



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:19 AM UTC

PDB ID : 9KN6 / pdb_00009kn6
EMDB ID : EMD-62454
Title : Structure of the HCV IRES-dependent pre-48S translation initiation complex with eIF1A, eIF5B, and eIF3
Authors : Iwasaki, W.; Kashiwagi, K.; Sakamoto, A.; Nishimoto, M.; Takahashi, M.; Machida, K.; Imataka, H.; Matsumoto, A.; Shichino, Y.; Iwasaki, S.; Imami, K.; Ito, T.
Deposited on : 2024-11-18
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

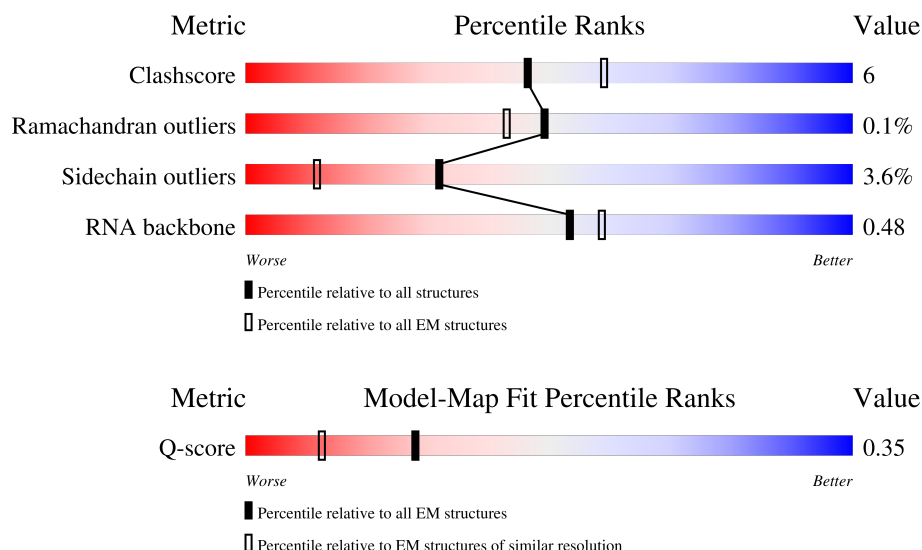
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1A	144	
2	5B	621	

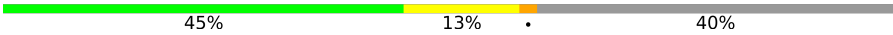
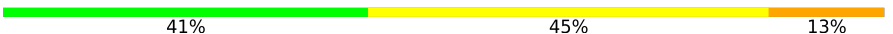
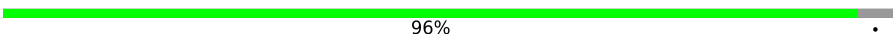
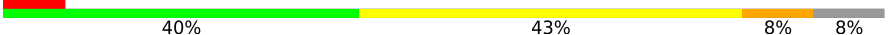
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Mol	Chain	Length	Quality of chain
3	SA	295	
4	SB	264	
5	SC	293	
6	SD	243	
7	SE	263	
8	SF	204	
9	SG	249	
10	SH	194	
11	SI	208	
12	SJ	194	
13	SK	165	
14	SL	158	
15	Sf	132	
16	SN	151	
17	SO	151	
18	SP	145	
19	SQ	146	
20	SR	135	
21	SS	152	
22	ST	145	
23	SU	119	
24	SV	83	
25	SW	130	
26	SX	143	
27	SY	133	

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Mol	Chain	Length	Quality of chain
28	SZ	125	
29	Sa	115	
30	Sb	84	
31	Sc	69	
32	Sd	56	
33	Se	59	
34	sh	156	
35	Sg	317	
36	zy	75	
37	Ln	25	
38	zz	332	
39	S2	1869	
40	3m	374	
41	3f	357	
42	3a	1382	
43	3e	445	
44	3c	913	
45	3h	352	
46	3d	548	
47	3k	218	
48	3l	564	

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 115376 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 Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	98	Total	C	N	O	S	0	0
			783	494	139	146	4		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5B	621	Total	C	N	O	S	0	0
			4917	3135	847	913	22		

- Molecule 3 is a protein called Small ribosomal subunit protein uS2.

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

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

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

- Molecule 5 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SC	219	Total	C	N	O	S	0	0
			1700	1100	292	298	10		

- Molecule 6 is a protein called 40S ribosomal protein S3.

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

- Molecule 7 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 8 is a protein called 40S ribosomal protein S5.

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

- Molecule 9 is a protein called 40S ribosomal protein S6.

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

- Molecule 10 is a protein called 40S ribosomal protein S7.

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

- Molecule 11 is a protein called 40S ribosomal protein S8.

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

- Molecule 12 is a protein called 40S ribosomal protein S9.

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

- Molecule 13 is a protein called 40S ribosomal protein S10.

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

- Molecule 14 is a protein called 40S ribosomal protein S11.

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

- Molecule 15 is a protein called 40S ribosomal protein S12.

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

- Molecule 16 is a protein called 40S ribosomal protein S13.

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

- Molecule 17 is a protein called 40S ribosomal protein S14.

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

- Molecule 18 is a protein called 40S ribosomal protein S15.

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

- Molecule 19 is a protein called 40S ribosomal protein S16.

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

- Molecule 20 is a protein called 40S ribosomal protein S17.

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

- Molecule 21 is a protein called 40S ribosomal protein S18.

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

- Molecule 22 is a protein called 40S ribosomal protein S19.

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

- Molecule 23 is a protein called 40S ribosomal protein S20.

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

- Molecule 24 is a protein called 40S ribosomal protein S21.

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

- Molecule 25 is a protein called 40S ribosomal protein S15a.

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

- Molecule 26 is a protein called 40S ribosomal protein S23.

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

- Molecule 27 is a protein called 40S ribosomal protein S24.

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

- Molecule 28 is a protein called 40S ribosomal protein S25.

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

- Molecule 29 is a protein called 40S ribosomal protein S26.

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

- Molecule 30 is a protein called 40S ribosomal protein S27.

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

- Molecule 31 is a protein called 40S ribosomal protein S28.

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

- Molecule 32 is a protein called 40S ribosomal protein S29.

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

- Molecule 33 is a protein called 40S ribosomal protein S30.

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

- Molecule 34 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 35 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 36 is a RNA chain called Initiator Met-tRNA-i.

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

- Molecule 37 is a protein called 60S ribosomal protein L41.

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

- Molecule 38 is a RNA chain called HCV-IRES RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	zz	306	Total	C	N	O	P	0	0
			6528	2909	1164	2149	306		

- Molecule 39 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	S2	1759	Total	C	N	O	P	4	0
			37626	16795	6759	12310	1762		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	3m	363	Total	C	N	O	S	0	0
			2639	1666	450	511	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3f	269	Total	C	N	O	S	0	0
			2063	1303	354	394	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	3a	592	Total	C	N	O	S	0	0
			4470	2835	796	818	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	3e	430	Total	C	N	O	S	0	0
			3224	2053	561	594	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	3c	543	Total	C	N	O	S	0	0
			3907	2452	716	716	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3h	318	Total	C	N	O	S	0	0
			2520	1599	431	475	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3d	55	Total	C	N	O	S	0	0
			343	220	64	58	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3k	215	Total	C	N	O	S	0	0
			1475	932	251	282	10		

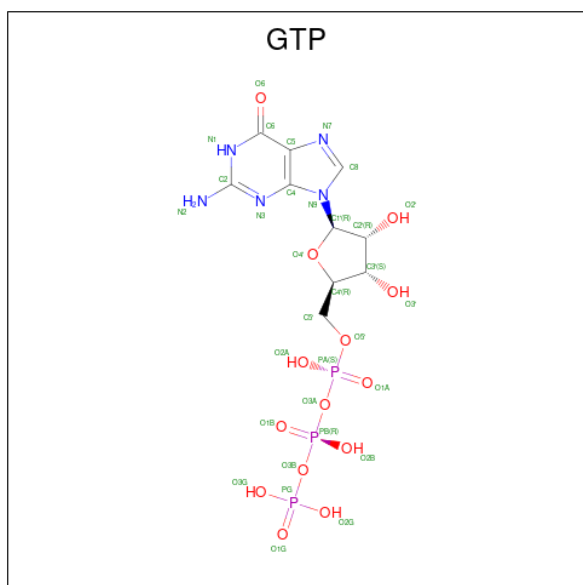
- Molecule 48 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	3l	520	Total	C	N	O	S	0	0
			4335	2808	715	793	19		

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

Mol	Chain	Residues	Atoms		AltConf
49	5B	1	Total	Mg	0
			1	1	
49	S2	7	Total	Mg	0
			7	7	

- Molecule 50 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



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

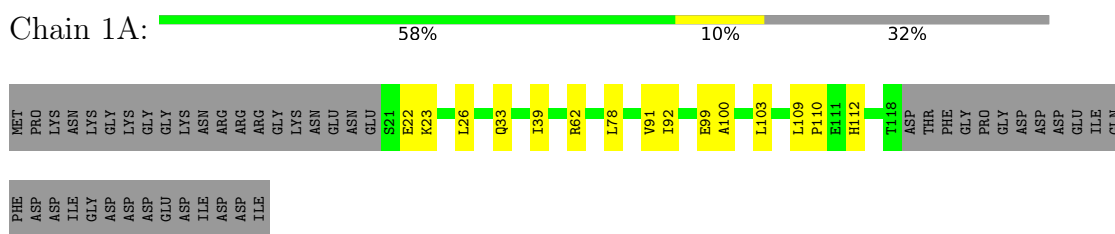
- Molecule 51 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

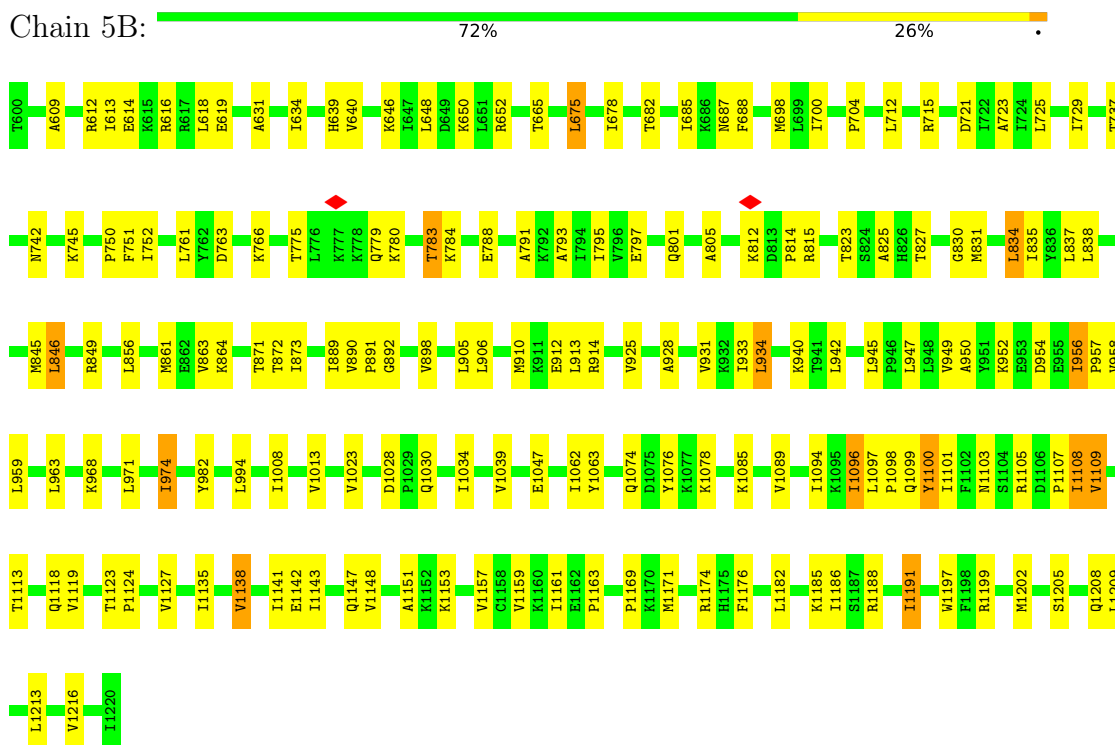
3 Residue-property plots [i](#)

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: Eukaryotic translation initiation factor 1A, X-chromosomal



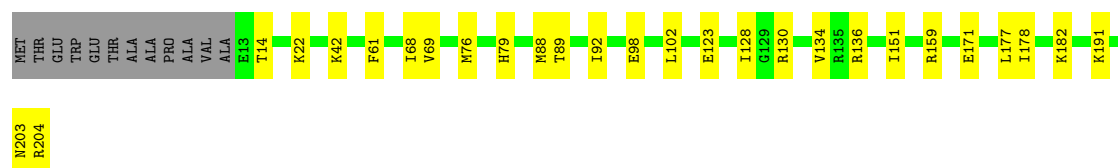
- Molecule 2: Eukaryotic translation initiation factor 5B



- Molecule 3: Small ribosomal subunit protein uS2

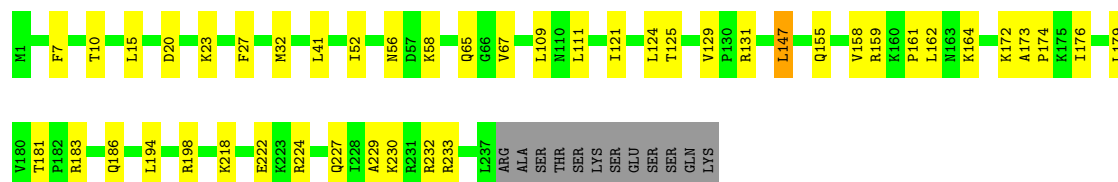


Chain SF:  81% 13% 6%



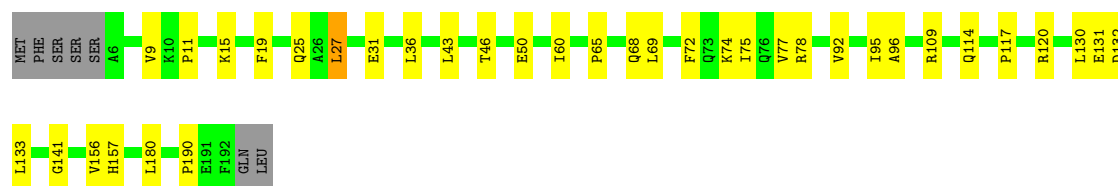
- Molecule 9: 40S ribosomal protein S6

Chain SG:  77% 18% 5%



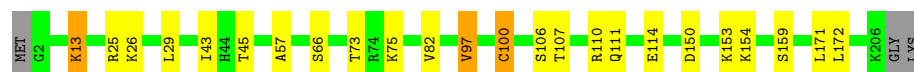
- Molecule 10: 40S ribosomal protein S7

Chain SH:  78% 18% 4%



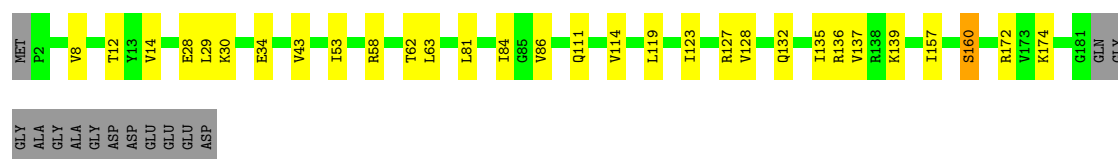
- Molecule 11: 40S ribosomal protein S8

Chain SI:  87% 10% 3%

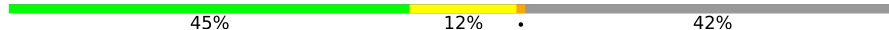


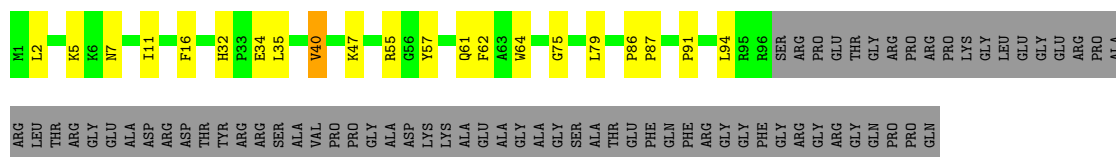
- Molecule 12: 40S ribosomal protein S9

Chain SJ:  77% 15% 8%

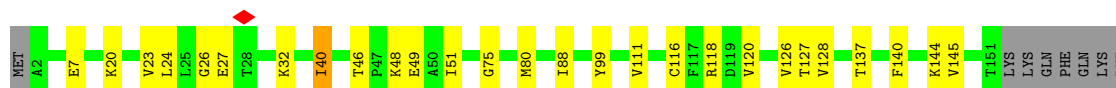
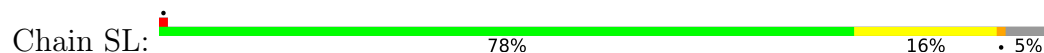


- Molecule 13: 40S ribosomal protein S10

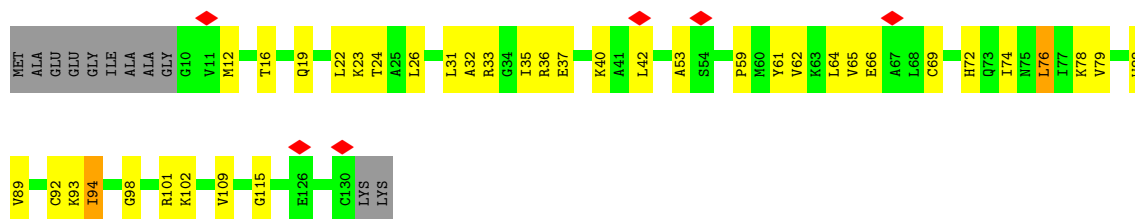
Chain SK:  45% 12% 43%



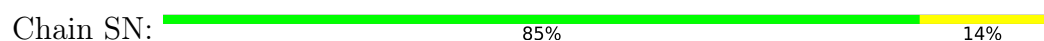
- Molecule 14: 40S ribosomal protein S11



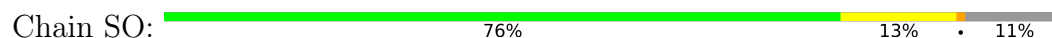
- Molecule 15: 40S ribosomal protein S12



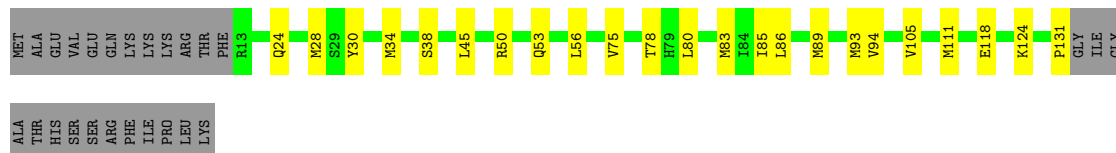
- Molecule 16: 40S ribosomal protein S13



- Molecule 17: 40S ribosomal protein S14



- Molecule 18: 40S ribosomal protein S15



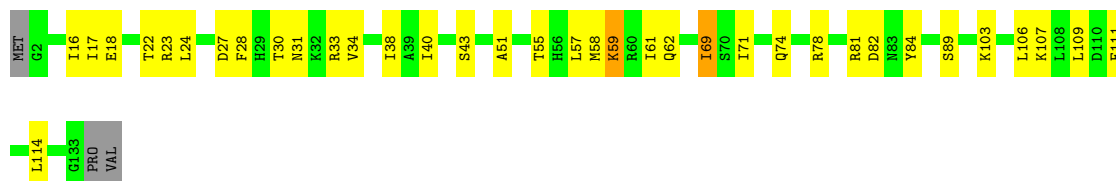
- Molecule 19: 40S ribosomal protein S16

Chain SQ:  84% 12% ..



- Molecule 20: 40S ribosomal protein S17

Chain SR:  71% 25% ..



- Molecule 21: 40S ribosomal protein S18

Chain SS:  80% 13% 6%



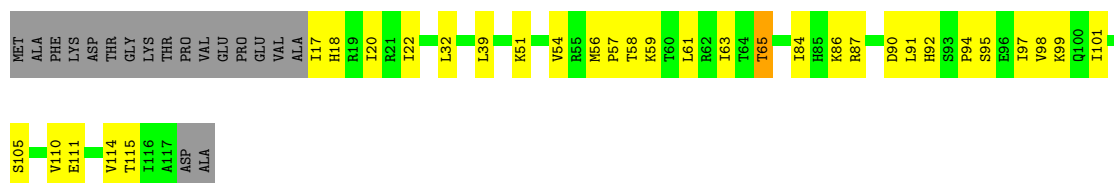
- Molecule 22: 40S ribosomal protein S19

Chain ST:  85% 13% .



- Molecule 23: 40S ribosomal protein S20

Chain SU:  58% 26% 15%



- Molecule 24: 40S ribosomal protein S21

Chain SV:  84% 14% .



- Molecule 25: 40S ribosomal protein S15a

Chain SW:  87% 12% .



- Molecule 26: 40S ribosomal protein S23

Chain SX: 85% 11% . .



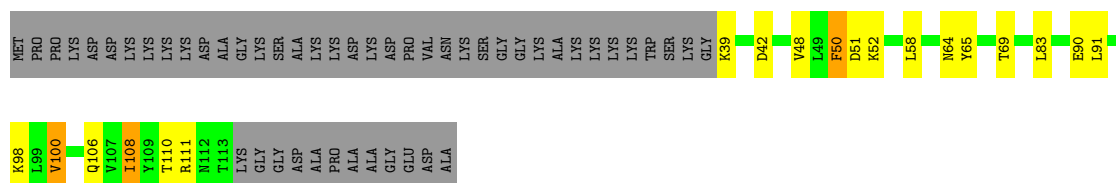
- Molecule 27: 40S ribosomal protein S24

Chain SY: 74% 19% 7%



- Molecule 28: 40S ribosomal protein S25

Chain SZ: 45% 13% . 40%



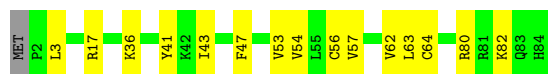
- Molecule 29: 40S ribosomal protein S26

Chain Sa: 78% 8% . 13%



- Molecule 30: 40S ribosomal protein S27

Chain Sb: 81% 18% .



- Molecule 31: 40S ribosomal protein S28

Chain Sc: 71% 19% 10%



- Molecule 32: 40S ribosomal protein S29

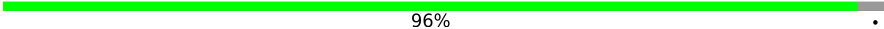
- LYS VAL HIS GLY SER LEU A7 Q22 K25 R31 R40 R41 V45 N58 SER

- | | | |
|-----|------|-----|
| LYS | ILE | MET |
| PRO | GLN | GLN |
| GLU | LYS | ILE |
| ASP | GLU | PHE |
| LYS | SER | VAL |
| | THR | LYS |
| | LEU | THR |
| | HIS | LEU |
| | LEU | THR |
| | VAL | GLY |
| | LEU | LYS |
| | ARG | THR |
| | LEU | ILE |
| | ARG | THR |
| | GLY | LEU |
| | GLY | GLU |
| | ALA | VAL |
| | LYS | GLU |
| | ARG | PRO |
| | LYS | SER |
| | LYS | ASP |
| | LYS | THR |
| | LYS | ILE |
| | SER | GLU |
| | TYR | ASN |
| | THR | VAL |
| | THR | LYS |
| | THR | LYS |
| | P88 | ALA |
| | K99 | LYS |
| | H93 | ILE |
| | K94 | GLN |
| | R95 | ASP |
| | K96 | LYS |
| | K97 | GLU |
| | V98 | GLY |
| | K99 | ILE |
| | L100 | PRO |
| | | PRO |
| | L103 | ASP |
| | | GLN |
| | Y106 | GLN |
| | K107 | ARG |
| | V108 | LEU |
| | D109 | ILE |
| | | PHE |
| | S115 | ALA |
| | | GLY |
| | R118 | LYS |
| | R119 | GLN |
| | | LEU |
| | C126 | GLU |
| | | ASP |
| | G129 | GLY |
| | V130 | ARG |
| | F131 | THR |
| | | LEU |
| | Y148 | SER |
| | | ASP |
| | | TYR |
| | | ASN |

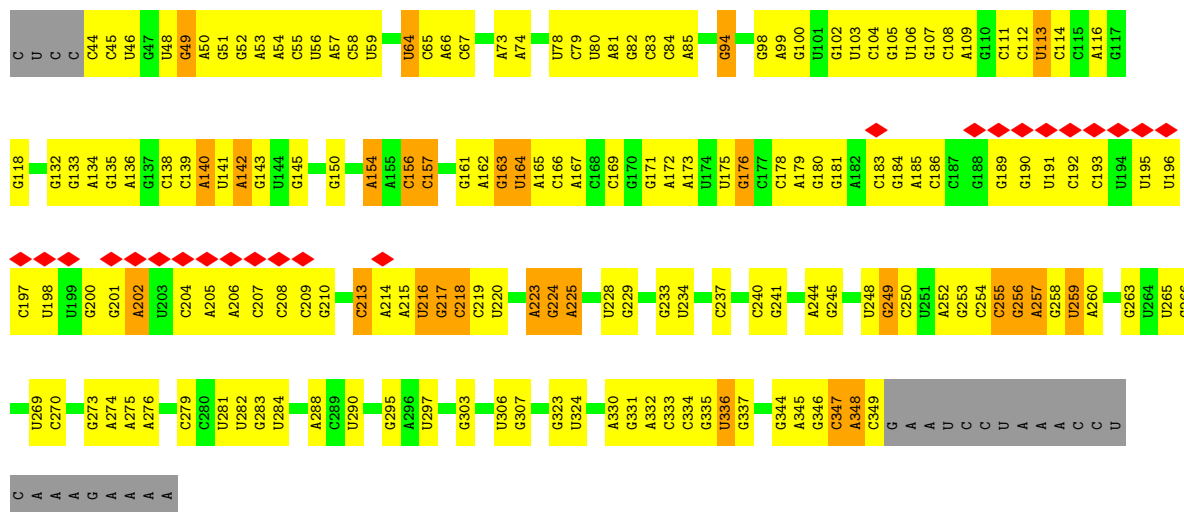
- | | | | | | | | | | |
|------|------|------|------|------|------|-----|-----|-----|------|
| L288 | F299 | T303 | V309 | W310 | I314 | GLY | THR | ARG | F156 | S157 | I164 | I165 | V166 | K172 | L173 | V174 | K175 | V176 | W177 | N178 | L179 | K185 | N186 | N187 | H188 | I189 | G190 | H191 | N192 | G193 | Y194 | L195 | D203 | G214 | M217 | T229 | L230 | D234 | I235 | I236 | K237 | A238 | Y246 | A251 | I256 | E262 | L270 | K271 | T287 | S288 | L289 | T297 | F106 | D107 | L108 | L109 | S110 | V111 | V121 | R125 | I129 | W132 | G136 | T141 | V142 | Q143 | D144 | E145 | S146 | W150 |
| Met | T2 | M5 | T10 | W17 | V18 | K30 | R36 | T39 | I40 | R57 | R60 | H64 | V70 | L87 | R88 | L89 | G95 | R99 | R100 | F101 | K106 | D107 | L108 | L109 | S110 | V111 | V121 | R125 | I129 | W132 | G136 | T141 | V142 | Q143 | D144 | E145 | S146 | W150 | |

- | | | | | | | | |
|----|----|----|----|----|----|----|-----|
| A1 | A4 | G5 | A6 | G7 | U8 | G9 | G10 | G11 | G12 | G15 | C16 | G17 | G18 | A19 | A20 | G21 | U24 | G25 | C26 | U27 | G28 | A34 | U35 | C40 | A41 | G42 | A43 | C47 | G48 | A49 | U50 | G51 | G52 | A53 | U54 | C55 | G56 | A57 | A58 | C61 | A62 | C65 | U66 | C67 | U68 | G69 | C70 | U71 | A72 | C73 | G74 | A75 |
|----|----|----|----|----|----|----|-----|

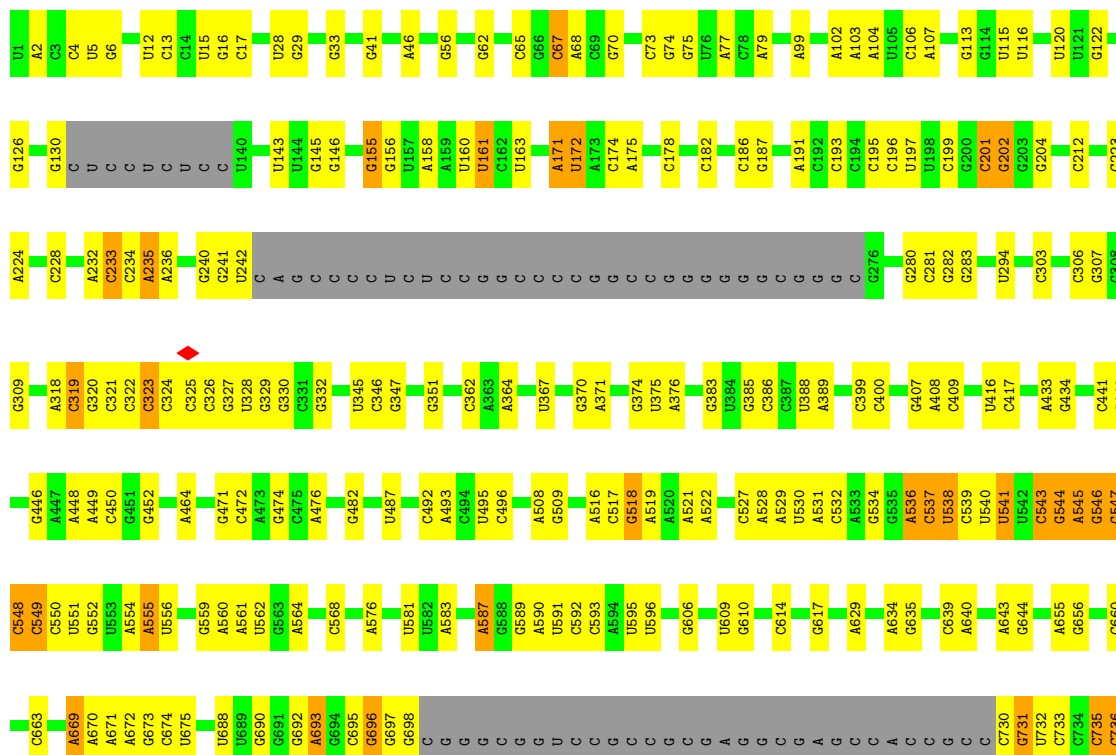
- WORLDWIDE
PDB
PROTEIN DATA BANK

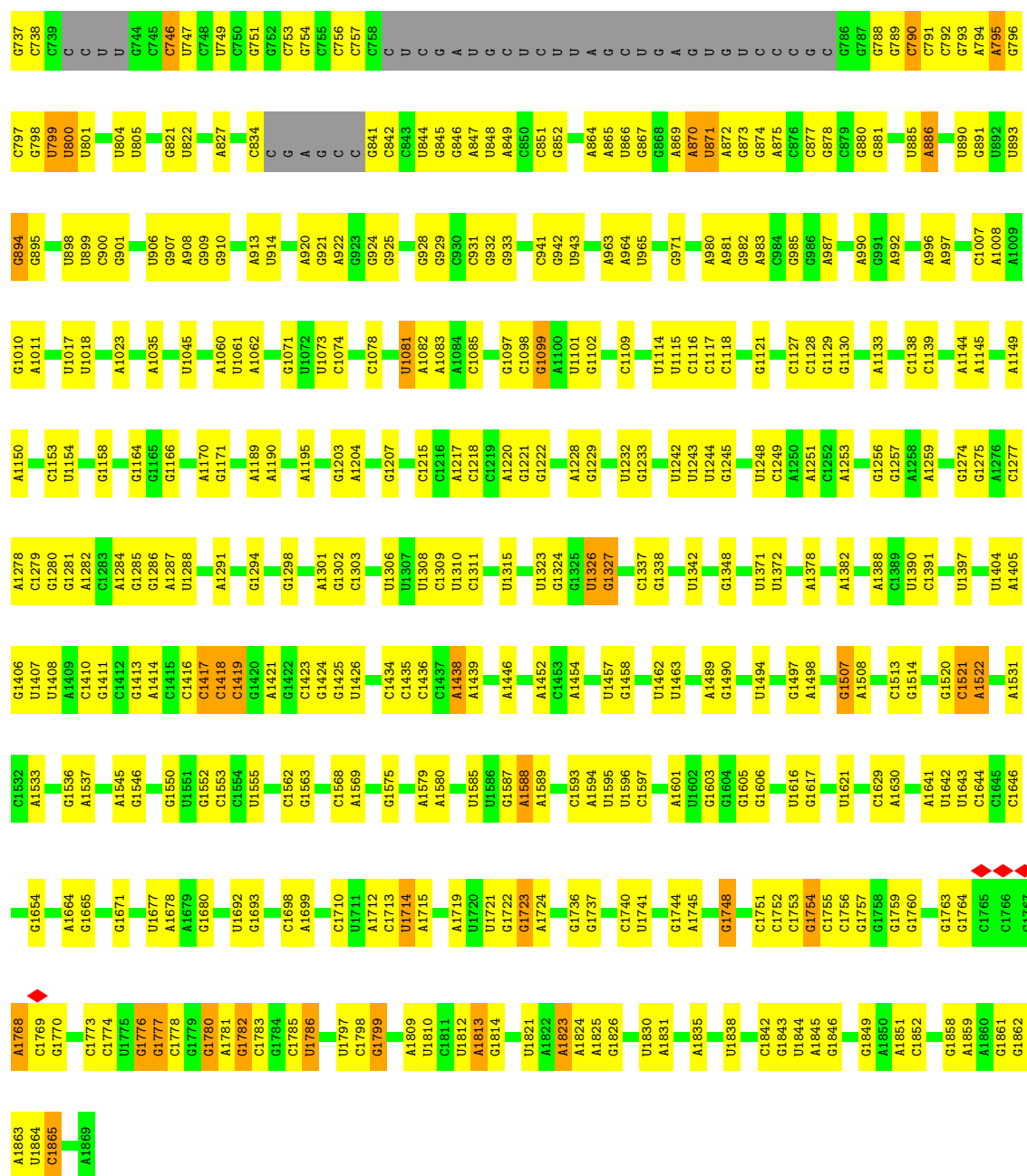
Chain Ln:  96% .

● Molecule 38: HCV-IRES RNA

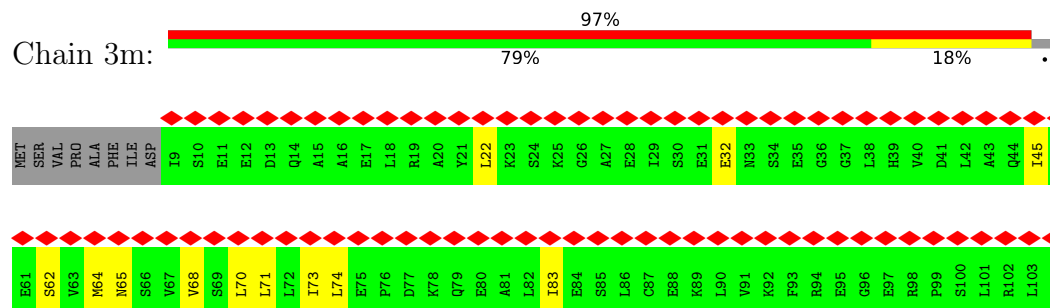
Chain zz:  7% 40% 43% 8% 8%

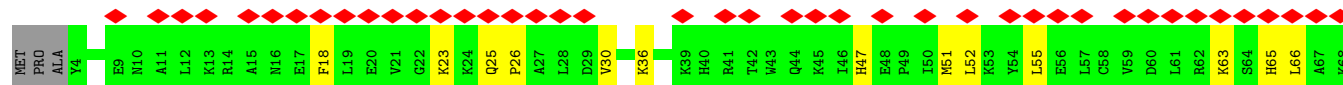
● Molecule 39: 18S ribosomal RNA

Chain S2:  61% 29% . 6%

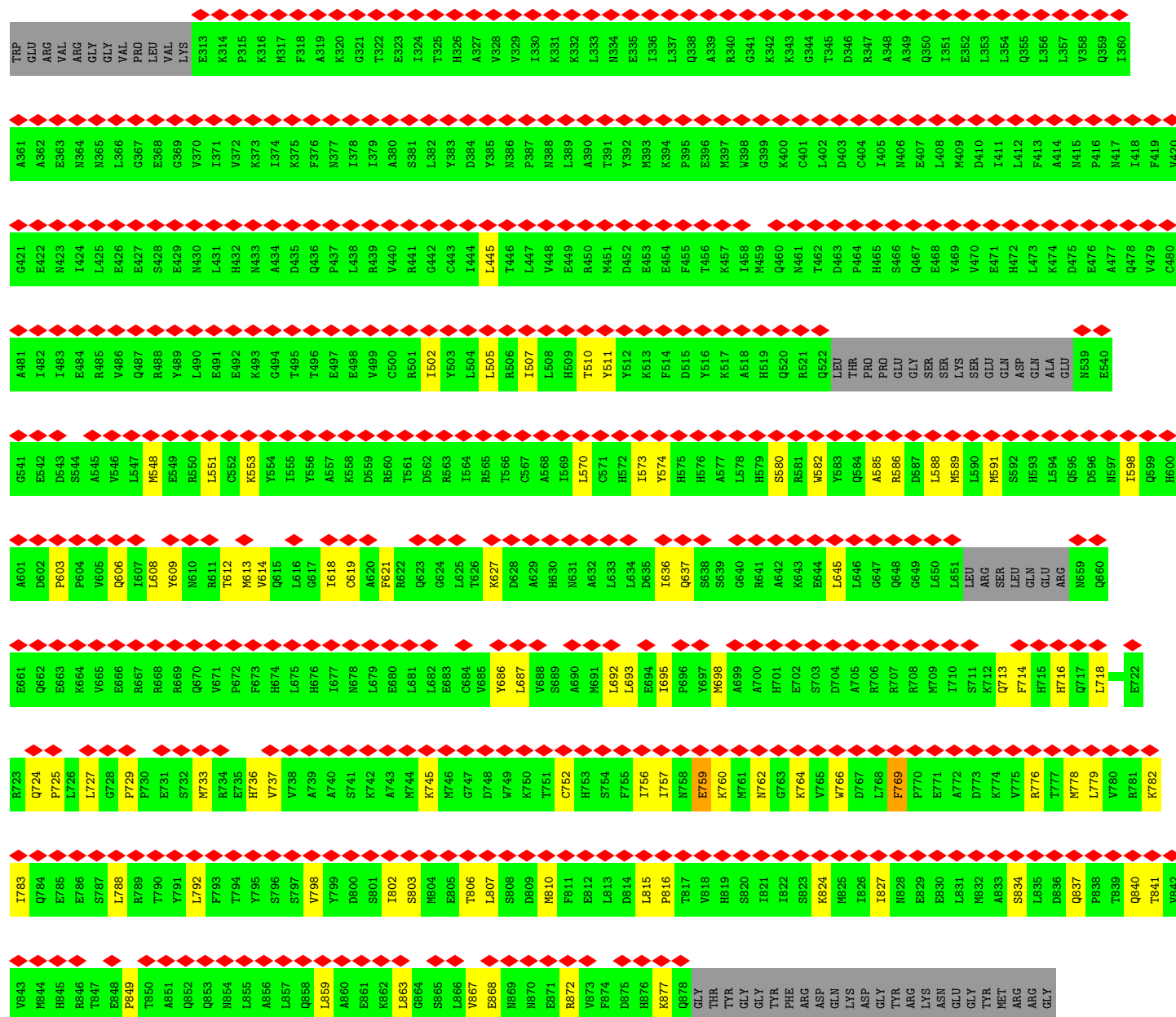


• Molecule 40: Eukaryotic translation initiation factor 3 subunit M





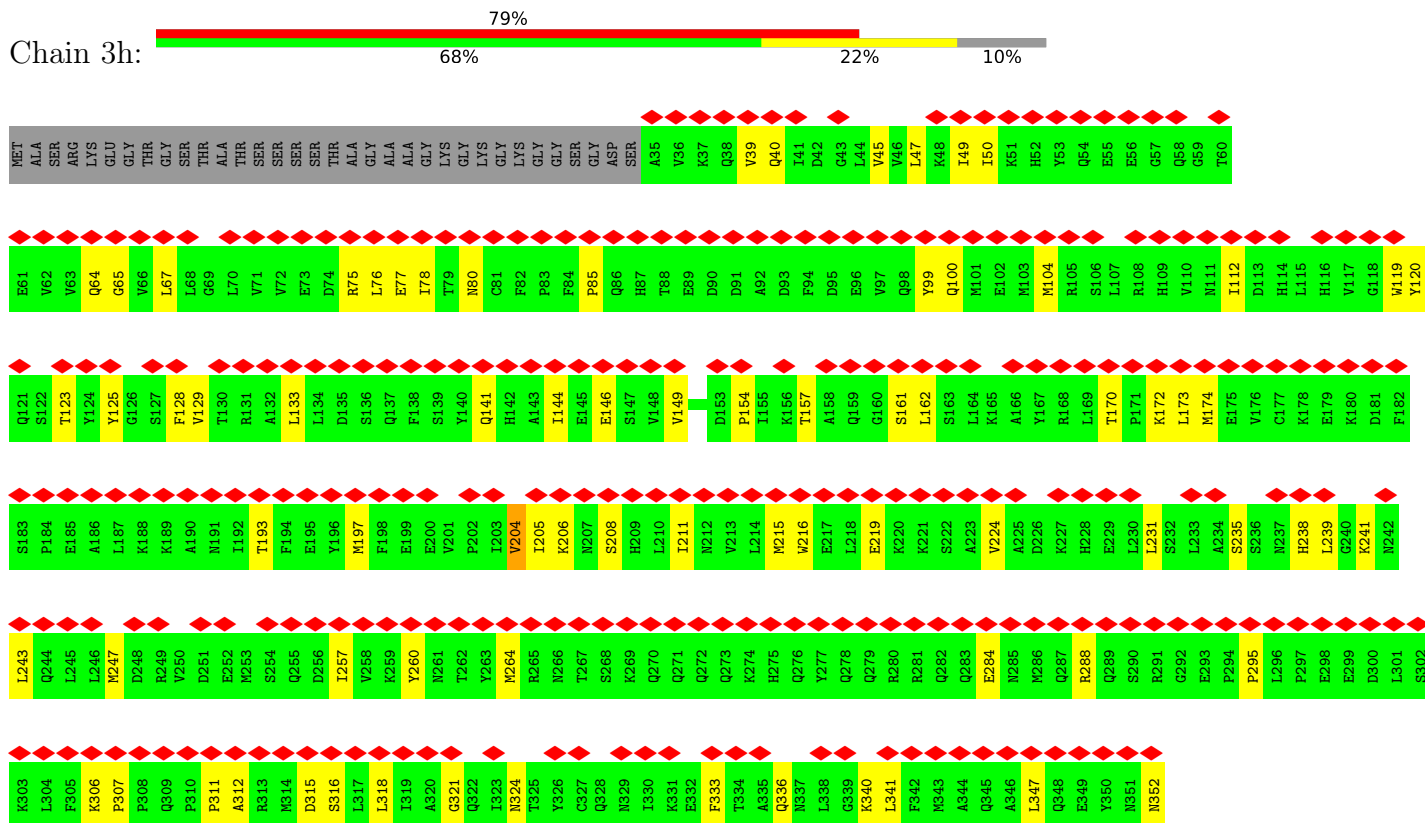




GLY
TYR
SER
GLN
GLN
GLN
SER
GLN
THR
ALA
TYR

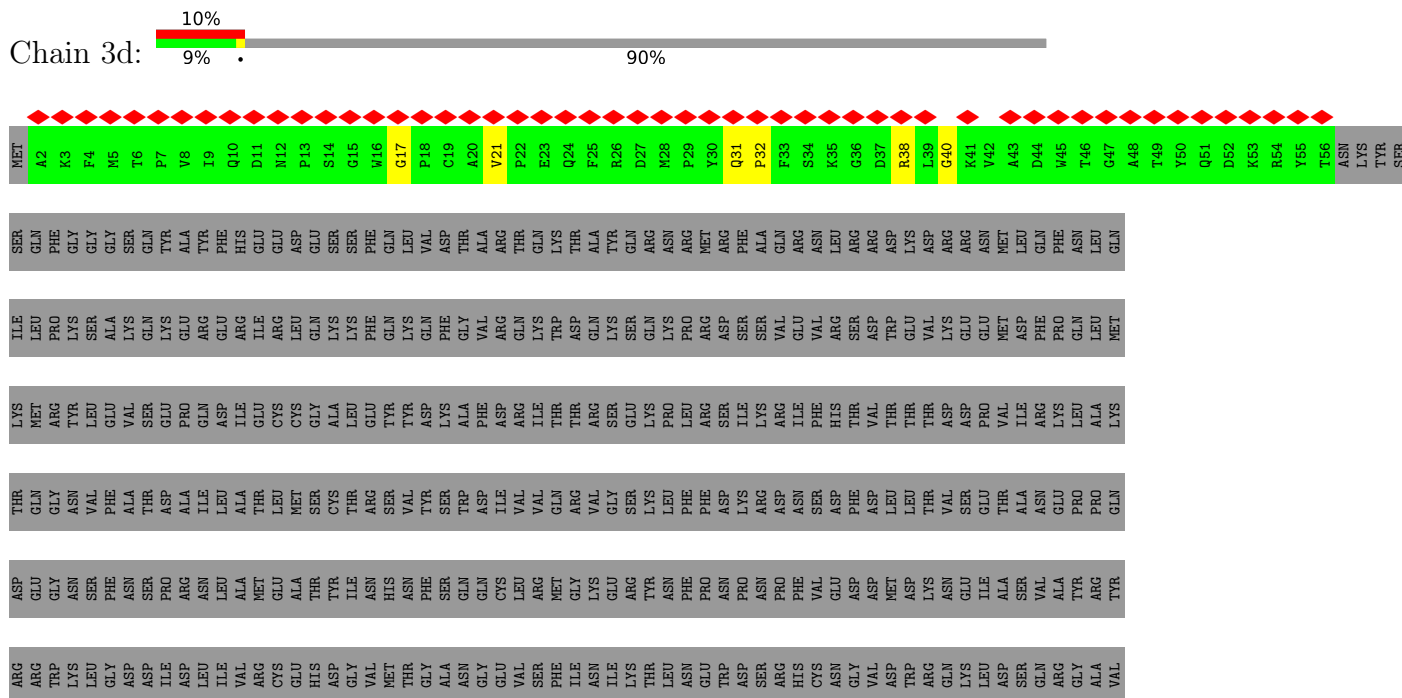
• Molecule 45: Eukaryotic translation initiation factor 3 subunit H

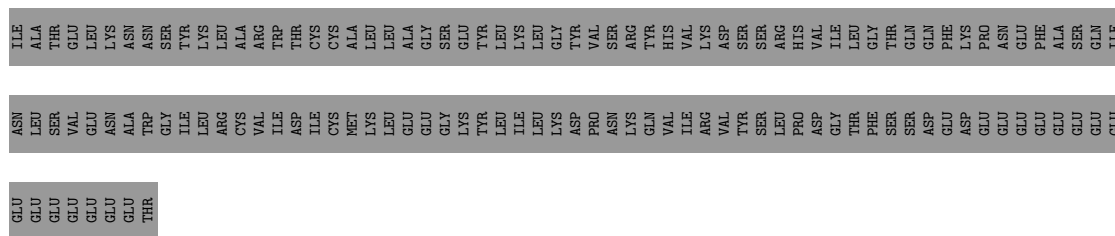
Chain 3h:



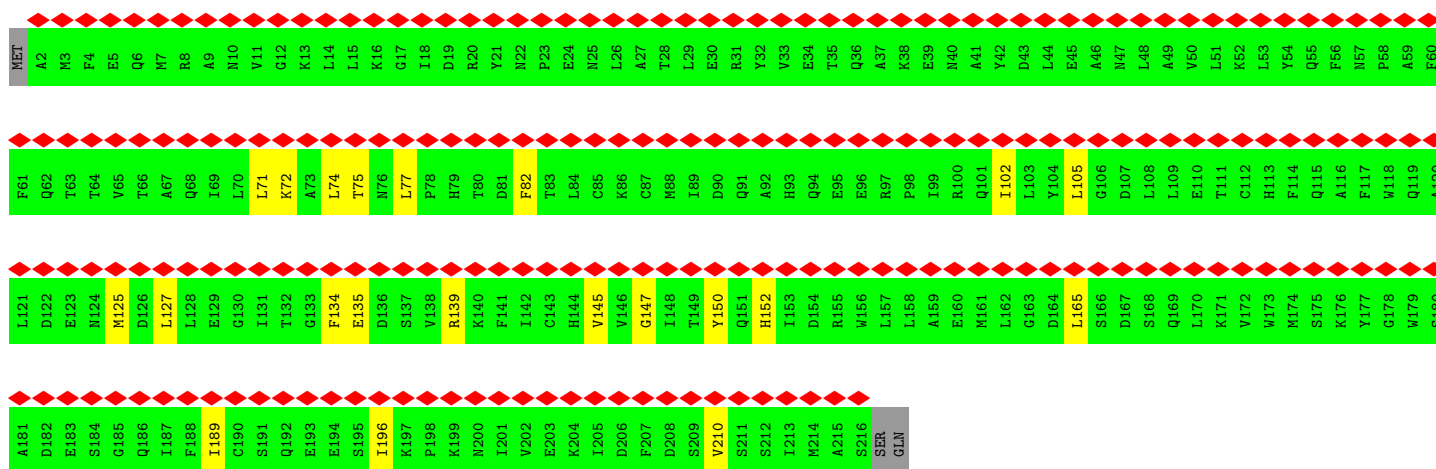
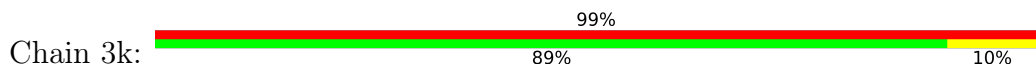
• Molecule 46: Eukaryotic translation initiation factor 3 subunit D

Chain 3d:

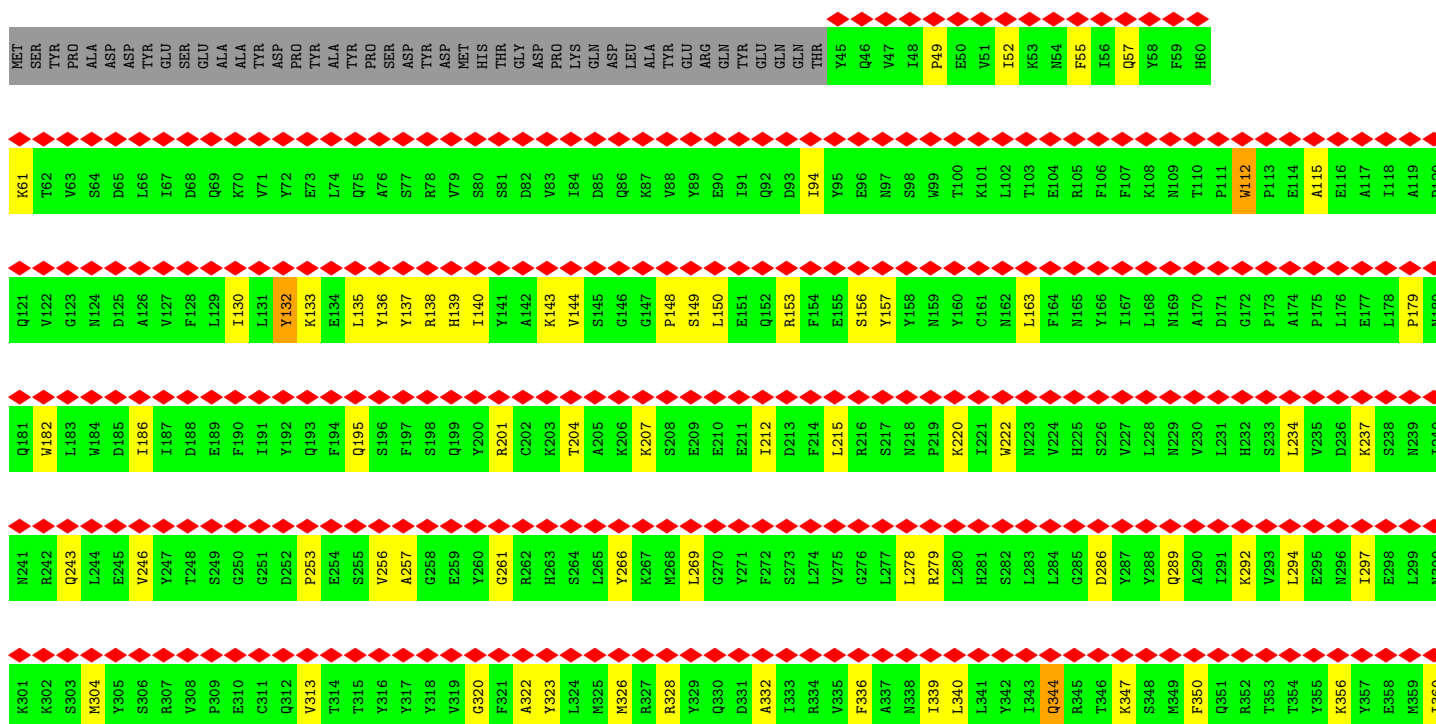




- Molecule 47: Eukaryotic translation initiation factor 3 subunit K



- Molecule 48: Eukaryotic translation initiation factor 3 subunit L





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19430	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.103	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.011	Depositor
Map size ($\text{\AA}$)	636.0, 636.0, 636.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.272, 1.272, 1.272	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1A	0.15	0/793	0.41	0/1061
2	5B	0.20	0/4999	0.54	0/6740
3	SA	0.19	0/1742	0.38	0/2367
4	SB	0.19	0/1749	0.36	0/2340
5	SC	0.20	0/1737	0.43	0/2347
6	SD	0.18	0/1784	0.40	0/2402
7	SE	0.20	0/2107	0.38	0/2836
8	SF	0.20	0/1540	0.42	0/2071
9	SG	0.17	0/1946	0.37	0/2590
10	SH	0.19	0/1529	0.42	0/2048
11	SI	0.18	0/1711	0.35	0/2282
12	SJ	0.18	0/1524	0.36	0/2035
13	SK	0.18	0/834	0.45	0/1125
14	SL	0.20	0/1241	0.37	0/1662
15	Sf	0.20	0/945	0.57	0/1269
16	SN	0.20	0/1226	0.39	0/1649
17	SO	0.19	0/1020	0.40	0/1368
18	SP	0.20	0/1003	0.49	0/1340
19	SQ	0.23	0/1133	0.49	0/1517
20	SR	0.22	0/1082	0.54	0/1452
21	SS	0.18	0/1202	0.42	0/1610
22	ST	0.20	0/1122	0.42	0/1504
23	SU	0.18	0/813	0.45	0/1092
24	SV	0.17	0/643	0.36	0/860
25	SW	0.21	0/1051	0.38	0/1406
26	SX	0.20	0/1116	0.43	0/1490
27	SY	0.19	0/1031	0.46	0/1370
28	SZ	0.24	0/607	0.58	0/815
29	Sa	0.22	0/817	0.39	0/1095
30	Sb	0.20	0/665	0.39	0/891
31	Sc	0.23	0/490	0.49	0/656
32	Sd	0.20	0/470	0.41	0/623

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Se	0.15	0/422	0.41	0/555
34	sh	0.18	0/533	0.44	0/706
35	Sg	0.16	0/2493	0.42	0/3394
36	zy	0.15	0/1798	0.32	0/2802
37	Ln	0.19	0/231	0.42	0/294
38	zz	0.16	0/7294	0.35	0/11371
39	S2	0.19	0/42073	0.31	0/65576
40	3m	0.14	0/2676	0.40	0/3635
41	3f	0.15	0/2099	0.40	0/2856
42	3a	0.16	0/4556	0.39	0/6205
43	3e	0.15	0/3288	0.39	0/4475
44	3c	0.15	0/3973	0.41	0/5406
45	3h	0.15	0/2571	0.39	0/3484
46	3d	0.14	0/354	0.36	0/488
47	3k	0.12	0/1502	0.36	0/2052
48	3l	0.15	0/4446	0.40	0/6013
All	All	0.18	0/121981	0.38	0/175225

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	783	0	793	8	0
2	5B	4917	0	5099	102	0
3	SA	1705	0	1706	21	0
4	SB	1722	0	1794	22	0
5	SC	1700	0	1784	11	0
6	SD	1756	0	1851	22	0
7	SE	2065	0	2169	14	0
8	SF	1518	0	1569	17	0
9	SG	1923	0	2089	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	SH	1506	0	1603	18	0
11	SI	1682	0	1769	14	0
12	SJ	1499	0	1618	14	0
13	SK	810	0	836	19	0
14	SL	1220	0	1289	16	0
15	Sf	935	0	964	29	0
16	SN	1202	0	1289	16	0
17	SO	1007	0	1032	10	0
18	SP	984	0	1033	15	0
19	SQ	1116	0	1185	9	0
20	SR	1068	0	1121	21	0
21	SS	1184	0	1244	11	0
22	ST	1103	0	1133	12	0
23	SU	803	0	873	16	0
24	SV	636	0	637	7	0
25	SW	1034	0	1080	12	0
26	SX	1098	0	1167	10	0
27	SY	1014	0	1082	15	0
28	SZ	601	0	662	12	0
29	Sa	803	0	850	7	0
30	Sb	651	0	672	7	0
31	Sc	488	0	514	10	0
32	Sd	459	0	452	5	0
33	Se	417	0	463	3	0
34	sh	522	0	530	9	0
35	Sg	2436	0	2393	43	0
36	zy	1607	0	815	25	0
37	Ln	230	0	276	0	0
38	zz	6528	0	3303	74	0
39	S2	37626	0	19015	268	0
40	3m	2639	0	2442	44	0
41	3f	2063	0	2054	53	0
42	3a	4470	0	4177	71	0
43	3e	3224	0	2925	45	0
44	3c	3907	0	3472	67	0
45	3h	2520	0	2445	53	0
46	3d	343	0	253	3	0
47	3k	1475	0	1239	14	0
48	3l	4335	0	4272	81	0
49	5B	1	0	0	0	0
49	S2	7	0	0	0	0
50	5B	32	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	Sa	1	0	0	0	0
51	sh	1	0	0	0	0
All	All	115376	0	93044	1275	0

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

All (1275) 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)
38:zz:259:U:H3	38:zz:274:A:N6	1.73	0.87
38:zz:256:G:N1	38:zz:276:A:N6	2.26	0.83
38:zz:259:U:H3	38:zz:274:A:H62	1.26	0.83
39:S2:885:U:H3	39:S2:901:G:H1	0.85	0.83
39:S2:1710:C:H42	39:S2:1823:A:H61	1.26	0.82
39:S2:197:U:H3	39:S2:202:G:H1	0.83	0.81
47:3k:125:MET:HE3	47:3k:125:MET:H	1.44	0.81
39:S2:1751:C:H42	39:S2:1782:G:H21	1.28	0.81
8:SF:130:ARG:HH22	38:zz:84:C:H42	1.30	0.77
35:Sg:87:LEU:HD21	35:Sg:111:VAL:HG11	1.67	0.77
2:5B:1094:ILE:HB	2:5B:1182:LEU:HB2	1.68	0.76
36:zy:10:G:H21	36:zy:24:U:H3	1.34	0.75
43:3e:251:PRO:HB2	43:3e:288:TYR:HB2	1.68	0.74
39:S2:1723:G:H2'	39:S2:1724:A:H8	1.52	0.73
39:S2:1764:G:O6	39:S2:1768:A:N7	2.21	0.73
38:zz:259:U:O4	38:zz:274:A:N7	2.22	0.73
24:SV:32:ILE:HD13	24:SV:60:ARG:HD2	1.72	0.72
41:3f:335:LEU:HB3	48:3l:547:ILE:HG21	1.72	0.72
40:3m:268:LEU:HD13	40:3m:273:ASN:HD21	1.55	0.71
44:3c:724:GLN:HE21	44:3c:727:LEU:HB2	1.56	0.71
43:3e:297:GLU:O	43:3e:301:VAL:HB	1.90	0.71
2:5B:721:ASP:HB2	2:5B:849:ARG:HH12	1.57	0.70
41:3f:206:LEU:HD21	42:3a:554:VAL:HG13	1.73	0.70
25:SW:106:THR:HG23	25:SW:108:ALA:H	1.55	0.70
40:3m:106:LEU:HD21	40:3m:127:LEU:HA	1.73	0.70
12:SJ:111:GLN:HE21	12:SJ:123:ILE:HG12	1.57	0.70
38:zz:176:G:H5'	42:3a:36:LYS:HD3	1.74	0.69
42:3a:472:VAL:HG23	44:3c:798:VAL:HG11	1.73	0.69
2:5B:1097:LEU:HD22	2:5B:1113:THR:HG23	1.74	0.69
2:5B:752:ILE:HD12	2:5B:838:LEU:HD23	1.74	0.69
14:SL:49:GLU:HB2	14:SL:118:ARG:HH12	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:S2:536:A:H3'	39:S2:537:C:H5''	1.73	0.68
42:3a:335:ARG:HB2	42:3a:340:ARG:HH21	1.56	0.68
38:zz:256:G:C6	38:zz:276:A:N6	2.61	0.68
36:zy:12:G:H1	36:zy:21:G:H22	1.42	0.68
21:SS:63:GLU:HB3	21:SS:66:ARG:HH21	1.58	0.68
39:S2:1723:G:H2'	39:S2:1724:A:C8	2.29	0.68
2:5B:665:THR:HG23	2:5B:704:PRO:HA	1.77	0.67
44:3c:762:ASN:HA	44:3c:766:TRP:HB2	1.75	0.67
10:SH:95:ILE:HD11	10:SH:133:LEU:HD13	1.77	0.67
40:3m:354:LEU:HD11	41:3f:283:LEU:HD22	1.77	0.67
2:5B:952:LYS:HG3	2:5B:954:ASP:H	1.60	0.66
45:3h:170:THR:HG22	45:3h:172:LYS:H	1.60	0.66
3:SA:122:LEU:HD13	3:SA:142:LEU:HD21	1.77	0.66
18:SP:118:GLU:HB2	21:SS:120:HIS:H	1.59	0.66
36:zy:19:A:H5'	36:zy:58:A:H61	1.60	0.66
17:SO:45:THR:HG22	17:SO:52:THR:HA	1.78	0.66
45:3h:312:ALA:HB3	45:3h:315:ASP:HB2	1.78	0.66
2:5B:956:ILE:HG13	2:5B:957:PRO:HD3	1.78	0.66
39:S2:197:U:O2	39:S2:202:G:N2	2.26	0.66
39:S2:240:G:H2'	39:S2:241:G:C8	2.31	0.66
42:3a:286:SER:HA	44:3c:729:PRO:HD3	1.78	0.66
35:Sg:256:ILE:HB	35:Sg:270:LEU:HB2	1.76	0.66
24:SV:14:PRO:HG2	24:SV:23:ILE:HD11	1.76	0.65
35:Sg:178:ASN:HB3	35:Sg:185:LYS:HD2	1.77	0.65
5:SC:104:ASP:HB3	5:SC:130:ILE:HD12	1.78	0.65
35:Sg:109:LEU:HD11	35:Sg:125:ARG:HG3	1.79	0.65
2:5B:863:VAL:HG12	2:5B:873:ILE:HG22	1.78	0.65
4:SB:33:VAL:HG23	4:SB:44:ILE:HB	1.79	0.65
39:S2:527:C:H2'	39:S2:528:A:H8	1.61	0.65
2:5B:752:ILE:HD13	2:5B:837:LEU:HG	1.78	0.65
14:SL:75:GLY:HA3	14:SL:88:ILE:HD12	1.78	0.65
2:5B:1118:GLN:HB2	2:5B:1153:LYS:HE3	1.79	0.65
25:SW:76:SER:HB3	39:S2:1158:G:H5''	1.77	0.65
39:S2:880:G:H1	39:S2:906:U:H3	1.45	0.65
2:5B:842:THR:HA	2:5B:846:LEU:HB2	1.78	0.64
45:3h:231:LEU:HA	45:3h:340:LYS:HZ1	1.62	0.64
23:SU:17:ILE:HD13	23:SU:94:PRO:HD3	1.80	0.64
48:3l:115:ALA:HB2	48:3l:133:LYS:HD3	1.79	0.64
2:5B:889:ILE:HD11	2:5B:956:ILE:HG22	1.80	0.64
43:3e:167:SER:HB3	46:3d:17:GLY:H	1.63	0.64
32:Sd:22:ARG:HG2	32:Sd:38:MET:HG2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:zz:141:U:H2'	38:zz:142:A:H4'	1.80	0.64
38:zz:347:C:H5''	38:zz:348:A:H5'	1.78	0.64
2:5B:892:GLY:HA2	2:5B:942:LEU:H	1.63	0.63
9:SG:131:ARG:HH12	9:SG:161:PRO:HD2	1.61	0.63
27:SY:116:LYS:HB3	39:S2:161:U:H5'	1.79	0.63
42:3a:55:LEU:HD11	42:3a:89:VAL:HG13	1.79	0.63
4:SB:49:VAL:HB	4:SB:62:LEU:HD21	1.79	0.63
19:SQ:102:GLU:HB2	19:SQ:105:LYS:HE3	1.79	0.63
16:SN:46:THR:HG22	16:SN:49:GLN:HG3	1.80	0.63
38:zz:65:C:H2'	38:zz:66:A:H8	1.64	0.63
40:3m:156:LEU:HD21	40:3m:160:LYS:HG3	1.81	0.63
44:3c:756:ILE:HG23	44:3c:757:ILE:HG12	1.80	0.63
39:S2:1101:U:H2'	39:S2:1102:G:H8	1.63	0.63
35:Sg:156:PHE:HE1	35:Sg:179:LEU:HD21	1.62	0.62
40:3m:270:HIS:HA	40:3m:273:ASN:HB2	1.81	0.62
42:3a:241:ILE:HD11	42:3a:282:VAL:HB	1.81	0.62
47:3k:135:GLU:HB3	47:3k:139:ARG:HH21	1.65	0.62
39:S2:874:G:H2'	39:S2:875:A:H8	1.65	0.62
15:Sf:64:LEU:HD11	34:sh:103:LEU:HB3	1.81	0.62
8:SF:123:GLU:HB2	31:Sc:59:LEU:HD12	1.81	0.62
48:3l:376:THR:HB	48:3l:461:ARG:HH22	1.64	0.62
2:5B:698:MET:HE2	2:5B:700:ILE:HD11	1.82	0.61
47:3k:77:LEU:HD11	47:3k:82:PHE:H	1.65	0.61
2:5B:1105:ARG:HH11	36:zy:71:U:H5	1.47	0.61
39:S2:587:A:H5'	39:S2:592:C:H41	1.64	0.61
9:SG:159:ARG:HG2	9:SG:173:ALA:HB2	1.83	0.61
44:3c:573:ILE:HD12	44:3c:585:ALA:HA	1.83	0.61
44:3c:687:LEU:HD21	44:3c:733:MET:HE2	1.83	0.61
30:Sb:17:ARG:HD2	39:S2:1127:C:H4'	1.83	0.61
30:Sb:36:LYS:HB3	30:Sb:43:ILE:HD12	1.83	0.61
48:3l:289:GLN:HA	48:3l:292:LYS:HB3	1.82	0.61
8:SF:128:ILE:HD11	31:Sc:68:LEU:HB3	1.83	0.60
43:3e:258:THR:HG22	43:3e:277:LEU:HD21	1.83	0.60
1:1A:33:GLN:HB3	1:1A:78:LEU:HD11	1.81	0.60
18:SP:86:LEU:H	18:SP:89:MET:HE3	1.66	0.60
35:Sg:172:LYS:HD3	35:Sg:193:GLY:H	1.66	0.60
42:3a:546:LYS:HE2	45:3h:216:TRP:HZ3	1.65	0.60
41:3f:337:VAL:HG11	45:3h:239:LEU:HD21	1.84	0.60
48:3l:458:SER:HA	48:3l:461:ARG:HE	1.66	0.60
13:SK:55:ARG:HG3	39:S2:1277:C:H4'	1.83	0.60
15:Sf:36:ARG:HH21	15:Sf:40:LYS:HZ1	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:S2:886:A:H61	39:S2:900:C:H42	1.49	0.60
43:3e:236:PHE:HD2	43:3e:257:LEU:HD13	1.67	0.60
15:Sf:69:CYS:HB2	15:Sf:74:ILE:HG22	1.83	0.60
29:Sa:26:CYS:HB3	29:Sa:77:CYS:SG	2.40	0.60
39:S2:528:A:H2'	39:S2:529:A:H8	1.67	0.60
9:SG:56:ASN:HD21	39:S2:155:G:H21	1.48	0.60
22:ST:124:THR:HG23	22:ST:127:GLY:H	1.67	0.60
2:5B:1171:MET:HB3	2:5B:1174:ARG:HB2	1.84	0.59
48:3l:432:HIS:HB3	48:3l:435:TYR:HB2	1.84	0.59
39:S2:1277:C:H2'	39:S2:1278:A:H8	1.66	0.59
41:3f:97:VAL:HG22	45:3h:47:LEU:HB3	1.84	0.59
48:3l:470:MET:HE1	48:3l:475:LEU:HB2	1.83	0.59
19:SQ:97:GLN:HB2	19:SQ:105:LYS:HD3	1.84	0.59
35:Sg:142:VAL:HG12	35:Sg:146:SER:HB3	1.85	0.59
40:3m:193:THR:HG23	40:3m:195:ASP:H	1.66	0.59
43:3e:303:PHE:HE2	44:3c:824:LYS:HG2	1.67	0.59
20:SR:28:PHE:HA	20:SR:55:THR:HG21	1.84	0.59
35:Sg:129:ILE:HB	35:Sg:142:VAL:HB	1.83	0.59
17:SO:34:PHE:HB3	17:SO:41:PHE:HB2	1.83	0.59
18:SP:34:MET:HE1	18:SP:45:LEU:HB2	1.84	0.59
2:5B:968:LYS:HA	2:5B:971:LEU:HG	1.85	0.59
39:S2:197:U:O4	39:S2:202:G:O6	2.21	0.59
48:3l:356:LYS:O	48:3l:360:ILE:HG13	2.02	0.59
44:3c:803:SER:HA	44:3c:841:THR:HG22	1.84	0.58
2:5B:725:LEU:HD21	2:5B:737:THR:HG23	1.86	0.58
2:5B:1141:ILE:HG23	2:5B:1159:VAL:HG12	1.85	0.58
6:SD:39:VAL:HG22	6:SD:48:ILE:HG13	1.85	0.58
39:S2:530:U:H3	39:S2:555:A:H2	1.51	0.58
48:3l:49:PRO:HD2	48:3l:52:ILE:HD12	1.85	0.58
9:SG:56:ASN:HD22	39:S2:156:G:H1'	1.68	0.58
39:S2:546:G:H4'	39:S2:547:G:H5'	1.85	0.58
39:S2:1769:C:H2'	39:S2:1770:G:C8	2.38	0.58
41:3f:108:ARG:HD3	45:3h:112:ILE:HG12	1.85	0.58
39:S2:1562:C:H2'	39:S2:1563:G:H8	1.69	0.58
2:5B:750:PRO:HG2	2:5B:846:LEU:HD11	1.86	0.58
39:S2:1513:C:H2'	39:S2:1514:G:H8	1.69	0.58
42:3a:186:LEU:HD11	42:3a:242:SER:HB2	1.85	0.58
43:3e:229:ARG:HA	43:3e:232:ILE:HD12	1.86	0.58
39:S2:527:C:H2'	39:S2:528:A:C8	2.39	0.58
44:3c:627:LYS:HA	44:3c:693:LEU:HD11	1.86	0.58
8:SF:102:LEU:HD11	28:SZ:100:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:zz:256:G:N2	38:zz:276:A:N1	2.52	0.58
39:S2:885:U:O4	39:S2:901:G:O6	2.22	0.58
43:3e:311:LYS:HE3	43:3e:315:CYS:HB2	1.86	0.58
44:3c:687:LEU:HA	44:3c:714:PHE:HZ	1.68	0.58
48:3l:289:GLN:CD	48:3l:289:GLN:H	2.12	0.58
31:Sc:12:ALA:HB1	31:Sc:32:VAL:HB	1.85	0.57
19:SQ:42:ILE:HG22	19:SQ:44:PRO:HD2	1.85	0.57
34:sh:118:ARG:HB2	34:sh:131:PHE:HB3	1.86	0.57
39:S2:609:U:H2'	39:S2:610:G:H8	1.69	0.57
43:3e:144:TYR:HB3	43:3e:175:SER:HB2	1.84	0.57
2:5B:845:MET:HG3	2:5B:846:LEU:HD22	1.85	0.57
20:SR:71:ILE:HD12	20:SR:74:GLN:HB3	1.84	0.57
40:3m:224:LEU:HD11	40:3m:245:VAL:HG11	1.85	0.57
6:SD:161:GLY:HA3	39:S2:1388:A:H61	1.68	0.57
18:SP:131:PRO:HD3	39:S2:1522:A:H62	1.69	0.57
39:S2:1010:G:H2'	39:S2:1011:A:H8	1.70	0.57
47:3k:150:TYR:HE1	48:3l:487:ARG:HH22	1.51	0.57
6:SD:70:THR:HB	6:SD:86:LEU:HG	1.85	0.57
20:SR:27:ASP:HB3	20:SR:30:THR:HG22	1.87	0.57
41:3f:252:ILE:HG22	45:3h:215:MET:HG2	1.86	0.57
14:SL:48:LYS:HA	14:SL:51:ILE:HG22	1.85	0.57
38:zz:184:G:H2'	38:zz:214:A:H61	1.68	0.57
2:5B:1142:GLU:HG2	2:5B:1147:GLN:HG2	1.87	0.57
39:S2:851:C:H5''	39:S2:852:G:H5'	1.87	0.57
43:3e:244:ASN:O	43:3e:248:THR:HG23	2.05	0.57
25:SW:6:VAL:HG23	25:SW:29:PRO:HG2	1.87	0.57
48:3l:313:VAL:HG22	48:3l:339:ILE:HD11	1.86	0.57
36:zy:57:A:H3'	36:zy:58:A:H8	1.69	0.57
42:3a:272:MET:HA	42:3a:275:TYR:HB2	1.85	0.57
44:3c:603:PRO:HA	44:3c:606:GLN:HB2	1.87	0.57
12:SJ:53:ILE:HD13	12:SJ:81:LEU:HD21	1.86	0.56
38:zz:216:U:H5'	42:3a:72:TYR:OH	2.05	0.56
39:S2:1536:G:H2'	39:S2:1537:A:H8	1.70	0.56
18:SP:75:VAL:HG12	18:SP:93:MET:HB3	1.87	0.56
43:3e:222:PHE:HB3	43:3e:232:ILE:HD11	1.87	0.56
9:SG:15:LEU:HD22	39:S2:155:G:H4'	1.87	0.56
13:SK:64:TRP:CE2	32:Sd:23:VAL:HG22	2.41	0.56
23:SU:32:LEU:HD21	23:SU:87:ARG:HG2	1.86	0.56
38:zz:55:C:H4'	38:zz:57:A:H62	1.70	0.56
38:zz:223:A:HO2'	38:zz:224:G:H8	1.51	0.56
39:S2:792:C:H2'	39:S2:793:G:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SG:52:ILE:HG23	9:SG:109:LEU:HD21	1.86	0.56
15:Sf:22:LEU:HD22	15:Sf:89:VAL:HG23	1.87	0.56
28:SZ:50:PHE:CZ	28:SZ:58:LEU:HD12	2.40	0.56
39:S2:1228:A:H2'	39:S2:1229:G:H8	1.70	0.56
35:Sg:214:GLY:HA2	35:Sg:236:ILE:HG12	1.87	0.56
38:zz:180:G:H2'	38:zz:181:G:C8	2.40	0.56
42:3a:476:ARG:HD3	44:3c:798:VAL:HG22	1.88	0.56
4:SB:137:LEU:HG	4:SB:215:VAL:HG22	1.87	0.56
13:SK:55:ARG:HB3	13:SK:57:TYR:HE2	1.71	0.56
39:S2:981:A:H2'	39:S2:982:G:C8	2.40	0.56
40:3m:65:ASN:HA	40:3m:68:VAL:HB	1.88	0.56
48:3l:243:GLN:HB3	48:3l:253:PRO:HB3	1.86	0.56
2:5B:1143:ILE:HG13	2:5B:1148:VAL:HG11	1.88	0.56
39:S2:1228:A:H2'	39:S2:1229:G:C8	2.41	0.56
40:3m:218:PHE:HA	40:3m:276:LYS:HE3	1.86	0.56
42:3a:26:PRO:O	42:3a:30:VAL:HG23	2.05	0.56
43:3e:309:GLN:HE21	43:3e:340:ILE:HG21	1.71	0.56
44:3c:445:LEU:HA	44:3c:502:ILE:HD11	1.88	0.56
39:S2:1244:U:H2'	39:S2:1245:G:H8	1.70	0.56
48:3l:457:LEU:HD13	48:3l:496:LYS:HE3	1.88	0.56
10:SH:60:ILE:HB	10:SH:92:VAL:HG22	1.88	0.56
12:SJ:135:ILE:HD11	12:SJ:157:ILE:HG23	1.88	0.56
16:SN:88:LEU:O	16:SN:92:ILE:HG13	2.06	0.56
2:5B:1143:ILE:HG12	2:5B:1157:VAL:HG12	1.88	0.55
27:SY:9:THR:HA	27:SY:23:MET:HE3	1.87	0.55
15:Sf:66:GLU:HA	15:Sf:69:CYS:SG	2.47	0.55
38:zz:260:A:H62	38:zz:273:G:H21	1.55	0.55
39:S2:880:G:N2	39:S2:906:U:O2	2.33	0.55
39:S2:1769:C:H2'	39:S2:1770:G:H8	1.71	0.55
40:3m:83:ILE:HG21	40:3m:119:VAL:HG13	1.88	0.55
10:SH:74:LYS:HG3	10:SH:75:ILE:HG23	1.89	0.55
48:3l:540:GLY:HA2	48:3l:543:PHE:CZ	2.42	0.55
7:SE:5:PRO:HD2	39:S2:446:G:H21	1.71	0.55
42:3a:523:LEU:HB3	45:3h:231:LEU:HG	1.89	0.55
42:3a:428:VAL:HG23	42:3a:429:PRO:HD3	1.89	0.55
15:Sf:24:THR:HB	15:Sf:115:GLY:HA3	1.88	0.55
18:SP:83:MET:HE2	18:SP:83:MET:HA	1.88	0.55
39:S2:322:C:H2'	39:S2:323:C:C6	2.42	0.55
47:3k:147:GLY:HA2	47:3k:189:ILE:HG21	1.89	0.55
5:SC:70:VAL:HG11	5:SC:93:ILE:HG23	1.89	0.55
39:S2:730:C:H2'	39:S2:731:G:H4'	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:3c:636:ILE:HG23	44:3c:645:LEU:HD23	1.89	0.55
48:3l:204:THR:HA	48:3l:207:LYS:HD2	1.88	0.55
18:SP:105:VAL:HG21	18:SP:111:MET:HE1	1.89	0.54
48:3l:347:LYS:HA	48:3l:350:PHE:HB2	1.89	0.54
2:5B:912:GLU:HG2	2:5B:914:ARG:H	1.72	0.54
7:SE:44:LEU:HD21	7:SE:70:ILE:HG21	1.88	0.54
39:S2:1764:G:C6	39:S2:1768:A:N7	2.74	0.54
45:3h:40:GLN:HB3	45:3h:206:LYS:HG2	1.89	0.54
13:SK:55:ARG:HB3	13:SK:57:TYR:CE2	2.43	0.54
35:Sg:174:VAL:HB	35:Sg:188:HIS:HB2	1.89	0.54
40:3m:120:ARG:HH21	40:3m:154:TRP:NE1	2.05	0.54
41:3f:247:ILE:HG12	45:3h:161:SER:HA	1.90	0.54
47:3k:102:ILE:HA	47:3k:105:LEU:HD12	1.90	0.54
40:3m:49:CYS:HA	40:3m:52:CYS:HB2	1.90	0.54
2:5B:634:ILE:HD12	2:5B:698:MET:HE3	1.89	0.54
2:5B:1127:VAL:HG22	2:5B:1182:LEU:HD22	1.89	0.54
2:5B:1138:VAL:HA	2:5B:1161:ILE:HA	1.89	0.54
18:SP:56:LEU:HD12	18:SP:80:LEU:HD12	1.90	0.54
44:3c:877:LYS:HG2	45:3h:264:MET:HE1	1.88	0.54
12:SJ:128:VAL:O	12:SJ:132:GLN:HG2	2.07	0.54
36:zy:27:U:H2'	36:zy:28:G:H8	1.71	0.54
38:zz:259:U:C4	38:zz:274:A:N7	2.76	0.54
39:S2:106:C:H2'	39:S2:107:A:H8	1.72	0.54
39:S2:877:C:H2'	39:S2:878:G:C8	2.42	0.54
41:3f:96:PRO:HA	41:3f:99:LEU:HB2	1.89	0.54
43:3e:346:ARG:HH12	44:3c:827:ILE:HD11	1.73	0.54
35:Sg:238:ALA:H	35:Sg:251:ALA:HB3	1.72	0.54
39:S2:528:A:H2'	39:S2:529:A:C8	2.43	0.54
43:3e:341:PHE:HE2	43:3e:360:LEU:HD22	1.73	0.54
45:3h:45:VAL:HG21	45:3h:78:ILE:HG22	1.90	0.54
2:5B:704:PRO:HG3	2:5B:712:LEU:HD12	1.89	0.54
4:SB:144:LYS:HB2	4:SB:208:HIS:HB3	1.90	0.54
39:S2:223:C:H2'	39:S2:224:A:C8	2.43	0.54
39:S2:1754:G:H1'	39:S2:1780:G:H1'	1.90	0.54
40:3m:273:ASN:O	40:3m:277:MET:HG2	2.08	0.54
9:SG:181:THR:HG22	9:SG:183:ARG:H	1.73	0.53
35:Sg:256:ILE:HD13	35:Sg:289:LEU:HD21	1.90	0.53
39:S2:756:C:H2'	39:S2:757:C:H6	1.73	0.53
48:3l:457:LEU:HD12	48:3l:493:PHE:HA	1.90	0.53
31:Sc:35:MET:HE2	31:Sc:35:MET:HA	1.89	0.53
39:S2:1756:C:H2'	39:S2:1757:G:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5B:650:LYS:HG2	2:5B:831:MET:HE3	1.90	0.53
5:SC:195:LEU:HD23	5:SC:224:THR:HG22	1.89	0.53
12:SJ:30:LYS:O	12:SJ:34:GLU:HG3	2.09	0.53
38:zz:145:G:H1	38:zz:248:U:H3	1.55	0.53
39:S2:1550:G:H3'	39:S2:1579:A:H61	1.73	0.53
4:SB:168:MET:O	4:SB:172:MET:HG3	2.08	0.53
39:S2:235:A:H2'	39:S2:236:A:C8	2.43	0.53
39:S2:1232:U:H2'	39:S2:1233:G:H8	1.72	0.53
2:5B:678:ILE:HD11	2:5B:698:MET:HG3	1.91	0.53
28:SZ:98:LYS:HB3	28:SZ:110:THR:HG23	1.89	0.53
3:SA:108:PHE:HB3	3:SA:140:VAL:HG21	1.91	0.53
26:SX:66:ILE:HG22	26:SX:68:LYS:HE3	1.90	0.53
38:zz:180:G:H2'	38:zz:181:G:H8	1.73	0.53
39:S2:1098:C:H2'	39:S2:1099:G:C8	2.44	0.53
39:S2:1281:G:H2'	39:S2:1282:A:C8	2.44	0.53
43:3e:312:LEU:HD23	43:3e:337:ARG:HE	1.73	0.53
45:3h:40:GLN:HA	45:3h:204:VAL:O	2.08	0.53
39:S2:1776:G:H2'	39:S2:1777:G:H4'	1.90	0.53
41:3f:283:LEU:HD23	42:3a:530:LEU:HD13	1.90	0.53
45:3h:45:VAL:O	45:3h:49:ILE:HG12	2.07	0.53
2:5B:834:LEU:O	2:5B:838:LEU:HG	2.07	0.53
21:SS:129:LEU:HD13	39:S2:1521:C:H5'	1.90	0.53
39:S2:864:A:H2'	39:S2:865:A:H8	1.74	0.53
41:3f:301:ASP:HB2	41:3f:304:VAL:HB	1.91	0.53
42:3a:98:GLU:HA	42:3a:153:LEU:HD21	1.91	0.53
45:3h:215:MET:HE2	45:3h:215:MET:HA	1.91	0.53
17:SO:95:ILE:HD11	17:SO:126:ILE:HD12	1.90	0.53
38:zz:65:C:H2'	38:zz:66:A:C8	2.42	0.53
39:S2:1536:G:H2'	39:S2:1537:A:C8	2.44	0.53
41:3f:354:LEU:HD12	44:3c:877:LYS:HZ2	1.73	0.53
48:3l:367:MET:O	48:3l:371:LEU:HD12	2.08	0.53
39:S2:848:U:H2'	39:S2:849:A:H8	1.73	0.53
39:S2:870:A:H4'	39:S2:871:U:H3'	1.90	0.52
13:SK:91:PRO:HG2	13:SK:94:LEU:HD12	1.92	0.52
14:SL:23:VAL:HG23	14:SL:26:GLY:H	1.74	0.52
1:1A:100:ALA:HA	1:1A:103:LEU:HD23	1.90	0.52
42:3a:161:LEU:HG	42:3a:174:TYR:HE2	1.75	0.52
4:SB:135:LEU:HD11	4:SB:217:MET:HE2	1.91	0.52
13:SK:11:ILE:HD11	13:SK:40:VAL:HG21	1.90	0.52
39:S2:963:A:H2'	39:S2:964:A:C8	2.44	0.52
40:3m:120:ARG:HH22	40:3m:150:TRP:CG	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:3f:106:TYR:HA	41:3f:116:VAL:HG21	1.91	0.52
12:SJ:136:ARG:HD3	12:SJ:160:SER:HA	1.92	0.52
39:S2:547:G:H2'	39:S2:549:C:H5	1.75	0.52
39:S2:1588:A:H2'	39:S2:1589:A:C8	2.44	0.52
47:3k:196:ILE:HG13	48:3l:522:TYR:HB3	1.91	0.52
48:3l:234:LEU:HD21	48:3l:269:LEU:HG	1.91	0.52
38:zz:104:C:H2'	38:zz:105:G:C8	2.44	0.52
39:S2:433:A:H2'	39:S2:434:G:C8	2.44	0.52
39:S2:791:C:H2'	39:S2:792:C:C6	2.44	0.52
40:3m:22:LEU:HD11	40:3m:45:ILE:HA	1.91	0.52
16:SN:49:GLN:HA	16:SN:52:VAL:HG12	1.91	0.52
35:Sg:191:HIS:CD2	35:Sg:195:LEU:HD11	2.44	0.52
48:3l:350:PHE:CD1	48:3l:360:ILE:HD13	2.45	0.52
29:Sa:79:ILE:HD11	39:S2:1864:U:H5'	1.91	0.52
38:zz:178:C:H2'	38:zz:179:A:H8	1.75	0.52
13:SK:2:LEU:HB2	39:S2:1315:U:H4'	1.91	0.52
35:Sg:39:THR:HG22	35:Sg:60:ARG:HB3	1.91	0.52
39:S2:1101:U:H2'	39:S2:1102:G:C8	2.45	0.52
7:SE:79:ASP:HB3	7:SE:82:TYR:HB2	1.91	0.52
22:ST:130:ASP:O	22:ST:134:ILE:HD12	2.09	0.52
36:zy:10:G:N2	36:zy:24:U:H3	2.04	0.52
39:S2:1010:G:H2'	39:S2:1011:A:C8	2.44	0.52
42:3a:398:PHE:HB2	42:3a:511:LEU:HD21	1.92	0.51
2:5B:872:THR:HG22	2:5B:934:LEU:HA	1.91	0.51
39:S2:907:G:H2'	39:S2:908:A:C8	2.45	0.51
41:3f:309:MET:HE2	41:3f:309:MET:HA	1.93	0.51
11:SI:106:SER:HB3	11:SI:171:LEU:HG	1.93	0.51
39:S2:794:A:H2'	39:S2:795:A:C8	2.46	0.51
45:3h:100:GLN:O	45:3h:104:MET:HG2	2.10	0.51
48:3l:535:VAL:HB	48:3l:538:ARG:HG2	1.92	0.51
9:SG:218:LYS:O	9:SG:222:GLU:HG2	2.11	0.51
10:SH:9:VAL:HG12	10:SH:11:PRO:HD3	1.91	0.51
39:S2:746:C:H4'	39:S2:747:U:H5'	1.92	0.51
42:3a:234:LEU:HD21	42:3a:274:ASN:HB3	1.92	0.51
48:3l:451:VAL:HA	48:3l:454:GLN:NE2	2.26	0.51
9:SG:27:PHE:HE2	9:SG:41:LEU:HD21	1.74	0.51
15:Sf:93:LYS:HG2	15:Sf:102:LYS:HB2	1.93	0.51
38:zz:98:G:H2'	38:zz:99:A:C8	2.46	0.51
38:zz:336:U:HO2'	38:zz:337:G:H8	1.58	0.51
39:S2:543:C:H3'	39:S2:544:G:H8	1.75	0.51
39:S2:669:A:H8	39:S2:1164:G:O2'	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:zy:12:G:H22	36:zy:21:G:N2	2.09	0.51
43:3e:384:ILE:HD12	43:3e:391:VAL:HG22	1.92	0.51
2:5B:1197:TRP:H	2:5B:1199:ARG:HH21	1.59	0.51
10:SH:117:PRO:HD2	10:SH:120:ARG:HG3	1.93	0.51
12:SJ:174:LYS:HG3	39:S2:560:A:H5'	1.92	0.51
40:3m:53:LEU:HD13	40:3m:64:MET:HE1	1.93	0.51
41:3f:351:ASN:HD21	45:3h:257:ILE:HD11	1.75	0.51
2:5B:1109:VAL:HG11	36:zy:74:C:H1'	1.91	0.51
42:3a:296:LEU:HD23	42:3a:322:VAL:HA	1.92	0.51
44:3c:806:THR:O	44:3c:810:MET:HG3	2.09	0.51
16:SN:25:TRP:CD2	30:Sb:82:LYS:HD3	2.46	0.51
38:zz:73:A:H2'	38:zz:74:A:H8	1.76	0.51
38:zz:178:C:H2'	38:zz:179:A:C8	2.46	0.51
39:S2:907:G:H2'	39:S2:908:A:H8	1.74	0.51
44:3c:598:ILE:HG21	44:3c:609:TYR:HD2	1.76	0.51
27:SY:41:ARG:HA	27:SY:55:ILE:HD11	1.92	0.51
38:zz:213:C:H2'	38:zz:214:A:C8	2.46	0.51
39:S2:1035:A:N6	39:S2:1081:U:H3	2.09	0.51
2:5B:1205:SER:HB2	2:5B:1208:GLN:HE21	1.75	0.50
3:SA:187:GLY:HA2	24:SV:45:ARG:HH11	1.76	0.50
36:zy:9:G:H3'	36:zy:10:G:C8	2.46	0.50
39:S2:1189:A:H2'	39:S2:1190:A:H8	1.76	0.50
39:S2:1545:A:H2'	39:S2:1546:G:C8	2.46	0.50
42:3a:247:GLN:O	42:3a:251:LYS:HG2	2.11	0.50
44:3c:574:TYR:HD2	44:3c:612:THR:HA	1.77	0.50
18:SP:24:GLN:O	18:SP:28:MET:HG2	2.10	0.50
35:Sg:299:PHE:HD1	35:Sg:309:VAL:HG12	1.76	0.50
48:3l:535:VAL:HG12	48:3l:538:ARG:H	1.76	0.50
48:3l:543:PHE:O	48:3l:547:ILE:HG13	2.11	0.50
2:5B:639:HIS:CD2	2:5B:640:VAL:HG12	2.47	0.50
2:5B:675:LEU:HA	2:5B:678:ILE:HB	1.94	0.50
39:S2:102:A:H4'	39:S2:104:A:C8	2.47	0.50
39:S2:1813:A:H3'	39:S2:1814:G:H8	1.76	0.50
48:3l:150:LEU:HD23	48:3l:153:ARG:HD2	1.93	0.50
4:SB:87:ILE:HG22	4:SB:101:HIS:HB2	1.93	0.50
12:SJ:114:VAL:HG22	12:SJ:119:LEU:HD12	1.94	0.50
2:5B:1124:PRO:HG2	2:5B:1185:LYS:HB3	1.94	0.50
3:SA:184:ARG:HH21	3:SA:191:ARG:HA	1.75	0.50
9:SG:229:ALA:HA	9:SG:232:ARG:HG2	1.93	0.50
39:S2:145:G:H2'	39:S2:146:G:C8	2.46	0.50
44:3c:613:MET:HE1	44:3c:636:ILE:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5B:1096:ILE:HG13	2:5B:1176:PHE:HZ	1.77	0.50
12:SJ:136:ARG:HE	12:SJ:139:LYS:HA	1.75	0.50
21:SS:84:LEU:HD12	21:SS:97:GLN:HB2	1.92	0.50
24:SV:38:GLU:OE1	24:SV:51:LYS:HD2	2.12	0.50
32:Sd:33:LYS:HE2	32:Sd:34:TYR:CZ	2.46	0.50
35:Sg:176:VAL:HB	35:Sg:186:THR:HB	1.93	0.50
41:3f:120:LEU:HD23	41:3f:131:VAL:HG11	1.93	0.50
36:zy:4:A:H2'	36:zy:5:G:C8	2.47	0.50
40:3m:62:SER:HB2	41:3f:222:GLY:H	1.76	0.50
43:3e:144:TYR:CZ	43:3e:178:LEU:HD13	2.47	0.50
43:3e:322:ASP:HB3	43:3e:325:LEU:HB2	1.94	0.50
6:SD:20:GLU:HB2	13:SK:64:TRP:CZ3	2.46	0.50
6:SD:31:GLU:HA	6:SD:107:TYR:HE2	1.77	0.50
13:SK:57:TYR:HB3	13:SK:75:GLY:HA2	1.93	0.50
27:SY:25:ILE:HD11	27:SY:73:GLY:HA3	1.93	0.50
29:Sa:51:ARG:HG2	31:Sc:62:GLU:HB3	1.94	0.50
39:S2:793:G:H2'	39:S2:794:A:O4'	2.12	0.50
39:S2:1279:C:H2'	39:S2:1280:G:H8	1.77	0.50
5:SC:139:LEU:HD11	5:SC:237:ALA:HB1	1.92	0.49
19:SQ:39:LEU:HD23	19:SQ:52:LEU:HD23	1.92	0.49
44:3c:588:LEU:HA	44:3c:591:MET:HB2	1.94	0.49
45:3h:119:TRP:HH2	45:3h:133:LEU:HG	1.76	0.49
48:3l:322:ALA:O	48:3l:326:MET:HG2	2.12	0.49
2:5B:791:ALA:O	2:5B:795:ILE:HG13	2.12	0.49
4:SB:67:PHE:O	4:SB:85:LYS:HA	2.11	0.49
11:SI:150:ASP:HA	11:SI:153:LYS:HD2	1.92	0.49
15:Sf:40:LYS:HD3	34:sh:129:GLY:HA3	1.93	0.49
40:3m:143:GLU:HB3	40:3m:146:GLN:HG3	1.93	0.49
42:3a:226:GLN:O	42:3a:230:LEU:HG	2.12	0.49
42:3a:326:THR:HA	42:3a:329:ILE:HD11	1.93	0.49
42:3a:329:ILE:HB	42:3a:367:ARG:HH11	1.76	0.49
28:SZ:50:PHE:HD1	28:SZ:51:ASP:H	1.60	0.49
40:3m:71:LEU:HD13	40:3m:74:LEU:HD12	1.94	0.49
42:3a:351:LYS:HG2	44:3c:725:PRO:HA	1.94	0.49
2:5B:1013:VAL:HG23	2:5B:1039:VAL:HG11	1.95	0.49
6:SD:42:THR:HG22	6:SD:44:THR:H	1.77	0.49
10:SH:36:LEU:HD21	10:SH:78:ARG:HD2	1.93	0.49
27:SY:110:ARG:HH21	27:SY:126:GLY:HA3	1.76	0.49
39:S2:5:U:H2'	39:S2:6:G:H8	1.77	0.49
42:3a:480:LEU:HB3	42:3a:482:VAL:HG12	1.94	0.49
13:SK:32:HIS:HE1	13:SK:34:GLU:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:S2:106:C:H2'	39:S2:107:A:C8	2.48	0.49
41:3f:256:CYS:HB3	45:3h:216:TRP:CE2	2.47	0.49
43:3e:349:GLN:HB2	44:3c:834:SER:HB2	1.94	0.49
3:SA:205:ARG:HH22	3:SA:210:ILE:HG13	1.78	0.49
15:Sf:16:THR:O	15:Sf:19:GLN:HG3	2.13	0.49
17:SO:30:VAL:HG23	17:SO:94:HIS:HB2	1.93	0.49
26:SX:72:VAL:HG13	26:SX:81:ILE:HG13	1.94	0.49
39:S2:70:G:H21	39:S2:79:A:H62	1.60	0.49
39:S2:196:C:H2'	39:S2:197:U:C6	2.47	0.49
39:S2:1759:G:H2'	39:S2:1760:G:C8	2.48	0.49
41:3f:343:LEU:HD12	48:3l:554:ASN:ND2	2.27	0.49
7:SE:61:VAL:HG12	7:SE:80:ILE:HD12	1.94	0.49
38:zz:248:U:H2'	38:zz:249:G:H8	1.78	0.49
48:3l:475:LEU:HD21	48:3l:479:LEU:HD12	1.94	0.49
2:5B:646:LYS:HG3	2:5B:825:ALA:HB1	1.95	0.49
5:SC:214:LEU:HD13	5:SC:244:ILE:HD11	1.94	0.49
7:SE:140:VAL:HG22	7:SE:146:THR:HG22	1.93	0.49
8:SF:89:THR:HA	8:SF:92:ILE:HD12	1.94	0.49
39:S2:1714:U:H2'	39:S2:1715:A:H8	1.77	0.49
40:3m:113:MET:HE1	40:3m:123:VAL:HG11	1.95	0.49
43:3e:351:ILE:HD11	43:3e:356:LEU:HD21	1.93	0.49
45:3h:67:LEU:HD13	45:3h:78:ILE:HG13	1.94	0.49
45:3h:336:GLN:O	45:3h:340:LYS:HG2	2.13	0.49
1:1A:62:ARG:HD3	1:1A:92:ILE:HG22	1.94	0.49
5:SC:207:ALA:HB2	39:S2:4:C:H4'	1.94	0.49
7:SE:247:THR:O	7:SE:251:GLU:HB3	2.13	0.49
19:SQ:19:ALA:HB2	19:SQ:75:GLY:HA3	1.94	0.49
27:SY:86:GLU:OE2	27:SY:87:PRO:HD2	2.12	0.49
40:3m:161:LYS:O	40:3m:165:LEU:HG	2.13	0.49
45:3h:67:LEU:HD22	45:3h:78:ILE:HG21	1.95	0.49
2:5B:793:ALA:O	2:5B:797:GLU:HG2	2.13	0.49
7:SE:146:THR:HG21	39:S2:122:G:H21	1.78	0.49
39:S2:1763:G:H2'	39:S2:1764:G:H8	1.76	0.49
2:5B:775:THR:O	2:5B:779:GLN:HG2	2.13	0.48
2:5B:925:VAL:HG21	2:5B:931:VAL:HG21	1.95	0.48
4:SB:68:GLU:HG3	4:SB:85:LYS:HG2	1.95	0.48
4:SB:165:ARG:O	4:SB:169:MET:HG3	2.13	0.48
33:Se:25:LYS:HA	33:Se:25:LYS:HD3	1.65	0.48
34:sh:119:ARG:HH12	34:sh:148:TYR:HD2	1.61	0.48
36:zy:4:A:H2'	36:zy:5:G:H8	1.77	0.48
38:zz:179:A:H2'	38:zz:180:G:H8	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SI:66:SER:HA	11:SI:73:THR:HG22	1.96	0.48
21:SS:54:LYS:HB2	21:SS:58:GLU:OE2	2.12	0.48
22:ST:71:GLY:O	22:ST:75:MET:HG2	2.13	0.48
26:SX:60:LYS:HG2	26:SX:114:ASP:O	2.13	0.48
36:zy:42:G:H2'	36:zy:43:A:C8	2.48	0.48
39:S2:321:C:H2'	39:S2:322:C:C6	2.48	0.48
42:3a:190:ARG:HB3	42:3a:193:GLU:HB2	1.94	0.48
44:3c:548:MET:HE2	44:3c:548:MET:HA	1.94	0.48
48:3l:475:LEU:HD22	48:3l:486:PHE:CD1	2.49	0.48
38:zz:179:A:H2'	38:zz:180:G:C8	2.48	0.48
39:S2:746:C:H1'	39:S2:747:U:H5	1.79	0.48
39:S2:1277:C:H2'	39:S2:1278:A:C8	2.48	0.48
44:3c:507:ILE:HG12	44:3c:511:TYR:HB3	1.95	0.48
45:3h:260:TYR:HE1	45:3h:311:PRO:HG2	1.77	0.48
45:3h:306:LYS:HD2	45:3h:307:PRO:HD2	1.94	0.48
10:SH:27:LEU:O	10:SH:31:GLU:HB2	2.13	0.48
16:SN:46:THR:HG23	16:SN:48:SER:H	1.77	0.48
27:SY:66:GLY:HA3	39:S2:581:U:H4'	1.95	0.48
35:Sg:57:ARG:HE	35:Sg:95:GLY:HA3	1.78	0.48
39:S2:1281:G:H2'	39:S2:1282:A:H8	1.78	0.48
39:S2:1773:C:H2'	39:S2:1774:C:O4'	2.14	0.48
44:3c:507:ILE:HA	44:3c:510:THR:HG22	1.96	0.48
48:3l:472:VAL:HG13	48:3l:486:PHE:HE2	1.78	0.48
2:5B:652:ARG:HA	2:5B:910:MET:SD	2.53	0.48
2:5B:1108:ILE:HD11	2:5B:1169:PRO:HB2	1.95	0.48
3:SA:18:PHE:CZ	3:SA:177:MET:HE1	2.49	0.48
6:SD:18:LYS:HZ2	6:SD:39:VAL:HB	1.78	0.48
38:zz:257:A:H1'	38:zz:259:U:H5	1.79	0.48
42:3a:279:VAL:HA	42:3a:282:VAL:HG12	1.96	0.48
44:3c:695:ILE:HD12	44:3c:745:LYS:HZ1	1.78	0.48
18:SP:124:LYS:HB3	18:SP:124:LYS:HE2	1.67	0.48
26:SX:101:LEU:HB3	26:SX:124:LYS:HB2	1.94	0.48
40:3m:120:ARG:HH21	40:3m:154:TRP:HE1	1.61	0.48
23:SU:20:ILE:HB	23:SU:91:LEU:HB2	1.96	0.48
39:S2:844:U:H2'	39:S2:845:G:H8	1.79	0.48
39:S2:1763:G:H2'	39:S2:1764:G:C8	2.49	0.48
43:3e:351:ILE:HG23	43:3e:391:VAL:HB	1.96	0.48
43:3e:291:PRO:HB2	43:3e:311:LYS:HZ3	1.78	0.48
45:3h:47:LEU:HA	45:3h:50:ILE:HB	1.96	0.48
2:5B:974:ILE:HG12	2:5B:1008:ILE:HD13	1.95	0.48
12:SJ:132:GLN:HB3	39:S2:562:U:H4'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:SU:20:ILE:HG13	23:SU:98:VAL:HG21	1.96	0.48
39:S2:232:A:H5''	39:S2:890:U:H3	1.78	0.48
44:3c:570:LEU:HD13	44:3c:608:LEU:HB3	1.96	0.48
9:SG:164:LYS:HB2	39:S2:67:C:N4	2.29	0.48
11:SI:110:ARG:O	11:SI:114:GLU:HG2	2.14	0.48
39:S2:1232:U:H2'	39:S2:1233:G:C8	2.48	0.48
40:3m:137:ILE:HG12	40:3m:171:ALA:HB1	1.95	0.48
41:3f:115:ARG:HH22	41:3f:183:SER:HB3	1.79	0.48
42:3a:201:LEU:HB3	42:3a:233:ARG:NH2	2.28	0.48
45:3h:65:GLY:HA3	45:3h:120:TYR:CE1	2.49	0.48
48:3l:140:ILE:HD12	48:3l:144:VAL:HG21	1.96	0.48
48:3l:362:LYS:O	48:3l:366:GLN:HG2	2.14	0.48
15:Sf:12:MET:HE3	15:Sf:16:THR:OG1	2.14	0.47
20:SR:111:PHE:O	20:SR:114:LEU:HD13	2.14	0.47
39:S2:1748:G:H1	39:S2:1786:U:H3	1.62	0.47
40:3m:230:LYS:HA	40:3m:233:GLU:HG3	1.95	0.47
42:3a:535:GLU:HG2	45:3h:224:VAL:HG21	1.96	0.47
7:SE:62:LYS:HA	7:SE:80:ILE:HD11	1.95	0.47
8:SF:88:MET:O	8:SF:92:ILE:HG13	2.14	0.47
16:SN:127:ARG:O	16:SN:131:THR:HG22	2.15	0.47
18:SP:53:GLN:H	18:SP:53:GLN:CD	2.21	0.47
38:zz:256:G:N1	38:zz:276:A:C6	2.82	0.47
2:5B:1188:ARG:HA	2:5B:1191:ILE:HG22	1.96	0.47
6:SD:123:LEU:HD11	6:SD:152:PHE:HB3	1.96	0.47
17:SO:120:ALA:HB2	29:Sa:53:ILE:HD13	1.96	0.47
38:zz:240:C:H2'	38:zz:241:G:C8	2.49	0.47
41:3f:115:ARG:NE	41:3f:117:ILE:HD11	2.30	0.47
41:3f:340:LEU:HD11	45:3h:243:LEU:HD11	1.96	0.47
43:3e:167:SER:HA	43:3e:170:TRP:HD1	1.80	0.47
43:3e:305:PHE:HE1	43:3e:343:THR:HG23	1.79	0.47
10:SH:109:ARG:HH21	39:S2:867:G:H21	1.61	0.47
22:ST:104:LEU:HD22	22:ST:121:ARG:HD2	1.96	0.47
27:SY:39:GLU:HA	27:SY:42:GLU:HG3	1.96	0.47
41:3f:91:VAL:O	41:3f:128:SER:HA	2.14	0.47
47:3k:152:HIS:CE1	48:3l:524:ASP:HB2	2.49	0.47
4:SB:136:ARG:HB2	4:SB:218:LEU:HD11	1.96	0.47
17:SO:117:ARG:O	17:SO:121:ARG:HG2	2.15	0.47
20:SR:103:LYS:HA	20:SR:106:LEU:HD12	1.97	0.47
36:zy:27:U:H2'	36:zy:28:G:C8	2.49	0.47
36:zy:57:A:H3'	36:zy:58:A:C8	2.48	0.47
39:S2:1405:A:H2'	39:S2:1406:G:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SD:101:GLN:HG3	6:SD:126:ILE:HD11	1.97	0.47
9:SG:7:PHE:HD2	9:SG:10:THR:HG22	1.78	0.47
38:zz:183:C:H2'	38:zz:184:G:C8	2.50	0.47
43:3e:239:GLN:HG3	43:3e:242:TYR:H	1.79	0.47
48:3l:137:TYR:CE2	48:3l:156:SER:HA	2.50	0.47
2:5B:1163:PRO:HG3	2:5B:1169:PRO:HB3	1.95	0.47
4:SB:222:LYS:HD2	4:SB:222:LYS:HA	1.71	0.47
8:SF:42:LYS:HD3	8:SF:42:LYS:HA	1.65	0.47
9:SG:186:GLN:HE22	39:S2:318:A:H61	1.62	0.47
19:SQ:31:LEU:HD21	19:SQ:33:LYS:HD2	1.97	0.47
20:SR:109:LEU:HG	20:SR:111:PHE:HD2	1.80	0.47
22:ST:78:ILE:HD11	39:S2:1587:G:C5	2.50	0.47
23:SU:94:PRO:HD2	23:SU:97:ILE:HD11	1.96	0.47
39:S2:201:C:H3'	39:S2:202:G:H8	1.79	0.47
39:S2:878:G:H22	39:S2:908:A:H2	1.62	0.47
39:S2:1417:C:H5''	39:S2:1418:C:C5	2.49	0.47
39:S2:1736:G:H2'	39:S2:1737:G:H8	1.79	0.47
39:S2:1858:G:H2'	39:S2:1859:A:H8	1.79	0.47
42:3a:319:SER:HA	42:3a:322:VAL:HG12	1.95	0.47
43:3e:414:ARG:HE	43:3e:417:MET:HG3	1.79	0.47
44:3c:687:LEU:HA	44:3c:714:PHE:CZ	2.47	0.47
48:3l:246:VAL:HG21	48:3l:256:VAL:HG21	1.97	0.47
48:3l:323:TYR:HB3	48:3l:332:ALA:HB2	1.96	0.47
4:SB:217:MET:HE3	4:SB:217:MET:HB2	1.69	0.47
36:zy:5:G:H2'	36:zy:6:A:H8	1.80	0.47
38:zz:205:A:H2'	38:zz:206:A:C8	2.50	0.47
39:S2:1007:C:H2'	39:S2:1008:A:C8	2.49	0.47
39:S2:1768:A:H2'	39:S2:1769:C:C6	2.50	0.47
40:3m:120:ARG:HE	40:3m:154:TRP:HE1	1.63	0.47
46:3d:31:GLN:HG2	46:3d:32:PRO:HD2	1.97	0.47
9:SG:224:ARG:HA	9:SG:227:GLN:OE1	2.15	0.47
39:S2:754:G:C6	39:S2:791:C:H1'	2.50	0.47
39:S2:1643:U:H2'	39:S2:1644:C:C6	2.49	0.47
2:5B:906:LEU:HD21	2:5B:931:VAL:HG22	1.97	0.47
21:SS:50:ILE:HD11	21:SS:63:GLU:HB2	1.97	0.47
39:S2:1144:A:H2'	39:S2:1145:A:C8	2.51	0.47
13:SK:86:PRO:HA	13:SK:87:PRO:HD3	1.83	0.46
39:S2:866:U:H2'	39:S2:867:G:C8	2.50	0.46
41:3f:172:TRP:HZ3	41:3f:174:ALA:HB2	1.80	0.46
44:3c:586:ARG:HD2	44:3c:586:ARG:HA	1.68	0.46
48:3l:294:LEU:HD22	48:3l:297:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:3l:320:GLY:HA3	48:3l:336:PHE:HE1	1.80	0.46
8:SF:130:ARG:NH2	38:zz:84:C:H42	2.07	0.46
9:SG:230:LYS:HA	9:SG:233:ARG:HE	1.80	0.46
20:SR:51:ALA:O	20:SR:55:THR:HG23	2.15	0.46
39:S2:1326:U:H4'	39:S2:1327:G:OP1	2.15	0.46
39:S2:1797:U:H2'	39:S2:1798:C:C6	2.49	0.46
42:3a:525:ALA:O	42:3a:529:VAL:HG12	2.15	0.46
48:3l:377:MET:HE1	48:3l:454:GLN:NE2	2.30	0.46
3:SA:80:ARG:O	3:SA:84:GLN:HG2	2.15	0.46
15:Sf:37:GLU:CD	15:Sf:37:GLU:H	2.23	0.46
21:SS:26:ILE:HA	21:SS:56:ALA:HB2	1.96	0.46
39:S2:595:U:H2'	39:S2:596:U:C6	2.50	0.46
39:S2:1677:U:H2'	39:S2:1678:A:H8	1.80	0.46
41:3f:103:VAL:HG23	45:3h:211:ILE:HG22	1.95	0.46
2:5B:1127:VAL:HG23	2:5B:1135:ILE:HD11	1.97	0.46
6:SD:8:LYS:HB3	23:SU:61:LEU:HD21	1.97	0.46
10:SH:141:GLY:HA2	16:SN:18:TYR:HE2	1.80	0.46
38:zz:139:C:H2'	38:zz:140:A:C8	2.50	0.46
39:S2:799:U:O2'	39:S2:800:U:H5''	2.16	0.46
39:S2:1845:A:H2'	39:S2:1846:G:C8	2.50	0.46
41:3f:353:LYS:HD2	41:3f:353:LYS:HA	1.65	0.46
48:3l:369:ALA:O	48:3l:373:ILE:HG13	2.15	0.46
2:5B:1199:ARG:HA	2:5B:1202:MET:HE3	1.98	0.46
4:SB:120:MET:HE1	39:S2:987:A:C6	2.50	0.46
6:SD:158:ILE:HG22	6:SD:189:MET:SD	2.55	0.46
9:SG:172:LYS:HE3	39:S2:65:C:H4'	1.98	0.46
15:Sf:33:ARG:HB2	15:Sf:109:VAL:HG22	1.96	0.46
39:S2:1845:A:H2'	39:S2:1846:G:H8	1.81	0.46
42:3a:63:LYS:HB3	42:3a:66:LEU:HD23	1.98	0.46
48:3l:464:LEU:HD11	48:3l:519:VAL:HG13	1.97	0.46
2:5B:823:THR:HG22	2:5B:830:GLY:HA3	1.96	0.46
4:SB:120:MET:HG3	4:SB:142:PHE:CE2	2.50	0.46
39:S2:1755:C:H2'	39:S2:1756:C:H6	1.80	0.46
42:3a:539:PRO:HG2	42:3a:542:ILE:HB	1.96	0.46
45:3h:288:ARG:HB2	45:3h:295:PRO:HA	1.98	0.46
11:SI:97:VAL:HG12	11:SI:100:CYS:HB3	1.97	0.46
26:SX:68:LYS:HB3	26:SX:91:LEU:HD22	1.97	0.46
28:SZ:64:ASN:HA	28:SZ:111:ARG:HD3	1.98	0.46
39:S2:1337:C:H2'	39:S2:1338:G:H8	1.81	0.46
41:3f:249:VAL:O	41:3f:253:MET:HG3	2.15	0.46
42:3a:514:MET:HE2	42:3a:514:MET:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:3e:211:ARG:O	43:3e:215:ILE:HG12	2.16	0.46
43:3e:355:MET:HE1	44:3c:837:GLN:HG2	1.97	0.46
44:3c:573:ILE:HD11	44:3c:588:LEU:HB3	1.98	0.46
44:3c:614:VAL:O	44:3c:618:ILE:HG12	2.16	0.46
2:5B:797:GLU:O	2:5B:801:GLN:HG2	2.15	0.46
3:SA:59:LEU:HD23	3:SA:59:LEU:HA	1.82	0.46
7:SE:31:PRO:HA	7:SE:81:THR:HB	1.98	0.46
13:SK:16:PHE:HE1	13:SK:91:PRO:HD3	1.80	0.46
38:zz:275:A:H2'	38:zz:276:A:H8	1.80	0.46
43:3e:403:GLN:O	43:3e:406:GLU:HG3	2.16	0.46
45:3h:125:TYR:CE2	45:3h:241:LYS:HB3	2.50	0.46
45:3h:260:TYR:CE1	45:3h:311:PRO:HG2	2.50	0.46
3:SA:210:ILE:O	3:SA:214:GLU:HG2	2.16	0.46
15:Sf:23:LYS:HA	15:Sf:23:LYS:HD3	1.78	0.46
35:Sg:106:LYS:HE3	35:Sg:107:ASP:H	1.81	0.46
35:Sg:125:ARG:HG2	35:Sg:150:TRP:CG	2.50	0.46
39:S2:893:U:H2'	39:S2:894:G:C8	2.51	0.46
2:5B:856:LEU:HG	2:5B:949:VAL:HG12	1.98	0.46
2:5B:1103:ASN:HB3	2:5B:1107:PRO:HG2	1.97	0.46
10:SH:114:GLN:NE2	39:S2:875:A:H1'	2.31	0.46
13:SK:57:TYR:HB3	13:SK:75:GLY:CA	2.46	0.46
38:zz:78:U:H2'	38:zz:79:C:C6	2.51	0.46
39:S2:980:A:H2'	39:S2:981:A:C8	2.50	0.46
39:S2:1736:G:H2'	39:S2:1737:G:C8	2.50	0.46
45:3h:141:GLN:HG3	45:3h:174:MET:HE2	1.98	0.46
47:3k:75:THR:HG22	47:3k:134:PHE:HD1	1.80	0.46
7:SE:11:ARG:HA	7:SE:28:ALA:HB2	1.98	0.45
15:Sf:36:ARG:HH21	15:Sf:40:LYS:NZ	2.11	0.45
15:Sf:36:ARG:HH22	39:S2:1310:U:P	2.39	0.45
22:ST:113:VAL:HG12	22:ST:123:LEU:HD12	1.98	0.45
39:S2:201:C:H3'	39:S2:202:G:C8	2.52	0.45
39:S2:551:U:H2'	39:S2:552:G:C8	2.51	0.45
39:S2:898:U:H2'	39:S2:899:U:C6	2.51	0.45
6:SD:67:ARG:HA	6:SD:70:THR:HG22	1.97	0.45
12:SJ:63:LEU:HD23	12:SJ:63:LEU:HA	1.84	0.45
14:SL:40:ILE:HD13	14:SL:40:ILE:HA	1.78	0.45
15:Sf:92:CYS:HA	15:Sf:102:LYS:HB3	1.97	0.45
28:SZ:90:GLU:OE1	28:SZ:91:LEU:HD12	2.16	0.45
38:zz:112:C:H2'	38:zz:113:U:O4'	2.15	0.45
38:zz:183:C:H2'	38:zz:184:G:H8	1.81	0.45
41:3f:217:VAL:HG13	41:3f:235:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:3f:327:LEU:HD12	45:3h:341:LEU:HD22	1.98	0.45
42:3a:225:SER:HA	42:3a:228:MET:HE3	1.99	0.45
48:3l:447:PHE:O	48:3l:451:VAL:HG13	2.16	0.45
39:S2:1418:C:H4'	39:S2:1419:C:H2'	1.99	0.45
48:3l:133:LYS:HA	48:3l:133:LYS:HD2	1.69	0.45
48:3l:286:ASP:HB3	48:3l:289:GLN:HG2	1.98	0.45
48:3l:471:PRO:HD2	48:3l:474:LYS:HD3	1.99	0.45
5:SC:73:MET:HE3	5:SC:96:PHE:HZ	1.80	0.45
11:SI:154:LYS:HD3	11:SI:154:LYS:HA	1.58	0.45
29:Sa:18:VAL:HG21	29:Sa:33:ASP:OD1	2.16	0.45
39:S2:1759:G:H2'	39:S2:1760:G:H8	1.80	0.45
44:3c:553:LYS:HA	44:3c:553:LYS:HD3	1.76	0.45
8:SF:136:ARG:HB2	8:SF:203:ASN:HD22	1.81	0.45
31:Sc:17:VAL:HG23	31:Sc:30:VAL:HG12	1.99	0.45
38:zz:172:A:H2'	38:zz:173:A:C8	2.52	0.45
39:S2:1457:U:H2'	39:S2:1458:G:H8	1.81	0.45
44:3c:863:LEU:O	44:3c:867:VAL:HG13	2.16	0.45
48:3l:545:ARG:HH12	48:3l:548:HIS:HB3	1.82	0.45
3:SA:32:PHE:CD1	39:S2:1097:G:H4'	2.51	0.45
6:SD:157:MET:HG2	6:SD:159:HIS:CE1	2.51	0.45
8:SF:22:LYS:HB3	8:SF:22:LYS:HE2	1.72	0.45
8:SF:79:HIS:CD2	8:SF:159:ARG:HD2	2.52	0.45
18:SP:85:ILE:HD12	18:SP:111:MET:HG2	1.99	0.45
19:SQ:50:LYS:HA	19:SQ:53:GLU:HG3	1.99	0.45
22:ST:97:LYS:HB2	22:ST:97:LYS:HE3	1.72	0.45
23:SU:59:LYS:HB2	23:SU:84:ILE:HB	1.98	0.45
39:S2:788:G:H2'	39:S2:789:G:C8	2.52	0.45
39:S2:845:G:H2'	39:S2:846:G:C8	2.51	0.45
39:S2:1244:U:H2'	39:S2:1245:G:C8	2.52	0.45
40:3m:189:LEU:HD23	40:3m:228:PRO:HG2	1.99	0.45
40:3m:251:SER:HA	40:3m:254:LYS:HE2	1.98	0.45
42:3a:47:HIS:O	42:3a:51:MET:HG2	2.16	0.45
43:3e:274:LEU:HD21	43:3e:300:TYR:CZ	2.52	0.45
44:3c:637:GLN:HB3	44:3c:686:TYR:CZ	2.52	0.45
2:5B:795:ILE:HA	2:5B:805:ALA:HB3	1.99	0.45
2:5B:905:LEU:HD11	2:5B:934:LEU:HD12	1.99	0.45
7:SE:182:MET:HE3	7:SE:192:ILE:HD11	1.97	0.45
11:SI:75:LYS:HE2	39:S2:303:C:H5''	1.99	0.45
14:SL:111:VAL:HG12	14:SL:140:PHE:HB2	1.98	0.45
15:Sf:53:ALA:HA	15:Sf:79:VAL:HG12	1.98	0.45
16:SN:91:LEU:HB3	16:SN:122:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:zy:17:G:H5'	36:zy:56:G:N2	2.32	0.45
39:S2:1189:A:H2'	39:S2:1190:A:C8	2.52	0.45
39:S2:1755:C:H2'	39:S2:1756:C:C6	2.52	0.45
43:3e:259:THR:HA	43:3e:332:PHE:HE2	1.81	0.45
1:1A:23:LYS:HD2	1:1A:23:LYS:HA	1.80	0.45
8:SF:68:ILE:HD11	8:SF:151:ILE:HD11	1.99	0.45
12:SJ:58:ARG:O	12:SJ:62:THR:HG23	2.17	0.45
14:SL:120:VAL:HG12	14:SL:145:VAL:HG11	1.99	0.45
19:SQ:48:GLN:HA	19:SQ:48:GLN:HE21	1.81	0.45
38:zz:80:U:H2'	38:zz:81:A:C8	2.52	0.45
38:zz:275:A:H2'	38:zz:276:A:C8	2.51	0.45
39:S2:928:G:H2'	39:S2:929:G:C8	2.51	0.45
44:3c:621:PHE:O	44:3c:778:MET:HE1	2.17	0.45
2:5B:613:ILE:HD11	2:5B:958:VAL:HG11	1.98	0.45
3:SA:38:ILE:HG12	3:SA:47:TYR:HD2	1.81	0.45
4:SB:63:LYS:HG3	4:SB:89:GLU:HA	1.98	0.45
5:SC:133:TYR:CD1	5:SC:216:MET:HA	2.51	0.45
11:SI:107:THR:O	11:SI:111:GLN:HG3	2.17	0.45
15:Sf:19:GLN:HB3	15:Sf:88:TRP:CE3	2.52	0.45
20:SR:31:ASN:ND2	20:SR:55:THR:HG22	2.32	0.45
38:zz:240:C:H2'	38:zz:241:G:H8	1.82	0.45
43:3e:353:ILE:HA	43:3e:356:LEU:HB2	1.99	0.45
47:3k:74:LEU:HD12	47:3k:77:LEU:HD22	1.99	0.45
48:3l:257:ALA:HB1	48:3l:261:GLY:HA3	1.99	0.45
8:SF:171:GLU:OE1	28:SZ:69:THR:HG21	2.17	0.45
18:SP:78:THR:HA	39:S2:1298:G:H4'	1.98	0.45
30:Sb:54:VAL:HG12	30:Sb:63:LEU:HD13	1.98	0.45
35:Sg:172:LYS:CD	35:Sg:193:GLY:H	2.30	0.45
38:zz:108:C:H2'	38:zz:109:A:C8	2.52	0.45
39:S2:538:U:H2'	39:S2:539:C:O4'	2.16	0.45
40:3m:236:LEU:HD12	40:3m:239:ASP:HB3	1.99	0.45
48:3l:139:HIS:HB3	48:3l:143:LYS:HE2	1.99	0.45
2:5B:1074:GLN:O	2:5B:1078:LYS:HG2	2.15	0.44
3:SA:34:MET:HE1	3:SA:162:PRO:HB3	2.00	0.44
13:SK:32:HIS:CE1	13:SK:34:GLU:HB3	2.52	0.44
15:Sf:94:ILE:HG13	15:Sf:98:GLY:HA2	1.99	0.44
35:Sg:106:LYS:HD2	35:Sg:106:LYS:HA	1.85	0.44
39:S2:885:U:H2'	39:S2:886:A:C8	2.52	0.44
39:S2:1629:C:H2'	39:S2:1630:A:H8	1.81	0.44
43:3e:289:LYS:HA	43:3e:289:LYS:HD3	1.77	0.44
44:3c:792:LEU:HD23	44:3c:792:LEU:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:3l:130:ILE:HG21	48:3l:163:LEU:HB2	1.98	0.44
48:3l:382:ILE:HG13	48:3l:383:ASP:H	1.82	0.44
15:Sf:65:VAL:HG12	15:Sf:76:LEU:HD21	1.99	0.44
38:zz:44:C:H2'	38:zz:45:C:C6	2.51	0.44
38:zz:224:G:H2'	38:zz:225:A:C8	2.53	0.44
39:S2:388:U:H2'	39:S2:389:A:C8	2.52	0.44
39:S2:561:A:H2'	39:S2:562:U:C6	2.52	0.44
39:S2:634:A:H2'	39:S2:635:G:H8	1.82	0.44
39:S2:1217:A:H2'	39:S2:1218:C:C6	2.52	0.44
39:S2:1616:U:H2'	39:S2:1617:G:C8	2.52	0.44
2:5B:723:ALA:O	2:5B:751:PHE:HA	2.17	0.44
12:SJ:28:GLU:HG2	12:SJ:43:VAL:HG11	1.99	0.44
39:S2:756:C:H2'	39:S2:757:C:C6	2.52	0.44
48:3l:135:LEU:HA	48:3l:138:ARG:HD3	1.99	0.44
1:1A:62:ARG:HB2	1:1A:91:VAL:O	2.17	0.44
15:Sf:78:LYS:HD2	15:Sf:78:LYS:HA	1.83	0.44
23:SU:58:THR:HG23	39:S2:1446:A:H5''	2.00	0.44
39:S2:186:C:H2'	39:S2:187:G:H8	1.82	0.44
39:S2:656:G:N2	39:S2:663:C:H5''	2.32	0.44
39:S2:941:C:H2'	39:S2:942:G:C8	2.53	0.44
40:3m:241:LEU:O	40:3m:245:VAL:HG12	2.16	0.44
41:3f:201:THR:O	41:3f:213:ILE:HA	2.18	0.44
43:3e:166:LEU:HD21	43:3e:195:THR:HG21	2.00	0.44
48:3l:457:LEU:O	48:3l:461:ARG:HG2	2.18	0.44
2:5B:933:ILE:HD13	2:5B:933:ILE:HA	1.85	0.44
2:5B:1100:TYR:HD2	2:5B:1101:ILE:HG22	1.82	0.44
2:5B:1103:ASN:CG	2:5B:1109:VAL:HG13	2.42	0.44
2:5B:1119:VAL:H	2:5B:1151:ALA:HB3	1.81	0.44
13:SK:11:ILE:HD13	13:SK:35:LEU:HD12	1.99	0.44
35:Sg:5:MET:HB2	35:Sg:270:LEU:HD21	2.00	0.44
39:S2:696:G:H5''	39:S2:735:C:H41	1.83	0.44
39:S2:982:G:H2'	39:S2:983:A:H8	1.81	0.44
44:3c:687:LEU:HD22	44:3c:737:VAL:HG21	1.99	0.44
45:3h:144:ILE:HG22	45:3h:146:GLU:H	1.83	0.44
2:5B:950:ALA:HB2	2:5B:959:LEU:HD22	1.99	0.44
23:SU:87:ARG:HA	23:SU:87:ARG:HD3	1.73	0.44
24:SV:55:ILE:HG21	24:SV:65:SER:HB2	1.99	0.44
35:Sg:121:VAL:HG11	35:Sg:165:ILE:HD11	1.99	0.44
35:Sg:246:TYR:HE2	35:Sg:262:GLU:HB3	1.82	0.44
41:3f:345:GLN:O	41:3f:348:ILE:HG13	2.16	0.44
42:3a:491:LEU:HD12	42:3a:491:LEU:HA	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:3e:400:PRO:HB3	44:3c:849:PRO:HB3	1.98	0.44
5:SC:63:VAL:HG23	5:SC:64:THR:HG23	1.98	0.44
15:Sf:93:LYS:HZ3	15:Sf:101:ARG:HE	1.65	0.44
15:Sf:93:LYS:NZ	15:Sf:101:ARG:HE	2.16	0.44
23:SU:63:ILE:HG22	23:SU:65:THR:HG22	2.00	0.44
25:SW:5:ASN:HB3	25:SW:8:ALA:HB3	1.99	0.44
36:zy:68:U:H2'	36:zy:69:G:C8	2.53	0.44
38:zz:200:G:H2'	38:zz:201:G:C8	2.53	0.44
39:S2:538:U:H3	39:S2:545:A:H2	1.65	0.44
39:S2:753:C:N4	39:S2:790:C:H42	2.16	0.44
39:S2:804:U:H2'	39:S2:805:U:H6	1.83	0.44
39:S2:1438:A:H2'	39:S2:1439:A:C8	2.52	0.44
39:S2:1798:C:H2'	39:S2:1799:G:O4'	2.17	0.44
42:3a:352:GLN:HA	42:3a:355:LEU:HG	2.00	0.44
2:5B:631:ALA:HB3	2:5B:928:ALA:HB1	1.99	0.44
4:SB:97:LEU:HD12	4:SB:232:HIS:CD2	2.53	0.44
6:SD:172:VAL:HG22	6:SD:185:LYS:HG2	2.00	0.44
7:SE:240:ARG:HE	7:SE:240:ARG:HB3	1.57	0.44
13:SK:5:LYS:HE3	13:SK:5:LYS:HB2	1.69	0.44
13:SK:7:ASN:O	13:SK:11:ILE:HG12	2.18	0.44
15:Sf:42:LEU:HD12	15:Sf:72:HIS:CD2	2.53	0.44
39:S2:1410:C:H2'	39:S2:1411:G:H8	1.83	0.44
42:3a:63:LYS:HD3	42:3a:63:LYS:HA	1.77	0.44
42:3a:455:LEU:HD23	42:3a:458:LEU:HD23	1.99	0.44
10:SH:43:LEU:HB3	10:SH:72:PHE:HE2	1.82	0.44
10:SH:46:THR:HG23	10:SH:65:PRO:HD3	2.00	0.44
34:sh:89:LYS:HD3	39:S2:1507:G:C2	2.53	0.44
35:Sg:17:TRP:CE2	35:Sg:303:THR:HB	2.53	0.44
42:3a:55:LEU:HD22	42:3a:93:TYR:CZ	2.53	0.44
42:3a:194:PHE:CE2	42:3a:243:MET:HG3	2.53	0.44
44:3c:589:MET:HE1	44:3c:612:THR:HG23	1.99	0.44
9:SG:32:MET:HE3	9:SG:65:GLN:HA	2.00	0.43
20:SR:17:ILE:HD13	20:SR:57:LEU:HB3	2.00	0.43
26:SX:29:LYS:HB2	26:SX:29:LYS:HE2	1.72	0.43
36:zy:5:G:H2'	36:zy:6:A:C8	2.53	0.43
38:zz:79:C:H2'	38:zz:80:U:C6	2.53	0.43
39:S2:441:C:H2'	39:S2:442:C:H6	1.83	0.43
39:S2:1531:A:H4'	39:S2:1605:G:H4'	2.00	0.43
41:3f:109:ARG:HH11	41:3f:114:ALA:HA	1.83	0.43
41:3f:115:ARG:HE	41:3f:117:ILE:HD11	1.82	0.43
45:3h:173:LEU:HD11	45:3h:197:MET:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SB:67:PHE:HD2	17:SO:47:LEU:HB3	1.84	0.43
11:SI:25:ARG:HD3	11:SI:25:ARG:HA	1.83	0.43
27:SY:110:ARG:O	27:SY:114:MET:HG3	2.17	0.43
28:SZ:52:LYS:HD2	28:SZ:52:LYS:HA	1.78	0.43
38:zz:66:A:H2'	38:zz:67:C:C6	2.53	0.43
38:zz:145:G:N2	38:zz:248:U:O2	2.43	0.43
39:S2:116:U:H3	39:S2:347:G:H1	1.66	0.43
40:3m:127:LEU:HD21	40:3m:140:ILE:HD12	1.99	0.43
42:3a:407:VAL:HA	42:3a:410:VAL:HG22	2.00	0.43
42:3a:437:LEU:HD23	42:3a:474:ALA:HB2	2.00	0.43
2:5B:982:TYR:O	2:5B:1034:ILE:HA	2.18	0.43
2:5B:1209:LEU:O	2:5B:1213:LEU:HG	2.18	0.43
3:SA:183:LEU:HD23	3:SA:183:LEU:HA	1.83	0.43
10:SH:130:LEU:HD21	10:SH:156:VAL:HG21	1.99	0.43
14:SL:127:THR:HB	14:SL:144:LYS:HG2	2.00	0.43
15:Sf:59:PRO:HA	15:Sf:62:VAL:HG22	2.00	0.43
16:SN:88:LEU:HD12	16:SN:88:LEU:HA	1.79	0.43
20:SR:109:LEU:HG	20:SR:111:PHE:CD2	2.54	0.43
36:zy:66:U:H2'	36:zy:67:C:C6	2.54	0.43
38:zz:156:C:HO2'	38:zz:157:C:H6	1.62	0.43
38:zz:193:C:H42	38:zz:202:A:H61	1.65	0.43
39:S2:674:C:H2'	39:S2:675:U:C6	2.53	0.43
39:S2:1756:C:H2'	39:S2:1757:G:H8	1.81	0.43
42:3a:532:LYS:HA	42:3a:532:LYS:HD2	1.91	0.43
44:3c:582:TRP:HB3	44:3c:619:CYS:SG	2.58	0.43
2:5B:1085:LYS:HE3	2:5B:1085:LYS:HB3	1.91	0.43
16:SN:55:ARG:HD3	30:Sb:47:PHE:CD2	2.53	0.43
31:Sc:59:LEU:HD23	31:Sc:59:LEU:HA	1.92	0.43
39:S2:15:U:H2'	39:S2:16:G:O4'	2.18	0.43
39:S2:1568:C:H2'	39:S2:1569:A:C8	2.54	0.43
44:3c:756:ILE:HG21	44:3c:783:ILE:HD13	2.00	0.43
47:3k:72:LYS:HD3	47:3k:72:LYS:HA	1.68	0.43
48:3l:148:PRO:HG2	48:3l:153:ARG:NH2	2.33	0.43
2:5B:1023:VAL:HG21	26:SX:50:ILE:HG21	1.99	0.43
3:SA:26:GLY:HA3	3:SA:150:THR:HG23	2.00	0.43
6:SD:227:LYS:HB3	6:SD:227:LYS:HE3	1.85	0.43
8:SF:204:ARG:NH1	31:Sc:60:GLU:HB2	2.33	0.43
10:SH:19:PHE:CE1	10:SH:50:GLU:HB2	2.54	0.43
11:SI:26:LYS:HD2	11:SI:29:LEU:HD23	2.00	0.43
16:SN:136:PRO:HG2	16:SN:139:TRP:HB2	2.00	0.43
20:SR:69:ILE:HD12	20:SR:69:ILE:HA	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26: SX:129: SER: HB3	39: S2:29: G: H4'	2.01	0.43
27: SY:100: LYS: HD2	27: SY:100: LYS: HA	1.70	0.43
35: Sg:256: ILE: HG23	35: Sg:289: LEU: HD11	1.99	0.43
39: S2:1844: U: H2'	39: S2:1845: A: C8	2.54	0.43
44: 3c:580: SER: HA	44: 3c:619: CYS: SG	2.58	0.43
45: 3h:321: GLY: HA2	45: 3h:324: ASN: ND2	2.33	0.43
14: SL:32: LYS: HD2	14: SL:32: LYS: HA	1.87	0.43
20: SR:16: ILE: HG23	20: SR:38: ILE: HD11	1.99	0.43
20: SR:18: GLU: HA	20: SR:71: ILE: HG22	2.00	0.43
38: zz:219: C: H2'	38: zz:220: U: C6	2.53	0.43
39: S2:656: G: H21	39: S2:663: C: H5''	1.83	0.43
41: 3f:98: ILE: HD13	41: 3f:131: VAL: HG11	2.01	0.43
41: 3f:183: SER: HA	41: 3f:186: ILE: HG12	2.01	0.43
2: 5B:1109: VAL: HA	2: 5B:1159: VAL: O	2.19	0.43
9: SG:20: ASP: OD2	9: SG:23: LYS: HG3	2.19	0.43
14: SL:24: LEU: HA	14: SL:27: GLU: HB3	1.99	0.43
39: S2:841: G: H2'	39: S2:842: C: C6	2.54	0.43
42: 3a:198: CYS: HB3	42: 3a:202: ARG: NH1	2.34	0.43
48: 3l:372: ALA: HA	48: 3l:398: MET: HE1	2.00	0.43
12: SJ:127: ARG: HD3	33: Se:31: ARG: HD3	2.01	0.43
22: ST:134: ILE: HD12	22: ST:134: ILE: H	1.82	0.43
23: SU:95: SER: O	23: SU:99: LYS: HG2	2.19	0.43
25: SW:28: ARG: HE	25: SW:28: ARG: HB3	1.69	0.43
35: Sg:289: LEU: HD23	35: Sg:289: LEU: HA	1.88	0.43
36: zy:24: U: H2'	36: zy:25: G: H8	1.83	0.43
39: S2:5: U: H2'	39: S2:6: G: C8	2.53	0.43
40: 3m:240: LEU: HD13	40: 3m:255: PHE: CE2	2.54	0.43
41: 3f:186: ILE: HA	41: 3f:189: TYR: HB2	2.00	0.43
48: 3l:112: TRP: HE1	48: 3l:132: TYR: HE1	1.65	0.43
48: 3l:278: LEU: HD12	48: 3l:279: ARG: N	2.34	0.43
2: 5B:648: LEU: HB3	2: 5B:652: ARG: NH1	2.33	0.43
7: SE:107: GLY: HA2	7: SE:189: LEU: HG	2.00	0.43
9: SG:58: LYS: HE2	9: SG:58: LYS: HB2	1.91	0.43
32: Sd:48: LYS: HE2	32: Sd:53: ILE: HG22	2.00	0.43
39: S2:441: C: H2'	39: S2:442: C: C6	2.54	0.43
39: S2:906: U: H2'	39: S2:907: G: C8	2.54	0.43
39: S2:964: A: H2'	39: S2:965: U: C6	2.54	0.43
39: S2:1593: C: H2'	39: S2:1594: A: H8	1.84	0.43
42: 3a:227: SER: HB3	42: 3a:268: LYS: HE2	2.00	0.43
2: 5B:940: LYS: HA	2: 5B:940: LYS: HD3	1.83	0.43
8: SF:171: GLU: CD	28: SZ:106: GLN: HE22	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:SU:22:ILE:HD13	23:SU:114:VAL:HG23	2.01	0.43
26:SX:58:GLU:H	26:SX:58:GLU:HG2	1.57	0.43
35:Sg:89:LEU:HD23	35:Sg:99:ARG:HG3	2.00	0.43
36:zy:17:G:H21	36:zy:55:C:H2'	1.83	0.43
36:zy:34:A:H2'	36:zy:35:U:H6	1.83	0.43
38:zz:217:G:H3'	38:zz:218:C:C5	2.54	0.43
38:zz:255:C:H2'	38:zz:256:G:C8	2.53	0.43
39:S2:388:U:H2'	39:S2:389:A:H8	1.84	0.43
39:S2:1413:G:H2'	39:S2:1414:A:H8	1.84	0.43
40:3m:70:LEU:HA	40:3m:73:ILE:HG22	2.00	0.43
41:3f:254:LYS:NZ	41:3f:271:GLN:HG2	2.34	0.43
42:3a:198:CYS:HB3	42:3a:202:ARG:HH12	1.84	0.43
42:3a:269:PRO:HA	42:3a:272:MET:SD	2.59	0.43
43:3e:233:ILE:O	43:3e:237:LEU:HB2	2.19	0.43
44:3c:752:CYS:O	44:3c:756:ILE:HG22	2.19	0.43
48:3l:179:PRO:HG2	48:3l:182:TRP:HB2	2.00	0.43
48:3l:454:GLN:HB3	48:3l:496:LYS:HE2	2.00	0.43
1:1A:110:PRO:HB2	1:1A:112:HIS:CE1	2.54	0.42
2:5B:648:LEU:HD21	2:5B:700:ILE:HG21	2.01	0.42
7:SE:33:THR:O	39:S2:120:U:H1'	2.19	0.42
14:SL:99:TYR:CE1	26:SX:13:LEU:HB3	2.54	0.42
17:SO:98:ARG:HG2	17:SO:99:ALA:O	2.19	0.42
18:SP:93:MET:HE3	18:SP:93:MET:HA	2.01	0.42
22:ST:129:ARG:HG3	39:S2:1416:C:OP1	2.19	0.42
38:zz:58:C:H2'	38:zz:59:U:C6	2.54	0.42
39:S2:518:G:H2'	39:S2:519:A:H8	1.84	0.42
39:S2:1128:C:H2'	39:S2:1129:G:C8	2.53	0.42
39:S2:1588:A:H2'	39:S2:1589:A:H8	1.84	0.42
41:3f:137:VAL:HG13	41:3f:152:PHE:HB3	2.00	0.42
42:3a:473:ASP:O	42:3a:477:HIS:HB2	2.19	0.42
45:3h:284:GLU:HG3	45:3h:288:ARG:HG2	2.00	0.42
10:SH:36:LEU:HD11	10:SH:78:ARG:HG2	2.01	0.42
11:SI:13:LYS:HB2	14:SL:137:THR:HG21	2.01	0.42
20:SR:24:LEU:HD23	20:SR:58:MET:SD	2.58	0.42
25:SW:115:GLU:HB2	25:SW:118:ARG:NH2	2.34	0.42
33:Se:40:ARG:HG2	33:Se:41:ARG:HG3	2.02	0.42
38:zz:163:G:O2'	38:zz:164:U:H5''	2.19	0.42
39:S2:201:C:H5''	39:S2:202:G:N7	2.34	0.42
39:S2:546:G:N2	39:S2:548:C:C2	2.87	0.42
39:S2:841:G:H2'	39:S2:842:C:H6	1.83	0.42
39:S2:1692:U:H2'	39:S2:1693:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:3c:598:ILE:HG13	44:3c:609:TYR:CD2	2.54	0.42
4:SB:97:LEU:HD13	4:SB:97:LEU:HA	1.93	0.42
24:SV:34:MET:HB2	24:SV:34:MET:HE3	1.77	0.42
38:zz:141:U:N3	38:zz:142:A:H1'	2.34	0.42
39:S2:1562:C:H2'	39:S2:1563:G:C8	2.51	0.42
42:3a:355:LEU:HA	42:3a:358:LEU:HG	2.01	0.42
43:3e:411:LEU:HG	44:3c:867:VAL:HG21	2.01	0.42
45:3h:39:VAL:HG12	45:3h:76:LEU:HB3	2.00	0.42
45:3h:260:TYR:OH	45:3h:316:SER:HB3	2.19	0.42
48:3l:157:TYR:HB2	48:3l:222:TRP:NE1	2.35	0.42
2:5B:1089:VAL:HG23	2:5B:1186:ILE:HG22	2.01	0.42
6:SD:109:LEU:HD21	6:SD:115:VAL:HG12	2.00	0.42
21:SS:27:ALA:HB2	21:SS:52:LEU:HD22	2.02	0.42
32:Sd:19:ARG:HD2	32:Sd:32:ARG:HD3	2.01	0.42
39:S2:693:A:C2	39:S2:737:G:H2'	2.54	0.42
6:SD:117:ARG:HA	6:SD:117:ARG:HD3	1.73	0.42
16:SN:135:LEU:HD23	16:SN:136:PRO:HD2	2.02	0.42
28:SZ:39:LYS:HD3	38:zz:94:G:H5'	2.01	0.42
39:S2:1310:U:H2'	39:S2:1311:C:C6	2.54	0.42
42:3a:183:LYS:HA	42:3a:183:LYS:HD3	1.86	0.42
42:3a:450:ILE:HD12	42:3a:450:ILE:HA	1.93	0.42
44:3c:692:LEU:HD22	44:3c:782:LYS:HG2	2.01	0.42
48:3l:367:MET:HA	48:3l:370:LEU:HG	2.01	0.42
48:3l:484:GLN:O	48:3l:488:ILE:HG12	2.19	0.42
3:SA:90:PHE:HD1	3:SA:179:ALA:HB2	1.84	0.42
3:SA:213:GLU:HG3	20:SR:84:TYR:CZ	2.54	0.42
5:SC:183:LYS:HD2	25:SW:95:PRO:HA	2.00	0.42
5:SC:196:ILE:HB	5:SC:223:TYR:HB2	2.00	0.42
9:SG:194:LEU:O	9:SG:198:ARG:HG3	2.20	0.42
19:SQ:14:GLY:HA3	19:SQ:86:GLN:HG2	2.01	0.42
24:SV:17:CYS:HB2	24:SV:56:CYS:HB3	2.01	0.42
25:SW:115:GLU:HA	25:SW:118:ARG:HB3	2.02	0.42
35:Sg:156:PHE:HA	35:Sg:165:ILE:HD12	2.02	0.42
39:S2:160:U:O2'	39:S2:161:U:H3'	2.20	0.42
39:S2:1073:U:H2'	39:S2:1074:C:H6	1.85	0.42
40:3m:240:LEU:HD13	40:3m:255:PHE:HE2	1.85	0.42
38:zz:154:A:C8	38:zz:228:U:H1'	2.54	0.42
39:S2:1407:U:H2'	39:S2:1408:U:C6	2.55	0.42
39:S2:1740:C:H2'	39:S2:1741:U:C6	2.55	0.42
42:3a:489:ARG:HE	42:3a:489:ARG:HB3	1.69	0.42
44:3c:815:LEU:HD11	44:3c:840:GLN:HE22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3h:154:PRO:HA	45:3h:157:THR:HG22	2.01	0.42
46:3d:38:ARG:HH21	46:3d:40:GLY:HA3	1.85	0.42
48:3l:135:LEU:O	48:3l:138:ARG:HG2	2.20	0.42
48:3l:328:ARG:HH12	48:3l:509:LEU:HA	1.85	0.42
48:3l:494:LYS:HD3	48:3l:498:LYS:HG2	2.01	0.42
2:5B:616:ARG:HA	2:5B:619:GLU:HG3	2.02	0.42
6:SD:18:LYS:NZ	6:SD:39:VAL:HB	2.34	0.42
14:SL:80:MET:HE1	14:SL:120:VAL:O	2.20	0.42
16:SN:112:LYS:HE2	16:SN:112:LYS:HB3	1.85	0.42
22:ST:29:LYS:HE3	22:ST:29:LYS:HB3	1.81	0.42
23:SU:39:LEU:HD22	23:SU:101:ILE:HG13	2.02	0.42
30:Sb:36:LYS:HZ3	30:Sb:80:ARG:HH12	1.67	0.42
35:Sg:17:TRP:HB2	35:Sg:36:ARG:HG3	2.02	0.42
38:zz:58:C:H2'	38:zz:59:U:H6	1.85	0.42
39:S2:171:A:H3'	39:S2:172:U:C6	2.54	0.42
39:S2:639:C:H2'	39:S2:640:A:C8	2.55	0.42
39:S2:1221:G:H2'	39:S2:1222:G:H8	1.83	0.42
39:S2:1390:U:H2'	39:S2:1391:C:H6	1.85	0.42
39:S2:1844:U:H2'	39:S2:1845:A:H8	1.85	0.42
40:3m:277:MET:O	40:3m:281:THR:HG23	2.19	0.42
43:3e:18:LEU:HA	43:3e:178:LEU:HD21	2.01	0.42
43:3e:319:LEU:HD13	43:3e:329:LEU:HA	2.02	0.42
6:SD:204:LEU:HD12	6:SD:204:LEU:HA	1.84	0.42
20:SR:34:VAL:O	20:SR:38:ILE:HG23	2.19	0.42
35:Sg:87:LEU:HB2	35:Sg:101:PHE:HB2	2.00	0.42
35:Sg:157:SER:HB3	35:Sg:164:ILE:HB	2.00	0.42
39:S2:804:U:H2'	39:S2:805:U:C6	2.55	0.42
39:S2:909:G:H2'	39:S2:910:G:C8	2.55	0.42
39:S2:1425:G:H2'	39:S2:1426:U:C6	2.55	0.42
41:3f:163:VAL:HA	45:3h:85:PRO:HG3	2.01	0.42
42:3a:439:LEU:HD11	42:3a:458:LEU:HD21	2.00	0.42
44:3c:757:ILE:HG21	44:3c:776:ARG:HD2	2.02	0.42
44:3c:769:PHE:HD1	44:3c:769:PHE:HA	1.73	0.42
48:3l:388:LEU:HD13	48:3l:388:LEU:HA	1.94	0.42
48:3l:498:LYS:HD2	48:3l:498:LYS:HA	1.77	0.42
2:5B:639:HIS:CG	2:5B:640:VAL:H	2.37	0.42
2:5B:729:ILE:HD13	2:5B:761:LEU:HD21	2.01	0.42
3:SA:49:ILE:HG21	3:SA:162:PRO:O	2.20	0.42
4:SB:153:THR:HB	4:SB:155:TYR:CE1	2.54	0.42
6:SD:27:ARG:HB3	13:SK:61:GLN:NE2	2.35	0.42
8:SF:178:ILE:HD13	8:SF:178:ILE:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:SZ:100:VAL:HB	28:SZ:108:ILE:HB	2.02	0.42
35:Sg:297:THR:HA	35:Sg:310:TRP:O	2.20	0.42
39:S2:1809:A:H2'	39:S2:1810:U:C6	2.55	0.42
41:3f:253:MET:HA	41:3f:256:CYS:SG	2.60	0.42
42:3a:23:LYS:HE3	42:3a:23:LYS:HB2	1.90	0.42
44:3c:759:GLU:H	44:3c:759:GLU:HG2	1.62	0.42
10:SH:65:PRO:HG2	10:SH:68:GLN:HB2	2.02	0.41
35:Sg:30:MET:HE3	35:Sg:30:MET:HB3	1.93	0.41
38:zz:215:A:H4'	42:3a:76:ASN:HD21	1.85	0.41
38:zz:216:U:H3	42:3a:69:GLU:HG2	1.84	0.41
38:zz:256:G:H1	38:zz:276:A:N6	2.09	0.41
41:3f:90:ARG:NH1	41:3f:196:ASN:HD21	2.18	0.41
48:3l:136:TYR:O	48:3l:139:HIS:HB2	2.20	0.41
2:5B:780:LYS:O	2:5B:784:LYS:HG2	2.20	0.41
9:SG:174:PRO:HB3	39:S2:65:C:C5	2.55	0.41
16:SN:46:THR:O	16:SN:50:ILE:HG12	2.20	0.41
17:SO:72:TYR:CZ	17:SO:76:LEU:HD21	2.55	0.41
21:SS:106:LYS:HD3	21:SS:106:LYS:HA	1.78	0.41
27:SY:61:ARG:HA	27:SY:61:ARG:HD2	1.82	0.41
39:S2:345:U:H2'	39:S2:346:C:C6	2.55	0.41
39:S2:495:U:H2'	39:S2:496:C:O4'	2.20	0.41
39:S2:931:C:H2'	39:S2:932:G:C8	2.55	0.41
41:3f:172:TRP:HE1	41:3f:187:HIS:HA	1.84	0.41
41:3f:202:VAL:HG22	41:3f:213:ILE:HD12	2.01	0.41
44:3c:608:LEU:HD12	44:3c:608:LEU:HA	1.90	0.41
44:3c:760:LYS:O	44:3c:764:LYS:HG3	2.19	0.41
48:3l:525:LYS:HB2	48:3l:525:LYS:HE2	1.80	0.41
1:1A:26:LEU:HD13	1:1A:99:GLU:HG2	2.02	0.41
2:5B:814:PRO:HD2	2:5B:815:ARG:NH1	2.36	0.41
2:5B:1062:ILE:HD12	2:5B:1062:ILE:HA	1.85	0.41
10:SH:157:HIS:HB3	10:SH:190:PRO:HG3	2.03	0.41
35:Sg:173:LEU:HD22	35:Sg:189:ILE:HG12	2.02	0.41
38:zz:44:C:H2'	38:zz:45:C:H6	1.85	0.41
38:zz:193:C:H42	38:zz:202:A:N6	2.19	0.41
39:S2:906:U:H2'	39:S2:907:G:H8	1.85	0.41
42:3a:18:PHE:HB3	42:3a:23:LYS:HG3	2.02	0.41
44:3c:788:LEU:HD11	44:3c:807:LEU:HD11	2.02	0.41
48:3l:157:TYR:HE2	48:3l:220:LYS:HZ1	1.69	0.41
2:5B:712:LEU:HA	2:5B:715:ARG:HG2	2.01	0.41
20:SR:33:ARG:HA	20:SR:33:ARG:HD3	1.88	0.41
27:SY:46:LYS:HE3	27:SY:46:LYS:HB3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:S2:996:A:H2'	39:S2:997:A:C8	2.55	0.41
40:3m:109:LEU:O	40:3m:113:MET:HG2	2.21	0.41
41:3f:159:LEU:HD11	45:3h:99:TYR:HD1	1.86	0.41
43:3e:417:MET:O	43:3e:421:ASN:HB2	2.21	0.41
44:3c:573:ILE:HD11	44:3c:588:LEU:HD23	2.01	0.41
48:3l:237:LYS:HG2	48:3l:266:TYR:HE1	1.84	0.41
20:SR:59:LYS:HE3	20:SR:59:LYS:HB3	1.72	0.41
20:SR:78:ARG:HA	20:SR:81:ARG:HG2	2.02	0.41
27:SY:37:LYS:HG2	27:SY:57:VAL:HG23	2.03	0.41
35:Sg:125:ARG:HA	35:Sg:150:TRP:HB3	2.01	0.41
39:S2:12:U:H2'	39:S2:13:C:C6	2.56	0.41
39:S2:551:U:H2'	39:S2:552:G:H8	1.86	0.41
39:S2:1221:G:H2'	39:S2:1222:G:C8	2.55	0.41
40:3m:233:GLU:HG2	40:3m:238:HIS:CG	2.56	0.41
42:3a:186:LEU:HD12	42:3a:186:LEU:HA	1.82	0.41
44:3c:745:LYS:HD3	44:3c:745:LYS:HA	1.73	0.41
8:SF:61:PHE:CE2	31:Sc:51:ARG:HB3	2.55	0.41
28:SZ:50:PHE:CD2	28:SZ:83:LEU:HD21	2.56	0.41
34:sh:99:LYS:HG3	34:sh:100:LEU:HD23	2.02	0.41
34:sh:107:LYS:NZ	34:sh:115:SER:HB2	2.36	0.41
35:Sg:217:MET:HA	35:Sg:229:THR:HA	2.01	0.41
35:Sg:230:LEU:HD13	35:Sg:230:LEU:HA	1.87	0.41
35:Sg:271:LYS:HE3	35:Sg:271:LYS:HB3	1.91	0.41
36:zy:18:G:H1'	36:zy:55:C:H1'	2.01	0.41
39:S2:924:G:H2'	39:S2:925:G:H8	1.85	0.41
39:S2:1203:G:H2'	39:S2:1204:A:C8	2.56	0.41
39:S2:1710:C:H42	39:S2:1823:A:N6	2.07	0.41
44:3c:548:MET:HE1	44:3c:551:LEU:HD13	2.02	0.41
45:3h:129:VAL:HG12	45:3h:318:LEU:HD12	2.01	0.41
47:3k:210:VAL:HG12	48:3l:548:HIS:CE1	2.55	0.41
2:5B:891:PRO:HG3	2:5B:945:LEU:HB2	2.03	0.41
3:SA:51:LEU:HD23	3:SA:51:LEU:HA	1.84	0.41
9:SG:52:ILE:HA	9:SG:111:LEU:HD23	2.03	0.41
10:SH:69:LEU:HD22	10:SH:96:ALA:HB2	2.02	0.41
14:SL:7:GLU:HG2	39:S2:375:U:H1'	2.02	0.41
15:Sf:19:GLN:HB3	15:Sf:88:TRP:HE3	1.85	0.41
15:Sf:26:LEU:HD13	15:Sf:31:LEU:HD21	2.01	0.41
23:SU:51:LYS:HB2	23:SU:90:ASP:HB2	2.01	0.41
23:SU:56:MET:HB2	23:SU:86:LYS:HB3	2.02	0.41
25:SW:88:LYS:H	25:SW:88:LYS:HG2	1.72	0.41
36:zy:12:G:H22	36:zy:21:G:H22	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:S2:374:G:H2'	39:S2:375:U:C6	2.56	0.41
39:S2:736:C:H2'	39:S2:737:G:C8	2.56	0.41
40:3m:62:SER:HB2	41:3f:222:GLY:N	2.34	0.41
41:3f:330:ASN:HD22	45:3h:341:LEU:HD21	1.86	0.41
42:3a:87:GLU:HG3	42:3a:173:LEU:HD22	2.02	0.41
42:3a:276:TYR:HB3	42:3a:299:LEU:HD12	2.03	0.41
42:3a:420:LYS:H	42:3a:420:LYS:HG2	1.71	0.41
43:3e:160:ALA:HB2	43:3e:191:ARG:HH12	1.85	0.41
43:3e:295:PHE:HB2	43:3e:311:LYS:HG2	2.03	0.41
44:3c:698:MET:HE2	44:3c:745:LYS:HE3	2.02	0.41
48:3l:201:ARG:HG2	48:3l:215:LEU:HD23	2.03	0.41
2:5B:913:LEU:HD23	2:5B:913:LEU:HA	1.90	0.41
3:SA:180:ARG:O	3:SA:184:ARG:HG3	2.21	0.41
4:SB:187:LYS:HB2	4:SB:187:LYS:HE3	1.86	0.41
11:SI:172:LEU:HD23	11:SI:172:LEU:HA	1.88	0.41
13:SK:47:LYS:HA	13:SK:47:LYS:HD2	1.89	0.41
15:Sf:35:ILE:HD13	15:Sf:61:TYR:CE1	2.56	0.41
16:SN:71:ILE:HG13	39:S2:1018:U:H5''	2.03	0.41
25:SW:115:GLU:HB2	25:SW:118:ARG:HH21	1.85	0.41
27:SY:38:THR:O	27:SY:42:GLU:HG3	2.20	0.41
27:SY:49:LYS:HE2	27:SY:49:LYS:HB2	1.88	0.41
31:Sc:40:ARG:HA	31:Sc:40:ARG:HD2	1.87	0.41
38:zz:64:U:H2'	38:zz:65:C:C6	2.56	0.41
42:3a:295:THR:HG22	42:3a:359:LEU:HD11	2.03	0.41
48:3l:55:PHE:HE1	48:3l:94:ILE:HG23	1.85	0.41
1:1A:109:LEU:HD12	1:1A:110:PRO:HD2	2.03	0.41
2:5B:1202:MET:HE3	2:5B:1202:MET:HB3	1.72	0.41
2:5B:1213:LEU:HA	2:5B:1216:VAL:HG12	2.03	0.41
16:SN:112:LYS:O	16:SN:116:ILE:HG12	2.21	0.41
29:Sa:5:ARG:HD3	39:S2:1865:C:O4'	2.21	0.41
30:Sb:41:TYR:CD1	38:zz:163:G:H2'	2.56	0.41
35:Sg:156:PHE:CE1	35:Sg:179:LEU:HD21	2.50	0.41
38:zz:78:U:H2'	38:zz:79:C:H6	1.86	0.41
39:S2:233:C:H2'	39:S2:234:C:C6	2.56	0.41
39:S2:367:U:H4'	39:S2:371:A:C8	2.56	0.41
39:S2:508:A:H3'	39:S2:509:G:H8	1.85	0.41
39:S2:521:A:H2'	39:S2:522:A:O4'	2.21	0.41
39:S2:980:A:H2'	39:S2:981:A:H8	1.85	0.41
39:S2:1323:U:H2'	39:S2:1324:G:C8	2.56	0.41
39:S2:1417:C:H2'	39:S2:1418:C:C4	2.56	0.41
41:3f:330:ASN:HD21	42:3a:520:ARG:HH21	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:3e:147:ALA:O	43:3e:151:LEU:HG	2.21	0.41
43:3e:274:LEU:O	43:3e:278:VAL:HG23	2.20	0.41
44:3c:815:LEU:HB3	44:3c:816:PRO:HD3	2.03	0.41
45:3h:123:THR:HG21	45:3h:128:PHE:HB3	2.02	0.41
48:3l:195:GLN:HA	48:3l:421:LEU:HD21	2.01	0.41
48:3l:207:LYS:HE2	48:3l:215:LEU:HD11	2.02	0.41
48:3l:340:LEU:O	48:3l:344:GLN:HG2	2.21	0.41
48:3l:391:ARG:HD3	48:3l:391:ARG:HA	1.88	0.41
2:5B:614:GLU:O	2:5B:618:LEU:HD13	2.21	0.41
2:5B:682:THR:HG23	2:5B:688:PHE:CE1	2.56	0.41
6:SD:31:GLU:HA	6:SD:107:TYR:CE2	2.56	0.41
22:ST:56:ARG:O	22:ST:60:THR:HG22	2.20	0.41
39:S2:241:G:H2'	39:S2:242:U:O4'	2.21	0.41
39:S2:753:C:H42	39:S2:790:C:H42	1.69	0.41
39:S2:1842:C:H2'	39:S2:1843:G:H8	1.86	0.41
40:3m:159:GLU:HA	40:3m:162:HIS:NE2	2.36	0.41
40:3m:354:LEU:HD13	40:3m:357:TRP:HE3	1.86	0.41
41:3f:118:GLY:HA3	41:3f:173:TYR:CZ	2.56	0.41
41:3f:248:GLY:HA2	45:3h:162:LEU:HD11	2.03	0.41
42:3a:486:HIS:ND1	44:3c:802:ILE:HA	2.36	0.41
2:5B:685:ILE:HG22	2:5B:687:ASN:H	1.85	0.40
2:5B:780:LYS:HB2	2:5B:783:THR:HG23	2.03	0.40
2:5B:1030:GLN:HB3	2:5B:1076:TYR:CE2	2.57	0.40
6:SD:209:SER:HB3	20:SR:40:ILE:HB	2.03	0.40
14:SL:111:VAL:HG11	14:SL:128:VAL:HG11	2.02	0.40
21:SS:98:VAL:HG23	21:SS:103:LEU:HG	2.02	0.40
29:Sa:10:ARG:HB2	29:Sa:33:ASP:OD2	2.21	0.40
35:Sg:165:ILE:HG22	35:Sg:177:TRP:HB2	2.02	0.40
39:S2:28:U:H2'	39:S2:29:G:H8	1.86	0.40
39:S2:223:C:H2'	39:S2:224:A:H8	1.85	0.40
39:S2:540:U:H2'	39:S2:541:U:H5	1.86	0.40
41:3f:163:VAL:HG22	45:3h:85:PRO:HG3	2.02	0.40
48:3l:518:GLU:HA	48:3l:533:THR:HB	2.02	0.40
2:5B:742:ASN:O	2:5B:745:LYS:HG3	2.21	0.40
2:5B:1096:ILE:HG13	2:5B:1176:PHE:CZ	2.56	0.40
4:SB:181:LEU:HA	4:SB:184:VAL:HG12	2.04	0.40
9:SG:121:ILE:HB	9:SG:124:LEU:HB3	2.04	0.40
35:Sg:146:SER:HA	35:Sg:177:TRP:HH2	1.86	0.40
38:zz:80:U:H2'	38:zz:81:A:H8	1.86	0.40
39:S2:416:U:H2'	39:S2:417:C:O4'	2.21	0.40
39:S2:1595:U:H2'	39:S2:1596:U:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:3l:57:GLN:HB3	48:3l:61:LYS:NZ	2.36	0.40
2:5B:766:LYS:HB2	2:5B:827:THR:HG23	2.03	0.40
2:5B:835:ILE:HA	2:5B:838:LEU:HD12	2.03	0.40
2:5B:890:VAL:HG12	2:5B:947:LEU:HD12	2.03	0.40
3:SA:170:SER:O	3:SA:174:MET:HG2	2.21	0.40
3:SA:207:PRO:HA	3:SA:210:ILE:HG22	2.03	0.40
9:SG:176:ILE:HD12	39:S2:77:A:H1'	2.02	0.40
21:SS:52:LEU:HD23	21:SS:52:LEU:HA	1.88	0.40
22:ST:27:LYS:HB2	22:ST:27:LYS:HE3	1.82	0.40
34:sh:126:CYS:HB3	34:sh:130:VAL:HG11	2.02	0.40
39:S2:241:G:O5'	39:S2:241:G:H8	2.05	0.40
39:S2:880:G:H2'	39:S2:881:G:H8	1.87	0.40
39:S2:1759:G:N2	39:S2:1774:C:H1'	2.36	0.40
40:3m:128:ILE:HG21	40:3m:167:LEU:HB3	2.03	0.40
40:3m:151:ILE:HA	40:3m:151:ILE:HD12	1.85	0.40
40:3m:160:LYS:HA	40:3m:160:LYS:HD2	1.86	0.40
41:3f:91:VAL:HG12	41:3f:236:THR:HB	2.02	0.40
41:3f:98:ILE:HG13	41:3f:99:LEU:N	2.35	0.40
47:3k:71:LEU:O	47:3k:75:THR:HG23	2.22	0.40
2:5B:864:LYS:HE2	2:5B:864:LYS:HB3	1.91	0.40
9:SG:147:LEU:H	9:SG:147:LEU:HD12	1.85	0.40
11:SI:45:THR:HG23	39:S2:307:G:O2'	2.22	0.40
17:SO:135:ILE:HD12	17:SO:135:ILE:HA	1.96	0.40
20:SR:58:MET:O	20:SR:62:GLN:HG2	2.21	0.40
23:SU:56:MET:HE3	23:SU:57:PRO:HD2	2.04	0.40
25:SW:19:LYS:HE2	25:SW:19:LYS:HB2	1.96	0.40
25:SW:111:MET:HE3	25:SW:116:ALA:HB2	2.04	0.40
34:sh:95:ARG:HH21	34:sh:97:LYS:HE3	1.87	0.40
39:S2:319:C:H2'	39:S2:320:G:O4'	2.21	0.40
39:S2:1593:C:H2'	39:S2:1594:A:C8	2.55	0.40
40:3m:65:ASN:HB3	41:3f:221:MET:SD	2.62	0.40
40:3m:212:LEU:HB2	40:3m:268:LEU:HD11	2.03	0.40
42:3a:25:GLN:HB2	42:3a:26:PRO:HD3	2.03	0.40
44:3c:573:ILE:HG23	44:3c:585:ALA:HB1	2.04	0.40
44:3c:859:LEU:HD21	45:3h:247:MET:HB2	2.04	0.40
45:3h:235:SER:HB2	45:3h:333:PHE:CE2	2.57	0.40
47:3k:139:ARG:HD3	47:3k:165:LEU:HD11	2.03	0.40
2:5B:609:ALA:HA	2:5B:612:ARG:HH21	1.85	0.40
2:5B:910:MET:O	2:5B:910:MET:HG3	2.22	0.40
11:SI:43:ILE:HG12	11:SI:57:ALA:HA	2.04	0.40
14:SL:20:LYS:HD2	14:SL:20:LYS:HA	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Sf:32:ALA:HB1	15:Sf:37:GLU:HB2	2.04	0.40
18:SP:30:TYR:O	18:SP:34:MET:HG2	2.22	0.40
35:Sg:101:PHE:CD1	35:Sg:136:GLY:HA2	2.56	0.40
38:zz:49:G:H2'	38:zz:50:A:C8	2.57	0.40
39:S2:375:U:H2'	39:S2:376:A:C8	2.57	0.40
39:S2:864:A:H2'	39:S2:865:A:C8	2.55	0.40
39:S2:1597:C:H4'	39:S2:1603:G:O6	2.21	0.40
39:S2:1641:A:H2'	39:S2:1642:U:O4'	2.21	0.40
42:3a:179:GLN:OE1	42:3a:231:GLU:HG3	2.22	0.40
42:3a:342:LEU:HD11	44:3c:718:LEU:HB3	2.03	0.40
43:3e:170:TRP:CH2	43:3e:214:LEU:HD22	2.56	0.40
44:3c:868:GLU:O	44:3c:872:ARG:HG3	2.21	0.40
45:3h:75:ARG:HG3	45:3h:77:GLU:HG3	2.03	0.40
45:3h:80:ASN:HD22	45:3h:112:ILE:HG21	1.87	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	1A	96/144 (67%)	88 (92%)	8 (8%)	0	100	100
2	5B	619/621 (100%)	580 (94%)	35 (6%)	4 (1%)	21	52
3	SA	214/295 (72%)	209 (98%)	5 (2%)	0	100	100
4	SB	210/264 (80%)	199 (95%)	11 (5%)	0	100	100
5	SC	217/293 (74%)	210 (97%)	7 (3%)	0	100	100
6	SD	224/243 (92%)	218 (97%)	6 (3%)	0	100	100
7	SE	258/263 (98%)	248 (96%)	10 (4%)	0	100	100
8	SF	190/204 (93%)	182 (96%)	8 (4%)	0	100	100
9	SG	235/249 (94%)	232 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	SH	185/194 (95%)	180 (97%)	5 (3%)	0	100	100
11	SI	203/208 (98%)	194 (96%)	9 (4%)	0	100	100
12	SJ	178/194 (92%)	175 (98%)	3 (2%)	0	100	100
13	SK	94/165 (57%)	86 (92%)	8 (8%)	0	100	100
14	SL	148/158 (94%)	144 (97%)	4 (3%)	0	100	100
15	Sf	119/132 (90%)	109 (92%)	10 (8%)	0	100	100
16	SN	147/151 (97%)	141 (96%)	6 (4%)	0	100	100
17	SO	133/151 (88%)	120 (90%)	13 (10%)	0	100	100
18	SP	117/145 (81%)	112 (96%)	5 (4%)	0	100	100
19	SQ	138/146 (94%)	133 (96%)	5 (4%)	0	100	100
20	SR	130/135 (96%)	123 (95%)	7 (5%)	0	100	100
21	SS	141/152 (93%)	134 (95%)	7 (5%)	0	100	100
22	ST	140/145 (97%)	139 (99%)	1 (1%)	0	100	100
23	SU	99/119 (83%)	94 (95%)	4 (4%)	1 (1%)	12	40
24	SV	81/83 (98%)	81 (100%)	0	0	100	100
25	SW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
26	SX	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
27	SY	122/133 (92%)	119 (98%)	3 (2%)	0	100	100
28	SZ	73/125 (58%)	69 (94%)	3 (4%)	1 (1%)	9	33
29	Sa	98/115 (85%)	95 (97%)	3 (3%)	0	100	100
30	Sb	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
31	Sc	60/69 (87%)	58 (97%)	2 (3%)	0	100	100
32	Sd	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
33	Se	50/59 (85%)	47 (94%)	3 (6%)	0	100	100
34	sh	62/156 (40%)	56 (90%)	6 (10%)	0	100	100
35	Sg	311/317 (98%)	292 (94%)	19 (6%)	0	100	100
37	Ln	22/25 (88%)	21 (96%)	1 (4%)	0	100	100
40	3m	361/374 (96%)	343 (95%)	18 (5%)	0	100	100
41	3f	267/357 (75%)	263 (98%)	4 (2%)	0	100	100
42	3a	590/1382 (43%)	563 (95%)	27 (5%)	0	100	100
43	3e	428/445 (96%)	413 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	3c	537/913 (59%)	517 (96%)	20 (4%)	0	100	100
45	3h	316/352 (90%)	304 (96%)	12 (4%)	0	100	100
46	3d	53/548 (10%)	49 (92%)	4 (8%)	0	100	100
47	3k	213/218 (98%)	206 (97%)	7 (3%)	0	100	100
48	3l	518/564 (92%)	503 (97%)	15 (3%)	0	100	100
All	All	8797/11419 (77%)	8431 (96%)	360 (4%)	6 (0%)	49	75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	5B	1099	GLN
2	5B	1108	ILE
2	5B	1098	PRO
23	SU	54	VAL
28	SZ	42	ASP
2	5B	1138	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	82/123 (67%)	80 (98%)	2 (2%)	43	65
2	5B	546/546 (100%)	523 (96%)	23 (4%)	26	55
3	SA	180/243 (74%)	173 (96%)	7 (4%)	28	56
4	SB	193/231 (84%)	189 (98%)	4 (2%)	47	67
5	SC	185/225 (82%)	180 (97%)	5 (3%)	39	63
6	SD	189/202 (94%)	180 (95%)	9 (5%)	23	52
7	SE	223/225 (99%)	215 (96%)	8 (4%)	31	58
8	SF	162/170 (95%)	154 (95%)	8 (5%)	22	51
9	SG	207/218 (95%)	199 (96%)	8 (4%)	28	56
10	SH	167/174 (96%)	160 (96%)	7 (4%)	26	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	SI	178/180 (99%)	173 (97%)	5 (3%)	38	62
12	SJ	160/168 (95%)	151 (94%)	9 (6%)	19	47
13	SK	87/136 (64%)	84 (97%)	3 (3%)	32	59
14	SL	134/142 (94%)	130 (97%)	4 (3%)	36	61
15	Sf	102/108 (94%)	100 (98%)	2 (2%)	48	68
16	SN	130/131 (99%)	129 (99%)	1 (1%)	73	79
17	SO	104/119 (87%)	100 (96%)	4 (4%)	29	57
18	SP	107/130 (82%)	104 (97%)	3 (3%)	38	62
19	SQ	116/121 (96%)	113 (97%)	3 (3%)	40	64
20	SR	119/122 (98%)	110 (92%)	9 (8%)	12	37
21	SS	124/132 (94%)	118 (95%)	6 (5%)	23	52
22	ST	112/115 (97%)	110 (98%)	2 (2%)	51	70
23	SU	93/107 (87%)	86 (92%)	7 (8%)	12	38
24	SV	67/67 (100%)	65 (97%)	2 (3%)	36	61
25	SW	112/113 (99%)	111 (99%)	1 (1%)	70	78
26	SX	113/115 (98%)	103 (91%)	10 (9%)	9	32
27	SY	108/115 (94%)	105 (97%)	3 (3%)	38	62
28	SZ	67/103 (65%)	62 (92%)	5 (8%)	12	38
29	Sa	87/98 (89%)	85 (98%)	2 (2%)	44	66
30	Sb	75/76 (99%)	69 (92%)	6 (8%)	11	36
31	Sc	55/62 (89%)	53 (96%)	2 (4%)	31	58
32	Sd	48/49 (98%)	48 (100%)	0	100	100
33	Se	42/48 (88%)	40 (95%)	2 (5%)	23	52
34	sh	57/140 (41%)	53 (93%)	4 (7%)	14	41
35	Sg	272/275 (99%)	257 (94%)	15 (6%)	19	48
37	Ln	23/24 (96%)	23 (100%)	0	100	100
40	3m	252/335 (75%)	246 (98%)	6 (2%)	43	65
41	3f	229/289 (79%)	221 (96%)	8 (4%)	32	58
42	3a	433/1259 (34%)	421 (97%)	12 (3%)	38	62
43	3e	302/406 (74%)	294 (97%)	8 (3%)	40	64
44	3c	343/811 (42%)	336 (98%)	7 (2%)	48	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	3h	272/310 (88%)	262 (96%)	10 (4%)	30	58
46	3d	19/494 (4%)	18 (95%)	1 (5%)	20	49
47	3k	121/193 (63%)	119 (98%)	2 (2%)	53	71
48	3l	475/515 (92%)	460 (97%)	15 (3%)	34	60
All	All	7272/9965 (73%)	7012 (96%)	260 (4%)	32	58

All (260) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	22	GLU
1	1A	39	ILE
2	5B	675	LEU
2	5B	763	ASP
2	5B	783	THR
2	5B	788	GLU
2	5B	812	LYS
2	5B	834	LEU
2	5B	846	LEU
2	5B	861	MET
2	5B	871	THR
2	5B	898	VAL
2	5B	934	LEU
2	5B	956	ILE
2	5B	963	LEU
2	5B	974	ILE
2	5B	994	LEU
2	5B	1028	ASP
2	5B	1047	GLU
2	5B	1063	TYR
2	5B	1096	ILE
2	5B	1100	TYR
2	5B	1109	VAL
2	5B	1123	THR
2	5B	1191	ILE
3	SA	23	THR
3	SA	38	ILE
3	SA	104	THR
3	SA	111	GLN
3	SA	197	VAL
3	SA	200	ASP
3	SA	211	GLU

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Mol	Chain	Res	Type
4	SB	140	VAL
4	SB	147	ASN
4	SB	186	ASN
4	SB	218	LEU
5	SC	121	ARG
5	SC	165	VAL
5	SC	188	CYS
5	SC	260	VAL
5	SC	263	LYS
6	SD	37	VAL
6	SD	42	THR
6	SD	54	ARG
6	SD	135	GLU
6	SD	153	VAL
6	SD	160	SER
6	SD	168	VAL
6	SD	208	VAL
6	SD	225	GLU
7	SE	12	VAL
7	SE	65	CYS
7	SE	115	THR
7	SE	131	VAL
7	SE	139	LEU
7	SE	177	THR
7	SE	208	VAL
7	SE	214	ASN
8	SF	14	THR
8	SF	69	VAL
8	SF	76	MET
8	SF	98	GLU
8	SF	134	VAL
8	SF	177	LEU
8	SF	182	LYS
8	SF	191	LYS
9	SG	67	VAL
9	SG	125	THR
9	SG	129	VAL
9	SG	147	LEU
9	SG	155	GLN
9	SG	158	VAL
9	SG	162	LEU
9	SG	179	LEU

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Mol	Chain	Res	Type
10	SH	15	LYS
10	SH	25	GLN
10	SH	27	LEU
10	SH	77	VAL
10	SH	131	GLU
10	SH	132	ASP
10	SH	180	LEU
11	SI	13	LYS
11	SI	82	VAL
11	SI	97	VAL
11	SI	100	CYS
11	SI	159	SER
12	SJ	8	VAL
12	SJ	12	THR
12	SJ	14	VAL
12	SJ	29	LEU
12	SJ	84	ILE
12	SJ	86	VAL
12	SJ	137	VAL
12	SJ	160	SER
12	SJ	172	ARG
13	SK	40	VAL
13	SK	62	PHE
13	SK	79	LEU
14	SL	40	ILE
14	SL	46	THR
14	SL	116	CYS
14	SL	126	VAL
15	Sf	76	LEU
15	Sf	94	ILE
16	SN	20	ARG
17	SO	47	LEU
17	SO	87	GLU
17	SO	103	ASN
17	SO	130	GLU
18	SP	38	SER
18	SP	50	ARG
18	SP	94	VAL
19	SQ	20	THR
19	SQ	48	GLN
19	SQ	66	VAL
20	SR	22	THR

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Mol	Chain	Res	Type
20	SR	23	ARG
20	SR	43	SER
20	SR	59	LYS
20	SR	61	ILE
20	SR	69	ILE
20	SR	82	ASP
20	SR	89	SER
20	SR	107	LYS
21	SS	64	VAL
21	SS	71	MET
21	SS	94	LYS
21	SS	103	LEU
21	SS	118	ARG
21	SS	136	THR
22	ST	9	VAL
22	ST	50	GLU
23	SU	18	HIS
23	SU	65	THR
23	SU	92	HIS
23	SU	105	SER
23	SU	110	VAL
23	SU	111	GLU
23	SU	115	THR
24	SV	34	MET
24	SV	69	ILE
25	SW	34	ILE
26	SX	25	LYS
26	SX	29	LYS
26	SX	32	LEU
26	SX	48	LYS
26	SX	58	GLU
26	SX	70	VAL
26	SX	72	VAL
26	SX	100	VAL
26	SX	102	VAL
26	SX	129	SER
27	SY	3	ASP
27	SY	99	LYS
27	SY	125	VAL
28	SZ	48	VAL
28	SZ	50	PHE
28	SZ	65	TYR

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Mol	Chain	Res	Type
28	SZ	100	VAL
28	SZ	108	ILE
29	Sa	29	CYS
29	Sa	79	ILE
30	Sb	3	LEU
30	Sb	53	VAL
30	Sb	56	CYS
30	Sb	57	VAL
30	Sb	62	VAL
30	Sb	64	CYS
31	Sc	43	ILE
31	Sc	61	SER
33	Se	22	GLN
33	Se	45	VAL
34	sh	93	HIS
34	sh	106	TYR
34	sh	130	VAL
34	sh	148	TYR
35	Sg	10	THR
35	Sg	18	VAL
35	Sg	40	ILE
35	Sg	64	HIS
35	Sg	70	VAL
35	Sg	132	TRP
35	Sg	141	THR
35	Sg	144	ASP
35	Sg	150	TRP
35	Sg	166	VAL
35	Sg	203	ASP
35	Sg	229	THR
35	Sg	230	LEU
35	Sg	234	ASP
35	Sg	287	THR
40	3m	32	GLU
40	3m	142	THR
40	3m	192	TYR
40	3m	205	HIS
40	3m	237	ILE
40	3m	274	MET
41	3f	97	VAL
41	3f	124	VAL
41	3f	155	ASN

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Mol	Chain	Res	Type
41	3f	168	LEU
41	3f	198	ILE
41	3f	255	THR
41	3f	262	VAL
41	3f	293	VAL
42	3a	52	LEU
42	3a	65	HIS
42	3a	155	GLU
42	3a	175	HIS
42	3a	176	ASP
42	3a	288	ASN
42	3a	332	THR
42	3a	370	LEU
42	3a	428	VAL
42	3a	452	PHE
42	3a	455	LEU
42	3a	554	VAL
43	3e	153	PHE
43	3e	223	PHE
43	3e	243	LEU
43	3e	253	ILE
43	3e	314	GLU
43	3e	324	PHE
43	3e	326	VAL
43	3e	414	ARG
44	3c	505	LEU
44	3c	713	GLN
44	3c	716	HIS
44	3c	736	HIS
44	3c	759	GLU
44	3c	769	PHE
44	3c	779	LEU
45	3h	64	GLN
45	3h	149	VAL
45	3h	193	THR
45	3h	204	VAL
45	3h	205	ILE
45	3h	208	SER
45	3h	219	GLU
45	3h	238	HIS
45	3h	347	LEU
45	3h	352	ASN

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Mol	Chain	Res	Type
46	3d	21	VAL
47	3k	127	LEU
47	3k	145	VAL
48	3l	112	TRP
48	3l	132	TYR
48	3l	149	SER
48	3l	186	ILE
48	3l	212	ILE
48	3l	304	MET
48	3l	344	GLN
48	3l	363	GLN
48	3l	441	LEU
48	3l	447	PHE
48	3l	497	MET
48	3l	523	ILE
48	3l	527	MET
48	3l	528	ILE
48	3l	548	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	87	ASN
2	5B	736	GLN
2	5B	984	GLN
2	5B	1118	GLN
3	SA	164	ASN
5	SC	136	HIS
6	SD	159	HIS
7	SE	67	GLN
7	SE	157	ASN
8	SF	203	ASN
9	SG	56	ASN
9	SG	187	HIS
10	SH	68	GLN
10	SH	97	GLN
12	SJ	140	GLN
13	SK	7	ASN
13	SK	42	ASN
13	SK	61	GLN
14	SL	5	GLN
14	SL	100	ASN

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Mol	Chain	Res	Type
16	SN	101	HIS
17	SO	32	HIS
17	SO	103	ASN
18	SP	79	HIS
20	SR	31	ASN
22	ST	137	GLN
23	SU	92	HIS
25	SW	98	GLN
26	SX	73	GLN
29	Sa	72	HIS
30	Sb	19	HIS
30	Sb	26	GLN
32	Sd	37	ASN
34	sh	139	HIS
35	Sg	4	GLN
35	Sg	51	ASN
35	Sg	147	HIS
35	Sg	181	ASN
35	Sg	191	HIS
35	Sg	222	ASN
35	Sg	272	GLN
40	3m	65	ASN
40	3m	257	GLN
40	3m	270	HIS
40	3m	273	ASN
41	3f	155	ASN
41	3f	330	ASN
41	3f	347	GLN
42	3a	76	ASN
42	3a	288	ASN
42	3a	412	ASN
42	3a	430	GLN
42	3a	518	GLN
42	3a	544	GLN
43	3e	239	GLN
43	3e	309	GLN
44	3c	519	HIS
44	3c	623	GLN
44	3c	637	GLN
44	3c	648	GLN
44	3c	674	HIS
44	3c	724	GLN

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Mol	Chain	Res	Type
44	3c	840	GLN
44	3c	853	GLN
44	3c	858	GLN
45	3h	80	ASN
45	3h	86	GLN
45	3h	191	ASN
45	3h	255	GLN
45	3h	276	GLN
45	3h	345	GLN
47	3k	76	ASN
47	3k	169	GLN
48	3l	86	GLN
48	3l	97	ASN
48	3l	218	ASN
48	3l	514	GLN
48	3l	529	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
36	zy	74/75 (98%)	26 (35%)	0
38	zz	305/332 (91%)	118 (38%)	0
39	S2	1748/1869 (93%)	325 (18%)	9 (0%)
All	All	2127/2276 (93%)	469 (22%)	9 (0%)

All (469) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
36	zy	5	G
36	zy	6	A
36	zy	8	U
36	zy	9	G
36	zy	10	G
36	zy	15	G
36	zy	16	C
36	zy	18	G
36	zy	19	A
36	zy	20	A
36	zy	40	C
36	zy	41	A
36	zy	47	C

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Mol	Chain	Res	Type
36	zy	48	G
36	zy	50	U
36	zy	51	G
36	zy	53	A
36	zy	54	U
36	zy	56	G
36	zy	57	A
36	zy	61	C
36	zy	62	A
36	zy	65	C
36	zy	71	U
36	zy	73	C
36	zy	74	C
38	zz	46	U
38	zz	48	U
38	zz	49	G
38	zz	51	G
38	zz	52	G
38	zz	53	A
38	zz	54	A
38	zz	56	U
38	zz	64	U
38	zz	82	G
38	zz	83	C
38	zz	85	A
38	zz	94	G
38	zz	100	G
38	zz	102	G
38	zz	103	U
38	zz	106	U
38	zz	107	G
38	zz	111	C
38	zz	113	U
38	zz	114	C
38	zz	116	A
38	zz	118	G
38	zz	132	G
38	zz	133	G
38	zz	134	A
38	zz	135	G
38	zz	136	A
38	zz	138	C

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Mol	Chain	Res	Type
38	zz	140	A
38	zz	142	A
38	zz	143	G
38	zz	150	G
38	zz	154	A
38	zz	156	C
38	zz	157	C
38	zz	161	G
38	zz	162	A
38	zz	163	G
38	zz	164	U
38	zz	165	A
38	zz	166	C
38	zz	167	A
38	zz	169	C
38	zz	171	G
38	zz	175	U
38	zz	176	G
38	zz	185	A
38	zz	186	C
38	zz	189	G
38	zz	190	G
38	zz	191	U
38	zz	192	C
38	zz	195	U
38	zz	196	U
38	zz	197	C
38	zz	198	U
38	zz	202	A
38	zz	204	C
38	zz	207	C
38	zz	208	C
38	zz	209	C
38	zz	210	G
38	zz	213	C
38	zz	216	U
38	zz	217	G
38	zz	218	C
38	zz	223	A
38	zz	224	G
38	zz	225	A
38	zz	229	G

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Mol	Chain	Res	Type
38	zz	233	G
38	zz	234	U
38	zz	237	C
38	zz	244	A
38	zz	245	G
38	zz	249	G
38	zz	250	C
38	zz	252	A
38	zz	253	G
38	zz	254	C
38	zz	255	C
38	zz	256	G
38	zz	257	A
38	zz	258	G
38	zz	259	U
38	zz	263	G
38	zz	265	U
38	zz	266	G
38	zz	269	U
38	zz	270	C
38	zz	279	C
38	zz	281	U
38	zz	282	U
38	zz	283	G
38	zz	284	U
38	zz	288	A
38	zz	290	U
38	zz	295	G
38	zz	297	U
38	zz	303	G
38	zz	306	U
38	zz	307	G
38	zz	323	G
38	zz	324	U
38	zz	330	A
38	zz	331	G
38	zz	332	A
38	zz	333	C
38	zz	334	C
38	zz	335	G
38	zz	336	U
38	zz	344	G

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Mol	Chain	Res	Type
38	zz	345	A
38	zz	346	G
38	zz	347	C
38	zz	348	A
38	zz	349	C
39	S2	2	A
39	S2	17	C
39	S2	33	G
39	S2	41	G
39	S2	46	A
39	S2	56	G
39	S2	62	G
39	S2	67	C
39	S2	68	A
39	S2	73	C
39	S2	74	G
39	S2	75	G
39	S2	99	A
39	S2	103	A
39	S2	113	G
39	S2	115	U
39	S2	126	G
39	S2	130	G
39	S2	143	U
39	S2	155	G
39	S2	158	A
39	S2	161	U
39	S2	163	U
39	S2	172	U
39	S2	175	A
39	S2	178	C
39	S2	182	C
39	S2	191	A
39	S2	193	C
39	S2	195	C
39	S2	199	C
39	S2	201	C
39	S2	202	G
39	S2	204	G
39	S2	212	C
39	S2	228	C
39	S2	233	C

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Mol	Chain	Res	Type
39	S2	235	A
39	S2	280	G
39	S2	281	C
39	S2	282	G
39	S2	283	G
39	S2	294	U
39	S2	306	C
39	S2	309	G
39	S2	319	C
39	S2	324	C
39	S2	325	C
39	S2	326	C
39	S2	327	G
39	S2	328	U
39	S2	329	G
39	S2	330	G
39	S2	332	G
39	S2	351	G
39	S2	362	C
39	S2	364	A
39	S2	370	G
39	S2	383	G
39	S2	385	G
39	S2	386	C
39	S2	399	C
39	S2	400	C
39	S2	407	G
39	S2	408	A
39	S2	409	C
39	S2	448	A
39	S2	449	A
39	S2	450	C
39	S2	452	G
39	S2	464	A
39	S2	471	G
39	S2	472	C
39	S2	474	G
39	S2	476	A
39	S2	482	G
39	S2	487	U
39	S2	492	C
39	S2	493	A

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Mol	Chain	Res	Type
39	S2	516	A
39	S2	517	C
39	S2	518	G
39	S2	532	C
39	S2	534	G
39	S2	536	A
39	S2	537	C
39	S2	538	U
39	S2	541	U
39	S2	543	C
39	S2	544	G
39	S2	545	A
39	S2	546	G
39	S2	547	G
39	S2	548	C
39	S2	549	C
39	S2	550	C
39	S2	554	A
39	S2	555	A
39	S2	556	U
39	S2	559	G
39	S2	564	A
39	S2	568	C
39	S2	576	A
39	S2	583	A
39	S2	587	A
39	S2	589	G
39	S2	590	A
39	S2	591	U
39	S2	593	C
39	S2	606	G
39	S2	614	C
39	S2	617	G
39	S2	629	A
39	S2	643	A
39	S2	644	G
39	S2	655	A
39	S2	660	C
39	S2	669	A
39	S2	670	A
39	S2	671	A
39	S2	672	A

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Mol	Chain	Res	Type
39	S2	673	G
39	S2	688	U
39	S2	690	G
39	S2	692	G
39	S2	693	A
39	S2	695	C
39	S2	696	G
39	S2	697	G
39	S2	698	G
39	S2	731	G
39	S2	732	U
39	S2	733	C
39	S2	735	C
39	S2	736	C
39	S2	738	C
39	S2	746	C
39	S2	749	U
39	S2	751	G
39	S2	790	C
39	S2	795	A
39	S2	796	G
39	S2	797	C
39	S2	798	G
39	S2	799	U
39	S2	800	U
39	S2	801	U
39	S2	821	G
39	S2	822	U
39	S2	827	A
39	S2	834	C
39	S2	847	A
39	S2	869	A
39	S2	870	A
39	S2	871	U
39	S2	872	A
39	S2	873	G
39	S2	886	A
39	S2	891	G
39	S2	894	G
39	S2	895	G
39	S2	913	A
39	S2	914	U

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Mol	Chain	Res	Type
39	S2	920	A
39	S2	921	G
39	S2	922	A
39	S2	933	G
39	S2	943	U
39	S2	971	G
39	S2	985	G
39	S2	990	A
39	S2	992	A
39	S2	1017	U
39	S2	1023	A
39	S2	1045	U
39	S2	1060	A
39	S2	1061	U
39	S2	1062	A
39	S2	1071	G
39	S2	1078	C
39	S2	1081	U
39	S2	1082	A
39	S2	1083	A
39	S2	1085	C
39	S2	1099	G
39	S2	1109	C
39	S2	1114	U
39	S2	1115	U
39	S2	1117	C
39	S2	1118	C
39	S2	1121	G
39	S2	1130	G
39	S2	1133	A
39	S2	1138	C
39	S2	1139	C
39	S2	1149	A
39	S2	1150	A
39	S2	1153	C
39	S2	1154	U
39	S2	1166	G
39	S2	1170	A
39	S2	1171	G
39	S2	1195	A
39	S2	1207	G
39	S2	1215	C

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Mol	Chain	Res	Type
39	S2	1220	A
39	S2	1242	U
39	S2	1243	U
39	S2	1248	U
39	S2	1249	C
39	S2	1251	A
39	S2	1253	A
39	S2	1256	G
39	S2	1257	G
39	S2	1259	A
39	S2	1274	G
39	S2	1275	G
39	S2	1284	A
39	S2	1285	G
39	S2	1286	G
39	S2	1287	A
39	S2	1288	U
39	S2	1291	A
39	S2	1294	G
39	S2	1301	A
39	S2	1302	G
39	S2	1303	C
39	S2	1306	U
39	S2	1308	U
39	S2	1309	C
39	S2	1326	U
39	S2	1327	G
39	S2	1342	U
39	S2	1348	G
39	S2	1371	U
39	S2	1372	U
39	S2	1378	A
39	S2	1382	A
39	S2	1397	U
39	S2	1404	U
39	S2	1417	C
39	S2	1418	C
39	S2	1419	C
39	S2	1421	A
39	S2	1423	C
39	S2	1424	G
39	S2	1434	C

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Mol	Chain	Res	Type
39	S2	1435	C
39	S2	1436	C
39	S2	1438	A
39	S2	1452	A
39	S2	1454	A
39	S2	1462	U
39	S2	1463	U
39	S2	1489	A
39	S2	1490	G
39	S2	1494	U
39	S2	1497	G
39	S2	1498	A
39	S2	1507	G
39	S2	1508	A
39	S2	1520	G
39	S2	1521	C
39	S2	1522	A
39	S2	1533	A
39	S2	1552	G
39	S2	1553	C
39	S2	1555	U
39	S2	1575	G
39	S2	1580	A
39	S2	1585	U
39	S2	1588	A
39	S2	1601	A
39	S2	1606	G
39	S2	1621	U
39	S2	1646	C
39	S2	1654	G
39	S2	1664	A
39	S2	1665	G
39	S2	1671	G
39	S2	1680	G
39	S2	1698	C
39	S2	1699	A
39	S2	1712	A
39	S2	1713	C
39	S2	1714	U
39	S2	1719	A
39	S2	1721	U
39	S2	1722	G

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Mol	Chain	Res	Type
39	S2	1723	G
39	S2	1744	G
39	S2	1745	A
39	S2	1748	G
39	S2	1752	C
39	S2	1753	C
39	S2	1754	G
39	S2	1768	A
39	S2	1776	G
39	S2	1777	G
39	S2	1778	C
39	S2	1780	G
39	S2	1781	A
39	S2	1782	G
39	S2	1783	C
39	S2	1785	C
39	S2	1786	U
39	S2	1799	G
39	S2	1812	U
39	S2	1813	A
39	S2	1821	U
39	S2	1823	A
39	S2	1824	A
39	S2	1825	A
39	S2	1826	G
39	S2	1830	U
39	S2	1831	A
39	S2	1835	A
39	S2	1838	U
39	S2	1849	G
39	S2	1851	A
39	S2	1852	C
39	S2	1861	G
39	S2	1862	G
39	S2	1863	A
39	S2	1865	C

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
39	S2	171	A
39	S2	174	C

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Mol	Chain	Res	Type
39	S2	323	C
39	S2	517	C
39	S2	531	A
39	S2	871	U
39	S2	1116	C
39	S2	1326	U
39	S2	1434	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
50	GTP	5B	1302	49	33,34,34	3.43	17 (51%)	50,54,54	1.75	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	GTP	5B	1302	49	-	4/22/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	5B	1302	GTP	C3'-C4'	-8.82	1.30	1.53
50	5B	1302	GTP	O4'-C4'	7.63	1.62	1.45
50	5B	1302	GTP	C4-N3	6.63	1.49	1.34
50	5B	1302	GTP	C2-N3	5.44	1.46	1.33
50	5B	1302	GTP	PA-O3A	4.89	1.64	1.59
50	5B	1302	GTP	PB-O3B	4.87	1.64	1.59
50	5B	1302	GTP	C2-N2	4.80	1.45	1.34
50	5B	1302	GTP	PB-O3A	4.80	1.64	1.59
50	5B	1302	GTP	O4'-C1'	-4.68	1.31	1.42
50	5B	1302	GTP	C5-N7	-2.92	1.33	1.39
50	5B	1302	GTP	O3'-C3'	2.84	1.50	1.43
50	5B	1302	GTP	O2'-C2'	-2.74	1.36	1.43
50	5B	1302	GTP	C2-N1	2.68	1.44	1.37
50	5B	1302	GTP	O6-C6	-2.54	1.18	1.23
50	5B	1302	GTP	C5-C6	2.46	1.53	1.44
50	5B	1302	GTP	C6-N1	2.31	1.43	1.38
50	5B	1302	GTP	C4-N9	-2.08	1.32	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	5B	1302	GTP	C5-C4-N3	-4.90	120.59	128.39
50	5B	1302	GTP	C1'-N9-C4	-4.48	113.24	126.49
50	5B	1302	GTP	C2-N3-C4	4.35	119.78	112.30
50	5B	1302	GTP	C1'-N9-C8	3.88	137.76	126.73
50	5B	1302	GTP	N9-C8-N7	-3.25	107.38	113.40
50	5B	1302	GTP	N9-C4-N3	3.05	132.06	125.95
50	5B	1302	GTP	C2-N1-C6	-2.75	120.11	125.11
50	5B	1302	GTP	C5-C6-N1	2.55	119.75	113.25
50	5B	1302	GTP	O6-C6-C5	-2.22	120.68	126.53
50	5B	1302	GTP	C8-N7-C5	2.21	108.20	104.26

There are no chirality outliers.

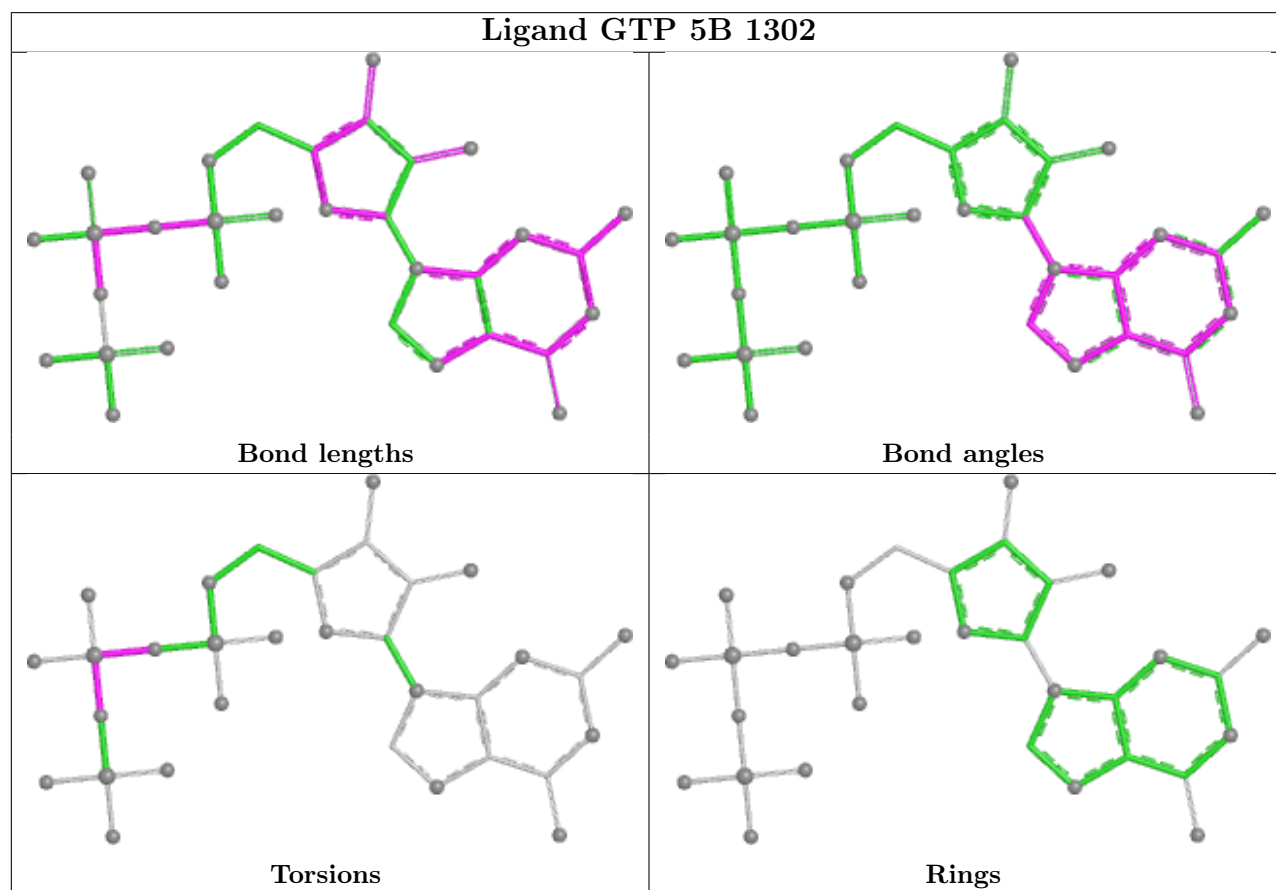
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	5B	1302	GTP	PG-O3B-PB-O2B
50	5B	1302	GTP	PA-O3A-PB-O3B
50	5B	1302	GTP	PG-O3B-PB-O1B
50	5B	1302	GTP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

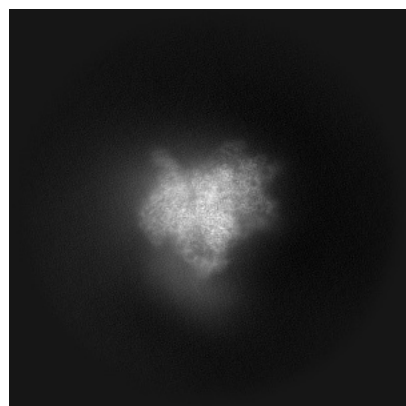
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62454. These allow visual inspection of the internal detail of the map and identification of artifacts.

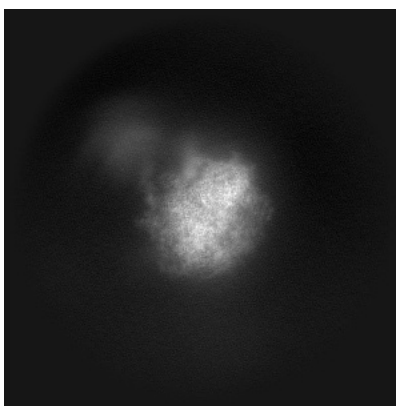
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

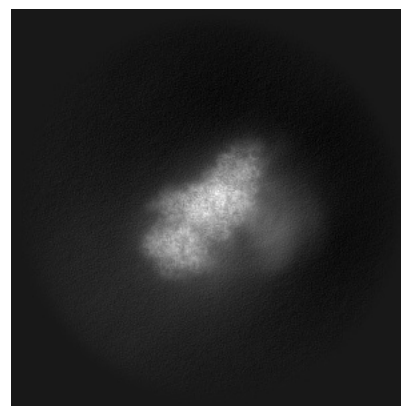
6.1.1 Primary map



X

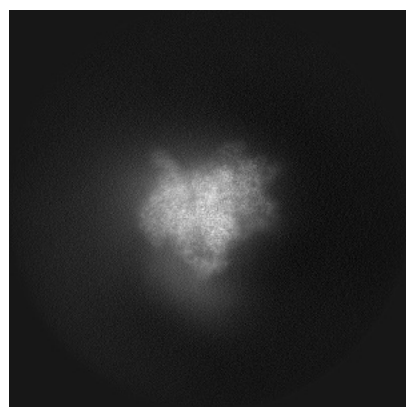


Y

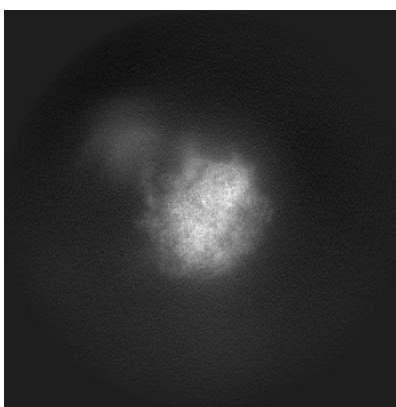


Z

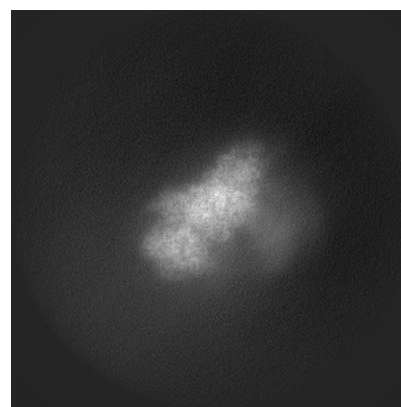
6.1.2 Raw map



X



Y

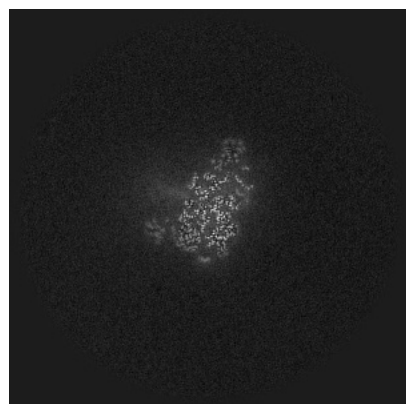


Z

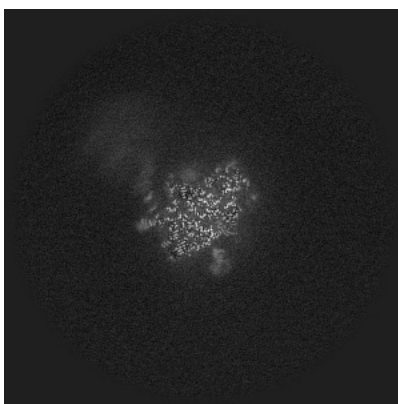
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

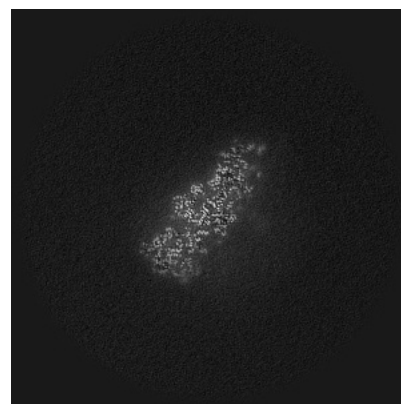
6.2.1 Primary map



X Index: 250

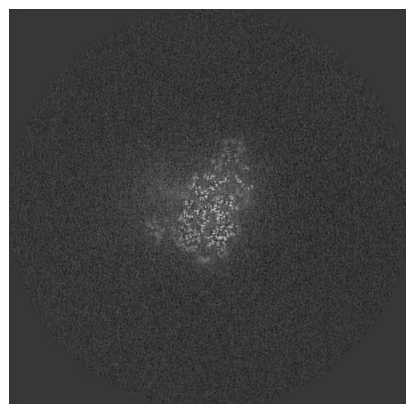


Y Index: 250

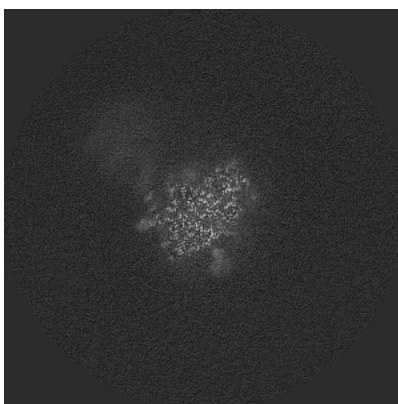


Z Index: 250

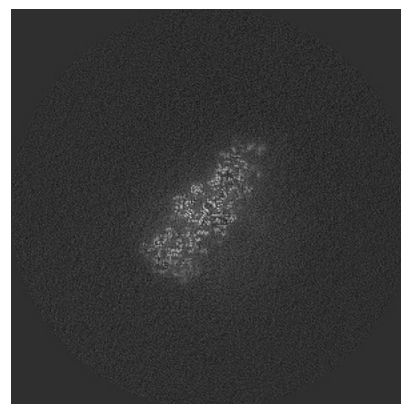
6.2.2 Raw map



X Index: 250



Y Index: 250

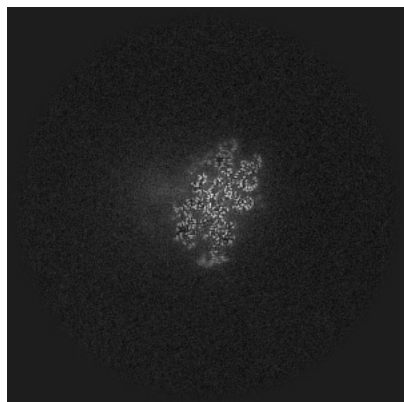


Z Index: 250

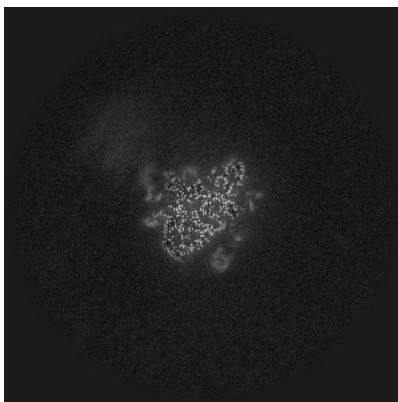
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

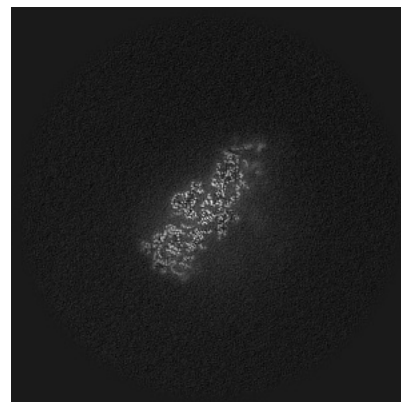
6.3.1 Primary map



X Index: 260

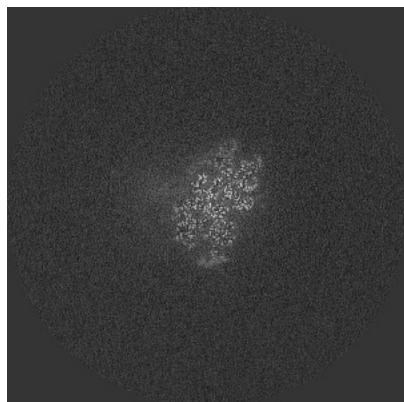


Y Index: 255

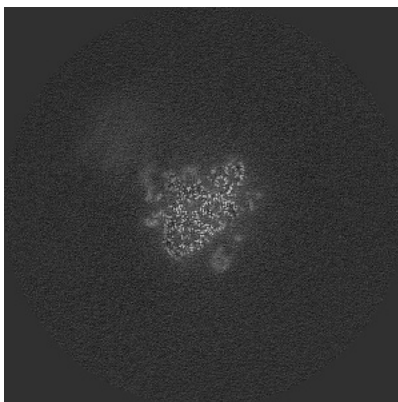


Z Index: 248

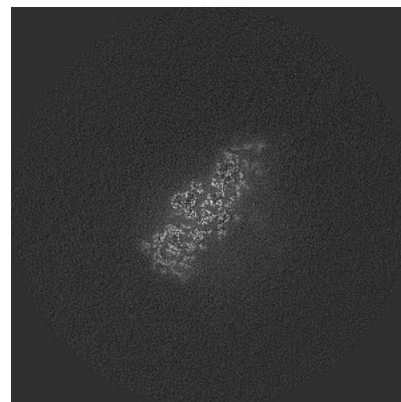
6.3.2 Raw map



X Index: 260



Y Index: 255

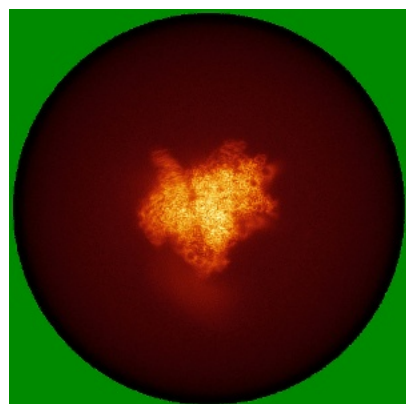


Z Index: 248

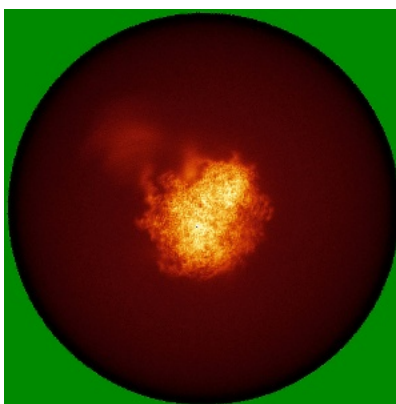
The images above show the largest variance slices of the map in three orthogonal directions.

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

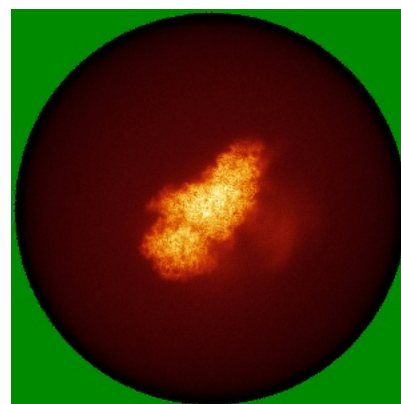
6.4.1 Primary map



X

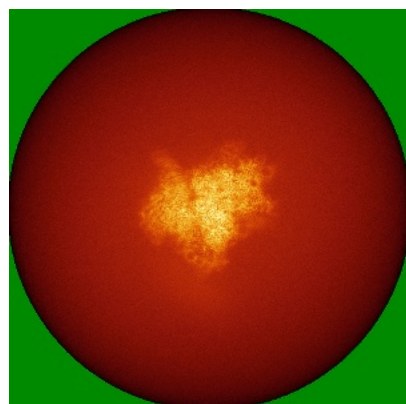


Y

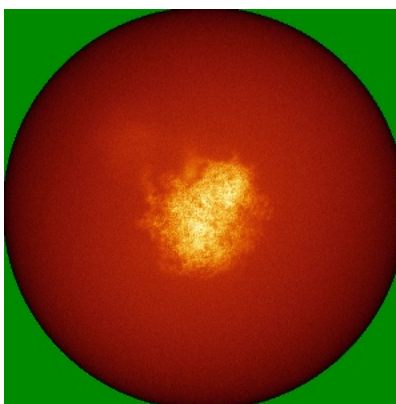


Z

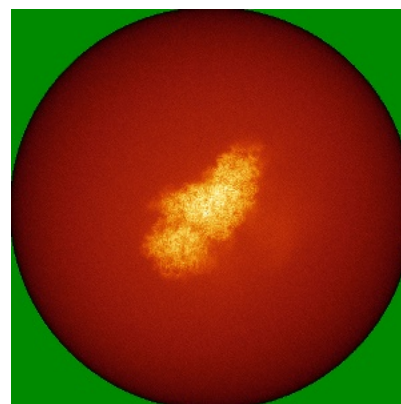
6.4.2 Raw map



X



Y

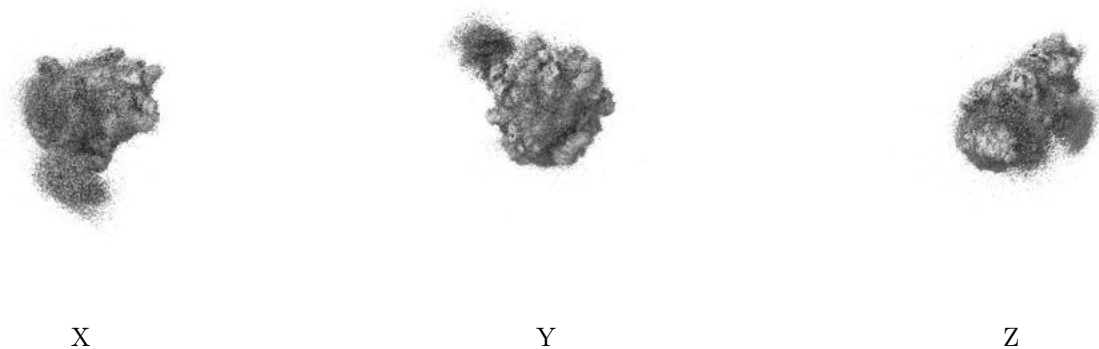


Z

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

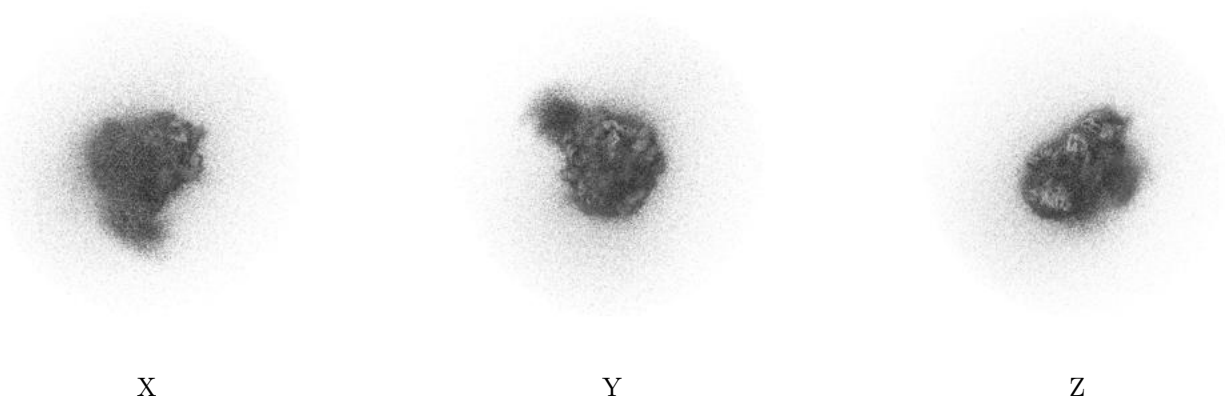
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

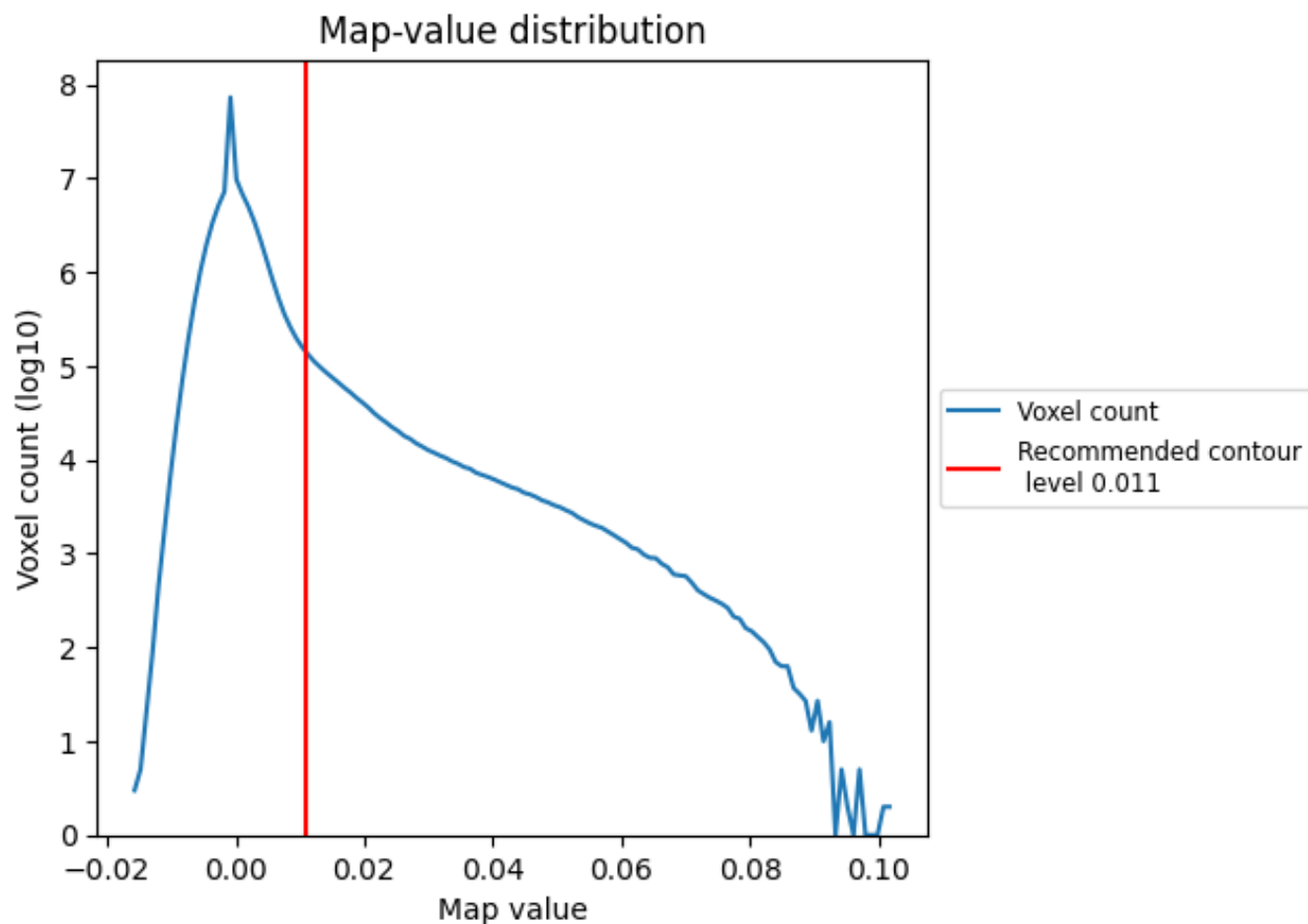
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

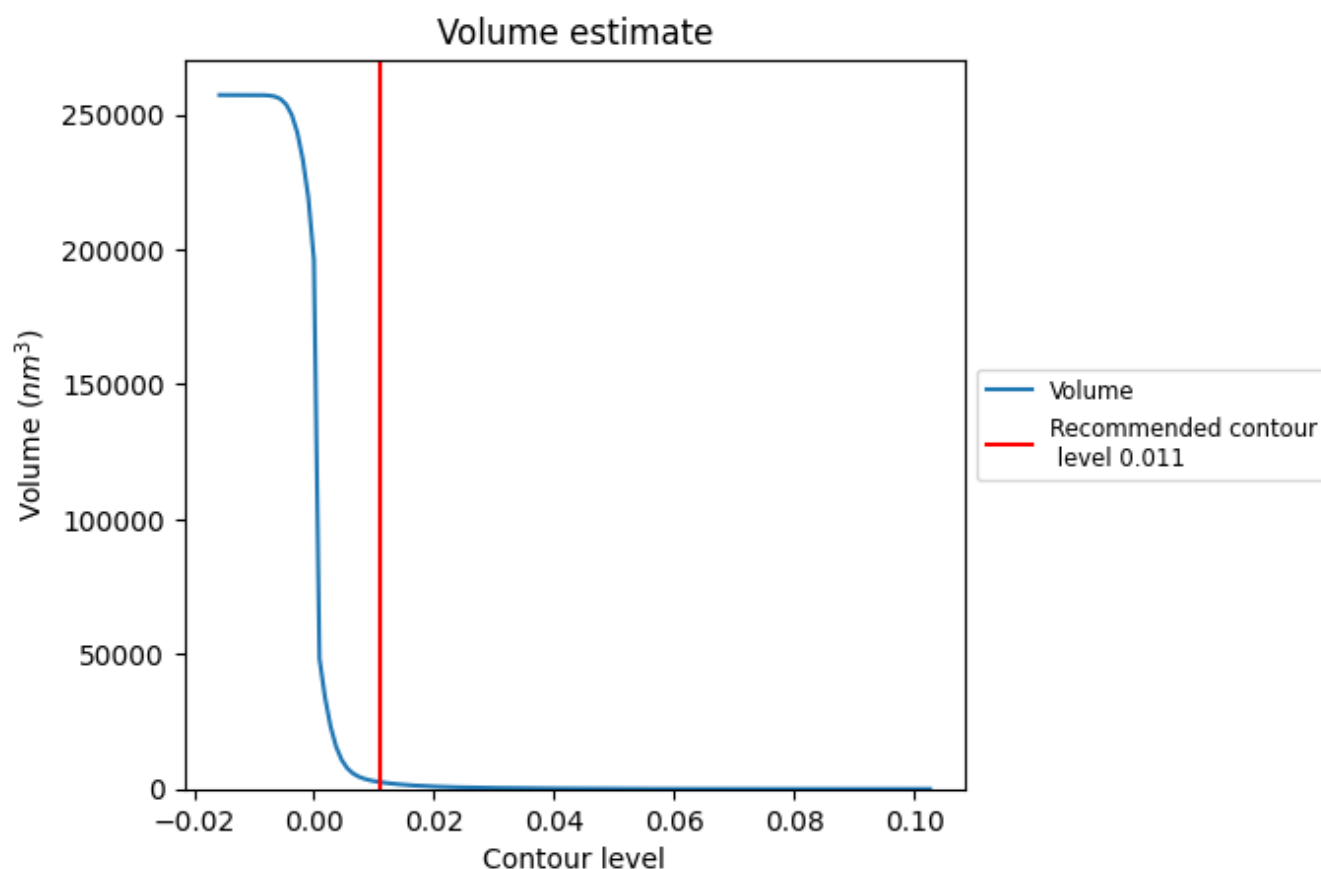
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

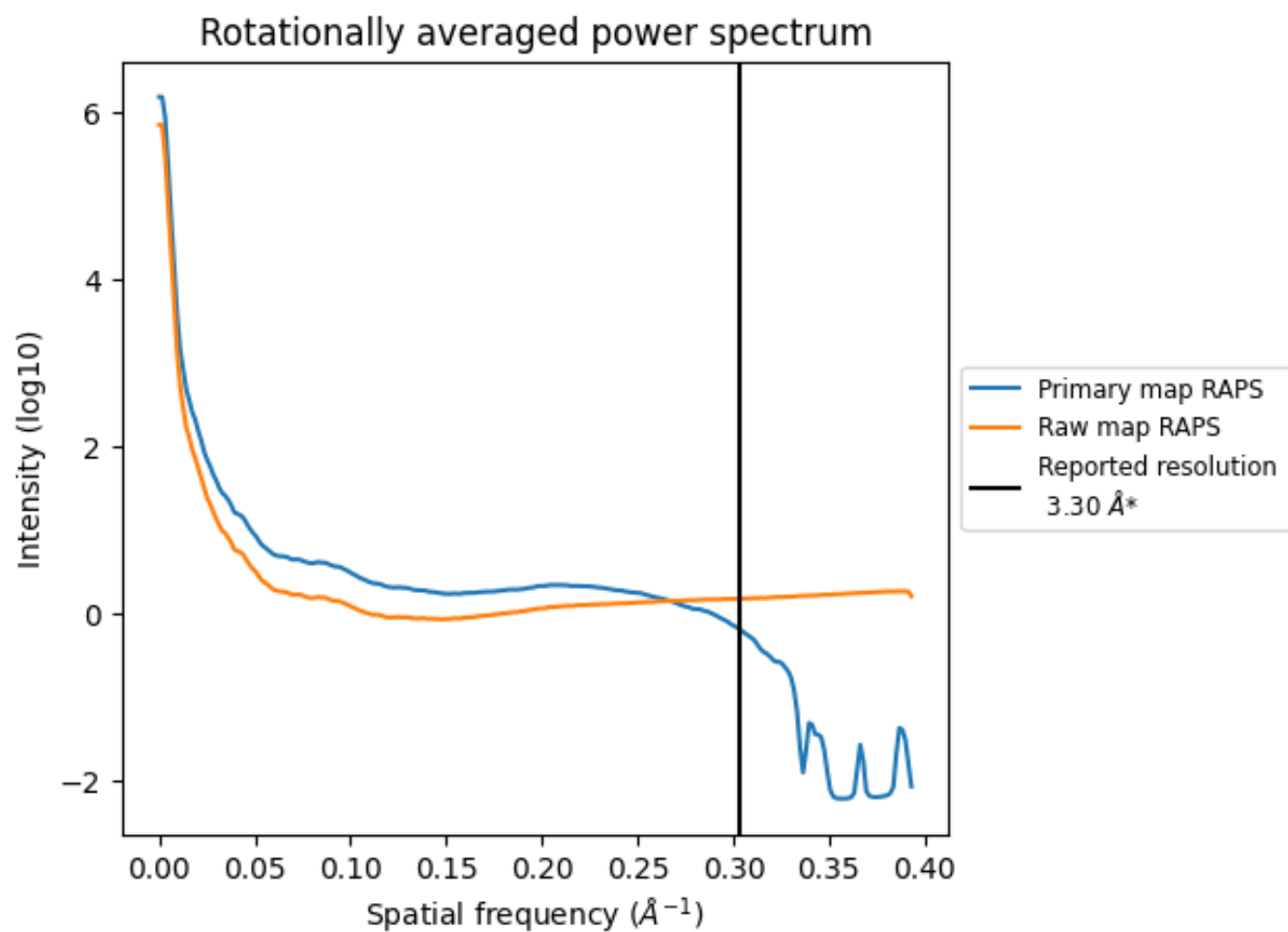
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2536 nm^3 ; this corresponds to an approximate mass of 2291 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](#)

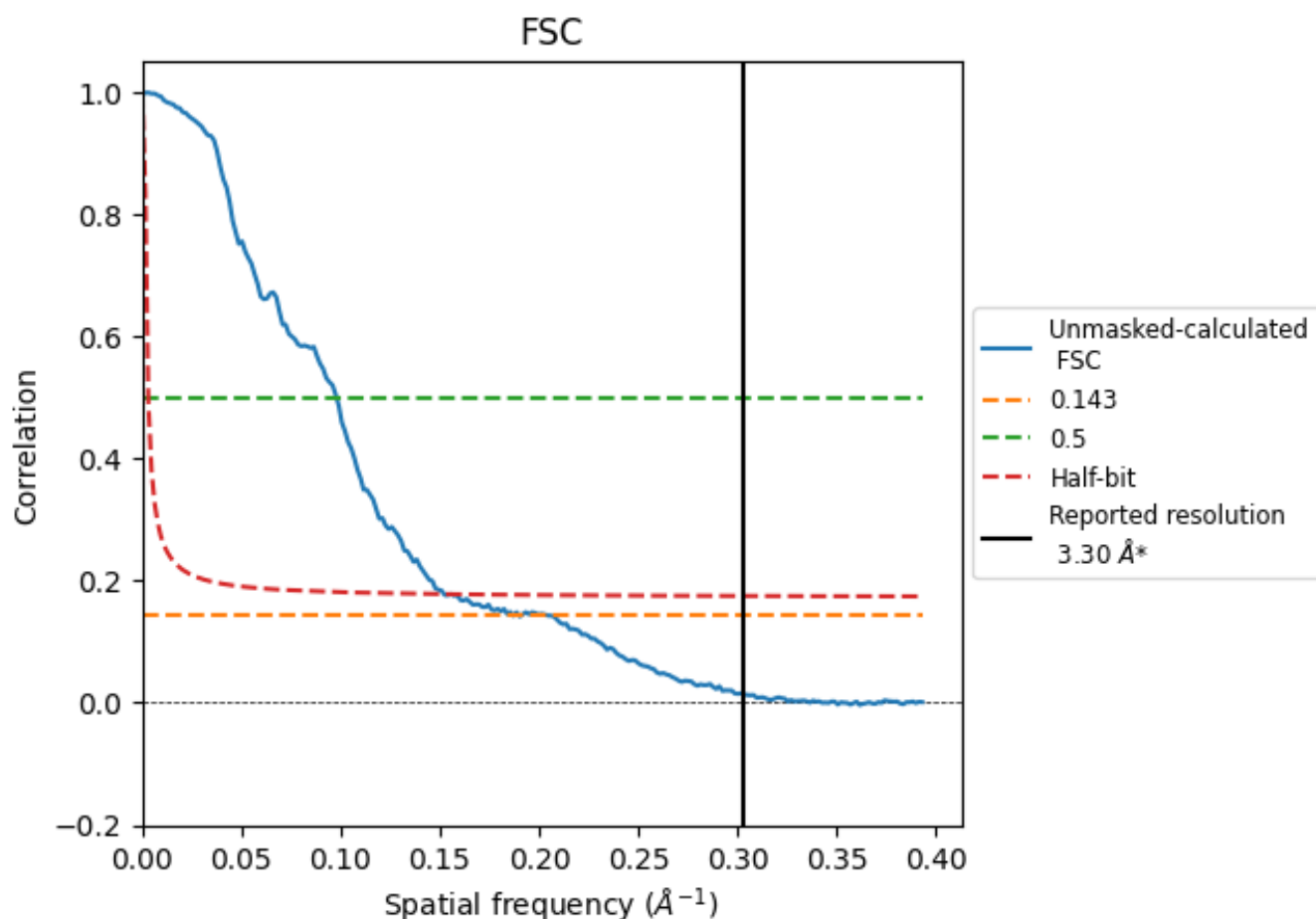


*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

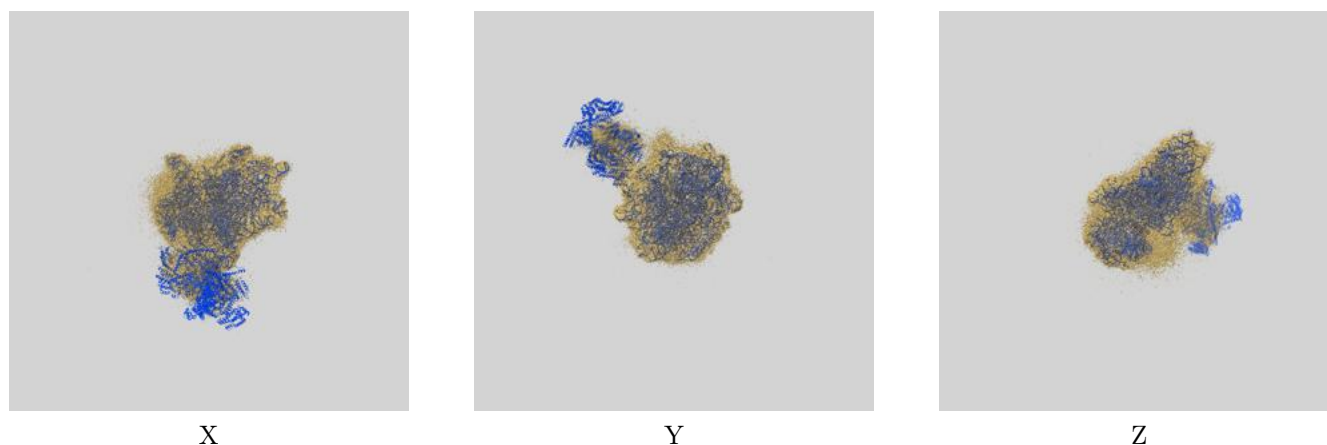
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.35	10.21	6.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.35 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

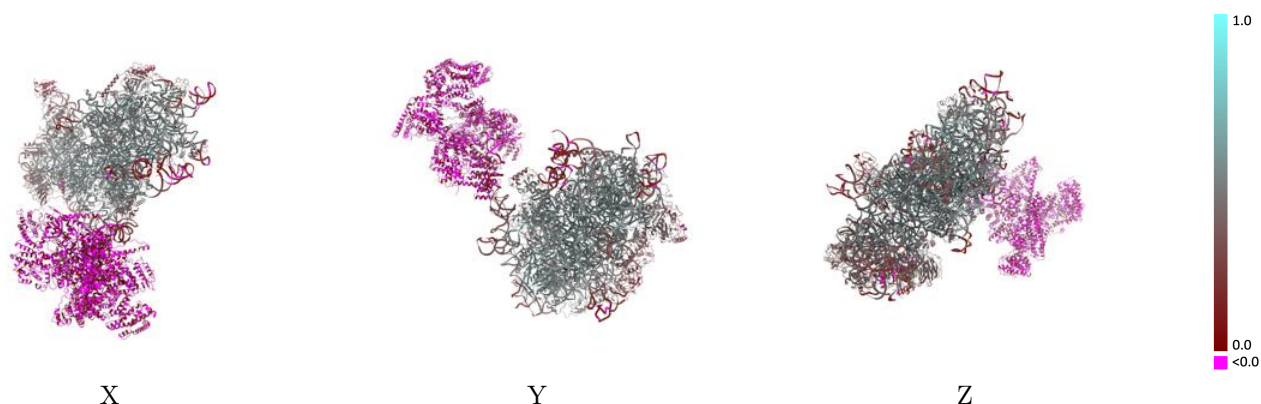
This section contains information regarding the fit between EMDB map EMD-62454 and PDB model 9KN6. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



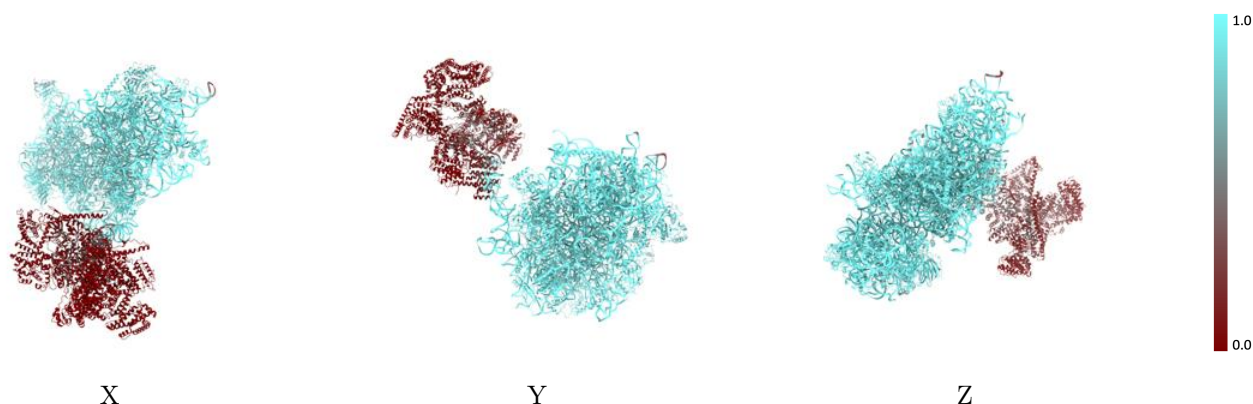
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



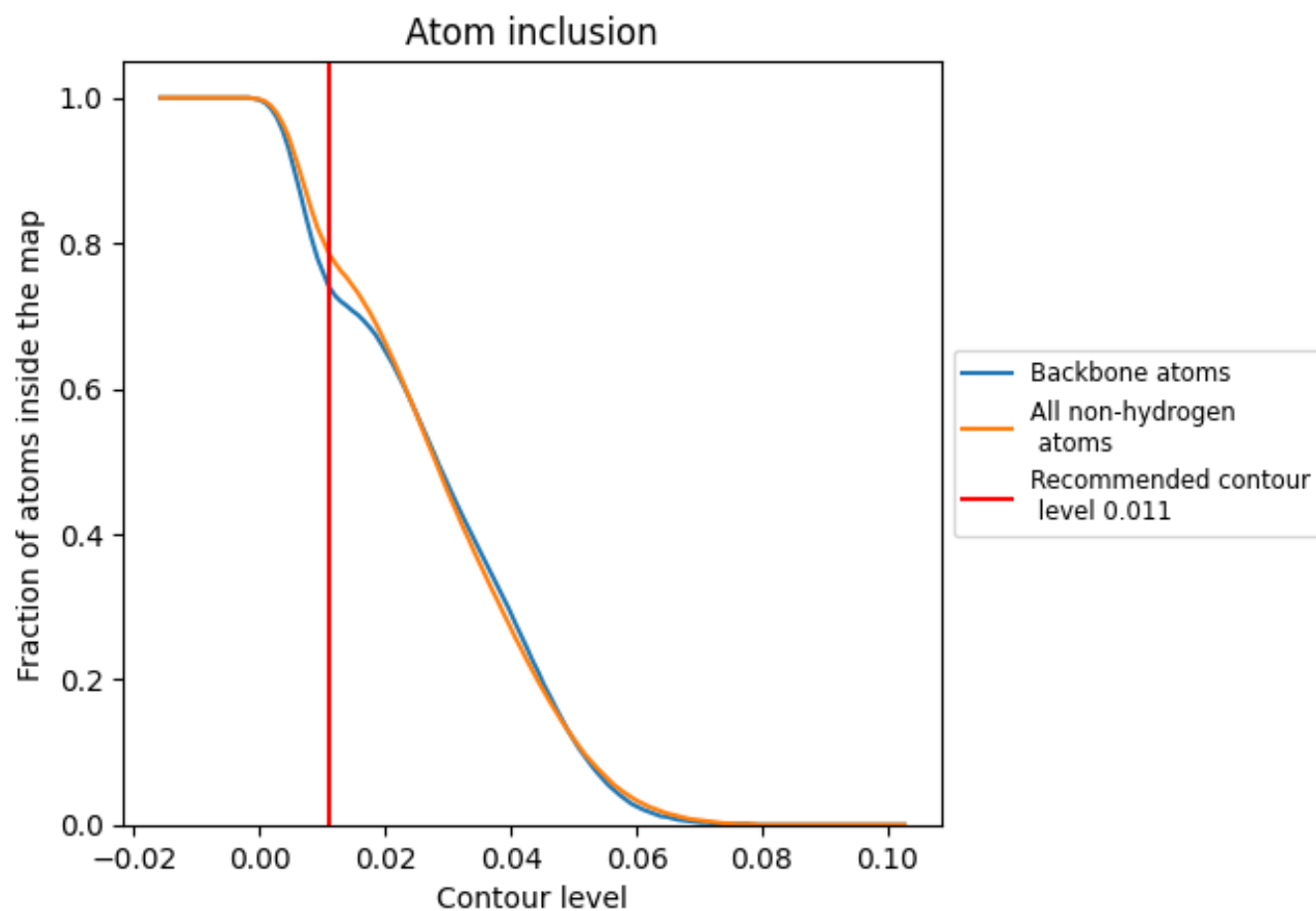
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.011).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 79% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7870	 0.3500
1A	 0.9900	 0.4410
3a	 0.1570	 0.0020
3c	 0.0930	 -0.0030
3d	 0.0270	 -0.0250
3e	 0.0200	 -0.0010
3f	 0.1090	 0.0040
3h	 0.1570	 -0.0020
3k	 0.0070	 0.0190
3l	 0.0110	 0.0050
3m	 0.0220	 0.0060
5B	 0.9480	 0.3550
Ln	 1.0000	 0.5100
S2	 0.9930	 0.4690
SA	 0.9970	 0.5080
SB	 0.9890	 0.5170
SC	 0.9990	 0.5310
SD	 0.9990	 0.4530
SE	 0.9980	 0.5250
SF	 0.9970	 0.5110
SG	 0.9780	 0.4420
SH	 0.9830	 0.4420
SI	 0.9800	 0.4850
SJ	 0.9980	 0.5190
SK	 0.9920	 0.3710
SL	 0.9870	 0.5100
SN	 1.0000	 0.5160
SO	 0.9980	 0.5260
SP	 0.9650	 0.3710
SQ	 0.9980	 0.4680
SR	 0.9960	 0.4510
SS	 0.9860	 0.4350
ST	 0.9850	 0.4160
SU	 0.9910	 0.4250
SV	 0.9980	 0.5180



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Chain	Atom inclusion	Q-score
SW	 0.9990	 0.5430
SX	 1.0000	 0.5390
SY	 0.9970	 0.4970
SZ	 0.9860	 0.4530
Sa	 1.0000	 0.5310
Sb	 0.9980	 0.4990
Sc	 1.0000	 0.5130
Sd	 1.0000	 0.4750
Se	 1.0000	 0.4750
Sf	 0.8300	 0.1640
Sg	 0.9800	 0.3610
sh	 0.9020	 0.2190
zy	 0.9820	 0.2600
zz	 0.9210	 0.3100