66	0.43
36:S2:1415:C:H2'	36:S2:1416:C:C6	2.53	0.43
36:S2:1772:C:H2'	36:S2:1773:C:C6	2.53	0.43
42:3e:113:LEU:HD12	42:3e:113:LEU:HA	1.81	0.43
42:3e:138:GLN:HB3	42:3e:143:ASN:HB3	2.00	0.43
43:3c:804:MET:HE3	43:3c:840:GLN:HG3	2.01	0.43
47:3l:324:LEU:HD12	47:3l:370:LEU:HD13	2.00	0.43
1:SA:13:GLU:O	1:SA:17:LYS:HG3	2.17	0.43
1:SA:183:LEU:HD23	1:SA:183:LEU:HA	1.88	0.43
8:SH:95:ILE:HD11	8:SH:133:LEU:HD13	1.99	0.43
25:SY:103:SER:HB3	25:SY:106:GLN:HB2	2.00	0.43
32:sh:89:LYS:HD3	36:S2:1507:G:C5	2.54	0.43
36:S2:1415:C:H2'	36:S2:1416:C:H6	1.84	0.43
36:S2:1845:A:H2'	36:S2:1846:G:H8	1.83	0.43
38:5B:991:LEU:HD21	38:5B:1008:ILE:HB	1.98	0.43
40:3f:97:VAL:HG21	44:3h:51:LYS:HD3	2.00	0.43
44:3h:68:LEU:HD11	44:3h:82:PHE:HD1	1.84	0.43
3:SC:127:PHE:CD1	3:SC:141:VAL:HG22	2.53	0.43
13:Sf:63:LYS:HD2	32:sh:108:VAL:HG13	1.99	0.43
17:SQ:113:ILE:HG12	17:SQ:120:LEU:HD12	2.00	0.43
33:Sg:17:TRP:HB2	33:Sg:36:ARG:HG3	2.00	0.43
33:Sg:194:TYR:CE2	33:Sg:212:LYS:HD2	2.53	0.43
36:S2:197:U:H2'	36:S2:198:U:O4'	2.18	0.43
36:S2:1232:U:H2'	36:S2:1233:G:C8	2.53	0.43
7:SG:175:LYS:HG3	36:S2:77:A:H2	1.84	0.43
11:SK:26:ASP:OD2	11:SK:29:MET:HG3	2.18	0.43
26:SZ:47:LEU:HB2	26:SZ:79:ILE:HG22	1.99	0.43
36:S2:752:G:H2'	36:S2:753:C:C6	2.53	0.43
36:S2:964:A:H2'	36:S2:965:U:C6	2.53	0.43
36:S2:1628:C:H2'	36:S2:1629:C:C6	2.54	0.43
37:zz:183:C:H2'	37:zz:184:G:C8	2.54	0.43
38:5B:639:HIS:CG	38:5B:640:VAL:H	2.36	0.43
38:5B:988:LEU:O	38:5B:992:GLU:HG3	2.19	0.43
40:3f:268:ASP:HB3	44:3h:336:GLN:HB2	2.00	0.43
43:3c:504:LEU:HD13	43:3c:564:ILE:HG21	2.01	0.43
44:3h:99:TYR:CE1	44:3h:103:MET:HE2	2.54	0.43
44:3h:119:TRP:HE1	44:3h:149:VAL:HG12	1.82	0.43
3:SC:74:LYS:HD3	3:SC:74:LYS:HA	1.69	0.43
7:SG:213:LEU:HD21	7:SG:217:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SI:57:ALA:HB2	9:SI:183:GLY:HA2	2.00	0.43
36:S2:230:A:H5''	36:S2:888:U:H1'	2.00	0.43
36:S2:382:C:H2'	36:S2:383:G:C8	2.54	0.43
43:3c:762:ASN:HA	43:3c:766:TRP:HB2	2.00	0.43
47:3l:137:TYR:CE2	47:3l:156:SER:HA	2.53	0.43
47:3l:403:LYS:HA	47:3l:403:LYS:HD2	1.89	0.43
13:Sf:56:CYS:SG	13:Sf:62:VAL:HG22	2.58	0.43
18:SR:48:ASN:ND2	36:S2:1452:A:H5''	2.34	0.43
36:S2:1629:C:C2	36:S2:1630:A:C8	3.07	0.43
38:5B:755:LEU:HB2	38:5B:820:LEU:HD21	2.00	0.43
43:3c:510:THR:HG22	43:3c:513:LYS:HE3	2.01	0.43
46:3k:179:TRP:CE2	46:3k:189:ILE:HG23	2.54	0.43
47:3l:168:LEU:HD21	47:3l:234:LEU:HG	2.00	0.43
14:SN:114:ARG:O	14:SN:118:ILE:HG13	2.18	0.43
24:SX:75:ILE:HD13	38:5B:1019:MET:CE	2.49	0.43
34:zy:12:G:H22	34:zy:21:G:N2	2.16	0.43
36:S2:96:C:H2'	36:S2:97:U:C6	2.53	0.43
36:S2:1227:G:C2	36:S2:1228:A:C8	3.07	0.43
36:S2:1434:C:H4'	36:S2:1435:C:OP2	2.17	0.43
36:S2:1736:G:H2'	36:S2:1737:G:H8	1.83	0.43
39:3m:218:PHE:HA	39:3m:276:LYS:HE3	2.01	0.43
42:3e:170:TRP:HE1	42:3e:210:GLN:NE2	2.17	0.43
43:3c:717:GLN:HA	43:3c:720:VAL:HG22	1.99	0.43
47:3l:237:LYS:HD2	47:3l:260:TYR:CD2	2.53	0.43
4:SD:70:THR:HB	4:SD:86:LEU:HG	2.01	0.43
7:SG:29:GLU:HA	7:SG:101:ILE:HD11	2.01	0.43
9:SI:124:LYS:HG3	9:SI:125:LYS:H	1.83	0.43
14:SN:25:TRP:CD1	28:Sb:82:LYS:HD2	2.53	0.43
17:SQ:72:VAL:HG21	17:SQ:84:ILE:HD11	2.00	0.43
18:SR:24:LEU:HD23	18:SR:24:LEU:HA	1.87	0.43
39:3m:18:LEU:HD12	39:3m:18:LEU:HA	1.85	0.43
40:3f:336:MET:HE3	40:3f:336:MET:HA	2.01	0.43
5:SE:11:ARG:HA	5:SE:28:ALA:HB2	2.01	0.43
9:SI:121:LEU:HD11	9:SI:166:PHE:CG	2.54	0.43
33:Sg:165:ILE:HG12	33:Sg:177:TRP:HB2	2.01	0.43
33:Sg:269:GLU:HB3	33:Sg:271:LYS:HZ1	1.83	0.43
36:S2:982:G:H2'	36:S2:983:A:C8	2.54	0.43
40:3f:187:HIS:CE1	40:3f:199:HIS:HB2	2.54	0.43
43:3c:718:LEU:HD23	43:3c:738:VAL:HG23	2.00	0.43
1:SA:51:LEU:HA	1:SA:54:THR:HG22	2.00	0.42
1:SA:81:ASN:HA	1:SA:84:GLN:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:SB:226:GLY:O	2:SB:230:GLU:HG3	2.18	0.42
3:SC:275:LYS:HD2	3:SC:275:LYS:HA	1.86	0.42
20:ST:123:LEU:HD23	20:ST:123:LEU:HA	1.84	0.42
36:S2:1723:G:N2	36:S2:1812:U:H3	2.17	0.42
37:zz:179:A:H2'	37:zz:180:G:C8	2.53	0.42
47:3l:325:MET:HE2	47:3l:326:MET:HG2	2.01	0.42
8:SH:63:PHE:HA	8:SH:95:ILE:O	2.19	0.42
16:SP:62:LYS:HD3	16:SP:62:LYS:HA	1.81	0.42
18:SR:29:HIS:HA	18:SR:32:LYS:HD3	2.00	0.42
23:SW:111:MET:HB2	23:SW:115:GLU:OE1	2.19	0.42
33:Sg:210:GLY:HA3	33:Sg:236:ILE:HG21	2.01	0.42
36:S2:319:C:H2'	36:S2:320:G:O4'	2.18	0.42
36:S2:1103:C:H2'	36:S2:1104:G:C8	2.54	0.42
36:S2:1144:A:H2'	36:S2:1145:A:C8	2.54	0.42
36:S2:1413:G:H2'	36:S2:1414:A:C8	2.53	0.42
37:zz:305:U:N3	37:zz:313:G:C6	2.87	0.42
38:5B:765:LYS:H	38:5B:779:GLN:HE22	1.66	0.42
38:5B:1042:GLU:H	38:5B:1042:GLU:HG2	1.61	0.42
38:5B:1186:ILE:HD12	38:5B:1213:LEU:HD21	2.01	0.42
39:3m:46:ILE:HD12	39:3m:46:ILE:HA	1.90	0.42
40:3f:348:ILE:HG13	44:3h:323:ILE:HG21	2.01	0.42
41:3a:192:ALA:O	41:3a:196:LYS:HG3	2.19	0.42
43:3c:574:TYR:O	43:3c:578:LEU:HB2	2.20	0.42
2:SB:83:LYS:HE2	2:SB:106:THR:HA	2.01	0.42
13:Sf:36:ARG:HD2	13:Sf:36:ARG:HA	1.89	0.42
27:Sa:10:ARG:HB2	27:Sa:33:ASP:OD2	2.18	0.42
32:sh:89:LYS:HD2	32:sh:89:LYS:HA	1.79	0.42
36:S2:1230:C:H2'	36:S2:1231:C:H6	1.83	0.42
37:zz:259:U:O2'	37:zz:260:A:H8	2.02	0.42
41:3a:91:ARG:HD3	41:3a:94:LEU:HD21	1.99	0.42
41:3a:268:LYS:HA	41:3a:268:LYS:HD3	1.87	0.42
44:3h:45:VAL:HG21	44:3h:78:ILE:HG22	2.02	0.42
5:SE:259:LYS:HB3	5:SE:259:LYS:HE3	1.73	0.42
18:SR:87:GLU:H	18:SR:87:GLU:CD	2.27	0.42
21:SU:104:ILE:HD13	21:SU:104:ILE:HA	1.85	0.42
36:S2:1203:G:H2'	36:S2:1204:A:C8	2.54	0.42
36:S2:1639:G:H2'	36:S2:1640:A:C8	2.54	0.42
37:zz:52:G:H2'	37:zz:53:A:H8	1.84	0.42
38:5B:1030:GLN:HB3	38:5B:1076:TYR:CE1	2.54	0.42
40:3f:92:VAL:HA	40:3f:129:VAL:HG13	2.01	0.42
43:3c:750:LYS:HA	43:3c:750:LYS:HD2	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3k:151:GLN:HE21	46:3k:191:SER:HA	1.83	0.42
47:3l:347:LYS:HA	47:3l:350:PHE:CD2	2.54	0.42
11:SK:14:LEU:HG	11:SK:34:GLU:OE2	2.18	0.42
36:S2:1189:A:H2'	36:S2:1190:A:H8	1.84	0.42
36:S2:1355:C:O2'	36:S2:1356:G:C8	2.73	0.42
36:S2:1621:U:O2'	36:S2:1622:U:H2'	2.18	0.42
38:5B:634:ILE:HD12	38:5B:700:ILE:HG13	2.00	0.42
3:SC:133:TYR:CE1	3:SC:216:MET:HA	2.54	0.42
16:SP:60:LEU:HD21	16:SP:94:VAL:HG22	2.01	0.42
18:SR:40:ILE:O	18:SR:40:ILE:HG22	2.19	0.42
27:Sa:5:ARG:HD3	36:S2:1865:C:O4'	2.19	0.42
36:S2:1758:G:H2'	36:S2:1759:G:C8	2.54	0.42
36:S2:1844:U:H2'	36:S2:1845:A:C8	2.55	0.42
43:3c:781:ARG:O	43:3c:785:GLU:HG2	2.20	0.42
15:SO:116:LEU:HD13	27:Sa:45:VAL:HG12	2.01	0.42
25:SY:25:ILE:HD12	25:SY:44:LEU:HD21	2.00	0.42
28:Sb:8:LEU:HD23	28:Sb:8:LEU:HA	1.82	0.42
36:S2:464:A:H5'	36:S2:465:A:C8	2.54	0.42
39:3m:22:LEU:HD12	39:3m:29:ILE:HD13	2.00	0.42
41:3a:48:GLU:HB3	41:3a:49:PRO:HD3	2.01	0.42
42:3e:360:LEU:HD23	42:3e:360:LEU:HA	1.89	0.42
46:3k:174:MET:SD	46:3k:187:ILE:HG21	2.60	0.42
47:3l:52:ILE:HA	47:3l:55:PHE:HB3	2.01	0.42
47:3l:412:LEU:HD23	47:3l:412:LEU:HA	1.79	0.42
4:SD:18:LYS:HB2	4:SD:18:LYS:HE2	1.80	0.42
4:SD:193:ASP:HA	4:SD:194:PRO:HD3	1.95	0.42
6:SF:91:ARG:HD2	26:SZ:103:HIS:CE1	2.54	0.42
15:SO:119:LEU:HD12	15:SO:119:LEU:HA	1.93	0.42
36:S2:1683:C:H2'	36:S2:1684:C:H6	1.85	0.42
37:zz:141:U:H2'	37:zz:142:A:C8	2.54	0.42
40:3f:90:ARG:NH2	40:3f:217:VAL:HG11	2.35	0.42
43:3c:611:ARG:HH21	43:3c:671:VAL:HG11	1.85	0.42
1:SA:180:ARG:NE	1:SA:184:ARG:HH12	2.18	0.42
5:SE:3:ARG:HG2	36:S2:447:A:H4'	2.00	0.42
7:SG:218:LYS:HB3	7:SG:218:LYS:HE3	1.79	0.42
23:SW:6:VAL:HG13	23:SW:29:PRO:HB2	2.02	0.42
36:S2:551:U:H2'	36:S2:552:G:C8	2.55	0.42
36:S2:563:G:O2'	36:S2:564:A:H8	2.02	0.42
36:S2:803:C:H2'	36:S2:804:U:C6	2.55	0.42
36:S2:1408:U:H2'	36:S2:1409:A:C8	2.55	0.42
38:5B:689:ASP:HB2	38:5B:692:ASN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:3c:469:TYR:HE2	43:3c:674:HIS:HB2	1.85	0.42
44:3h:331:LYS:HE3	44:3h:331:LYS:HB3	1.91	0.42
1:SA:34:MET:HE3	1:SA:154:LEU:HD21	2.01	0.42
1:SA:130:ASP:O	1:SA:133:PRO:HD2	2.20	0.42
2:SB:181:LEU:HA	2:SB:184:VAL:HG22	2.02	0.42
6:SF:151:ILE:HD13	6:SF:151:ILE:HA	1.86	0.42
7:SG:133:LEU:HD22	36:S2:65:C:C2	2.55	0.42
7:SG:174:PRO:HB3	36:S2:65:C:C5	2.55	0.42
8:SH:86:LYS:HG2	8:SH:87:PHE:HD1	1.85	0.42
36:S2:844:U:H2'	36:S2:845:G:C8	2.55	0.42
37:zz:59:U:H2'	37:zz:60:G:C8	2.55	0.42
37:zz:243:G:H2'	37:zz:244:A:C8	2.55	0.42
38:5B:637:LEU:HD23	38:5B:740:SER:HB3	2.02	0.42
47:3l:489:GLN:HA	47:3l:492:VAL:HG22	2.01	0.42
1:SA:118:GLU:HG3	3:SC:65:LYS:HG3	2.01	0.41
9:SI:141:ARG:HD3	9:SI:145:ILE:HG22	2.02	0.41
13:Sf:35:ILE:HG12	13:Sf:61:TYR:HE1	1.83	0.41
14:SN:118:ILE:HG12	14:SN:121:ARG:HH21	1.85	0.41
15:SO:129:ILE:HG21	27:Sa:44:ILE:HG21	2.02	0.41
19:SS:66:ARG:O	19:SS:70:ILE:HG13	2.21	0.41
28:Sb:24:LEU:HD12	28:Sb:24:LEU:HA	1.86	0.41
33:Sg:235:ILE:O	33:Sg:252:THR:HA	2.20	0.41
36:S2:909:G:H2'	36:S2:910:G:C8	2.55	0.41
36:S2:1277:C:H2'	36:S2:1278:A:C8	2.52	0.41
36:S2:1763:G:H2'	36:S2:1764:G:C8	2.55	0.41
38:5B:685:ILE:HG21	38:5B:836:TYR:HD1	1.85	0.41
38:5B:833:SER:O	38:5B:837:LEU:HD13	2.20	0.41
42:3e:209:GLN:HA	42:3e:212:THR:HG23	2.01	0.41
43:3c:565:ARG:NH2	43:3c:566:THR:HG22	2.35	0.41
43:3c:637:GLN:HG2	43:3c:686:TYR:CD2	2.55	0.41
44:3h:119:TRP:NE1	44:3h:149:VAL:HG12	2.35	0.41
44:3h:274:LYS:O	44:3h:278:GLN:HG3	2.19	0.41
44:3h:329:ASN:O	44:3h:332:GLU:HG3	2.20	0.41
15:SO:31:CYS:HB2	15:SO:93:LEU:HD13	2.02	0.41
17:SQ:42:ILE:HD13	17:SQ:42:ILE:HA	1.80	0.41
18:SR:16:ILE:HD12	18:SR:38:ILE:HD11	2.01	0.41
26:SZ:98:LYS:HB3	26:SZ:98:LYS:HE3	1.76	0.41
33:Sg:260:ASP:HB3	33:Sg:265:ILE:HG23	2.02	0.41
36:S2:496:C:H2'	36:S2:497:C:C6	2.55	0.41
39:3m:25:LYS:HA	39:3m:25:LYS:HD3	1.82	0.41
39:3m:124:TYR:HB3	39:3m:154:TRP:CH2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:3m:176:LYS:HA	39:3m:176:LYS:HD3	1.71	0.41
39:3m:280:LEU:HD23	39:3m:280:LEU:HA	1.91	0.41
40:3f:107:GLU:HB2	44:3h:210:LEU:HD22	2.01	0.41
42:3e:341:PHE:HB3	42:3e:374:LEU:HD11	2.00	0.41
44:3h:152:TYR:HE1	44:3h:157:THR:HG21	1.85	0.41
47:3l:287:TYR:O	47:3l:291:ILE:HG12	2.20	0.41
47:3l:389:GLN:H	47:3l:389:GLN:HG3	1.72	0.41
4:SD:107:TYR:HD1	4:SD:107:TYR:HA	1.70	0.41
5:SE:60:GLU:O	5:SE:64:ILE:HG13	2.20	0.41
5:SE:158:ASP:HB2	5:SE:173:ILE:O	2.21	0.41
10:SJ:101:LYS:HA	10:SJ:101:LYS:HD3	1.73	0.41
13:Sf:58:GLU:O	13:Sf:62:VAL:HG23	2.20	0.41
14:SN:5:HIS:HB3	14:SN:117:LEU:HD13	2.02	0.41
15:SO:142:ARG:NH2	27:Sa:27:ALA:HB2	2.35	0.41
36:S2:280:G:O6	36:S2:891:G:H1'	2.20	0.41
36:S2:874:G:H2'	36:S2:875:A:C8	2.53	0.41
38:5B:643:GLY:O	38:5B:647:ILE:HG22	2.19	0.41
41:3a:41:ARG:HH12	41:3a:76:ASN:HB3	1.84	0.41
41:3a:202:ARG:NH1	41:3a:233:ARG:HH21	2.17	0.41
47:3l:474:LYS:HD2	47:3l:474:LYS:HA	1.86	0.41
6:SF:42:LYS:HD3	6:SF:42:LYS:HA	1.86	0.41
11:SK:30:PRO:HA	11:SK:41:PRO:HB3	2.01	0.41
13:Sf:91:LEU:HD11	36:S2:1284:A:C6	2.55	0.41
14:SN:72:LEU:HD22	14:SN:72:LEU:HA	1.87	0.41
21:SU:61:LEU:O	21:SU:81:GLN:HA	2.21	0.41
29:Sc:12:ALA:HB1	29:Sc:32:VAL:HB	2.01	0.41
32:sh:105:TYR:CD1	32:sh:118:ARG:HD3	2.56	0.41
36:S2:1272:C:H2'	36:S2:1273:C:C6	2.55	0.41
46:3k:204:LYS:HD3	46:3k:204:LYS:HA	1.89	0.41
6:SF:204:ARG:HG2	15:SO:72:TYR:CE1	2.56	0.41
7:SG:52:ILE:HG23	7:SG:109:LEU:HD21	2.03	0.41
15:SO:147:ARG:HA	27:Sa:28:ARG:HH11	1.85	0.41
17:SQ:45:ARG:HA	17:SQ:45:ARG:HD2	1.92	0.41
19:SS:40:TYR:HE2	19:SS:71:MET:HG3	1.86	0.41
24:SX:4:CYS:HB3	36:S2:1161:U:OP2	2.20	0.41
25:SY:37:LYS:HA	25:SY:40:ILE:HG22	2.02	0.41
34:zy:34:A:H2'	34:zy:35:U:H6	1.85	0.41
40:3f:251:LEU:HD22	44:3h:162:LEU:HB2	2.02	0.41
42:3e:136:LYS:O	42:3e:140:GLU:HG2	2.19	0.41
42:3e:409:LYS:HG2	47:3l:388:LEU:HD22	2.02	0.41
43:3c:504:LEU:HA	43:3c:507:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:3c:760:LYS:HG3	43:3c:764:LYS:HD3	2.03	0.41
43:3c:814:ASP:CG	43:3c:816:PRO:HD2	2.44	0.41
46:3k:91:GLN:O	46:3k:95:GLU:HG2	2.21	0.41
47:3l:563:ARG:HG3	47:3l:564:PRO:HD3	2.02	0.41
4:SD:72:VAL:HG11	11:SK:70:TYR:HE1	1.86	0.41
11:SK:35:LEU:HD23	11:SK:35:LEU:HA	1.86	0.41
23:SW:66:THR:OG1	23:SW:68:ARG:HG3	2.20	0.41
31:Se:51:LYS:HE3	31:Se:51:LYS:HB3	1.84	0.41
36:S2:15:U:H2'	36:S2:16:G:O4'	2.19	0.41
41:3a:61:LEU:O	41:3a:62:ARG:HG2	2.21	0.41
41:3a:389:ASP:HA	41:3a:392:ASN:HD21	1.85	0.41
42:3e:348:HIS:NE2	43:3c:837:GLN:HB2	2.36	0.41
42:3e:358:ASP:O	42:3e:359:LYS:HG2	2.21	0.41
4:SD:198:ILE:HD13	4:SD:198:ILE:HA	1.88	0.41
7:SG:149:LYS:HE3	7:SG:149:LYS:HB3	1.88	0.41
7:SG:164:LYS:HB2	36:S2:67:C:C4	2.56	0.41
7:SG:207:ALA:O	7:SG:211:LYS:HG2	2.20	0.41
9:SI:10:LYS:HB3	9:SI:10:LYS:HE3	1.79	0.41
13:Sf:32:ALA:HB2	13:Sf:112:LYS:HZ2	1.86	0.41
13:Sf:94:ILE:HG23	13:Sf:98:GLY:HA2	2.03	0.41
14:SN:62:GLN:HB2	14:SN:65:PHE:HB2	2.02	0.41
18:SR:33:ARG:HA	18:SR:33:ARG:HD3	1.80	0.41
18:SR:58:MET:HE2	18:SR:58:MET:HB2	1.69	0.41
29:Sc:63:ARG:HD3	29:Sc:66:ARG:HH21	1.86	0.41
36:S2:160:U:O2'	36:S2:161:U:H3'	2.20	0.41
36:S2:1643:U:H2'	36:S2:1644:C:C6	2.54	0.41
37:zz:313:G:H2'	37:zz:314:C:C6	2.56	0.41
43:3c:624:GLY:HA2	43:3c:778:MET:HE1	2.03	0.41
44:3h:228:HIS:CE1	44:3h:230:LEU:HD13	2.56	0.41
46:3k:213:ILE:H	46:3k:213:ILE:HG13	1.63	0.41
47:3l:101:LYS:HB2	47:3l:101:LYS:HE2	1.83	0.41
47:3l:310:GLU:H	47:3l:310:GLU:HG3	1.61	0.41
47:3l:324:LEU:HD23	47:3l:324:LEU:HA	1.91	0.41
2:SB:146:ARG:HE	2:SB:206:PRO:HG2	1.86	0.41
3:SC:91:SER:HB2	3:SC:156:ILE:HG23	2.01	0.41
12:SL:82:MET:HG3	12:SL:85:THR:HG23	2.02	0.41
16:SP:57:LEU:HD11	16:SP:86:LEU:HD12	2.02	0.41
22:SV:42:VAL:HG13	22:SV:43:THR:HG23	2.03	0.41
36:S2:803:C:H2'	36:S2:804:U:H6	1.86	0.41
36:S2:1410:C:H2'	36:S2:1411:G:H8	1.85	0.41
36:S2:1593:C:H2'	36:S2:1594:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:S2:1714:U:H2'	36:S2:1715:A:H8	1.84	0.41
37:zz:245:G:H2'	37:zz:246:A:C8	2.55	0.41
39:3m:98:ARG:HE	39:3m:100:SER:HB2	1.85	0.41
41:3a:41:ARG:HD2	41:3a:41:ARG:HA	1.69	0.41
42:3e:182:TRP:HB2	42:3e:225:HIS:CD2	2.55	0.41
42:3e:183:ASP:HA	42:3e:186:MET:HE2	2.02	0.41
42:3e:342:GLU:CD	42:3e:378:ALA:HB2	2.46	0.41
47:3l:277:LEU:HD21	47:3l:293:VAL:HG21	2.02	0.41
2:SB:133:TYR:CE1	2:SB:221:PRO:HD2	2.56	0.41
5:SE:106:LYS:HE3	5:SE:106:LYS:HB2	1.87	0.41
8:SH:127:ASP:O	8:SH:131:GLU:HG3	2.21	0.41
9:SI:125:LYS:HD3	9:SI:125:LYS:HA	1.74	0.41
10:SJ:136:ARG:HD3	10:SJ:160:SER:HA	2.03	0.41
10:SJ:151:LEU:HD23	10:SJ:151:LEU:HA	1.85	0.41
12:SL:96:ILE:HD12	24:SX:10:ALA:HB1	2.03	0.41
12:SL:99:TYR:CD1	24:SX:13:LEU:HD23	2.55	0.41
14:SN:94:LYS:HB2	14:SN:94:LYS:HE3	1.71	0.41
33:Sg:120:ILE:HD13	33:Sg:120:ILE:HA	1.77	0.41
36:S2:106:C:H2'	36:S2:107:A:C8	2.55	0.41
36:S2:841:G:H2'	36:S2:842:C:H6	1.85	0.41
36:S2:1407:U:H2'	36:S2:1408:U:C6	2.56	0.41
36:S2:1809:A:H2'	36:S2:1810:U:C6	2.55	0.41
37:zz:308:C:H2'	37:zz:309:G:C8	2.55	0.41
38:5B:739:GLU:O	38:5B:743:LEU:HG	2.20	0.41
38:5B:877:LEU:HB3	38:5B:927:ALA:HA	2.02	0.41
40:3f:157:TYR:CZ	40:3f:169:ILE:HG12	2.56	0.41
40:3f:337:VAL:HG13	44:3h:330:ILE:HD11	2.03	0.41
46:3k:114:PHE:HA	46:3k:117:PHE:HB3	2.02	0.41
47:3l:552:GLU:HG3	47:3l:555:ARG:HH11	1.85	0.41
2:SB:123:ALA:HB2	2:SB:165:ARG:HG3	2.02	0.41
4:SD:201:LYS:HE3	4:SD:201:LYS:HB2	1.89	0.41
9:SI:151:GLU:O	9:SI:154:LYS:HG2	2.21	0.41
10:SJ:144:ILE:HD13	10:SJ:144:ILE:HA	1.85	0.41
19:SS:87:GLN:HB3	19:SS:95:TYR:CE2	2.56	0.41
25:SY:36:PRO:HG2	25:SY:39:GLU:HB2	2.03	0.41
36:S2:51:U:H2'	36:S2:52:G:H8	1.86	0.41
36:S2:1406:G:H2'	36:S2:1407:U:C6	2.55	0.41
37:zz:193:C:H42	37:zz:202:A:H61	1.69	0.41
38:5B:757:LYS:HD3	50:5B:1302:GTP:C5	2.55	0.41
38:5B:1138:VAL:HG23	38:5B:1159:VAL:HB	2.03	0.41
39:3m:254:LYS:HB3	39:3m:254:LYS:HE3	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:3c:584:GLN:HE22	45:3d:2:ALA:HB3	1.86	0.41
44:3h:219:GLU:HA	44:3h:222:SER:HB3	2.01	0.41
47:3l:322:ALA:O	47:3l:326:MET:HB2	2.21	0.41
1:SA:32:PHE:CD2	36:S2:1097:G:H4'	2.56	0.40
2:SB:231:LEU:HA	2:SB:231:LEU:HD23	1.80	0.40
5:SE:173:ILE:HD11	5:SE:235:TRP:CD2	2.56	0.40
6:SF:99:ILE:HD11	26:SZ:106:GLN:HE21	1.86	0.40
9:SI:136:ILE:HD13	9:SI:136:ILE:HA	1.92	0.40
11:SK:65:ARG:HG2	30:Sd:22:ARG:O	2.20	0.40
19:SS:106:LYS:HA	19:SS:106:LYS:HD3	1.84	0.40
23:SW:101:PHE:HA	23:SW:113:HIS:CE1	2.56	0.40
24:SX:3:LYS:HB3	24:SX:3:LYS:HE2	1.89	0.40
29:Sc:13:ARG:CZ	29:Sc:35:MET:HE1	2.50	0.40
33:Sg:271:LYS:HE3	33:Sg:271:LYS:HB3	1.94	0.40
36:S2:1347:U:H2'	36:S2:1348:G:N3	2.35	0.40
36:S2:1705:C:H2'	36:S2:1706:G:C8	2.56	0.40
38:5B:1110:MET:O	38:5B:1158:CYS:HA	2.21	0.40
41:3a:531:ALA:O	41:3a:535:GLU:HG2	2.20	0.40
42:3e:229:ARG:HA	42:3e:229:ARG:HD2	1.78	0.40
1:SA:126:ASP:O	1:SA:130:ASP:HB2	2.22	0.40
13:Sf:124:ILE:HD13	13:Sf:124:ILE:HA	1.86	0.40
34:zy:59:A:H2'	34:zy:60:C:O4'	2.22	0.40
36:S2:50:A:H1'	38:5B:868:GLY:HA3	2.03	0.40
36:S2:900:C:H2'	36:S2:901:G:H8	1.86	0.40
36:S2:1862:G:H1'	36:S2:1863:A:H2'	2.03	0.40
38:5B:1131:ASN:CG	38:5B:1132:PHE:H	2.29	0.40
41:3a:158:ARG:HH21	41:3a:161:LEU:HG	1.86	0.40
44:3h:249:ARG:HD2	44:3h:319:ILE:HG23	2.03	0.40
46:3k:72:LYS:HD2	46:3k:72:LYS:HA	1.75	0.40
46:3k:124:ASN:O	46:3k:127:LEU:HG	2.22	0.40
5:SE:66:MET:HE1	36:S2:502:C:OP2	2.21	0.40
12:SL:45:LYS:HE3	12:SL:45:LYS:HB2	1.83	0.40
12:SL:93:LEU:HD23	12:SL:93:LEU:HA	1.93	0.40
14:SN:112:LYS:HB3	14:SN:112:LYS:HE2	1.77	0.40
17:SQ:15:ARG:HH22	36:S2:1444:U:P	2.44	0.40
24:SX:85:VAL:HG21	24:SX:91:LEU:HD13	2.04	0.40
27:Sa:45:VAL:HG11	27:Sa:53:ILE:HG13	2.03	0.40
29:Sc:16:LYS:HB2	29:Sc:16:LYS:HE3	1.80	0.40
31:Se:53:LYS:HD3	31:Se:53:LYS:HA	1.80	0.40
36:S2:1531:A:H2'	36:S2:1532:C:C6	2.57	0.40
37:zz:79:C:H2'	37:zz:80:U:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:zz:177:C:H2'	37:zz:178:C:C6	2.56	0.40
38:5B:905:LEU:HB3	38:5B:919:TYR:HB3	2.03	0.40
38:5B:1093:LYS:HB3	38:5B:1115:GLU:HG3	2.03	0.40
39:3m:268:LEU:HD22	39:3m:273:ASN:HD22	1.86	0.40
41:3a:171:GLU:HG2	41:3a:175:HIS:NE2	2.36	0.40
42:3e:276:ASP:HA	42:3e:279:LYS:HD2	2.03	0.40
44:3h:141:GLN:HA	44:3h:144:ILE:O	2.22	0.40
46:3k:76:ASN:HB3	46:3k:79:HIS:NE2	2.36	0.40
1:SA:176:TRP:CE3	1:SA:177:MET:HG2	2.56	0.40
7:SG:220:ALA:O	7:SG:224:ARG:HG2	2.22	0.40
9:SI:106:SER:HB3	9:SI:171:LEU:HG	2.03	0.40
18:SR:100:PRO:HD3	18:SR:120:THR:O	2.21	0.40
21:SU:99:LYS:HA	21:SU:99:LYS:HD2	1.98	0.40
23:SW:79:PHE:O	23:SW:124:LYS:HA	2.22	0.40
24:SX:101:LEU:HB3	24:SX:124:LYS:HB2	2.03	0.40
33:Sg:64:HIS:ND1	33:Sg:65:PHE:HD1	2.20	0.40
33:Sg:297:THR:HA	33:Sg:310:TRP:O	2.21	0.40
36:S2:1667:U:H2'	36:S2:1668:U:C6	2.57	0.40
38:5B:707:GLU:HA	38:5B:713:ARG:HH22	1.85	0.40
38:5B:965:HIS:HA	38:5B:968:LYS:HG2	2.03	0.40
41:3a:212:HIS:HA	41:3a:217:ALA:HB3	2.03	0.40
41:3a:436:ILE:HD13	41:3a:462:VAL:HG21	2.02	0.40
42:3e:225:HIS:CE1	42:3e:227:LYS:HB3	2.57	0.40
3:SC:216:MET:HE2	3:SC:216:MET:HB2	1.95	0.40
9:SI:60:LEU:HA	9:SI:60:LEU:HD23	1.86	0.40
10:SJ:33:GLY:HA3	31:Se:38:TYR:CG	2.56	0.40
14:SN:78:LYS:HD2	14:SN:78:LYS:HA	1.90	0.40
21:SU:40:ILE:HD12	21:SU:40:ILE:HA	1.82	0.40
33:Sg:42:MET:CE	33:Sg:92:LEU:HD23	2.52	0.40
34:zy:10:G:H1	34:zy:44:G:N2	2.19	0.40
34:zy:22:C:H2'	34:zy:23:G:C8	2.56	0.40
34:zy:64:C:H2'	34:zy:65:C:H6	1.86	0.40
36:S2:429:C:H2'	36:S2:430:C:H6	1.87	0.40
36:S2:600:G:H2'	36:S2:601:G:H8	1.86	0.40
36:S2:1306:U:C4	36:S2:1307:U:C4	3.10	0.40
37:zz:77:G:H2'	37:zz:78:U:C6	2.57	0.40
38:5B:613:ILE:HG22	38:5B:616:ARG:NH1	2.37	0.40
38:5B:695:ILE:HD13	38:5B:695:ILE:HA	1.83	0.40
38:5B:1124:PRO:HG2	38:5B:1185:LYS:HB3	2.03	0.40
41:3a:7:ARG:HA	41:3a:8:PRO:HD2	1.99	0.40
41:3a:235:VAL:HA	41:3a:238:ASP:OD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:3a:338:ILE:H	41:3a:338:ILE:HG12	1.63	0.40
43:3c:602:ASP:HB3	43:3c:604:PRO:HD2	2.04	0.40
44:3h:169:LEU:HD12	44:3h:169:LEU:HA	1.78	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	SA	214/295 (72%)	206 (96%)	8 (4%)	0	100	100
2	SB	210/264 (80%)	201 (96%)	9 (4%)	0	100	100
3	SC	218/293 (74%)	212 (97%)	6 (3%)	0	100	100
4	SD	224/243 (92%)	221 (99%)	3 (1%)	0	100	100
5	SE	258/263 (98%)	244 (95%)	14 (5%)	0	100	100
6	SF	190/204 (93%)	182 (96%)	8 (4%)	0	100	100
7	SG	235/249 (94%)	232 (99%)	3 (1%)	0	100	100
8	SH	185/194 (95%)	181 (98%)	4 (2%)	0	100	100
9	SI	203/208 (98%)	195 (96%)	8 (4%)	0	100	100
10	SJ	178/194 (92%)	176 (99%)	2 (1%)	0	100	100
11	SK	94/165 (57%)	89 (95%)	5 (5%)	0	100	100
12	SL	148/158 (94%)	141 (95%)	7 (5%)	0	100	100
13	Sf	119/132 (90%)	108 (91%)	11 (9%)	0	100	100
14	SN	147/151 (97%)	139 (95%)	8 (5%)	0	100	100
15	SO	133/151 (88%)	123 (92%)	10 (8%)	0	100	100
16	SP	117/145 (81%)	113 (97%)	4 (3%)	0	100	100
17	SQ	138/146 (94%)	135 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	SR	130/135 (96%)	123 (95%)	7 (5%)	0	100	100
19	SS	141/152 (93%)	136 (96%)	5 (4%)	0	100	100
20	ST	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
21	SU	99/119 (83%)	96 (97%)	2 (2%)	1 (1%)	13	47
22	SV	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
23	SW	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
24	SX	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
25	SY	122/133 (92%)	119 (98%)	3 (2%)	0	100	100
26	SZ	73/125 (58%)	68 (93%)	5 (7%)	0	100	100
27	Sa	98/115 (85%)	97 (99%)	1 (1%)	0	100	100
28	Sb	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
29	Sc	60/69 (87%)	55 (92%)	5 (8%)	0	100	100
30	Sd	50/56 (89%)	46 (92%)	4 (8%)	0	100	100
31	Se	50/59 (85%)	47 (94%)	3 (6%)	0	100	100
32	sh	62/156 (40%)	60 (97%)	2 (3%)	0	100	100
33	Sg	311/317 (98%)	295 (95%)	16 (5%)	0	100	100
35	Ln	22/25 (88%)	21 (96%)	1 (4%)	0	100	100
38	5B	619/621 (100%)	589 (95%)	29 (5%)	1 (0%)	44	75
39	3m	361/374 (96%)	342 (95%)	19 (5%)	0	100	100
40	3f	267/357 (75%)	262 (98%)	5 (2%)	0	100	100
41	3a	590/1382 (43%)	568 (96%)	22 (4%)	0	100	100
42	3e	428/445 (96%)	411 (96%)	16 (4%)	1 (0%)	44	75
43	3c	537/913 (59%)	519 (97%)	18 (3%)	0	100	100
44	3h	315/352 (90%)	304 (96%)	11 (4%)	0	100	100
45	3d	53/548 (10%)	50 (94%)	3 (6%)	0	100	100
46	3k	213/218 (98%)	198 (93%)	15 (7%)	0	100	100
47	3l	518/564 (92%)	503 (97%)	15 (3%)	0	100	100
All	All	8698/11275 (77%)	8354 (96%)	341 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	SU	54	VAL

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Mol	Chain	Res	Type
38	5B	1138	VAL
42	3e	264	ASN

### 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	SA	180/243 (74%)	172 (96%)	8 (4%)	24	57
2	SB	193/231 (84%)	185 (96%)	8 (4%)	26	59
3	SC	186/225 (83%)	170 (91%)	16 (9%)	8	33
4	SD	189/202 (94%)	177 (94%)	12 (6%)	15	46
5	SE	223/225 (99%)	214 (96%)	9 (4%)	27	59
6	SF	162/170 (95%)	157 (97%)	5 (3%)	35	66
7	SG	207/218 (95%)	202 (98%)	5 (2%)	44	71
8	SH	167/174 (96%)	157 (94%)	10 (6%)	16	48
9	SI	178/180 (99%)	167 (94%)	11 (6%)	15	47
10	SJ	160/168 (95%)	153 (96%)	7 (4%)	24	57
11	SK	87/136 (64%)	83 (95%)	4 (5%)	23	56
12	SL	134/142 (94%)	132 (98%)	2 (2%)	60	81
13	Sf	102/108 (94%)	97 (95%)	5 (5%)	21	54
14	SN	130/131 (99%)	121 (93%)	9 (7%)	13	43
15	SO	104/119 (87%)	94 (90%)	10 (10%)	7	28
16	SP	107/130 (82%)	104 (97%)	3 (3%)	38	68
17	SQ	116/121 (96%)	109 (94%)	7 (6%)	16	48
18	SR	119/122 (98%)	115 (97%)	4 (3%)	32	63
19	SS	124/132 (94%)	118 (95%)	6 (5%)	21	55
20	ST	112/115 (97%)	108 (96%)	4 (4%)	30	62
21	SU	93/107 (87%)	89 (96%)	4 (4%)	25	57
22	SV	67/67 (100%)	66 (98%)	1 (2%)	60	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	SW	112/113 (99%)	104 (93%)	8 (7%)	12	42
24	SX	113/115 (98%)	105 (93%)	8 (7%)	12	42
25	SY	108/115 (94%)	103 (95%)	5 (5%)	23	56
26	SZ	67/103 (65%)	64 (96%)	3 (4%)	23	56
27	Sa	87/98 (89%)	81 (93%)	6 (7%)	13	43
28	Sb	75/76 (99%)	72 (96%)	3 (4%)	27	59
29	Sc	55/62 (89%)	52 (94%)	3 (6%)	18	51
30	Sd	46/49 (94%)	44 (96%)	2 (4%)	25	57
31	Se	42/48 (88%)	40 (95%)	2 (5%)	21	55
32	sh	57/140 (41%)	56 (98%)	1 (2%)	54	77
33	Sg	272/275 (99%)	260 (96%)	12 (4%)	24	57
35	Ln	23/24 (96%)	18 (78%)	5 (22%)	1	4
38	5B	546/546 (100%)	536 (98%)	10 (2%)	54	77
39	3m	251/335 (75%)	243 (97%)	8 (3%)	34	65
40	3f	228/289 (79%)	219 (96%)	9 (4%)	27	60
41	3a	439/1259 (35%)	419 (95%)	20 (5%)	23	56
42	3e	301/406 (74%)	288 (96%)	13 (4%)	25	57
43	3c	347/811 (43%)	330 (95%)	17 (5%)	21	54
44	3h	271/310 (87%)	260 (96%)	11 (4%)	26	59
45	3d	20/494 (4%)	19 (95%)	1 (5%)	20	54
46	3k	120/193 (62%)	116 (97%)	4 (3%)	33	64
47	3l	474/515 (92%)	455 (96%)	19 (4%)	27	59
All	All	7194/9842 (73%)	6874 (96%)	320 (4%)	26	57

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	SA	8	LEU
1	SA	38	ILE
1	SA	112	ILE
1	SA	136	GLU
1	SA	142	LEU
1	SA	192	GLU
1	SA	201	LEU

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Mol	Chain	Res	Type
1	SA	209	GLU
2	SB	25	PHE
2	SB	52	THR
2	SB	91	VAL
2	SB	105	LEU
2	SB	111	CYS
2	SB	169	MET
2	SB	225	LEU
2	SB	228	LEU
3	SC	105	GLU
3	SC	112	VAL
3	SC	120	GLN
3	SC	155	ILE
3	SC	157	LEU
3	SC	161	SER
3	SC	163	VAL
3	SC	185	THR
3	SC	191	VAL
3	SC	192	LEU
3	SC	196	ILE
3	SC	227	ARG
3	SC	233	LEU
3	SC	248	TYR
3	SC	268	GLU
3	SC	270	THR
4	SD	16	ILE
4	SD	20	GLU
4	SD	42	THR
4	SD	54	ARG
4	SD	66	ILE
4	SD	84	VAL
4	SD	93	THR
4	SD	101	GLN
4	SD	149	SER
4	SD	172	VAL
4	SD	176	LEU
4	SD	221	THR
5	SE	115	THR
5	SE	129	ILE
5	SE	146	THR
5	SE	164	LEU
5	SE	217	SER

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Mol	Chain	Res	Type
5	SE	222	LEU
5	SE	228	ILE
5	SE	248	ILE
5	SE	250	GLU
6	SF	70	GLU
6	SF	103	LEU
6	SF	149	GLN
6	SF	168	THR
6	SF	195	GLU
7	SG	67	VAL
7	SG	113	ILE
7	SG	158	VAL
7	SG	162	LEU
7	SG	212	LEU
8	SH	27	LEU
8	SH	46	THR
8	SH	49	LYS
8	SH	51	ILE
8	SH	72	PHE
8	SH	76	GLN
8	SH	119	SER
8	SH	121	THR
8	SH	130	LEU
8	SH	184	ASP
9	SI	5	ARG
9	SI	14	THR
9	SI	36	THR
9	SI	76	THR
9	SI	91	VAL
9	SI	95	THR
9	SI	107	THR
9	SI	111	GLN
9	SI	159	SER
9	SI	174	CYS
9	SI	189	VAL
10	SJ	53	ILE
10	SJ	61	LEU
10	SJ	71	LEU
10	SJ	112	THR
10	SJ	117	LEU
10	SJ	122	SER
10	SJ	137	VAL

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Mol	Chain	Res	Type
11	SK	40	VAL
11	SK	71	LEU
11	SK	76	ILE
11	SK	90	VAL
12	SL	22	ARG
12	SL	80	MET
13	Sf	33	ARG
13	Sf	43	ASP
13	Sf	69	CYS
13	Sf	95	ASP
13	Sf	124	ILE
14	SN	22	VAL
14	SN	24	THR
14	SN	62	GLN
14	SN	63	VAL
14	SN	72	LEU
14	SN	87	ASP
14	SN	102	LEU
14	SN	103	GLU
14	SN	145	THR
15	SO	21	VAL
15	SO	27	VAL
15	SO	57	THR
15	SO	88	LEU
15	SO	90	ILE
15	SO	91	THR
15	SO	97	LEU
15	SO	100	THR
15	SO	116	LEU
15	SO	143	LYS
16	SP	23	ASP
16	SP	121	ILE
16	SP	126	VAL
17	SQ	18	THR
17	SQ	20	THR
17	SQ	42	ILE
17	SQ	61	GLU
17	SQ	102	GLU
17	SQ	104	SER
17	SQ	110	ASP
18	SR	37	GLU
18	SR	43	SER

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Mol	Chain	Res	Type
18	SR	88	VAL
18	SR	106	LEU
19	SS	31	THR
19	SS	38	ARG
19	SS	67	VAL
19	SS	71	MET
19	SS	83	PHE
19	SS	136	THR
20	ST	51	ASN
20	ST	88	MET
20	ST	114	GLU
20	ST	123	LEU
21	SU	39	LEU
21	SU	40	ILE
21	SU	95	SER
21	SU	104	ILE
22	SV	13	VAL
23	SW	11	LEU
23	SW	25	VAL
23	SW	74	VAL
23	SW	80	ASP
23	SW	83	LEU
23	SW	105	THR
23	SW	115	GLU
23	SW	121	THR
24	SX	32	LEU
24	SX	95	GLU
24	SX	100	VAL
24	SX	102	VAL
24	SX	105	PHE
24	SX	123	VAL
24	SX	125	VAL
24	SX	127	ASN
25	SY	17	LEU
25	SY	39	GLU
25	SY	72	PHE
25	SY	74	MET
25	SY	125	VAL
26	SZ	65	TYR
26	SZ	69	THR
26	SZ	110	THR
27	Sa	3	LYS

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Mol	Chain	Res	Type
27	Sa	21	ILE
27	Sa	23	CYS
27	Sa	24	THR
27	Sa	64	LEU
27	Sa	79	ILE
28	Sb	27	SER
28	Sb	53	VAL
28	Sb	57	VAL
29	Sc	9	ILE
29	Sc	18	LEU
29	Sc	43	ILE
30	Sd	5	GLN
30	Sd	55	LEU
31	Se	22	GLN
31	Se	29	THR
32	sh	103	LEU
33	Sg	24	THR
33	Sg	64	HIS
33	Sg	79	LEU
33	Sg	113	PHE
33	Sg	132	TRP
33	Sg	135	LEU
33	Sg	137	VAL
33	Sg	151	VAL
33	Sg	182	CYS
33	Sg	207	CYS
33	Sg	217	MET
33	Sg	246	TYR
35	Ln	6	ARG
35	Ln	7	LYS
35	Ln	13	LEU
35	Ln	14	LYS
35	Ln	20	MET
38	5B	651	LEU
38	5B	665	THR
38	5B	803	LEU
38	5B	808	PHE
38	5B	816	THR
38	5B	947	LEU
38	5B	1065	LEU
38	5B	1101	ILE
38	5B	1129	SER

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Mol	Chain	Res	Type
38	5B	1199	ARG
39	3m	64	MET
39	3m	72	LEU
39	3m	83	ILE
39	3m	117	THR
39	3m	151	ILE
39	3m	207	CYS
39	3m	257	GLN
39	3m	269	LEU
40	3f	99	LEU
40	3f	119	THR
40	3f	129	VAL
40	3f	148	VAL
40	3f	160	HIS
40	3f	178	ASP
40	3f	252	ILE
40	3f	272	VAL
40	3f	337	VAL
41	3a	40	HIS
41	3a	41	ARG
41	3a	59	VAL
41	3a	72	TYR
41	3a	73	GLN
41	3a	157	TYR
41	3a	220	LEU
41	3a	229	HIS
41	3a	243	MET
41	3a	262	LEU
41	3a	283	PHE
41	3a	344	MET
41	3a	361	LEU
41	3a	374	MET
41	3a	395	GLU
41	3a	399	ASN
41	3a	415	ARG
41	3a	424	LEU
41	3a	481	GLN
41	3a	523	LEU
42	3e	17	HIS
42	3e	19	VAL
42	3e	131	LEU
42	3e	201	VAL

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Mol	Chain	Res	Type
42	3e	221	VAL
42	3e	255	ARG
42	3e	296	VAL
42	3e	341	PHE
42	3e	348	HIS
42	3e	356	LEU
42	3e	362	MET
42	3e	375	ILE
42	3e	380	LEU
43	3c	505	LEU
43	3c	549	GLU
43	3c	572	HIS
43	3c	575	HIS
43	3c	593	HIS
43	3c	598	ILE
43	3c	674	HIS
43	3c	679	LEU
43	3c	684	CYS
43	3c	711	SER
43	3c	773	ASP
43	3c	810	MET
43	3c	818	VAL
43	3c	834	SER
43	3c	842	VAL
43	3c	844	MET
43	3c	847	THR
44	3h	44	LEU
44	3h	75	ARG
44	3h	97	VAL
44	3h	152	TYR
44	3h	214	LEU
44	3h	256	ASP
44	3h	280	ARG
44	3h	301	LEU
44	3h	343	MET
44	3h	347	LEU
44	3h	350	TYR
45	3d	10	GLN
46	3k	109	LEU
46	3k	161	MET
46	3k	196	ILE
46	3k	213	ILE

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Mol	Chain	Res	Type
47	3l	73	GLU
47	3l	79	VAL
47	3l	110	THR
47	3l	138	ARG
47	3l	168	LEU
47	3l	169	ASN
47	3l	225	HIS
47	3l	336	PHE
47	3l	349	MET
47	3l	353	THR
47	3l	359	MET
47	3l	388	LEU
47	3l	398	MET
47	3l	419	LYS
47	3l	425	VAL
47	3l	451	VAL
47	3l	482	THR
47	3l	497	MET
47	3l	539	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	SA	50	ASN
2	SB	43	ASN
2	SB	186	ASN
3	SC	172	ASN
4	SD	226	GLN
5	SE	138	HIS
5	SE	201	HIS
5	SE	216	ASN
6	SF	203	ASN
7	SG	70	HIS
7	SG	197	GLN
8	SH	114	GLN
8	SH	163	GLN
10	SJ	140	GLN
12	SL	11	GLN
16	SP	32	GLN
17	SQ	77	HIS
19	SS	42	HIS
19	SS	101	ASN

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Mol	Chain	Res	Type
23	SW	56	HIS
24	SX	31	HIS
30	Sd	26	ASN
31	Se	15	GLN
33	Sg	14	HIS
33	Sg	285	GLN
38	5B	666	GLN
38	5B	731	HIS
38	5B	736	GLN
38	5B	1144	ASN
38	5B	1175	HIS
39	3m	146	GLN
39	3m	205	HIS
40	3f	177	HIS
40	3f	342	ASN
41	3a	10	ASN
41	3a	76	ASN
41	3a	180	GLN
41	3a	288	ASN
41	3a	297	HIS
41	3a	392	ASN
41	3a	441	GLN
41	3a	481	GLN
41	3a	544	GLN
42	3e	17	HIS
42	3e	354	ASN
43	3c	670	GLN
43	3c	716	HIS
43	3c	724	GLN
44	3h	40	GLN
44	3h	98	GLN
44	3h	212	ASN
44	3h	228	HIS
44	3h	270	GLN
44	3h	279	GLN
44	3h	282	GLN
44	3h	285	ASN
47	3l	69	GLN
47	3l	169	ASN
47	3l	199	GLN
47	3l	218	ASN
47	3l	263	HIS

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Mol	Chain	Res	Type
47	3l	289	GLN
47	3l	344	GLN
47	3l	364	ASN
47	3l	366	GLN
47	3l	368	HIS
47	3l	443	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	zy	74/75 (98%)	26 (35%)	0
36	S2	1747/1869 (93%)	327 (18%)	7 (0%)
37	zz	312/332 (93%)	114 (36%)	0
All	All	2133/2276 (93%)	467 (21%)	7 (0%)

All (467) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	zy	5	G
34	zy	8	U
34	zy	9	G
34	zy	15	G
34	zy	16	C
34	zy	17	G
34	zy	18	G
34	zy	19	A
34	zy	20	A
34	zy	21	G
34	zy	23	G
34	zy	39	C
34	zy	41	A
34	zy	42	G
34	zy	47	C
34	zy	52	G
34	zy	54	U
34	zy	56	G
34	zy	57	A
34	zy	60	C
34	zy	61	C
34	zy	62	A
34	zy	65	C

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Mol	Chain	Res	Type
34	zy	72	A
34	zy	73	C
34	zy	74	C
36	S2	2	A
36	S2	4	C
36	S2	17	C
36	S2	33	G
36	S2	41	G
36	S2	44	U
36	S2	45	A
36	S2	46	A
36	S2	56	G
36	S2	59	U
36	S2	62	G
36	S2	67	C
36	S2	68	A
36	S2	73	C
36	S2	74	G
36	S2	75	G
36	S2	99	A
36	S2	103	A
36	S2	113	G
36	S2	114	G
36	S2	115	U
36	S2	126	G
36	S2	130	G
36	S2	143	U
36	S2	149	A
36	S2	161	U
36	S2	163	U
36	S2	167	G
36	S2	172	U
36	S2	178	C
36	S2	191	A
36	S2	193	C
36	S2	194	C
36	S2	195	C
36	S2	199	C
36	S2	200	G
36	S2	202	G
36	S2	211	G
36	S2	228	C

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Mol	Chain	Res	Type
36	S2	229	A
36	S2	230	A
36	S2	281	C
36	S2	282	G
36	S2	283	G
36	S2	294	U
36	S2	302	A
36	S2	306	C
36	S2	309	G
36	S2	319	C
36	S2	324	C
36	S2	325	C
36	S2	326	C
36	S2	327	G
36	S2	328	U
36	S2	329	G
36	S2	330	G
36	S2	335	G
36	S2	347	G
36	S2	362	C
36	S2	364	A
36	S2	370	G
36	S2	383	G
36	S2	385	G
36	S2	386	C
36	S2	407	G
36	S2	408	A
36	S2	409	C
36	S2	421	G
36	S2	448	A
36	S2	449	A
36	S2	450	C
36	S2	464	A
36	S2	471	G
36	S2	472	C
36	S2	474	G
36	S2	482	G
36	S2	487	U
36	S2	492	C
36	S2	493	A
36	S2	516	A
36	S2	517	C

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Mol	Chain	Res	Type
36	S2	518	G
36	S2	525	A
36	S2	532	C
36	S2	536	A
36	S2	537	C
36	S2	538	U
36	S2	539	C
36	S2	540	U
36	S2	541	U
36	S2	543	C
36	S2	545	A
36	S2	546	G
36	S2	547	G
36	S2	548	C
36	S2	549	C
36	S2	550	C
36	S2	554	A
36	S2	555	A
36	S2	563	G
36	S2	564	A
36	S2	568	C
36	S2	576	A
36	S2	583	A
36	S2	587	A
36	S2	589	G
36	S2	590	A
36	S2	591	U
36	S2	614	C
36	S2	617	G
36	S2	628	A
36	S2	629	A
36	S2	643	A
36	S2	644	G
36	S2	655	A
36	S2	659	G
36	S2	660	C
36	S2	663	C
36	S2	669	A
36	S2	670	A
36	S2	671	A
36	S2	672	A
36	S2	673	G

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Mol	Chain	Res	Type
36	S2	684	G
36	S2	688	U
36	S2	690	G
36	S2	692	G
36	S2	693	A
36	S2	695	C
36	S2	696	G
36	S2	697	G
36	S2	698	G
36	S2	731	G
36	S2	732	U
36	S2	733	C
36	S2	735	C
36	S2	736	C
36	S2	738	C
36	S2	746	C
36	S2	748	C
36	S2	749	U
36	S2	756	C
36	S2	790	C
36	S2	795	A
36	S2	796	G
36	S2	799	U
36	S2	801	U
36	S2	821	G
36	S2	822	U
36	S2	827	A
36	S2	834	C
36	S2	847	A
36	S2	870	A
36	S2	871	U
36	S2	872	A
36	S2	873	G
36	S2	878	G
36	S2	886	A
36	S2	891	G
36	S2	913	A
36	S2	914	U
36	S2	920	A
36	S2	922	A
36	S2	933	G
36	S2	934	G

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Mol	Chain	Res	Type
36	S2	943	U
36	S2	971	G
36	S2	985	G
36	S2	990	A
36	S2	992	A
36	S2	1017	U
36	S2	1023	A
36	S2	1045	U
36	S2	1058	A
36	S2	1061	U
36	S2	1062	A
36	S2	1081	U
36	S2	1082	A
36	S2	1083	A
36	S2	1085	C
36	S2	1109	C
36	S2	1114	U
36	S2	1115	U
36	S2	1117	C
36	S2	1118	C
36	S2	1121	G
36	S2	1133	A
36	S2	1138	C
36	S2	1149	A
36	S2	1150	A
36	S2	1153	C
36	S2	1154	U
36	S2	1171	G
36	S2	1195	A
36	S2	1207	G
36	S2	1208	A
36	S2	1215	C
36	S2	1221	G
36	S2	1242	U
36	S2	1243	U
36	S2	1249	C
36	S2	1251	A
36	S2	1253	A
36	S2	1256	G
36	S2	1257	G
36	S2	1258	A
36	S2	1259	A

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Mol	Chain	Res	Type
36	S2	1264	C
36	S2	1274	G
36	S2	1275	G
36	S2	1285	G
36	S2	1286	G
36	S2	1288	U
36	S2	1295	A
36	S2	1301	A
36	S2	1302	G
36	S2	1303	C
36	S2	1308	U
36	S2	1309	C
36	S2	1322	G
36	S2	1326	U
36	S2	1327	G
36	S2	1342	U
36	S2	1343	U
36	S2	1355	C
36	S2	1356	G
36	S2	1357	A
36	S2	1371	U
36	S2	1372	U
36	S2	1378	A
36	S2	1391	C
36	S2	1397	U
36	S2	1404	U
36	S2	1417	C
36	S2	1418	C
36	S2	1419	C
36	S2	1420	G
36	S2	1421	A
36	S2	1422	G
36	S2	1423	C
36	S2	1424	G
36	S2	1434	C
36	S2	1435	C
36	S2	1436	C
36	S2	1437	C
36	S2	1438	A
36	S2	1454	A
36	S2	1462	U
36	S2	1463	U

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Mol	Chain	Res	Type
36	S2	1464	C
36	S2	1478	U
36	S2	1489	A
36	S2	1490	G
36	S2	1494	U
36	S2	1497	G
36	S2	1498	A
36	S2	1507	G
36	S2	1508	A
36	S2	1509	U
36	S2	1520	G
36	S2	1521	C
36	S2	1522	A
36	S2	1523	C
36	S2	1533	A
36	S2	1575	G
36	S2	1580	A
36	S2	1585	U
36	S2	1588	A
36	S2	1601	A
36	S2	1606	G
36	S2	1621	U
36	S2	1646	C
36	S2	1654	G
36	S2	1657	G
36	S2	1658	G
36	S2	1661	A
36	S2	1662	U
36	S2	1664	A
36	S2	1665	G
36	S2	1671	G
36	S2	1680	G
36	S2	1683	C
36	S2	1699	A
36	S2	1712	A
36	S2	1713	C
36	S2	1714	U
36	S2	1719	A
36	S2	1721	U
36	S2	1722	G
36	S2	1723	G
36	S2	1744	G

*Continued on next page...*

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Mol	Chain	Res	Type
36	S2	1745	A
36	S2	1748	G
36	S2	1752	C
36	S2	1753	C
36	S2	1754	G
36	S2	1768	A
36	S2	1776	G
36	S2	1777	G
36	S2	1778	C
36	S2	1779	G
36	S2	1780	G
36	S2	1781	A
36	S2	1782	G
36	S2	1783	C
36	S2	1784	G
36	S2	1786	U
36	S2	1799	G
36	S2	1812	U
36	S2	1813	A
36	S2	1820	G
36	S2	1821	U
36	S2	1823	A
36	S2	1824	A
36	S2	1825	A
36	S2	1826	G
36	S2	1829	G
36	S2	1835	A
36	S2	1838	U
36	S2	1849	G
36	S2	1851	A
36	S2	1852	C
36	S2	1861	G
36	S2	1862	G
36	S2	1863	A
36	S2	1864	U
36	S2	1865	C
37	zz	46	U
37	zz	48	U
37	zz	49	G
37	zz	59	U
37	zz	62	C
37	zz	82	G

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Mol	Chain	Res	Type
37	zz	83	C
37	zz	85	A
37	zz	94	G
37	zz	102	G
37	zz	106	U
37	zz	111	C
37	zz	116	A
37	zz	121	C
37	zz	123	C
37	zz	124	C
37	zz	125	C
37	zz	133	G
37	zz	134	A
37	zz	135	G
37	zz	137	G
37	zz	138	C
37	zz	141	U
37	zz	150	G
37	zz	154	A
37	zz	156	C
37	zz	157	C
37	zz	161	G
37	zz	162	A
37	zz	163	G
37	zz	164	U
37	zz	165	A
37	zz	166	C
37	zz	167	A
37	zz	169	C
37	zz	171	G
37	zz	172	A
37	zz	175	U
37	zz	184	G
37	zz	185	A
37	zz	186	C
37	zz	187	C
37	zz	188	G
37	zz	189	G
37	zz	191	U
37	zz	192	C
37	zz	195	U
37	zz	196	U

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Mol	Chain	Res	Type
37	zz	197	C
37	zz	198	U
37	zz	202	A
37	zz	204	C
37	zz	207	C
37	zz	208	C
37	zz	209	C
37	zz	210	G
37	zz	213	C
37	zz	216	U
37	zz	217	G
37	zz	223	A
37	zz	224	G
37	zz	225	A
37	zz	228	U
37	zz	229	G
37	zz	232	C
37	zz	233	G
37	zz	234	U
37	zz	237	C
37	zz	244	A
37	zz	245	G
37	zz	246	A
37	zz	253	G
37	zz	258	G
37	zz	260	A
37	zz	265	U
37	zz	266	G
37	zz	270	C
37	zz	275	A
37	zz	277	G
37	zz	280	C
37	zz	281	U
37	zz	282	U
37	zz	284	U
37	zz	288	A
37	zz	289	C
37	zz	290	U
37	zz	295	G
37	zz	296	A
37	zz	297	U
37	zz	301	G

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Mol	Chain	Res	Type
37	zz	304	C
37	zz	306	U
37	zz	307	G
37	zz	308	C
37	zz	312	U
37	zz	315	C
37	zz	318	G
37	zz	325	C
37	zz	329	U
37	zz	330	A
37	zz	331	G
37	zz	332	A
37	zz	333	C
37	zz	334	C
37	zz	337	G
37	zz	338	C
37	zz	339	A
37	zz	345	A
37	zz	349	C
37	zz	352	A
37	zz	353	U
37	zz	354	C
37	zz	355	C
37	zz	356	U

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	S2	282	G
36	S2	517	C
36	S2	531	A
36	S2	871	U
36	S2	1326	U
36	S2	1355	C
36	S2	1434	C

## 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 12 ligands modelled in this entry, 11 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
50	GTP	5B	1302	49	26,34,34	3.55	13 (50%)	32,54,54	1.67	8 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	GTP	5B	1302	49	-	3/18/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	5B	1302	GTP	C3'-C4'	-8.52	1.31	1.53
50	5B	1302	GTP	O4'-C4'	7.65	1.62	1.45
50	5B	1302	GTP	O4'-C1'	-7.21	1.31	1.41
50	5B	1302	GTP	C2-N3	5.51	1.46	1.33
50	5B	1302	GTP	C4-N3	5.07	1.49	1.37
50	5B	1302	GTP	C2-N2	4.71	1.45	1.34
50	5B	1302	GTP	C6-N1	3.60	1.43	1.37
50	5B	1302	GTP	O3'-C3'	3.01	1.50	1.43
50	5B	1302	GTP	C5-C6	3.01	1.53	1.47
50	5B	1302	GTP	O2'-C2'	-2.86	1.36	1.43
50	5B	1302	GTP	C2-N1	2.67	1.44	1.37
50	5B	1302	GTP	C5-C4	-2.51	1.36	1.43
50	5B	1302	GTP	O6-C6	-2.34	1.18	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	5B	1302	GTP	PB-O3B-PG	-3.64	120.32	132.83
50	5B	1302	GTP	C3'-C2'-C1'	3.54	106.30	100.98
50	5B	1302	GTP	C5-C6-N1	3.50	120.12	113.95
50	5B	1302	GTP	C2-N1-C6	-2.85	119.84	125.10
50	5B	1302	GTP	C8-N7-C5	2.72	108.17	102.99
50	5B	1302	GTP	PA-O3A-PB	-2.68	123.62	132.83
50	5B	1302	GTP	C2'-C3'-C4'	2.49	107.48	102.64
50	5B	1302	GTP	O6-C6-C5	-2.16	120.16	124.37

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	5B	1302	GTP	PG-O3B-PB-O2B
50	5B	1302	GTP	O4'-C4'-C5'-O5'
50	5B	1302	GTP	PG-O3B-PB-O1B

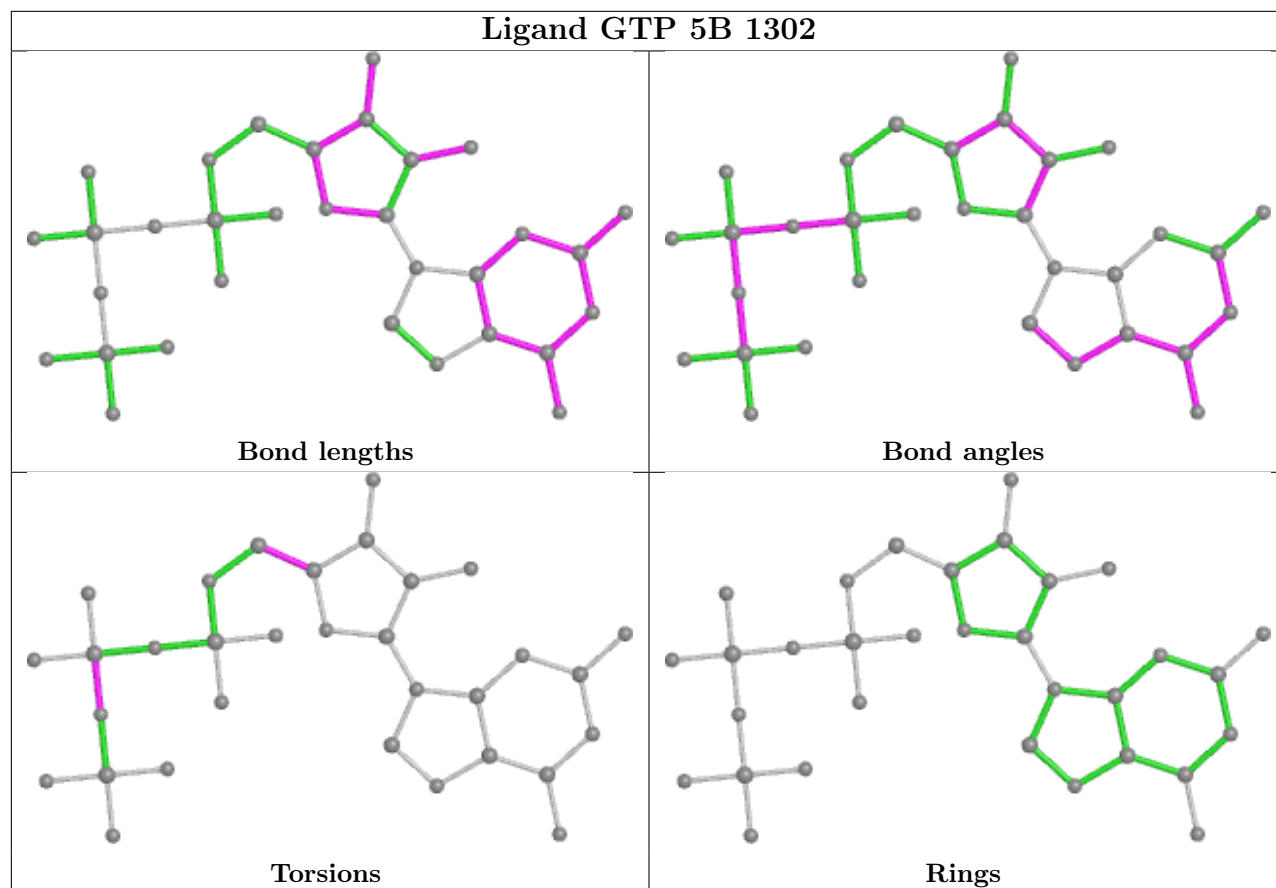
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	5B	1302	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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.

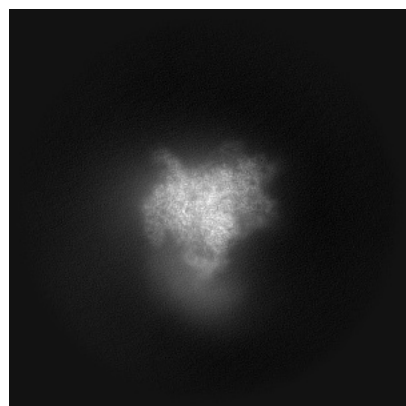
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62535. These allow visual inspection of the internal detail of the map and identification of artifacts.

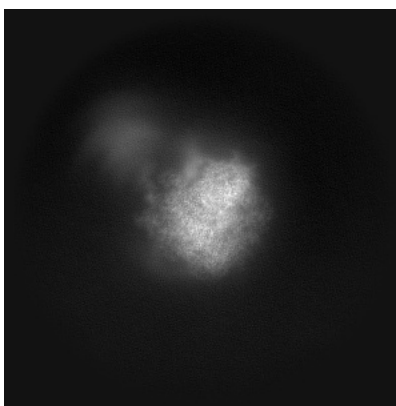
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

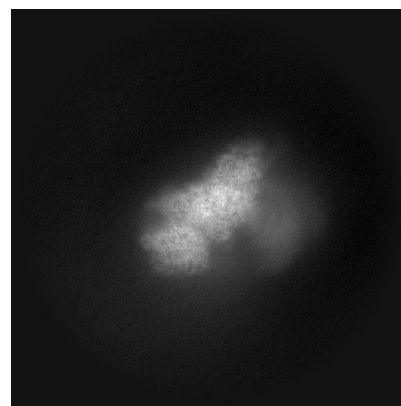
#### 6.1.1 Primary map



X

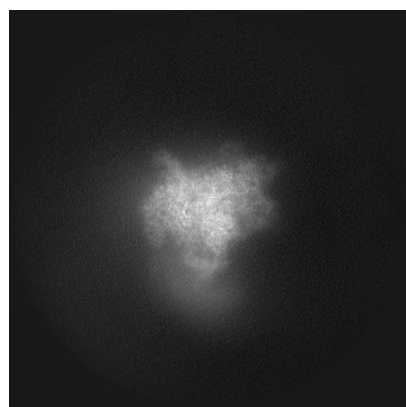


Y

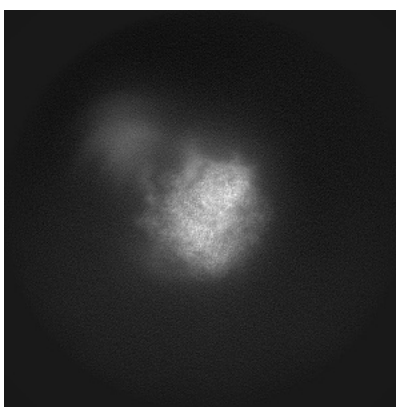


Z

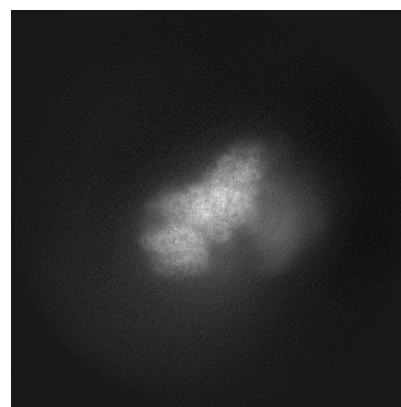
#### 6.1.2 Raw map



X



Y

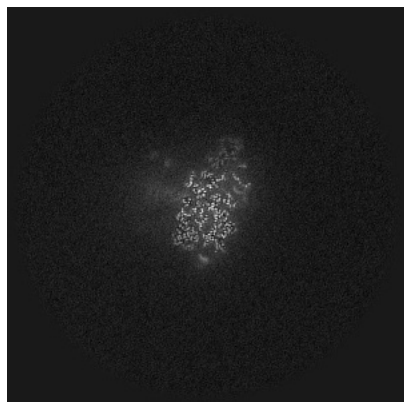


Z

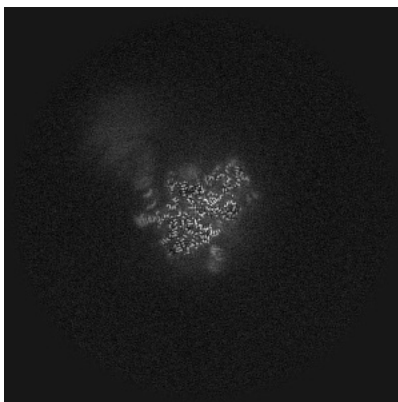
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

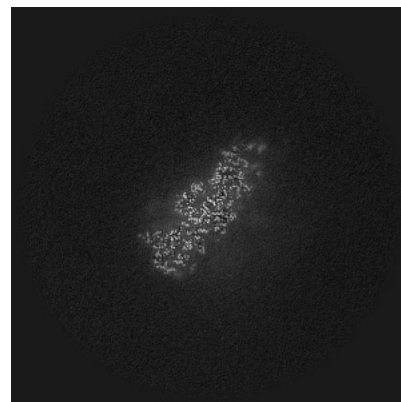
### 6.2.1 Primary map



X Index: 250

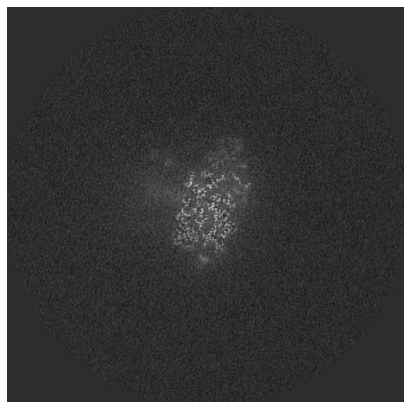


Y Index: 250

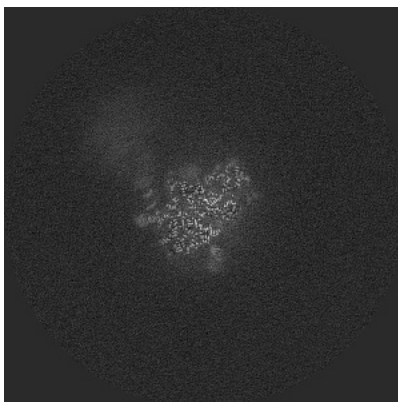


Z Index: 250

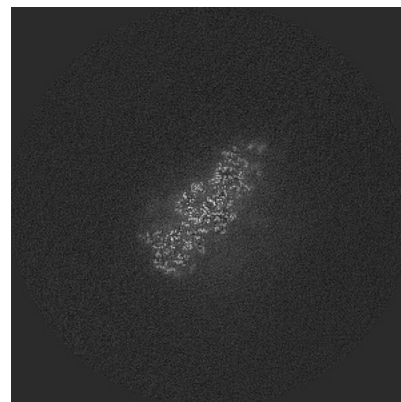
### 6.2.2 Raw map



X Index: 250



Y Index: 250

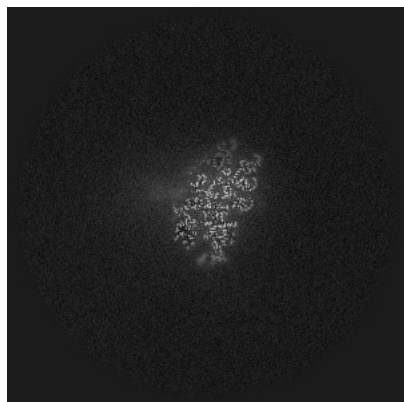


Z Index: 250

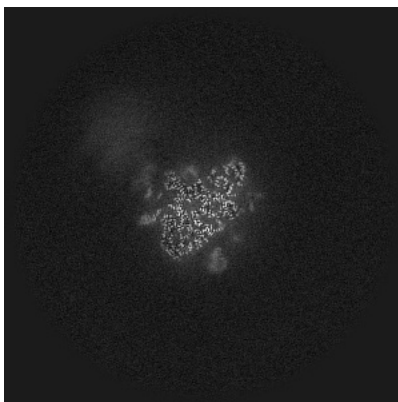
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

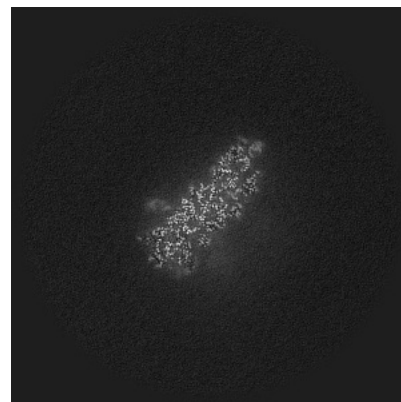
### 6.3.1 Primary map



X Index: 259

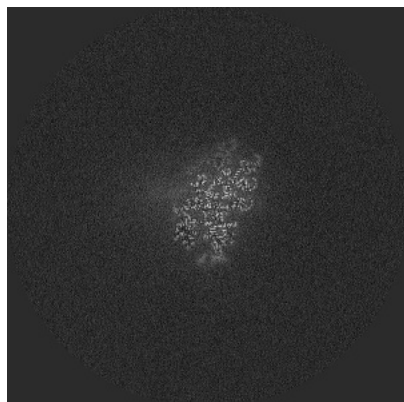


Y Index: 254

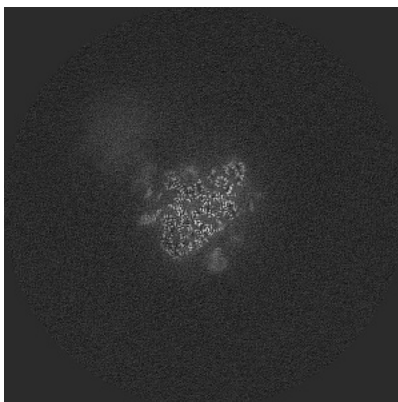


Z Index: 258

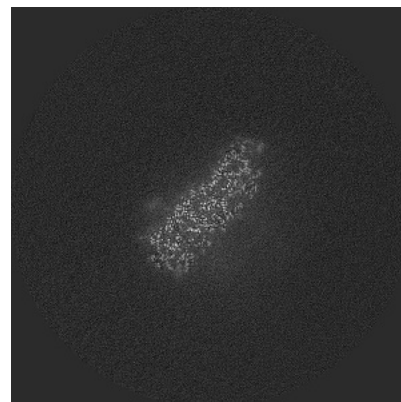
### 6.3.2 Raw map



X Index: 259



Y Index: 254

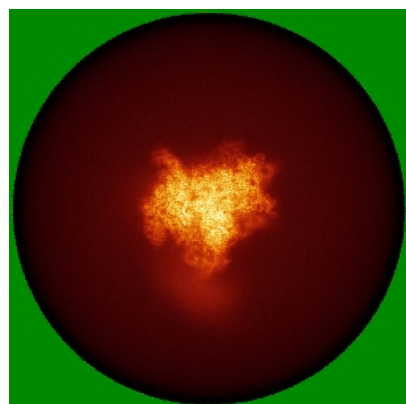


Z Index: 256

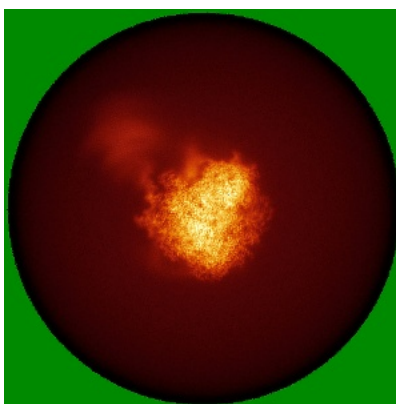
The images above show the largest variance slices of the map in three orthogonal directions.

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

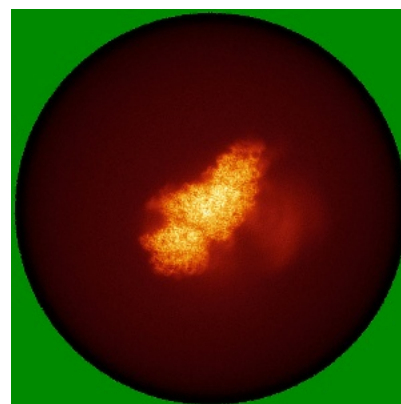
### 6.4.1 Primary map



X

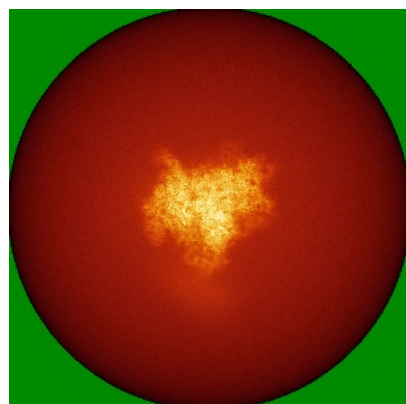


Y

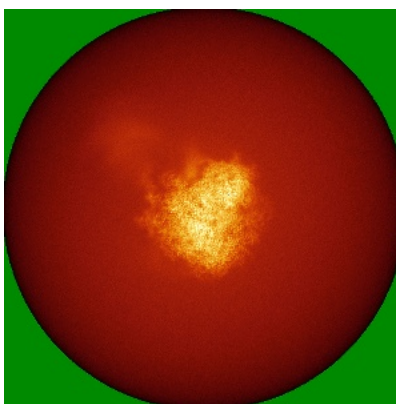


Z

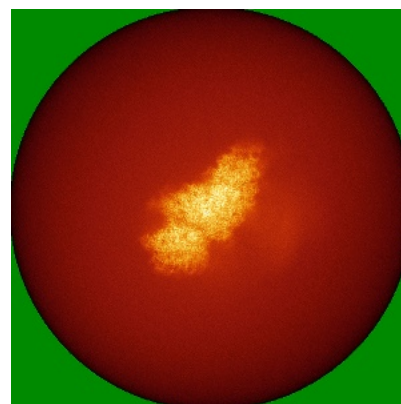
### 6.4.2 Raw map



X



Y



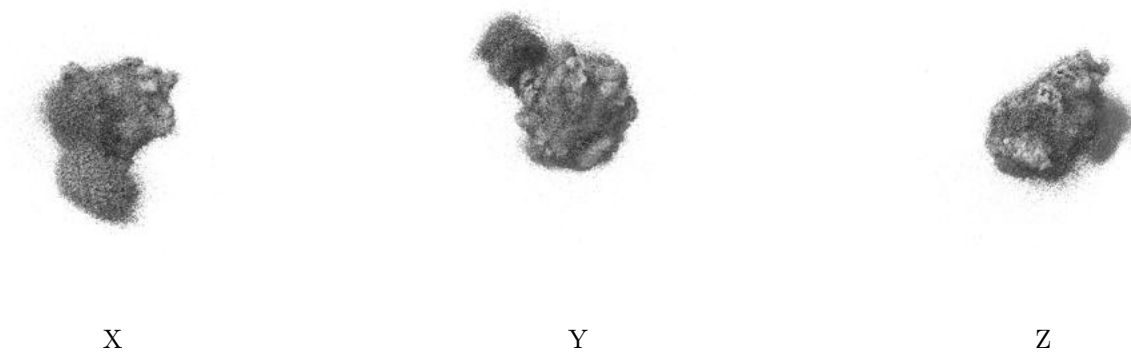
Z

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.



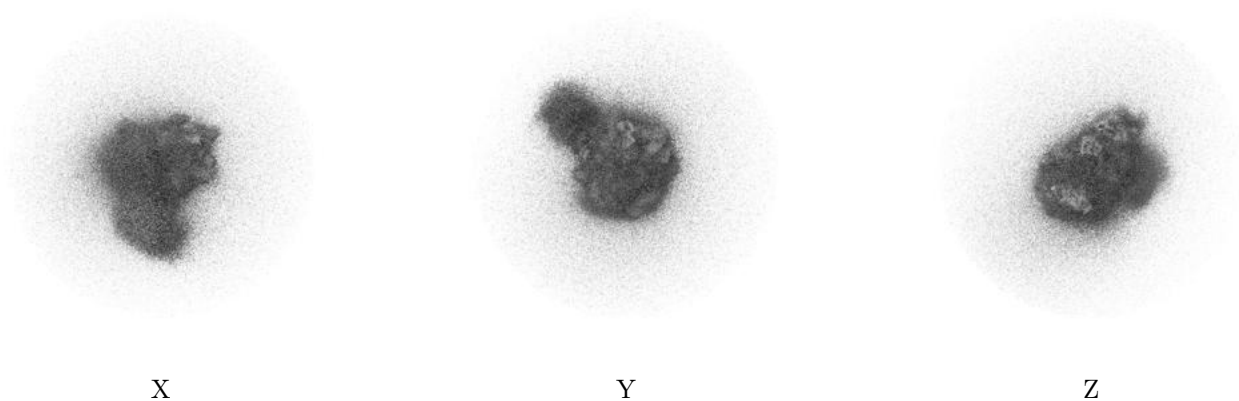
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

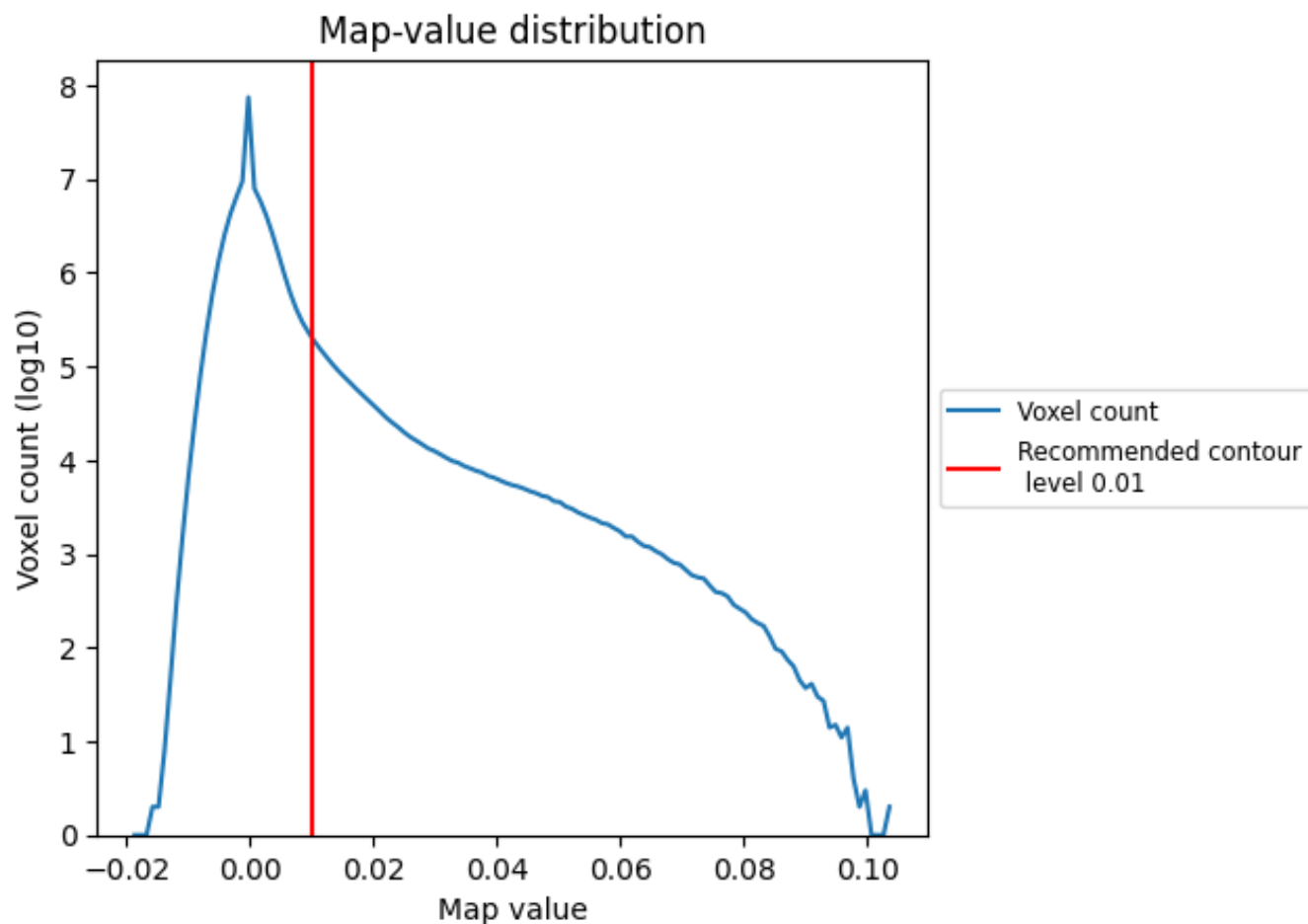
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

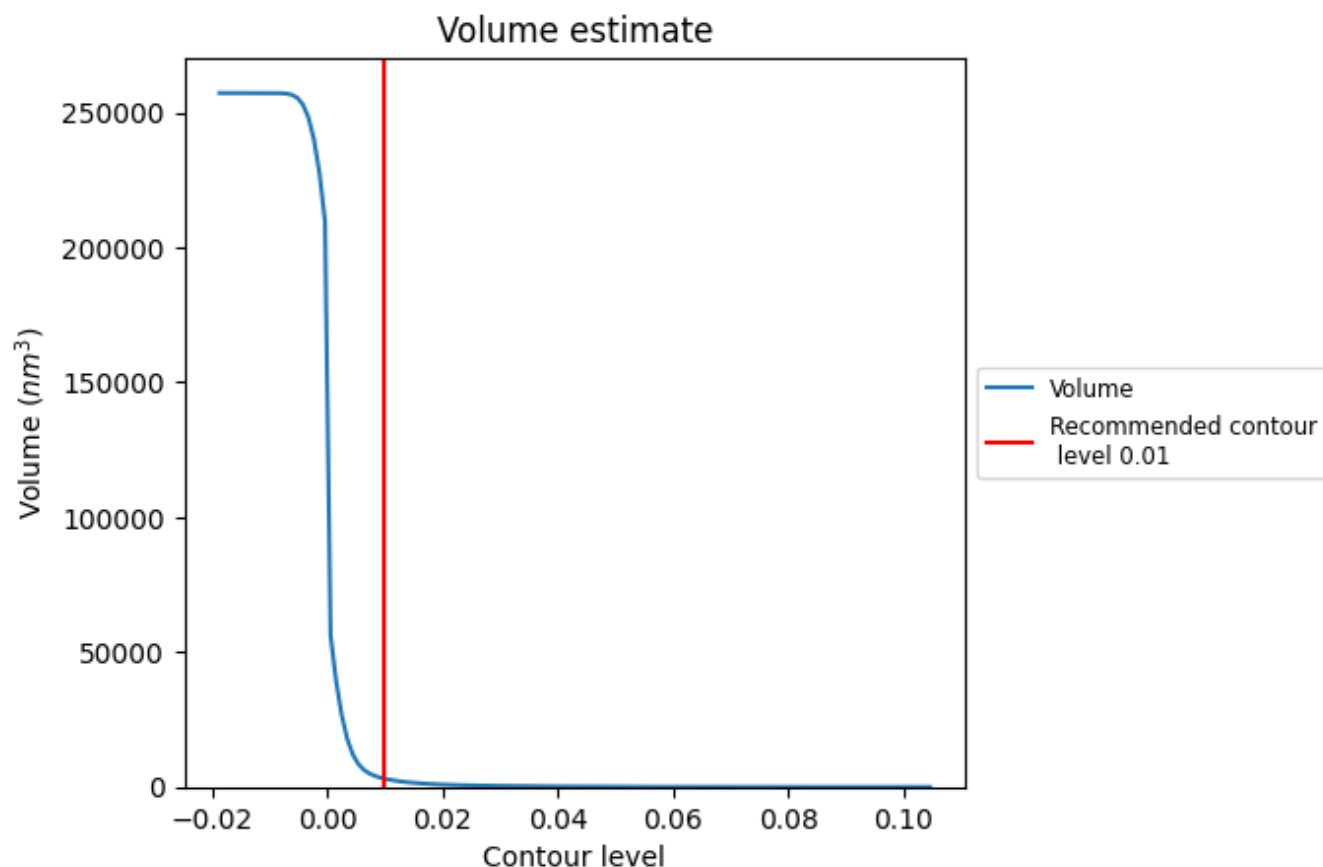
This section contains the results of statistical analysis of the map.

### 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](#)

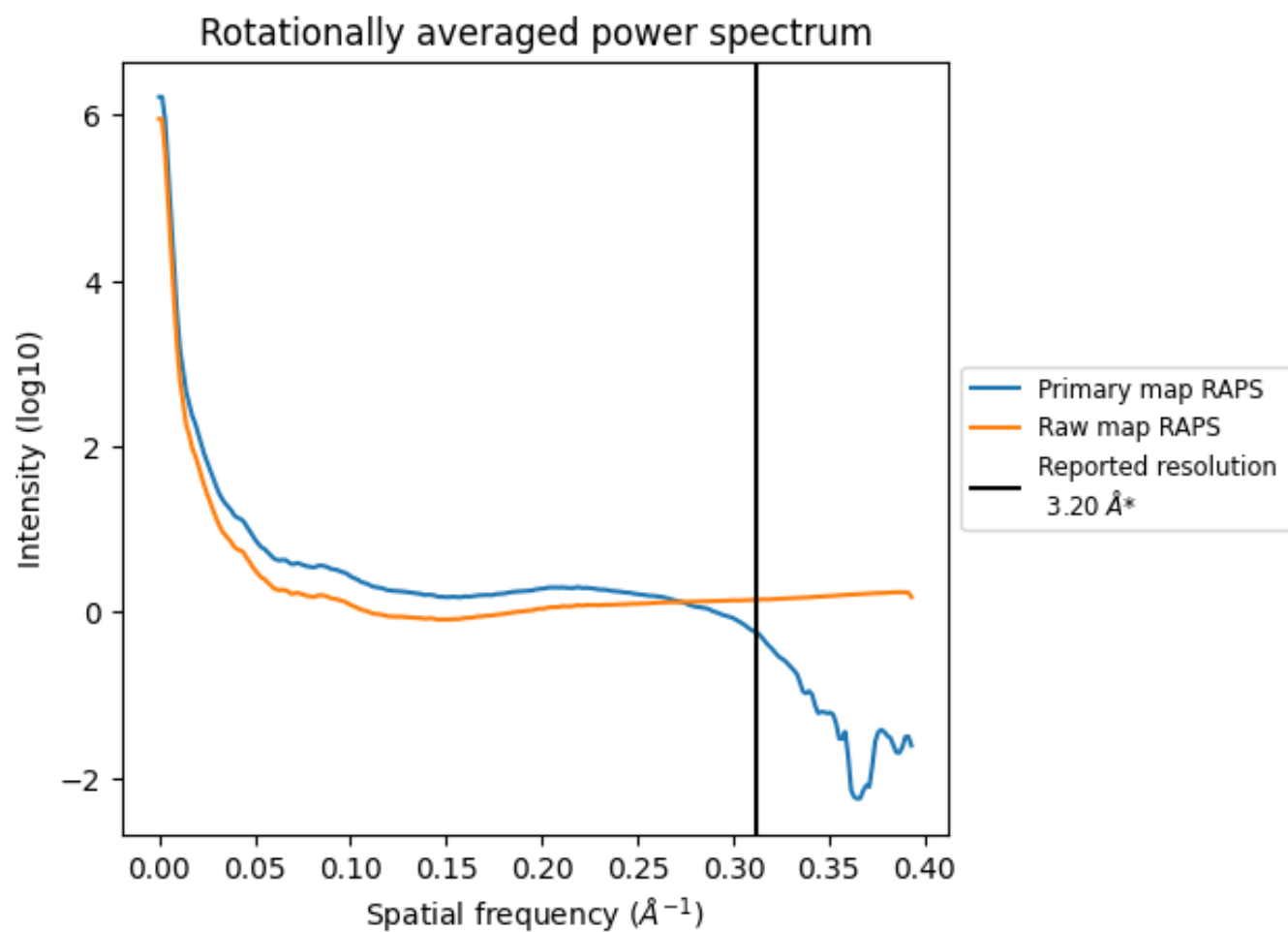


The volume at the recommended contour level is 3045 nm<sup>3</sup>; this corresponds to an approximate mass of 2751 kDa.

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 ⓘ

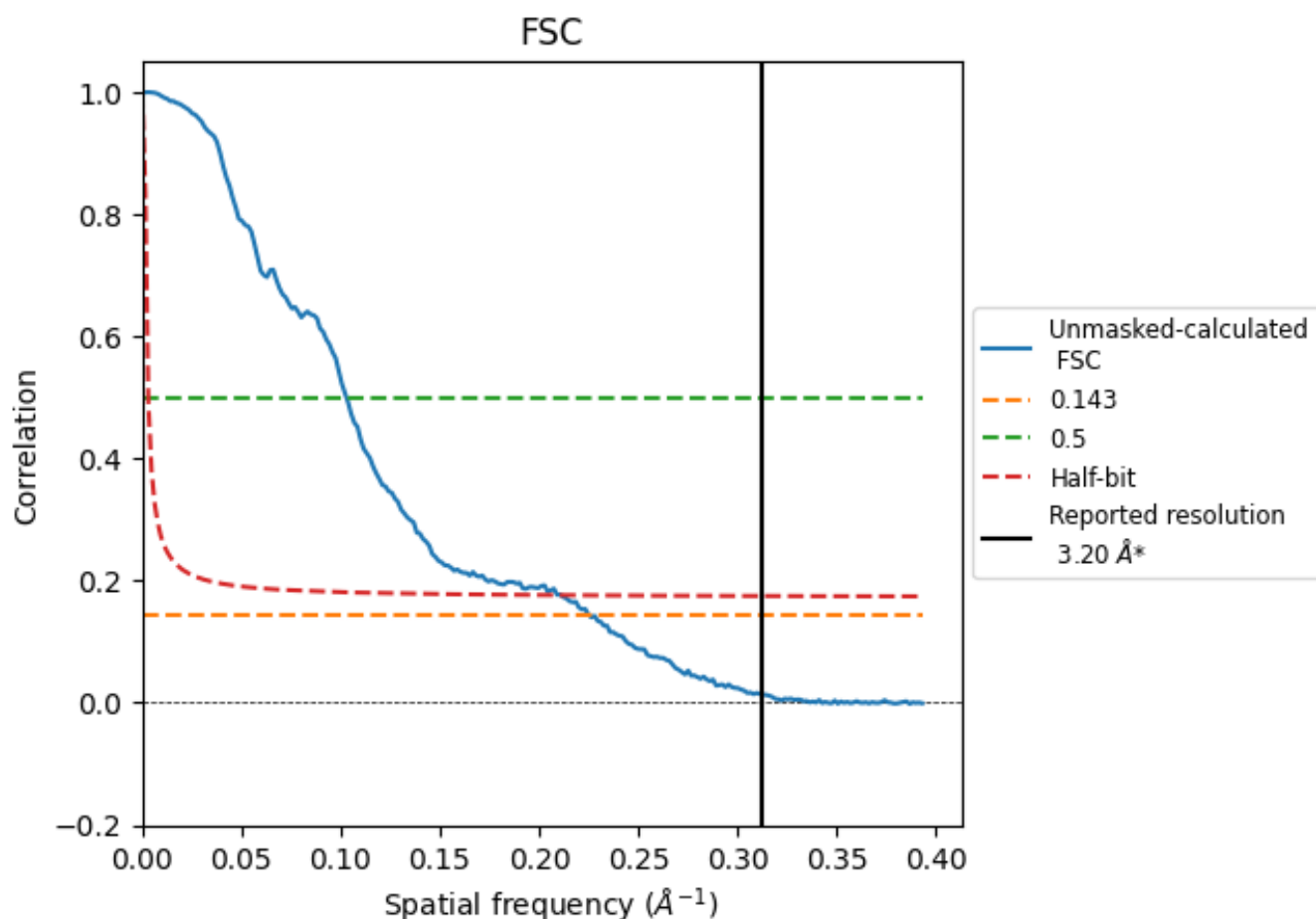


\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.312 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

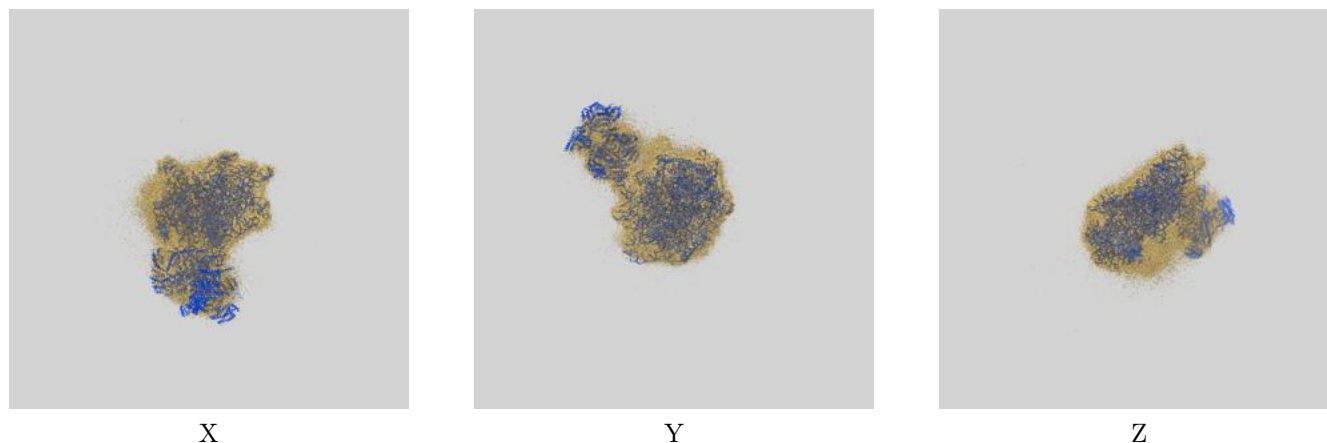
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.44	9.72	4.74

\*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 4.44 differs from the reported value 3.2 by more than 10 %

## 9 Map-model fit [i](#)

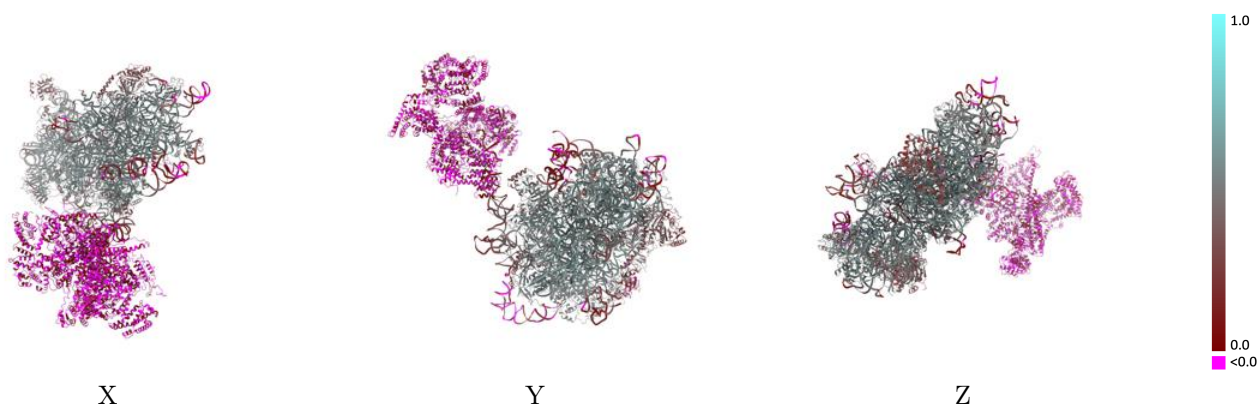
This section contains information regarding the fit between EMDB map EMD-62535 and PDB model 9KRP. Per-residue inclusion information can be found in section [3](#) on page [13](#).

### 9.1 Map-model overlay [i](#)



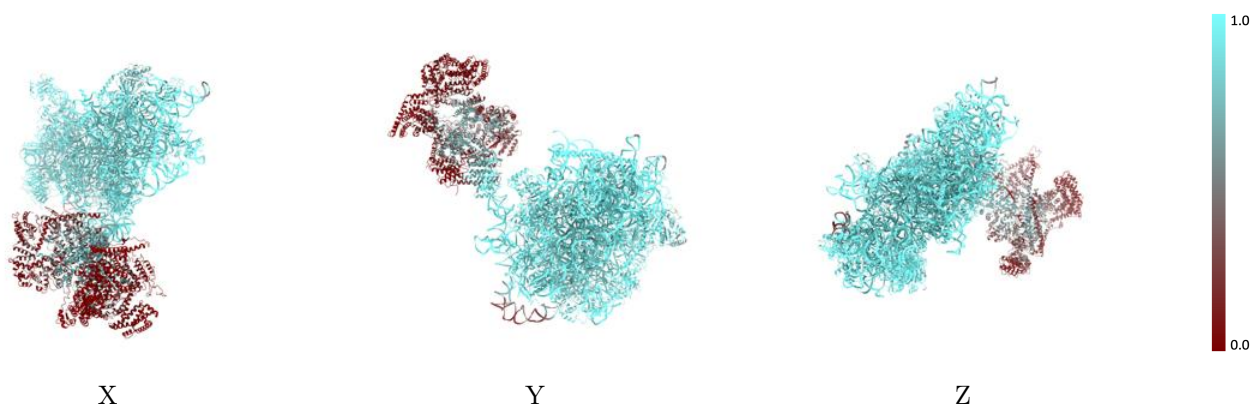
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



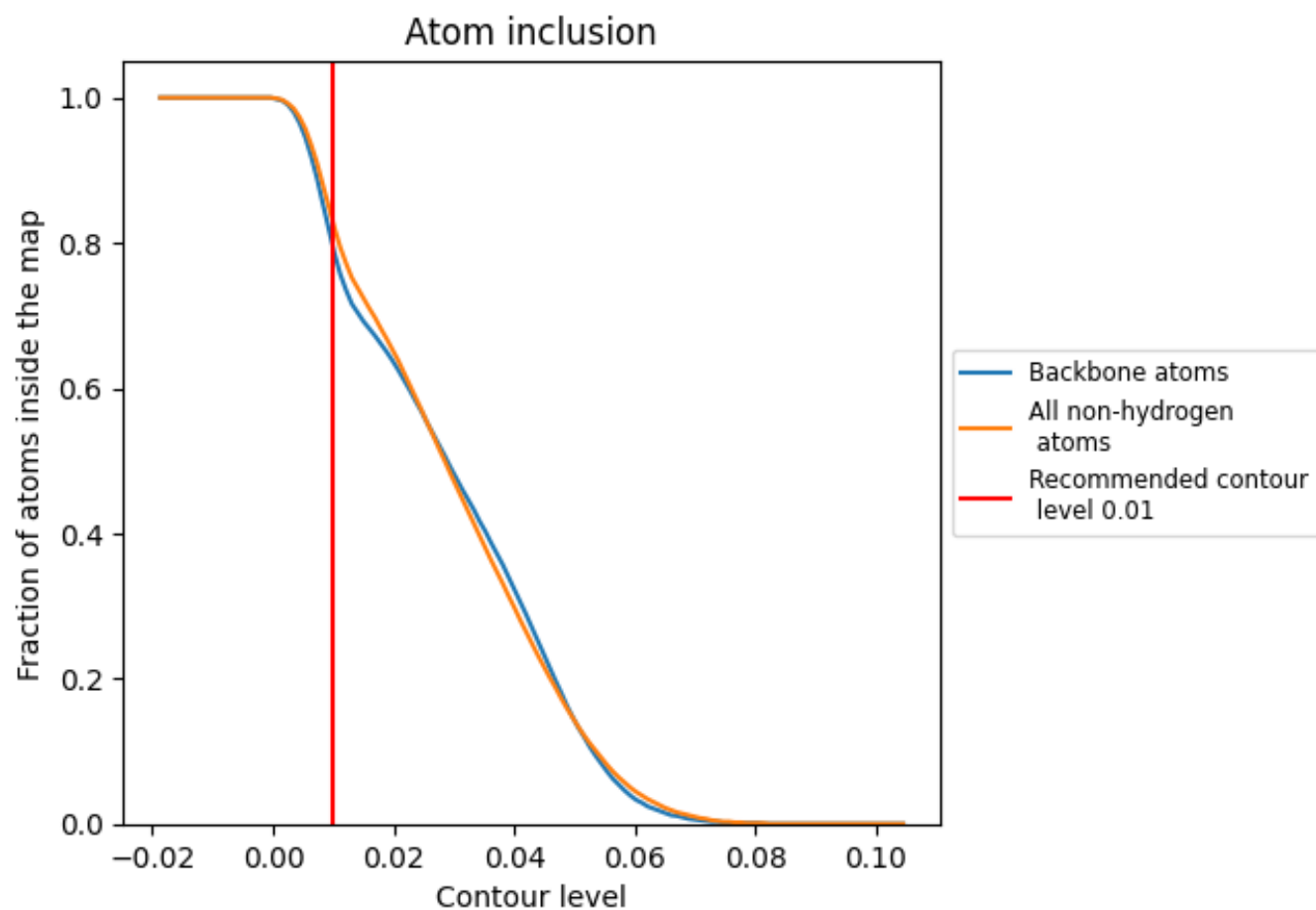
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 79% of all backbone atoms, 83% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8270	 0.3580
3a	 0.5240	 0.0190
3c	 0.4240	 0.0120
3d	 0.0470	 0.0250
3e	 0.1810	 0.0060
3f	 0.3850	 0.0040
3h	 0.4830	 0.0210
3k	 0.0320	 0.0090
3l	 0.0870	 0.0110
3m	 0.1150	 0.0200
5B	 0.9210	 0.3030
Ln	 1.0000	 0.5180
S2	 0.9960	 0.4870
SA	 0.9990	 0.5280
SB	 0.9900	 0.4820
SC	 1.0000	 0.5350
SD	 0.9980	 0.4970
SE	 1.0000	 0.5350
SF	 0.9980	 0.5060
SG	 0.9910	 0.4440
SH	 0.9970	 0.4600
SI	 0.9880	 0.4940
SJ	 1.0000	 0.5210
SK	 0.9980	 0.4680
SL	 0.9970	 0.5170
SN	 0.9990	 0.5230
SO	 0.9970	 0.5240
SP	 0.9940	 0.4890
SQ	 0.9960	 0.5030
SR	 0.9980	 0.4940
SS	 0.9870	 0.5040
ST	 0.9950	 0.5100
SU	 0.9960	 0.4850
SV	 1.0000	 0.5170
SW	 1.0000	 0.5230



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Chain	Atom inclusion	Q-score
SX	 0.9990	 0.5230
SY	 0.9970	 0.4910
SZ	 0.9930	 0.4690
Sa	 1.0000	 0.5290
Sb	 1.0000	 0.5110
Sc	 1.0000	 0.4890
Sd	 1.0000	 0.5460
Se	 1.0000	 0.4780
Sf	 0.9570	 0.3170
Sg	 0.9910	 0.4520
sh	 0.9630	 0.3680
zy	 0.9890	 0.3030
zz	 0.7870	 0.1850