Full wwPDB EM Validation Report ⓘ

Apr 22, 2024 – 03:16 PM JST

PDB ID	:	8XXN
EMDB ID	:	EMD-38754
Title	:	Cryo-EM structure of the human 43S ribosome with PDCD4
Authors	:	Ye, X.; Huang, Z.; Li, Y.; Wang, M.; Cheng, J.
Deposited on	:	2024-01-18
Resolution	:	3.60 Å(reported)
Based on initial model	:	7A09

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

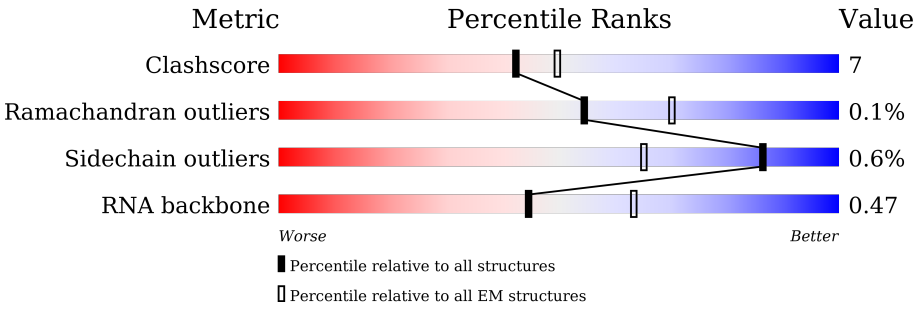
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	Ln	25	96%
2	S2	1869	53% 31% 8% 8%
3	SA	295	58% 17% 25%
4	SB	264	67% 14% 19%
5	SD	243	80% 14% 7%
6	SE	263	85% 14%
7	SF	204	71% 22% 7%

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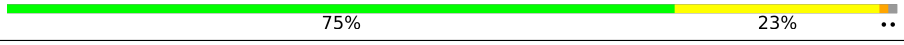
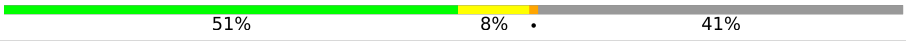
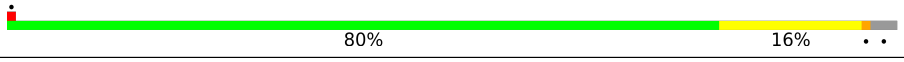
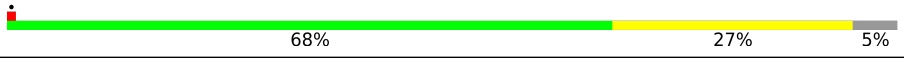
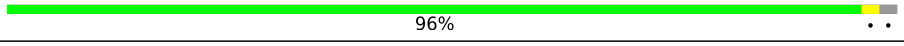
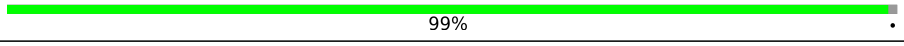
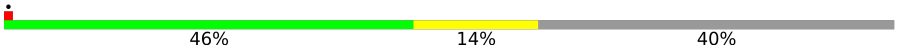
Mol	Chain	Length	Quality of chain
8	SH	194	
9	SI	208	
10	SK	165	
11	SL	158	
12	SP	145	
13	SQ	146	
14	SR	135	
15	SS	152	
16	ST	145	
17	SU	119	
18	SV	83	
19	SX	143	
20	Sa	115	
21	Sc	69	
22	Sd	56	
23	Sg	317	
24	SC	293	
25	SG	249	
26	SJ	194	
27	SM	132	
28	SN	151	
29	SO	151	
30	SW	130	
31	SY	133	
32	SZ	125	

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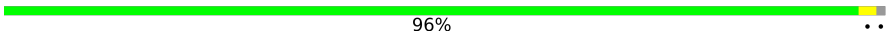
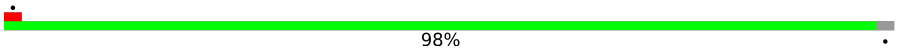
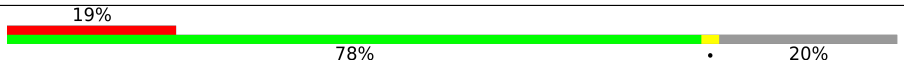
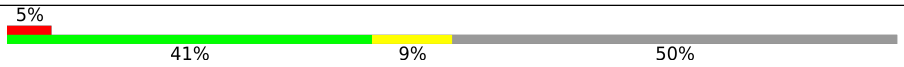
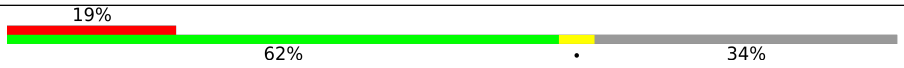
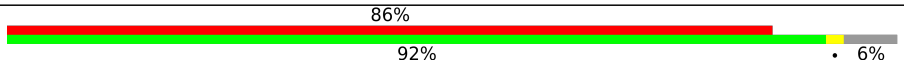
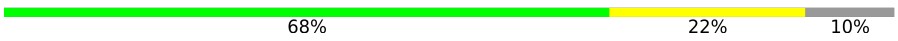
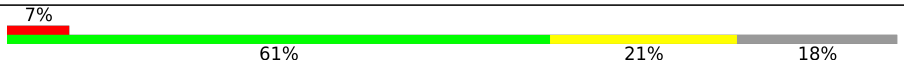
Mol	Chain	Length	Quality of chain
33	Sb	84	
34	Se	59	
35	Sf	156	
36	C1	113	
37	4A	406	
38	CD	469	
39	3A	1382	
40	3B	814	
41	3C	913	
42	3E	445	
43	3F	357	
44	3G	320	
45	3H	352	
46	3I	325	
47	3K	218	
48	3L	564	
49	3M	374	
50	3N	548	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 114565 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 60S ribosomal protein L41.

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

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S2	1723	Total	C	N	O	P	0	0
			36535	16298	6533	11982	1722		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SA	221	Total	C	N	O	S	0	0
			1741	1106	305	322	8		

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 6 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 10 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 11 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SL	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 12 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SP	121	Total	C	N	O	S	0	0
			985	623	185	170	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SQ	144	Total	C	N	O	S	0	0
			1142	726	216	197	3		

- Molecule 14 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SR	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 15 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 16 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 17 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SU	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 18 is a protein called 40S ribosomal protein S21.

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

- Molecule 19 is a protein called 40S ribosomal protein S23.

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

- Molecule 20 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 22 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Sd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 23 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 24 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 25 is a protein called 40S ribosomal protein S6.

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

- Molecule 26 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 27 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SM	122	Total	C	N	O	S	0	0
			940	590	164	177	9		

- Molecule 28 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 29 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SO	140	Total	C	N	O	S	0	0
			1049	642	204	197	6		

- Molecule 30 is a protein called 40S ribosomal protein S15a.

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

- Molecule 31 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SY	131	Total	C	N	O	S	0	0
			1065	673	209	178	5		

- Molecule 32 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 33 is a protein called 40S ribosomal protein S27.

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

- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	C1	90	Total	C	N	O	0	0
			443	262	90	91		

- Molecule 37 is a protein called Eukaryotic initiation factor 4A-I.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	4A	342	Total	C	N	O	0	0
			1691	1007	342	342		

- Molecule 38 is a protein called Programmed cell death protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	CD	347	Total	C	N	O	0	0
			1841	1100	368	373		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	3A	692	Total	C	N	O	S	0	0
			5379	3374	980	1003	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	3B	536	Total	C	N	O	S	0	0
			2966	1801	580	580	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3C	625	Total	C	N	O	S	0	0
			5070	3204	898	933	35		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	3E	416	Total	C	N	O	S	0	0
			3437	2202	585	630	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	3F	269	Total	C	N	O	S	0	0
			2090	1317	356	405	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
44	3G	84	Total	C	N	O	0	0
			667	418	120	129		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3H	295	Total	C	N	O	S	0	0
			2413	1532	417	449	15		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
46	3I	305	Total	C	N	O	0	0
			1497	887	305	305		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3K	217	Total	C	N	O	S	0	0
			1750	1116	288	334	12		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	3L	372	Total	C	N	O	S	0	0
			3111	2011	520	563	17		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3M	338	Total	C	N	O	S	0	0
			2705	1727	457	504	17		

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3N	447	Total	C	N	O	S	0	0
			3617	2279	625	691	22		

- Molecule 51 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
51	S2	22	Total	Mg	0
			22	22	
51	SG	1	Total	Mg	0
			1	1	

- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

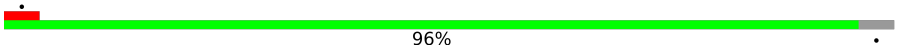
Mol	Chain	Residues	Atoms		AltConf
52	Sa	1	Total	Zn	0
			1	1	
52	Sd	1	Total	Zn	0
			1	1	
52	Sf	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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

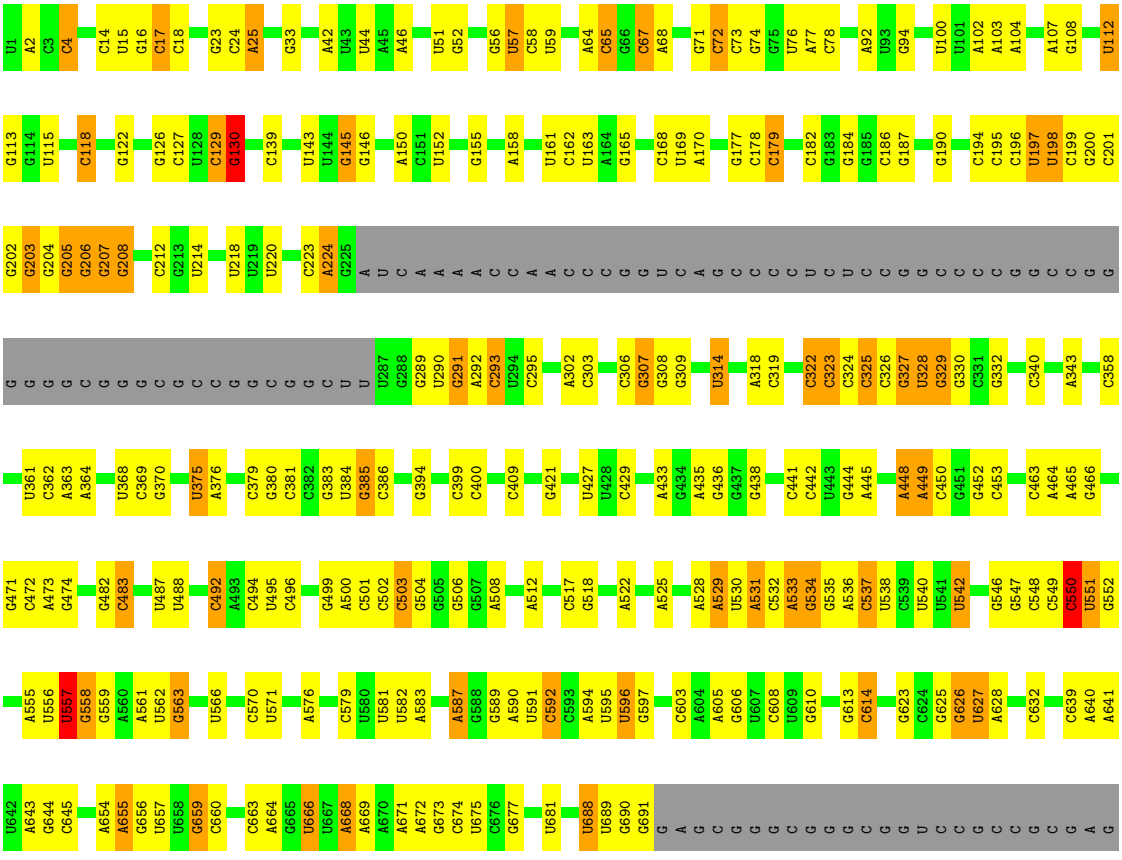
- Molecule 1: 60S ribosomal protein L41

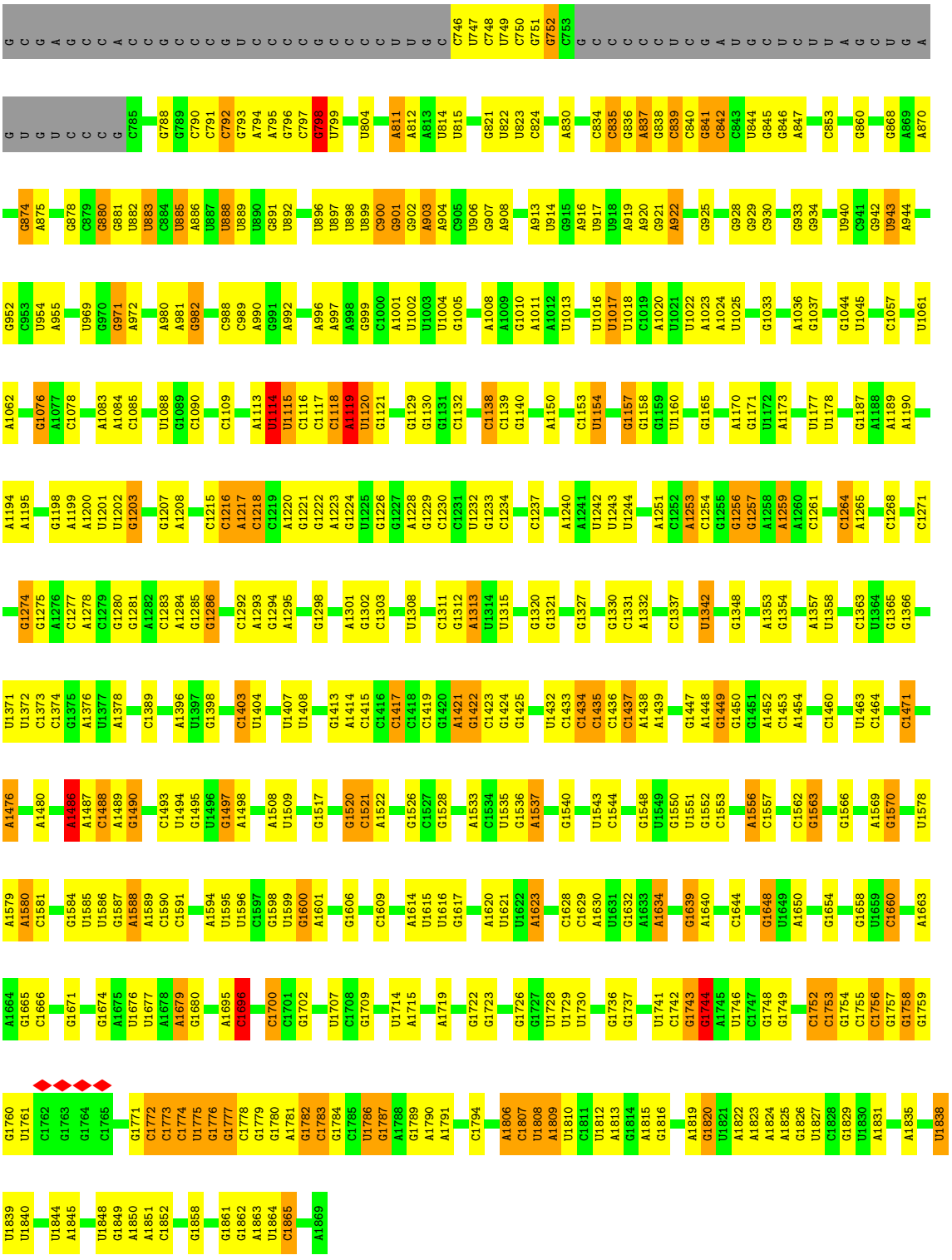
Chain Ln:



- Molecule 2: 18S rRNA

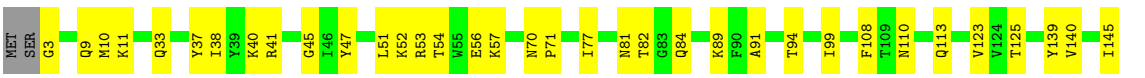
Chain S2:

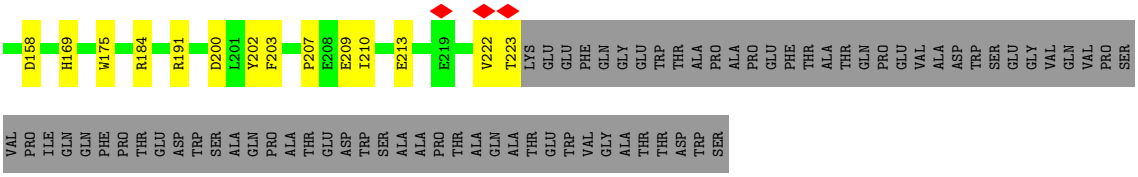




• Molecule 3: 40S ribosomal protein SA

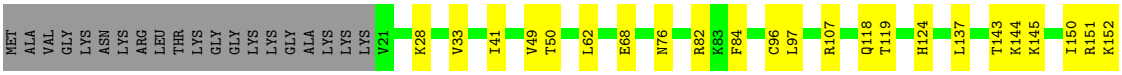
Chain SA:





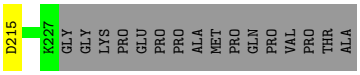
• Molecule 4: 40S ribosomal protein S3a

Chain SB:



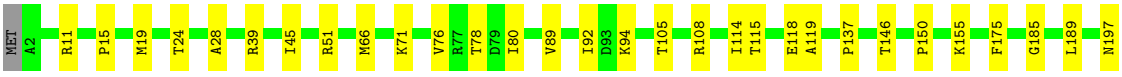
• Molecule 5: 40S ribosomal protein S3

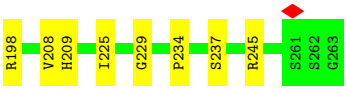
Chain SD:



• Molecule 6: 40S ribosomal protein S4, X isoform

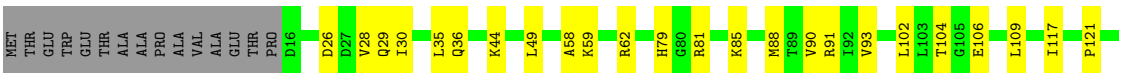
Chain SE:

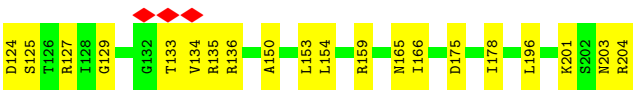




• Molecule 7: 40S ribosomal protein S5

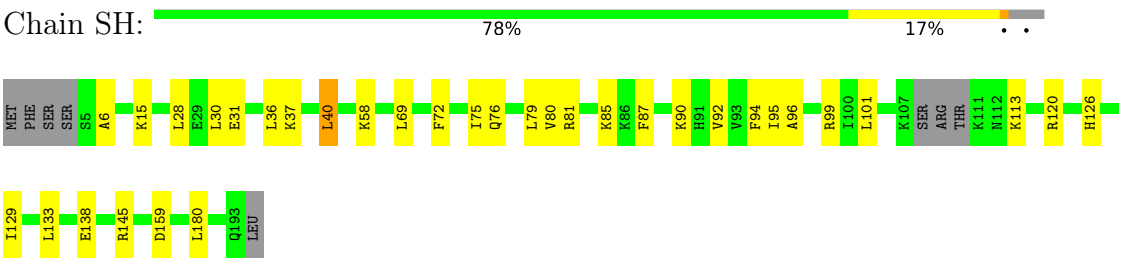
Chain SF:





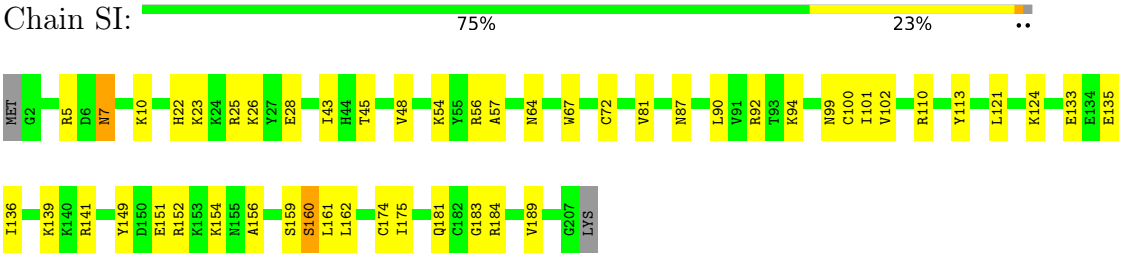
• Molecule 8: 40S ribosomal protein S7

Chain SH:



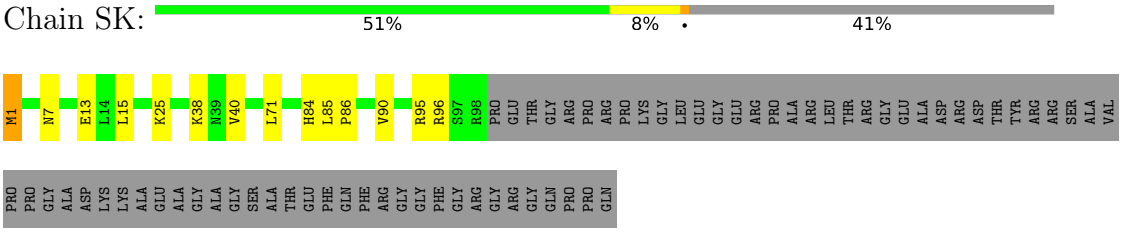
• Molecule 9: 40S ribosomal protein S8

Chain SI:



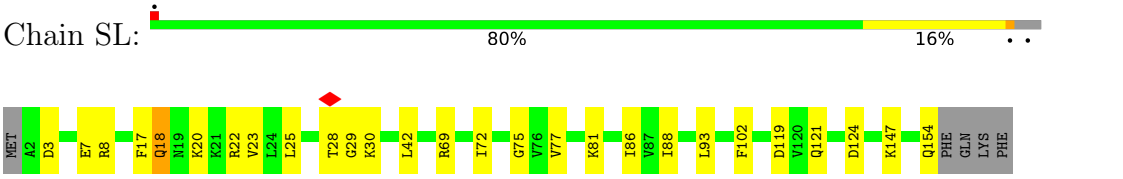
• Molecule 10: 40S ribosomal protein S10

Chain SK:



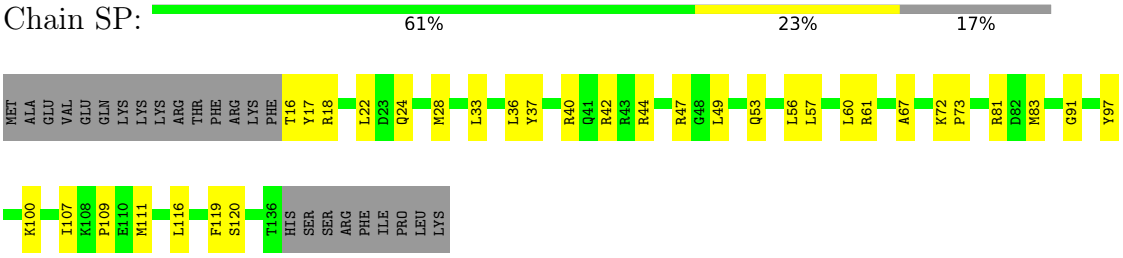
• Molecule 11: 40S ribosomal protein S11

Chain SL:



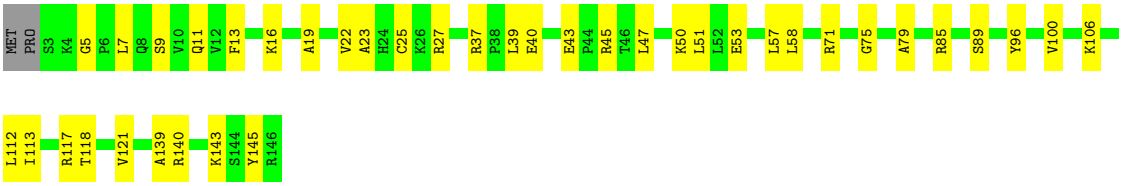
• Molecule 12: 40S ribosomal protein S15

Chain SP:

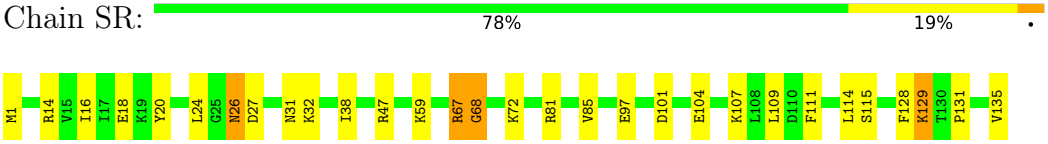


• Molecule 13: 40S ribosomal protein S16

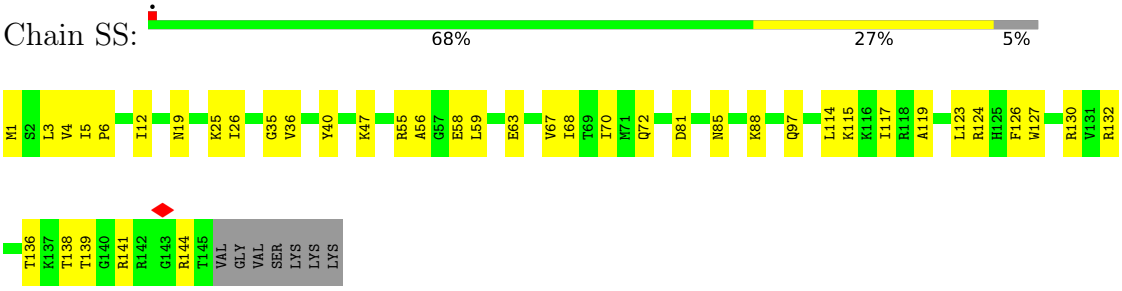
Chain SQ:



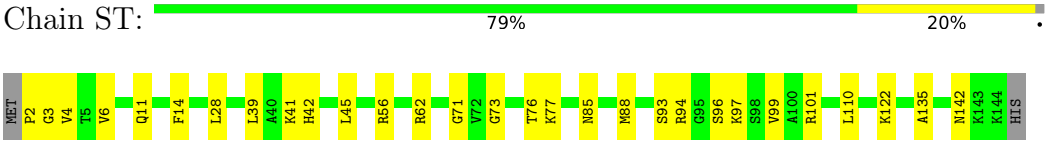
• Molecule 14: 40S ribosomal protein S17



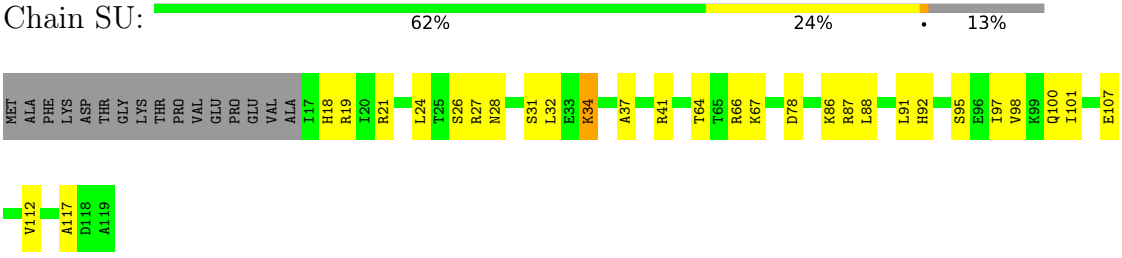
• Molecule 15: 40S ribosomal protein S18



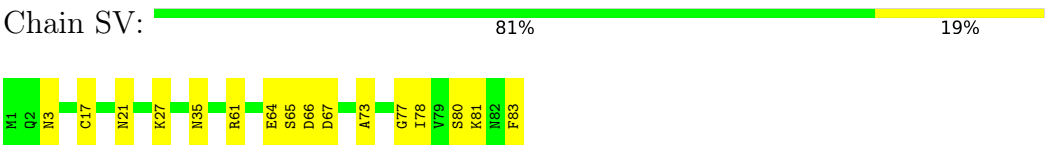
• Molecule 16: 40S ribosomal protein S19



• Molecule 17: 40S ribosomal protein S20

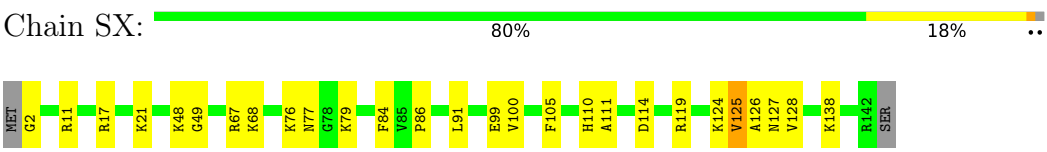


• Molecule 18: 40S ribosomal protein S21



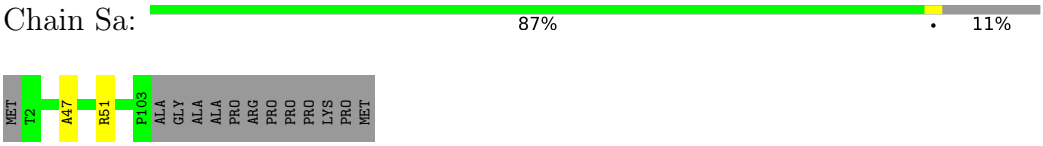
• Molecule 19: 40S ribosomal protein S23

Chain SX:



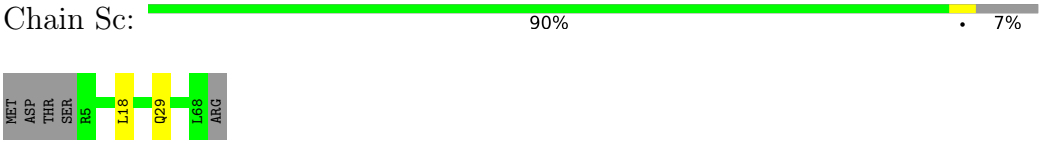
• Molecule 20: 40S ribosomal protein S26

Chain Sa:



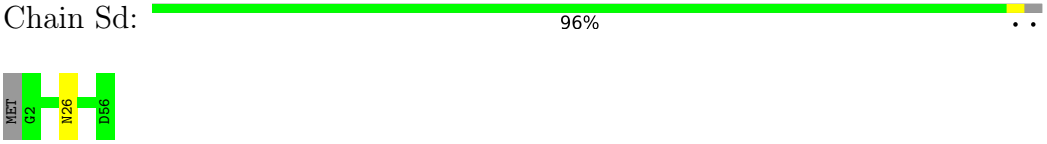
• Molecule 21: 40S ribosomal protein S28

Chain Sc:



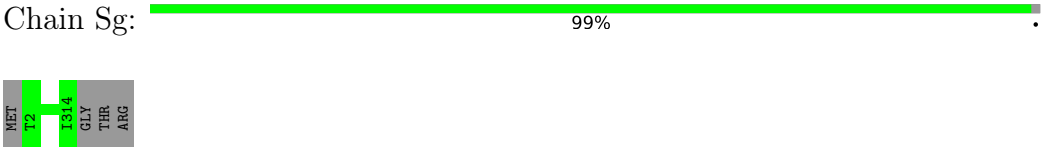
• Molecule 22: 40S ribosomal protein S29

Chain Sd:



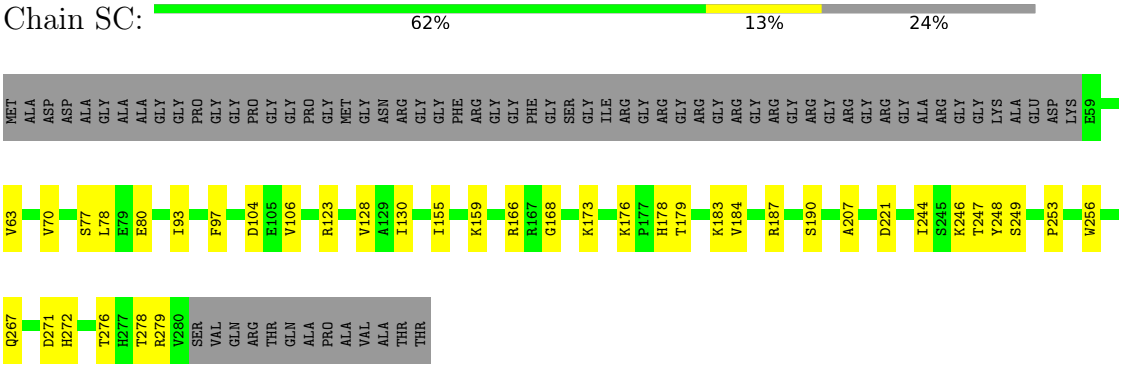
• Molecule 23: Receptor of activated protein C kinase 1

Chain Sg:



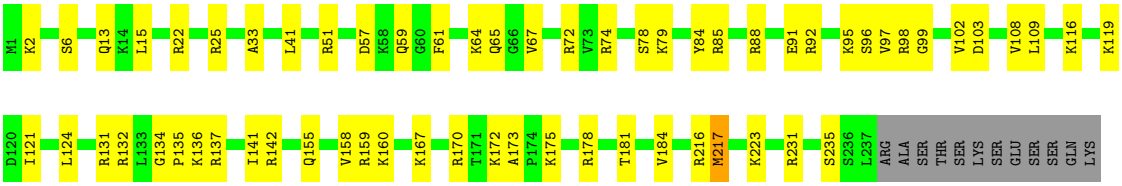
• Molecule 24: 40S ribosomal protein S2

Chain SC:

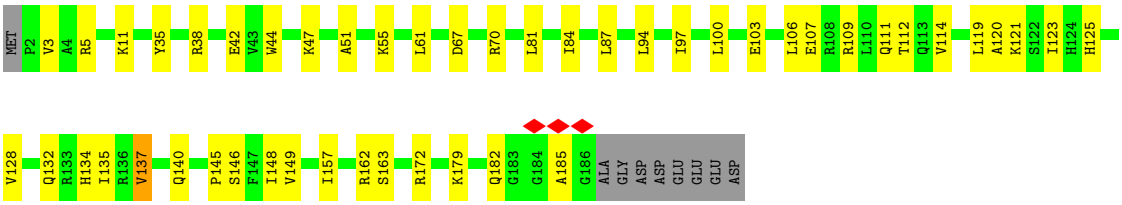


• Molecule 25: 40S ribosomal protein S6

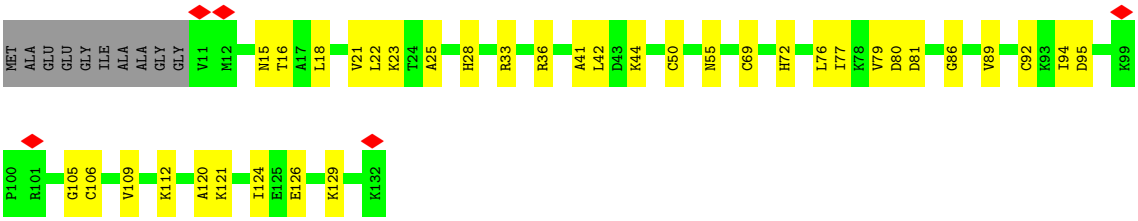
Chain SG:



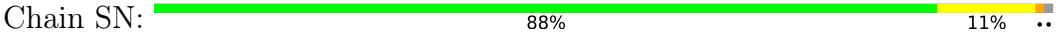
• Molecule 26: 40S ribosomal protein S9

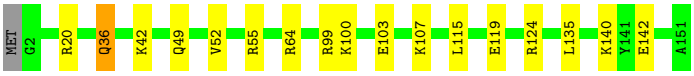


• Molecule 27: 40S ribosomal protein S12

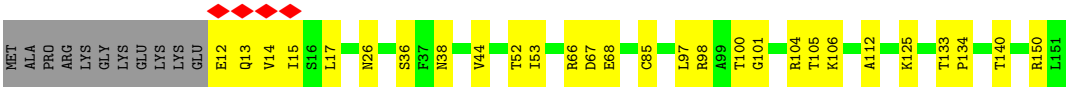


• Molecule 28: 40S ribosomal protein S13

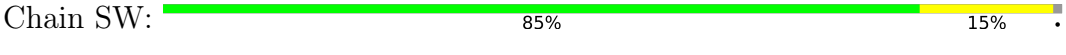


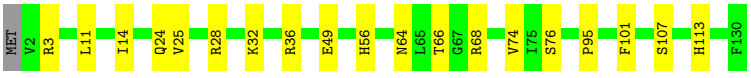


• Molecule 29: 40S ribosomal protein S14



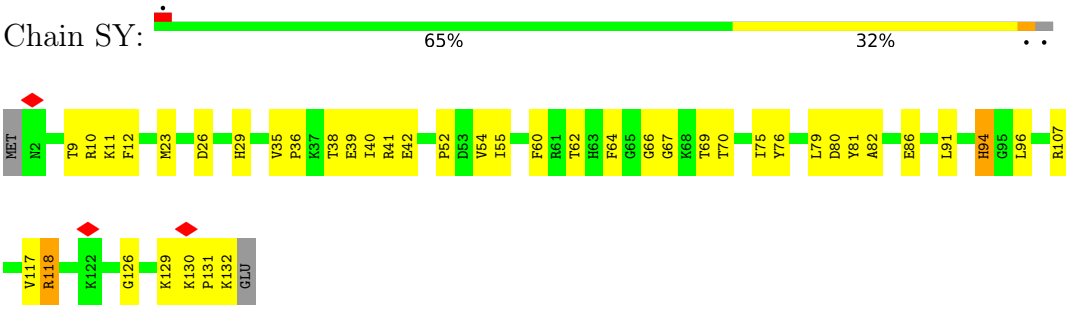
• Molecule 30: 40S ribosomal protein S15a





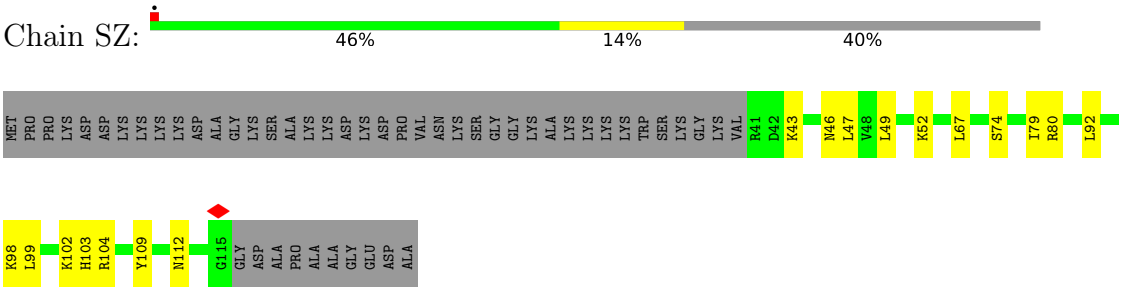
• Molecule 31: 40S ribosomal protein S24

Chain SY:



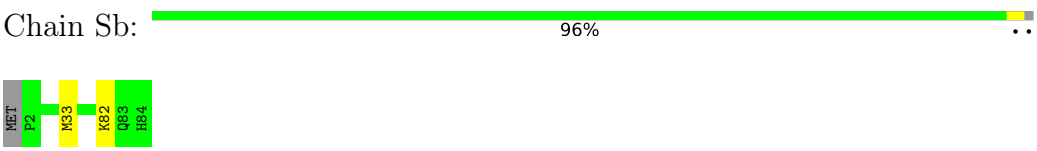
• Molecule 32: 40S ribosomal protein S25

Chain SZ:



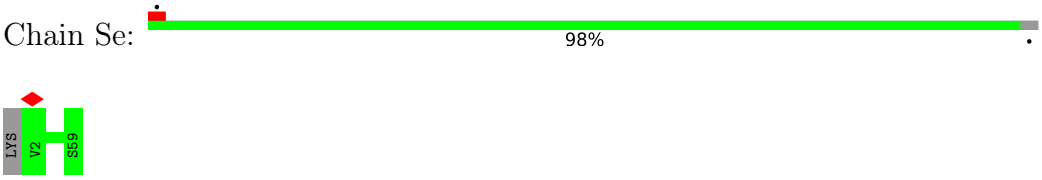
• Molecule 33: 40S ribosomal protein S27

Chain Sb:



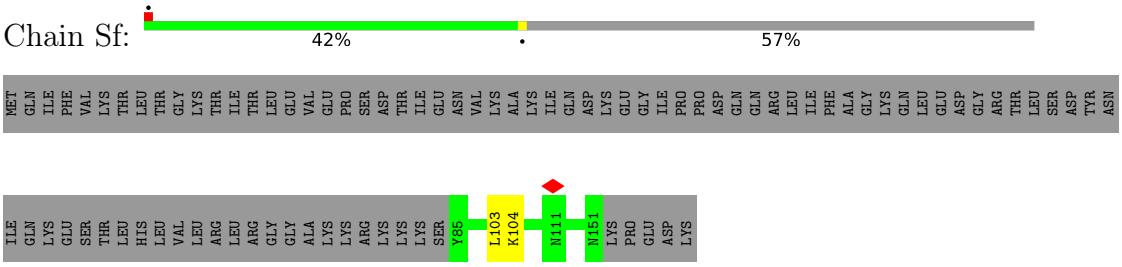
• Molecule 34: 40S ribosomal protein S30

Chain Se:



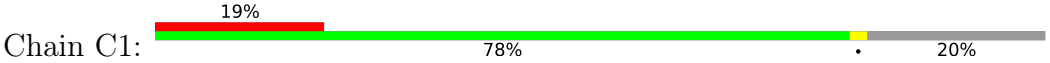
• Molecule 35: Ubiquitin-40S ribosomal protein S27a

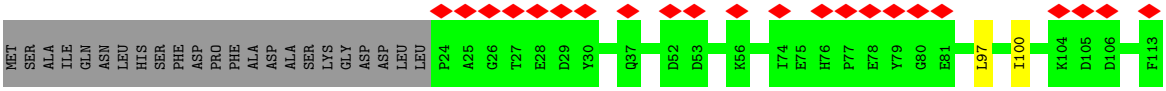
Chain Sf:



• Molecule 36: Eukaryotic translation initiation factor 1

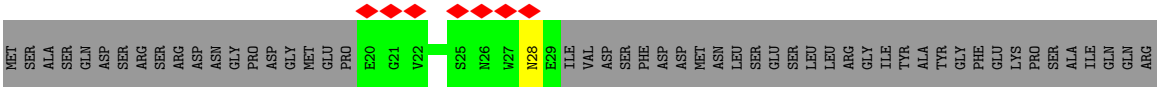
Chain C1:

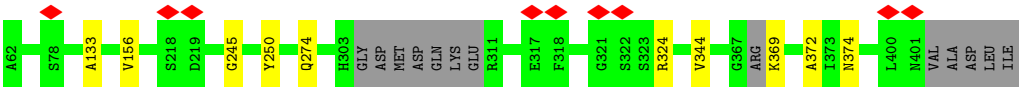




• Molecule 37: Eukaryotic initiation factor 4A-I

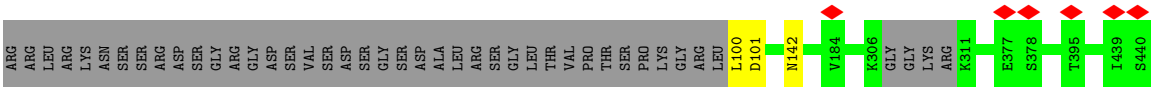
Chain 4A:

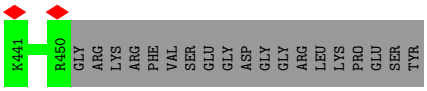




• Molecule 38: Programmed cell death protein 4

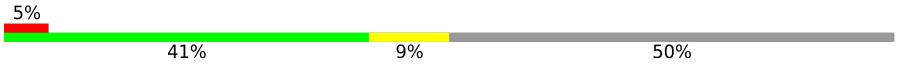
Chain CD:

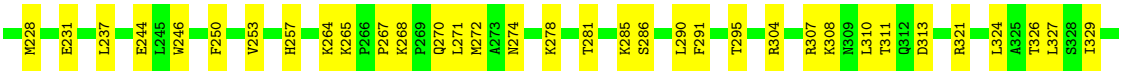


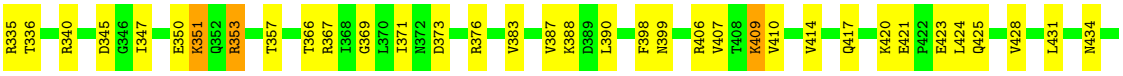


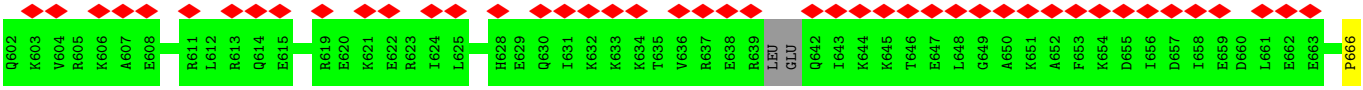
• Molecule 39: Eukaryotic translation initiation factor 3 subunit A

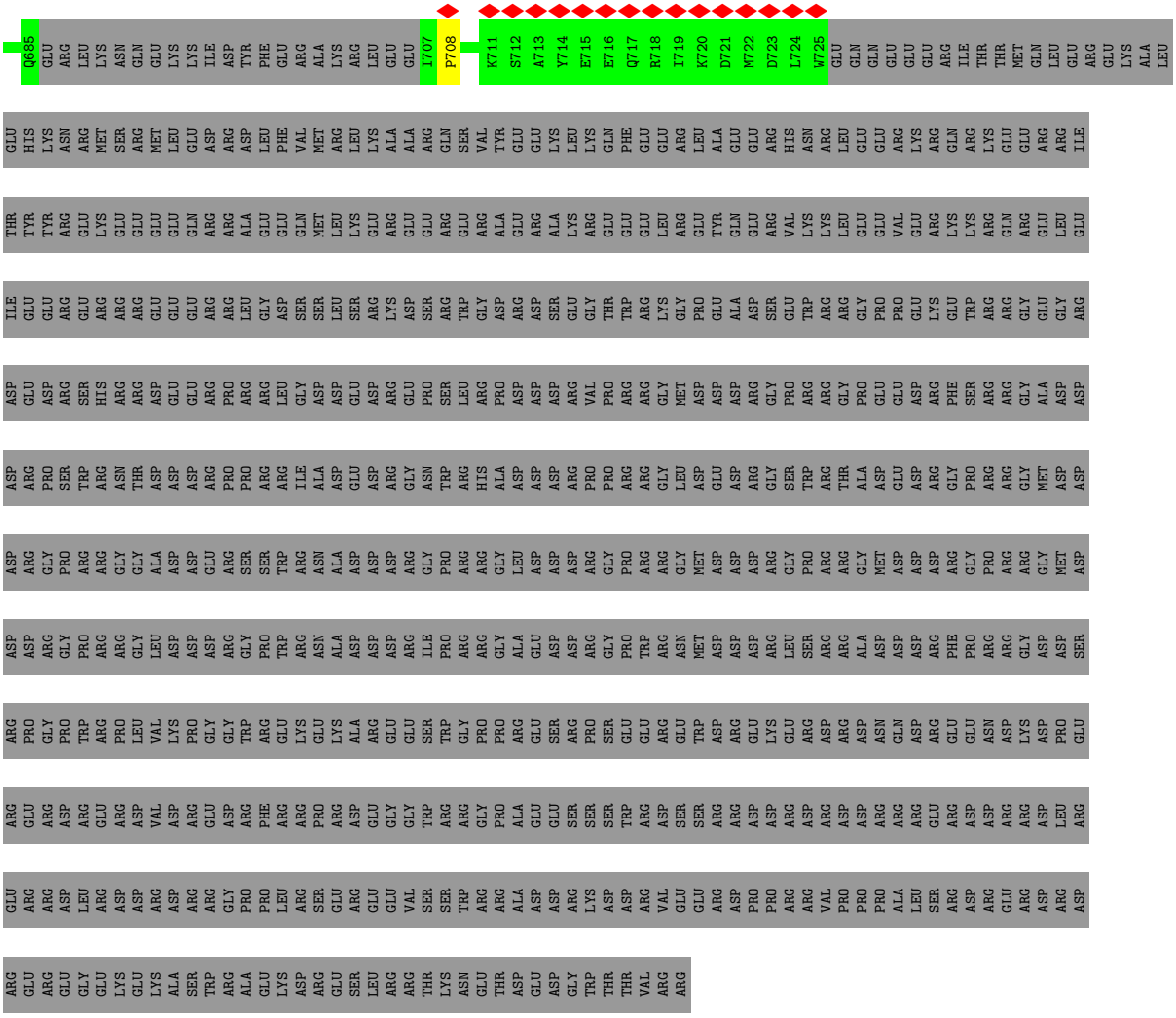
Chain 3A:





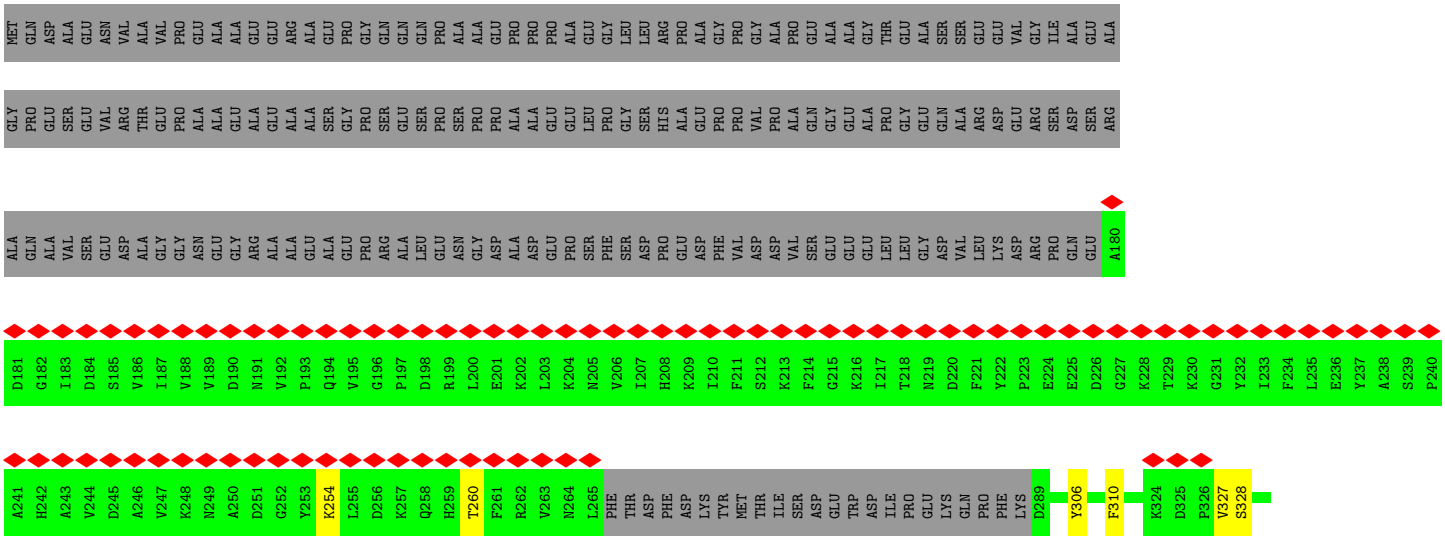


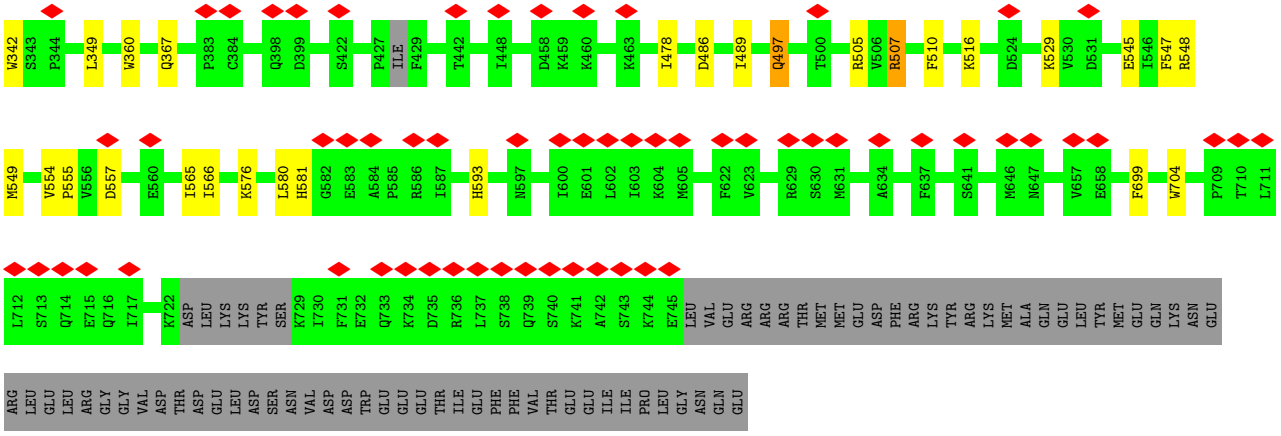




• Molecule 40: Eukaryotic translation initiation factor 3 subunit B

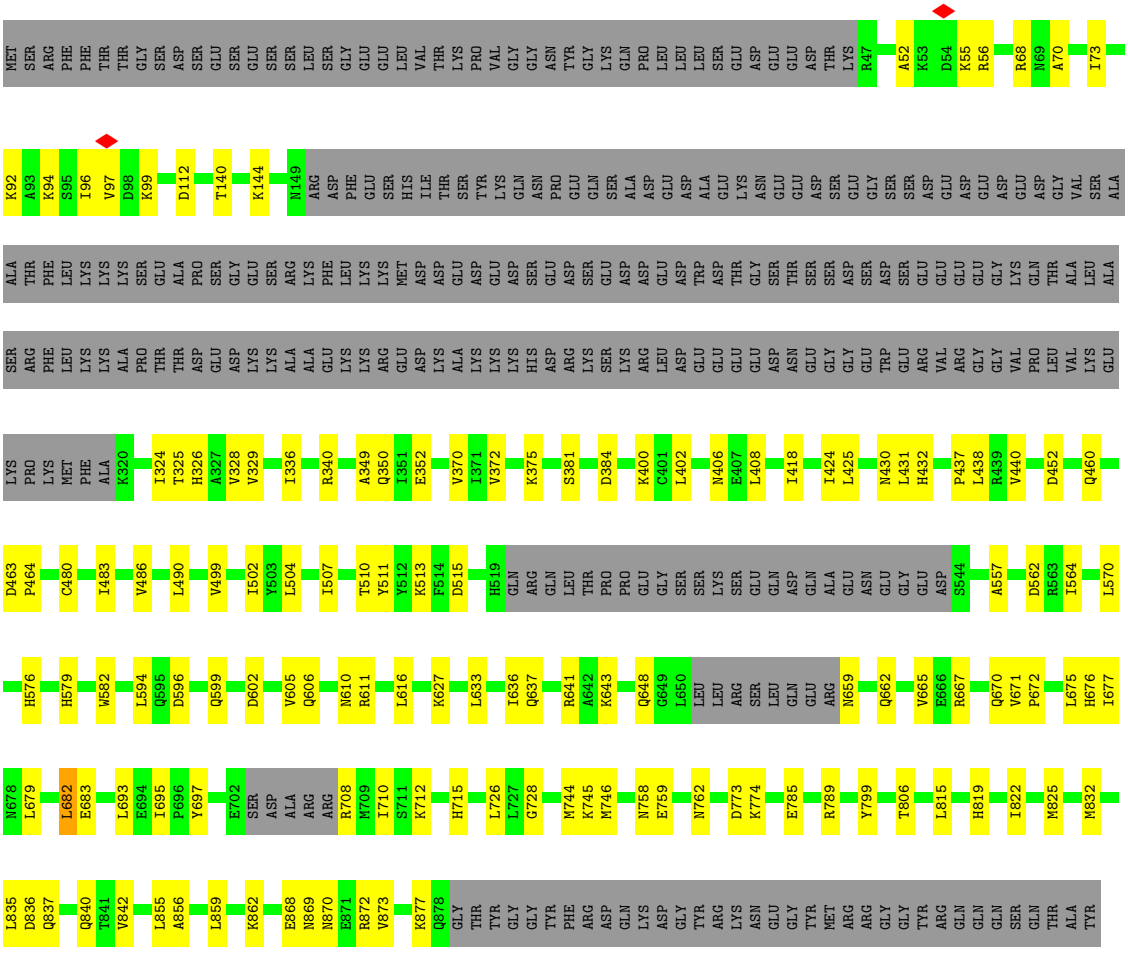
Chain 3B:





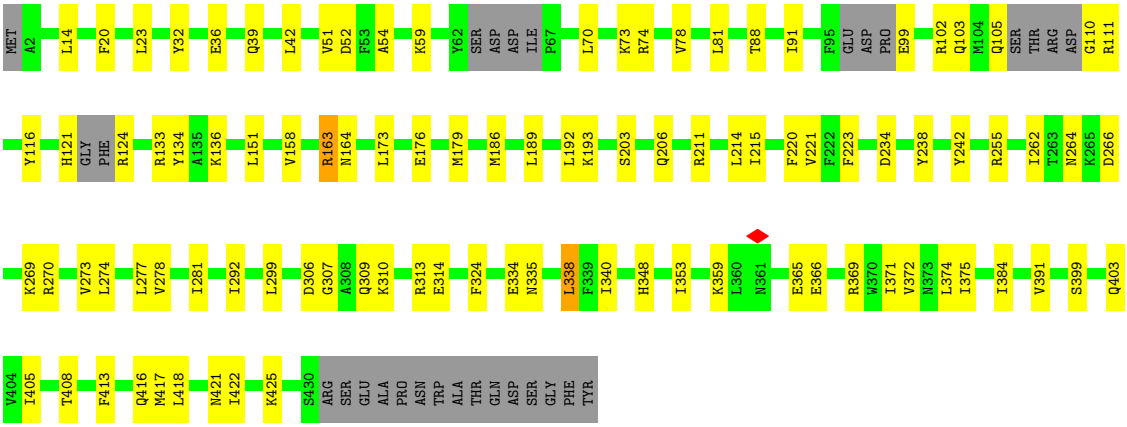
• Molecule 41: Eukaryotic translation initiation factor 3 subunit C

Chain 3C:

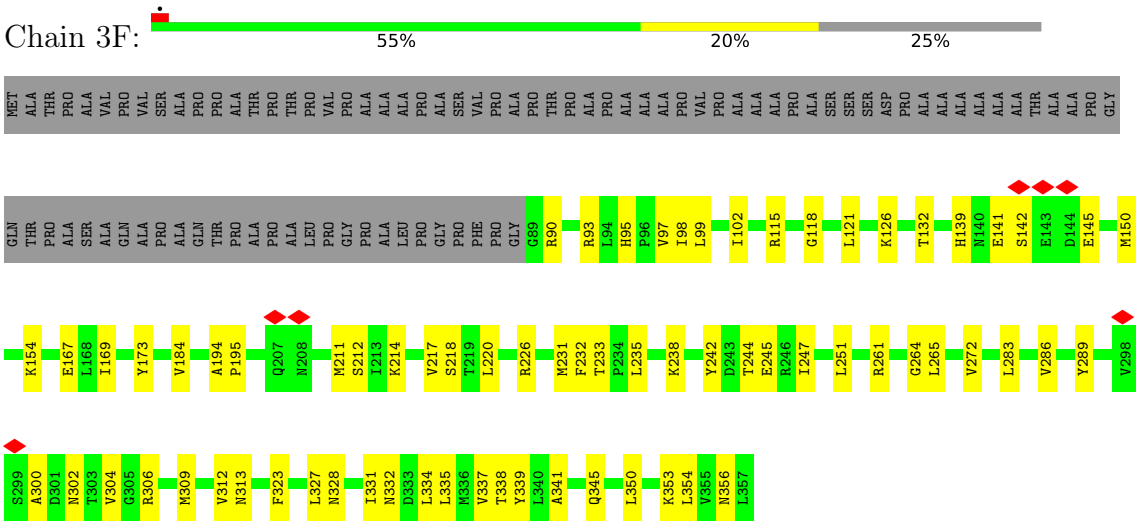


• Molecule 42: Eukaryotic translation initiation factor 3 subunit E

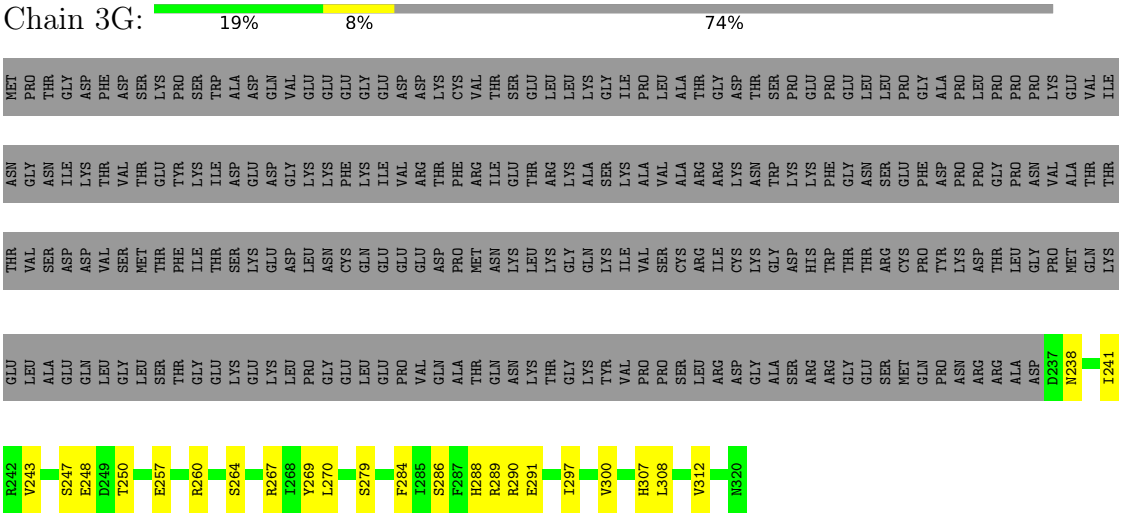
Chain 3E:



• Molecule 43: Eukaryotic translation initiation factor 3 subunit F

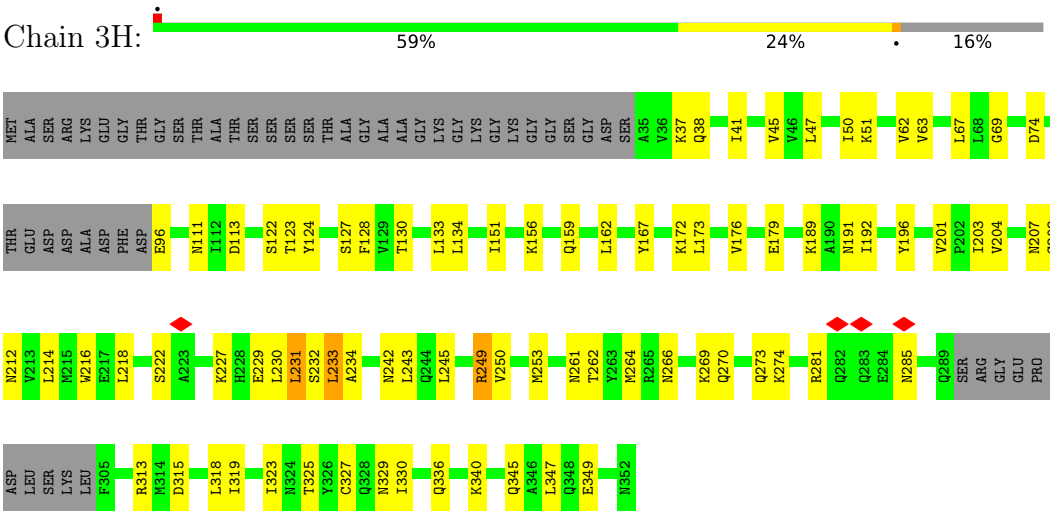


• Molecule 44: Eukaryotic translation initiation factor 3 subunit G



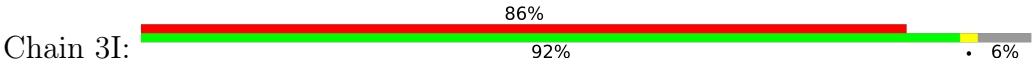
• Molecule 45: Eukaryotic translation initiation factor 3 subunit H

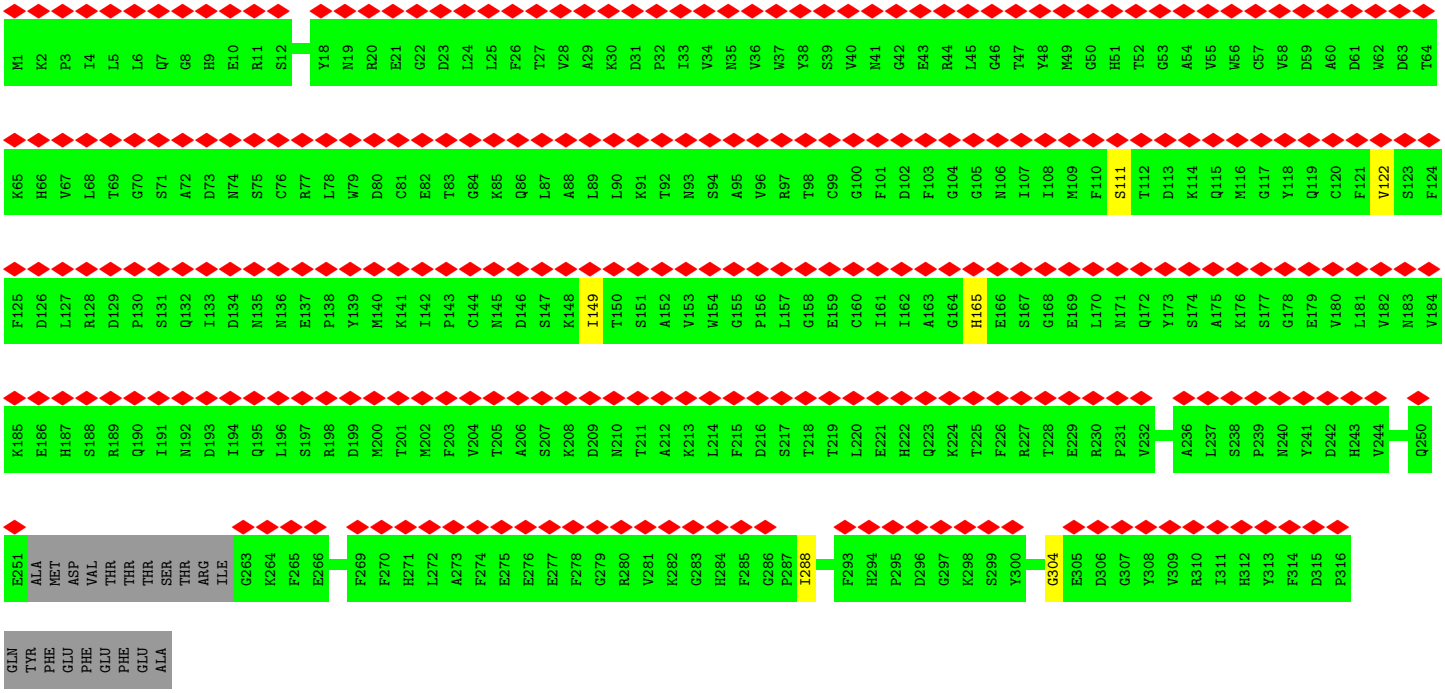
Chain 3H:



• Molecule 46: Eukaryotic translation initiation factor 3 subunit I

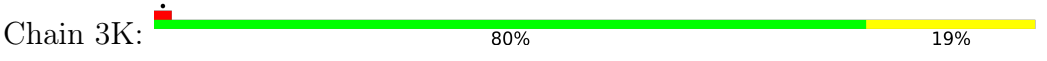
Chain 3I:

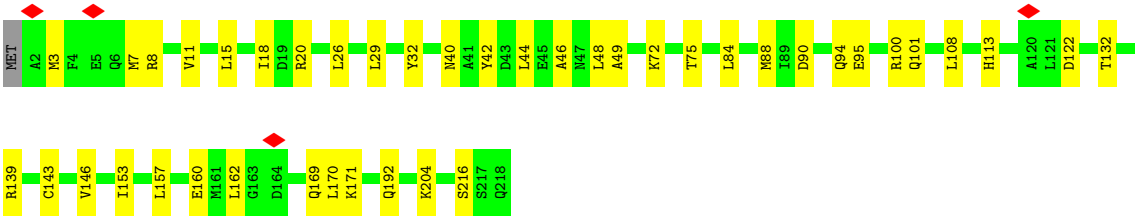




• Molecule 47: Eukaryotic translation initiation factor 3 subunit K

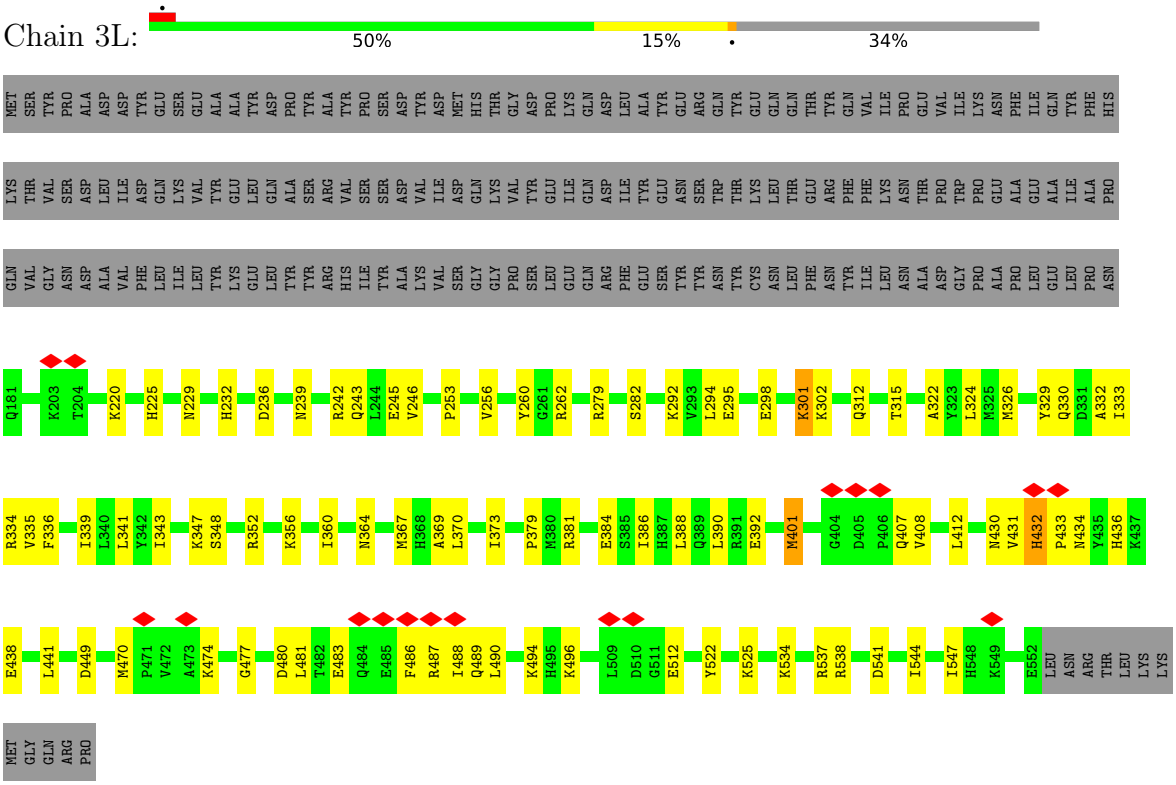
Chain 3K:





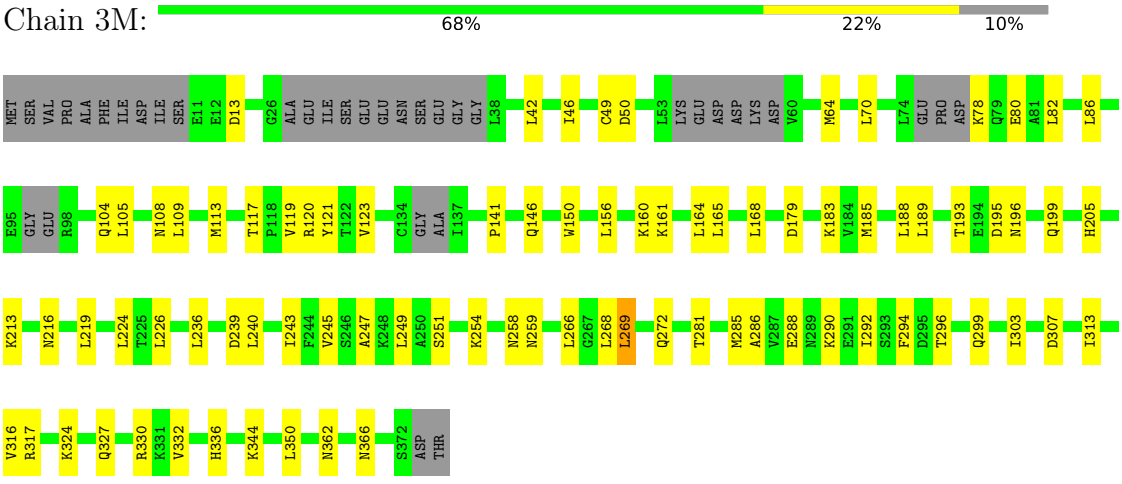
• Molecule 48: Eukaryotic translation initiation factor 3 subunit L

Chain 3L:



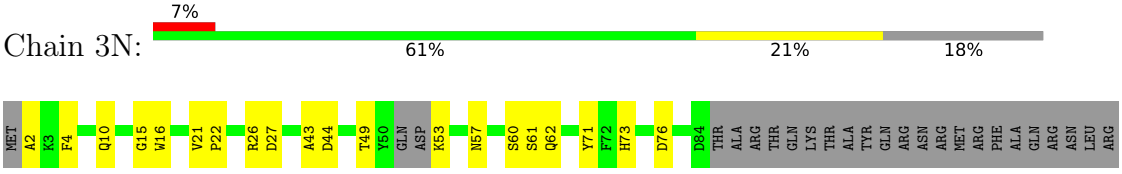
• Molecule 49: Eukaryotic translation initiation factor 3 subunit M

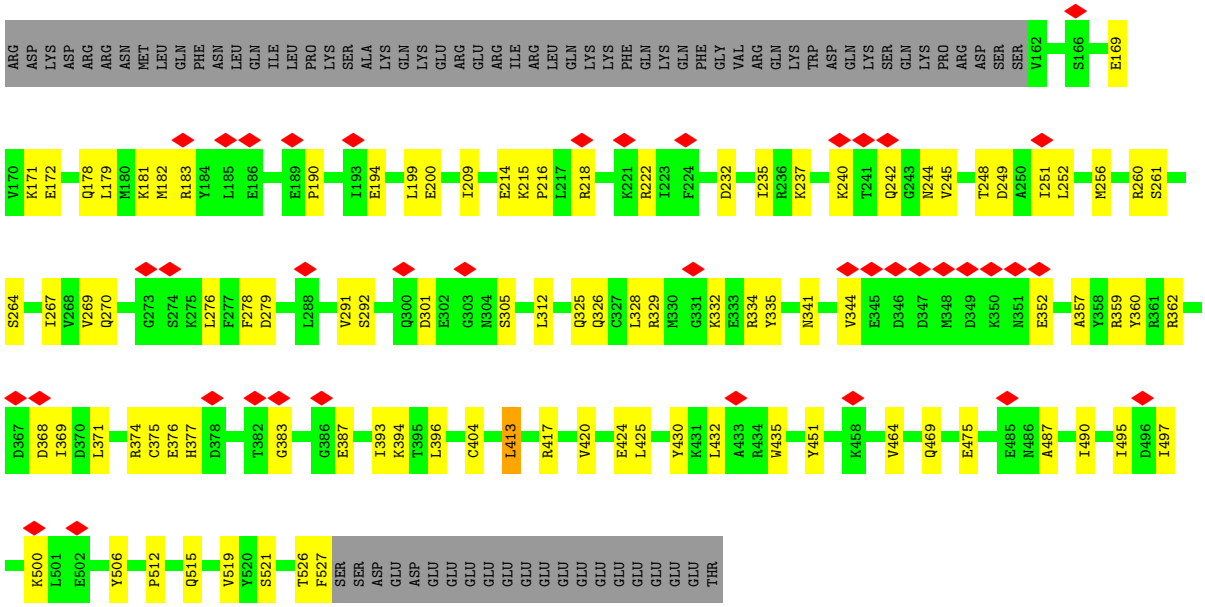
Chain 3M:



• Molecule 50: Eukaryotic translation initiation factor 3 subunit D

Chain 3N:




ARG ASP LYS ASP ARG ARG ASN MET LEU GLN PHE ASN LEU GLN ILE LEU PRO LYS SER ALA LYS GLN LYS GLU ARG GLU ARG ILE ARG LEU GLN LYS LYS PHE GLN LYS GLN PHE GLY VAL ARG GLN LYS TRP ASP GLN LYS SER GLN LYS PRO ARG ASP SER SER V162 S166 E169
V170 K171 E172 Q178 L179 M180 K181 M182 R183 Y184 L185 E186 E189 P190 I193 E194 L199 E200 I209 E214 K215 P216 L217 R218 K221 R222 I223 F224 D232 I235 R236 K237 K240 T241 Q242 G243 N244 V245 T248 D249 A250 I251 L252 M256 R260 S261
S264 I267 V268 V269 Q270 G273 S274 K275 L276 F277 F278 D279 L288 V291 S292 Q300 D301 E302 G303 N304 S305 L312 Q325 Q326 C327 L328 R329 M330 G331 K332 E333 R334 Y335 N341 V344 E345 D346 D347 M348 D349 K350 M351 E352 A357 Y358 R359 Y360 R361 R362
D367 D368 I369 D370 L371 R374 C375 E376 H377 D378 T382 G383 G386 E387 I393 K394 T395 L396 C404 L413 R417 V420 E424 L425 Y430 K431 L432 A433 R434 W435 Y451 K458 V464 Q469 E475 E485 N486 A487 I490 I495 D496 I497
K500 L501 E502 Y506 P512 Q515 V519 Y520 S521 T526 F527 SER SER ASP GLU ASP GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12788	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.375	Depositor
Minimum map value	-0.228	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	481.32, 481.32, 481.32	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.146, 1.146, 1.146	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	Ln	0.29	0/231	0.77	0/294
2	S2	0.60	0/40840	1.06	173/63635 (0.3%)
3	SA	0.39	0/1778	0.64	0/2416
4	SB	0.37	0/1765	0.68	0/2362
5	SD	0.39	0/1793	0.74	0/2414
6	SE	0.36	0/2118	0.65	0/2849
7	SF	0.35	0/1516	0.72	1/2037 (0.0%)
8	SH	0.34	0/1519	0.69	1/2033 (0.0%)
9	SI	0.36	0/1715	0.75	0/2287
10	SK	0.36	0/851	0.70	2/1147 (0.2%)
11	SL	0.39	0/1268	0.59	0/1696
12	SP	0.36	0/1003	0.80	0/1342
13	SQ	0.39	0/1160	0.76	2/1553 (0.1%)
14	SR	0.37	0/1105	0.75	1/1484 (0.1%)
15	SS	0.32	0/1216	0.72	0/1628
16	ST	0.34	0/1131	0.69	0/1515
17	SU	0.36	0/827	0.71	0/1110
18	SV	0.38	0/643	0.69	0/860
19	SX	0.43	0/1116	0.66	0/1490
20	Sa	0.40	0/836	0.73	0/1121
21	Sc	0.37	0/508	0.84	1/680 (0.1%)
22	Sd	0.43	0/470	0.74	0/623
23	Sg	0.30	0/2493	0.68	0/3394
24	SC	0.43	0/1762	0.68	1/2381 (0.0%)
25	SG	0.31	0/1946	0.71	1/2590 (0.0%)
26	SJ	0.40	0/1550	0.72	1/2069 (0.0%)
27	SM	0.34	0/950	0.75	0/1275
28	SN	0.37	0/1232	0.67	0/1656
29	SO	0.37	0/1062	0.67	0/1425
30	SW	0.39	0/1051	0.63	0/1406
31	SY	0.35	0/1083	0.72	0/1438
32	SZ	0.32	0/604	0.83	1/810 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Sb	0.36	0/665	0.69	0/891
34	Se	0.31	0/465	0.64	0/612
35	Sf	0.29	0/560	0.73	1/745 (0.1%)
36	C1	0.25	0/442	0.58	0/611
37	4A	0.25	0/1687	0.53	0/2344
38	CD	0.33	0/1846	0.53	0/2550
39	3A	0.28	0/5463	0.64	4/7394 (0.1%)
40	3B	0.27	0/2981	0.54	1/4115 (0.0%)
41	3C	0.31	0/5154	0.69	5/6942 (0.1%)
42	3E	0.29	0/3503	0.66	2/4728 (0.0%)
43	3F	0.29	0/2126	0.64	0/2890
44	3G	0.33	0/680	0.69	1/916 (0.1%)
45	3H	0.27	0/2458	0.65	2/3313 (0.1%)
46	3I	0.25	0/1495	0.48	0/2073
47	3K	0.26	0/1785	0.58	1/2414 (0.0%)
48	3L	0.29	0/3187	0.68	3/4299 (0.1%)
49	3M	0.28	0/2743	0.65	2/3697 (0.1%)
50	3N	0.29	0/3699	0.63	2/5001 (0.0%)
All	All	0.44	0/120081	0.83	209/170555 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	SF	0	2
9	SI	0	1
14	SR	0	1
19	SX	0	5
21	Sc	0	1
26	SJ	0	1
32	SZ	0	1
33	Sb	0	2
43	3F	0	1
45	3H	0	1
48	3L	0	2
All	All	0	18

There are no bond length outliers.

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S2	1772	C	N3-C2-O2	-14.58	111.70	121.90
2	S2	1772	C	N1-C2-O2	14.18	127.41	118.90
2	S2	501	C	N1-C2-O2	13.09	126.75	118.90
2	S2	501	C	C2-N1-C1'	12.99	133.09	118.80
2	S2	293	C	N1-C2-O2	12.27	126.26	118.90
2	S2	557	U	N3-C2-O2	-12.18	113.68	122.20
2	S2	883	U	N3-C2-O2	-10.98	114.52	122.20
2	S2	293	C	C2-N1-C1'	10.79	130.67	118.80
2	S2	1437	C	C2-N1-C1'	10.25	130.08	118.80
2	S2	501	C	N3-C2-O2	-9.99	114.91	121.90
2	S2	882	U	N1-C2-O2	9.98	129.78	122.80
2	S2	1437	C	N1-C2-O2	9.83	124.80	118.90
2	S2	501	C	C6-N1-C1'	-9.76	109.08	120.80
2	S2	549	C	N3-C2-O2	-9.61	115.17	121.90
2	S2	882	U	N3-C2-O2	-9.39	115.63	122.20
2	S2	1453	C	C2-N1-C1'	9.32	129.05	118.80
2	S2	1772	C	C6-N1-C2	-9.26	116.60	120.30
2	S2	293	C	N3-C2-O2	-9.04	115.57	121.90
2	S2	1453	C	N1-C2-O2	8.49	124.00	118.90
2	S2	883	U	N1-C2-O2	8.49	128.74	122.80
2	S2	1696	C	N1-C2-O2	8.45	123.97	118.90
2	S2	1696	C	N3-C2-O2	-8.44	115.99	121.90
2	S2	1139	C	C2-N1-C1'	8.42	128.06	118.80
2	S2	118	C	N1-C2-O2	8.39	123.93	118.90
2	S2	883	U	C2-N1-C1'	8.31	127.67	117.70
2	S2	1139	C	N3-C2-O2	-8.28	116.10	121.90
2	S2	557	U	N1-C2-N3	8.27	119.86	114.90
2	S2	557	U	C2-N3-C4	-8.22	122.07	127.00
2	S2	1139	C	N1-C2-O2	7.96	123.67	118.90
2	S2	882	U	C2-N1-C1'	7.92	127.20	117.70
2	S2	1696	C	C2-N1-C1'	7.82	127.40	118.80
2	S2	293	C	C6-N1-C1'	-7.81	111.43	120.80
2	S2	494	C	N1-C2-O2	7.76	123.56	118.90
2	S2	1437	C	N3-C2-O2	-7.75	116.47	121.90
2	S2	1772	C	C2-N1-C1'	7.70	127.27	118.80
2	S2	118	C	C2-N1-C1'	7.70	127.27	118.80
2	S2	178	C	N1-C2-O2	7.37	123.32	118.90
50	3N	368	ASP	CB-CG-OD1	7.36	124.92	118.30
2	S2	1261	C	N1-C2-O2	7.35	123.31	118.90
2	S2	118	C	N3-C2-O2	-7.26	116.82	121.90
2	S2	842	C	C2-N1-C1'	7.26	126.78	118.80
2	S2	632	C	C2-N1-C1'	7.24	126.77	118.80
2	S2	195	C	N3-C2-O2	-7.21	116.85	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S2	1437	C	C6-N1-C2	-7.10	117.46	120.30
2	S2	427	U	C2-N1-C1'	7.10	126.22	117.70
13	SQ	7	LEU	CA-CB-CG	7.05	131.53	115.30
2	S2	1520	G	C4-N9-C1'	7.04	135.65	126.50
2	S2	1437	C	C6-N1-C1'	-7.01	112.38	120.80
41	3C	682	LEU	CA-CB-CG	6.97	131.32	115.30
2	S2	1520	G	N3-C4-N9	6.96	130.17	126.00
48	3L	412	LEU	CA-CB-CG	6.93	131.24	115.30
2	S2	548	C	C2-N1-C1'	6.84	126.32	118.80
41	3C	452	ASP	CB-CG-OD1	6.80	124.42	118.30
2	S2	1119	A	O4'-C1'-N9	6.75	113.60	108.20
2	S2	1389	C	C6-N1-C2	-6.69	117.62	120.30
2	S2	1453	C	C6-N1-C1'	-6.68	112.78	120.80
2	S2	1016	U	N3-C2-O2	-6.67	117.53	122.20
8	SH	40	LEU	CA-CB-CG	6.63	130.55	115.30
2	S2	688	U	P-O3'-C3'	6.62	127.64	119.70
2	S2	537	C	C2-N1-C1'	6.61	126.07	118.80
2	S2	130	G	N3-C4-C5	-6.55	125.33	128.60
2	S2	1016	U	C2-N1-C1'	6.52	125.53	117.70
2	S2	130	G	N3-C4-N9	6.52	129.91	126.00
2	S2	632	C	C6-N1-C2	-6.51	117.70	120.30
26	SJ	61	LEU	CA-CB-CG	6.48	130.21	115.30
2	S2	130	G	C4-N9-C1'	6.47	134.92	126.50
2	S2	548	C	N1-C2-O2	6.39	122.74	118.90
2	S2	1453	C	N3-C2-O2	-6.39	117.42	121.90
2	S2	1807	C	N3-C2-O2	-6.37	117.44	121.90
2	S2	1520	G	C8-N9-C1'	-6.36	118.73	127.00
2	S2	178	C	N3-C2-O2	-6.35	117.45	121.90
2	S2	1173	A	C6-N1-C2	-6.35	114.79	118.60
21	Sc	18	LEU	CA-CB-CG	6.35	129.90	115.30
2	S2	1261	C	N3-C2-O2	-6.33	117.47	121.90
2	S2	322	C	N1-C2-O2	6.32	122.69	118.90
2	S2	1417	C	N3-C2-O2	-6.31	117.48	121.90
2	S2	1807	C	C6-N1-C2	-6.30	117.78	120.30
2	S2	592	C	C2-N1-C1'	6.29	125.71	118.80
2	S2	1389	C	C2-N1-C1'	6.29	125.72	118.80
2	S2	1139	C	C6-N1-C2	-6.27	117.79	120.30
41	3C	746	MET	CG-SD-CE	6.26	110.22	100.20
2	S2	1016	U	N1-C2-O2	6.24	127.17	122.80
2	S2	501	C	C6-N1-C2	-6.21	117.82	120.30
2	S2	293	C	C5-C6-N1	6.20	124.10	121.00
2	S2	1591	C	N1-C2-O2	6.20	122.62	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	3A	164	LEU	CA-CB-CG	6.19	129.53	115.30
2	S2	1199	A	N1-C6-N6	-6.17	114.89	118.60
2	S2	427	U	N3-C2-O2	-6.17	117.88	122.20
2	S2	1696	C	C6-N1-C2	-6.16	117.83	120.30
25	SG	217	MET	CA-CB-CG	6.13	123.72	113.30
40	3B	507	ARG	CG-CD-NE	6.08	124.56	111.80
45	3H	233	LEU	CA-CB-CG	6.06	129.25	115.30
2	S2	1437	C	C5-C6-N1	6.06	124.03	121.00
2	S2	1292	C	N1-C2-O2	6.03	122.52	118.90
2	S2	293	C	C6-N1-C2	-6.00	117.90	120.30
50	3N	413	LEU	CA-CB-CG	5.99	129.06	115.30
2	S2	179	C	N1-C2-O2	5.97	122.48	118.90
2	S2	178	C	C2-N1-C1'	5.96	125.36	118.80
2	S2	427	U	N1-C2-O2	5.93	126.95	122.80
2	S2	842	C	C5-C6-N1	5.92	123.96	121.00
39	3A	511	LEU	CA-CB-CG	5.88	128.83	115.30
2	S2	57	U	N3-C2-O2	-5.87	118.09	122.20
2	S2	1173	A	C5-C6-N1	5.85	120.62	117.70
2	S2	1271	C	N1-C2-O2	5.83	122.40	118.90
45	3H	231	LEU	CA-CB-CG	5.83	128.70	115.30
2	S2	632	C	C5-C6-N1	5.82	123.91	121.00
2	S2	882	U	C5-C6-N1	5.81	125.61	122.70
42	3E	338	LEU	CA-CB-CG	5.79	128.62	115.30
2	S2	1471	C	C2-N1-C1'	5.79	125.17	118.80
2	S2	1520	G	N3-C4-C5	-5.78	125.71	128.60
41	3C	832	MET	CA-CB-CG	5.75	123.08	113.30
49	3M	266	LEU	CA-CB-CG	5.75	128.51	115.30
2	S2	1315	U	N1-C2-O2	5.73	126.81	122.80
2	S2	194	C	N1-C2-O2	5.72	122.33	118.90
2	S2	1154	U	C2-N1-C1'	5.72	124.56	117.70
39	3A	666	PRO	N-CA-CB	5.71	110.15	103.30
2	S2	534	G	N1-C2-N2	-5.67	111.09	116.20
2	S2	1018	U	N1-C2-O2	5.66	126.76	122.80
39	3A	708	PRO	N-CA-CB	5.66	110.09	103.30
2	S2	494	C	N3-C2-O2	-5.64	117.95	121.90
2	S2	1139	C	C6-N1-C1'	-5.62	114.06	120.80
13	SQ	58	LEU	CA-CB-CG	5.62	128.22	115.30
2	S2	659	G	C4-N9-C1'	5.58	133.75	126.50
10	SK	1	MET	CG-SD-CE	5.57	109.12	100.20
2	S2	549	C	N1-C2-N3	5.57	123.10	119.20
2	S2	325	C	C2-N1-C1'	5.55	124.91	118.80
2	S2	1471	C	C6-N1-C2	-5.55	118.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S2	1460	C	C2-N1-C1'	5.54	124.89	118.80
2	S2	550	C	C6-N1-C1'	5.52	127.42	120.80
2	S2	549	C	C6-N1-C1'	5.52	127.42	120.80
35	Sf	103	LEU	CA-CB-CG	5.52	127.99	115.30
2	S2	1408	U	C2-N1-C1'	5.51	124.32	117.70
47	3K	3	MET	CA-CB-CG	5.51	122.66	113.30
2	S2	1330	G	C3'-C2'-C1'	-5.50	97.10	101.50
2	S2	666	U	C2-N1-C1'	5.49	124.28	117.70
2	S2	883	U	C6-N1-C2	-5.47	117.72	121.00
41	3C	836	ASP	CB-CG-OD1	5.47	123.22	118.30
2	S2	1700	C	O5'-P-OP1	-5.47	100.78	105.70
7	SF	26	ASP	CB-CG-OD1	5.47	123.22	118.30
2	S2	291	G	P-O3'-C3'	5.46	126.25	119.70
2	S2	882	U	C6-N1-C2	-5.46	117.72	121.00
2	S2	550	C	C5-C4-N4	5.45	124.01	120.20
2	S2	1315	U	N3-C2-O2	-5.44	118.39	122.20
2	S2	592	C	N1-C2-O2	5.42	122.15	118.90
2	S2	1453	C	C5-C6-N1	5.42	123.71	121.00
2	S2	659	G	C8-N9-C1'	-5.41	119.96	127.00
2	S2	1434	C	P-O3'-C3'	5.39	126.17	119.70
2	S2	130	G	C8-N9-C1'	-5.39	119.99	127.00
14	SR	68	GLY	N-CA-C	-5.38	99.65	113.10
2	S2	195	C	C6-N1-C2	-5.36	118.15	120.30
2	S2	1865	C	C6-N1-C2	-5.36	118.15	120.30
48	3L	379	PRO	C-N-CA	5.36	135.09	121.70
2	S2	798	G	N3-C4-N9	5.34	129.21	126.00
2	S2	1707	U	N3-C2-O2	-5.34	118.46	122.20
10	SK	84	HIS	C-N-CA	5.34	135.04	121.70
2	S2	322	C	N3-C2-O2	-5.33	118.17	121.90
2	S2	1315	U	C2-N1-C1'	5.33	124.09	117.70
2	S2	494	C	C2-N1-C1'	5.32	124.66	118.80
2	S2	1453	C	C6-N1-C2	-5.32	118.17	120.30
2	S2	882	U	C5-C4-O4	5.32	129.09	125.90
2	S2	1244	U	N3-C2-O2	-5.31	118.48	122.20
2	S2	501	C	C5-C6-N1	5.31	123.66	121.00
2	S2	1018	U	C2-N1-C1'	5.30	124.07	117.70
2	S2	1257	G	N1-C6-O6	-5.30	116.72	119.90
2	S2	1022	U	C2-N1-C1'	5.30	124.06	117.70
2	S2	118	C	C6-N1-C2	-5.28	118.19	120.30
2	S2	118	C	C6-N1-C1'	-5.27	114.47	120.80
2	S2	531	A	OP1-P-O3'	5.27	116.80	105.20
2	S2	549	C	N3-C4-N4	-5.27	114.31	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S2	1218	C	C5-C6-N1	5.27	123.63	121.00
2	S2	529	A	N1-C6-N6	-5.27	115.44	118.60
2	S2	814	U	N1-C2-O2	5.27	126.49	122.80
2	S2	814	U	N3-C2-O2	-5.26	118.52	122.20
2	S2	1460	C	C6-N1-C2	-5.26	118.20	120.30
2	S2	1415	C	C2-N1-C1'	5.26	124.58	118.80
2	S2	1114	U	O4'-C1'-N1	5.25	112.40	108.20
2	S2	358	C	C2-N1-C1'	5.25	124.57	118.80
2	S2	340	C	N1-C2-O2	5.24	122.04	118.90
2	S2	548	C	C6-N1-C1'	-5.24	114.51	120.80
2	S2	1234	C	C5-C6-N1	5.23	123.62	121.00
49	3M	269	LEU	CA-CB-CG	5.23	127.33	115.30
2	S2	1018	U	N3-C2-O2	-5.22	118.54	122.20
2	S2	579	C	N1-C2-O2	5.21	122.03	118.90
2	S2	853	C	N1-C2-O2	5.21	122.03	118.90
2	S2	557	U	N1-C2-O2	5.20	126.44	122.80
2	S2	548	C	C5-C6-N1	5.18	123.59	121.00
2	S2	1157	G	N3-C4-C5	-5.16	126.02	128.60
2	S2	542	U	N1-C2-O2	5.15	126.41	122.80
2	S2	1486	A	O4'-C1'-N9	5.15	112.32	108.20
2	S2	804	U	C5-C6-N1	5.14	125.27	122.70
2	S2	842	C	C6-N1-C2	-5.14	118.24	120.30
2	S2	1660	C	C2-N1-C1'	5.14	124.46	118.80
24	SC	63	VAL	C-N-CA	5.14	134.56	121.70
44	3G	270	LEU	CA-CB-CG	5.14	127.13	115.30
2	S2	205	G	N1-C6-O6	-5.14	116.82	119.90
2	S2	314	U	N3-C2-O2	-5.13	118.61	122.20
2	S2	112	U	P-O3'-C3'	5.11	125.83	119.70
2	S2	537	C	N1-C2-O2	5.10	121.96	118.90
2	S2	1292	C	N3-C2-O2	-5.09	118.34	121.90
2	S2	358	C	C6-N1-C2	-5.09	118.27	120.30
2	S2	1696	C	C6-N1-C1'	-5.08	114.71	120.80
2	S2	1744	G	C4-N9-C1'	-5.08	119.90	126.50
48	3L	449	ASP	CB-CG-OD1	5.08	122.87	118.30
2	S2	815	U	N3-C2-O2	-5.07	118.65	122.20
42	3E	314	GLU	CA-CB-CG	5.07	124.55	113.40
2	S2	549	C	C5-C4-N4	5.05	123.74	120.20
2	S2	1271	C	C2-N1-C1'	5.04	124.34	118.80
32	SZ	47	LEU	CA-CB-CG	5.04	126.89	115.30
2	S2	1744	G	O4'-C1'-N9	5.00	112.20	108.20

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
43	3F	194	ALA	Peptide
45	3H	196	TYR	Peptide
48	3L	401	MET	Peptide
48	3L	432	HIS	Peptide
7	SF	133	THR	Peptide
7	SF	79	HIS	Peptide
9	SI	159	SER	Peptide
26	SJ	137	VAL	Peptide
14	SR	67	ARG	Peptide
19	SX	119	ARG	Sidechain
19	SX	124	LYS	Peptide
19	SX	125	VAL	Peptide
19	SX	126	ALA	Peptide
19	SX	86	PRO	Peptide
32	SZ	46	ASN	Peptide
33	Sb	33	MET	Peptide
33	Sb	82	LYS	Peptide
21	Sc	29	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ln	230	0	276	0	0
2	S2	36535	0	18416	320	0
3	SA	1741	0	1746	32	0
4	SB	1738	0	1809	24	0
5	SD	1765	0	1865	23	0
6	SE	2076	0	2177	22	0
7	SF	1495	0	1549	26	0
8	SH	1497	0	1590	18	0
9	SI	1686	0	1772	40	0
10	SK	827	0	854	8	0
11	SL	1247	0	1323	20	0
12	SP	985	0	1031	25	0
13	SQ	1142	0	1213	25	0
14	SR	1090	0	1149	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	SS	1198	0	1261	30	0
16	ST	1112	0	1146	18	0
17	SU	817	0	882	18	0
18	SV	636	0	637	12	0
19	SX	1098	0	1167	14	0
20	Sa	821	0	870	0	0
21	Sc	506	0	536	0	0
22	Sd	459	0	448	0	0
23	Sg	2436	0	2393	0	0
24	SC	1725	0	1813	27	0
25	SG	1923	0	2088	42	0
26	SJ	1525	0	1640	34	0
27	SM	940	0	965	23	0
28	SN	1208	0	1294	14	0
29	SO	1049	0	1073	16	0
30	SW	1034	0	1080	13	0
31	SY	1065	0	1142	34	0
32	SZ	598	0	656	14	0
33	Sb	651	0	672	0	0
34	Se	459	0	503	0	0
35	Sf	548	0	555	0	0
36	C1	443	0	201	2	0
37	4A	1691	0	753	5	0
38	CD	1841	0	998	4	0
39	3A	5379	0	5155	83	0
40	3B	2966	0	1764	19	0
41	3C	5070	0	5110	91	0
42	3E	3437	0	3433	68	0
43	3F	2090	0	2092	56	0
44	3G	667	0	647	16	0
45	3H	2413	0	2411	69	0
46	3I	1497	0	676	3	0
47	3K	1750	0	1717	28	0
48	3L	3111	0	3085	59	0
49	3M	2705	0	2759	52	0
50	3N	3617	0	3495	71	0
51	S2	22	0	0	0	0
51	SG	1	0	0	0	0
52	Sa	1	0	0	0	0
52	Sd	1	0	0	0	0
52	Sf	1	0	0	0	0
All	All	114565	0	93887	1340	0

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

All (1340) 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)
41:3C:697:TYR:HH	41:3C:708:ARG:N	1.57	1.03
2:S2:886:A:N6	2:S2:901:G:C4	2.31	0.98
2:S2:885:U:H3	2:S2:901:G:H1	1.07	0.96
2:S2:1609:C:H42	2:S2:1630:A:H61	1.02	0.93
42:3E:99:GLU:O	42:3E:103:GLN:HB2	1.66	0.93
2:S2:1752:C:C4	2:S2:1779:G:N2	2.38	0.91
9:SI:99:ASN:HA	9:SI:175:ILE:O	1.71	0.91
39:3A:518:GLN:O	39:3A:522:GLN:HB2	1.71	0.90
2:S2:1548:G:C6	2:S2:1586:U:O4	2.28	0.87
38:CD:100:LEU:HD12	38:CD:101:ASP:N	1.92	0.84
48:3L:401:MET:HB2	48:3L:408:VAL:HG22	1.60	0.83
2:S2:533:A:H61	2:S2:550:C:N4	1.77	0.83
7:SF:127:ARG:HG3	7:SF:129:GLY:H	1.44	0.83
43:3F:331:ILE:O	43:3F:335:LEU:HB2	1.81	0.81
50:3N:252:LEU:O	50:3N:256:MET:HB2	1.81	0.80
11:SL:18:GLN:HA	11:SL:18:GLN:HE21	1.44	0.80
15:SS:115:LYS:HD3	15:SS:126:PHE:HB2	1.62	0.80
3:SA:209:GLU:O	3:SA:213:GLU:HB2	1.82	0.79
2:S2:1755:C:N4	2:S2:1756:C:N4	2.31	0.78
2:S2:1115:U:C2	2:S2:1118:C:N4	2.51	0.78
7:SF:134:VAL:HG13	7:SF:135:ARG:HG2	1.65	0.78
2:S2:886:A:N6	2:S2:901:G:C5	2.53	0.76
2:S2:1755:C:C4	2:S2:1756:C:N4	2.54	0.76
2:S2:1115:U:N3	2:S2:1118:C:N4	2.33	0.76
2:S2:323:C:H2'	2:S2:327:G:H22	1.51	0.76
2:S2:1609:C:N4	2:S2:1630:A:H61	1.83	0.76
2:S2:533:A:N6	2:S2:550:C:N4	2.33	0.75
44:3G:257:GLU:HG3	44:3G:260:ARG:HH22	1.50	0.75
10:SK:7:ASN:HD22	10:SK:40:VAL:HG12	1.52	0.75
50:3N:359:ARG:HB3	50:3N:375:CYS:HB2	1.67	0.75
41:3C:862:LYS:HD2	45:3H:250:VAL:HG11	1.68	0.74
9:SI:152:ARG:O	9:SI:156:ALA:HB2	1.88	0.73
2:S2:384:U:O4	9:SI:5:ARG:NH2	2.23	0.72
13:SQ:53:GLU:O	13:SQ:57:LEU:HB3	1.89	0.72
2:S2:1752:C:N3	2:S2:1779:G:N1	2.36	0.72
50:3N:169:GLU:HB2	50:3N:521:SER:HB2	1.72	0.72
2:S2:1609:C:H42	2:S2:1630:A:N6	1.83	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1752:C:C2	2:S2:1779:G:N1	2.57	0.71
2:S2:1752:C:N3	2:S2:1779:G:C2	2.58	0.71
9:SI:67:TRP:HE1	9:SI:162:LEU:HD21	1.54	0.71
15:SS:12:ILE:HD12	15:SS:19:ASN:HD21	1.56	0.71
12:SP:83:MET:HB3	12:SP:116:LEU:HD13	1.72	0.70
2:S2:570:C:H4'	31:SY:36:PRO:HG3	1.73	0.70
2:S2:952:G:H21	29:SO:52:THR:HG21	1.57	0.70
2:S2:57:U:O2	2:S2:500:A:N7	2.25	0.69
16:ST:85:ASN:HB2	16:ST:88:MET:HB2	1.73	0.69
2:S2:748:C:H42	2:S2:795:A:N6	1.89	0.69
50:3N:73:HIS:HB3	50:3N:76:ASP:HB3	1.73	0.69
39:3A:513:SER:OG	39:3A:517:GLU:OE2	2.10	0.68
39:3A:446:ILE:HD12	39:3A:512:GLN:HE21	1.59	0.68
2:S2:1755:C:N4	2:S2:1756:C:H41	1.92	0.68
50:3N:194:GLU:HB2	50:3N:360:TYR:HB2	1.74	0.68
2:S2:1609:C:N3	2:S2:1630:A:N1	2.41	0.68
39:3A:270:GLN:HE21	39:3A:274:ASN:HD22	1.42	0.68
41:3C:140:THR:OG1	41:3C:144:LYS:NZ	2.27	0.67
43:3F:345:GLN:OE1	48:3L:537:ARG:NH1	2.27	0.67
40:3B:565:ILE:HA	40:3B:581:HIS:HA	1.77	0.67
49:3M:156:LEU:HB2	49:3M:161:LYS:HE2	1.74	0.67
5:SD:59:LEU:HD11	44:3G:308:LEU:HD11	1.76	0.67
27:SM:41:ALA:O	27:SM:44:LYS:C	2.34	0.66
2:S2:748:C:N4	2:S2:795:A:N6	2.42	0.66
27:SM:22:LEU:HD21	27:SM:89:VAL:HA	1.78	0.66
49:3M:196:ASN:HB2	49:3M:199:GLN:HE21	1.59	0.66
50:3N:357:ALA:HB3	50:3N:377:HIS:HB2	1.77	0.66
36:C1:97:LEU:O	36:C1:100:ILE:O	2.14	0.66
2:S2:506:G:OP1	31:SY:108:LYS:NZ	2.28	0.65
8:SH:95:ILE:HD11	8:SH:133:LEU:HD13	1.78	0.65
27:SM:41:ALA:O	27:SM:44:LYS:O	2.14	0.65
50:3N:22:PRO:O	50:3N:26:ARG:NH1	2.30	0.65
45:3H:130:THR:H	45:3H:133:LEU:HB2	1.62	0.64
2:S2:1017:U:H5'	28:SN:55:ARG:HE	1.62	0.64
9:SI:113:TYR:HD2	9:SI:121:LEU:HD22	1.61	0.64
7:SF:29:GLN:HG3	50:3N:475:GLU:HG3	1.79	0.64
45:3H:62:VAL:HA	45:3H:122:SER:O	1.97	0.64
3:SA:53:ARG:HG2	18:SV:83:PHE:HD2	1.63	0.64
15:SS:141:ARG:HA	15:SS:144:ARG:HB2	1.77	0.64
2:S2:1488:C:O2'	2:S2:1490:G:OP2	2.16	0.63
26:SJ:114:VAL:HG21	26:SJ:135:ILE:HD13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:SY:130:LYS:HG3	31:SY:131:PRO:HD3	1.81	0.63
44:3G:300:VAL:HG13	44:3G:312:VAL:HG21	1.81	0.63
50:3N:21:VAL:HG12	50:3N:26:ARG:HH12	1.63	0.63
2:S2:1138:C:O2'	18:SV:61:ARG:NH1	2.31	0.63
4:SB:68:GLU:HA	4:SB:84:PHE:O	1.98	0.63
8:SH:58:LYS:HB2	8:SH:90:LYS:HG2	1.80	0.63
37:4A:250:TYR:HA	37:4A:374:ASN:O	1.98	0.63
40:3B:342:TRP:HA	40:3B:349:LEU:HA	1.80	0.63
2:S2:1752:C:C4	2:S2:1779:G:C2	2.86	0.63
2:S2:1562:C:H2'	2:S2:1563:G:H8	1.64	0.63
49:3M:224:LEU:HD11	49:3M:245:VAL:HG11	1.81	0.63
2:S2:533:A:N6	2:S2:550:C:H42	1.93	0.63
4:SB:198:GLU:HB2	4:SB:210:VAL:HG21	1.80	0.63
43:3F:302:ASN:OD1	43:3F:306:ARG:NH1	2.32	0.63
11:SL:42:LEU:HD13	11:SL:72:ILE:HD11	1.81	0.62
2:S2:24:C:OP1	26:SJ:11:LYS:NZ	2.27	0.62
2:S2:1658:G:OP2	2:S2:1660:C:N4	2.32	0.62
9:SI:100:CYS:O	9:SI:174:CYS:HA	1.99	0.62
3:SA:91:ALA:O	3:SA:94:THR:O	2.16	0.62
5:SD:137:VAL:HG22	5:SD:151:LYS:HG2	1.81	0.62
3:SA:200:ASP:HA	3:SA:203:PHE:HD2	1.63	0.62
14:SR:111:PHE:HB3	14:SR:114:LEU:HD21	1.79	0.62
40:3B:505:ARG:HE	40:3B:554:VAL:HB	1.65	0.62
39:3A:321:ARG:HD2	39:3A:423:GLU:HG3	1.82	0.62
41:3C:633:LEU:HA	41:3C:636:ILE:HG22	1.80	0.62
41:3C:855:LEU:HD13	45:3H:243:LEU:HD22	1.81	0.62
2:S2:1543:U:OP1	13:SQ:37:ARG:NH2	2.33	0.62
43:3F:218:SER:HB3	43:3F:220:LEU:HD23	1.82	0.62
31:SY:82:ALA:O	31:SY:86:GLU:HB3	1.99	0.62
2:S2:1005:G:OP2	4:SB:162:ARG:NH2	2.33	0.62
2:S2:1548:G:O6	2:S2:1586:U:C4	2.53	0.62
6:SE:11:ARG:NH1	6:SE:24:THR:OG1	2.33	0.62
43:3F:264:GLY:HA2	45:3H:204:VAL:HA	1.82	0.62
18:SV:35:ASN:OD1	24:SC:267:GLN:NE2	2.33	0.61
49:3M:80:GLU:HB3	49:3M:119:VAL:HG21	1.81	0.61
2:S2:1569:A:OP2	16:ST:97:LYS:NZ	2.33	0.61
3:SA:207:PRO:HA	3:SA:210:ILE:HB	1.82	0.61
2:S2:529:A:N6	2:S2:557:U:H3	1.99	0.61
43:3F:261:ARG:HE	45:3H:208:SER:HA	1.66	0.61
2:S2:380:G:OP2	9:SI:181:GLN:NE2	2.33	0.61
4:SB:143:THR:HG1	4:SB:205:TYR:HE2	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SE:185:GLY:H	6:SE:189:LEU:HD13	1.66	0.61
15:SS:85:ASN:OD1	15:SS:97:GLN:NE2	2.34	0.61
41:3C:507:ILE:O	41:3C:511:TYR:HB3	1.99	0.61
41:3C:659:ASN:OD1	41:3C:662:GLN:NE2	2.34	0.61
43:3F:332:ASN:ND2	48:3L:522:TYR:OH	2.34	0.61
2:S2:1759:G:N2	2:S2:1773:C:OP1	2.33	0.61
9:SI:101:ILE:HD13	9:SI:174:CYS:HB3	1.83	0.61
3:SA:38:ILE:HD11	3:SA:47:TYR:HB3	1.83	0.60
44:3G:267:ARG:HB2	44:3G:286:SER:HB3	1.83	0.60
6:SE:19:MET:SD	6:SE:51:ARG:NH2	2.74	0.60
49:3M:117:THR:HG23	49:3M:120:ARG:H	1.66	0.60
19:SX:68:LYS:HB3	19:SX:91:LEU:HD22	1.83	0.60
42:3E:353:ILE:HD11	42:3E:391:VAL:HG23	1.82	0.60
2:S2:925:G:H1	2:S2:1017:U:H3	0.81	0.60
2:S2:1160:U:O4	19:SX:2:GLY:N	2.34	0.60
45:3H:47:LEU:HD13	45:3H:50:ILE:HD11	1.84	0.60
2:S2:1781:A:O2'	2:S2:1782:G:N7	2.31	0.60
3:SA:40:LYS:NZ	14:SR:101:ASP:OD2	2.34	0.60
26:SJ:112:THR:HG22	26:SJ:123:ILE:HD11	1.84	0.60
2:S2:1536:G:H2'	2:S2:1537:A:H8	1.66	0.60
26:SJ:182:GLN:O	26:SJ:185:ALA:O	2.19	0.60
31:SY:82:ALA:O	31:SY:86:GLU:CB	2.50	0.60
43:3F:184:VAL:HG12	43:3F:232:PHE:HE1	1.66	0.60
50:3N:222:ARG:HG3	50:3N:325:GLN:HG3	1.83	0.60
2:S2:919:A:OP2	28:SN:64:ARG:NH2	2.32	0.59
9:SI:57:ALA:HB2	9:SI:183:GLY:HA2	1.84	0.59
41:3C:637:GLN:HE22	41:3C:683:GLU:HA	1.65	0.59
8:SH:101:LEU:HD13	8:SH:120:ARG:HG2	1.84	0.59
48:3L:341:LEU:HD12	48:3L:343:ILE:H	1.66	0.59
29:SO:44:VAL:HG13	29:SO:53:ILE:HB	1.85	0.59
50:3N:244:ASN:HD21	50:3N:369:ILE:HA	1.66	0.59
15:SS:25:LYS:HD2	15:SS:55:ARG:HD3	1.83	0.59
43:3F:283:LEU:HA	43:3F:286:VAL:HG12	1.83	0.59
2:S2:860:G:H21	30:SW:107:SER:HB2	1.67	0.59
39:3A:443:VAL:HG12	39:3A:493:PHE:HE2	1.67	0.59
49:3M:121:TYR:HE1	49:3M:164:LEU:HB2	1.68	0.59
45:3H:38:GLN:HA	45:3H:201:VAL:HB	1.85	0.59
2:S2:1274:G:OP1	10:SK:1:MET:N	2.34	0.59
6:SE:197:ASN:HB3	6:SE:209:HIS:HB2	1.84	0.59
7:SF:102:LEU:HD23	32:SZ:67:LEU:HD23	1.84	0.59
41:3C:641:ARG:HH21	50:3N:49:THR:HG23	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:3F:323:PHE:HZ	45:3H:345:GLN:HA	1.68	0.59
5:SD:42:THR:HG23	5:SD:45:ARG:H	1.67	0.59
48:3L:480:ASP:HB3	48:3L:486:PHE:HB3	1.83	0.59
7:SF:59:LYS:HB2	7:SF:62:ARG:HE	1.68	0.58
45:3H:242:ASN:HA	45:3H:245:LEU:HD12	1.85	0.58
24:SC:104:ASP:HB3	24:SC:130:ILE:HG13	1.85	0.58
39:3A:373:ASP:HA	39:3A:376:ARG:HG2	1.85	0.58
45:3H:38:GLN:NE2	45:3H:74:ASP:O	2.35	0.58
2:S2:71:G:O6	25:SG:170:ARG:NH2	2.37	0.58
2:S2:528:A:H2'	2:S2:529:A:H8	1.67	0.58
2:S2:1744:G:O2'	2:S2:1789:G:N2	2.35	0.58
49:3M:327:GLN:O	49:3M:330:ARG:NH1	2.36	0.58
2:S2:394:G:H5'	11:SL:81:LYS:HD3	1.85	0.58
2:S2:1358:U:OP2	24:SC:123:ARG:NH2	2.36	0.58
7:SF:35:LEU:HG	7:SF:117:ILE:HG13	1.85	0.58
10:SK:13:GLU:OE2	10:SK:38:LYS:NZ	2.36	0.58
48:3L:470:MET:HB2	48:3L:474:LYS:HB3	1.85	0.58
2:S2:77:A:OP2	25:SG:155:GLN:NE2	2.36	0.58
5:SD:211:VAL:O	14:SR:20:TYR:OH	2.21	0.58
27:SM:126:GLU:OE1	27:SM:129:LYS:NZ	2.37	0.58
39:3A:55:LEU:HD21	39:3A:71:LEU:HD21	1.85	0.58
39:3A:511:LEU:HD23	39:3A:512:GLN:HG3	1.86	0.58
41:3C:94:LYS:HE2	41:3C:99:LYS:HG2	1.85	0.58
11:SL:22:ARG:NH1	11:SL:23:VAL:O	2.36	0.58
39:3A:387:VAL:HA	39:3A:390:LEU:HD23	1.86	0.58
39:3A:572:ARG:NH1	45:3H:111:ASN:OD1	2.36	0.58
42:3E:274:LEU:HA	42:3E:277:LEU:HD12	1.84	0.58
2:S2:399:C:O4'	19:SX:11:ARG:NH1	2.35	0.58
6:SE:66:MET:SD	6:SE:78:THR:OG1	2.62	0.58
39:3A:366:THR:HG23	39:3A:369:GLY:H	1.69	0.58
49:3M:156:LEU:HD23	49:3M:160:LYS:HE2	1.86	0.58
25:SG:74:ARG:NH1	25:SG:96:SER:OG	2.37	0.58
39:3A:514:MET:HG3	39:3A:516:SER:H	1.68	0.58
2:S2:880:G:H3'	2:S2:881:G:H8	1.69	0.58
4:SB:107:ARG:NH1	29:SO:133:THR:O	2.36	0.58
5:SD:106:ARG:HD2	5:SD:173:ARG:HB3	1.86	0.58
43:3F:212:SER:O	43:3F:214:LYS:NZ	2.34	0.58
17:SU:98:VAL:HA	17:SU:101:ILE:HB	1.86	0.57
11:SL:75:GLY:HA3	11:SL:88:ILE:HD12	1.86	0.57
42:3E:255:ARG:HB2	42:3E:292:ILE:HD11	1.85	0.57
2:S2:129:C:H4'	2:S2:130:G:H5'	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SD:94:ARG:NH1	38:CD:142:ASN:OD1	2.36	0.57
30:SW:24:GLN:NE2	30:SW:64:ASN:OD1	2.36	0.57
43:3F:97:VAL:HG12	45:3H:47:LEU:HB3	1.85	0.57
12:SP:67:ALA:HB2	12:SP:73:PRO:HG3	1.87	0.57
24:SC:168:GLY:N	24:SC:179:THR:O	2.34	0.57
43:3F:356:ASN:OD1	45:3H:313:ARG:NH2	2.38	0.57
2:S2:1228:A:H2'	2:S2:1229:G:C8	2.39	0.57
9:SI:87:ASN:HB3	9:SI:90:LEU:HD23	1.85	0.57
39:3A:537:ILE:HD11	43:3F:304:VAL:HG11	1.86	0.57
2:S2:522:A:H5"	26:SJ:145:PRO:HD2	1.85	0.57
2:S2:1374:C:O2'	2:S2:1464:C:O2	2.22	0.57
2:S2:1644:C:H4'	13:SQ:140:ARG:HB2	1.86	0.57
41:3C:480:CYS:SG	41:3C:513:LYS:NZ	2.78	0.57
50:3N:218:ARG:O	50:3N:326:GLN:NE2	2.38	0.57
2:S2:1679:A:N6	7:SF:58:ALA:O	2.38	0.57
7:SF:28:VAL:HG21	7:SF:109:LEU:HB2	1.86	0.57
31:SY:126:GLY:HA2	31:SY:129:LYS:HB2	1.87	0.57
50:3N:245:VAL:HG12	50:3N:276:LEU:HB3	1.87	0.57
50:3N:291:VAL:HG12	50:3N:312:LEU:HD13	1.87	0.57
2:S2:1284:A:N6	2:S2:1313:A:O2'	2.38	0.57
42:3E:102:ARG:O	42:3E:105:GLN:NE2	2.38	0.57
2:S2:1756:C:O2	2:S2:1776:G:C6	2.58	0.56
15:SS:139:THR:O	15:SS:144:ARG:NH2	2.37	0.56
41:3C:507:ILE:HA	41:3C:510:THR:HG22	1.86	0.56
49:3M:213:LYS:HZ1	49:3M:269:LEU:HG	1.70	0.56
2:S2:587:A:H5'	2:S2:592:C:H42	1.70	0.56
2:S2:1277:C:H2'	2:S2:1278:A:H8	1.70	0.56
3:SA:41:ARG:HH11	3:SA:45:GLY:HA2	1.71	0.56
19:SX:128:VAL:HG13	19:SX:138:LYS:HE3	1.88	0.56
24:SC:166:ARG:HB2	24:SC:248:TYR:HD1	1.69	0.56
31:SY:60:PHE:HA	31:SY:70:THR:O	2.05	0.56
46:3I:149:ILE:HA	46:3I:165:HIS:HA	1.87	0.56
49:3M:249:LEU:HD23	49:3M:281:THR:HG21	1.87	0.56
2:S2:1228:A:H2'	2:S2:1229:G:H8	1.69	0.56
4:SB:150:ILE:HG23	14:SR:131:PRO:HA	1.88	0.56
7:SF:125:SER:HB2	7:SF:203:ASN:HD21	1.69	0.56
39:3A:523:LEU:HG	45:3H:347:LEU:HD13	1.88	0.56
40:3B:478:ILE:HG22	40:3B:497:GLN:HG3	1.86	0.56
43:3F:90:ARG:HA	43:3F:235:LEU:HD22	1.87	0.56
2:S2:1566:G:H1	16:ST:97:LYS:HE2	1.70	0.56
45:3H:173:LEU:HA	45:3H:176:VAL:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3M:141:PRO:HB2	49:3M:146:GLN:HG2	1.86	0.56
50:3N:487:ALA:HA	50:3N:490:ILE:HD12	1.88	0.56
2:S2:919:A:O2'	2:S2:1020:A:N6	2.37	0.56
9:SI:7:ASN:HD22	9:SI:7:ASN:C	2.09	0.56
40:3B:545:GLU:HA	40:3B:557:ASP:O	2.05	0.56
41:3C:486:VAL:HG13	41:3C:502:ILE:HD11	1.87	0.56
41:3C:710:ILE:O	41:3C:715:HIS:NE2	2.39	0.56
10:SK:85:LEU:HD12	10:SK:86:PRO:HD2	1.88	0.56
24:SC:178:HIS:ND1	24:SC:221:ASP:OD2	2.32	0.56
44:3G:238:ASN:O	44:3G:290:ARG:NH1	2.39	0.56
2:S2:1076:G:OP2	28:SN:107:LYS:NZ	2.33	0.56
2:S2:1216:C:N4	2:S2:1342:U:OP1	2.33	0.56
2:S2:1228:A:O2'	2:S2:1634:A:N3	2.37	0.56
25:SG:59:GLN:OE1	25:SG:72:ARG:NH2	2.38	0.56
49:3M:104:GLN:NE2	49:3M:108:ASN:OD1	2.39	0.56
49:3M:258:ASN:OD1	49:3M:259:ASN:ND2	2.39	0.56
50:3N:267:ILE:HD11	50:3N:278:PHE:HB3	1.87	0.56
2:S2:94:G:HO2'	2:S2:508:A:HO2'	1.49	0.55
2:S2:748:C:N4	2:S2:795:A:H61	2.03	0.55
2:S2:750:C:H41	2:S2:793:G:H21	1.54	0.55
31:SY:54:VAL:HG22	31:SY:76:TYR:HB2	1.89	0.55
40:3B:549:MET:HA	40:3B:554:VAL:HG22	1.87	0.55
48:3L:364:ASN:HA	48:3L:367:MET:HG2	1.87	0.55
2:S2:379:C:O2	9:SI:5:ARG:NH1	2.40	0.55
2:S2:1422:G:H1'	2:S2:1424:G:C8	2.41	0.55
12:SP:22:LEU:HD11	12:SP:109:PRO:HB3	1.89	0.55
2:S2:444:G:O6	9:SI:26:LYS:NZ	2.39	0.55
2:S2:677:G:OP1	28:SN:124:ARG:NH1	2.39	0.55
41:3C:759:GLU:HA	41:3C:762:ASN:HB2	1.87	0.55
48:3L:333:ILE:HB	48:3L:381:ARG:HG3	1.89	0.55
48:3L:430:ASN:H	48:3L:436:HIS:HE1	1.55	0.55
50:3N:171:LYS:HB2	50:3N:519:VAL:HG13	1.88	0.55
2:S2:1115:U:O2'	2:S2:1117:C:OP2	2.25	0.55
28:SN:49:GLN:HA	28:SN:52:VAL:HG12	1.88	0.55
39:3A:68:LYS:HD2	39:3A:159:GLN:HG2	1.88	0.55
2:S2:205:G:H2'	2:S2:206:G:H8	1.72	0.55
39:3A:407:VAL:HA	39:3A:410:VAL:HG12	1.89	0.55
41:3C:460:GLN:NE2	41:3C:670:GLN:O	2.39	0.55
42:3E:309:GLN:HB2	42:3E:359:LYS:HE3	1.89	0.55
44:3G:269:TYR:HB2	44:3G:284:PHE:HB2	1.88	0.55
47:3K:44:LEU:HD21	48:3L:294:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:3L:256:VAL:HG23	48:3L:260:TYR:HD2	1.71	0.55
50:3N:413:LEU:HB3	50:3N:420:VAL:HG21	1.88	0.55
2:S2:885:U:O4	2:S2:901:G:O6	2.24	0.55
2:S2:943:U:OP1	4:SB:214:LYS:NZ	2.40	0.55
2:S2:1354:G:N2	2:S2:1357:A:OP2	2.38	0.55
3:SA:3:GLY:N	3:SA:56:GLU:OE2	2.38	0.55
29:SO:26:ASN:HD22	29:SO:125:LYS:HD3	1.71	0.55
48:3L:370:LEU:HD13	48:3L:373:ILE:HD11	1.87	0.55
2:S2:922:A:OP2	30:SW:3:ARG:NH2	2.39	0.55
3:SA:108:PHE:HB3	3:SA:140:VAL:HG11	1.88	0.55
25:SG:6:SER:HA	25:SG:13:GLN:HG2	1.87	0.55
41:3C:602:ASP:HB3	41:3C:605:VAL:HG22	1.89	0.55
44:3G:247:SER:HB3	44:3G:250:THR:HG23	1.89	0.55
2:S2:528:A:H2'	2:S2:529:A:C8	2.42	0.55
4:SB:224:GLU:OE1	4:SB:227:LYS:N	2.36	0.55
27:SM:42:LEU:O	27:SM:72:HIS:NE2	2.40	0.55
40:3B:576:LYS:HA	40:3B:593:HIS:HA	1.88	0.55
11:SL:23:VAL:HG12	11:SL:25:LEU:H	1.73	0.54
48:3L:295:GLU:HB2	48:3L:298:GLU:HB2	1.89	0.54
8:SH:36:LEU:O	8:SH:40:LEU:HB3	2.08	0.54
39:3A:87:GLU:OE1	39:3A:91:ARG:NH1	2.40	0.54
39:3A:520:ARG:HB3	45:3H:234:ALA:HB2	1.88	0.54
47:3K:153:ILE:HB	47:3K:157:LEU:HD11	1.90	0.54
2:S2:1753:C:H5'	2:S2:1780:G:H22	1.72	0.54
12:SP:18:ARG:NH1	15:SS:88:LYS:O	2.40	0.54
15:SS:26:ILE:HA	15:SS:56:ALA:HB2	1.90	0.54
41:3C:641:ARG:NH2	50:3N:44:ASP:OD2	2.41	0.54
45:3H:123:THR:HG21	45:3H:128:PHE:HB3	1.90	0.54
2:S2:1838:U:O2	29:SO:150:ARG:NH1	2.40	0.54
9:SI:67:TRP:HD1	9:SI:189:VAL:HG11	1.73	0.54
13:SQ:9:SER:HA	13:SQ:25:CYS:O	2.08	0.54
13:SQ:11:GLN:HA	13:SQ:23:ALA:O	2.07	0.54
25:SG:88:ARG:HB2	25:SG:91:GLU:HB2	1.90	0.54
41:3C:662:GLN:HA	41:3C:665:VAL:HG12	1.90	0.54
42:3E:51:VAL:HG11	42:3E:74:ARG:HB2	1.89	0.54
2:S2:1084:A:OP1	2:S2:1858:G:O2'	2.24	0.54
15:SS:141:ARG:O	15:SS:144:ARG:C	2.45	0.54
26:SJ:3:VAL:HG13	26:SJ:5:ARG:HH11	1.73	0.54
39:3A:310:LEU:HG	39:3A:311:THR:HG22	1.88	0.54
39:3A:420:LYS:HD2	39:3A:421:GLU:HG2	1.89	0.54
2:S2:453:C:O2'	25:SG:92:ARG:O	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1130:G:OP2	2:S2:1130:G:N2	2.29	0.54
3:SA:52:LYS:HB2	14:SR:109:LEU:HD13	1.90	0.54
7:SF:30:ILE:HG23	7:SF:117:ILE:HD11	1.90	0.54
8:SH:80:VAL:HG23	8:SH:92:VAL:HG13	1.90	0.54
17:SU:21:ARG:HD3	17:SU:88:LEU:HD12	1.90	0.54
19:SX:77:ASN:O	19:SX:79:LYS:NZ	2.40	0.54
42:3E:88:THR:HG21	42:3E:134:TYR:HB2	1.90	0.54
48:3L:388:LEU:O	48:3L:392:GLU:N	2.40	0.54
2:S2:752:G:OP1	2:S2:792:C:O2'	2.24	0.54
9:SI:25:ARG:HB2	9:SI:28:GLU:HG3	1.90	0.54
9:SI:151:GLU:HA	9:SI:154:LYS:HG2	1.89	0.54
2:S2:613:G:O2'	2:S2:627:U:OP2	2.25	0.53
2:S2:925:G:O6	2:S2:1017:U:O4	2.26	0.53
19:SX:84:PHE:HB3	19:SX:105:PHE:HE2	1.72	0.53
42:3E:405:ILE:HA	42:3E:408:THR:HG22	1.90	0.53
49:3M:213:LYS:HD3	49:3M:268:LEU:HA	1.91	0.53
2:S2:67:C:OP1	25:SG:160:LYS:NZ	2.41	0.53
2:S2:571:U:O2'	31:SY:60:PHE:O	2.25	0.53
2:S2:1396:A:N7	2:S2:1449:G:O6	2.41	0.53
4:SB:190:PRO:HB3	39:3A:17:GLU:HG3	1.89	0.53
32:SZ:99:LEU:HG	32:SZ:109:TYR:HE1	1.72	0.53
37:4A:344:VAL:O	37:4A:372:ALA:HA	2.09	0.53
2:S2:1203:G:H1	2:S2:1696:C:H5	1.57	0.53
7:SF:90:VAL:HA	7:SF:93:VAL:HG12	1.91	0.53
39:3A:270:GLN:O	39:3A:274:ASN:ND2	2.41	0.53
48:3L:483:GLU:OE1	48:3L:489:GLN:NE2	2.41	0.53
2:S2:1584:G:OP1	16:ST:77:LYS:NZ	2.41	0.53
12:SP:91:GLY:N	12:SP:107:ILE:O	2.41	0.53
2:S2:1024:A:OP2	28:SN:124:ARG:NH2	2.42	0.53
48:3L:232:HIS:O	48:3L:236:ASP:HB2	2.08	0.53
2:S2:835:C:N4	31:SY:9:THR:O	2.42	0.53
39:3A:483:ARG:NH2	41:3C:799:TYR:O	2.41	0.53
41:3C:68:ARG:NH1	41:3C:112:ASP:OD2	2.42	0.53
41:3C:336:ILE:O	41:3C:350:GLN:NE2	2.41	0.53
41:3C:815:LEU:HD12	41:3C:819:HIS:HE1	1.73	0.53
42:3E:262:ILE:O	42:3E:335:ASN:ND2	2.41	0.53
2:S2:795:A:H2'	2:S2:796:G:H8	1.74	0.53
4:SB:82:ARG:NH1	4:SB:191:ASP:OD2	2.42	0.53
41:3C:504:LEU:HB2	41:3C:564:ILE:HG23	1.91	0.53
41:3C:606:GLN:O	41:3C:610:ASN:ND2	2.42	0.53
41:3C:869:ASN:OD1	45:3H:261:ASN:ND2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1562:C:H2'	2:S2:1563:G:C8	2.43	0.53
3:SA:37:TYR:OH	3:SA:57:LYS:NZ	2.42	0.53
15:SS:138:THR:HA	15:SS:141:ARG:HH21	1.74	0.53
41:3C:596:ASP:O	41:3C:599:GLN:NE2	2.42	0.53
42:3E:369:ARG:NH2	48:3L:480:ASP:OD1	2.42	0.53
47:3K:95:GLU:HG3	47:3K:100:ARG:HH21	1.73	0.53
2:S2:289:G:OP1	6:SE:155:LYS:NZ	2.40	0.53
2:S2:562:U:H2'	2:S2:563:G:C8	2.44	0.53
2:S2:969:U:O2	2:S2:971:G:N1	2.42	0.53
5:SD:195:THR:OG1	5:SD:197:LYS:NZ	2.41	0.53
9:SI:48:VAL:HG11	9:SI:54:LYS:HD2	1.91	0.53
31:SY:29:HIS:O	31:SY:67:GLY:HA2	2.09	0.53
41:3C:326:HIS:HA	41:3C:329:VAL:HG12	1.89	0.53
43:3F:121:LEU:HB3	43:3F:167:GLU:HG2	1.91	0.53
47:3K:95:GLU:HA	47:3K:100:ARG:HE	1.74	0.53
2:S2:1548:G:O6	2:S2:1586:U:O4	2.26	0.53
5:SD:119:CYS:HA	5:SD:122:VAL:HG22	1.92	0.53
2:S2:385:G:O2'	9:SI:10:LYS:NZ	2.41	0.52
2:S2:1650:A:H5"	13:SQ:139:ALA:HB2	1.92	0.52
26:SJ:94:LEU:HD23	26:SJ:97:ILE:HD12	1.90	0.52
2:S2:122:G:H21	6:SE:146:THR:HG21	1.74	0.52
37:4A:133:ALA:HA	37:4A:156:VAL:O	2.09	0.52
40:3B:486:ASP:HB2	40:3B:489:ILE:HB	1.91	0.52
43:3F:289:TYR:OH	43:3F:300:ALA:O	2.24	0.52
45:3H:229:GLU:O	45:3H:232:SER:OG	2.28	0.52
2:S2:840:C:H4'	2:S2:841:G:H5"	1.92	0.52
7:SF:81:ARG:O	7:SF:85:LYS:NZ	2.34	0.52
26:SJ:182:GLN:O	26:SJ:185:ALA:C	2.47	0.52
2:S2:1004:U:H2'	2:S2:1005:G:H8	1.74	0.52
9:SI:149:TYR:HA	9:SI:152:ARG:HB2	1.91	0.52
29:SO:97:LEU:HD11	29:SO:112:ALA:HB1	1.91	0.52
45:3H:270:GLN:OE1	45:3H:274:LYS:NZ	2.42	0.52
47:3K:40:ASN:ND2	47:3K:132:THR:O	2.42	0.52
48:3L:256:VAL:O	48:3L:260:TYR:HB2	2.10	0.52
2:S2:880:G:O6	2:S2:906:U:O2	2.28	0.52
2:S2:1232:U:H2'	2:S2:1233:G:C8	2.45	0.52
2:S2:1424:G:H2'	2:S2:1425:G:H8	1.74	0.52
5:SD:213:PRO:HB3	14:SR:20:TYR:HE1	1.75	0.52
39:3A:336:THR:OG1	39:3A:340:ARG:NH1	2.42	0.52
39:3A:428:VAL:HA	39:3A:431:LEU:HD12	1.90	0.52
42:3E:14:LEU:O	50:3N:10:GLN:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:SS:141:ARG:O	15:SS:144:ARG:O	2.27	0.52
26:SJ:67:ASP:HB3	26:SJ:70:ARG:HB3	1.92	0.52
31:SY:41:ARG:NH1	31:SY:52:PRO:O	2.42	0.52
49:3M:294:PHE:HB2	49:3M:330:ARG:HB3	1.92	0.52
12:SP:81:ARG:NH1	12:SP:120:SER:OG	2.42	0.52
31:SY:10:ARG:O	31:SY:11:LYS:C	2.48	0.52
2:S2:1398:G:H22	2:S2:1448:A:H2	1.58	0.52
13:SQ:19:ALA:HB2	13:SQ:75:GLY:HA3	1.92	0.52
45:3H:218:LEU:O	45:3H:222:SER:CB	2.58	0.52
2:S2:1353:A:OP1	3:SA:139:TYR:OH	2.26	0.52
41:3C:381:SER:HA	41:3C:384:ASP:HB2	1.90	0.52
3:SA:184:ARG:HB3	3:SA:191:ARG:HE	1.74	0.52
25:SG:181:THR:HG22	25:SG:184:VAL:HG23	1.92	0.52
26:SJ:103:GLU:O	26:SJ:107:GLU:HG2	2.10	0.52
42:3E:54:ALA:HB1	42:3E:70:LEU:HD21	1.91	0.52
49:3M:285:MET:HA	49:3M:288:GLU:HG2	1.92	0.52
2:S2:71:G:H2'	2:S2:72:C:H4'	1.91	0.51
2:S2:198:U:O2	2:S2:203:G:O6	2.28	0.51
30:SW:32:LYS:O	30:SW:36:ARG:HG2	2.09	0.51
37:4A:274:GLN:HA	37:4A:324:ARG:O	2.09	0.51
41:3C:627:LYS:HA	41:3C:693:LEU:HD21	1.91	0.51
42:3E:52:ASP:OD1	42:3E:52:ASP:N	2.43	0.51
47:3K:20:ARG:HE	47:3K:49:ALA:HB2	1.75	0.51
2:S2:102:A:H4'	2:S2:104:A:C8	2.45	0.51
39:3A:373:ASP:OD1	39:3A:376:ARG:NH1	2.44	0.51
41:3C:773:ASP:OD1	41:3C:774:LYS:N	2.43	0.51
43:3F:95:HIS:HB2	43:3F:98:ILE:HG12	1.92	0.51
2:S2:492:C:OP2	31:SY:107:ARG:NH2	2.43	0.51
24:SC:184:VAL:HG11	24:SC:247:THR:HB	1.92	0.51
50:3N:222:ARG:HH11	50:3N:352:GLU:HA	1.74	0.51
50:3N:245:VAL:HG11	50:3N:495:ILE:HD11	1.93	0.51
50:3N:292:SER:HG	50:3N:404:CYS:HG	1.57	0.51
2:S2:1548:G:C6	2:S2:1586:U:C4	2.98	0.51
16:ST:96:SER:HB3	16:ST:99:VAL:HG22	1.92	0.51
24:SC:272:HIS:O	24:SC:276:THR:OG1	2.21	0.51
39:3A:41:ARG:HH21	39:3A:77:ILE:HD11	1.74	0.51
43:3F:99:LEU:HD22	45:3H:218:LEU:HD21	1.92	0.51
48:3L:486:PHE:HA	48:3L:489:GLN:HB2	1.91	0.51
2:S2:868:G:OP2	2:S2:868:G:N2	2.35	0.51
2:S2:1486:A:H2'	2:S2:1487:A:C8	2.45	0.51
2:S2:1808:U:H2'	2:S2:1809:A:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:SU:26:SER:OG	17:SU:27:ARG:N	2.44	0.51
24:SC:130:ILE:HD13	24:SC:159:LYS:HG2	1.93	0.51
29:SO:98:ARG:HH21	29:SO:134:PRO:HG2	1.75	0.51
41:3C:340:ARG:NE	41:3C:384:ASP:OD2	2.42	0.51
42:3E:193:LYS:HE3	42:3E:214:LEU:HD21	1.91	0.51
50:3N:526:THR:HG23	50:3N:527:PHE:HD1	1.76	0.51
42:3E:372:VAL:HG11	48:3L:481:LEU:HD11	1.93	0.51
50:3N:270:GLN:NE2	50:3N:279:ASP:OD2	2.38	0.51
2:S2:1535:U:O4	7:SF:159:ARG:NE	2.33	0.51
7:SF:49:LEU:HD21	13:SQ:47:LEU:HA	1.93	0.51
8:SH:138:GLU:H	8:SH:159:ASP:HB2	1.76	0.51
16:ST:42:HIS:HB3	16:ST:93:SER:HB2	1.93	0.51
43:3F:251:LEU:HD22	45:3H:162:LEU:HB2	1.93	0.51
11:SL:18:GLN:HA	11:SL:18:GLN:NE2	2.22	0.51
25:SG:85:ARG:HH12	31:SY:118:ARG:NE	2.09	0.51
39:3A:9:GLU:HG3	39:3A:46:ILE:HG12	1.91	0.51
39:3A:398:PHE:HD2	39:3A:509:PRO:HB2	1.76	0.51
47:3K:216:SER:OG	48:3L:534:LYS:NZ	2.38	0.51
2:S2:307:G:N2	9:SI:45:THR:O	2.43	0.51
6:SE:11:ARG:HA	6:SE:28:ALA:HB2	1.93	0.51
39:3A:37:SER:O	39:3A:41:ARG:NH1	2.43	0.51
42:3E:39:GLN:HA	42:3E:42:LEU:HD12	1.92	0.51
50:3N:178:GLN:HA	50:3N:181:LYS:HG2	1.93	0.51
50:3N:269:VAL:O	50:3N:506:TYR:N	2.38	0.51
2:S2:837:A:N6	31:SY:9:THR:OG1	2.41	0.51
2:S2:1036:A:N3	2:S2:1844:U:O2'	2.42	0.51
5:SD:45:ARG:HE	5:SD:83:SER:HA	1.77	0.51
11:SL:119:ASP:O	11:SL:147:LYS:NZ	2.44	0.51
15:SS:68:ILE:HG23	15:SS:72:GLN:HE22	1.76	0.51
49:3M:269:LEU:HD12	49:3M:272:GLN:H	1.75	0.51
2:S2:691:G:N2	2:S2:691:G:OP2	2.37	0.50
2:S2:1536:G:H2'	2:S2:1537:A:C8	2.44	0.50
3:SA:158:ASP:OD1	18:SV:65:SER:OG	2.24	0.50
39:3A:278:LYS:O	39:3A:281:THR:OG1	2.27	0.50
41:3C:672:PRO:HD2	41:3C:675:LEU:HD12	1.91	0.50
41:3C:815:LEU:O	41:3C:819:HIS:ND1	2.30	0.50
42:3E:36:GLU:HG3	50:3N:4:PHE:HB3	1.92	0.50
42:3E:384:ILE:HG13	42:3E:391:VAL:HG13	1.93	0.50
47:3K:101:GLN:NE2	47:3K:122:ASP:OD1	2.44	0.50
2:S2:67:C:OP2	25:SG:172:LYS:NZ	2.44	0.50
2:S2:1758:G:O2'	2:S2:1774:C:N4	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:SG:2:LYS:HB2	25:SG:108:VAL:HG23	1.93	0.50
31:SY:91:LEU:O	31:SY:94:HIS:O	2.30	0.50
39:3A:311:THR:OG1	39:3A:313:ASP:OD1	2.30	0.50
14:SR:104:GLU:HA	14:SR:107:LYS:HG2	1.94	0.50
39:3A:468:GLU:HA	39:3A:471:ILE:HG12	1.94	0.50
42:3E:32:TYR:HB2	50:3N:2:ALA:HA	1.94	0.50
48:3L:332:ALA:HA	48:3L:335:VAL:HG12	1.93	0.50
24:SC:253:PRO:HA	24:SC:256:TRP:CG	2.47	0.50
26:SJ:114:VAL:HG23	26:SJ:119:LEU:HD13	1.94	0.50
39:3A:448:GLN:HB2	49:3M:324:LYS:HB3	1.91	0.50
49:3M:189:LEU:HB3	49:3M:226:LEU:HG	1.92	0.50
50:3N:301:ASP:OD2	50:3N:305:SER:OG	2.21	0.50
2:S2:907:G:H2'	2:S2:908:A:H8	1.75	0.50
2:S2:1280:G:H2'	2:S2:1281:G:H8	1.77	0.50
15:SS:4:VAL:HG13	15:SS:5:ILE:HG22	1.92	0.50
40:3B:507:ARG:HB2	40:3B:547:PHE:HZ	1.76	0.50
45:3H:242:ASN:HD22	45:3H:330:ILE:HG22	1.76	0.50
2:S2:944:A:H5"	29:SO:134:PRO:HB3	1.92	0.50
4:SB:124:HIS:HA	4:SB:137:LEU:O	2.10	0.50
11:SL:17:PHE:O	11:SL:20:LYS:NZ	2.44	0.50
26:SJ:146:SER:O	26:SJ:146:SER:OG	2.26	0.50
39:3A:464:ALA:HA	39:3A:467:LEU:HD12	1.93	0.50
40:3B:306:TYR:HA	40:3B:704:TRP:HA	1.94	0.50
42:3E:78:VAL:HA	42:3E:81:LEU:HD12	1.94	0.50
45:3H:134:LEU:HD11	45:3H:318:LEU:HD11	1.94	0.50
2:S2:561:A:O2'	26:SJ:134:HIS:NE2	2.36	0.50
3:SA:81:ASN:HA	3:SA:84:GLN:HB2	1.92	0.50
3:SA:200:ASP:HB2	14:SR:85:VAL:HG23	1.94	0.50
25:SG:121:ILE:HG21	25:SG:124:LEU:HD22	1.93	0.50
41:3C:424:ILE:HG23	41:3C:425:LEU:H	1.76	0.50
42:3E:365:GLU:OE2	48:3L:474:LYS:NZ	2.44	0.50
49:3M:303:ILE:HB	49:3M:307:ASP:HB3	1.94	0.50
2:S2:1580:A:OP1	17:SU:86:LYS:NZ	2.43	0.50
2:S2:1714:U:H2'	2:S2:1715:A:H8	1.76	0.50
16:ST:11:GLN:HA	16:ST:14:PHE:HB3	1.93	0.50
16:ST:76:THR:HG23	16:ST:94:ARG:HE	1.76	0.50
41:3C:712:LYS:HE2	41:3C:715:HIS:HD2	1.77	0.50
43:3F:272:VAL:HG11	45:3H:336:GLN:HE22	1.77	0.50
48:3L:490:LEU:O	48:3L:494:LYS:HG2	2.12	0.50
2:S2:201:C:H3'	2:S2:202:G:H21	1.78	0.49
6:SE:137:PRO:HB2	6:SE:150:PRO:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:SQ:85:ARG:NH2	13:SQ:118:THR:OG1	2.45	0.49
25:SG:57:ASP:OD1	25:SG:61:PHE:N	2.44	0.49
32:SZ:74:SER:HA	32:SZ:79:ILE:HB	1.94	0.49
2:S2:433:A:H5"	9:SI:22:HIS:HB3	1.94	0.49
2:S2:928:G:H2'	2:S2:929:G:C8	2.47	0.49
6:SE:208:VAL:HG21	6:SE:225:ILE:HD11	1.93	0.49
8:SH:76:GLN:HE21	8:SH:94:PHE:HB2	1.77	0.49
9:SI:92:ARG:O	9:SI:94:LYS:NZ	2.46	0.49
42:3E:136:LYS:HA	50:3N:16:TRP:HZ2	1.76	0.49
44:3G:243:VAL:HG22	44:3G:312:VAL:HG13	1.94	0.49
2:S2:207:G:H3'	2:S2:208:G:H8	1.78	0.49
2:S2:375:U:H2'	2:S2:376:A:C8	2.47	0.49
2:S2:533:A:H2'	2:S2:534:G:C8	2.47	0.49
13:SQ:39:LEU:HG	13:SQ:51:LEU:HD12	1.94	0.49
39:3A:350:GLU:OE1	39:3A:353:ARG:NE	2.44	0.49
45:3H:207:ASN:ND2	45:3H:212:ASN:OD1	2.45	0.49
50:3N:260:ARG:HB2	50:3N:430:TYR:HD2	1.77	0.49
2:S2:1286:G:N2	2:S2:1312:G:O2'	2.42	0.49
12:SP:24:GLN:O	12:SP:28:MET:HG3	2.13	0.49
49:3M:64:MET:HG3	49:3M:105:LEU:HD11	1.94	0.49
50:3N:329:ARG:HB2	50:3N:332:LYS:HD3	1.94	0.49
14:SR:1:MET:SD	14:SR:1:MET:N	2.79	0.49
17:SU:26:SER:HB3	17:SU:32:LEU:HD13	1.93	0.49
41:3C:610:ASN:HD21	50:3N:43:ALA:HB3	1.78	0.49
41:3C:637:GLN:NE2	41:3C:682:LEU:HD23	2.27	0.49
15:SS:124:ARG:O	15:SS:127:TRP:C	2.51	0.49
32:SZ:74:SER:OG	32:SZ:79:ILE:O	2.24	0.49
39:3A:162:ASP:O	39:3A:165:ARG:NE	2.42	0.49
44:3G:243:VAL:HG13	44:3G:312:VAL:HG22	1.94	0.49
47:3K:7:MET:HB2	47:3K:32:TYR:HE1	1.77	0.49
27:SM:18:LEU:HA	27:SM:21:VAL:HG22	1.95	0.49
50:3N:209:ILE:HD11	50:3N:214:GLU:HA	1.94	0.49
50:3N:396:LEU:HD12	50:3N:424:GLU:HG3	1.95	0.49
2:S2:1277:C:H2'	2:S2:1278:A:C8	2.48	0.49
12:SP:56:LEU:HD23	12:SP:60:LEU:HD23	1.95	0.49
13:SQ:117:ARG:HE	13:SQ:121:VAL:HG11	1.77	0.49
24:SC:155:ILE:O	24:SC:159:LYS:HG3	2.12	0.49
24:SC:187:ARG:HH12	24:SC:190:SER:HA	1.77	0.49
2:S2:1217:A:H2'	2:S2:1218:C:C6	2.48	0.49
2:S2:1588:A:H2'	2:S2:1589:A:C8	2.48	0.49
4:SB:143:THR:OG1	4:SB:144:LYS:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SF:88:MET:HG3	7:SF:91:ARG:HH21	1.78	0.49
12:SP:37:TYR:O	12:SP:42:ARG:NH1	2.45	0.49
15:SS:36:VAL:HG13	15:SS:40:TYR:HD2	1.78	0.49
19:SX:110:HIS:ND1	19:SX:111:ALA:O	2.46	0.49
44:3G:248:GLU:OE2	44:3G:279:SER:N	2.44	0.49
48:3L:360:ILE:O	48:3L:364:ASN:ND2	2.46	0.49
48:3L:386:ILE:HG13	48:3L:390:LEU:HD21	1.94	0.49
2:S2:907:G:H2'	2:S2:908:A:C8	2.48	0.48
2:S2:981:A:H2'	2:S2:982:G:C8	2.47	0.48
2:S2:1004:U:H2'	2:S2:1005:G:C8	2.48	0.48
6:SE:118:GLU:OE2	6:SE:237:SER:N	2.39	0.48
26:SJ:128:VAL:O	26:SJ:132:GLN:HG2	2.12	0.48
41:3C:667:ARG:HA	41:3C:670:GLN:HG2	1.94	0.48
43:3F:226:ARG:NH1	49:3M:13:ASP:OD2	2.46	0.48
48:3L:243:GLN:HG2	48:3L:253:PRO:HD2	1.95	0.48
50:3N:245:VAL:HG23	50:3N:371:LEU:HA	1.95	0.48
2:S2:302:A:N3	9:SI:64:ASN:ND2	2.60	0.48
3:SA:89:LYS:HB2	3:SA:202:TYR:CE1	2.48	0.48
15:SS:81:ASP:OD1	15:SS:81:ASP:N	2.45	0.48
47:3K:11:VAL:HG13	47:3K:15:LEU:HD12	1.95	0.48
47:3K:162:LEU:HG	47:3K:170:LEU:HD11	1.95	0.48
48:3L:477:GLY:O	48:3L:481:LEU:HB2	2.13	0.48
2:S2:641:A:O2'	2:S2:645:C:OP1	2.30	0.48
2:S2:1850:A:H2'	2:S2:1851:A:C8	2.48	0.48
6:SE:115:THR:HG23	6:SE:118:GLU:H	1.78	0.48
12:SP:91:GLY:HA2	12:SP:107:ILE:O	2.13	0.48
36:C1:97:LEU:O	36:C1:100:ILE:C	2.52	0.48
39:3A:399:ASN:HA	49:3M:317:ARG:HH21	1.78	0.48
49:3M:251:SER:HA	49:3M:254:LYS:HG2	1.95	0.48
50:3N:432:LEU:HA	50:3N:435:TRP:HE3	1.78	0.48
2:S2:448:A:H5"	9:SI:25:ARG:HA	1.94	0.48
2:S2:1617:G:N1	2:S2:1620:A:OP2	2.46	0.48
5:SD:131:ALA:HA	5:SD:191:PRO:HD3	1.94	0.48
12:SP:91:GLY:CA	12:SP:107:ILE:O	2.61	0.48
28:SN:140:LYS:HZ1	28:SN:142:GLU:HG2	1.79	0.48
39:3A:290:LEU:HA	39:3A:329:ILE:HG12	1.95	0.48
2:S2:197:U:OP2	2:S2:203:G:N2	2.46	0.48
2:S2:940:U:H3	2:S2:1002:U:H3	1.61	0.48
9:SI:152:ARG:O	9:SI:156:ALA:CB	2.61	0.48
27:SM:50:CYS:O	27:SM:76:LEU:HA	2.13	0.48
31:SY:79:LEU:HD11	31:SY:96:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:3B:310:PHE:HA	40:3B:699:PHE:HA	1.95	0.48
48:3L:245:GLU:HB3	48:3L:436:HIS:HD2	1.79	0.48
2:S2:218:U:O2	9:SI:184:ARG:NH1	2.43	0.48
2:S2:303:C:O2	9:SI:184:ARG:NH2	2.44	0.48
2:S2:463:C:O2	2:S2:466:G:N2	2.43	0.48
43:3F:142:SER:HB2	43:3F:145:GLU:HB3	1.95	0.48
47:3K:108:LEU:HB2	47:3K:113:HIS:HB2	1.96	0.48
2:S2:198:U:O2	2:S2:203:G:C6	2.66	0.48
2:S2:1311:C:OP2	27:SM:36:ARG:NH2	2.46	0.48
6:SE:105:THR:O	6:SE:245:ARG:NH2	2.38	0.48
13:SQ:13:PHE:HA	13:SQ:22:VAL:HA	1.96	0.48
41:3C:325:THR:OG1	41:3C:326:HIS:N	2.38	0.48
46:3I:111:SER:HA	46:3I:122:VAL:HA	1.96	0.48
50:3N:383:GLY:HA3	50:3N:387:GLU:HG3	1.95	0.48
2:S2:4:C:H4'	24:SC:207:ALA:HB2	1.95	0.48
2:S2:746:C:HO2'	2:S2:798:G:H1	1.60	0.48
8:SH:69:LEU:HD13	8:SH:96:ALA:HB2	1.96	0.48
16:ST:2:PRO:HA	16:ST:3:GLY:HA3	1.74	0.48
27:SM:92:CYS:HB3	27:SM:94:ILE:HG12	1.96	0.48
45:3H:325:THR:O	45:3H:329:ASN:ND2	2.46	0.48
2:S2:1714:U:H2'	2:S2:1715:A:C8	2.49	0.48
8:SH:126:HIS:HA	8:SH:129:ILE:HG22	1.95	0.48
25:SG:159:ARG:HE	25:SG:173:ALA:HB2	1.78	0.48
30:SW:14:ILE:HG22	30:SW:25:VAL:HG11	1.95	0.48
41:3C:370:VAL:HB	41:3C:431:LEU:HD12	1.95	0.48
42:3E:111:ARG:O	42:3E:111:ARG:NH1	2.46	0.48
42:3E:306:ASP:OD1	42:3E:307:GLY:N	2.47	0.48
2:S2:668:A:H5"	2:S2:1198:G:H4'	1.96	0.48
9:SI:110:ARG:HG3	9:SI:121:LEU:HD23	1.94	0.48
17:SU:97:ILE:HD12	17:SU:100:GLN:HE21	1.79	0.48
24:SC:128:VAL:HG11	24:SC:155:ILE:HG22	1.95	0.48
39:3A:335:ARG:HH21	41:3C:745:LYS:HB3	1.79	0.48
42:3E:422:ILE:HA	42:3E:425:LYS:HG2	1.96	0.48
43:3F:334:LEU:HA	43:3F:337:VAL:HG12	1.94	0.48
45:3H:62:VAL:HG22	45:3H:123:THR:HA	1.96	0.48
45:3H:124:TYR:HE2	45:3H:245:LEU:HD11	1.79	0.48
45:3H:151:ILE:HD13	45:3H:167:TYR:HD2	1.79	0.48
47:3K:84:LEU:O	47:3K:88:MET:HG2	2.13	0.48
2:S2:329:G:H2'	2:S2:330:G:C8	2.48	0.47
2:S2:563:G:H1	2:S2:592:C:H5	1.62	0.47
2:S2:1741:U:N3	2:S2:1794:C:N4	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SL:18:GLN:HE21	11:SL:18:GLN:CA	2.20	0.47
25:SG:65:GLN:HE21	25:SG:65:GLN:HB2	1.55	0.47
26:SJ:149:VAL:HG11	26:SJ:157:ILE:HD11	1.95	0.47
43:3F:169:ILE:HG13	43:3F:195:PRO:HG3	1.96	0.47
2:S2:1543:U:OP2	16:ST:62:ARG:NH2	2.36	0.47
6:SE:175:PHE:HE2	6:SE:198:ARG:HD2	1.78	0.47
27:SM:89:VAL:HG21	27:SM:109:VAL:HG21	1.95	0.47
42:3E:151:LEU:HD11	50:3N:16:TRP:HZ3	1.78	0.47
48:3L:336:PHE:HA	48:3L:339:ILE:HG22	1.97	0.47
3:SA:33:GLN:NE2	18:SV:64:GLU:OE2	2.48	0.47
7:SF:165:ASN:OD1	7:SF:166:ILE:N	2.47	0.47
39:3A:489:ARG:HH12	41:3C:806:THR:HG21	1.79	0.47
41:3C:637:GLN:HE21	41:3C:682:LEU:HD23	1.80	0.47
42:3E:186:MET:HA	42:3E:189:LEU:HD12	1.96	0.47
49:3M:46:ILE:HG21	49:3M:82:LEU:HD11	1.96	0.47
49:3M:120:ARG:HH22	49:3M:150:TRP:HE1	1.62	0.47
49:3M:290:LYS:HE3	49:3M:336:HIS:HA	1.96	0.47
2:S2:996:A:H2'	2:S2:997:A:C8	2.49	0.47
13:SQ:16:LYS:HG2	13:SQ:79:ALA:HA	1.96	0.47
39:3A:324:LEU:HD12	39:3A:424:LEU:HD13	1.95	0.47
41:3C:499:VAL:HA	41:3C:502:ILE:HG22	1.96	0.47
50:3N:21:VAL:HG12	50:3N:26:ARG:NH1	2.29	0.47
2:S2:223:C:H2'	2:S2:224:A:C8	2.49	0.47
2:S2:656:G:N2	2:S2:663:C:H5"	2.29	0.47
38:CD:100:LEU:HD12	38:CD:101:ASP:CA	2.43	0.47
39:3A:559:LYS:O	39:3A:563:LYS:NZ	2.47	0.47
42:3E:399:SER:O	42:3E:403:GLN:NE2	2.48	0.47
47:3K:192:GLN:NE2	48:3L:512:GLU:OE2	2.48	0.47
48:3L:384:GLU:HB3	48:3L:525:LYS:HG3	1.96	0.47
2:S2:503:C:H3'	2:S2:504:G:H8	1.80	0.47
2:S2:557:U:H2'	2:S2:558:G:C8	2.49	0.47
2:S2:1013:U:OP1	2:S2:1129:G:O2'	2.29	0.47
6:SE:45:ILE:HB	6:SE:80:ILE:HG23	1.97	0.47
25:SG:134:GLY:HA3	25:SG:158:VAL:HG11	1.97	0.47
27:SM:23:LYS:HA	27:SM:23:LYS:HD3	1.70	0.47
39:3A:228:MET:HA	39:3A:231:GLU:HG3	1.97	0.47
42:3E:215:ILE:HD11	42:3E:242:TYR:HB3	1.97	0.47
50:3N:200:GLU:HB2	50:3N:328:LEU:HD23	1.96	0.47
2:S2:1230:C:OP1	15:SS:130:ARG:NH2	2.47	0.47
3:SA:82:THR:O	3:SA:82:THR:OG1	2.30	0.47
8:SH:145:ARG:NH2	30:SW:49:GLU:OE1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SI:67:TRP:HE3	9:SI:72:CYS:HB3	1.80	0.47
14:SR:20:TYR:HE2	14:SR:38:ILE:HB	1.80	0.47
14:SR:32:LYS:HD2	14:SR:47:ARG:HH21	1.80	0.47
19:SX:67:ARG:NH2	19:SX:114:ASP:OD2	2.34	0.47
25:SG:137:ARG:HD2	25:SG:178:ARG:HD2	1.96	0.47
27:SM:15:ASN:OD1	27:SM:16:THR:N	2.47	0.47
29:SO:101:GLY:HA2	29:SO:106:LYS:HD3	1.96	0.47
41:3C:582:TRP:HE1	41:3C:616:LEU:HG	1.79	0.47
41:3C:648:GLN:HE22	41:3C:677:ILE:H	1.63	0.47
42:3E:211:ARG:O	42:3E:215:ILE:HG12	2.14	0.47
42:3E:270:ARG:HA	42:3E:273:VAL:HG12	1.97	0.47
43:3F:309:MET:HA	43:3F:312:VAL:HG22	1.97	0.47
48:3L:367:MET:HA	48:3L:370:LEU:HB2	1.97	0.47
48:3L:544:ILE:HA	48:3L:547:ILE:HG12	1.97	0.47
2:S2:375:U:H2'	2:S2:376:A:H8	1.80	0.47
5:SD:70:THR:HG22	5:SD:86:LEU:HD13	1.97	0.47
5:SD:213:PRO:HB3	14:SR:20:TYR:CE1	2.50	0.47
24:SC:70:VAL:HG11	24:SC:93:ILE:HG12	1.97	0.47
26:SJ:38:ARG:NH1	26:SJ:42:GLU:OE2	2.48	0.47
30:SW:11:LEU:HD12	30:SW:74:VAL:HB	1.96	0.47
41:3C:375:LYS:HB3	41:3C:408:LEU:HD12	1.97	0.47
44:3G:289:ARG:HG3	44:3G:291:GLU:H	1.80	0.47
48:3L:279:ARG:HA	48:3L:282:SER:HB2	1.97	0.47
2:S2:145:G:H2'	2:S2:146:G:C8	2.50	0.47
2:S2:186:C:H2'	2:S2:187:G:H8	1.80	0.47
25:SG:216:ARG:O	25:SG:217:MET:HG3	2.15	0.47
39:3A:153:LEU:HD23	39:3A:184:PHE:CE1	2.50	0.47
43:3F:265:LEU:HB2	45:3H:203:ILE:HB	1.95	0.47
45:3H:218:LEU:O	45:3H:222:SER:OG	2.29	0.47
2:S2:165:G:OP2	2:S2:165:G:N2	2.40	0.47
2:S2:1221:G:O2'	2:S2:1676:U:O2	2.28	0.47
2:S2:1570:G:HO2'	2:S2:1614:A:HO2'	1.63	0.47
3:SA:123:VAL:HG22	3:SA:145:ILE:HB	1.97	0.47
7:SF:201:LYS:HA	7:SF:204:ARG:NE	2.30	0.47
25:SG:33:ALA:HA	25:SG:51:ARG:HG3	1.97	0.47
29:SO:12:GLU:HA	29:SO:13:GLN:HA	1.65	0.47
41:3C:695:ILE:HG21	41:3C:744:MET:HG3	1.97	0.47
49:3M:292:ILE:HB	49:3M:332:VAL:HB	1.97	0.47
5:SD:67:ARG:HD3	10:SK:96:ARG:HB2	1.96	0.46
24:SC:271:ASP:OD1	24:SC:271:ASP:N	2.43	0.46
27:SM:80:ASP:OD1	27:SM:81:ASP:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:SM:120:ALA:O	27:SM:124:ILE:HG12	2.15	0.46
32:SZ:99:LEU:HD23	32:SZ:102:LYS:HB2	1.96	0.46
41:3C:570:LEU:HD21	41:3C:594:LEU:HG	1.96	0.46
50:3N:57:ASN:O	50:3N:60:SER:OG	2.34	0.46
2:S2:449:A:N1	25:SG:88:ARG:NH2	2.64	0.46
2:S2:1806:A:H2'	2:S2:1807:C:C6	2.51	0.46
24:SC:183:LYS:HG2	30:SW:95:PRO:HA	1.97	0.46
41:3C:324:ILE:HG22	41:3C:325:THR:H	1.80	0.46
42:3E:413:PHE:O	42:3E:416:GLN:HG3	2.15	0.46
49:3M:120:ARG:HA	49:3M:123:VAL:HG12	1.97	0.46
2:S2:614:C:O2'	2:S2:626:G:N2	2.48	0.46
2:S2:1550:G:H3'	2:S2:1579:A:H61	1.80	0.46
3:SA:110:ASN:HB3	3:SA:113:GLN:HG3	1.98	0.46
8:SH:81:ARG:HG2	8:SH:85:LYS:NZ	2.31	0.46
24:SC:166:ARG:HB2	24:SC:248:TYR:CD1	2.49	0.46
26:SJ:81:LEU:HA	26:SJ:84:ILE:HG22	1.97	0.46
42:3E:189:LEU:O	42:3E:193:LYS:HG2	2.16	0.46
45:3H:123:THR:OG1	45:3H:127:SER:O	2.33	0.46
2:S2:17:C:O2'	2:S2:1194:A:N1	2.45	0.46
2:S2:980:A:H2'	2:S2:981:A:C8	2.51	0.46
2:S2:1819:A:H2'	2:S2:1820:G:C8	2.50	0.46
5:SD:136:VAL:HG22	5:SD:186:VAL:HG23	1.97	0.46
6:SE:15:PRO:HG3	6:SE:39:ARG:HD2	1.97	0.46
31:SY:26:ASP:HA	31:SY:69:THR:O	2.15	0.46
31:SY:62:THR:HA	31:SY:69:THR:HA	1.98	0.46
41:3C:837:GLN:O	41:3C:840:GLN:NE2	2.48	0.46
2:S2:942:G:H2'	2:S2:943:U:C6	2.51	0.46
15:SS:6:PRO:HG2	15:SS:58:GLU:HG2	1.97	0.46
31:SY:12:PHE:HD2	31:SY:23:MET:HE3	1.80	0.46
39:3A:383:VAL:HB	39:3A:388:LYS:HD3	1.97	0.46
44:3G:264:SER:OG	44:3G:288:HIS:ND1	2.42	0.46
45:3H:231:LEU:HA	45:3H:340:LYS:HG2	1.97	0.46
47:3K:29:LEU:HD11	47:3K:46:ALA:HB1	1.98	0.46
49:3M:193:THR:OG1	49:3M:195:ASP:OD1	2.29	0.46
2:S2:1119:A:H5"	2:S2:1120:U:C5	2.50	0.46
4:SB:28:LYS:HA	4:SB:50:THR:HA	1.98	0.46
14:SR:97:GLU:N	14:SR:97:GLU:OE1	2.48	0.46
48:3L:330:GLN:O	48:3L:334:ARG:NH1	2.41	0.46
2:S2:328:U:O2'	2:S2:329:G:O5'	2.33	0.46
2:S2:1579:A:O2'	2:S2:1581:C:OP2	2.26	0.46
7:SF:175:ASP:HA	7:SF:178:ILE:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SI:135:GLU:O	9:SI:139:LYS:HG3	2.16	0.46
13:SQ:53:GLU:O	13:SQ:57:LEU:CB	2.63	0.46
38:CD:100:LEU:HD12	38:CD:100:LEU:C	2.34	0.46
39:3A:244:GLU:HB3	39:3A:246:TRP:CH2	2.50	0.46
42:3E:51:VAL:HG22	42:3E:73:LYS:HZ2	1.81	0.46
42:3E:266:ASP:HB3	42:3E:269:LYS:HE2	1.97	0.46
45:3H:63:VAL:HG22	45:3H:122:SER:OG	2.15	0.46
48:3L:348:SER:HB3	48:3L:352:ARG:HB2	1.97	0.46
2:S2:557:U:H5'	2:S2:558:G:H8	1.80	0.46
42:3E:111:ARG:HA	42:3E:111:ARG:HD2	1.84	0.46
45:3H:281:ARG:O	45:3H:285:ASN:ND2	2.49	0.46
2:S2:1189:A:H2'	2:S2:1190:A:C8	2.51	0.46
11:SL:28:THR:HA	11:SL:29:GLY:HA2	1.62	0.46
18:SV:77:GLY:HA2	18:SV:81:LYS:HE3	1.98	0.46
29:SO:100:THR:HG21	29:SO:104:ARG:HE	1.81	0.46
48:3L:432:HIS:CD2	48:3L:433:PRO:HD2	2.51	0.46
2:S2:441:C:H2'	2:S2:442:C:C6	2.50	0.46
2:S2:880:G:O6	2:S2:906:U:C2	2.69	0.46
2:S2:1752:C:N4	2:S2:1779:G:N2	2.63	0.46
2:S2:1758:G:HO2'	2:S2:1774:C:H41	1.63	0.46
5:SD:67:ARG:O	5:SD:70:THR:OG1	2.29	0.46
16:ST:28:LEU:HA	16:ST:110:LEU:HD21	1.98	0.46
16:ST:56:ARG:HA	16:ST:56:ARG:HD3	1.81	0.46
39:3A:19:LEU:HD21	39:3A:57:LEU:HD21	1.97	0.46
42:3E:163:ARG:HD3	42:3E:164:ASN:HB2	1.97	0.46
42:3E:203:SER:OG	42:3E:206:GLN:OE1	2.28	0.46
45:3H:123:THR:OG1	45:3H:124:TYR:N	2.49	0.46
45:3H:250:VAL:HA	45:3H:253:MET:HG3	1.97	0.46
2:S2:795:A:H2'	2:S2:796:G:C8	2.51	0.45
6:SE:92:ILE:O	6:SE:94:LYS:N	2.47	0.45
13:SQ:50:LYS:HA	13:SQ:50:LYS:HD3	1.82	0.45
26:SJ:121:LYS:HG2	40:3B:510:PHE:HD2	1.80	0.45
32:SZ:98:LYS:NZ	32:SZ:112:ASN:HA	2.31	0.45
42:3E:264:ASN:OD1	42:3E:270:ARG:NH1	2.49	0.45
43:3F:244:THR:HA	43:3F:247:ILE:HG22	1.97	0.45
46:3I:288:ILE:HA	46:3I:304:GLY:HA2	1.97	0.45
2:S2:168:C:H5'	25:SG:131:ARG:HH11	1.81	0.45
30:SW:101:PHE:HA	30:SW:113:HIS:HE1	1.81	0.45
39:3A:267:PRO:HG2	39:3A:272:MET:SD	2.56	0.45
45:3H:245:LEU:HB3	45:3H:249:ARG:HH21	1.81	0.45
45:3H:345:GLN:NE2	45:3H:349:GLU:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:3L:541:ASP:HA	48:3L:544:ILE:HG12	1.97	0.45
8:SH:30:LEU:HD21	8:SH:79:LEU:HD22	1.97	0.45
31:SY:114:MET:HA	31:SY:117:VAL:HG12	1.97	0.45
39:3A:286:SER:HA	41:3C:728:GLY:HA2	1.98	0.45
39:3A:597:ARG:NH1	39:3A:598:GLU:OE2	2.49	0.45
41:3C:659:ASN:HA	41:3C:662:GLN:HE22	1.81	0.45
42:3E:307:GLY:HA2	42:3E:310:LYS:HG2	1.97	0.45
43:3F:327:LEU:HD13	47:3K:204:LYS:HE2	1.98	0.45
43:3F:341:ALA:HB1	45:3H:327:CYS:SG	2.57	0.45
2:S2:198:U:H2'	2:S2:199:C:H2'	1.99	0.45
2:S2:1171:G:O2'	2:S2:1187:G:O6	2.25	0.45
2:S2:1435:C:H41	17:SU:92:HIS:CE1	2.35	0.45
2:S2:1497:G:O6	10:SK:25:LYS:NZ	2.45	0.45
2:S2:1556:A:O2'	2:S2:1557:C:O4'	2.31	0.45
2:S2:1562:C:H5"	16:ST:71:GLY:HA3	1.99	0.45
19:SX:49:GLY:O	19:SX:99:GLU:HA	2.16	0.45
41:3C:418:ILE:HG12	41:3C:438:LEU:HD23	1.97	0.45
42:3E:371:ILE:HA	42:3E:374:LEU:HD12	1.98	0.45
43:3F:306:ARG:NH2	49:3M:219:LEU:HD11	2.31	0.45
45:3H:218:LEU:O	45:3H:222:SER:HB2	2.15	0.45
50:3N:249:ASP:OD2	50:3N:376:GLU:N	2.42	0.45
3:SA:169:HIS:HA	3:SA:203:PHE:CD1	2.51	0.45
12:SP:57:LEU:O	12:SP:61:ARG:HG3	2.17	0.45
15:SS:1:MET:HG3	32:SZ:49:LEU:HD11	1.98	0.45
15:SS:35:GLY:O	15:SS:97:GLN:NE2	2.50	0.45
40:3B:516:LYS:HE2	40:3B:529:LYS:HB3	1.99	0.45
42:3E:189:LEU:HD11	42:3E:221:VAL:HG11	1.98	0.45
42:3E:234:ASP:HA	42:3E:238:TYR:HD2	1.80	0.45
43:3F:242:TYR:H	43:3F:245:GLU:HB2	1.81	0.45
45:3H:113:ASP:OD1	45:3H:113:ASP:N	2.49	0.45
45:3H:262:THR:O	45:3H:266:ASN:ND2	2.50	0.45
50:3N:190:PRO:HA	50:3N:362:ARG:O	2.16	0.45
4:SB:119:THR:H	4:SB:143:THR:HG22	1.81	0.45
11:SL:7:GLU:HG2	11:SL:8:ARG:H	1.81	0.45
15:SS:3:LEU:HD12	15:SS:4:VAL:HG12	1.98	0.45
27:SM:86:GLY:HA3	27:SM:105:GLY:HA3	1.97	0.45
41:3C:557:ALA:HB2	50:3N:27:ASP:HB3	1.98	0.45
43:3F:211:MET:HE2	45:3H:214:LEU:HA	1.99	0.45
44:3G:289:ARG:HE	44:3G:290:ARG:H	1.64	0.45
45:3H:227:LYS:HD2	45:3H:230:LEU:HD23	1.98	0.45
49:3M:205:HIS:HE1	49:3M:236:LEU:HD21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:3N:393:ILE:O	50:3N:394:LYS:HD2	2.17	0.45
2:S2:1421:A:H5"	2:S2:1422:G:C4	2.51	0.45
13:SQ:5:GLY:N	13:SQ:27:ARG:HH22	2.15	0.45
15:SS:59:LEU:HD12	15:SS:63:GLU:HG3	1.98	0.45
26:SJ:140:GLN:NE2	31:SY:64:PHE:O	2.50	0.45
41:3C:480:CYS:HA	41:3C:483:ILE:HG22	1.98	0.45
42:3E:299:LEU:HD13	42:3E:340:ILE:HG22	1.99	0.45
2:S2:186:C:H2'	2:S2:187:G:C8	2.52	0.45
24:SC:77:SER:O	24:SC:80:GLU:N	2.39	0.45
37:4A:245:GLY:O	37:4A:369:LYS:N	2.50	0.45
39:3A:250:PHE:HB2	41:3C:726:LEU:HD12	1.98	0.45
39:3A:367:ARG:O	39:3A:371:ILE:HG12	2.17	0.45
41:3C:96:ILE:HG13	41:3C:97:VAL:H	1.81	0.45
41:3C:515:ASP:OD1	41:3C:515:ASP:N	2.44	0.45
45:3H:269:LYS:HA	45:3H:269:LYS:HD3	1.79	0.45
2:S2:483:C:H5'	19:SX:48:LYS:HG3	1.98	0.45
2:S2:1736:G:H2'	2:S2:1737:G:C8	2.52	0.45
25:SG:85:ARG:HH12	31:SY:118:ARG:HE	1.65	0.45
47:3K:7:MET:HB2	47:3K:32:TYR:CE1	2.52	0.45
50:3N:199:LEU:O	50:3N:335:TYR:N	2.49	0.45
50:3N:215:LYS:HB3	50:3N:215:LYS:HE2	1.72	0.45
2:S2:57:U:OP1	2:S2:504:G:O2'	2.33	0.45
2:S2:1521:C:OP2	15:SS:136:THR:OG1	2.35	0.45
6:SE:71:LYS:HA	6:SE:76:VAL:HA	1.99	0.45
11:SL:22:ARG:NH2	11:SL:28:THR:OG1	2.50	0.45
15:SS:119:ALA:O	15:SS:123:LEU:HB2	2.17	0.45
25:SG:84:TYR:HD1	25:SG:95:LYS:HD2	1.82	0.45
47:3K:90:ASP:O	47:3K:94:GLN:HB2	2.16	0.45
47:3K:139:ARG:NH2	47:3K:169:GLN:OE1	2.50	0.45
48:3L:312:GLN:HA	48:3L:315:THR:HG22	1.98	0.45
50:3N:497:ILE:HA	50:3N:500:LYS:HG2	1.99	0.45
2:S2:380:G:P	9:SI:56:ARG:HH22	2.40	0.44
2:S2:874:G:H2'	2:S2:875:A:H8	1.81	0.44
2:S2:1220:A:N3	2:S2:1677:U:O2'	2.40	0.44
2:S2:1648:G:O2'	2:S2:1674:G:O6	2.23	0.44
13:SQ:13:PHE:HB3	13:SQ:22:VAL:HG12	1.99	0.44
26:SJ:87:LEU:HD13	26:SJ:100:LEU:HD21	1.99	0.44
43:3F:132:THR:OG1	43:3F:167:GLU:OE2	2.35	0.44
2:S2:15:U:H2'	2:S2:16:G:O4'	2.17	0.44
2:S2:152:U:O4'	25:SG:132:ARG:NH1	2.51	0.44
26:SJ:106:LEU:HD23	26:SJ:109:ARG:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:SJ:179:LYS:HA	26:SJ:182:GLN:HG2	1.99	0.44
39:3A:327:LEU:O	39:3A:434:ASN:ND2	2.50	0.44
41:3C:576:HIS:O	41:3C:579:HIS:C	2.56	0.44
42:3E:334:GLU:O	42:3E:338:LEU:HG	2.17	0.44
43:3F:118:GLY:HA3	43:3F:173:TYR:CZ	2.51	0.44
2:S2:562:U:O4	26:SJ:172:ARG:NH2	2.50	0.44
2:S2:690:G:OP2	2:S2:690:G:N2	2.45	0.44
8:SH:87:PHE:HB3	8:SH:90:LYS:HE2	1.99	0.44
11:SL:77:VAL:HG22	11:SL:86:ILE:HD12	1.99	0.44
39:3A:591:LYS:HA	39:3A:591:LYS:HD2	1.82	0.44
40:3B:327:VAL:HA	40:3B:328:SER:HA	1.58	0.44
49:3M:313:ILE:O	49:3M:317:ARG:HG2	2.16	0.44
50:3N:232:ASP:HB3	50:3N:235:ILE:HB	1.99	0.44
2:S2:902:G:O2'	2:S2:903:A:O4'	2.35	0.44
2:S2:1839:U:H2'	2:S2:1840:U:C6	2.52	0.44
13:SQ:113:ILE:HD12	13:SQ:117:ARG:HG3	2.00	0.44
18:SV:3:ASN:HA	24:SC:173:LYS:HD3	2.00	0.44
26:SJ:84:ILE:HD11	26:SJ:148:ILE:HG21	1.99	0.44
41:3C:490:LEU:HD12	41:3C:502:ILE:HG21	1.99	0.44
43:3F:328:ASN:HA	43:3F:331:ILE:HG12	1.99	0.44
49:3M:362:ASN:O	49:3M:366:ASN:ND2	2.50	0.44
50:3N:248:THR:H	50:3N:251:ILE:HD11	1.82	0.44
2:S2:551:U:H2'	2:S2:552:G:C4	2.52	0.44
2:S2:1600:G:H4'	32:SZ:43:LYS:HE3	1.99	0.44
6:SE:229:GLY:HA3	6:SE:234:PRO:HA	2.00	0.44
25:SG:98:ARG:NH2	25:SG:103:ASP:OD1	2.50	0.44
28:SN:140:LYS:NZ	28:SN:142:GLU:HG2	2.32	0.44
50:3N:200:GLU:OE2	50:3N:334:ARG:NH2	2.50	0.44
2:S2:118:C:H1'	2:S2:445:A:C5	2.53	0.44
2:S2:482:G:H5'	19:SX:76:LYS:HB3	1.98	0.44
2:S2:495:U:H2'	2:S2:496:C:O4'	2.18	0.44
2:S2:1268:C:HO2'	12:SP:97:TYR:HH	1.61	0.44
2:S2:1438:A:H2'	2:S2:1439:A:C8	2.52	0.44
9:SI:81:VAL:HG12	9:SI:102:VAL:HG12	2.00	0.44
27:SM:55:ASN:HB2	27:SM:81:ASP:HA	2.00	0.44
31:SY:38:THR:O	31:SY:42:GLU:HG2	2.18	0.44
31:SY:80:ASP:OD1	31:SY:81:TYR:N	2.50	0.44
47:3K:8:ARG:HA	47:3K:8:ARG:HD3	1.80	0.44
48:3L:431:VAL:HA	48:3L:434:ASN:HA	1.99	0.44
2:S2:1566:G:O6	16:ST:101:ARG:NH2	2.51	0.44
18:SV:17:CYS:O	18:SV:21:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:3A:257:HIS:NE2	39:3A:357:THR:O	2.50	0.44
41:3C:504:LEU:HD22	41:3C:564:ILE:HG12	1.99	0.44
41:3C:758:ASN:N	41:3C:758:ASN:OD1	2.49	0.44
43:3F:231:MET:SD	43:3F:231:MET:N	2.91	0.44
50:3N:252:LEU:O	50:3N:256:MET:CB	2.59	0.44
2:S2:1628:C:H2'	2:S2:1629:C:C6	2.52	0.44
2:S2:1744:G:H1'	2:S2:1790:A:N6	2.33	0.44
2:S2:1786:U:O2'	2:S2:1787:G:H8	2.01	0.44
5:SD:195:THR:HG23	5:SD:197:LYS:HG2	2.00	0.44
14:SR:14:ARG:O	14:SR:18:GLU:HG3	2.18	0.44
39:3A:264:LYS:HB3	39:3A:265:LYS:HZ2	1.83	0.44
41:3C:745:LYS:HA	41:3C:745:LYS:HD2	1.81	0.44
50:3N:328:LEU:HD11	50:3N:393:ILE:HG13	2.00	0.44
2:S2:1232:U:H2'	2:S2:1233:G:H8	1.83	0.44
3:SA:51:LEU:HA	3:SA:54:THR:HG22	2.00	0.44
4:SB:175:GLU:HG3	4:SB:193:ILE:HG12	1.99	0.44
5:SD:177:LEU:O	5:SD:179:GLN:N	2.51	0.44
7:SF:104:THR:HG23	7:SF:106:GLU:HB3	1.99	0.44
26:SJ:35:TYR:HD2	26:SJ:112:THR:HG21	1.82	0.44
30:SW:66:THR:HG23	30:SW:68:ARG:HB2	2.00	0.44
2:S2:199:C:O2'	2:S2:201:C:OP2	2.36	0.43
2:S2:1240:A:C6	12:SP:100:LYS:HB2	2.53	0.43
4:SB:41:ILE:HG12	4:SB:76:ASN:HB2	1.99	0.43
26:SJ:51:ALA:O	26:SJ:55:LYS:HG2	2.18	0.43
26:SJ:137:VAL:O	26:SJ:140:GLN:N	2.47	0.43
27:SM:79:VAL:HG22	27:SM:80:ASP:H	1.83	0.43
28:SN:100:LYS:HA	28:SN:103:GLU:HG3	2.00	0.43
39:3A:514:MET:HB3	39:3A:517:GLU:HG3	1.98	0.43
39:3A:571:ARG:HA	39:3A:574:THR:HG22	2.00	0.43
42:3E:223:PHE:HB3	42:3E:324:PHE:HB3	2.00	0.43
43:3F:353:LYS:HE3	48:3L:544:ILE:HD12	2.00	0.43
49:3M:46:ILE:HD11	49:3M:86:LEU:HD13	1.98	0.43
49:3M:49:CYS:SG	49:3M:50:ASP:N	2.91	0.43
2:S2:534:G:H2'	2:S2:535:G:C8	2.54	0.43
2:S2:747:U:N3	2:S2:796:G:N1	2.66	0.43
17:SU:28:ASN:HD21	17:SU:31:SER:HB3	1.84	0.43
24:SC:106:VAL:HG22	24:SC:128:VAL:HG22	1.99	0.43
24:SC:246:LYS:HA	24:SC:249:SER:HB3	1.98	0.43
24:SC:278:THR:HA	24:SC:279:ARG:HA	1.71	0.43
40:3B:566:ILE:N	40:3B:580:LEU:O	2.50	0.43
45:3H:69:GLY:HA3	45:3H:78:ILE:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3H:87:HIS:NE2	45:3H:96:GLU:OE1	2.49	0.43
2:S2:906:U:H2'	2:S2:907:G:H8	1.83	0.43
2:S2:906:U:H2'	2:S2:907:G:C8	2.54	0.43
2:S2:1403:C:N4	2:S2:1433:C:OP1	2.48	0.43
2:S2:1775:U:H2'	2:S2:1776:G:C2	2.53	0.43
13:SQ:143:LYS:HE2	13:SQ:145:TYR:HE1	1.83	0.43
29:SO:14:VAL:HG11	29:SO:17:LEU:HB2	2.00	0.43
31:SY:82:ALA:O	31:SY:86:GLU:HB2	2.18	0.43
39:3A:519:ILE:HG13	39:3A:520:ARG:HD2	1.99	0.43
41:3C:430:ASN:ND2	41:3C:437:PRO:O	2.47	0.43
42:3E:14:LEU:HD21	42:3E:220:PHE:CE2	2.54	0.43
43:3F:93:ARG:HA	43:3F:238:LYS:O	2.18	0.43
45:3H:273:GLN:OE1	45:3H:274:LYS:NZ	2.38	0.43
2:S2:681:U:O2'	2:S2:1160:U:OP1	2.32	0.43
2:S2:1201:U:H2'	2:S2:1202:U:C6	2.54	0.43
2:S2:1777:G:H2'	2:S2:1778:C:H6	1.83	0.43
11:SL:3:ASP:OD1	11:SL:3:ASP:N	2.51	0.43
17:SU:64:THR:HA	17:SU:78:ASP:O	2.19	0.43
19:SX:17:ARG:O	19:SX:21:LYS:HB2	2.19	0.43
24:SC:78:LEU:HB2	24:SC:97:PHE:CD2	2.53	0.43
28:SN:20:ARG:HH21	30:SW:56:HIS:HB3	1.82	0.43
28:SN:36:GLN:HE21	28:SN:36:GLN:HA	1.83	0.43
40:3B:254:LYS:HA	40:3B:260:THR:HA	2.01	0.43
4:SB:150:ILE:O	4:SB:151:ARG:HG2	2.18	0.43
6:SE:89:VAL:HG21	6:SE:119:ALA:HA	1.99	0.43
18:SV:27:LYS:HA	18:SV:27:LYS:HD3	1.77	0.43
24:SC:244:ILE:O	24:SC:247:THR:HG22	2.18	0.43
31:SY:11:LYS:O	31:SY:23:MET:HA	2.18	0.43
32:SZ:92:LEU:HD11	32:SZ:109:TYR:CZ	2.53	0.43
40:3B:548:ARG:HB2	40:3B:555:PRO:HD2	2.00	0.43
42:3E:110:GLY:N	42:3E:158:VAL:O	2.50	0.43
3:SA:123:VAL:HA	3:SA:145:ILE:O	2.18	0.43
7:SF:121:PRO:HB3	7:SF:196:LEU:HD11	2.00	0.43
39:3A:335:ARG:NH2	41:3C:745:LYS:HB3	2.33	0.43
43:3F:312:VAL:HG11	49:3M:350:LEU:HG	2.00	0.43
49:3M:179:ASP:OD1	49:3M:216:ASN:ND2	2.47	0.43
2:S2:65:C:N4	25:SG:134:GLY:O	2.35	0.43
9:SI:67:TRP:HA	9:SI:189:VAL:HG12	2.01	0.43
9:SI:133:GLU:HA	9:SI:136:ILE:HB	2.01	0.43
17:SU:37:ALA:O	17:SU:41:ARG:HG3	2.17	0.43
39:3A:340:ARG:HH21	39:3A:345:ASP:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:3C:430:ASN:HB3	41:3C:438:LEU:HD12	2.01	0.43
42:3E:422:ILE:HG21	43:3F:354:LEU:HD11	2.01	0.43
47:3K:72:LYS:O	47:3K:75:THR:OG1	2.29	0.43
50:3N:216:PRO:HA	50:3N:464:VAL:HG12	2.01	0.43
2:S2:380:G:N1	2:S2:383:G:OP2	2.44	0.43
2:S2:750:C:N4	2:S2:752:G:OP2	2.51	0.43
3:SA:125:THR:HG22	3:SA:175:TRP:HE1	1.82	0.43
8:SH:129:ILE:HD11	8:SH:180:LEU:HD13	2.00	0.43
12:SP:111:MET:HG2	12:SP:119:PHE:CZ	2.53	0.43
31:SY:35:VAL:HG13	31:SY:40:ILE:HD11	2.01	0.43
41:3C:611:ARG:NH2	41:3C:675:LEU:O	2.46	0.43
42:3E:372:VAL:HA	42:3E:375:ILE:HG12	1.99	0.43
43:3F:356:ASN:ND2	45:3H:191:ASN:OD1	2.52	0.43
48:3L:333:ILE:HG13	48:3L:334:ARG:HD2	2.01	0.43
50:3N:179:LEU:HA	50:3N:182:MET:HE1	2.01	0.43
2:S2:1815:A:H3'	2:S2:1816:G:H8	1.84	0.43
17:SU:18:HIS:HB3	17:SU:117:ALA:HB2	2.01	0.43
25:SG:136:LYS:NZ	25:SG:175:LYS:O	2.48	0.43
26:SJ:134:HIS:ND1	26:SJ:163:SER:HB2	2.34	0.43
39:3A:307:ARG:HD2	39:3A:310:LEU:HB3	2.00	0.43
39:3A:520:ARG:HG3	45:3H:233:LEU:HD12	2.00	0.43
50:3N:341:ASN:HB3	50:3N:344:VAL:HG22	2.00	0.43
2:S2:435:A:OP1	9:SI:23:LYS:NZ	2.50	0.43
2:S2:1158:G:H5"	30:SW:76:SER:HB2	2.01	0.43
2:S2:1407:U:H4'	13:SQ:71:ARG:NH2	2.34	0.43
42:3E:59:LYS:HA	42:3E:59:LYS:HD3	1.83	0.43
47:3K:143:CYS:HA	47:3K:146:VAL:HG12	2.01	0.43
2:S2:888:U:H2'	2:S2:900:C:H42	1.83	0.42
2:S2:1781:A:H3'	2:S2:1783:C:C4	2.54	0.42
29:SO:44:VAL:HG11	29:SO:85:CYS:SG	2.59	0.42
39:3A:281:THR:HB	39:3A:285:LYS:NZ	2.34	0.42
41:3C:52:ALA:HA	41:3C:55:LYS:HG2	2.00	0.42
49:3M:109:LEU:O	49:3M:113:MET:HG3	2.19	0.42
2:S2:1222:G:H2'	2:S2:1223:A:C8	2.54	0.42
9:SI:81:VAL:HA	9:SI:102:VAL:HG12	2.01	0.42
11:SL:121:GLN:N	11:SL:124:ASP:OD2	2.43	0.42
12:SP:33:LEU:HD12	12:SP:33:LEU:HA	1.90	0.42
25:SG:142:ARG:HE	25:SG:142:ARG:HB3	1.73	0.42
27:SM:69:CYS:O	27:SM:72:HIS:C	2.57	0.42
41:3C:835:LEU:HA	41:3C:842:VAL:HA	2.01	0.42
41:3C:837:GLN:HB2	42:3E:348:HIS:HD2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3K:26:LEU:HA	47:3K:29:LEU:HB2	2.01	0.42
48:3L:369:ALA:O	48:3L:373:ILE:HG23	2.19	0.42
50:3N:261:SER:O	50:3N:515:GLN:NE2	2.45	0.42
2:S2:1010:G:H2'	2:S2:1011:A:C8	2.54	0.42
13:SQ:89:SER:HB3	13:SQ:112:LEU:HD13	1.99	0.42
14:SR:128:PHE:CD2	14:SR:129:LYS:HG3	2.54	0.42
39:3A:594:LEU:HD22	39:3A:597:ARG:HH21	1.84	0.42
47:3K:48:LEU:HD12	48:3L:292:LYS:HB3	2.02	0.42
49:3M:213:LYS:HD2	49:3M:213:LYS:HA	1.70	0.42
2:S2:656:G:H21	2:S2:663:C:H5"	1.85	0.42
3:SA:77:ILE:HG12	3:SA:99:ILE:HB	2.01	0.42
19:SX:77:ASN:O	19:SX:79:LYS:N	2.52	0.42
25:SG:116:LYS:HE3	25:SG:116:LYS:HB3	1.78	0.42
47:3K:157:LEU:HA	47:3K:160:GLU:HG3	2.01	0.42
2:S2:67:C:H42	25:SG:167:LYS:HB3	1.85	0.42
2:S2:988:C:O2'	4:SB:118:GLN:O	2.37	0.42
15:SS:67:VAL:HA	15:SS:70:ILE:HG22	2.00	0.42
18:SV:66:ASP:OD1	18:SV:67:ASP:N	2.53	0.42
18:SV:80:SER:HB3	18:SV:83:PHE:HB3	2.02	0.42
25:SG:67:VAL:HB	25:SG:99:GLY:HA2	2.00	0.42
39:3A:406:ARG:O	39:3A:409:LYS:HG3	2.19	0.42
41:3C:785:GLU:OE1	41:3C:789:ARG:NH1	2.29	0.42
41:3C:870:ASN:HA	41:3C:873:VAL:HG22	2.00	0.42
42:3E:136:LYS:NZ	50:3N:15:GLY:O	2.51	0.42
43:3F:93:ARG:HB3	43:3F:238:LYS:HZ3	1.84	0.42
44:3G:264:SER:HG	44:3G:288:HIS:CE1	2.33	0.42
48:3L:356:LYS:HD2	48:3L:356:LYS:HA	1.84	0.42
6:SE:19:MET:SD	6:SE:108:ARG:HD2	2.59	0.42
12:SP:44:ARG:O	12:SP:47:ARG:C	2.58	0.42
27:SM:95:ASP:OD1	27:SM:95:ASP:N	2.53	0.42
31:SY:129:LYS:HA	31:SY:129:LYS:HD3	1.78	0.42
39:3A:304:ARG:O	39:3A:308:LYS:NZ	2.39	0.42
41:3C:402:LEU:O	41:3C:406:ASN:ND2	2.52	0.42
41:3C:868:GLU:OE1	41:3C:872:ARG:NH1	2.53	0.42
42:3E:176:GLU:HA	42:3E:179:MET:SD	2.59	0.42
43:3F:345:GLN:NE2	45:3H:327:CYS:SG	2.93	0.42
2:S2:14:C:H5'	24:SC:190:SER:OG	2.19	0.42
2:S2:1758:G:HO2'	2:S2:1774:C:N4	2.16	0.42
7:SF:91:ARG:HD2	32:SZ:103:HIS:CE1	2.55	0.42
12:SP:36:LEU:HD23	12:SP:36:LEU:HA	1.93	0.42
26:SJ:44:TRP:HA	26:SJ:47:LYS:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:SN:99:ARG:NH2	28:SN:119:GLU:OE2	2.43	0.42
39:3A:268:LYS:HB3	39:3A:271:LEU:HG	2.02	0.42
39:3A:321:ARG:HA	39:3A:424:LEU:HD21	2.02	0.42
43:3F:335:LEU:O	43:3F:338:THR:OG1	2.32	0.42
5:SD:87:TYR:CD1	44:3G:307:HIS:HA	2.55	0.42
14:SR:26:ASN:O	14:SR:26:ASN:ND2	2.45	0.42
15:SS:47:LYS:HD3	15:SS:47:LYS:HA	1.86	0.42
26:SJ:121:LYS:H	26:SJ:125:HIS:HD2	1.66	0.42
29:SO:14:VAL:H	29:SO:15:ILE:HA	1.84	0.42
31:SY:39:GLU:HA	31:SY:42:GLU:HG2	2.01	0.42
39:3A:291:PHE:O	39:3A:295:THR:HG23	2.20	0.42
41:3C:400:LYS:HE3	41:3C:400:LYS:HB2	1.80	0.42
41:3C:877:LYS:HG2	45:3H:264:MET:HE1	2.01	0.42
2:S2:78:C:H1'	25:SG:175:LYS:HG3	2.01	0.42
2:S2:1253:A:H4'	2:S2:1254:C:H5"	2.01	0.42
2:S2:1528:G:O2'	2:S2:1666:C:OP1	2.36	0.42
2:S2:1615:U:O4	12:SP:40:ARG:NH1	2.53	0.42
5:SD:95:GLY:HA2	5:SD:101:GLN:NE2	2.35	0.42
16:ST:3:GLY:HA2	16:ST:4:VAL:HA	1.89	0.42
26:SJ:120:ALA:HB1	26:SJ:125:HIS:CD2	2.55	0.42
41:3C:56:ARG:NH1	41:3C:92:LYS:O	2.53	0.42
41:3C:562:ASP:HB2	50:3N:71:TYR:HD1	1.84	0.42
42:3E:309:GLN:OE1	42:3E:313:ARG:NH2	2.53	0.42
47:3K:171:LYS:HD2	47:3K:171:LYS:HA	1.77	0.42
48:3L:225:HIS:O	48:3L:229:ASN:ND2	2.53	0.42
50:3N:425:LEU:HA	50:3N:432:LEU:HD21	2.02	0.42
2:S2:1216:C:HO2'	13:SQ:145:TYR:HH	1.66	0.42
18:SV:73:ALA:HB1	18:SV:78:ILE:HB	2.01	0.42
25:SG:2:LYS:HB3	25:SG:15:LEU:HD11	2.00	0.42
42:3E:369:ARG:HH22	48:3L:477:GLY:HA2	1.84	0.42
42:3E:417:MET:O	42:3E:421:ASN:ND2	2.53	0.42
50:3N:242:GLN:HE21	50:3N:362:ARG:NH2	2.18	0.42
2:S2:1471:C:H42	2:S2:1476:A:N6	2.18	0.41
2:S2:1598:G:H5"	32:SZ:80:ARG:HD3	2.02	0.41
5:SD:170:THR:HG22	5:SD:187:LYS:HG2	2.02	0.41
15:SS:114:LEU:HA	15:SS:117:ILE:HG22	2.02	0.41
17:SU:34:LYS:HE3	17:SU:107:GLU:HG2	2.01	0.41
39:3A:101:THR:HG22	39:3A:149:TRP:HB3	2.02	0.41
40:3B:360:TRP:HA	40:3B:367:GLN:HA	2.02	0.41
41:3C:431:LEU:HG	41:3C:432:HIS:CD2	2.55	0.41
47:3K:18:ILE:HD12	48:3L:262:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:3L:324:LEU:HD11	48:3L:370:LEU:HB3	2.02	0.41
49:3M:185:MET:SD	49:3M:188:LEU:HD22	2.60	0.41
49:3M:344:LYS:HD3	49:3M:344:LYS:HA	1.82	0.41
2:S2:57:U:O2'	2:S2:499:G:N3	2.50	0.41
2:S2:581:U:H4'	31:SY:66:GLY:HA2	2.02	0.41
2:S2:1551:U:OP2	2:S2:1579:A:N6	2.53	0.41
2:S2:1777:G:H2'	2:S2:1778:C:C6	2.54	0.41
4:SB:33:VAL:HG12	4:SB:96:CYS:HB2	2.01	0.41
4:SB:49:VAL:HB	4:SB:62:LEU:HD21	2.02	0.41
9:SI:94:LYS:HE2	9:SI:94:LYS:HB2	1.82	0.41
12:SP:16:THR:OG1	12:SP:17:TYR:N	2.53	0.41
17:SU:19:ARG:HA	17:SU:91:LEU:O	2.19	0.41
42:3E:366:GLU:HA	42:3E:369:ARG:HB2	2.03	0.41
45:3H:233:LEU:HD23	45:3H:340:LYS:HB3	2.02	0.41
45:3H:315:ASP:OD1	45:3H:315:ASP:N	2.53	0.41
48:3L:537:ARG:HH21	48:3L:538:ARG:NH1	2.18	0.41
49:3M:243:ILE:HA	49:3M:247:ALA:HB3	2.02	0.41
50:3N:172:GLU:HG2	50:3N:519:VAL:HG12	2.01	0.41
2:S2:24:C:O2'	2:S2:25:A:O5'	2.38	0.41
2:S2:375:U:H1'	11:SL:7:GLU:OE2	2.20	0.41
2:S2:587:A:OP2	26:SJ:172:ARG:NH2	2.53	0.41
2:S2:811:A:H2'	2:S2:812:A:C8	2.56	0.41
7:SF:44:LYS:HD2	7:SF:44:LYS:HA	1.77	0.41
11:SL:29:GLY:HA3	11:SL:30:LYS:HA	1.62	0.41
16:ST:6:VAL:HG12	16:ST:135:ALA:HB2	2.01	0.41
42:3E:20:PHE:HA	42:3E:23:LEU:HB2	2.03	0.41
43:3F:217:VAL:O	43:3F:233:THR:OG1	2.34	0.41
43:3F:313:ASN:HB2	49:3M:336:HIS:HB2	2.01	0.41
49:3M:239:ASP:OD1	49:3M:240:LEU:N	2.52	0.41
2:S2:1037:G:H4'	2:S2:1845:A:H4'	2.02	0.41
2:S2:1337:C:H4'	17:SU:67:LYS:O	2.21	0.41
4:SB:145:LYS:NZ	14:SR:135:VAL:O	2.33	0.41
7:SF:127:ARG:HB3	7:SF:136:ARG:HB2	2.02	0.41
8:SH:72:PHE:O	8:SH:75:ILE:O	2.37	0.41
9:SI:160:SER:OG	9:SI:161:LEU:N	2.53	0.41
41:3C:463:ASP:HA	41:3C:464:PRO:HD3	1.97	0.41
41:3C:671:VAL:HG23	41:3C:676:HIS:CD2	2.56	0.41
42:3E:262:ILE:HG12	42:3E:335:ASN:HB3	2.03	0.41
43:3F:115:ARG:C	43:3F:139:HIS:HE2	2.24	0.41
2:S2:1226:G:N1	2:S2:1639:G:OP2	2.50	0.41
2:S2:1268:C:O2'	12:SP:97:TYR:OH	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1595:U:H2'	2:S2:1596:U:C6	2.55	0.41
4:SB:152:LYS:HE2	4:SB:152:LYS:HB3	1.83	0.41
8:SH:6:ALA:HB2	8:SH:28:LEU:HD22	2.01	0.41
9:SI:139:LYS:HB2	9:SI:141:ARG:HE	1.85	0.41
12:SP:72:LYS:H	12:SP:72:LYS:HD2	1.85	0.41
41:3C:515:ASP:OD1	41:3C:579:HIS:NE2	2.50	0.41
41:3C:822:ILE:HA	41:3C:825:MET:SD	2.61	0.41
42:3E:99:GLU:OE2	42:3E:116:TYR:OH	2.37	0.41
42:3E:173:LEU:HD11	42:3E:192:LEU:HD22	2.03	0.41
47:3K:8:ARG:NH2	47:3K:42:TYR:O	2.43	0.41
48:3L:243:GLN:HA	48:3L:246:VAL:HG22	2.02	0.41
48:3L:329:TYR:HA	48:3L:332:ALA:HB3	2.01	0.41
50:3N:413:LEU:HB2	50:3N:417:ARG:HH11	1.83	0.41
2:S2:1115:U:H3	2:S2:1118:C:N4	2.17	0.41
2:S2:1748:G:H1	2:S2:1786:U:H3	1.67	0.41
7:SF:124:ASP:N	7:SF:124:ASP:OD1	4.31	0.41
44:3G:241:ILE:HD12	44:3G:297:ILE:HD11	2.03	0.41
45:3H:156:LYS:HA	45:3H:159:GLN:HG3	2.02	0.41
2:S2:639:C:H2'	2:S2:640:A:C8	2.56	0.41
2:S2:674:C:H2'	2:S2:675:U:C6	2.56	0.41
2:S2:1113:A:H2'	2:S2:1114:U:C6	2.56	0.41
2:S2:1540:G:OP1	16:ST:39:LEU:HD23	2.20	0.41
3:SA:222:VAL:HG13	3:SA:223:THR:HG23	2.03	0.41
4:SB:222:LYS:NZ	4:SB:223:PHE:O	2.45	0.41
6:SE:114:ILE:HB	6:SE:118:GLU:HB3	2.02	0.41
8:SH:113:LYS:HD2	8:SH:113:LYS:HA	1.91	0.41
17:SU:24:LEU:HD13	17:SU:112:VAL:HG22	2.03	0.41
17:SU:32:LEU:HD23	17:SU:87:ARG:HD2	2.02	0.41
25:SG:64:LYS:HB2	25:SG:97:VAL:HG11	2.01	0.41
26:SJ:111:GLN:HE21	26:SJ:123:ILE:HG12	1.86	0.41
28:SN:115:LEU:O	28:SN:119:GLU:HG2	2.21	0.41
31:SY:55:ILE:HG23	31:SY:75:ILE:HG13	2.03	0.41
43:3F:98:ILE:O	43:3F:102:ILE:HG12	2.20	0.41
43:3F:139:HIS:CE1	43:3F:141:GLU:HB2	2.55	0.41
49:3M:117:THR:HG23	49:3M:120:ARG:N	2.33	0.41
49:3M:296:THR:HA	49:3M:299:GLN:HG3	2.03	0.41
2:S2:107:A:H2'	2:S2:108:G:C8	2.56	0.41
2:S2:746:C:O2'	2:S2:798:G:N1	2.51	0.41
2:S2:1232:U:H3	2:S2:1526:G:H1	1.69	0.41
3:SA:89:LYS:HD3	14:SR:81:ARG:HH22	1.86	0.41
5:SD:215:ASP:OD1	5:SD:215:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:SQ:40:GLU:OE1	13:SQ:40:GLU:N	2.53	0.41
41:3C:324:ILE:HB	41:3C:328:VAL:HG11	2.02	0.41
50:3N:264:SER:HB3	50:3N:512:PRO:HB3	2.02	0.41
2:S2:839:C:H41	31:SY:10:ARG:HA	1.86	0.41
2:S2:844:U:H2'	2:S2:845:G:H8	1.85	0.41
2:S2:1189:A:H2'	2:S2:1190:A:H8	1.85	0.41
2:S2:1432:U:H4'	2:S2:1437:C:C2	2.56	0.41
8:SH:31:GLU:O	8:SH:37:LYS:HE2	2.21	0.41
10:SK:90:VAL:O	10:SK:95:ARG:NE	2.54	0.41
11:SL:93:LEU:HG	11:SL:102:PHE:HB3	2.02	0.41
14:SR:27:ASP:O	14:SR:31:ASN:ND2	2.30	0.41
17:SU:95:SER:HA	17:SU:98:VAL:HG22	2.03	0.41
25:SG:231:ARG:O	25:SG:235:SER:OG	2.31	0.41
27:SM:25:ALA:HA	27:SM:28:HIS:CE1	2.56	0.41
29:SO:14:VAL:N	29:SO:15:ILE:HA	2.36	0.41
32:SZ:67:LEU:HD23	32:SZ:67:LEU:HA	1.91	0.41
39:3A:53:LYS:HA	39:3A:53:LYS:HD3	1.88	0.41
39:3A:237:LEU:HD11	39:3A:253:VAL:HG13	2.03	0.41
40:3B:548:ARG:HD3	40:3B:555:PRO:HB2	2.01	0.41
42:3E:121:HIS:CD2	42:3E:124:ARG:HH12	2.39	0.41
42:3E:278:VAL:HA	42:3E:281:ILE:HG22	2.03	0.41
48:3L:438:GLU:HA	48:3L:441:LEU:HG	2.03	0.41
48:3L:487:ARG:HA	48:3L:488:ILE:HA	1.72	0.41
49:3M:286:ALA:HA	49:3M:292:ILE:HD11	2.03	0.41
2:S2:51:U:H2'	2:S2:52:G:C8	2.55	0.41
2:S2:921:G:N1	30:SW:28:ARG:HD2	2.36	0.41
2:S2:1259:A:H1'	2:S2:1264:C:N4	2.36	0.41
12:SP:49:LEU:HD23	12:SP:53:GLN:HG3	2.03	0.41
16:ST:73:GLY:HA2	16:ST:76:THR:HG22	2.03	0.41
25:SG:223:LYS:HD2	25:SG:223:LYS:HA	1.89	0.41
27:SM:112:LYS:HE2	27:SM:112:LYS:HB2	1.91	0.41
41:3C:349:ALA:HA	41:3C:352:GLU:HG2	2.03	0.41
45:3H:172:LYS:HD2	45:3H:192:ILE:HD12	2.02	0.41
49:3M:165:LEU:HD12	49:3M:168:LEU:HD12	2.02	0.41
50:3N:61:SER:OG	50:3N:62:GLN:N	2.54	0.41
2:S2:654:A:OP2	2:S2:655:A:O2'	2.27	0.40
2:S2:1284:A:O2'	27:SM:106:CYS:SG	2.66	0.40
10:SK:15:LEU:HD21	10:SK:71:LEU:HD13	2.03	0.40
11:SL:154:GLN:NE2	28:SN:135:LEU:O	2.50	0.40
12:SP:111:MET:HA	15:SS:117:ILE:HD11	2.02	0.40
13:SQ:45:ARG:HD3	13:SQ:45:ARG:HA	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:SQ:96:TYR:HA	13:SQ:100:VAL:HG22	2.01	0.40
25:SG:41:LEU:HD12	25:SG:41:LEU:HA	1.87	0.40
25:SG:135:PRO:HB2	25:SG:141:ILE:HD13	2.02	0.40
39:3A:417:GLN:HB2	39:3A:420:LYS:HB3	2.03	0.40
45:3H:41:ILE:HD11	45:3H:45:VAL:HG11	2.02	0.40
48:3L:322:ALA:O	48:3L:326:MET:HG3	2.21	0.40
49:3M:78:LYS:HA	49:3M:78:LYS:HD2	1.95	0.40
2:S2:150:A:N6	2:S2:169:U:O2	2.54	0.40
2:S2:834:C:H42	2:S2:839:C:H42	1.70	0.40
2:S2:1265:A:O2'	2:S2:1327:G:OP2	2.34	0.40
2:S2:1743:G:H21	2:S2:1791:A:H62	1.69	0.40
3:SA:91:ALA:O	3:SA:94:THR:C	2.60	0.40
7:SF:153:LEU:HD23	7:SF:153:LEU:HA	1.92	0.40
14:SR:114:LEU:HB3	14:SR:115:SER:H	1.57	0.40
19:SX:100:VAL:HG12	19:SX:125:VAL:HA	2.02	0.40
24:SC:176:LYS:HA	24:SC:176:LYS:HD3	1.76	0.40
25:SG:22:ARG:HH21	25:SG:25:ARG:NH1	2.19	0.40
29:SO:36:SER:C	29:SO:38:ASN:H	2.25	0.40
39:3A:446:ILE:HD13	49:3M:316:VAL:HG21	2.03	0.40
42:3E:408:THR:HG21	43:3F:339:TYR:HE2	1.86	0.40
43:3F:97:VAL:HG11	45:3H:51:LYS:HB2	2.03	0.40
43:3F:247:ILE:HG13	45:3H:227:LYS:HE3	2.03	0.40
45:3H:176:VAL:HA	45:3H:179:GLU:HG2	2.02	0.40
45:3H:319:ILE:O	45:3H:323:ILE:HG12	2.22	0.40
50:3N:237:LYS:HA	50:3N:240:LYS:HG2	2.03	0.40
50:3N:248:THR:HG22	50:3N:374:ARG:HB3	2.02	0.40
50:3N:451:TYR:HE2	50:3N:469:GLN:HB2	1.86	0.40
2:S2:595:U:H2'	2:S2:596:U:C6	2.56	0.40
2:S2:1365:G:H2'	2:S2:1366:G:C8	2.55	0.40
2:S2:1623:A:N7	15:SS:132:ARG:HB3	2.36	0.40
3:SA:70:ASN:HA	3:SA:71:PRO:HD2	1.98	0.40
14:SR:59:LYS:HE3	14:SR:59:LYS:HB2	1.91	0.40
25:SG:102:VAL:HG21	25:SG:109:LEU:HD21	2.03	0.40
27:SM:18:LEU:HD22	27:SM:77:ILE:HG21	2.03	0.40
39:3A:326:THR:HA	39:3A:329:ILE:HG13	2.04	0.40
39:3A:414:VAL:O	39:3A:425:GLN:NE2	2.37	0.40
41:3C:70:ALA:HA	41:3C:73:ILE:HG12	2.03	0.40
41:3C:856:ALA:HA	41:3C:859:LEU:HD12	2.02	0.40
45:3H:67:LEU:HD23	45:3H:78:ILE:HG13	2.03	0.40
48:3L:239:ASN:OD1	48:3L:242:ARG:NH1	2.55	0.40
48:3L:301:LYS:HE3	48:3L:302:LYS:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3M:42:LEU:HD13	49:3M:70:LEU:HD11	2.03	0.40
2:S2:582:U:OP1	26:SJ:162:ARG:NH1	2.54	0.40
2:S2:1025:U:OP1	2:S2:1090:C:O2'	2.32	0.40
2:S2:1594:A:H5"	32:SZ:104:ARG:HB3	2.02	0.40
2:S2:1616:U:O4	12:SP:40:ARG:NH1	2.54	0.40
3:SA:9:GLN:HG3	3:SA:10:MET:H	1.85	0.40
9:SI:43:ILE:HA	9:SI:56:ARG:O	2.22	0.40
14:SR:16:ILE:HG22	14:SR:24:LEU:HD11	2.04	0.40
15:SS:124:ARG:O	15:SS:127:TRP:O	2.40	0.40
25:SG:78:SER:OG	25:SG:79:LYS:N	2.53	0.40
39:3A:550:HIS:CE1	45:3H:216:TRP:HB3	2.57	0.40
41:3C:643:LYS:HB3	41:3C:679:LEU:HD21	2.04	0.40
42:3E:88:THR:HG22	42:3E:91:ILE:HD13	2.03	0.40
42:3E:418:LEU:HD11	43:3F:350:LEU:HD22	2.03	0.40
43:3F:265:LEU:N	45:3H:203:ILE:O	2.51	0.40
45:3H:210:LEU:O	45:3H:214:LEU:HD23	2.22	0.40
48:3L:253:PRO:HA	48:3L:256:VAL:HG12	2.02	0.40
2:S2:17:C:H2'	2:S2:18:C:C6	2.57	0.40
2:S2:1177:U:H2'	2:S2:1178:U:C6	2.56	0.40
2:S2:1256:G:C8	17:SU:66:ARG:HB2	2.57	0.40
2:S2:1413:G:H2'	2:S2:1414:A:H8	1.87	0.40
2:S2:1589:A:H2'	2:S2:1590:C:C6	2.57	0.40
4:SB:97:LEU:HB3	4:SB:232:HIS:CD2	2.56	0.40
5:SD:48:ILE:HB	5:SD:86:LEU:HG	2.04	0.40
7:SF:150:ALA:O	7:SF:154:LEU:HG	2.22	0.40
14:SR:67:ARG:HB3	14:SR:68:GLY:H	1.58	0.40
32:SZ:99:LEU:HA	32:SZ:109:TYR:HD1	1.86	0.40
39:3A:129:LEU:HA	39:3A:132:VAL:HG22	2.02	0.40
39:3A:271:LEU:HA	39:3A:274:ASN:HD21	1.87	0.40
39:3A:347:ILE:HG22	39:3A:351:LYS:HE2	2.03	0.40
41:3C:372:VAL:HG13	41:3C:440:VAL:HG11	2.04	0.40
43:3F:150:MET:O	43:3F:154:LYS:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ln	22/25 (88%)	22 (100%)	0	0	100	100
3	SA	219/295 (74%)	205 (94%)	13 (6%)	1 (0%)	29	68
4	SB	212/264 (80%)	193 (91%)	19 (9%)	0	100	100
5	SD	225/243 (93%)	205 (91%)	19 (8%)	1 (0%)	34	71
6	SE	260/263 (99%)	245 (94%)	15 (6%)	0	100	100
7	SF	187/204 (92%)	163 (87%)	24 (13%)	0	100	100
8	SH	182/194 (94%)	157 (86%)	23 (13%)	2 (1%)	14	53
9	SI	204/208 (98%)	179 (88%)	23 (11%)	2 (1%)	15	55
10	SK	96/165 (58%)	85 (88%)	11 (12%)	0	100	100
11	SL	151/158 (96%)	137 (91%)	14 (9%)	0	100	100
12	SP	119/145 (82%)	114 (96%)	5 (4%)	0	100	100
13	SQ	142/146 (97%)	126 (89%)	15 (11%)	1 (1%)	22	61
14	SR	133/135 (98%)	118 (89%)	14 (10%)	1 (1%)	19	59
15	SS	143/152 (94%)	129 (90%)	14 (10%)	0	100	100
16	ST	141/145 (97%)	127 (90%)	13 (9%)	1 (1%)	22	61
17	SU	101/119 (85%)	92 (91%)	9 (9%)	0	100	100
18	SV	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
19	SX	139/143 (97%)	122 (88%)	16 (12%)	1 (1%)	22	61
20	Sa	100/115 (87%)	89 (89%)	10 (10%)	1 (1%)	15	55
21	Sc	62/69 (90%)	45 (73%)	17 (27%)	0	100	100
22	Sd	53/56 (95%)	46 (87%)	7 (13%)	0	100	100
23	Sg	311/317 (98%)	267 (86%)	44 (14%)	0	100	100
24	SC	220/293 (75%)	204 (93%)	16 (7%)	0	100	100
25	SG	235/249 (94%)	218 (93%)	17 (7%)	0	100	100
26	SJ	183/194 (94%)	169 (92%)	14 (8%)	0	100	100
27	SM	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
28	SN	148/151 (98%)	142 (96%)	6 (4%)	0	100	100
29	SO	138/151 (91%)	128 (93%)	9 (6%)	1 (1%)	22	61
30	SW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	SY	129/133 (97%)	117 (91%)	12 (9%)	0	100	100
32	SZ	73/125 (58%)	58 (80%)	15 (20%)	0	100	100
33	Sb	81/84 (96%)	67 (83%)	14 (17%)	0	100	100
34	Se	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
35	Sf	65/156 (42%)	54 (83%)	11 (17%)	0	100	100
36	C1	88/113 (78%)	80 (91%)	8 (9%)	0	100	100
37	4A	334/406 (82%)	319 (96%)	14 (4%)	1 (0%)	41	75
38	CD	343/469 (73%)	327 (95%)	16 (5%)	0	100	100
39	3A	682/1382 (49%)	658 (96%)	23 (3%)	1 (0%)	51	83
40	3B	528/814 (65%)	503 (95%)	25 (5%)	0	100	100
41	3C	615/913 (67%)	581 (94%)	34 (6%)	0	100	100
42	3E	406/445 (91%)	387 (95%)	19 (5%)	0	100	100
43	3F	267/357 (75%)	253 (95%)	14 (5%)	0	100	100
44	3G	82/320 (26%)	79 (96%)	3 (4%)	0	100	100
45	3H	289/352 (82%)	268 (93%)	21 (7%)	0	100	100
46	3I	301/325 (93%)	288 (96%)	13 (4%)	0	100	100
47	3K	215/218 (99%)	200 (93%)	15 (7%)	0	100	100
48	3L	370/564 (66%)	342 (92%)	28 (8%)	0	100	100
49	3M	326/374 (87%)	316 (97%)	10 (3%)	0	100	100
50	3N	441/548 (80%)	420 (95%)	21 (5%)	0	100	100
All	All	10145/13101 (77%)	9404 (93%)	727 (7%)	14 (0%)	54	83

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	SD	178	ARG
8	SH	15	LYS
9	SI	160	SER
37	4A	28	ASN
19	SX	127	ASN
29	SO	140	THR
8	SH	99	ARG
13	SQ	43	GLU
39	3A	351	LYS
3	SA	11	LYS

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Mol	Chain	Res	Type
16	ST	45	LEU
9	SI	124	LYS
14	SR	129	LYS
20	Sa	47	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ln	23/24 (96%)	23 (100%)	0	100	100
3	SA	183/243 (75%)	183 (100%)	0	100	100
4	SB	195/231 (84%)	195 (100%)	0	100	100
5	SD	190/202 (94%)	189 (100%)	1 (0%)	88	95
6	SE	224/225 (100%)	224 (100%)	0	100	100
7	SF	159/170 (94%)	158 (99%)	1 (1%)	86	94
8	SH	166/174 (95%)	166 (100%)	0	100	100
9	SI	178/180 (99%)	177 (99%)	1 (1%)	86	94
10	SK	89/136 (65%)	89 (100%)	0	100	100
11	SL	137/142 (96%)	135 (98%)	2 (2%)	65	84
12	SP	107/130 (82%)	107 (100%)	0	100	100
13	SQ	119/121 (98%)	118 (99%)	1 (1%)	81	91
14	SR	122/122 (100%)	120 (98%)	2 (2%)	62	83
15	SS	126/132 (96%)	126 (100%)	0	100	100
16	ST	113/115 (98%)	110 (97%)	3 (3%)	44	73
17	SU	94/107 (88%)	93 (99%)	1 (1%)	73	88
18	SV	67/67 (100%)	67 (100%)	0	100	100
19	SX	113/115 (98%)	113 (100%)	0	100	100
20	Sa	89/98 (91%)	88 (99%)	1 (1%)	73	88
21	Sc	57/62 (92%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	Sd	48/49 (98%)	47 (98%)	1 (2%)	53 78
23	Sg	272/275 (99%)	272 (100%)	0	100 100
24	SC	188/225 (84%)	188 (100%)	0	100 100
25	SG	207/218 (95%)	206 (100%)	1 (0%)	88 95
26	SJ	161/168 (96%)	161 (100%)	0	100 100
27	SM	102/108 (94%)	100 (98%)	2 (2%)	55 79
28	SN	130/131 (99%)	128 (98%)	2 (2%)	65 84
29	SO	110/119 (92%)	106 (96%)	4 (4%)	35 67
30	SW	112/113 (99%)	112 (100%)	0	100 100
31	SY	113/115 (98%)	110 (97%)	3 (3%)	44 73
32	SZ	66/103 (64%)	65 (98%)	1 (2%)	65 84
33	Sb	75/76 (99%)	75 (100%)	0	100 100
34	Se	47/48 (98%)	47 (100%)	0	100 100
35	Sf	60/140 (43%)	59 (98%)	1 (2%)	60 82
38	CD	37/404 (9%)	37 (100%)	0	100 100
39	3A	544/1259 (43%)	540 (99%)	4 (1%)	84 93
40	3B	90/702 (13%)	89 (99%)	1 (1%)	73 88
41	3C	553/811 (68%)	553 (100%)	0	100 100
42	3E	380/406 (94%)	378 (100%)	2 (0%)	88 95
43	3F	237/289 (82%)	236 (100%)	1 (0%)	91 97
44	3G	70/277 (25%)	70 (100%)	0	100 100
45	3H	269/310 (87%)	266 (99%)	3 (1%)	73 88
47	3K	192/193 (100%)	192 (100%)	0	100 100
48	3L	342/515 (66%)	337 (98%)	5 (2%)	65 84
49	3M	304/335 (91%)	303 (100%)	1 (0%)	92 97
50	3N	398/494 (81%)	396 (100%)	2 (0%)	88 95
All	All	7658/10679 (72%)	7611 (99%)	47 (1%)	86 94

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	SD	76	ARG
7	SF	36	GLN

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Mol	Chain	Res	Type
9	SI	7	ASN
11	SL	18	GLN
11	SL	69	ARG
13	SQ	106	LYS
14	SR	26	ASN
14	SR	72	LYS
16	ST	41	LYS
16	ST	122	LYS
16	ST	142	ASN
17	SU	34	LYS
20	Sa	51	ARG
22	Sd	26	ASN
25	SG	119	LYS
27	SM	33	ARG
27	SM	121	LYS
28	SN	36	GLN
28	SN	42	LYS
29	SO	66	ARG
29	SO	67	ASP
29	SO	68	GLU
29	SO	105	THR
31	SY	94	HIS
31	SY	118	ARG
31	SY	132	LYS
32	SZ	52	LYS
35	Sf	104	LYS
39	3A	353	ARG
39	3A	409	LYS
39	3A	546	LYS
39	3A	559	LYS
40	3B	497	GLN
42	3E	133	ARG
42	3E	163	ARG
43	3F	126	LYS
45	3H	37	LYS
45	3H	189	LYS
45	3H	249	ARG
48	3L	220	LYS
48	3L	301	LYS
48	3L	347	LYS
48	3L	407	GLN
48	3L	496	LYS

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Mol	Chain	Res	Type
49	3M	183	LYS
50	3N	53	LYS
50	3N	183	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
7	SF	203	ASN
10	SK	7	ASN
11	SL	18	GLN
12	SP	98	ASN
15	SS	85	ASN
15	SS	97	GLN
18	SV	35	ASN
23	Sg	104	HIS
24	SC	267	GLN
25	SG	110	ASN
25	SG	155	GLN
26	SJ	113	GLN
28	SN	36	GLN
39	3A	270	GLN
39	3A	512	GLN
41	3C	630	HIS
41	3C	637	GLN
41	3C	869	ASN
43	3F	332	ASN
43	3F	347	GLN
45	3H	38	GLN
45	3H	261	ASN
48	3L	364	ASN
48	3L	432	HIS
48	3L	436	HIS
49	3M	199	GLN
49	3M	205	HIS
49	3M	366	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	S2	1701/1869 (91%)	433 (25%)	4 (0%)

All (433) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	S2	2	A
2	S2	4	C
2	S2	17	C
2	S2	23	G
2	S2	25	A
2	S2	33	G
2	S2	42	A
2	S2	44	U
2	S2	46	A
2	S2	56	G
2	S2	58	C
2	S2	59	U
2	S2	64	A
2	S2	65	C
2	S2	67	C
2	S2	68	A
2	S2	72	C
2	S2	73	C
2	S2	74	G
2	S2	76	U
2	S2	92	A
2	S2	100	U
2	S2	103	A
2	S2	113	G
2	S2	115	U
2	S2	126	G
2	S2	127	C
2	S2	129	C
2	S2	130	G
2	S2	139	C
2	S2	143	U
2	S2	145	G
2	S2	155	G
2	S2	158	A
2	S2	161	U
2	S2	162	C
2	S2	163	U
2	S2	170	A
2	S2	177	G
2	S2	179	C
2	S2	182	C
2	S2	184	G

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Mol	Chain	Res	Type
2	S2	190	G
2	S2	196	C
2	S2	197	U
2	S2	198	U
2	S2	200	G
2	S2	203	G
2	S2	204	G
2	S2	206	G
2	S2	207	G
2	S2	208	G
2	S2	212	C
2	S2	214	U
2	S2	220	U
2	S2	224	A
2	S2	290	U
2	S2	291	G
2	S2	292	A
2	S2	293	C
2	S2	295	C
2	S2	306	C
2	S2	307	G
2	S2	308	G
2	S2	309	G
2	S2	314	U
2	S2	318	A
2	S2	319	C
2	S2	322	C
2	S2	323	C
2	S2	324	C
2	S2	325	C
2	S2	326	C
2	S2	327	G
2	S2	328	U
2	S2	329	G
2	S2	332	G
2	S2	343	A
2	S2	361	U
2	S2	362	C
2	S2	363	A
2	S2	364	A
2	S2	368	U
2	S2	369	C

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Mol	Chain	Res	Type
2	S2	370	G
2	S2	375	U
2	S2	381	C
2	S2	385	G
2	S2	386	C
2	S2	400	C
2	S2	409	C
2	S2	421	G
2	S2	429	C
2	S2	436	G
2	S2	438	G
2	S2	448	A
2	S2	449	A
2	S2	450	C
2	S2	452	G
2	S2	464	A
2	S2	465	A
2	S2	471	G
2	S2	472	C
2	S2	473	A
2	S2	474	G
2	S2	483	C
2	S2	487	U
2	S2	488	U
2	S2	492	C
2	S2	502	C
2	S2	503	C
2	S2	512	A
2	S2	517	C
2	S2	518	G
2	S2	525	A
2	S2	530	U
2	S2	531	A
2	S2	532	C
2	S2	533	A
2	S2	536	A
2	S2	537	C
2	S2	538	U
2	S2	540	U
2	S2	542	U
2	S2	546	G
2	S2	547	G

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Mol	Chain	Res	Type
2	S2	550	C
2	S2	551	U
2	S2	555	A
2	S2	556	U
2	S2	557	U
2	S2	558	G
2	S2	559	G
2	S2	563	G
2	S2	566	U
2	S2	576	A
2	S2	583	A
2	S2	587	A
2	S2	589	G
2	S2	590	A
2	S2	591	U
2	S2	594	A
2	S2	596	U
2	S2	597	G
2	S2	603	C
2	S2	605	A
2	S2	606	G
2	S2	608	C
2	S2	610	G
2	S2	614	C
2	S2	623	G
2	S2	625	G
2	S2	626	G
2	S2	627	U
2	S2	628	A
2	S2	643	A
2	S2	644	G
2	S2	655	A
2	S2	657	U
2	S2	659	G
2	S2	660	C
2	S2	664	A
2	S2	666	U
2	S2	668	A
2	S2	669	A
2	S2	671	A
2	S2	672	A
2	S2	673	G

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Mol	Chain	Res	Type
2	S2	688	U
2	S2	689	U
2	S2	749	U
2	S2	751	G
2	S2	752	G
2	S2	788	G
2	S2	790	C
2	S2	791	C
2	S2	792	C
2	S2	794	A
2	S2	797	C
2	S2	798	G
2	S2	799	U
2	S2	811	A
2	S2	821	G
2	S2	822	U
2	S2	823	U
2	S2	824	C
2	S2	830	A
2	S2	835	C
2	S2	836	G
2	S2	837	A
2	S2	838	G
2	S2	839	C
2	S2	841	G
2	S2	842	C
2	S2	846	G
2	S2	847	A
2	S2	870	A
2	S2	874	G
2	S2	878	G
2	S2	880	G
2	S2	883	U
2	S2	885	U
2	S2	888	U
2	S2	889	U
2	S2	891	G
2	S2	892	U
2	S2	896	U
2	S2	897	U
2	S2	898	U
2	S2	899	U

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Mol	Chain	Res	Type
2	S2	900	C
2	S2	901	G
2	S2	903	A
2	S2	904	A
2	S2	913	A
2	S2	914	U
2	S2	916	A
2	S2	917	U
2	S2	920	A
2	S2	922	A
2	S2	930	C
2	S2	933	G
2	S2	934	G
2	S2	943	U
2	S2	954	U
2	S2	955	A
2	S2	971	G
2	S2	972	A
2	S2	982	G
2	S2	989	C
2	S2	990	A
2	S2	992	A
2	S2	999	G
2	S2	1001	A
2	S2	1008	A
2	S2	1017	U
2	S2	1023	A
2	S2	1033	G
2	S2	1044	G
2	S2	1045	U
2	S2	1057	C
2	S2	1061	U
2	S2	1062	A
2	S2	1076	G
2	S2	1078	C
2	S2	1083	A
2	S2	1085	C
2	S2	1088	U
2	S2	1109	C
2	S2	1114	U
2	S2	1115	U
2	S2	1116	C

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Mol	Chain	Res	Type
2	S2	1118	C
2	S2	1119	A
2	S2	1120	U
2	S2	1121	G
2	S2	1132	C
2	S2	1138	C
2	S2	1140	G
2	S2	1150	A
2	S2	1153	C
2	S2	1154	U
2	S2	1157	G
2	S2	1165	G
2	S2	1170	A
2	S2	1195	A
2	S2	1200	A
2	S2	1203	G
2	S2	1207	G
2	S2	1208	A
2	S2	1215	C
2	S2	1216	C
2	S2	1217	A
2	S2	1224	G
2	S2	1237	C
2	S2	1242	U
2	S2	1243	U
2	S2	1251	A
2	S2	1253	A
2	S2	1256	G
2	S2	1257	G
2	S2	1259	A
2	S2	1264	C
2	S2	1274	G
2	S2	1275	G
2	S2	1283	C
2	S2	1285	G
2	S2	1286	G
2	S2	1293	A
2	S2	1294	G
2	S2	1295	A
2	S2	1298	G
2	S2	1301	A
2	S2	1302	G

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Mol	Chain	Res	Type
2	S2	1303	C
2	S2	1308	U
2	S2	1313	A
2	S2	1320	G
2	S2	1321	G
2	S2	1331	C
2	S2	1332	A
2	S2	1342	U
2	S2	1348	G
2	S2	1363	C
2	S2	1371	U
2	S2	1372	U
2	S2	1373	C
2	S2	1376	A
2	S2	1378	A
2	S2	1403	C
2	S2	1404	U
2	S2	1417	C
2	S2	1419	C
2	S2	1421	A
2	S2	1422	G
2	S2	1423	C
2	S2	1435	C
2	S2	1436	C
2	S2	1447	G
2	S2	1449	G
2	S2	1450	G
2	S2	1452	A
2	S2	1454	A
2	S2	1463	U
2	S2	1476	A
2	S2	1480	A
2	S2	1486	A
2	S2	1488	C
2	S2	1489	A
2	S2	1490	G
2	S2	1493	C
2	S2	1494	U
2	S2	1495	G
2	S2	1497	G
2	S2	1498	A
2	S2	1508	A

Continued on next page...

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Mol	Chain	Res	Type
2	S2	1509	U
2	S2	1517	G
2	S2	1520	G
2	S2	1521	C
2	S2	1522	A
2	S2	1533	A
2	S2	1537	A
2	S2	1544	C
2	S2	1552	G
2	S2	1553	C
2	S2	1556	A
2	S2	1563	G
2	S2	1570	G
2	S2	1578	U
2	S2	1580	A
2	S2	1585	U
2	S2	1587	G
2	S2	1588	A
2	S2	1599	U
2	S2	1600	G
2	S2	1601	A
2	S2	1606	G
2	S2	1621	U
2	S2	1623	A
2	S2	1632	G
2	S2	1634	A
2	S2	1639	G
2	S2	1640	A
2	S2	1648	G
2	S2	1654	G
2	S2	1663	A
2	S2	1665	G
2	S2	1671	G
2	S2	1679	A
2	S2	1680	G
2	S2	1695	A
2	S2	1696	C
2	S2	1700	C
2	S2	1702	G
2	S2	1709	G
2	S2	1719	A
2	S2	1722	G

Continued on next page...

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Mol	Chain	Res	Type
2	S2	1723	G
2	S2	1726	G
2	S2	1728	U
2	S2	1729	U
2	S2	1730	U
2	S2	1742	C
2	S2	1743	G
2	S2	1744	G
2	S2	1746	U
2	S2	1749	G
2	S2	1752	C
2	S2	1753	C
2	S2	1754	G
2	S2	1756	C
2	S2	1757	G
2	S2	1758	G
2	S2	1760	G
2	S2	1761	U
2	S2	1771	G
2	S2	1772	C
2	S2	1773	C
2	S2	1774	C
2	S2	1775	U
2	S2	1776	G
2	S2	1777	G
2	S2	1782	G
2	S2	1783	C
2	S2	1784	G
2	S2	1786	U
2	S2	1787	G
2	S2	1806	A
2	S2	1808	U
2	S2	1809	A
2	S2	1810	U
2	S2	1812	U
2	S2	1813	A
2	S2	1820	G
2	S2	1822	A
2	S2	1823	A
2	S2	1824	A
2	S2	1825	A
2	S2	1826	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S2	1827	U
2	S2	1829	G
2	S2	1831	A
2	S2	1835	A
2	S2	1838	U
2	S2	1848	U
2	S2	1849	G
2	S2	1852	C
2	S2	1861	G
2	S2	1862	G
2	S2	1863	A
2	S2	1864	U
2	S2	1865	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	S2	112	U
2	S2	291	G
2	S2	688	U
2	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 26 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

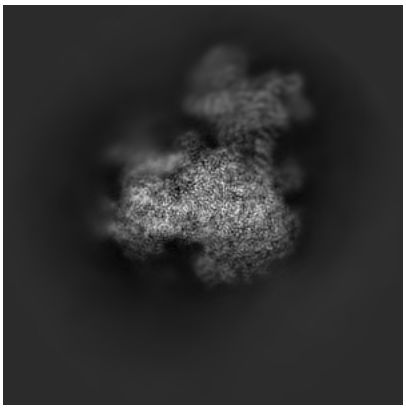
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38754. These allow visual inspection of the internal detail of the map and identification of artifacts.

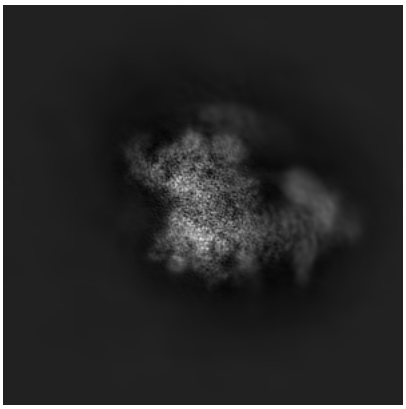
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

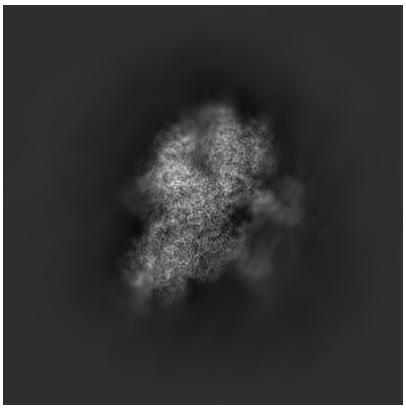
6.1.1 Primary map



X

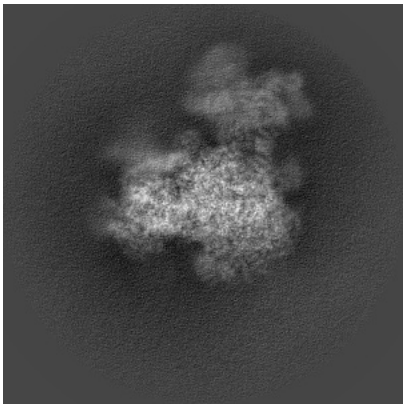


Y

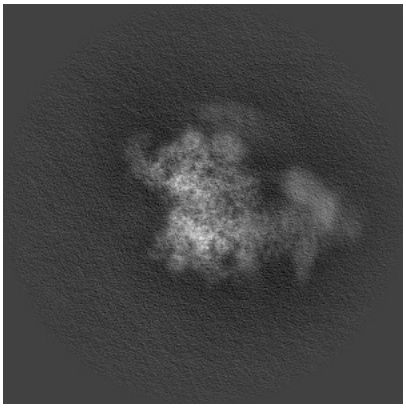


Z

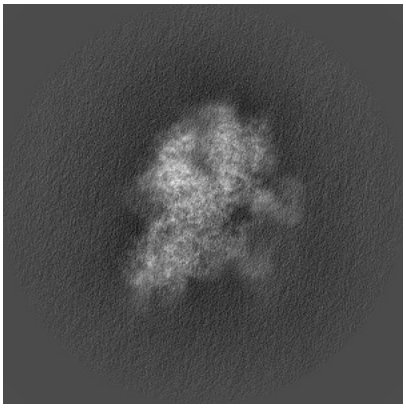
6.1.2 Raw map



X



Y



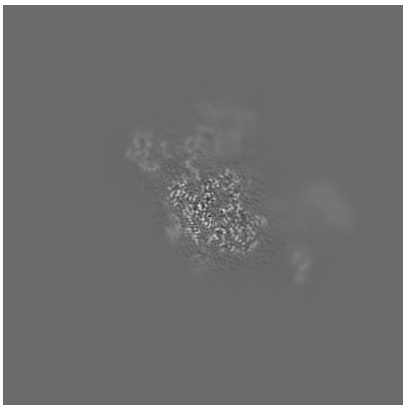
Z

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

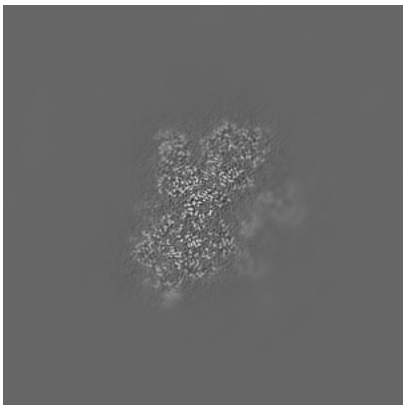
6.2 Central slices (i)

6.2.1 Primary map

X Index: 210

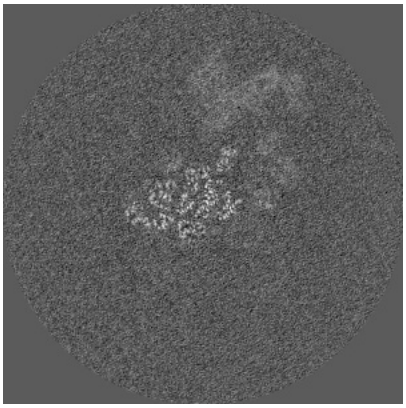


Y Index: 210

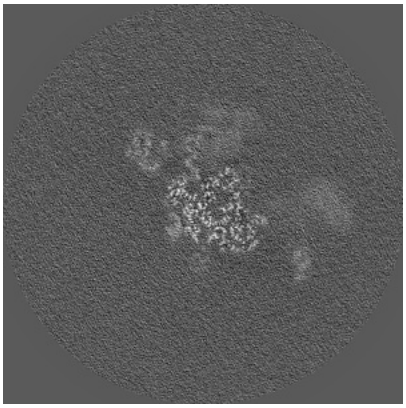


Z Index: 210

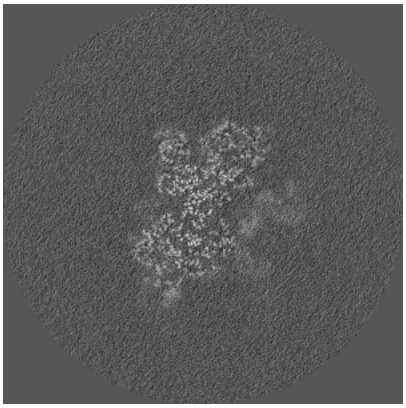
6.2.2 Raw map



X Index: 210



Y Index: 210

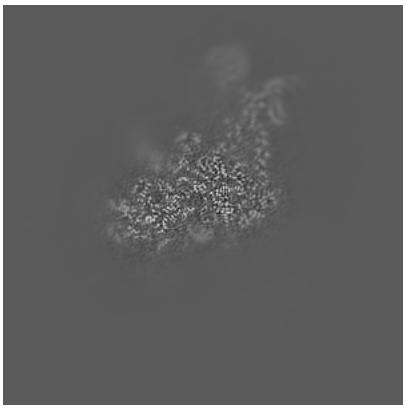


Z Index: 210

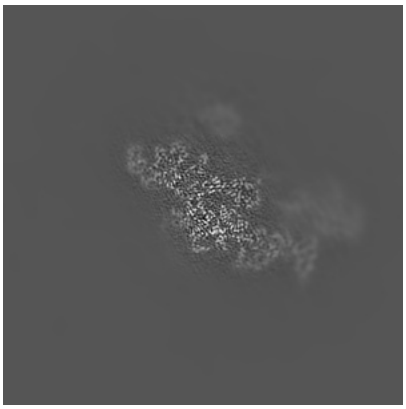
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

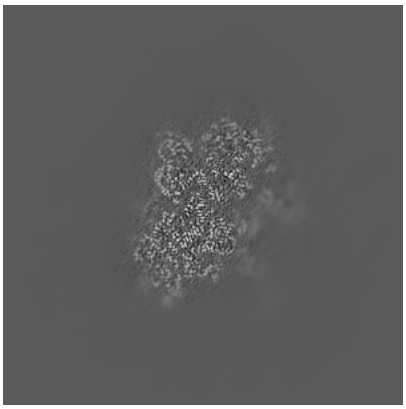
6.3.1 Primary map



X Index: 183

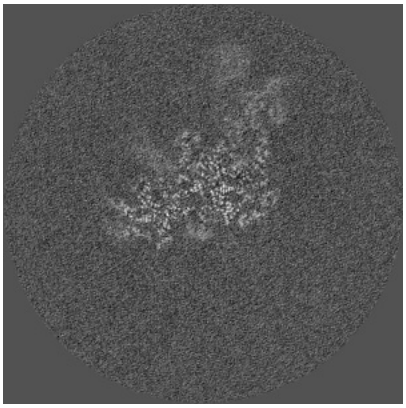


Y Index: 231

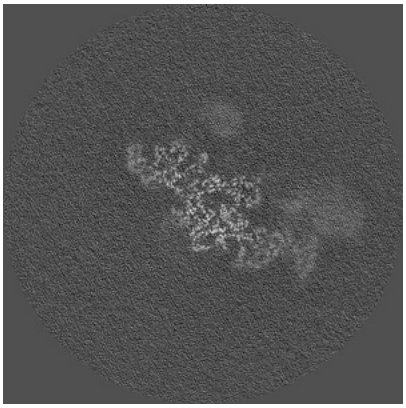


Z Index: 207

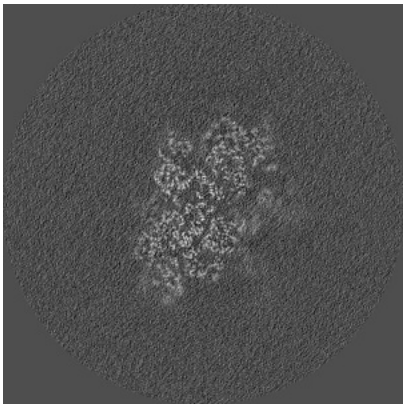
6.3.2 Raw map



X Index: 182



Y Index: 231

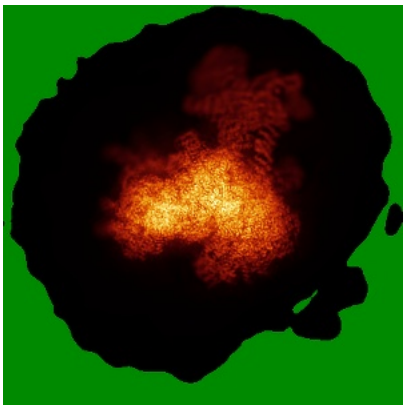


Z Index: 206

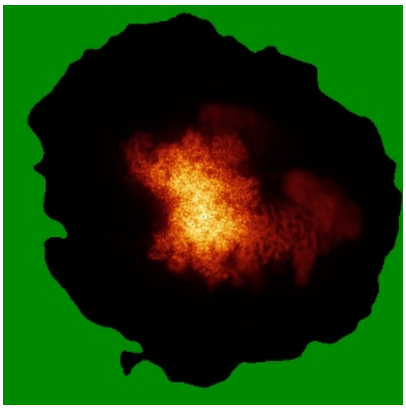
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

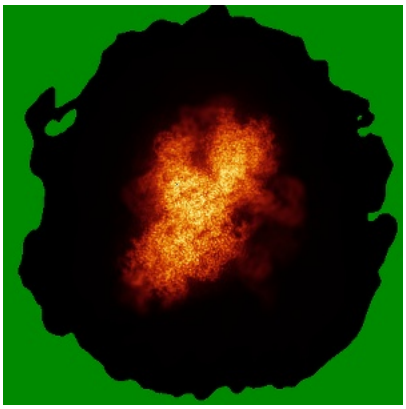
6.4.1 Primary map



X

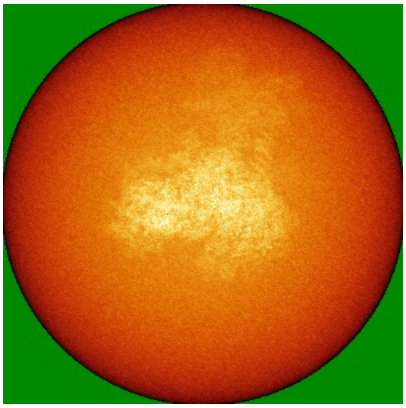


Y

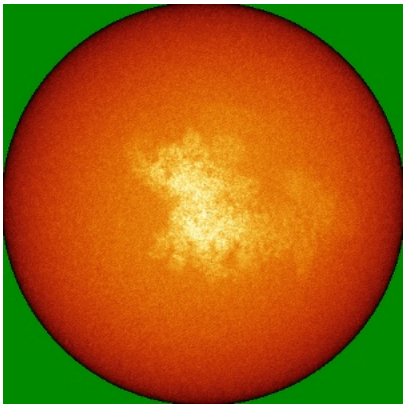


Z

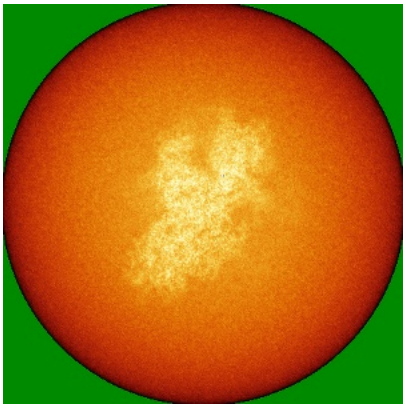
6.4.2 Raw map



X



Y

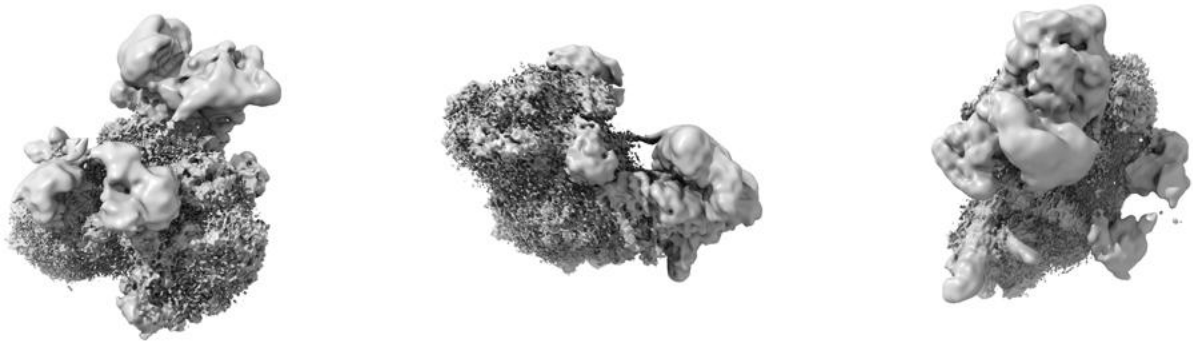


Z

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)

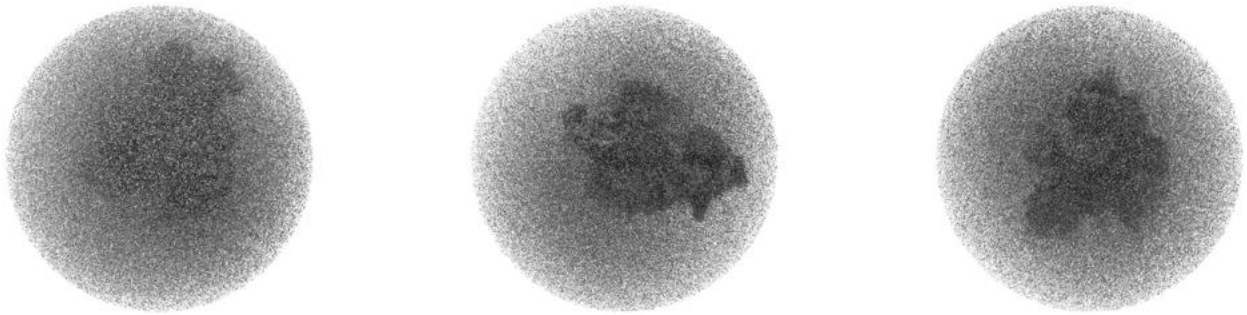
6.5.1 Primary map



X Y Z

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



X Y Z

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.

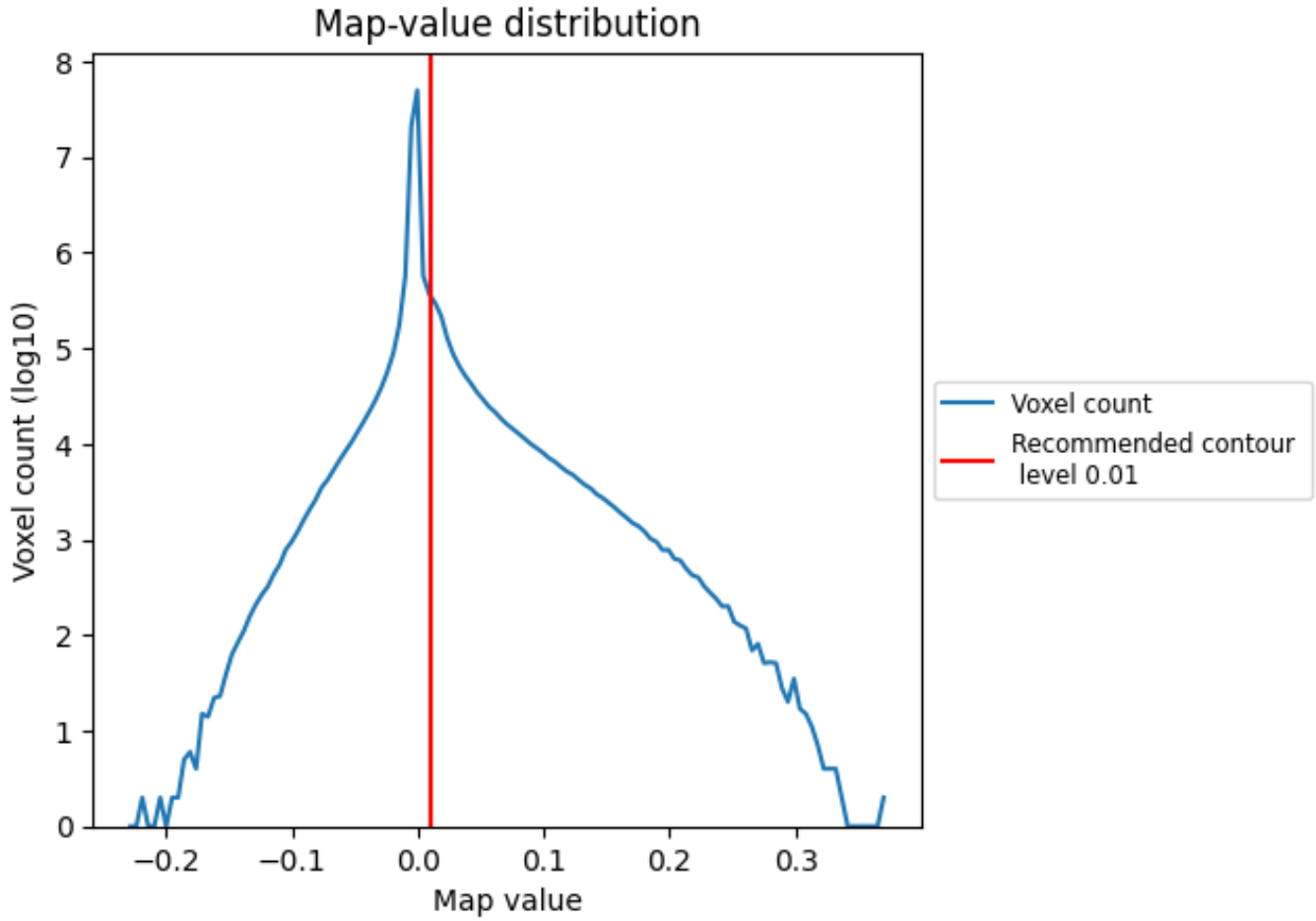
6.6 Mask visualisation (i)

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

7 Map analysis

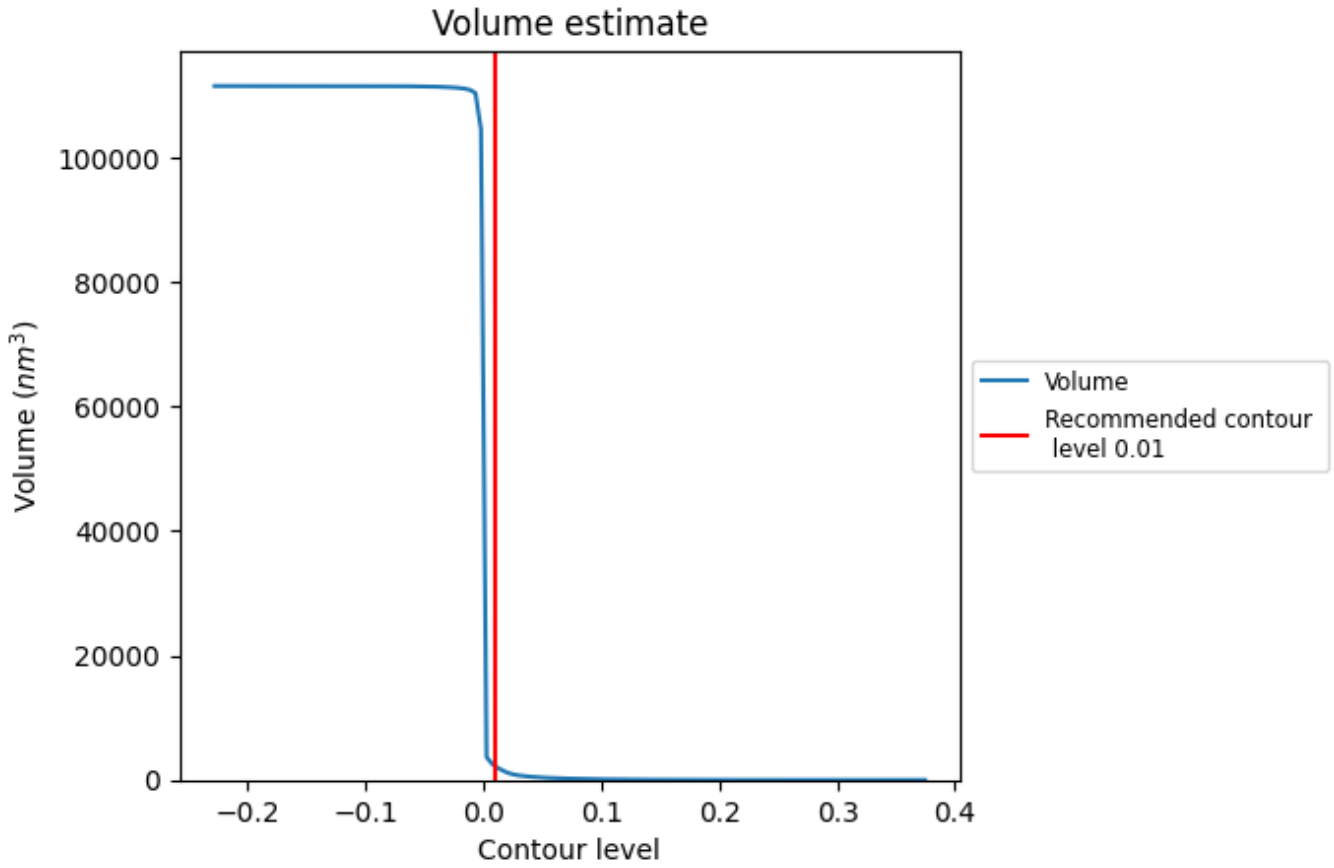
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

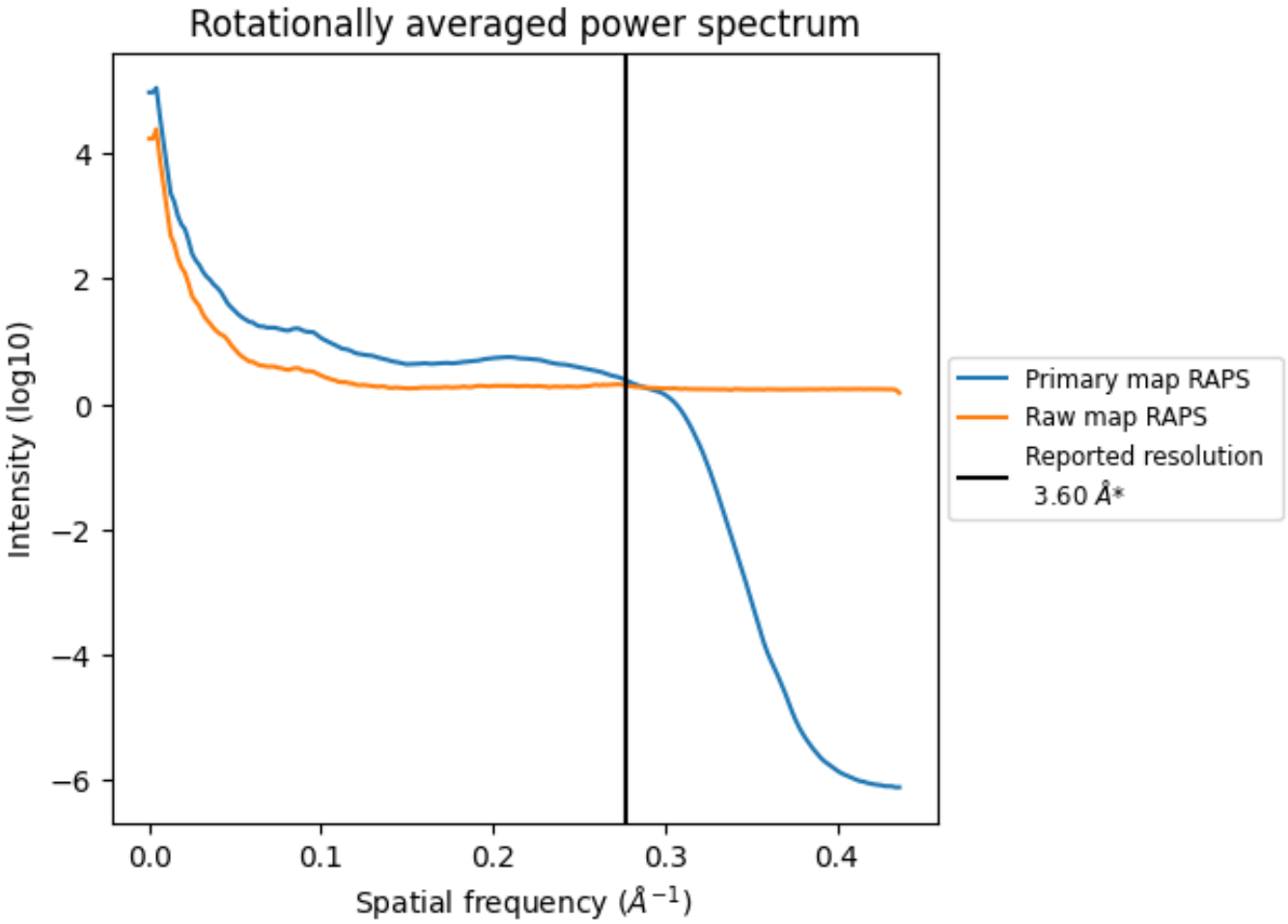
7.2 Volume estimate



The volume at the recommended contour level is 2214 nm^3; this corresponds to an approximate mass of 2000 kDa.

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

7.3 Rotationally averaged power spectrum (i)

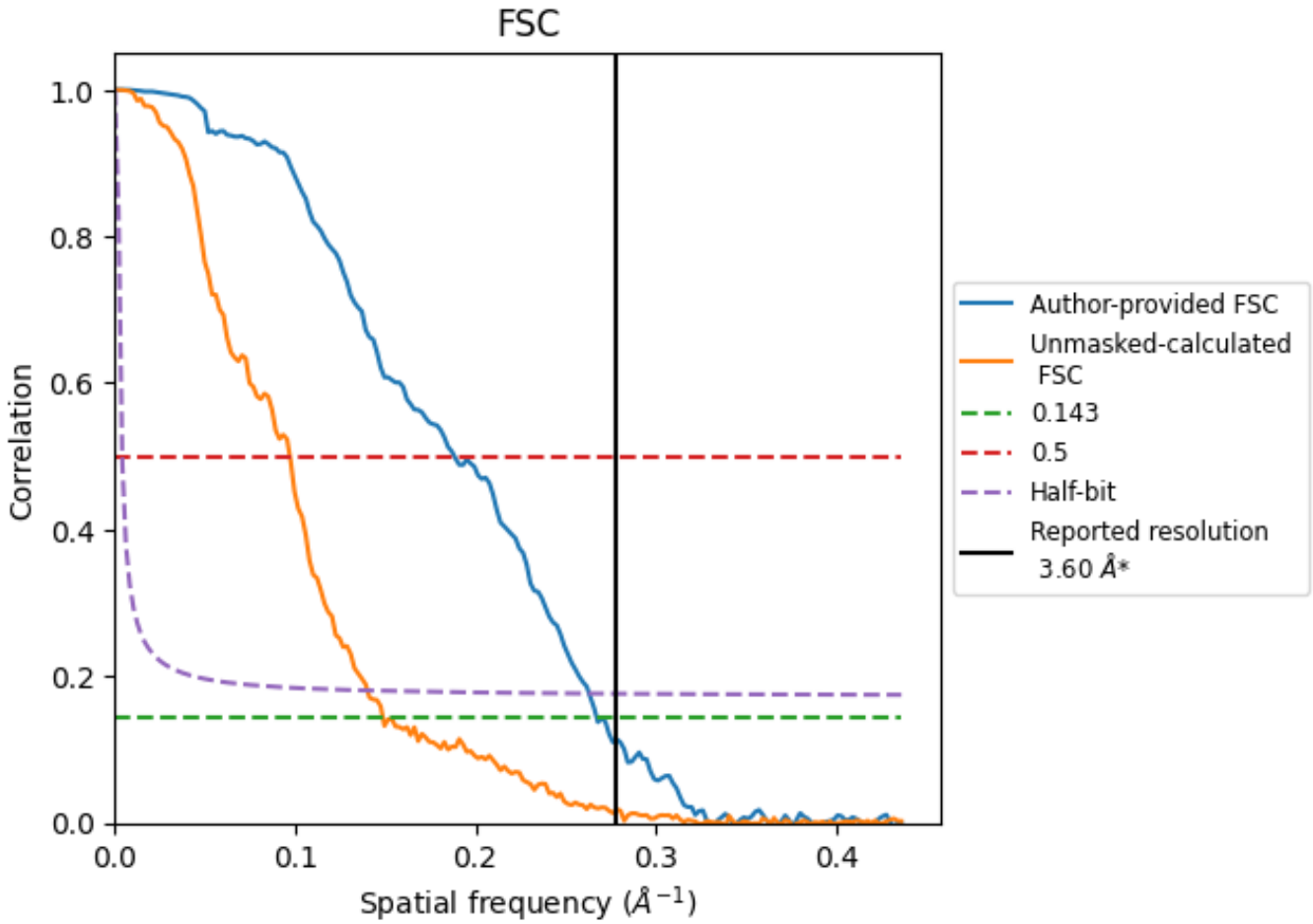


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

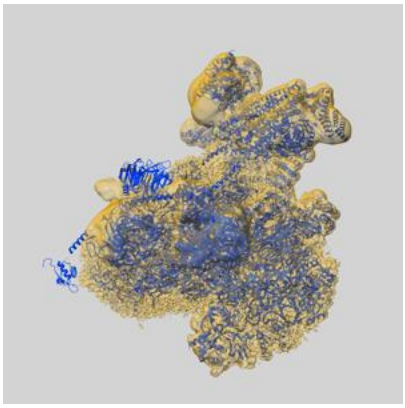
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.74	5.31	3.80
Unmasked-calculated*	6.72	10.29	7.13

*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 6.72 differs from the reported value 3.6 by more than 10 %

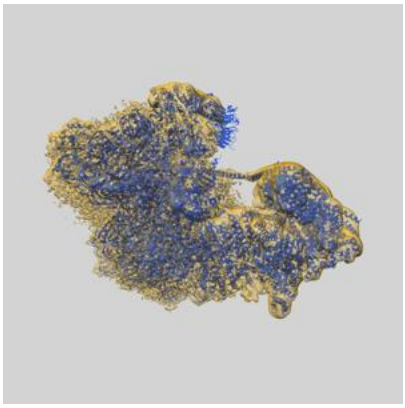
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38754 and PDB model 8XXN. Per-residue inclusion information can be found in section 3 on page 13.

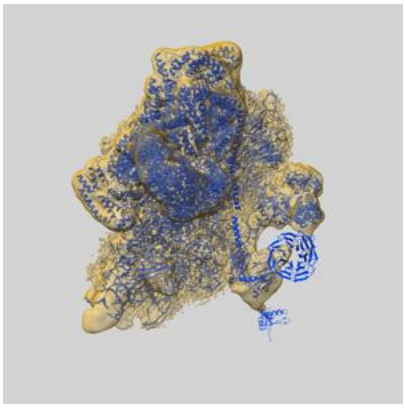
9.1 Map-model overlay



X



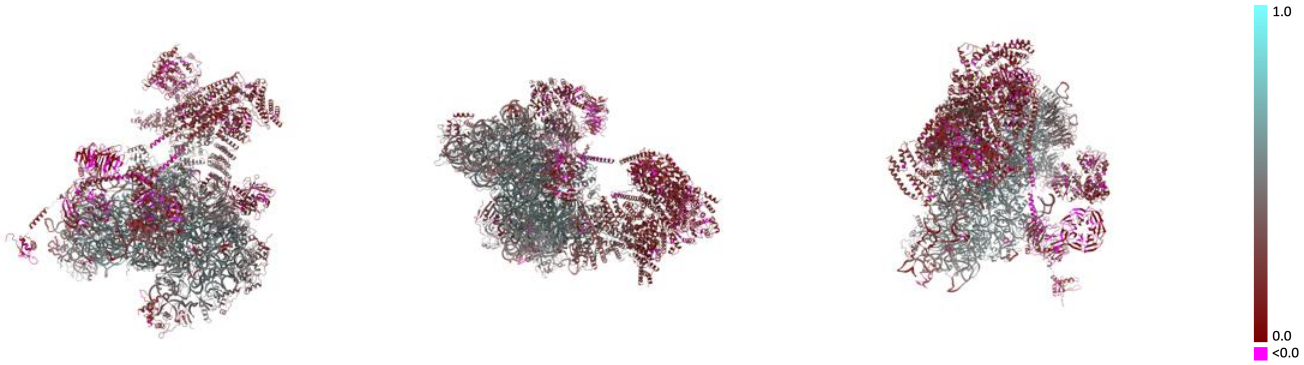
Y



Z

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.

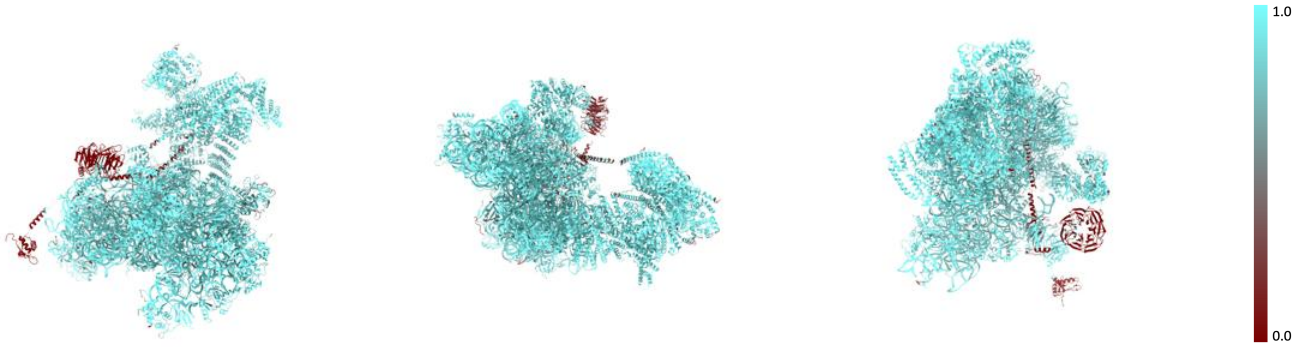
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

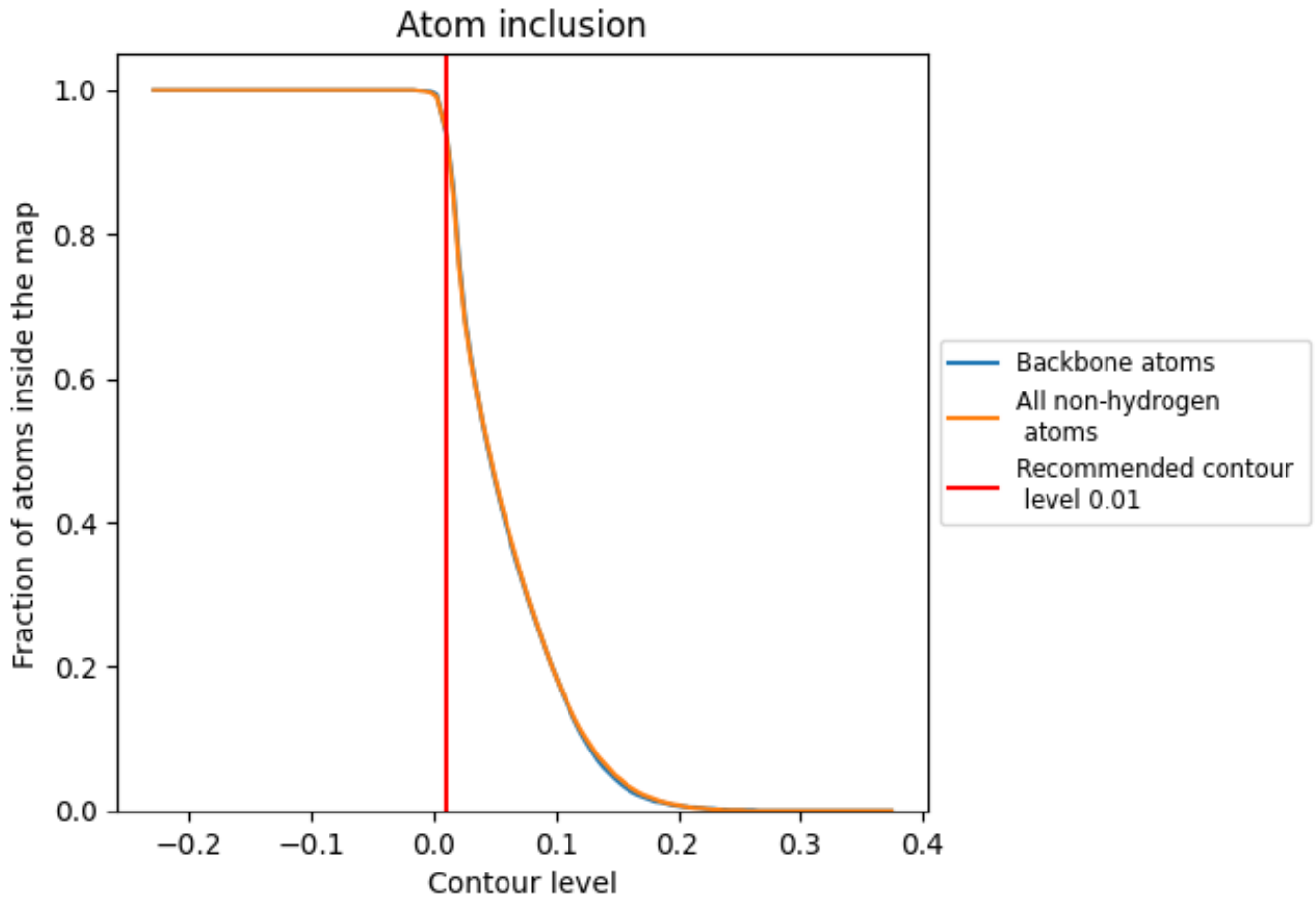
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (i)



At the recommended contour level, 94% of all backbone atoms, 94% 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	0.9450	0.3740
3A	0.9040	0.2270
3B	0.7020	0.1290
3C	0.9470	0.3030
3E	0.9700	0.1700
3F	0.9620	0.1150
3G	0.9830	0.3040
3H	0.9600	0.1330
3I	0.0760	0.0340
3K	0.9530	0.1120
3L	0.9440	0.1020
3M	0.9870	0.1520
3N	0.8220	0.1860
4A	0.9480	0.1480
C1	0.6820	0.2590
CD	0.9670	0.2320
Ln	0.8520	0.3970
S2	0.9900	0.4850
SA	0.9610	0.4950
SB	0.9770	0.4800
SC	0.9740	0.5270
SD	0.9720	0.4950
SE	0.9830	0.5260
SF	0.9510	0.4530
SG	0.9840	0.4140
SH	0.9690	0.4300
SI	0.9780	0.4550
SJ	0.9730	0.5110
SK	0.9790	0.4530
SL	0.9600	0.5040
SM	0.9200	0.2250
SN	0.9800	0.5050
SO	0.9430	0.4670
SP	0.9570	0.4420
SQ	0.9600	0.4990

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
SR	0.9500	0.4640
SS	0.9470	0.4140
ST	0.9690	0.4540
SU	0.9640	0.4310
SV	0.9840	0.5070
SW	0.9810	0.5560
SX	0.9800	0.5370
SY	0.9560	0.4710
SZ	0.9190	0.3480
Sa	0.9730	0.5240
Sb	0.9560	0.4980
Sc	0.9360	0.4050
Sd	0.9820	0.5310
Se	0.9370	0.4670
Sf	0.9480	0.3020
Sg	0.9820	0.3780