



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:49 PM UTC

PDB ID : 7UQB / pdb_00007uqb
EMDB ID : EMD-26686
Title : Nucleoplasmic pre-60S intermediate of the Nog2 containing pre-rotation state from a SPB1-D52A strain with AIF4
Authors : Sekulski, K.; Cruz, V.E.; Weirich, C.S.; Erzberger, J.P.
Deposited on : 2022-04-19
Resolution : 2.43 Å(reported)
Based on initial model : 3JCT

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:

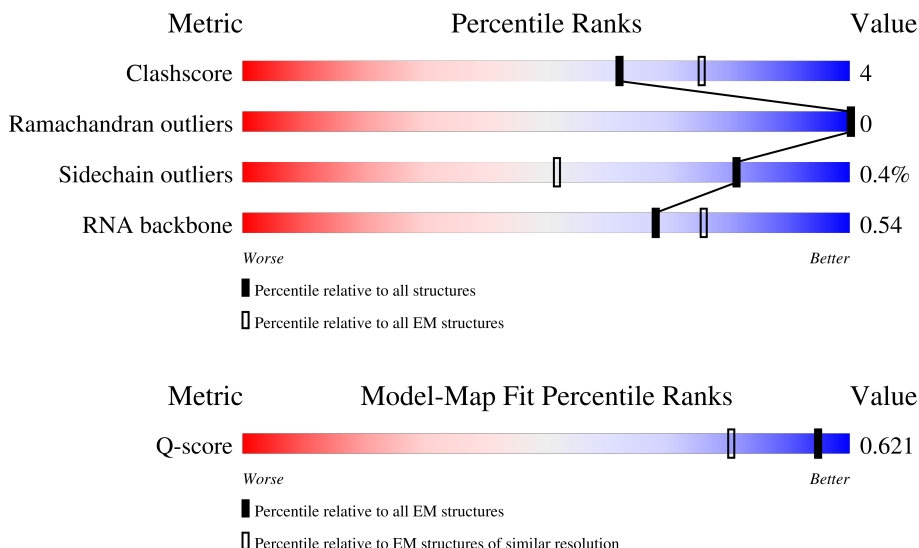
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.43 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	5787 (1.94 - 2.93)

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

Mol	Chain	Length	Quality of chain
1	A	254	
2	1	3396	
3	2	158	

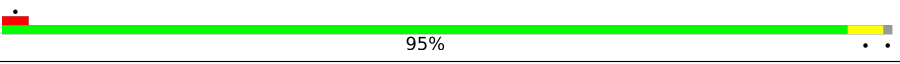
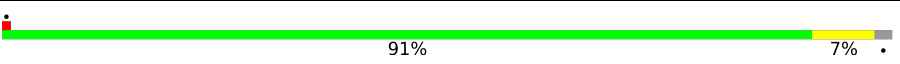
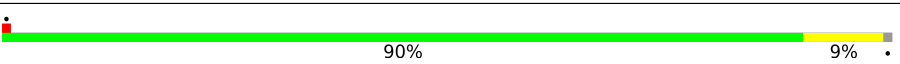
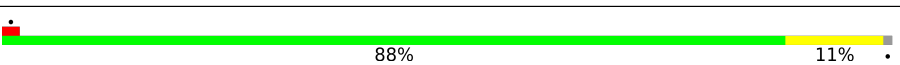
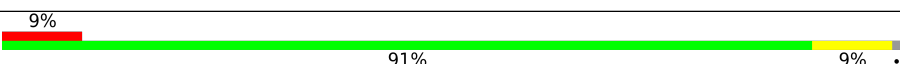
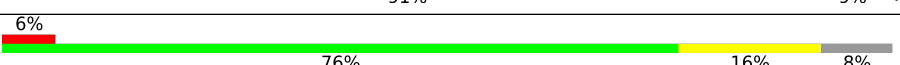
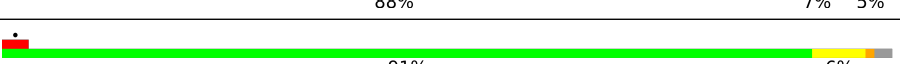
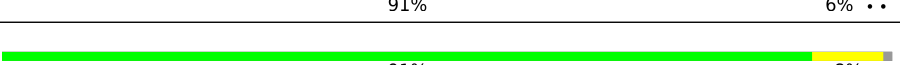
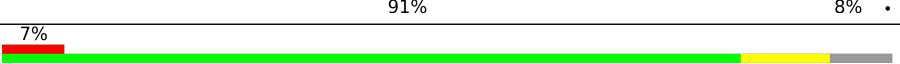
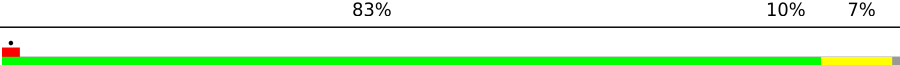
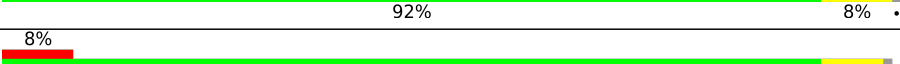
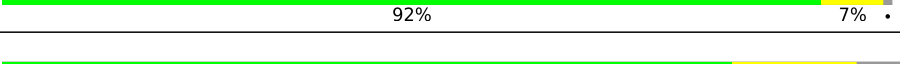
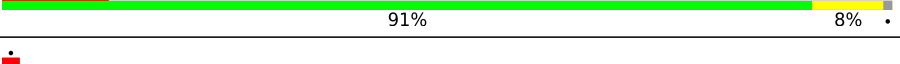
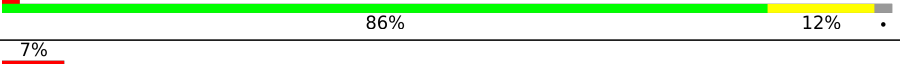
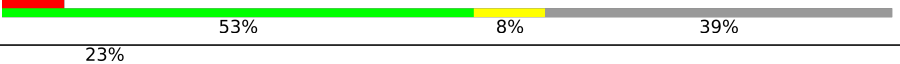
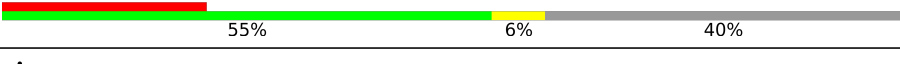
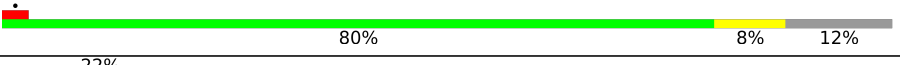
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Mol	Chain	Length	Quality of chain
4	3	121	
5	5	120	
6	6	74	
7	8	165	
8	9	175	
9	B	387	
10	C	362	
11	D	297	
12	E	176	
13	F	244	
14	G	256	
15	H	191	
16	I	166	
17	J	174	
18	K	376	
19	L	199	
20	M	138	
21	N	204	
22	O	199	
23	P	184	
24	Q	186	
25	R	189	
26	S	172	
27	T	160	
28	U	121	

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Mol	Chain	Length	Quality of chain
29	V	137	
30	W	236	
31	X	142	
32	Y	127	
33	Z	136	
34	a	149	
35	b	647	
36	c	105	
37	d	113	
38	e	130	
39	f	107	
40	g	121	
41	h	120	
42	i	100	
43	j	88	
44	k	78	
45	l	51	
46	m	486	
47	n	605	
48	o	220	
49	p	92	
50	q	455	
51	r	261	
52	s	77	
53	t	322	

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Mol	Chain	Length	Quality of chain
54	u	199	
55	v	344	
56	w	201	
57	x	514	
58	y	245	
59	z	106	
60	4	593	

2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 157949 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	213	Total	C	N	O	S	0	0
			1634	1023	326	284	1		

- Molecule 2 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	2991	Total	C	N	O	P	0	0
			64042	28618	11563	20870	2991		

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 5 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	73	Total	C	N	O	S	0	0
			645	395	133	114	3		

- Molecule 6 is a RNA chain called ITS2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	58	Total	C	N	O	P	0	0
			1227	550	210	409	58		

- Molecule 7 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	158	Total	C	N	O	S	0	0
			1196	750	216	228	2		

- Molecule 8 is a protein called Ribosome biogenesis protein ALB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	118	Total	C	N	O		0	0
			937	590	181	166			

- Molecule 9 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 10 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	361	Total	C	N	O	S	0	0
			2749	1730	522	494	3		

- Molecule 11 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	270	Total	C	N	O	S	0	0
			2180	1379	382	417	2		

- Molecule 12 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	155	Total	C	N	O	S	0	0
			1230	795	221	213	1		

- Molecule 13 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	219	Total	C	N	O	S	0	0
			1761	1138	320	302	1		

- Molecule 14 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	224	Total	C	N	O	S	0	0
			1753	1122	314	314	3		

- Molecule 15 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 16 is a protein called Bud site selection protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	131	Total	C	N	O	S	0	0
			1059	662	195	198	4		

- Molecule 17 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	171	Total	C	N	O	S	0	0
			1368	856	256	252	4		

- Molecule 18 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	268	Total	C	N	O	S	0	0
			2155	1387	355	409	4		

- Molecule 19 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	180	Total	C	N	O	S	0	0
			1438	892	296	250			

- Molecule 20 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 21 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	189	Total	C	N	O	S	0	0
			1620	1016	342	261	1		

- Molecule 22 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 23 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	P	175	Total	C	N	O	0	0
			1388	862	277	249		

- Molecule 24 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	147	Total	C	N	O	S	0	0
			1136	718	219	198	1		

- Molecule 25 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	R	156	Total	C	N	O	0	0
			1258	781	265	212		

- Molecule 26 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 27 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	114	Total	C	N	O	S	0	0
			905	568	175	159	3		

- Molecule 28 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	U	106	Total	C	N	O	0	0
			844	545	138	161		

- Molecule 29 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 30 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	234	Total	C	N	O	S	0	0
			1888	1194	323	365	6		

- Molecule 31 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	139	Total	C	N	O	S	0	0
			1088	697	194	195	2		

- Molecule 32 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 33 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Z	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 34 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	92	Total	C	N	O	S	0	0
			731	477	129	124	1		

- Molecule 35 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	642	Total	C	N	O	S	0	0
			5185	3251	938	970	26		

- Molecule 36 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 37 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	107	Total	C	N	O	S	0	0
			873	553	165	154	1		

- Molecule 38 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 39 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 40 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

- Molecule 41 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 42 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 43 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

- Molecule 44 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	77	Total	C	N	O	S	0	0
			612	391	115	106			

- Molecule 45 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 46 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	466	Total	C	N	O	S	0	0
			3754	2372	681	691	10		

- Molecule 47 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	369	Total	C	N	O	S	0	0
			3014	1954	521	530	9		

- Molecule 48 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	133	Total	C	N	O	S	0	0
			1107	716	198	189	4		

- Molecule 49 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 50 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	156	Total	C	N	O	S	0	0
			1298	821	233	243	1		

- Molecule 51 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	230	Total	C	N	O	S	0	0
			1860	1177	352	324	7		

- Molecule 52 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	72	Total	C	N	O	S	0	0
			602	377	118	104	3		

- Molecule 53 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	287	Total	C	N	O	S	0	0
			2306	1459	427	417	3		

- Molecule 54 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	150	Total	C	N	O	S	0	0
			1265	793	253	210	9		

- Molecule 55 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	v	293	Total	C	N	O	S	0	0
			2366	1512	415	422	17		

- Molecule 56 is a protein called Ribosome biogenesis regulatory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	w	194	Total	C	N	O	S	0	0
			1541	965	277	294	5		

- Molecule 57 is a protein called RSA4 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	504	Total	C	N	O	S	0	0
			3927	2468	695	743	21		

- Molecule 58 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	y	244	Total	C	N	O	S	0	0
			1849	1146	319	377	7		

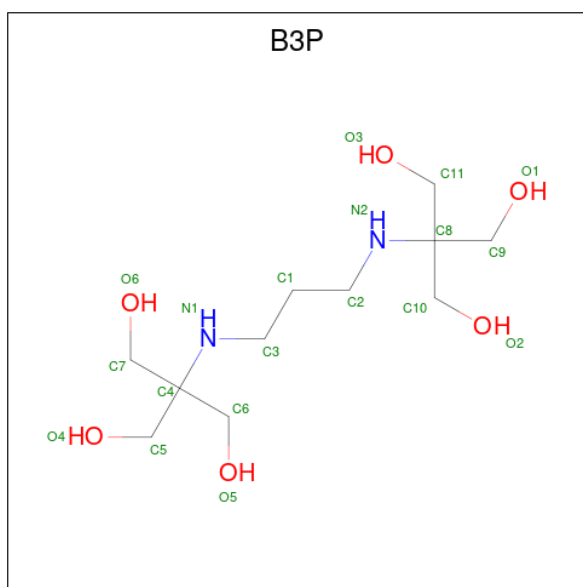
- Molecule 59 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	z	87	Total	C	N	O	S	0	0
			714	444	142	127	1		

- Molecule 60 is a protein called Probable metalloprotease ARX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	4	538	Total	C	N	O	S	0	0
			4166	2633	718	800	15		

- Molecule 61 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: C₁₁H₂₆N₂O₆).



Mol	Chain	Residues	Atoms				AltConf
61	1	1	Total	C	N	O	0
			19	11	2	6	
61	1	1	Total	C	N	O	0
			19	11	2	6	
61	1	1	Total	C	N	O	0
			19	11	2	6	

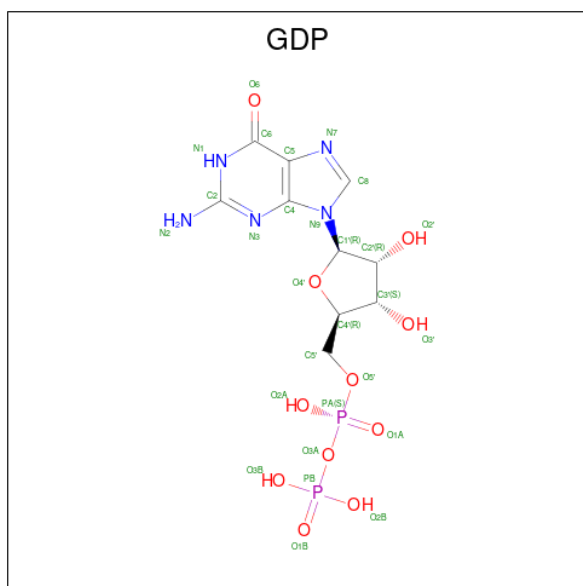
- Molecule 62 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
62	1	76	Total	Mg	0
			76	76	
62	2	1	Total	Mg	0
			1	1	
62	R	1	Total	Mg	0
			1	1	
62	V	1	Total	Mg	0
			1	1	
62	b	1	Total	Mg	0
			1	1	
62	m	1	Total	Mg	0
			1	1	

- Molecule 63 is ZINC ION (CCD ID: ZN) (formula: Zn).

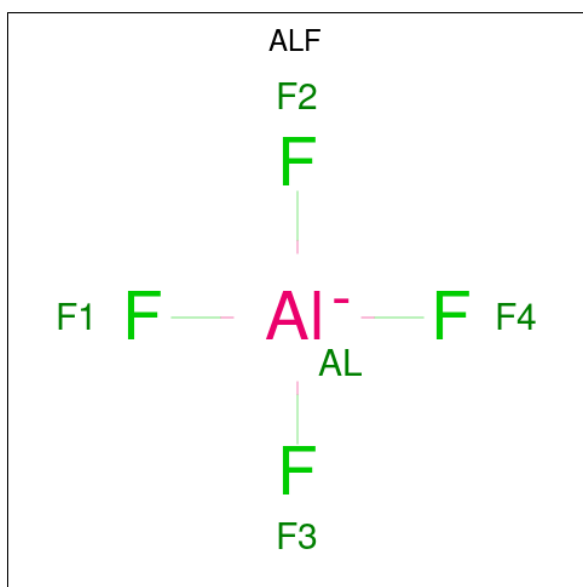
Mol	Chain	Residues	Atoms		AltConf
63	I	1	Total	Zn	0
			1	1	
63	g	1	Total	Zn	0
			1	1	
63	j	1	Total	Zn	0
			1	1	
63	p	1	Total	Zn	0
			1	1	
63	u	1	Total	Zn	0
			1	1	

- Molecule 64 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
64	b	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	m	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 65 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
65	m	1	Total	Al	F	0
			5	1	4	

- Molecule 66 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
66	m	1	Total	K	0
			1	1	

- Molecule 67 is water.

Mol	Chain	Residues	Atoms		AltConf
67	A	2	Total	O	0
			2	2	
67	1	340	Total	O	0
			340	340	
67	2	7	Total	O	0
			7	7	
67	B	2	Total	O	0
			2	2	
67	C	1	Total	O	0
			1	1	
67	F	3	Total	O	0
			3	3	
67	N	2	Total	O	0
			2	2	

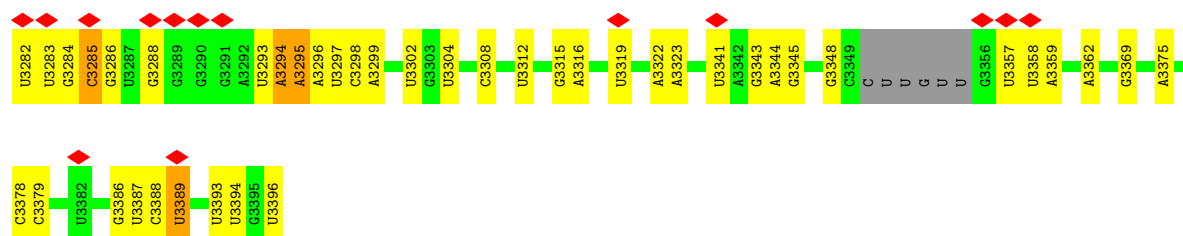
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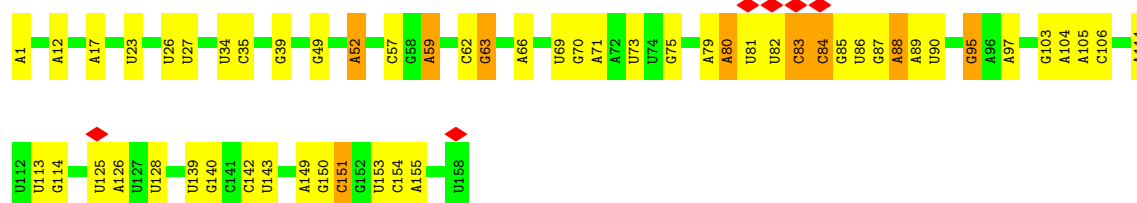
Mol	Chain	Residues	Atoms		AltConf
67	O	1	Total 1	O 1	0
67	R	1	Total 1	O 1	0
67	V	3	Total 3	O 3	0
67	X	1	Total 1	O 1	0
67	b	3	Total 3	O 3	0
67	d	1	Total 1	O 1	0
67	j	4	Total 4	O 4	0
67	m	3	Total 3	O 3	0



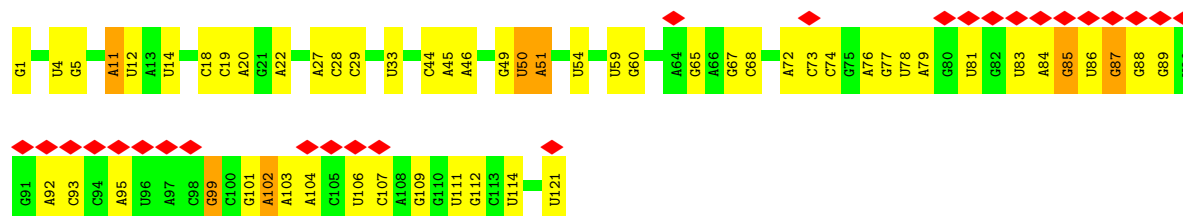




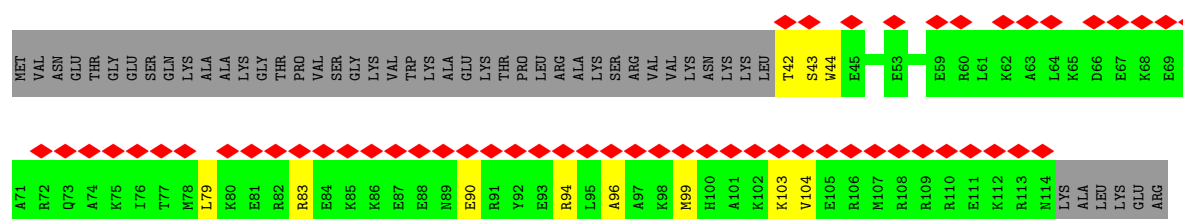
• Molecule 3: 5.8S rRNA



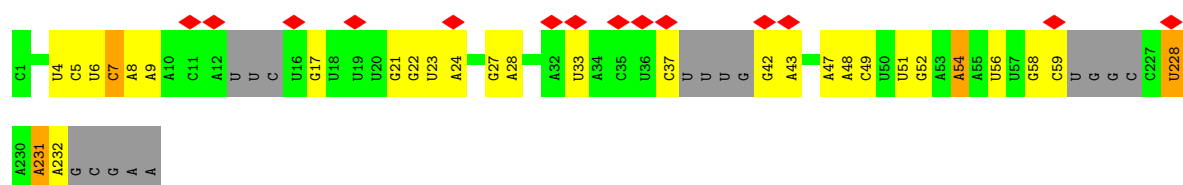
• Molecule 4: 5S rRNA



• Molecule 5: rRNA-processing protein

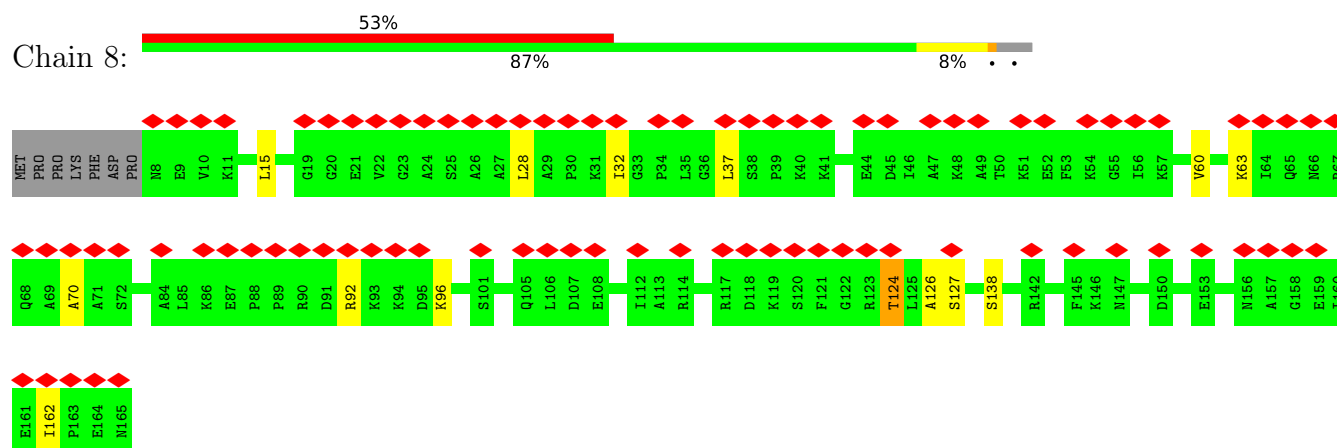


• Molecule 6: ITS2 rRNA



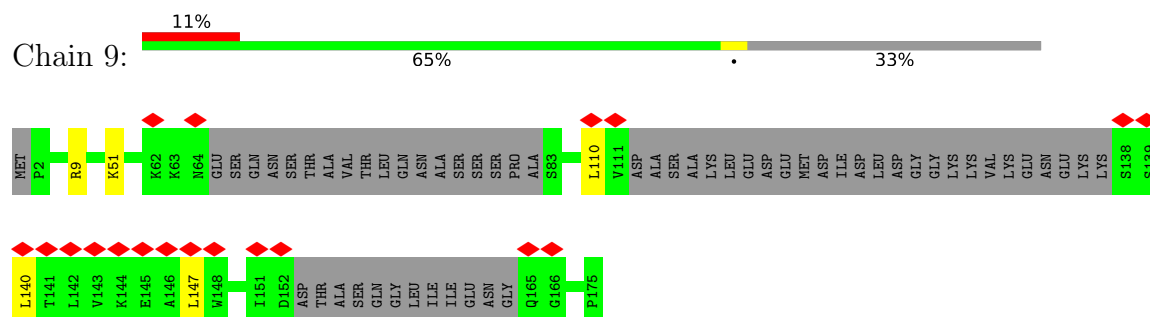
- Molecule 7: 60S ribosomal protein L12-A

Chain 8:



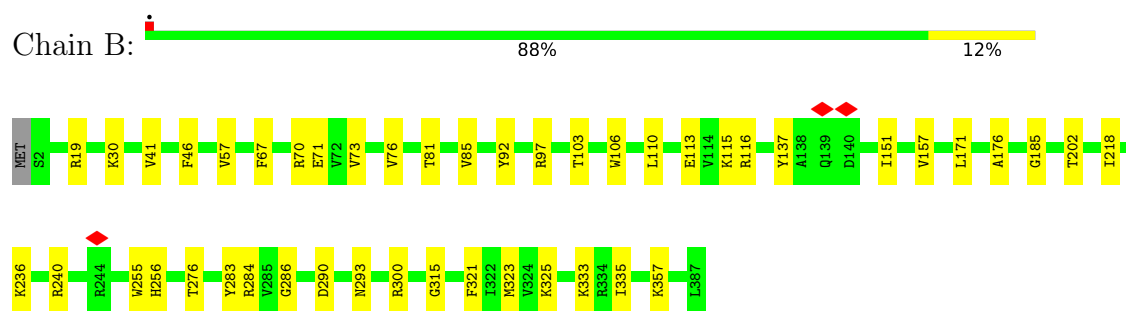
- Molecule 8: Ribosome biogenesis protein ALB1

Chain 9:



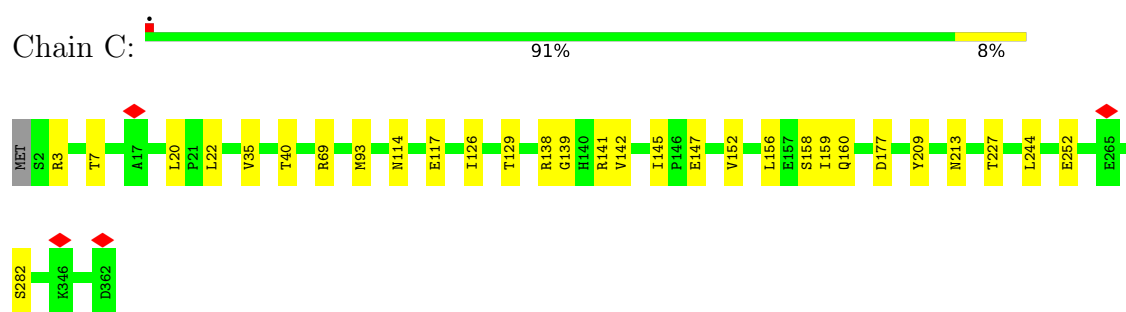
- Molecule 9: 60S ribosomal protein L3

Chain B:

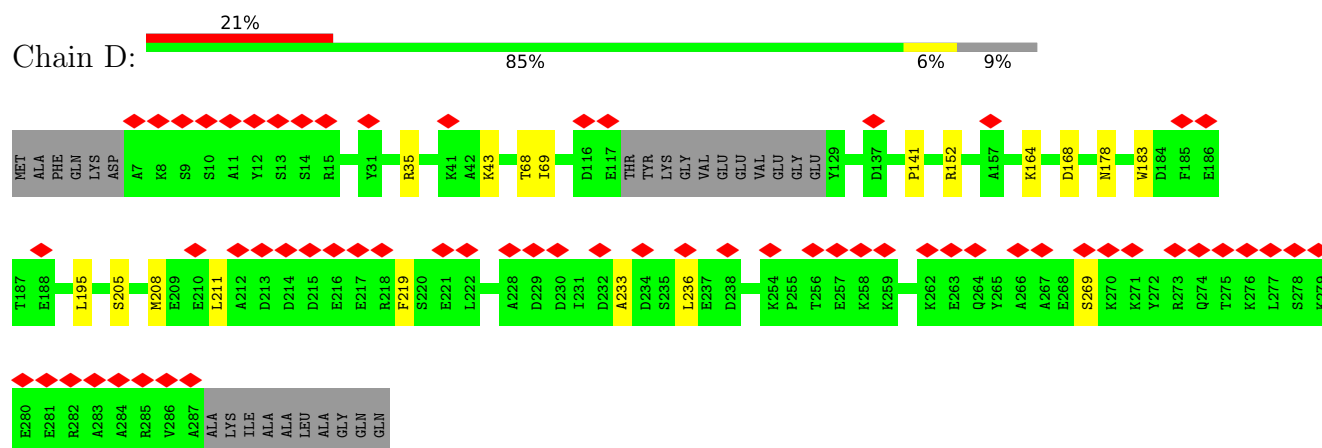


- Molecule 10: 60S ribosomal protein L4-A

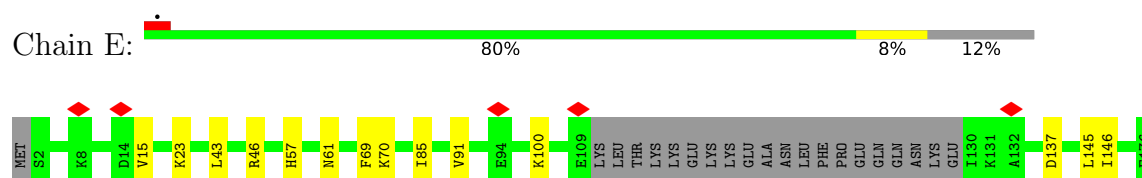
Chain C:



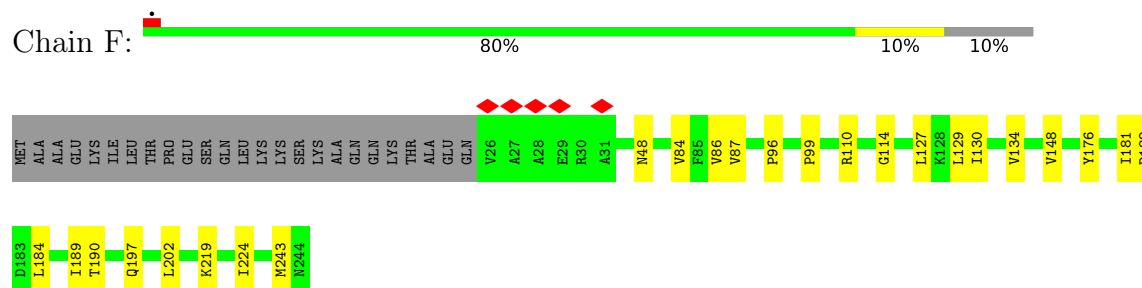
- Molecule 11: 60S ribosomal protein L5



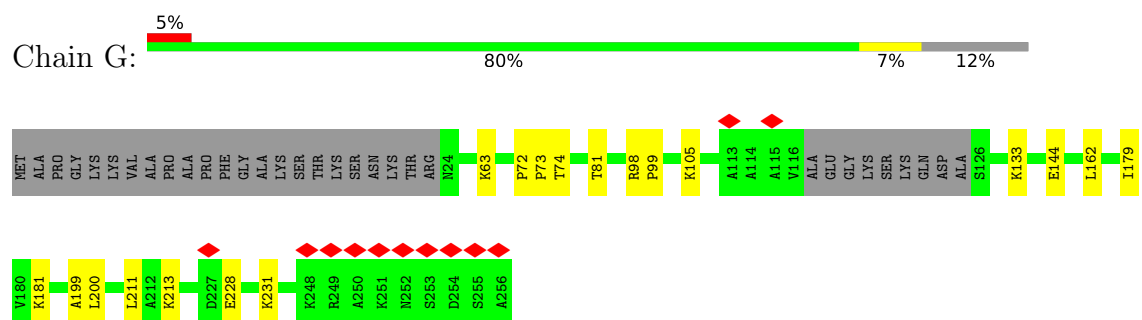
- Molecule 12: 60S ribosomal protein L6-A



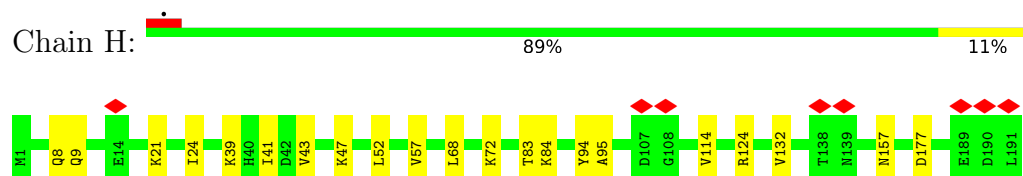
- Molecule 13: 60S ribosomal protein L7-A



- Molecule 14: 60S ribosomal protein L8-A

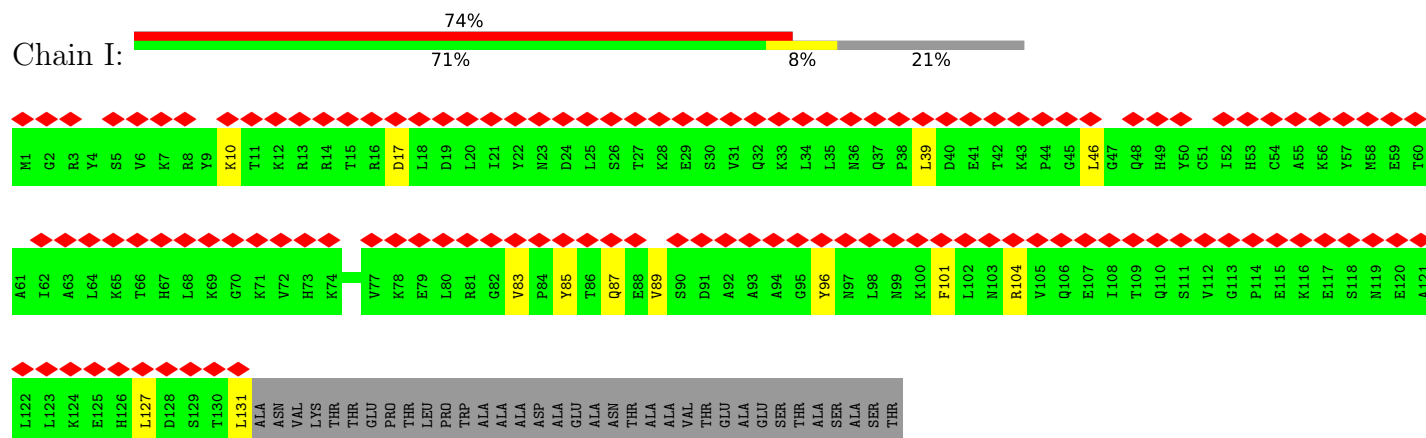


- Molecule 15: 60S ribosomal protein L9-A



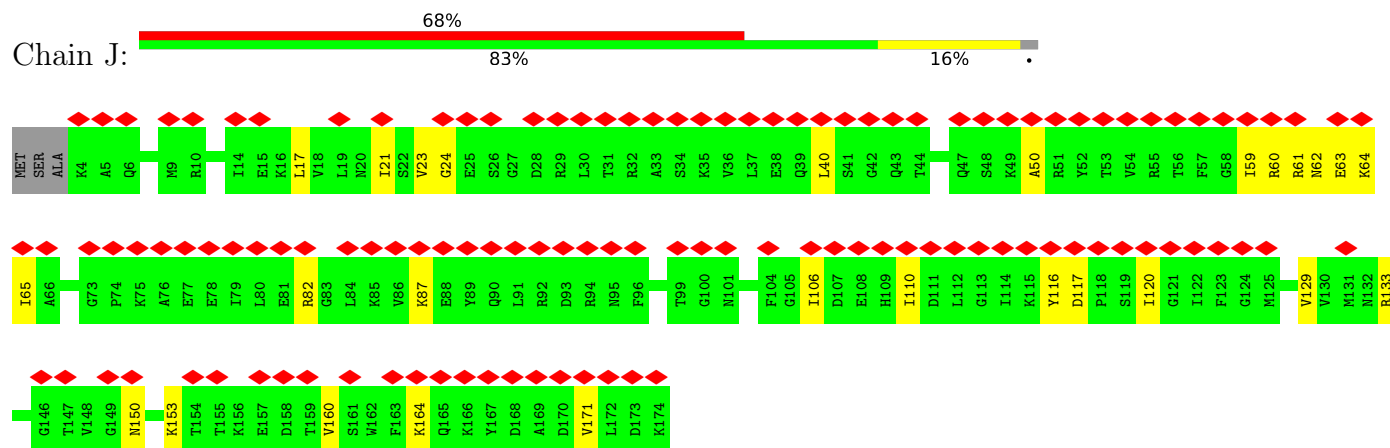
- Molecule 16: Bud site selection protein 20

Chain I:



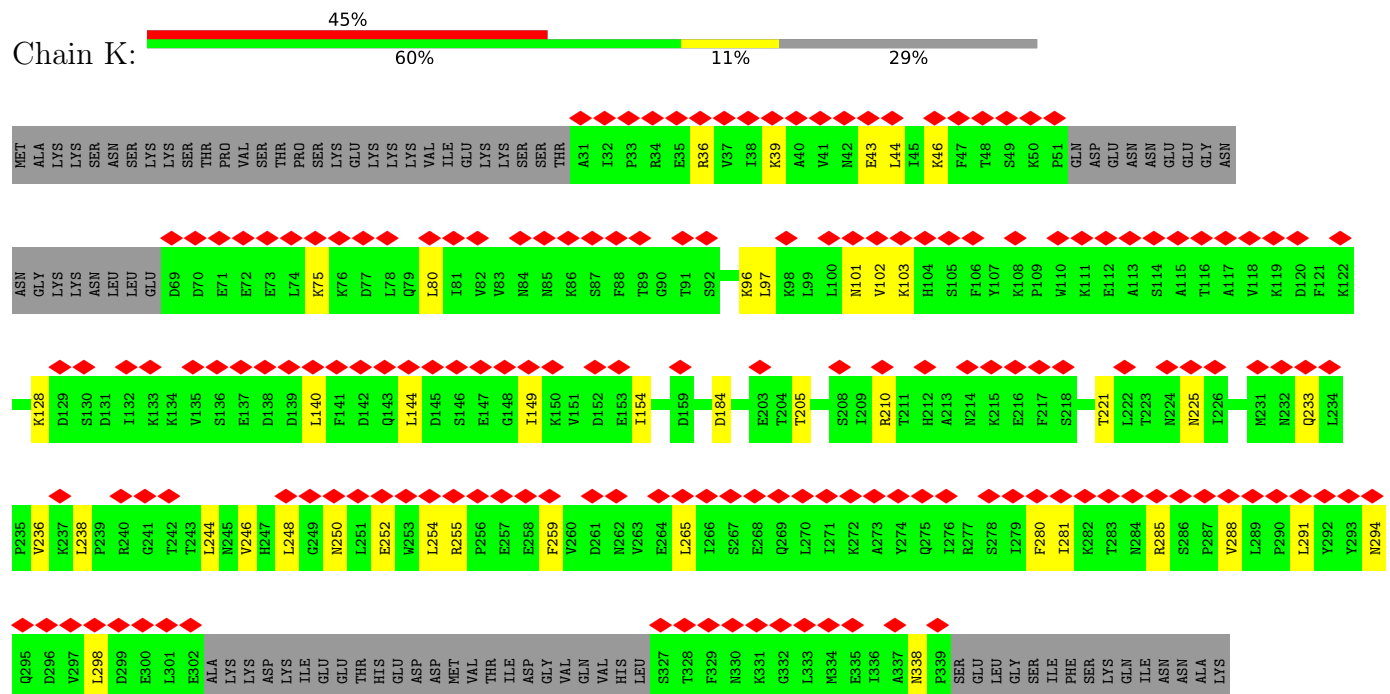
- Molecule 17: 60S ribosomal protein L11-A

Chain J:



- Molecule 18: Proteasome-interacting protein CIC1

Chain K:



LYS
ARG
SER
SER
GLU
LEU
GLU
LYS
GLU
SER
SER
SER
GLU
ALA
VAL
LYS
LYS
ALA
LYS
SER

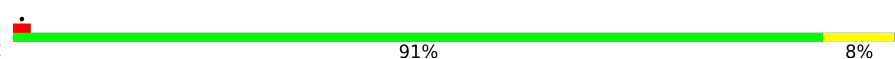
- Molecule 19: 60S ribosomal protein L13-A

Chain L: 

MET
ALA
ILE
SER
LYS
ASN
LEU
PRO
ILE
LYS
SER
ASN
HIS
PHE
R15
W18
Q19
E20
D27
K31
R36
I46
R73
A90
I95
Q106
N129
G130
K131
A132
P133
E134
T144
A151
T152
E164
G181
E184
K185
R186
A187
R188
E189
K190
A191

E192
A193
E194
ALA
GLU
LYS
LYS
LYS

- Molecule 20: 60S ribosomal protein L14-A

Chain M: 

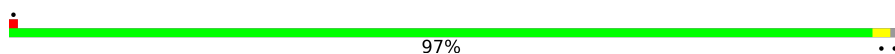
MET
S2
T3
D4
S5
I6
V7
K8
N11
K25
L32
G48
V53
Q62
W94
R106
K137
A138

- Molecule 21: 60S ribosomal protein L15-A

Chain N: 

MET
G2
A3
Y4
K5
Y6
L7
R12
V18
R65
R71
F76
LYS
GLY
ALA
THR
TYR
GLY
LYS
PRO
THR
ASN
GLN
GLY
VAL
ASN
E91
L116
N117
S126
Y129
V155
H158
A161
R162
T183
K184
A185
G186
R187
K204

- Molecule 22: 60S ribosomal protein L16-A

Chain O: 

MET
SER
Y3
K12
R49
L84
K171
Y199

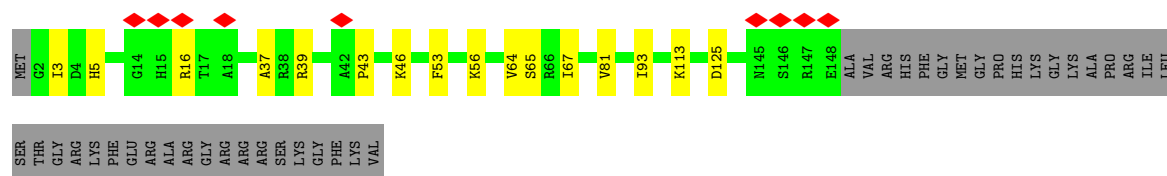
- Molecule 23: 60S ribosomal protein L17-A

Chain P: 

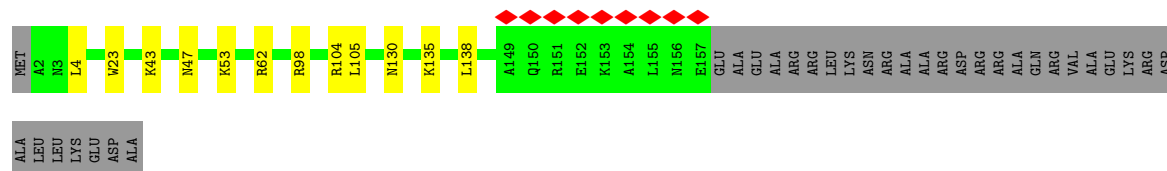
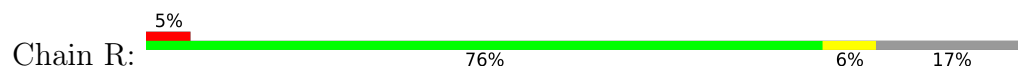
MET
A2
R3
L22
I36
E49
R56
I67
G68
R69
E75
Q92
L95
A98
L107
A122
P123
K124
Q125
R126
E140
S141
S142
P143
I146
E147
L148
E152
E155
ALA
VAL
ALA
LYS
LYS
ALA
ALA
GLU
LYS
K164
R167
A184

- Molecule 24: 60S ribosomal protein L18-A

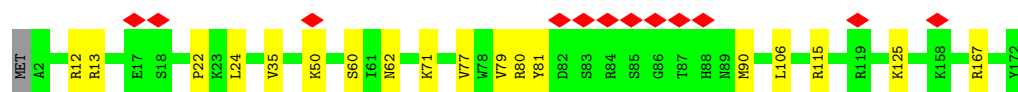
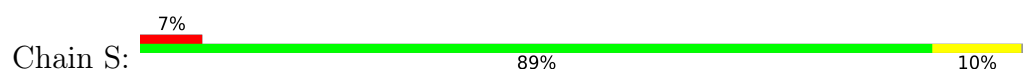
Chain Q: 



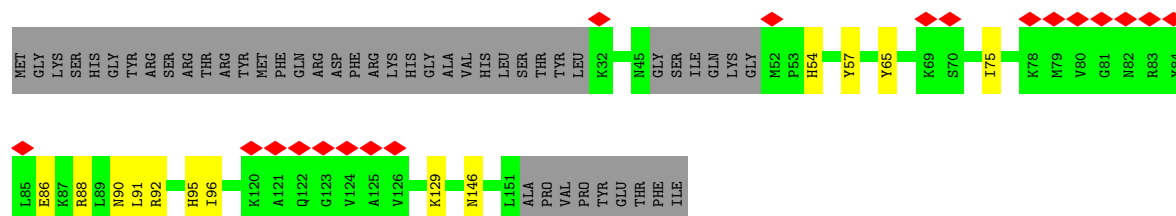
- Molecule 25: 60S ribosomal protein L19-A



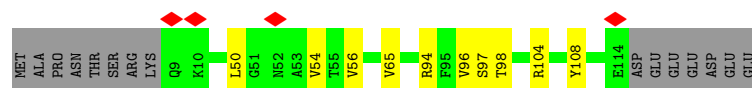
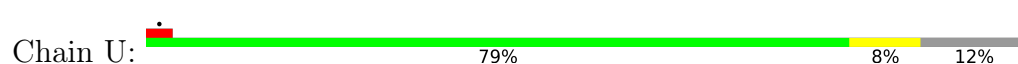
- Molecule 26: 60S ribosomal protein L20-A



- Molecule 27: 60S ribosomal protein L21-A



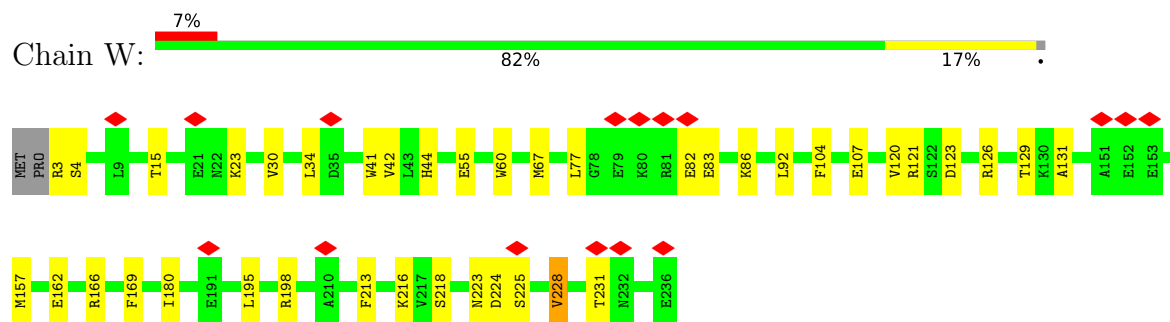
- Molecule 28: 60S ribosomal protein L22-A



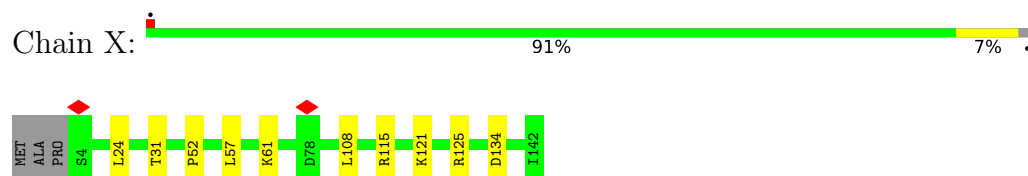
- Molecule 29: 60S ribosomal protein L23-A



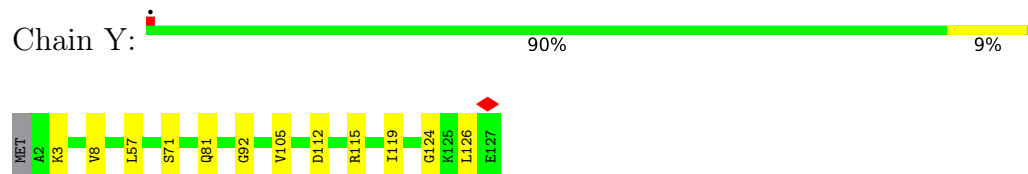
- Molecule 30: Ribosome assembly factor MRT4



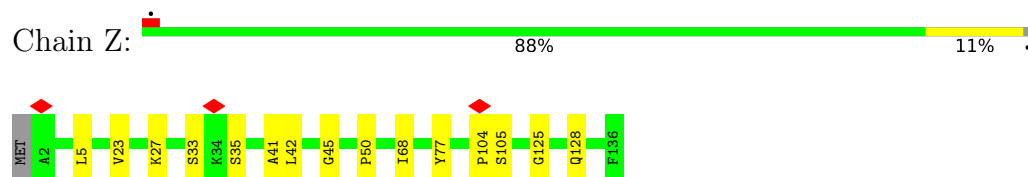
- Molecule 31: 60S ribosomal protein L25



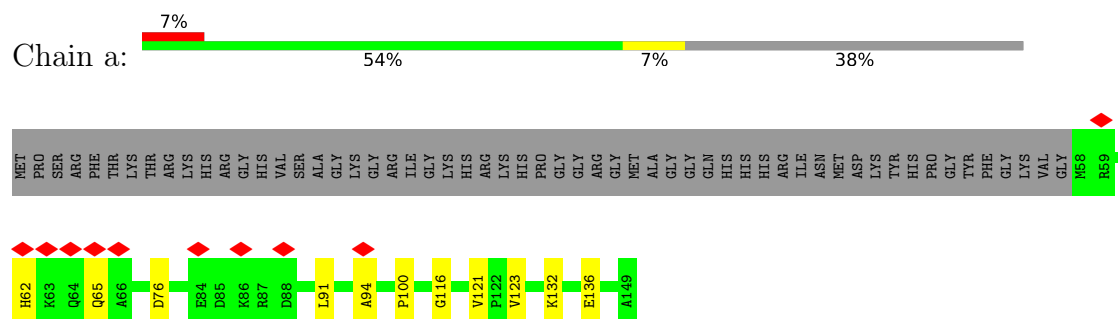
- Molecule 32: 60S ribosomal protein L26-A



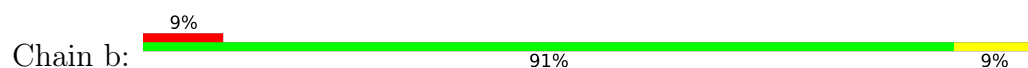
- Molecule 33: 60S ribosomal protein L27-A

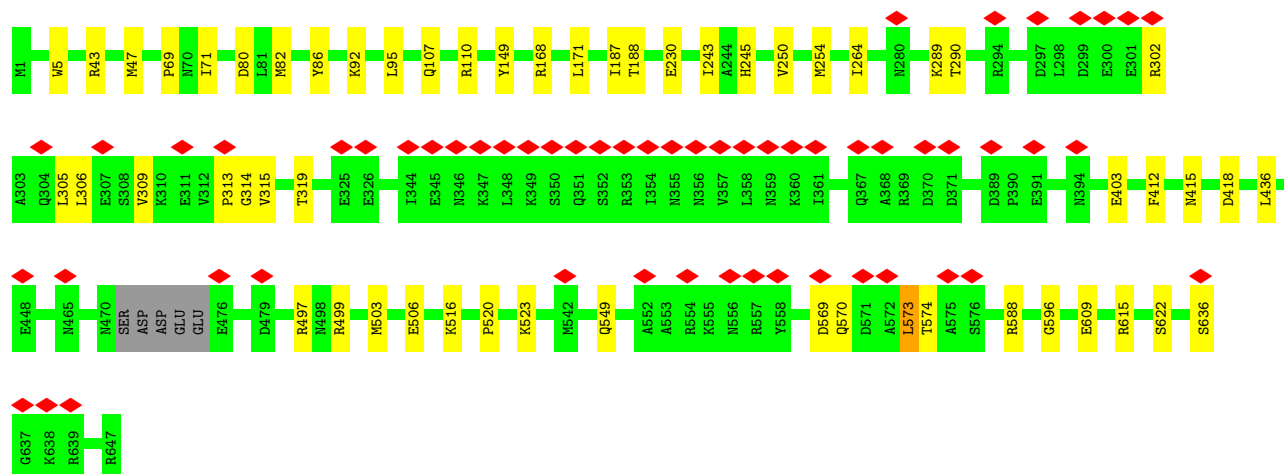


- Molecule 34: 60S ribosomal protein L28

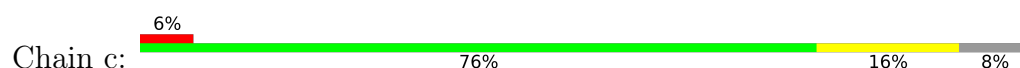


- Molecule 35: Nucleolar GTP-binding protein 1

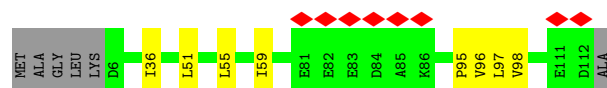
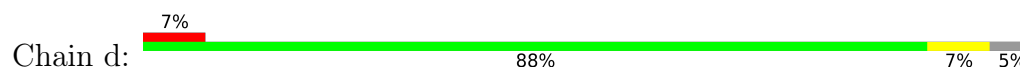




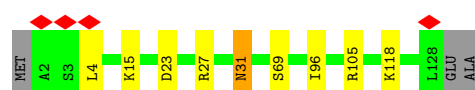
- Molecule 36: 60S ribosomal protein L30



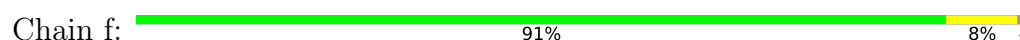
- Molecule 37: 60S ribosomal protein L31-A



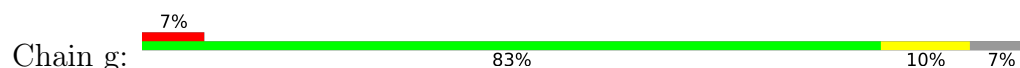
- Molecule 38: 60S ribosomal protein L32

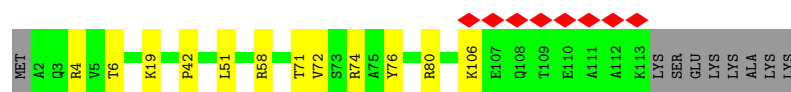


- Molecule 39: 60S ribosomal protein L33-A

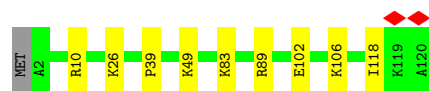
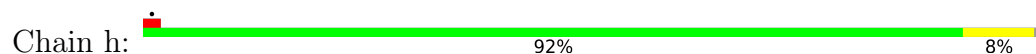


- Molecule 40: 60S ribosomal protein L34-A

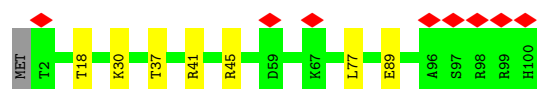




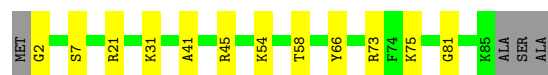
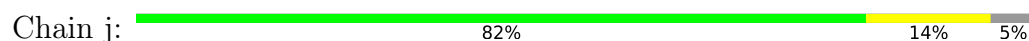
- Molecule 41: 60S ribosomal protein L35-A



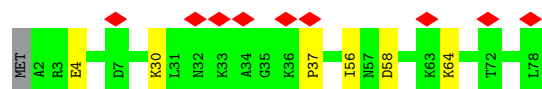
- Molecule 42: 60S ribosomal protein L36-A



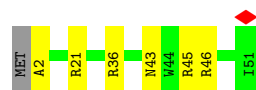
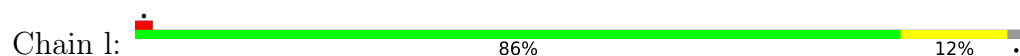
- Molecule 43: 60S ribosomal protein L37-A



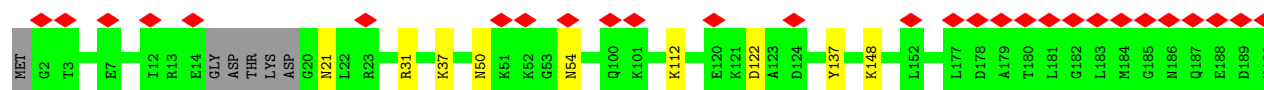
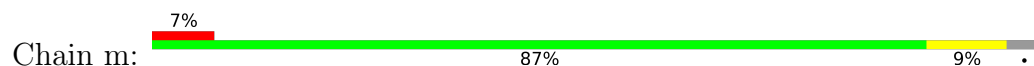
- Molecule 44: 60S ribosomal protein L38

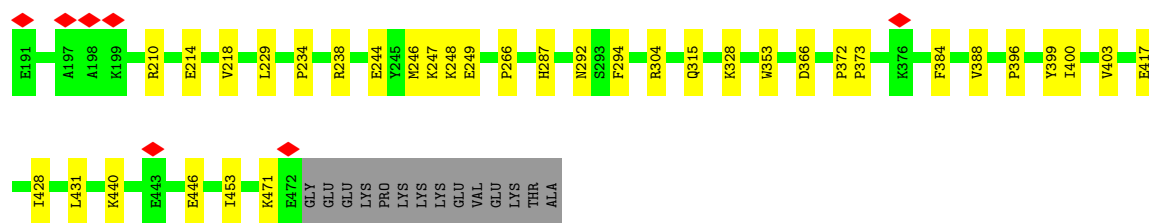


- Molecule 45: 60S ribosomal protein L39

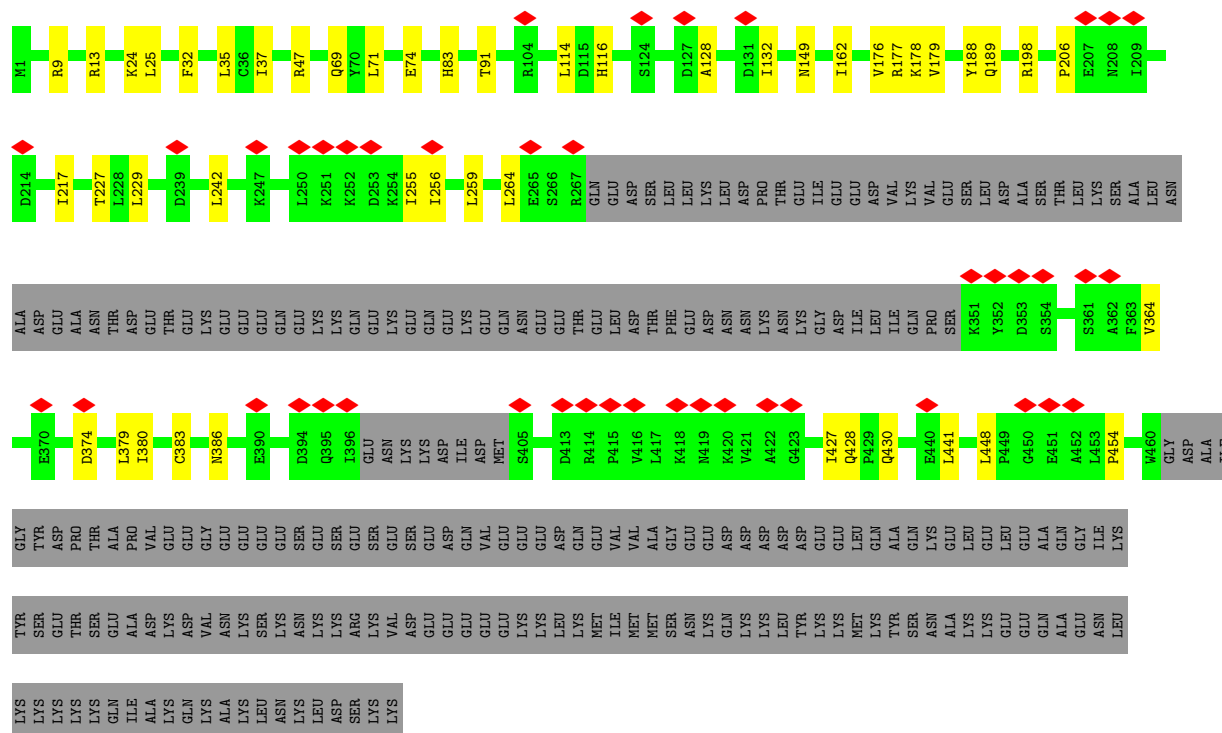


- Molecule 46: Nucleolar GTP-binding protein 2

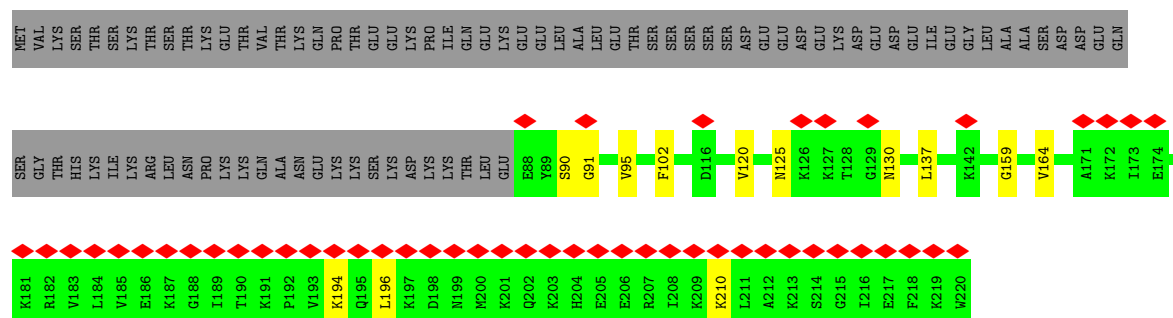




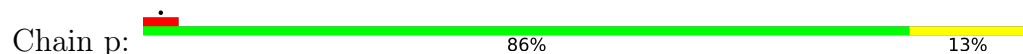
• Molecule 47: Pescadillo homolog



• Molecule 48: Ribosome biogenesis protein 15

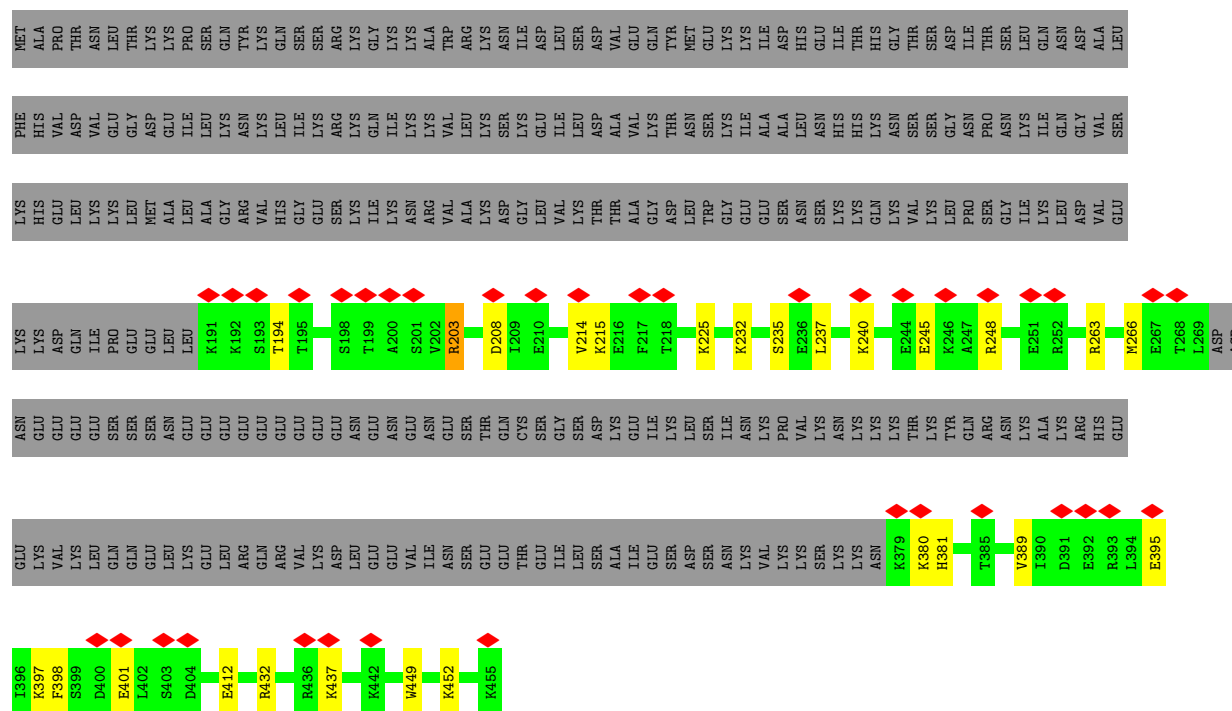


• Molecule 49: 60S ribosomal protein L43-A

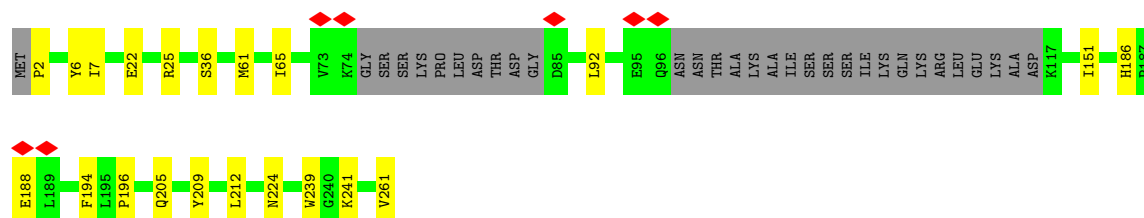
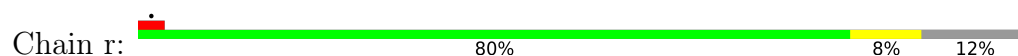




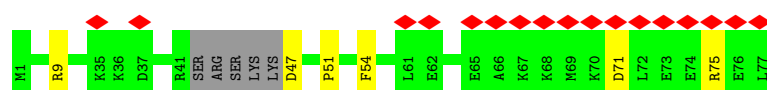
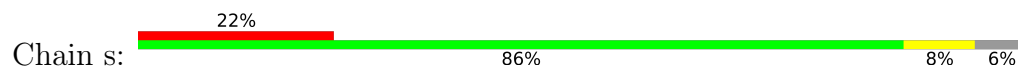
• Molecule 50: Ribosome biogenesis protein NOP53



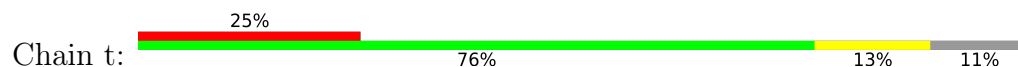
• Molecule 51: Ribosome biogenesis protein NSA2

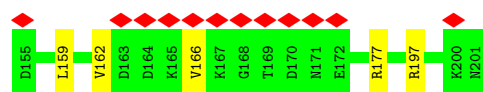


• Molecule 52: Nuclear GTP-binding protein NUG1

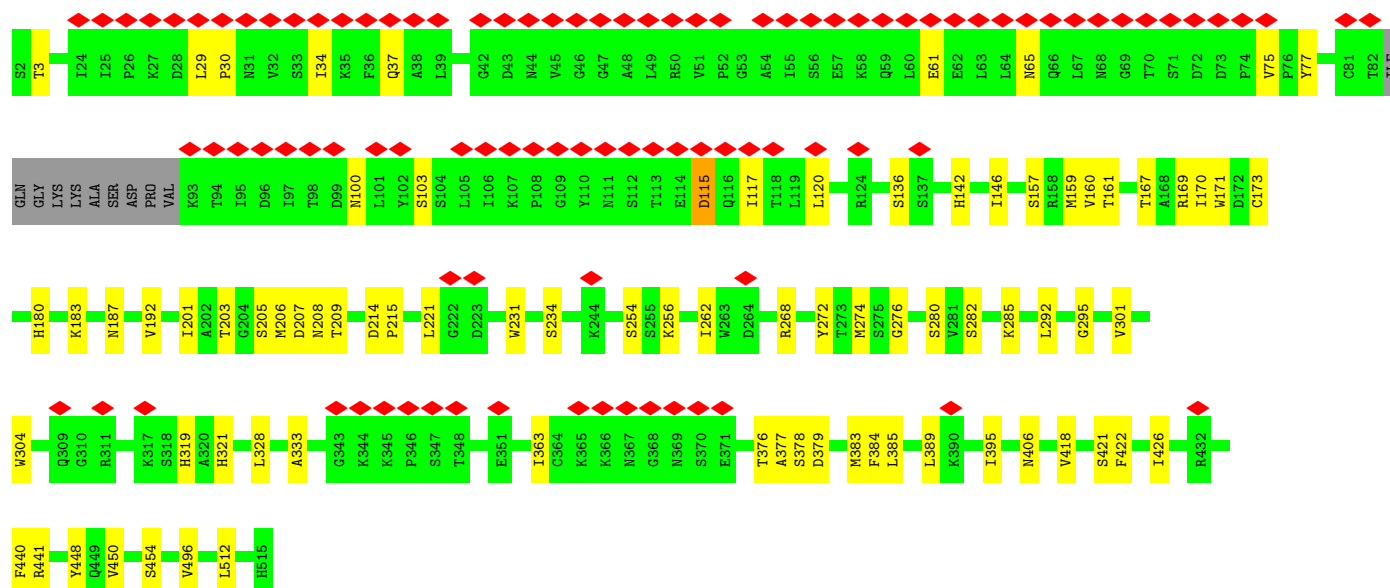
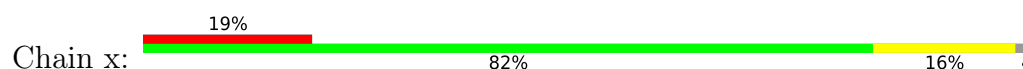


• Molecule 53: Ribosome biogenesis protein RLP7

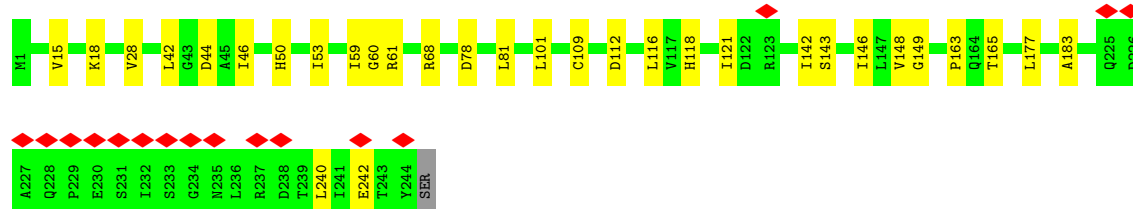
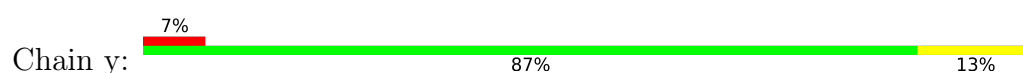




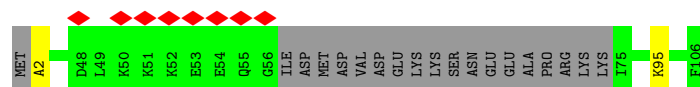
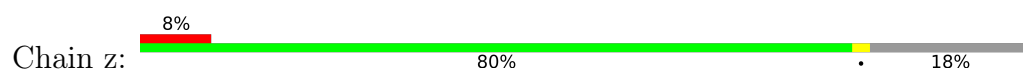
• Molecule 57: RSA4 isoform 1



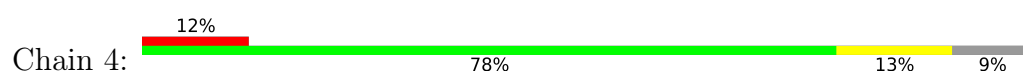
• Molecule 58: Eukaryotic translation initiation factor 6

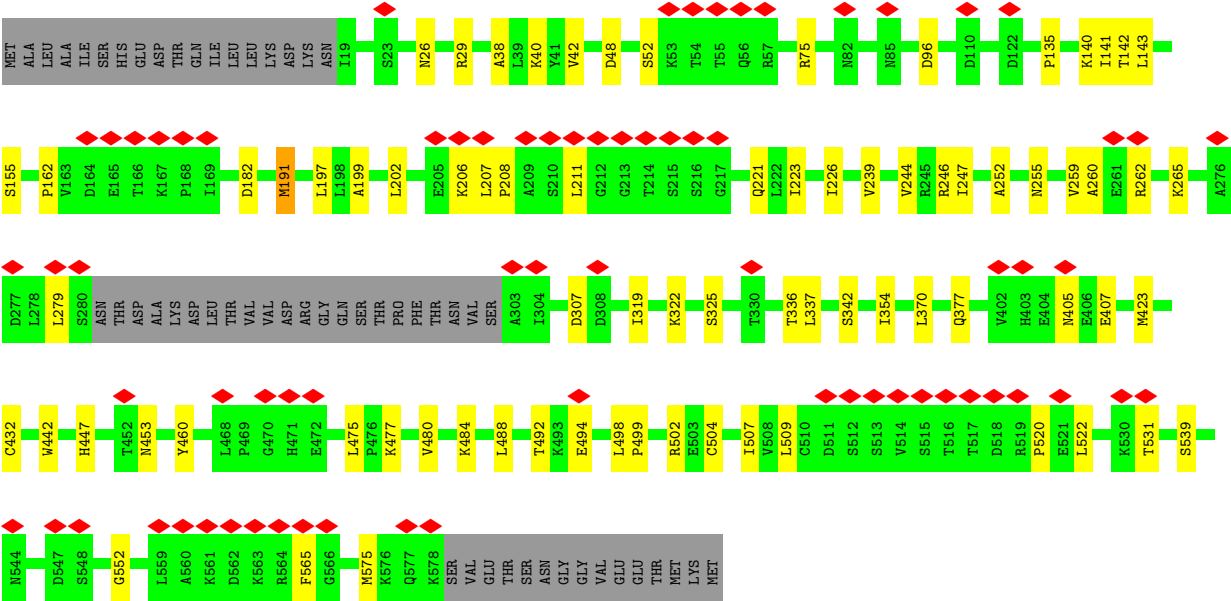


• Molecule 59: UPF0642 protein YBL028C



• Molecule 60: Probable metalloprotease ARX1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	414994	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.440	Depositor
Minimum map value	-0.221	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.032	Depositor
Map size ($\text{\AA}$)	427.19998, 427.19998, 427.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 1MA, K, 5MC, ZN, OMU, B3P, MG, OMG, OMC, A2M, ALF, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/1666	0.36	0/2241
2	1	0.16	0/70382	0.31	0/109722
3	2	0.15	0/3724	0.30	0/5798
4	3	0.10	0/2861	0.22	0/4457
5	5	0.13	0/649	0.24	0/848
6	6	0.13	0/1367	0.28	0/2118
7	8	0.12	0/1210	0.29	0/1627
8	9	0.11	0/948	0.24	0/1264
9	B	0.14	0/3152	0.35	0/4239
10	C	0.13	0/2801	0.32	0/3792
11	D	0.11	0/2227	0.27	0/3004
12	E	0.13	0/1251	0.33	0/1682
13	F	0.14	0/1798	0.33	0/2420
14	G	0.14	0/1784	0.32	0/2408
15	H	0.13	0/1539	0.34	0/2073
16	I	0.12	0/1075	0.29	0/1443
17	J	0.11	0/1389	0.31	0/1860
18	K	0.11	0/2190	0.29	0/2955
19	L	0.12	0/1460	0.31	0/1960
20	M	0.14	0/1074	0.32	0/1446
21	N	0.14	0/1654	0.33	0/2213
22	O	0.17	0/1585	0.33	0/2128
23	P	0.14	0/1410	0.37	0/1893
24	Q	0.12	0/1153	0.28	0/1555
25	R	0.13	0/1275	0.28	0/1702
26	S	0.12	0/1473	0.29	0/1980
27	T	0.12	0/916	0.27	0/1226
28	U	0.13	0/861	0.37	0/1167
29	V	0.14	0/1018	0.35	0/1369
30	W	0.11	0/1920	0.29	0/2586
31	X	0.13	0/1103	0.34	0/1484
32	Y	0.12	0/1004	0.33	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Z	0.12	0/1118	0.29	0/1497
34	a	0.11	0/747	0.25	0/1008
35	b	0.14	0/5270	0.32	0/7080
36	c	0.13	0/751	0.29	0/1008
37	d	0.13	0/887	0.32	0/1191
38	e	0.12	0/1041	0.31	0/1394
39	f	0.15	0/868	0.35	0/1168
40	g	0.14	0/891	0.33	0/1191
41	h	0.14	0/978	0.29	0/1301
42	i	0.12	0/778	0.29	0/1034
43	j	0.15	0/680	0.35	0/901
44	k	0.12	0/618	0.29	0/826
45	l	0.14	0/443	0.33	0/588
46	m	0.13	0/3828	0.31	0/5154
47	n	0.13	0/3085	0.31	0/4166
48	o	0.11	0/1129	0.30	0/1502
49	p	0.15	0/701	0.35	0/934
50	q	0.14	0/1321	0.35	0/1766
51	r	0.13	0/1892	0.31	0/2528
52	s	0.13	0/608	0.26	0/798
53	t	0.13	0/2333	0.30	0/3128
54	u	0.14	0/1287	0.32	0/1711
55	v	0.12	0/2410	0.31	0/3220
56	w	0.12	0/1565	0.28	0/2108
57	x	0.12	0/4022	0.35	0/5460
58	y	0.13	0/1872	0.34	0/2548
59	z	0.13	0/721	0.26	0/948
60	4	0.12	0/4242	0.29	0/5758
All	All	0.14	0/166005	0.31	0/239917

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

Mol	Chain	#Chirality outliers	#Planarity outliers
54	u	0	1
56	w	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	u	75	ARG	Sidechain
56	w	46	ARG	Sidechain

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	A	1634	0	1685	13	0
2	1	64042	0	32235	452	0
3	2	3353	0	1695	27	0
4	3	2579	0	1304	23	0
5	5	645	0	688	6	0
6	6	1227	0	622	18	0
7	8	1196	0	1257	11	0
8	9	937	0	1008	5	0
9	B	3081	0	3165	28	0
10	C	2749	0	2863	33	0
11	D	2180	0	2134	16	0
12	E	1230	0	1320	13	0
13	F	1761	0	1843	15	0
14	G	1753	0	1845	20	0
15	H	1518	0	1587	13	0
16	I	1059	0	1089	11	0
17	J	1368	0	1401	21	0
18	K	2155	0	2230	38	0
19	L	1438	0	1493	9	0
20	M	1059	0	1154	10	0
21	N	1620	0	1679	16	0
22	O	1555	0	1659	3	0
23	P	1388	0	1423	22	0
24	Q	1136	0	1214	21	0
25	R	1258	0	1342	9	0
26	S	1437	0	1475	14	0
27	T	905	0	957	19	0
28	U	844	0	855	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	V	1003	0	1048	4	0
30	W	1888	0	1917	23	0
31	X	1088	0	1175	6	0
32	Y	993	0	1081	8	0
33	Z	1092	0	1155	8	0
34	a	731	0	773	7	0
35	b	5185	0	5250	39	0
36	c	743	0	797	10	0
37	d	873	0	914	5	0
38	e	1020	0	1090	11	0
39	f	850	0	880	6	0
40	g	881	0	945	11	0
41	h	969	0	1078	7	0
42	i	771	0	849	5	0
43	j	665	0	668	8	0
44	k	612	0	682	4	0
45	l	436	0	475	7	0
46	m	3754	0	3823	32	0
47	n	3014	0	3094	35	0
48	o	1107	0	1159	9	0
49	p	694	0	734	8	0
50	q	1298	0	1343	24	0
51	r	1860	0	1965	17	0
52	s	602	0	661	4	0
53	t	2306	0	2454	36	0
54	u	1265	0	1314	14	0
55	v	2366	0	2452	43	0
56	w	1541	0	1597	21	0
57	x	3927	0	3893	49	0
58	y	1849	0	1836	19	0
59	z	714	0	760	2	0
60	4	4166	0	4248	50	0
61	1	57	0	78	5	0
62	1	76	0	0	0	0
62	2	1	0	0	0	0
62	R	1	0	0	0	0
62	V	1	0	0	0	0
62	b	1	0	0	0	0
62	m	1	0	0	0	0
63	I	1	0	0	0	0
63	g	1	0	0	0	0
63	j	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	p	1	0	0	0	0
63	u	1	0	0	0	0
64	b	28	0	12	1	0
64	m	28	0	12	0	0
65	m	5	0	0	1	0
66	m	1	0	0	0	0
67	1	340	0	0	2	0
67	2	7	0	0	0	0
67	A	2	0	0	0	0
67	B	2	0	0	0	0
67	C	1	0	0	0	0
67	F	3	0	0	0	0
67	N	2	0	0	0	0
67	O	1	0	0	0	0
67	R	1	0	0	0	0
67	V	3	0	0	0	0
67	X	1	0	0	0	0
67	b	3	0	0	0	0
67	d	1	0	0	0	0
67	j	4	0	0	0	0
67	m	3	0	0	0	0
All	All	157949	0	125434	1196	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 4.

All (1196) 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)
10:C:142:VAL:CB	10:C:145:ILE:HD12	1.46	1.41
24:Q:3:ILE:HD11	24:Q:5:HIS:CE1	1.69	1.28
10:C:142:VAL:CB	10:C:145:ILE:CD1	2.23	1.16
55:v:132:THR:HG22	55:v:226:ILE:HG21	1.21	1.13
55:v:132:THR:HG22	55:v:226:ILE:CG2	1.82	1.08
10:C:142:VAL:CA	10:C:145:ILE:HD12	1.85	1.06
10:C:142:VAL:HG12	10:C:145:ILE:CD1	1.85	1.06
10:C:142:VAL:HA	10:C:145:ILE:CD1	1.88	1.02
23:P:107:LEU:HB3	23:P:152:GLU:OE2	1.61	1.00
10:C:142:VAL:HB	10:C:145:ILE:HD12	1.01	1.00
55:v:132:THR:CG2	55:v:226:ILE:HG21	1.91	0.99
10:C:142:VAL:CG1	10:C:145:ILE:CD1	2.40	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:3:ILE:CD1	24:Q:5:HIS:CE1	2.45	0.98
10:C:142:VAL:HG12	10:C:145:ILE:HD11	1.43	0.98
15:H:94:TYR:HA	15:H:177:ASP:OD1	1.63	0.98
10:C:142:VAL:CA	10:C:145:ILE:CD1	2.42	0.95
28:U:98:THR:HG22	28:U:104:ARG:HH11	1.27	0.95
18:K:254:LEU:O	18:K:259:PHE:HE2	1.49	0.94
10:C:142:VAL:HB	10:C:145:ILE:CD1	1.89	0.94
27:T:91:LEU:CD2	56:w:159:LEU:HD13	1.97	0.94
51:r:92:LEU:HD13	57:x:231:TRP:CZ2	2.03	0.92
12:E:15:VAL:CG2	38:e:4:LEU:HD11	1.99	0.92
23:P:107:LEU:HD22	23:P:152:GLU:OE2	1.69	0.92
24:Q:3:ILE:HD11	24:Q:5:HIS:HE1	1.31	0.90
2:1:2203:U:H3	2:1:2239:G:H1	1.12	0.90
17:J:21:ILE:HG22	17:J:23:VAL:HG23	1.53	0.90
23:P:107:LEU:CB	23:P:152:GLU:OE2	2.20	0.90
50:q:225:LYS:HE2	50:q:395:GLU:OE2	1.72	0.90
10:C:142:VAL:HA	10:C:145:ILE:HD11	1.56	0.87
55:v:132:THR:CG2	55:v:226:ILE:CG2	2.53	0.84
2:1:173:G:H1	2:1:245:U:H3	0.84	0.84
27:T:91:LEU:HD21	56:w:159:LEU:HD13	1.59	0.83
60:4:492:THR:HG22	60:4:494:GLU:H	1.43	0.83
20:M:11:ASN:O	20:M:11:ASN:OD1	1.97	0.83
2:1:1132:C:H2'	2:1:1133:A2M:H8	1.61	0.82
2:1:2442:G:H1	2:1:2505:U:H3	1.23	0.82
28:U:98:THR:HG22	28:U:104:ARG:NH1	1.94	0.81
47:n:427:ILE:HG22	47:n:428:GLN:N	1.93	0.81
55:v:187:GLN:NE2	56:w:46:ARG:HH22	1.80	0.80
12:E:15:VAL:HG22	38:e:4:LEU:HD11	1.62	0.79
51:r:92:LEU:HD13	57:x:231:TRP:HZ2	1.46	0.79
23:P:107:LEU:CD2	23:P:152:GLU:OE2	2.30	0.79
53:t:312:VAL:HG12	53:t:313:ASP:N	1.96	0.77
60:4:447:HIS:CD2	60:4:492:THR:OG1	2.38	0.76
29:V:96:GLU:OE2	54:u:24:ASN:HB2	1.85	0.76
30:W:44:HIS:HB2	30:W:216:LYS:HB2	1.68	0.76
35:b:609:GLU:HG3	45:l:36:ARG:HB3	1.68	0.76
10:C:209:TYR:HE1	10:C:227:THR:HG22	1.50	0.75
18:K:254:LEU:O	18:K:259:PHE:CE2	2.39	0.75
12:E:15:VAL:CG2	38:e:4:LEU:CD1	2.65	0.74
16:I:17:ASP:OD2	54:u:23:ARG:HD2	1.87	0.74
53:t:312:VAL:HG12	53:t:313:ASP:H	1.50	0.74
16:I:96:TYR:OH	54:u:2:ARG:NH2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:970:A:H61	2:1:1111:U:H3	1.34	0.73
47:n:427:ILE:CG2	47:n:428:GLN:H	2.00	0.73
23:P:107:LEU:HD22	23:P:152:GLU:CD	2.13	0.73
47:n:427:ILE:CG2	47:n:428:GLN:N	2.51	0.73
7:8:15:LEU:HD23	7:8:28:LEU:HD11	1.71	0.73
2:1:3268:A:OP1	12:E:46:ARG:NH2	2.23	0.72
28:U:98:THR:CG2	28:U:104:ARG:HH11	2.01	0.72
6:6:229:U:H5	53:t:278:SER:HG	1.38	0.72
56:w:8:ASN:O	56:w:8:ASN:OD1	2.07	0.72
50:q:214:VAL:HG12	50:q:215:LYS:H	1.56	0.70
51:r:92:LEU:CD1	57:x:231:TRP:CZ2	2.74	0.70
2:1:2919:A:H61	2:1:2927:C:H42	1.37	0.70
32:Y:112:ASP:OD1	32:Y:115:ARG:HB2	1.91	0.70
29:V:87:ARG:HH22	29:V:137:VAL:HG21	1.55	0.69
2:1:2830:G:H2'	2:1:2831:G:C8	2.28	0.69
7:8:15:LEU:CD2	7:8:28:LEU:HD11	2.21	0.69
60:4:155:SER:HB3	60:4:504:CYS:HB3	1.74	0.69
2:1:799:G:O2'	19:L:18:TRP:NE1	2.25	0.69
2:1:1481:A:N3	2:1:1858:A:O2'	2.26	0.69
21:N:116:LEU:O	21:N:117:ASN:OD1	2.11	0.69
55:v:205:LYS:HB2	55:v:226:ILE:HD11	1.74	0.69
58:y:68:ARG:NH2	58:y:112:ASP:O	2.25	0.69
2:1:2875:U:H3	2:1:2952:G:HO2'	1.39	0.69
26:S:79:VAL:HG11	26:S:106:LEU:HD21	1.75	0.68
2:1:2248:C:H2'	46:m:304:ARG:HH21	1.59	0.68
53:t:312:VAL:CG1	53:t:313:ASP:H	2.07	0.68
20:M:25:LYS:HE2	20:M:62:GLN:HA	1.76	0.68
32:Y:3:LYS:HD2	32:Y:8:VAL:HG23	1.74	0.68
2:1:86:G:N2	2:1:99:A:OP2	2.26	0.67
2:1:838:G:O6	49:p:4:ARG:NH2	2.28	0.67
55:v:132:THR:HG22	55:v:226:ILE:HG23	1.76	0.67
27:T:92:ARG:HB2	27:T:95:HIS:HD2	1.60	0.67
2:1:2940:A:H2'	9:B:255:TRP:HB3	1.77	0.67
2:1:2966:G:O6	46:m:31:ARG:NH2	2.28	0.67
27:T:91:LEU:HD23	56:w:159:LEU:HD13	1.76	0.67
13:F:110:ARG:HB3	24:Q:3:ILE:HG22	1.77	0.66
35:b:573:LEU:HD11	60:4:259:VAL:HA	1.78	0.66
22:O:12:LYS:O	26:S:167:ARG:NH2	2.25	0.66
2:1:1570:U:H1'	53:t:279:GLY:HA2	1.78	0.65
55:v:187:GLN:NE2	56:w:46:ARG:NH2	2.43	0.65
51:r:92:LEU:CD1	57:x:231:TRP:HZ2	2.08	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:2771:U:H2'	2:1:2772:C:H2'	1.78	0.65
15:H:83:THR:HG23	15:H:84:LYS:HG3	1.79	0.65
60:4:319:ILE:O	60:4:504:CYS:HA	1.97	0.65
2:1:925:A:N6	2:1:2415:C:OP1	2.30	0.64
17:J:21:ILE:CG2	17:J:23:VAL:HG23	2.25	0.64
48:o:95:VAL:HG12	48:o:164:VAL:HG22	1.78	0.64
2:1:2764:C:N3	2:1:2794:G:C2	2.66	0.64
10:C:209:TYR:CE1	10:C:227:THR:HG22	2.31	0.64
18:K:255:ARG:O	18:K:259:PHE:CD2	2.49	0.64
2:1:3045:G:OP1	9:B:19:ARG:NH2	2.30	0.64
6:6:229:U:H5	53:t:278:SER:OG	1.80	0.64
2:1:687:U:OP2	19:L:36:ARG:NH2	2.30	0.64
6:6:229:U:C5	53:t:278:SER:OG	2.50	0.63
23:P:125:GLN:HB3	23:P:141:SER:HB2	1.80	0.63
53:t:312:VAL:CG1	53:t:313:ASP:N	2.61	0.63
10:C:20:LEU:HD11	10:C:252:GLU:HG3	1.79	0.63
55:v:220:ARG:NH1	56:w:10:PRO:O	2.32	0.63
60:4:492:THR:HG22	60:4:494:GLU:N	2.14	0.63
2:1:1437:OMC:HM22	10:C:93:MET:HG3	1.80	0.63
2:1:1661:G:H2'	2:1:1662:G:C8	2.34	0.63
50:q:395:GLU:O	50:q:395:GLU:HG2	1.99	0.63
3:2:66:A:OP1	41:h:10:ARG:NH2	2.32	0.62
10:C:142:VAL:CG1	10:C:145:ILE:HD11	2.14	0.62
50:q:214:VAL:HG12	50:q:215:LYS:N	2.13	0.62
28:U:96:VAL:HG12	28:U:97:SER:N	2.15	0.62
55:v:162:LEU:O	55:v:166:ARG:HB2	2.00	0.62
55:v:73:SER:OG	55:v:74:PRO:HD3	2.00	0.62
2:1:728:G:H5'	24:Q:43:PRO:HB2	1.80	0.62
47:n:9:ARG:HG2	47:n:13:ARG:HH21	1.65	0.62
60:4:423:MET:HE1	60:4:432:CYS:HB2	1.81	0.61
12:E:15:VAL:HG23	38:e:4:LEU:HD11	1.80	0.61
12:E:15:VAL:HG22	38:e:4:LEU:CD1	2.27	0.61
2:1:68:C:OP2	2:1:301:G:N2	2.33	0.61
1:A:21:ARG:HD3	2:1:824:C:H5''	1.82	0.61
1:A:135:ILE:HD12	1:A:149:ARG:HE	1.65	0.61
16:I:83:VAL:O	54:u:47:ARG:NH2	2.33	0.61
35:b:171:LEU:HD22	35:b:250:VAL:HG13	1.80	0.61
4:3:89:G:N2	4:3:92:A:OP1	2.34	0.61
34:a:100:PRO:HG2	34:a:123:VAL:HG12	1.81	0.61
30:W:86:LYS:NZ	30:W:223:ASN:OD1	2.31	0.61
55:v:147:ALA:HB3	55:v:186:ILE:HD13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:n:428:GLN:NE2	47:n:448:LEU:O	2.34	0.61
34:a:76:ASP:HB3	34:a:116:GLY:HA3	1.81	0.60
60:4:221:GLN:NE2	60:4:307:ASP:O	2.33	0.60
18:K:144:LEU:HB3	18:K:149:ILE:HB	1.82	0.60
35:b:187:ILE:HG13	35:b:188:THR:HG23	1.83	0.60
2:1:2717:U:OP2	2:1:2753:G:O2'	2.19	0.60
15:H:57:VAL:HG23	15:H:68:LEU:HD13	1.84	0.60
60:4:75:ARG:NH2	60:4:575:MET:SD	2.72	0.60
6:6:228:U:O2	53:t:148:ARG:NH2	2.35	0.60
2:1:2514:U:OP2	2:1:2586:G:N2	2.31	0.60
6:6:7:C:H5	6:6:21:G:H1	1.46	0.60
18:K:103:LYS:HG2	18:K:265:LEU:HD22	1.84	0.60
32:Y:57:LEU:O	32:Y:105:VAL:HG12	2.02	0.60
47:n:255:ILE:HG22	47:n:256:ILE:HG12	1.84	0.59
47:n:427:ILE:HG22	47:n:428:GLN:H	1.60	0.59
2:1:1448:U:H2'	2:1:1449:A2M:H8	1.84	0.59
2:1:2898:G:N2	51:r:7:ILE:H	2.00	0.59
57:x:34:ILE:HG22	57:x:117:ILE:HB	1.84	0.59
6:6:51:U:O2'	6:6:54:A:N7	2.34	0.59
3:2:128:U:O4	47:n:47:ARG:NH2	2.35	0.59
57:x:61:GLU:O	57:x:65:ASN:ND2	2.36	0.59
2:1:3348:G:H1	2:1:3357:U:H3	1.50	0.59
2:1:1725:C:H5''	49:p:36:ARG:HH12	1.68	0.59
2:1:2442:G:N2	2:1:2505:U:O2	2.31	0.59
36:c:17:VAL:HG11	36:c:92:ILE:HD12	1.83	0.59
2:1:1778:G:O2'	2:1:1780:G:OP2	2.19	0.59
9:B:67:PHE:HA	9:B:70:ARG:HD2	1.84	0.59
18:K:255:ARG:O	18:K:259:PHE:HD2	1.85	0.59
20:M:48:GLY:HA3	20:M:53:VAL:HB	1.83	0.59
51:r:22:GLU:OE2	51:r:25:ARG:NH2	2.34	0.59
2:1:562:C:H5''	26:S:71:LYS:HD2	1.83	0.59
35:b:264:ILE:HD12	35:b:302:ARG:HD3	1.84	0.59
44:k:30:LYS:O	44:k:37:PRO:HA	2.03	0.59
2:1:1940:G:H21	2:1:3362:A:H8	1.51	0.59
2:1:3275:U:O2'	39:f:99:ARG:NH1	2.36	0.59
9:B:110:LEU:O	9:B:115:LYS:NZ	2.32	0.59
35:b:43:ARG:HB3	35:b:47:MET:HE3	1.84	0.59
55:v:102:PHE:HB2	55:v:114:ILE:HG22	1.84	0.59
2:1:2426:U:H3	2:1:2603:G:H1	1.51	0.59
18:K:254:LEU:HB2	18:K:259:PHE:CZ	2.38	0.59
2:1:2797:C:OP1	56:w:197:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:2219:A:H2'	2:1:2220:A2M:H8	1.86	0.58
2:1:3021:A:H2	2:1:3033:A:H62	1.51	0.58
7:8:92:ARG:O	7:8:96:LYS:NZ	2.33	0.58
15:H:94:TYR:CA	15:H:177:ASP:OD1	2.46	0.58
2:1:654:C:OP1	38:e:27:ARG:NH2	2.36	0.58
2:1:2901:G:O2'	2:1:3024:A:N1	2.36	0.58
46:m:50:ASN:OD1	46:m:54:ASN:N	2.36	0.58
2:1:3234:A:H2	2:1:3253:G:H22	1.52	0.58
18:K:140:LEU:HD12	18:K:154:ILE:HD11	1.85	0.58
2:1:172:G:H1	2:1:246:U:H3	1.50	0.58
2:1:2699:G:OP1	55:v:62:ARG:NH2	2.35	0.58
32:Y:57:LEU:HB3	32:Y:105:VAL:CG1	2.33	0.58
35:b:569:ASP:O	60:4:262:ARG:NH2	2.37	0.58
50:q:214:VAL:CG1	50:q:215:LYS:H	2.16	0.58
2:1:361:A:O3'	43:j:45:ARG:NH2	2.37	0.58
2:1:2547:A:O2'	2:1:2549:G:OP1	2.21	0.58
35:b:5:TRP:CD1	35:b:69:PRO:HG3	2.39	0.58
35:b:80:ASP:OD2	35:b:245:HIS:NE2	2.37	0.58
51:r:2:PRO:HB2	51:r:6:TYR:CG	2.39	0.58
57:x:136:SER:N	57:x:512:LEU:O	2.37	0.58
2:1:1635:G:N2	2:1:1638:A:OP2	2.33	0.58
4:3:67:G:H1	4:3:111:U:H3	1.52	0.58
9:B:113:GLU:HG2	9:B:176:ALA:HB2	1.86	0.58
11:D:141:PRO:HD2	56:w:86:VAL:HG21	1.85	0.58
18:K:250:ASN:ND2	18:K:252:GLU:OE1	2.36	0.58
53:t:197:GLY:HA3	53:t:314:ILE:HB	1.84	0.58
2:1:1261:G:H4'	2:1:1278:A:H2	1.69	0.57
2:1:1568:U:H5'	50:q:437:LYS:HB2	1.86	0.57
3:2:103:G:OP2	3:2:105:A:O2'	2.22	0.57
4:3:81:U:O2	4:3:99:G:O6	2.22	0.57
14:G:74:THR:CG2	21:N:18:VAL:HG22	2.33	0.57
24:Q:65:SER:CB	24:Q:93:ILE:HG21	2.35	0.57
35:b:497:ARG:NH2	54:u:123:ASP:OD1	2.32	0.57
55:v:106:PHE:HB3	55:v:244:MET:HE2	1.86	0.57
60:4:244:VAL:HG22	60:4:319:ILE:HG23	1.84	0.57
2:1:1696:A:H2'	2:1:1697:A:C8	2.39	0.57
24:Q:65:SER:HA	24:Q:93:ILE:HD13	1.87	0.57
57:x:221:LEU:O	57:x:268:ARG:NH1	2.35	0.57
2:1:1566:A:H2	50:q:432:ARG:HB2	1.70	0.57
2:1:2659:G:OP1	55:v:14:ARG:NH2	2.33	0.57
11:D:205:SER:OG	11:D:233:ALA:O	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1295:G:O2'	26:S:115:ARG:NH1	2.37	0.57
2:1:1746:U:O2'	44:k:4:GLU:OE1	2.22	0.57
14:G:74:THR:HG21	21:N:18:VAL:HG21	1.86	0.57
17:J:24:GLY:HA2	17:J:65:ILE:HG23	1.87	0.57
30:W:162:GLU:OE1	30:W:166:ARG:NH1	2.38	0.57
60:4:202:LEU:HB3	60:4:520:PRO:HB2	1.86	0.57
9:B:92:TYR:HB2	9:B:157:VAL:HB	1.87	0.57
18:K:236:VAL:CG1	18:K:244:LEU:HD21	2.34	0.57
47:n:179:VAL:HG21	47:n:379:LEU:HD11	1.86	0.57
2:1:1897:G:OP2	16:I:10:LYS:NZ	2.37	0.57
35:b:107:GLN:OE1	35:b:110:ARG:NH2	2.38	0.57
35:b:415:ASN:ND2	35:b:418:ASP:OD1	2.37	0.57
39:f:56:SER:O	39:f:63:LYS:NZ	2.37	0.57
2:1:600:G:N2	2:1:603:A:OP2	2.36	0.57
2:1:658:G:N7	67:1:3510:HOH:O	2.32	0.57
57:x:187:ASN:HB3	57:x:206:MET:HB3	1.85	0.57
2:1:2401:A:H5'	2:1:2402:A:H5''	1.87	0.57
55:v:145:GLY:HA3	55:v:186:ILE:HD12	1.87	0.57
2:1:1620:U:H2'	2:1:1621:A:C8	2.40	0.57
2:1:1667:A:H2'	2:1:1668:G:C8	2.40	0.57
2:1:3233:C:H2'	2:1:3234:A:C8	2.40	0.57
2:1:2777:G:O6	34:a:62:HIS:ND1	2.37	0.56
26:S:22:PRO:O	27:T:146:ASN:ND2	2.38	0.56
30:W:82:GLU:HG2	30:W:83:GLU:HG3	1.86	0.56
2:1:1858:A:H1'	40:g:4:ARG:HD3	1.85	0.56
6:6:229:U:OP2	53:t:49:ARG:NH1	2.38	0.56
53:t:77:ARG:NH2	53:t:303:ASN:OD1	2.39	0.56
14:G:74:THR:HG21	21:N:18:VAL:CG2	2.35	0.56
60:4:26:ASN:OD1	60:4:29:ARG:NH1	2.39	0.56
2:1:1639:C:OP2	40:g:74:ARG:NH1	2.32	0.56
2:1:3252:G:H2'	2:1:3253:G:C8	2.41	0.56
10:C:69:ARG:HD2	35:b:636:SER:HA	1.88	0.56
2:1:1786:G:H2'	2:1:1787:A:C8	2.41	0.56
55:v:286:GLN:OE1	55:v:289:LYS:NZ	2.37	0.56
60:4:202:LEU:HD21	60:4:509:LEU:HB3	1.88	0.56
24:Q:65:SER:CA	24:Q:93:ILE:HD13	2.36	0.56
60:4:197:LEU:HD22	60:4:226:ILE:HD12	1.87	0.55
2:1:394:G:N1	2:1:397:A:OP2	2.38	0.55
2:1:674:G:O6	24:Q:56:LYS:NZ	2.39	0.55
9:B:71:GLU:OE2	9:B:357:LYS:NZ	2.38	0.55
55:v:54:LYS:HB3	55:v:57:MET:HE3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:w:19:VAL:HG22	56:w:30:ASP:HB3	1.89	0.55
2:1:1241:U:O2'	46:m:148:LYS:NZ	2.38	0.55
2:1:99:A:H2'	2:1:100:A:C8	2.41	0.55
2:1:1813:A:OP2	50:q:380:LYS:NZ	2.34	0.55
3:2:63:G:O2'	41:h:49:LYS:NZ	2.34	0.55
2:1:2875:U:N3	2:1:2952:G:O2'	2.36	0.55
47:n:178:LYS:HB2	47:n:189:GLN:HB3	1.89	0.55
57:x:161:THR:HB	57:x:171:TRP:HE1	1.71	0.55
5:5:79:LEU:HD13	5:5:83:ARG:HH21	1.71	0.55
6:6:7:C:OP2	18:K:128:LYS:NZ	2.32	0.55
1:A:80:GLU:HG3	49:p:66:GLY:HA2	1.89	0.55
2:1:1348:U:OP1	24:Q:39:ARG:NH1	2.40	0.55
60:4:211:LEU:HD13	60:4:552:GLY:HA3	1.89	0.55
2:1:266:A:OP1	21:N:5:LYS:NZ	2.36	0.55
2:1:3295:A:H2'	2:1:3296:A:C8	2.42	0.55
14:G:213:LYS:NZ	48:o:159:GLY:O	2.36	0.55
33:Z:125:GLY:O	33:Z:128:GLN:NE2	2.39	0.55
57:x:256:LYS:HD2	57:x:280:SER:HB2	1.87	0.55
7:8:15:LEU:C	7:8:15:LEU:HD12	2.32	0.54
57:x:160:VAL:HG21	57:x:201:ILE:HG21	1.89	0.54
2:1:12:A:H2'	2:1:13:A:C8	2.43	0.54
2:1:784:A:C6	24:Q:93:ILE:HG22	2.42	0.54
49:p:70:THR:HG22	49:p:71:VAL:N	2.23	0.54
60:4:507:ILE:HD12	60:4:522:LEU:HD11	1.89	0.54
2:1:1596:C:H2'	2:1:1597:C:C6	2.42	0.54
2:1:2396:G:H2'	2:1:2398:A:H5'	1.88	0.54
4:3:44:C:H4'	11:D:152:ARG:HG3	1.90	0.54
7:8:15:LEU:HD11	7:8:60:VAL:HB	1.89	0.54
18:K:221:THR:O	18:K:225:ASN:ND2	2.40	0.54
18:K:298:LEU:HD21	48:o:196:LEU:HD11	1.90	0.54
2:1:655:C:H2'	2:1:656:A:H8	1.73	0.54
17:J:63:GLU:HG2	17:J:64:LYS:N	2.23	0.54
27:T:91:LEU:CD2	56:w:159:LEU:HB2	2.37	0.54
50:q:225:LYS:CE	50:q:395:GLU:OE2	2.52	0.54
9:B:85:VAL:HG22	9:B:202:THR:HG22	1.88	0.54
18:K:254:LEU:C	18:K:259:PHE:CE2	2.86	0.54
30:W:126:ARG:O	30:W:129:THR:OG1	2.24	0.54
40:g:71:THR:HG22	40:g:72:VAL:O	2.07	0.54
2:1:1571:A:OP2	53:t:284:ASN:ND2	2.40	0.54
2:1:1717:U:H2'	2:1:1718:G:C8	2.43	0.54
2:1:2926:A:H2'	2:1:2927:C:C6	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:114:ASN:HB2	10:C:117:GLU:HG3	1.89	0.54
34:a:132:LYS:NZ	34:a:136:GLU:OE2	2.41	0.54
42:i:45:ARG:NH2	42:i:89:GLU:OE2	2.40	0.54
46:m:122:ASP:OD1	57:x:441:ARG:NH2	2.41	0.54
4:3:12:U:OP2	4:3:68:C:O2'	2.26	0.54
57:x:192:VAL:HG12	57:x:203:THR:HG22	1.90	0.54
58:y:163:PRO:HA	58:y:183:ALA:HB1	1.90	0.54
2:1:1949:G:OP1	25:R:104:ARG:NH1	2.40	0.54
2:1:2692:A:HO2'	2:1:2693:C:H6	1.54	0.54
47:n:380:ILE:O	47:n:383:CYS:C	2.51	0.54
21:N:155:VAL:O	21:N:162:ARG:NH2	2.36	0.54
56:w:22:ASP:OD2	56:w:25:ASN:ND2	2.41	0.54
2:1:2898:G:H22	51:r:7:ILE:H	1.54	0.53
21:N:183:THR:HG22	21:N:187:ARG:HB2	1.89	0.53
60:4:42:VAL:HG21	60:4:141:ILE:HG21	1.88	0.53
2:1:567:G:H2'	2:1:568:G:C8	2.43	0.53
2:1:1657:C:O2'	2:1:1797:A:OP2	2.19	0.53
25:R:98:ARG:NH2	25:R:130:ASN:OD1	2.35	0.53
2:1:908:OMG:N2	2:1:2609:A:OP1	2.38	0.53
23:P:36:ILE:HD11	23:P:95:LEU:HD11	1.90	0.53
32:Y:57:LEU:HB3	32:Y:105:VAL:HG13	1.91	0.53
50:q:203:ARG:NH2	50:q:208:ASP:OD1	2.41	0.53
2:1:2317:A:H5''	2:1:2318:U:H3'	1.90	0.53
31:X:52:PRO:HD3	50:q:194:THR:HG22	1.91	0.53
46:m:229:LEU:HD21	46:m:238:ARG:CG	2.38	0.53
46:m:353:TRP:HA	46:m:366:ASP:O	2.08	0.53
11:D:205:SER:HB2	11:D:236:LEU:HD12	1.90	0.53
12:E:43:LEU:HD11	12:E:85:ILE:HG13	1.91	0.53
16:I:17:ASP:OD2	54:u:23:ARG:CD	2.55	0.53
47:n:176:VAL:O	47:n:177:ARG:NH1	2.38	0.53
55:v:185:THR:HG23	55:v:200:LEU:HD12	1.91	0.53
2:1:1207:G:O2'	51:r:36:SER:OG	2.27	0.53
2:1:3153:U:H3	2:1:3293:U:H3	1.57	0.53
2:1:675:C:O2'	2:1:679:U:OP1	2.25	0.53
2:1:2357:A:H2'	2:1:2358:A:C8	2.43	0.53
9:B:218:ILE:HG12	9:B:276:THR:HG23	1.91	0.53
35:b:506:GLU:HA	37:d:97:LEU:HD13	1.90	0.53
43:j:21:ARG:NH2	43:j:41:ALA:O	2.38	0.53
35:b:549:GLN:OE1	35:b:549:GLN:O	2.26	0.53
47:n:162:ILE:HG12	47:n:229:LEU:HD23	1.91	0.53
2:1:2522:G:O2'	2:1:2524:A:OP2	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:231:A:O2'	53:t:49:ARG:NH2	2.41	0.53
40:g:71:THR:HG22	40:g:72:VAL:N	2.23	0.53
46:m:400:ILE:HG13	46:m:428:ILE:HD11	1.91	0.53
2:1:3322:A:H2'	2:1:3323:A:C8	2.44	0.52
6:6:28:A:OP1	48:o:125:ASN:ND2	2.40	0.52
33:Z:23:VAL:HG12	33:Z:45:GLY:HA3	1.92	0.52
35:b:254:MET:HE1	35:b:309:VAL:HG21	1.91	0.52
57:x:377:ALA:HA	57:x:383:MET:HG2	1.90	0.52
2:1:87:U:H2'	2:1:88:A:H8	1.74	0.52
2:1:2160:G:H2'	2:1:2161:G:H8	1.75	0.52
2:1:3153:U:OP2	2:1:3293:U:O2'	2.28	0.52
17:J:164:LYS:HE3	17:J:171:VAL:HG23	1.91	0.52
60:4:239:VAL:HB	60:4:322:LYS:HB2	1.90	0.52
2:1:283:G:H2'	2:1:284:A:C8	2.45	0.52
2:1:358:G:N2	2:1:361:A:OP2	2.39	0.52
2:1:662:U:H2'	2:1:663:OMC:C6	2.44	0.52
10:C:209:TYR:CE1	10:C:227:THR:CG2	2.92	0.52
35:b:302:ARG:HA	35:b:305:LEU:HD12	1.91	0.52
2:1:3050:U:O2'	54:u:16:GLY:O	2.18	0.52
11:D:178:ASN:HA	11:D:183:TRP:CD2	2.45	0.52
55:v:72:MET:HB3	55:v:110:ILE:HG13	1.91	0.52
2:1:1659:U:H2'	2:1:1660:C:C6	2.45	0.52
26:S:77:VAL:HG11	26:S:106:LEU:HD22	1.92	0.52
2:1:1616:U:H2'	2:1:1617:G:C8	2.44	0.52
2:1:1621:A:H2'	2:1:1622:U:C6	2.45	0.52
2:1:2417:OMU:HM22	2:1:2418:G:H3'	1.91	0.52
2:1:3070:A:OP1	25:R:62:ARG:NH1	2.40	0.52
4:3:4:U:H2'	4:3:5:G:H8	1.75	0.52
32:Y:71:SER:N	32:Y:81:GLN:O	2.33	0.52
43:j:54:LYS:O	43:j:58:THR:HB	2.10	0.52
50:q:397:LYS:NZ	50:q:412:GLU:OE2	2.43	0.52
60:4:199:ALA:HB2	60:4:522:LEU:HD22	1.91	0.52
60:4:247:ILE:HD12	60:4:252:ALA:HA	1.92	0.52
2:1:91:G:H22	2:1:94:G:H3'	1.74	0.52
2:1:563:U:H2'	2:1:564:G:H8	1.74	0.52
2:1:2585:G:OP1	50:q:452:LYS:NZ	2.38	0.52
2:1:3165:A:H62	2:1:3285:C:H42	1.57	0.52
15:H:8:GLN:HB3	15:H:72:LYS:HD2	1.92	0.52
35:b:71:ILE:HG13	35:b:82:MET:HE3	1.91	0.52
39:f:14:LEU:HD11	39:f:31:LYS:HB2	1.90	0.52
50:q:398:PHE:HB2	50:q:401:GLU:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:t:75:ILE:HD12	53:t:156:PRO:HG2	1.91	0.52
57:x:426:ILE:HB	57:x:440:PHE:HB2	1.92	0.52
41:h:102:GLU:HG3	41:h:106:LYS:HE3	1.92	0.51
47:n:259:LEU:C	47:n:259:LEU:HD12	2.34	0.51
57:x:333:ALA:HB2	57:x:363:ILE:HD12	1.91	0.51
60:4:197:LEU:HD23	60:4:223:ILE:HD13	1.91	0.51
2:1:900:G:H1'	2:1:1589:A:N6	2.24	0.51
6:6:8:A:O2'	53:t:97:LYS:NZ	2.40	0.51
55:v:50:SER:HB2	55:v:57:MET:HG3	1.91	0.51
10:C:7:THR:OG1	10:C:147:GLU:OE2	2.25	0.51
11:D:164:LYS:HE3	11:D:195:LEU:HD21	1.92	0.51
23:P:98:ALA:HB2	23:P:148:LEU:HD11	1.92	0.51
1:A:117:GLU:HG2	1:A:124:GLY:H	1.75	0.51
13:F:86:VAL:O	13:F:114:GLY:HA2	2.09	0.51
28:U:96:VAL:CG1	28:U:97:SER:N	2.72	0.51
2:1:531:G:H2'	2:1:532:A:C8	2.46	0.51
2:1:664:U:H2'	2:1:665:A:C8	2.45	0.51
23:P:122:ALA:HB3	23:P:143:PRO:HB2	1.93	0.51
39:f:49:ILE:HD11	39:f:71:VAL:HG22	1.93	0.51
57:x:234:SER:HG	57:x:254:SER:HG	1.50	0.51
17:J:160:VAL:HG13	17:J:171:VAL:HG21	1.93	0.51
23:P:49:GLU:OE2	23:P:92:GLN:NE2	2.44	0.51
60:4:48:ASP:HA	60:4:52:SER:HB2	1.93	0.51
2:1:100:A:H2'	2:1:101:G:N3	2.25	0.51
3:2:52:A:H5'	45:l:21:ARG:HD3	1.92	0.51
14:G:133:LYS:HB2	14:G:199:ALA:HB3	1.93	0.51
2:1:173:G:O6	2:1:245:U:O4	2.29	0.51
2:1:1615:C:H2'	2:1:1616:U:C6	2.46	0.51
2:1:2585:G:N2	14:G:63:LYS:HG2	2.25	0.51
2:1:2768:U:H2'	2:1:2769:A:H8	1.75	0.51
3:2:49:G:O2'	41:h:39:PRO:O	2.29	0.51
2:1:1194:G:H2'	2:1:1195:A:C8	2.46	0.51
2:1:1907:C:O2	9:B:240:ARG:NH2	2.42	0.51
10:C:156:LEU:HD12	10:C:159:ILE:HD12	1.93	0.51
57:x:29:LEU:HD12	57:x:30:PRO:HD2	1.93	0.51
2:1:1553:U:H4'	2:1:1554:U:H5'	1.93	0.50
6:6:9:A:H5'	53:t:97:LYS:HE3	1.94	0.50
53:t:208:ILE:HD12	53:t:251:ILE:HG12	1.93	0.50
4:3:103:A:H2'	4:3:104:A:H8	1.76	0.50
7:8:63:LYS:HG3	7:8:70:ALA:HB3	1.93	0.50
14:G:74:THR:CG2	21:N:18:VAL:CG2	2.87	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:v:185:THR:CG2	55:v:200:LEU:HD12	2.41	0.50
2:1:974:G:OP1	24:Q:16:ARG:NH2	2.44	0.50
10:C:282:SER:OG	24:Q:125:ASP:OD2	2.29	0.50
17:J:133:ARG:NH1	17:J:153:LYS:O	2.44	0.50
18:K:102:VAL:HA	18:K:265:LEU:HD23	1.94	0.50
51:r:151:ILE:HD11	51:r:212:LEU:HD13	1.92	0.50
2:1:3358:U:H2'	2:1:3359:A:H8	1.76	0.50
8:9:147:LEU:HD12	60:4:279:LEU:HD13	1.92	0.50
10:C:160:GLN:NE2	10:C:213:ASN:O	2.44	0.50
35:b:570:GLN:NE2	60:4:260:ALA:O	2.38	0.50
2:1:163:C:H2'	2:1:164:A:C8	2.47	0.50
5:5:96:ALA:HA	5:5:104:VAL:HG21	1.92	0.50
13:F:96:PRO:HB2	13:F:99:PRO:HD2	1.93	0.50
18:K:39:LYS:O	18:K:43:GLU:HG2	2.11	0.50
50:q:263:ARG:HA	50:q:266:MET:HE2	1.94	0.50
23:P:107:LEU:CA	23:P:152:GLU:OE2	2.60	0.50
38:e:96:ILE:HG21	38:e:105:ARG:HG2	1.94	0.50
57:x:61:GLU:OE2	57:x:65:ASN:ND2	2.34	0.50
2:1:2883:U:H2'	2:1:2884:C:H6	1.77	0.50
10:C:126:ILE:O	10:C:129:THR:OG1	2.28	0.50
55:v:173:GLN:NE2	55:v:174:ASP:O	2.44	0.50
57:x:276:GLY:H	57:x:304:TRP:HH2	1.60	0.50
1:A:109:GLU:HG2	1:A:138:GLY:HA2	1.94	0.50
2:1:2403:G:H2'	2:1:2404:A:H8	1.76	0.50
18:K:210:ARG:O	18:K:225:ASN:ND2	2.44	0.50
35:b:149:TYR:HB2	46:m:137:TYR:HB3	1.94	0.50
58:y:15:VAL:HA	58:y:61:ARG:HG2	1.93	0.50
2:1:3192:U:H2'	2:1:3193:C:C6	2.47	0.49
10:C:139:GLY:O	10:C:141:ARG:NH1	2.45	0.49
12:E:70:LYS:HB3	12:E:146:ILE:HD11	1.94	0.49
27:T:91:LEU:CD1	27:T:96:ILE:CG2	2.90	0.49
37:d:51:LEU:HB3	37:d:55:LEU:HD23	1.93	0.49
57:x:378:SER:OG	57:x:379:ASP:N	2.45	0.49
60:4:142:THR:HG23	60:4:155:SER:HB2	1.94	0.49
3:2:12:A:OP1	23:P:3:ARG:NH1	2.44	0.49
25:R:105:LEU:HD23	25:R:138:LEU:HD23	1.93	0.49
34:a:94:ALA:HB2	34:a:121:VAL:HG22	1.93	0.49
35:b:290:THR:HG21	35:b:319:THR:HB	1.95	0.49
2:1:1:G:N2	6:6:232:A:OP2	2.44	0.49
2:1:664:U:H2'	2:1:665:A:H8	1.76	0.49
2:1:1083:G:H2'	2:1:1084:A:H8	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:W:169:PHE:O	30:W:198:ARG:NH1	2.39	0.49
47:n:206:PRO:HG2	53:t:228:VAL:HB	1.94	0.49
55:v:139:PRO:HB3	55:v:180:HIS:NE2	2.27	0.49
2:1:426:G:OP1	38:e:15:LYS:NZ	2.45	0.49
2:1:2095:G:H2'	2:1:2096:A:H8	1.77	0.49
47:n:188:TYR:O	47:n:198:ARG:HA	2.12	0.49
56:w:43:ASN:OD1	56:w:44:ALA:N	2.44	0.49
2:1:3067:C:H3'	25:R:62:ARG:HH22	1.76	0.49
3:2:71:A:H61	3:2:81:U:H5'	1.78	0.49
17:J:40:LEU:CD1	17:J:82:ARG:NH2	2.75	0.49
24:Q:64:VAL:HG23	24:Q:93:ILE:HD11	1.94	0.49
2:1:1573:G:O6	47:n:91:THR:OG1	2.26	0.49
2:1:2822:U:H3'	2:1:2823:G:H2'	1.94	0.49
4:3:87:G:H2'	4:3:88:G:C8	2.47	0.49
5:5:42:THR:OG1	5:5:43:SER:N	2.46	0.49
47:n:380:ILE:O	47:n:383:CYS:O	2.31	0.49
27:T:91:LEU:CD2	56:w:159:LEU:CD1	2.83	0.49
2:1:655:C:H2'	2:1:656:A:C8	2.46	0.49
2:1:2660:G:OP1	2:1:2750:U:O2'	2.30	0.49
2:1:2768:U:H2'	2:1:2769:A:C8	2.48	0.49
18:K:75:LYS:HE2	18:K:285:ARG:HG3	1.95	0.49
27:T:91:LEU:HD23	56:w:159:LEU:CD1	2.42	0.49
30:W:120:VAL:O	30:W:121:ARG:NH1	2.43	0.49
57:x:301:VAL:HG21	57:x:376:THR:HG21	1.95	0.49
2:1:2821:C:OP1	2:1:2822:U:O2'	2.29	0.49
2:1:3180:A:OP1	22:O:171:LYS:NZ	2.39	0.49
3:2:153:U:OP1	14:G:63:LYS:NZ	2.46	0.49
2:1:1592:G:OP1	40:g:58:ARG:NH2	2.43	0.49
2:1:1646:G:O2'	2:1:1808:G:N2	2.42	0.49
2:1:3302:U:H3	2:1:3312:U:H3	1.60	0.49
4:3:1:G:H1'	11:D:269:SER:HB2	1.94	0.49
47:n:24:LYS:NZ	47:n:69:GLN:OE1	2.42	0.49
58:y:28:VAL:HG12	58:y:50:HIS:HB3	1.94	0.49
2:1:986:PSU:H5''	13:F:129:LEU:HD11	1.94	0.48
2:1:2746:A:H5'	11:D:178:ASN:OD1	2.12	0.48
2:1:275:U:H2'	2:1:276:U:C6	2.48	0.48
2:1:571:U:H2'	2:1:572:A:H8	1.79	0.48
2:1:2821:C:O2'	2:1:2943:G:N2	2.45	0.48
2:1:3013:U:H2'	2:1:3014:U:C6	2.49	0.48
9:B:57:VAL:HG22	9:B:73:VAL:HG22	1.95	0.48
25:R:105:LEU:HD22	25:R:135:LYS:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:n:374:ASP:OD1	47:n:374:ASP:N	2.43	0.48
57:x:61:GLU:OE1	57:x:77:TYR:N	2.46	0.48
13:F:224:ILE:HD11	26:S:35:VAL:HG12	1.94	0.48
15:H:41:ILE:HG22	15:H:43:VAL:HG13	1.96	0.48
55:v:149:ASP:O	55:v:155:LYS:NZ	2.31	0.48
2:1:808:A:H61	2:1:932:U:H3	1.61	0.48
2:1:2412:G:H2'	2:1:2413:A:H8	1.78	0.48
2:1:2722:U:H4'	55:v:257:MET:HB2	1.94	0.48
2:1:3199:G:H5''	20:M:6:ILE:HD13	1.95	0.48
6:6:37:C:H42	6:6:42:G:H1	1.61	0.48
2:1:2585:G:H1	14:G:63:LYS:HZ3	1.62	0.48
2:1:2966:G:H2'	2:1:2967:A:C8	2.48	0.48
2:1:3026:G:H4'	51:r:2:PRO:HD3	1.95	0.48
4:3:87:G:H2'	4:3:88:G:H8	1.78	0.48
8:9:140:LEU:HD22	32:Y:92:GLY:HA2	1.95	0.48
10:C:142:VAL:HG12	10:C:145:ILE:HD13	1.87	0.48
17:J:21:ILE:CG2	17:J:23:VAL:CG2	2.91	0.48
28:U:94:ARG:HB3	28:U:108:TYR:CZ	2.49	0.48
13:F:184:LEU:HD21	13:F:202:LEU:HD21	1.94	0.48
35:b:499:ARG:HG3	35:b:503:MET:HE2	1.95	0.48
47:n:242:LEU:HD13	47:n:264:LEU:HD23	1.96	0.48
53:t:211:ARG:HH21	53:t:322:ASN:HA	1.79	0.48
2:1:2936:A:H2'	2:1:2937:G:C8	2.49	0.48
9:B:283:TYR:N	9:B:323:MET:O	2.45	0.48
15:H:9:GLN:HB3	15:H:52:LEU:HD11	1.94	0.48
26:S:12:ARG:HB3	26:S:24:LEU:HD23	1.94	0.48
33:Z:104:PRO:HA	33:Z:105:SER:HA	1.54	0.48
2:1:2628:A:N6	2:1:2651:G:O6	2.47	0.48
3:2:154:C:H5''	14:G:181:LYS:HD2	1.96	0.48
30:W:41:TRP:HZ3	30:W:231:THR:HG21	1.79	0.48
30:W:123:ASP:HB2	30:W:213:PHE:HB2	1.95	0.48
53:t:179:LEU:HD12	53:t:183:VAL:HB	1.96	0.48
2:1:129:U:H2'	2:1:130:A:C8	2.48	0.48
2:1:2357:A:H2'	2:1:2358:A:H8	1.79	0.48
2:1:3015:G:OP2	59:z:2:ALA:N	2.47	0.48
16:I:39:LEU:HB3	16:I:46:LEU:HD12	1.95	0.48
17:J:59:ILE:HG21	17:J:65:ILE:HD11	1.95	0.48
19:L:27:ASP:OD2	19:L:31:LYS:NZ	2.45	0.48
25:R:23:TRP:HB2	25:R:53:LYS:HE2	1.95	0.48
35:b:171:LEU:HD21	35:b:243:ILE:HG12	1.95	0.48
40:g:42:PRO:HB2	40:g:51:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:t:71:GLU:OE2	53:t:74:ARG:NH2	2.44	0.48
53:t:150:PRO:HB2	53:t:153:VAL:HG21	1.95	0.48
2:1:712:G:OP2	34:a:65:GLN:NE2	2.47	0.48
2:1:2367:A:H2'	2:1:2368:A:C8	2.48	0.48
6:6:27:G:OP1	48:o:130:ASN:ND2	2.43	0.48
7:8:15:LEU:CD1	7:8:60:VAL:HB	2.44	0.48
12:E:100:LYS:NZ	12:E:137:ASP:OD1	2.43	0.48
36:c:16:LEU:HA	36:c:19:LYS:HG2	1.95	0.48
57:x:282:SER:N	57:x:295:GLY:O	2.46	0.48
2:1:314:U:H2'	2:1:315:C:C6	2.50	0.47
23:P:22:LEU:HD12	23:P:146:ILE:HD12	1.96	0.47
47:n:364:VAL:HG22	47:n:386:ASN:HB2	1.95	0.47
2:1:651:G:O2'	2:1:1435:A:OP1	2.32	0.47
2:1:984:G:N1	2:1:1139:G:OP1	2.32	0.47
2:1:1718:G:H2'	2:1:1719:G:H8	1.79	0.47
23:P:126:ARG:HA	23:P:140:GLU:HG2	1.96	0.47
36:c:14:LEU:O	36:c:18:ILE:HG12	2.14	0.47
2:1:2272:G:C6	46:m:471:LYS:HB3	2.49	0.47
2:1:2515:A:N1	2:1:2594:C:N4	2.60	0.47
9:B:171:LEU:HD21	9:B:333:LYS:HB2	1.95	0.47
15:H:95:ALA:N	15:H:177:ASP:OD1	2.47	0.47
2:1:1226:G:H2'	2:1:1227:C:C6	2.49	0.47
2:1:2095:G:H2'	2:1:2096:A:C8	2.50	0.47
47:n:189:GLN:HB2	47:n:198:ARG:HG2	1.97	0.47
60:4:453:ASN:OD1	60:4:453:ASN:N	2.47	0.47
2:1:787:G:H2'	2:1:788:C:C6	2.49	0.47
2:1:3379:C:H4'	9:B:315:GLY:HA2	1.97	0.47
23:P:148:LEU:HD12	23:P:148:LEU:C	2.39	0.47
24:Q:67:ILE:HG23	24:Q:81:VAL:HG21	1.97	0.47
47:n:25:LEU:HD12	47:n:32:PHE:HD1	1.79	0.47
51:r:196:PRO:HG2	51:r:224:ASN:HB3	1.97	0.47
2:1:407:A:C2	3:2:17:A:H1'	2.50	0.47
2:1:616:G:H2'	2:1:617:G:C8	2.49	0.47
2:1:806:A:N6	2:1:936:A:O4'	2.48	0.47
2:1:1210:U:H5	30:W:3:ARG:HG2	1.80	0.47
2:1:1597:C:H5'	2:1:1696:A:H1'	1.97	0.47
2:1:2683:U:H2'	2:1:2684:C:H6	1.79	0.47
2:1:3343:G:O2'	2:1:3362:A:N6	2.47	0.47
33:Z:50:PRO:HD3	33:Z:68:ILE:HG12	1.95	0.47
53:t:207:LEU:HG	53:t:271:PHE:CD2	2.50	0.47
2:1:2523:A:OP1	31:X:31:THR:OG1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:59:A:O2'	31:X:61:LYS:NZ	2.42	0.47
4:3:29:C:H2'	4:3:51:A:H61	1.79	0.47
11:D:69:ILE:HG22	55:v:135:VAL:HG13	1.97	0.47
17:J:17:LEU:HD13	17:J:129:VAL:HG22	1.97	0.47
18:K:280:PHE:HB3	18:K:288:VAL:HB	1.96	0.47
49:p:38:ASP:HA	49:p:45:LYS:HA	1.97	0.47
57:x:205:SER:OG	57:x:206:MET:N	2.48	0.47
57:x:221:LEU:HB3	57:x:268:ARG:HH12	1.80	0.47
2:1:424:G:O2'	38:e:23:ASP:OD2	2.30	0.47
2:1:1568:U:H3'	50:q:437:LYS:HE3	1.97	0.47
2:1:1572:U:O2'	47:n:83:HIS:NE2	2.38	0.47
2:1:3295:A:H2'	2:1:3296:A:H8	1.80	0.47
54:u:2:ARG:NH1	58:y:78:ASP:OD2	2.48	0.47
60:4:475:LEU:HB2	60:4:480:VAL:HB	1.97	0.47
2:1:831:G:O2'	2:1:1864:A:N3	2.44	0.47
2:1:1097:G:O5'	27:T:129:LYS:NZ	2.48	0.47
2:1:1718:G:H2'	2:1:1719:G:C8	2.50	0.47
9:B:284:ARG:NH1	9:B:293:ASN:O	2.47	0.47
51:r:186:HIS:CE1	51:r:188:GLU:HB3	2.49	0.47
53:t:85:LYS:HD3	53:t:96:GLY:HA2	1.96	0.47
2:1:33:G:OP1	21:N:71:ARG:NH2	2.48	0.46
2:1:710:A:H2'	2:1:711:A:C8	2.50	0.46
2:1:2220:A2M:H3'	2:1:2221:G:H8	1.79	0.46
46:m:229:LEU:HD22	46:m:234:PRO:O	2.15	0.46
50:q:214:VAL:CG1	50:q:215:LYS:N	2.75	0.46
54:u:45:ASN:HB3	54:u:48:LYS:HB2	1.96	0.46
60:4:141:ILE:O	60:4:155:SER:HA	2.15	0.46
2:1:498:A:OP1	39:f:86:ARG:NH1	2.48	0.46
2:1:646:A:H1'	2:1:2375:G:C6	2.50	0.46
2:1:2654:C:H2'	2:1:2655:U:C2	2.51	0.46
2:1:2723:U:H2'	2:1:2724:OMU:H6	1.98	0.46
2:1:2769:A:H2'	2:1:2770:G:C8	2.49	0.46
2:1:2831:G:H2'	2:1:2832:C:C6	2.51	0.46
27:T:75:ILE:HG23	27:T:86:GLU:HG3	1.96	0.46
35:b:289:LYS:HG2	64:b:801:GDP:C6	2.50	0.46
36:c:22:LYS:N	36:c:94:GLU:O	2.44	0.46
2:1:226:C:H2'	2:1:227:G:O4'	2.16	0.46
2:1:2570:U:H4'	2:1:2571:U:H2'	1.95	0.46
2:1:2730:G:O6	46:m:315:GLN:NE2	2.40	0.46
3:2:26:U:H2'	3:2:27:U:C6	2.51	0.46
14:G:144:GLU:OE2	21:N:6:TYR:OH	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S:13:ARG:NH2	26:S:50:LYS:O	2.48	0.46
44:k:56:ILE:HG22	44:k:58:ASP:H	1.80	0.46
2:1:815:G:OP2	43:j:31:LYS:NZ	2.47	0.46
2:1:2191:PSU:O2'	46:m:292:ASN:OD1	2.32	0.46
2:1:2661:G:OP1	11:D:35:ARG:NH1	2.34	0.46
17:J:61:ARG:NH1	17:J:62:ASN:OD1	2.48	0.46
17:J:87:LYS:HG2	17:J:106:ILE:HD11	1.98	0.46
2:1:2620:G:O6	56:w:126:LYS:NZ	2.47	0.46
61:1:3403:B3P:O5	61:1:3403:B3P:O4	2.28	0.46
3:2:63:G:H22	3:2:97:A:H2	1.63	0.46
4:3:27:A:H2'	4:3:28:C:C6	2.50	0.46
9:B:290:ASP:HB3	9:B:293:ASN:HB3	1.95	0.46
23:P:56:ARG:NH2	23:P:75:GLU:OE2	2.41	0.46
31:X:108:LEU:N	31:X:125:ARG:O	2.47	0.46
47:n:35:LEU:HB3	47:n:71:LEU:HD11	1.98	0.46
47:n:427:ILE:HG23	47:n:428:GLN:H	1.80	0.46
57:x:207:ASP:OD1	57:x:209:THR:OG1	2.29	0.46
57:x:274:MET:HE1	57:x:292:LEU:HD22	1.97	0.46
58:y:142:ILE:HG13	58:y:148:VAL:HG12	1.98	0.46
2:1:29:C:H4'	2:1:62:A:H4'	1.96	0.46
2:1:656:A:H2'	2:1:657:A:C8	2.51	0.46
14:G:200:LEU:HD12	14:G:200:LEU:HA	1.82	0.46
18:K:294:ASN:OD1	18:K:294:ASN:N	2.48	0.46
28:U:50:LEU:HD22	28:U:54:VAL:HB	1.97	0.46
35:b:313:PRO:HA	35:b:314:GLY:HA2	1.57	0.46
50:q:215:LYS:HB2	50:q:381:HIS:CG	2.51	0.46
2:1:2681:U:H2'	2:1:2682:C:H6	1.81	0.46
61:1:3403:B3P:H31	61:1:3403:B3P:H62	1.68	0.46
19:L:106:GLN:HB3	42:i:18:THR:HB	1.98	0.46
26:S:80:ARG:NH1	52:s:47:ASP:OD1	2.49	0.46
45:l:43:ASN:HB3	45:l:46:ARG:HD2	1.97	0.46
55:v:185:THR:HG22	55:v:200:LEU:HB2	1.98	0.46
60:4:135:PRO:HB3	60:4:162:PRO:HD3	1.97	0.46
2:1:1220:U:H2'	5:5:44:TRP:NE1	2.30	0.46
2:1:1480:G:O2'	2:1:1871:U:O4	2.31	0.46
2:1:1555:U:O2'	2:1:1556:C:H2'	2.16	0.46
2:1:2344:U:H2'	2:1:2345:A:C8	2.51	0.46
2:1:2812:C:H2'	2:1:2813:A:C8	2.51	0.46
2:1:2922:G:O3'	46:m:210:ARG:NH2	2.45	0.46
2:1:2964:G:N2	2:1:2967:A:OP2	2.34	0.46
29:V:18:PRO:HA	29:V:51:ALA:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:W:42:VAL:HG23	30:W:218:SER:HB3	1.96	0.46
35:b:264:ILE:HD12	35:b:302:ARG:HH11	1.81	0.46
48:o:90:SER:OG	48:o:91:GLY:N	2.49	0.46
56:w:30:ASP:OD1	56:w:30:ASP:N	2.47	0.46
60:4:246:ARG:HE	60:4:265:LYS:HD3	1.81	0.46
2:1:3296:A:H2'	2:1:3297:U:H6	1.81	0.46
17:J:63:GLU:HG2	17:J:64:LYS:H	1.79	0.46
40:g:76:TYR:HB3	40:g:80:ARG:HB2	1.97	0.46
2:1:1805:C:H2'	2:1:1806:A:H8	1.82	0.45
2:1:2433:U:H1'	21:N:125:SER:HB3	1.98	0.45
17:J:23:VAL:HG12	17:J:23:VAL:O	2.15	0.45
30:W:131:ALA:HB2	30:W:195:LEU:HD21	1.98	0.45
16:I:127:LEU:O	16:I:131:LEU:HB2	2.16	0.45
36:c:49:PRO:HG2	36:c:52:ARG:HB3	1.98	0.45
53:t:180:THR:H	53:t:183:VAL:HB	1.81	0.45
2:1:289:A:H2'	2:1:290:G:H8	1.81	0.45
2:1:1176:C:H2'	2:1:1177:G:N2	2.31	0.45
2:1:2315:G:H4'	2:1:2316:G:C4	2.52	0.45
4:3:4:U:H2'	4:3:5:G:C8	2.50	0.45
18:K:80:LEU:HB3	18:K:246:VAL:HB	1.99	0.45
18:K:238:LEU:HD23	18:K:244:LEU:HD11	1.98	0.45
35:b:403:GLU:HG3	35:b:412:PHE:HB3	1.98	0.45
46:m:244:GLU:HA	46:m:247:LYS:HG2	1.99	0.45
46:m:287:HIS:HB3	46:m:294:PHE:HB3	1.97	0.45
55:v:28:LYS:NZ	55:v:163:ASP:OD2	2.35	0.45
60:4:342:SER:HA	60:4:354:ILE:HG23	1.98	0.45
60:4:447:HIS:CD2	60:4:492:THR:HG1	2.34	0.45
60:4:484:LYS:HE3	60:4:488:LEU:HD21	1.99	0.45
2:1:8:C:H2'	2:1:9:U:C6	2.52	0.45
2:1:501:A:H2'	2:1:502:U:C6	2.51	0.45
2:1:806:A:H2'	2:1:807:A2M:C8	2.46	0.45
2:1:1136:A:H2'	2:1:1137:C:C6	2.52	0.45
2:1:1497:C:O2'	2:1:1602:A:N3	2.47	0.45
2:1:1619:A:H2'	2:1:1620:U:O4'	2.16	0.45
2:1:2930:A:H2'	2:1:2931:C:C6	2.51	0.45
3:2:151:C:H2'	50:q:449:TRP:CZ3	2.52	0.45
17:J:50:ALA:HB3	17:J:63:GLU:H	1.82	0.45
19:L:189:GLU:HA	19:L:192:GLU:HG2	1.98	0.45
23:P:107:LEU:CG	23:P:152:GLU:OE2	2.64	0.45
30:W:60:TRP:HZ3	30:W:107:GLU:HG3	1.81	0.45
46:m:229:LEU:HD21	46:m:238:ARG:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:86:G:O2'	2:1:98:G:O6	2.26	0.45
2:1:348:A:N3	2:1:352:A:O2'	2.50	0.45
2:1:435:C:H5''	8:9:51:LYS:HE2	1.98	0.45
2:1:1193:A:OP1	22:O:49:ARG:NH1	2.36	0.45
2:1:2402:A:H1'	2:1:2403:G:C8	2.50	0.45
16:I:89:VAL:HG22	16:I:101:PHE:HE1	1.82	0.45
2:1:297:G:OP2	2:1:297:G:N2	2.39	0.45
2:1:585:A:H2'	2:1:586:C:C6	2.51	0.45
2:1:733:G:N2	2:1:736:A:OP2	2.47	0.45
2:1:1259:A:C8	30:W:67:MET:HB2	2.52	0.45
2:1:1261:G:H4'	2:1:1278:A:C2	2.49	0.45
2:1:1450:OMG:HM23	2:1:1450:OMG:H1'	1.82	0.45
2:1:2203:U:O2	2:1:2239:G:N2	2.39	0.45
14:G:228:GLU:HA	14:G:231:LYS:HE2	1.99	0.45
1:A:101:VAL:HG22	1:A:165:VAL:HG22	1.99	0.45
2:1:3209:A:C5	20:M:106:ARG:HD3	2.51	0.45
10:C:35:VAL:HG21	10:C:244:LEU:HD21	1.97	0.45
57:x:385:LEU:O	57:x:395:ILE:N	2.50	0.45
2:1:1666:G:H2'	2:1:1667:A:C8	2.52	0.45
2:1:2438:A:H2'	2:1:2439:A:C8	2.52	0.45
2:1:2949:U:H2'	2:1:2950:G:C8	2.52	0.45
2:1:2986:U:H2'	2:1:2987:A:H8	1.81	0.45
2:1:3218:A:H5''	2:1:3219:G:C5	2.52	0.45
4:3:84:A:N3	4:3:85:G:N2	2.65	0.45
10:C:142:VAL:CA	10:C:145:ILE:HD11	2.27	0.45
53:t:87:LYS:HD3	53:t:87:LYS:HA	1.78	0.45
2:1:1257:C:H2'	2:1:1258:U:O4'	2.17	0.45
2:1:1867:A:H2'	2:1:1868:G:C8	2.51	0.45
2:1:2585:G:H22	14:G:63:LYS:HG2	1.81	0.45
9:B:41:VAL:HA	9:B:185:GLY:HA3	1.98	0.45
10:C:3:ARG:NE	10:C:22:LEU:O	2.44	0.45
24:Q:16:ARG:HG3	24:Q:53:PHE:HB3	1.98	0.45
33:Z:5:LEU:HD11	36:c:35:ARG:HD2	1.99	0.45
44:k:64:LYS:HE2	44:k:64:LYS:HB3	1.78	0.45
46:m:328:LYS:NZ	65:m:802:ALF:F1	2.37	0.45
49:p:46:THR:OG1	49:p:57:CYS:SG	2.65	0.45
57:x:170:ILE:HB	57:x:180:HIS:HB2	1.98	0.45
1:A:104:LEU:HD22	1:A:136:ILE:HD11	1.99	0.45
2:1:1301:A:O2'	2:1:1302:A:O4'	2.35	0.45
2:1:3294:A:H2'	2:1:3295:A:O4'	2.17	0.45
27:T:91:LEU:HD13	27:T:96:ILE:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:j:66:TYR:OH	43:j:73:ARG:NH2	2.50	0.45
55:v:49:LEU:HD12	55:v:100:MET:HE1	1.98	0.45
57:x:37:GLN:O	57:x:120:LEU:HA	2.17	0.45
1:A:7:ASN:OD1	1:A:10:LYS:NZ	2.50	0.44
2:1:1281:G:H2'	2:1:1282:G:H8	1.82	0.44
11:D:164:LYS:NZ	11:D:168:ASP:OD2	2.50	0.44
17:J:150:ASN:HA	17:J:153:LYS:HE3	1.99	0.44
27:T:91:LEU:HD13	27:T:96:ILE:HG23	1.99	0.44
47:n:427:ILE:HG22	47:n:428:GLN:O	2.17	0.44
51:r:241:LYS:HE2	51:r:261:VAL:HG12	1.98	0.44
57:x:406:ASN:ND2	57:x:448:TYR:O	2.49	0.44
1:A:9:ARG:NH2	2:1:912:G:OP2	2.47	0.44
2:1:1475:A:OP2	35:b:516:LYS:NZ	2.36	0.44
2:1:2108:C:H1'	2:1:3344:A:C8	2.52	0.44
9:B:300:ARG:HB2	35:b:436:LEU:HD13	1.98	0.44
18:K:338:ASN:HB3	53:t:266:PHE:CD2	2.52	0.44
32:Y:119:ILE:HG22	32:Y:124:GLY:HA3	1.98	0.44
46:m:37:LYS:HE3	46:m:37:LYS:HB2	1.84	0.44
2:1:417:A:H2'	2:1:418:A:C8	2.53	0.44
2:1:3145:C:OP1	8:9:9:ARG:NH1	2.44	0.44
2:1:3388:C:H5''	2:1:3389:U:H5'	1.98	0.44
16:I:85:TYR:HA	16:I:89:VAL:HG21	2.00	0.44
47:n:37:ILE:HD11	47:n:217:ILE:HG23	1.98	0.44
2:1:1278:A:O2'	30:W:15:THR:O	2.31	0.44
2:1:2103:U:H2'	2:1:2104:A:C8	2.53	0.44
2:1:2731:U:O2	46:m:112:LYS:NZ	2.39	0.44
2:1:2880:PSU:H5'	9:B:236:LYS:HD3	2.00	0.44
2:1:3066:U:H2'	2:1:3067:C:C6	2.53	0.44
14:G:81:THR:HG22	14:G:179:ILE:HG22	2.00	0.44
30:W:34:LEU:HD11	30:W:77:LEU:HD23	1.99	0.44
58:y:118:HIS:HE2	58:y:146:ILE:HD12	1.82	0.44
1:A:128:ARG:HG3	2:1:2177:G:H2'	2.00	0.44
2:1:616:G:H2'	2:1:617:G:H8	1.83	0.44
2:1:786:A:H4'	2:1:787:G:H5'	1.99	0.44
2:1:1288:U:H2'	2:1:1289:G:C8	2.52	0.44
2:1:1492:G:N7	45:l:2:ALA:N	2.65	0.44
2:1:1743:G:H2'	2:1:1744:G:H8	1.82	0.44
2:1:2883:U:H2'	2:1:2884:C:C6	2.52	0.44
11:D:68:THR:CG2	55:v:132:THR:OG1	2.65	0.44
27:T:88:ARG:HB2	56:w:162:VAL:HB	1.99	0.44
2:1:1497:C:H2'	2:1:1498:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:3244:A:OP1	9:B:97:ARG:NH2	2.42	0.44
2:1:294:U:H4'	42:i:77:LEU:HD23	2.00	0.44
2:1:1447:G:H3'	23:P:67:ILE:HD11	1.99	0.44
2:1:1497:C:H2'	2:1:1498:A:H8	1.82	0.44
2:1:1597:C:H2'	2:1:1598:G:C8	2.53	0.44
2:1:2616:C:H5''	2:1:2617:U:H5'	2.00	0.44
2:1:3000:A:H2'	2:1:3001:C:C6	2.52	0.44
3:2:95:G:O2'	43:j:81:GLY:O	2.30	0.44
35:b:520:PRO:HG2	35:b:523:LYS:HB2	1.99	0.44
37:d:96:VAL:HG12	37:d:98:VAL:HG13	1.99	0.44
51:r:205:GLN:HB2	51:r:209:TYR:HD2	1.82	0.44
54:u:18:GLY:HA3	54:u:31:PHE:O	2.17	0.44
2:1:946:U:H2'	2:1:947:G:H8	1.83	0.44
2:1:1498:A:H2'	2:1:1499:C:C6	2.52	0.44
2:1:1616:U:H2'	2:1:1617:G:H8	1.83	0.44
2:1:2652:U:H2'	2:1:2653:C:C6	2.52	0.44
2:1:3386:G:H2'	2:1:3387:U:C6	2.53	0.44
3:2:142:C:H2'	3:2:143:U:C6	2.53	0.44
4:3:45:A:H2'	4:3:46:A:H8	1.83	0.44
33:Z:41:ALA:HB2	33:Z:77:TYR:HE1	1.83	0.44
2:1:158:G:H2'	2:1:159:A:H8	1.83	0.44
2:1:1276:U:O2'	2:1:1277:C:H5'	2.18	0.44
2:1:2694:A:H2'	2:1:2695:A:C8	2.53	0.44
18:K:101:ASN:HB3	18:K:233:GLN:HG2	1.99	0.44
38:e:69:SER:OG	38:e:118:LYS:NZ	2.51	0.44
47:n:430:GLN:NE2	47:n:454:PRO:O	2.42	0.44
57:x:268:ARG:HD3	57:x:268:ARG:HA	1.79	0.44
60:4:40:LYS:HG2	60:4:531:THR:HG22	1.99	0.44
2:1:1913:A:N3	2:1:2120:A:H2'	2.33	0.43
2:1:2609:A:H2'	2:1:2610:G:C8	2.53	0.43
7:8:126:ALA:HB2	7:8:162:ILE:HG13	1.98	0.43
13:F:48:ASN:ND2	13:F:182:ASP:OD2	2.51	0.43
43:j:75:LYS:HE2	43:j:75:LYS:HB3	1.89	0.43
48:o:194:LYS:HE2	48:o:194:LYS:HB2	1.90	0.43
2:1:110:G:OP2	19:L:73:ARG:NH2	2.41	0.43
2:1:1766:G:OP1	60:4:377:GLN:NE2	2.49	0.43
2:1:2412:G:H2'	2:1:2413:A:C8	2.53	0.43
2:1:2627:C:O2'	17:J:60:ARG:NH2	2.51	0.43
41:h:83:LYS:O	41:h:89:ARG:NH1	2.40	0.43
46:m:246:MET:HE2	46:m:246:MET:HB3	1.85	0.43
48:o:120:VAL:HG13	48:o:137:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:2793:OMG:H2'	2:1:2794:G:H4'	1.99	0.43
3:2:149:A:H2'	3:2:150:G:C8	2.53	0.43
4:3:77:G:N2	4:3:102:A:OP2	2.43	0.43
5:5:90:GLU:HG2	5:5:94:ARG:HE	1.83	0.43
5:5:99:MET:HE3	5:5:103:LYS:HE2	1.99	0.43
18:K:238:LEU:HD23	18:K:244:LEU:CD1	2.48	0.43
28:U:56:VAL:HG22	28:U:65:VAL:HG22	1.99	0.43
31:X:115:ARG:HD3	31:X:121:LYS:HE3	2.00	0.43
53:t:181:LYS:HE2	53:t:181:LYS:HB2	1.79	0.43
54:u:50:LYS:HG3	54:u:55:PHE:CE2	2.52	0.43
1:A:203:ALA:HB1	2:1:2146:C:H5''	2.00	0.43
2:1:374:A:H1'	2:1:375:A:H5''	1.99	0.43
2:1:659:G:N7	67:1:3524:HOH:O	2.37	0.43
2:1:1568:U:H4'	2:1:1569:U:O5'	2.18	0.43
2:1:1810:A:H2'	2:1:1811:G:C8	2.54	0.43
2:1:3209:A:C4	20:M:106:ARG:HD3	2.53	0.43
3:2:69:U:H2'	3:2:70:G:O4'	2.18	0.43
13:F:176:TYR:CZ	13:F:197:GLN:HG2	2.52	0.43
18:K:36:ARG:HG2	18:K:291:LEU:CD2	2.48	0.43
23:P:123:PRO:HB2	35:b:615:ARG:HD2	1.99	0.43
26:S:77:VAL:HG12	26:S:79:VAL:HG13	1.99	0.43
47:n:128:ALA:O	47:n:132:ILE:HG23	2.18	0.43
53:t:102:LYS:HB2	53:t:131:GLU:HG3	2.00	0.43
55:v:53:LYS:HE3	55:v:56:ASP:HB2	1.98	0.43
60:4:182:ASP:OD1	60:4:539:SER:OG	2.32	0.43
2:1:439:C:O2'	2:1:494:G:N2	2.52	0.43
2:1:1841:A:H1'	45:l:45:ARG:HH22	1.83	0.43
2:1:2994:A:O2'	3:2:1:A:N1	2.42	0.43
2:1:3023:U:H2'	2:1:3024:A:H8	1.84	0.43
2:1:3089:C:H2'	2:1:3090:U:O4'	2.18	0.43
2:1:3233:C:H2'	2:1:3234:A:H8	1.82	0.43
3:2:88:A:H2'	3:2:89:A:C8	2.54	0.43
12:E:145:LEU:HD23	12:E:145:LEU:HA	1.88	0.43
25:R:43:LYS:O	25:R:47:ASN:ND2	2.51	0.43
30:W:30:VAL:HG13	30:W:104:PHE:HZ	1.83	0.43
42:i:37:THR:CG2	42:i:41:ARG:CZ	2.97	0.43
53:t:207:LEU:HG	53:t:271:PHE:CE2	2.52	0.43
57:x:319:HIS:CE1	57:x:384:PHE:HD2	2.37	0.43
2:1:67:A:O2'	2:1:315:C:O2	2.35	0.43
2:1:2272:G:C5	46:m:471:LYS:HB3	2.54	0.43
10:C:142:VAL:HA	10:C:145:ILE:CG1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:94:TYR:HA	15:H:177:ASP:CG	2.40	0.43
18:K:140:LEU:CD1	18:K:154:ILE:HD11	2.49	0.43
26:S:60:SER:OG	26:S:62:ASN:OD1	2.36	0.43
35:b:596:GLY:HA3	60:4:460:TYR:CZ	2.53	0.43
46:m:248:LYS:NZ	46:m:249:GLU:OE2	2.36	0.43
60:4:140:LYS:HD2	60:4:502:ARG:HB2	1.99	0.43
2:1:1437:OMC:HM23	2:1:1437:OMC:H1'	1.78	0.43
2:1:2242:A:O2'	2:1:2244:A:OP1	2.36	0.43
13:F:189:ILE:HG23	13:F:190:THR:HG23	2.01	0.43
15:H:114:VAL:HB	15:H:124:ARG:HB2	2.01	0.43
30:W:224:ASP:OD1	30:W:225:SER:N	2.51	0.43
55:v:37:SER:OG	55:v:92:SER:O	2.28	0.43
55:v:123:LYS:HB2	55:v:229:ARG:HG2	2.01	0.43
2:1:925:A:N1	2:1:2414:G:H2'	2.33	0.43
2:1:1263:A:N6	7:8:138:SER:HB3	2.33	0.43
2:1:2344:U:H2'	2:1:2345:A:H8	1.83	0.43
2:1:2765:C:H42	2:1:2793:OMG:HN1	1.66	0.43
2:1:2801:A:H2'	46:m:21:ASN:HB3	2.01	0.43
35:b:86:TYR:O	35:b:149:TYR:OH	2.30	0.43
58:y:44:ASP:OD1	58:y:44:ASP:N	2.51	0.43
2:1:3:U:O2'	6:6:232:A:H8	2.01	0.43
2:1:123:A:OP1	14:G:105:LYS:NZ	2.40	0.43
2:1:2253:G:H2'	2:1:2254:U:C6	2.54	0.43
2:1:3099:C:H42	2:1:3135:U:H3	1.65	0.43
2:1:3267:A:H2'	12:E:69:PHE:CZ	2.54	0.43
4:3:78:U:H2'	4:3:79:A:H8	1.83	0.43
37:d:36:ILE:HD12	37:d:59:ILE:HD11	2.00	0.43
46:m:372:PRO:HA	46:m:373:PRO:HD3	1.93	0.43
57:x:157:SER:HA	57:x:173:CYS:HB2	2.00	0.43
1:A:127:ALA:HB2	1:A:134:VAL:HG23	2.01	0.43
2:1:1253:U:H5'	2:1:1254:C:H5'	2.01	0.43
2:1:1667:A:H2'	2:1:1668:G:H8	1.83	0.43
4:3:59:U:H2'	4:3:60:G:C8	2.53	0.43
9:B:76:VAL:HG12	9:B:325:LYS:HA	2.01	0.43
15:H:47:LYS:NZ	20:M:5:SER:O	2.45	0.43
30:W:55:GLU:OE2	30:W:121:ARG:NH2	2.41	0.43
33:Z:27:LYS:HB3	33:Z:42:LEU:HB2	2.01	0.43
35:b:168:ARG:HE	58:y:242:GLU:CD	2.26	0.43
35:b:622:SER:HB3	45:l:46:ARG:HH11	1.83	0.43
53:t:158:LYS:HB2	53:t:158:LYS:HE3	1.82	0.43
2:1:428:A:H2'	2:1:429:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:79:A:C6	3:2:80:A:H1'	2.54	0.42
6:6:7:C:N4	18:K:184:ASP:OD2	2.41	0.42
13:F:130:ILE:HD12	13:F:134:VAL:HG11	2.01	0.42
14:G:98:ARG:HA	14:G:99:PRO:HD3	1.89	0.42
16:I:104:ARG:HD2	16:I:104:ARG:HA	1.73	0.42
18:K:97:LEU:HD11	18:K:205:THR:HB	2.01	0.42
43:j:2:GLY:O	43:j:7:SER:OG	2.29	0.42
50:q:214:VAL:CG1	50:q:389:VAL:HG21	2.48	0.42
2:1:80:G:H2'	2:1:81:C:H6	1.84	0.42
2:1:1740:U:H4'	2:1:1741:A:H5'	1.99	0.42
2:1:1877:U:H5''	2:1:1878:G:O4'	2.18	0.42
2:1:2160:G:H2'	2:1:2161:G:C8	2.54	0.42
2:1:2167:A:H2'	2:1:2168:A:C8	2.54	0.42
2:1:2347:OMU:H2'	2:1:2348:A:O4'	2.19	0.42
2:1:2429:G:H2'	2:1:2430:A:H8	1.84	0.42
17:J:117:ASP:HB2	17:J:120:ILE:HG13	2.01	0.42
18:K:44:LEU:HD23	18:K:44:LEU:HA	1.85	0.42
57:x:100:ASN:ND2	57:x:103:SER:H	2.16	0.42
2:1:978:G:O2'	2:1:1103:A:N1	2.47	0.42
2:1:1288:U:H2'	2:1:1289:G:H8	1.82	0.42
2:1:1666:G:H2'	2:1:1667:A:H8	1.83	0.42
2:1:2552:C:H2'	36:c:50:VAL:HG11	2.01	0.42
61:1:3401:B3P:H112	61:1:3401:B3P:H21	1.69	0.42
8:9:110:LEU:HD12	8:9:110:LEU:HA	1.87	0.42
21:N:158:HIS:HB3	21:N:161:ALA:HB3	2.02	0.42
27:T:54:HIS:HB3	27:T:57:TYR:HD2	1.84	0.42
33:Z:33:SER:OG	33:Z:35:SER:O	2.28	0.42
38:e:31:ASN:OD1	38:e:31:ASN:N	2.49	0.42
40:g:71:THR:CG2	40:g:72:VAL:N	2.83	0.42
46:m:396:PRO:HA	46:m:399:TYR:HD2	1.83	0.42
56:w:30:ASP:HB2	56:w:32:ASN:HD22	1.84	0.42
60:4:207:LEU:HD12	60:4:208:PRO:HD2	2.02	0.42
60:4:279:LEU:HD23	60:4:477:LYS:HD3	2.01	0.42
60:4:322:LYS:HG2	60:4:502:ARG:HG3	2.01	0.42
2:1:630:A:H2'	2:1:631:U:C6	2.55	0.42
2:1:945:C:H2'	2:1:946:U:C6	2.54	0.42
2:1:2427:U:H2'	2:1:2428:U:C6	2.54	0.42
2:1:2764:C:C2	2:1:2794:G:N2	2.87	0.42
2:1:2986:U:H2'	2:1:2987:A:C8	2.54	0.42
61:1:3401:B3P:H31	61:1:3401:B3P:H71	1.83	0.42
3:2:83:C:H4'	3:2:84:C:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:32:ILE:HG23	7:8:37:LEU:HB2	2.01	0.42
13:F:87:VAL:HG11	13:F:243:MET:HE1	2.02	0.42
20:M:32:LEU:HD11	20:M:94:TRP:CD1	2.55	0.42
52:s:51:PRO:HG2	52:s:54:PHE:HB2	2.01	0.42
57:x:142:HIS:CE1	57:x:169:ARG:HG2	2.53	0.42
2:1:284:A:C5	2:1:285:A:H1'	2.54	0.42
2:1:595:G:N2	2:1:609:G:OP1	2.47	0.42
2:1:898:OMU:HM23	2:1:898:OMU:H1'	1.83	0.42
2:1:1129:A:H2'	2:1:1130:A:O4'	2.19	0.42
2:1:1153:A:N1	2:1:2371:G:O2'	2.47	0.42
2:1:1305:U:C4	9:B:256:HIS:HB3	2.55	0.42
2:1:2611:U:H2'	2:1:2612:U:C6	2.55	0.42
2:1:2959:OMC:HM23	2:1:2959:OMC:H1'	1.89	0.42
2:1:3121:U:H1'	2:1:3122:A:H5''	2.00	0.42
13:F:84:VAL:HG21	13:F:127:LEU:HD11	2.00	0.42
47:n:74:GLU:OE2	47:n:116:HIS:NE2	2.44	0.42
57:x:321:HIS:CG	57:x:379:ASP:HB3	2.54	0.42
60:4:191:MET:HE1	60:4:319:ILE:HB	2.02	0.42
2:1:127:G:H2'	2:1:128:G:H8	1.83	0.42
2:1:1195:A:OP2	52:s:9:ARG:NH1	2.51	0.42
2:1:2408:U:H2'	2:1:2409:G:C8	2.55	0.42
2:1:2738:A:H2'	2:1:2739:A:C8	2.54	0.42
2:1:3096:C:H2'	2:1:3097:C:C6	2.54	0.42
35:b:588:ARG:HG2	45:l:21:ARG:CZ	2.50	0.42
47:n:114:LEU:HB2	47:n:227:THR:HG21	2.02	0.42
57:x:421:SER:OG	57:x:422:PHE:N	2.53	0.42
2:1:798:G:H21	19:L:15:ARG:HH22	1.68	0.42
2:1:2842:U:O2'	2:1:2845:A:N7	2.52	0.42
2:1:3315:G:P	9:B:116:ARG:HH22	2.43	0.42
10:C:152:VAL:HG21	10:C:156:LEU:HD22	2.01	0.42
19:L:144:THR:HG21	41:h:118:ILE:HG21	2.02	0.42
29:V:135:VAL:HG22	58:y:101:LEU:HA	2.00	0.42
36:c:42:ILE:HD11	36:c:67:VAL:HG22	2.01	0.42
46:m:21:ASN:OD1	46:m:21:ASN:N	2.50	0.42
46:m:214:GLU:O	46:m:218:VAL:HG13	2.19	0.42
55:v:51:ALA:HA	55:v:54:LYS:HD2	2.00	0.42
2:1:297:G:O6	21:N:12:ARG:NH1	2.50	0.42
2:1:2739:A:H2'	2:1:2740:A:C8	2.55	0.42
3:2:57:C:H4'	3:2:63:G:N7	2.34	0.42
24:Q:37:ALA:HB1	24:Q:46:LYS:HD3	2.00	0.42
26:S:81:TYR:HE2	26:S:90:MET:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:p:70:THR:CG2	49:p:71:VAL:N	2.82	0.42
2:1:1699:A:H2'	2:1:1700:G:C8	2.55	0.42
2:1:2115:G:H22	2:1:2120:A:H1'	1.85	0.42
2:1:2997:G:OP2	59:z:95:LYS:NZ	2.38	0.42
4:3:101:G:N7	55:v:95:LYS:NZ	2.56	0.42
57:x:167:THR:HG22	57:x:183:LYS:HA	2.01	0.42
58:y:42:LEU:HD13	58:y:46:ILE:HD11	2.02	0.42
58:y:143:SER:HB2	58:y:165:THR:HG23	2.02	0.42
60:4:96:ASP:HB2	60:4:140:LYS:HE2	2.02	0.42
2:1:377:A:H1'	2:1:392:G:N2	2.35	0.42
2:1:1534:A:H2'	2:1:1535:A:C8	2.55	0.42
2:1:1791:C:H2'	2:1:1792:C:C6	2.55	0.42
2:1:2862:U:H1'	35:b:92:LYS:HE3	2.02	0.42
2:1:3308:C:O2'	23:P:69:ARG:O	2.29	0.42
3:2:139:U:H2'	3:2:140:G:H8	1.85	0.42
20:M:32:LEU:HD11	20:M:94:TRP:CG	2.55	0.42
23:P:107:LEU:HA	23:P:152:GLU:OE2	2.20	0.42
27:T:91:LEU:HD12	27:T:96:ILE:CG2	2.50	0.42
36:c:24:THR:HG22	36:c:91:SER:HB3	2.02	0.42
54:u:78:PRO:HB3	58:y:81:LEU:HG	2.02	0.42
55:v:50:SER:HB2	55:v:57:MET:HE2	2.02	0.42
57:x:262:ILE:HD12	57:x:272:TYR:HB2	2.00	0.42
57:x:285:LYS:HG2	57:x:328:LEU:HG	2.01	0.42
2:1:148:G:OP2	21:N:4:TYR:OH	2.31	0.41
2:1:1426:C:H4'	10:C:40:THR:HG23	2.02	0.41
2:1:1831:U:O2'	3:2:114:G:OP1	2.23	0.41
2:1:2529:A:H2'	2:1:2530:G:O4'	2.20	0.41
12:E:23:LYS:HA	12:E:23:LYS:HD3	1.93	0.41
17:J:50:ALA:N	17:J:63:GLU:O	2.52	0.41
51:r:61:MET:O	51:r:65:ILE:HG12	2.20	0.41
2:1:129:U:H2'	2:1:130:A:H8	1.85	0.41
2:1:629:U:H2'	2:1:630:A:C8	2.55	0.41
2:1:1169:A:H5''	13:F:219:LYS:HD3	2.02	0.41
2:1:2201:G:O6	2:1:2241:U:O4	2.38	0.41
2:1:2969:A:H2'	2:1:2970:C:O4'	2.20	0.41
2:1:3072:C:H2'	2:1:3073:A:O4'	2.21	0.41
2:1:3343:G:H21	2:1:3362:A:H2	1.65	0.41
9:B:103:THR:CG2	9:B:151:ILE:CG1	2.98	0.41
12:E:57:HIS:HE1	12:E:61:ASN:HA	1.85	0.41
15:H:21:LYS:HG3	20:M:8:LYS:HG3	2.01	0.41
30:W:92:LEU:HB2	30:W:228:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:507:U:H2'	2:1:508:U:C6	2.56	0.41
2:1:3298:C:C2	2:1:3299:A:C8	3.09	0.41
10:C:158:SER:HA	10:C:213:ASN:HB2	2.03	0.41
11:D:211:LEU:HD23	11:D:211:LEU:HA	1.88	0.41
17:J:110:ILE:HD13	17:J:116:TYR:HB2	2.02	0.41
18:K:80:LEU:HB2	18:K:248:LEU:HD21	2.02	0.41
2:1:36:C:O2'	2:1:934:G:N3	2.50	0.41
2:1:82:C:H2'	2:1:83:U:O4'	2.20	0.41
2:1:436:A:H2'	2:1:437:G:H8	1.84	0.41
2:1:818:C:H2'	2:1:819:U:O4'	2.20	0.41
2:1:1201:C:H2'	2:1:1202:A:C2	2.56	0.41
2:1:2929:C:H2'	2:1:2930:A:O4'	2.20	0.41
14:G:162:LEU:HD23	21:N:7:LEU:HD11	2.01	0.41
15:H:24:ILE:HD11	15:H:39:LYS:HD2	2.03	0.41
18:K:80:LEU:CD1	18:K:281:ILE:HD13	2.50	0.41
21:N:65:ARG:HG3	21:N:129:TYR:CE2	2.55	0.41
30:W:157:MET:HG2	30:W:180:ILE:HD12	2.02	0.41
31:X:57:LEU:HD23	31:X:61:LYS:HG2	2.01	0.41
41:h:26:LYS:HB3	41:h:26:LYS:HE2	1.85	0.41
49:p:13:LYS:HE3	49:p:14:TYR:CZ	2.55	0.41
54:u:73:GLN:HG2	54:u:75:ARG:NH2	2.35	0.41
56:w:40:ASP:OD1	56:w:41:SER:N	2.54	0.41
58:y:53:ILE:HG12	58:y:59:ILE:HG22	2.02	0.41
2:1:821:U:H2'	2:1:822:G:H8	1.85	0.41
2:1:1675:G:H2'	2:1:1676:A:H8	1.86	0.41
2:1:2685:C:H2'	2:1:2686:A:H8	1.86	0.41
2:1:2724:OMU:HM23	2:1:2724:OMU:H1'	1.68	0.41
2:1:3138:U:OP2	9:B:30:LYS:HG3	2.20	0.41
3:2:154:C:H2'	3:2:155:A:H8	1.85	0.41
11:D:208:MET:HG3	11:D:219:PHE:CE1	2.55	0.41
19:L:90:ALA:HB1	19:L:95:ILE:HB	2.02	0.41
46:m:446:GLU:H	46:m:446:GLU:HG2	1.64	0.41
53:t:205:ARG:HG2	53:t:251:ILE:HG21	2.03	0.41
58:y:109:CYS:HB2	58:y:149:GLY:HA2	2.01	0.41
58:y:116:LEU:HG	58:y:177:LEU:HD21	2.01	0.41
58:y:240:LEU:HD23	58:y:240:LEU:HA	1.87	0.41
2:1:266:A:H2'	42:i:30:LYS:HE3	2.03	0.41
2:1:506:U:H2'	2:1:507:U:O4'	2.21	0.41
2:1:668:G:H2'	2:1:669:U:H6	1.84	0.41
2:1:748:U:H2'	2:1:749:C:C6	2.55	0.41
2:1:961:C:H3'	2:1:962:A:H8	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:2279:A:H2	2:1:2314:PSU:HN3	1.68	0.41
2:1:2717:U:C2'	2:1:2718:U:H5'	2.51	0.41
2:1:2882:U:H2'	2:1:2883:U:C6	2.55	0.41
2:1:2958:A:H2'	2:1:2959:OMC:H6	1.85	0.41
2:1:3274:A:H5''	2:1:3276:G:OP2	2.21	0.41
9:B:286:GLY:HA3	9:B:321:PHE:CZ	2.56	0.41
11:D:43:LYS:HB3	55:v:168:GLU:HG2	2.03	0.41
14:G:200:LEU:HD23	14:G:211:LEU:HD13	2.02	0.41
35:b:306:LEU:HD23	35:b:306:LEU:HA	1.96	0.41
46:m:384:PHE:HE1	46:m:403:VAL:HG22	1.85	0.41
48:o:210:LYS:HE3	48:o:210:LYS:HB3	1.95	0.41
50:q:245:GLU:OE1	50:q:248:ARG:NH2	2.54	0.41
53:t:31:ILE:O	53:t:35:GLU:HG2	2.20	0.41
57:x:389:LEU:HD13	57:x:389:LEU:HA	1.93	0.41
58:y:18:LYS:HE2	58:y:60:GLY:HA2	2.02	0.41
2:1:541:U:H2'	2:1:542:G:C8	2.56	0.41
2:1:818:C:O2'	2:1:2138:A:N1	2.53	0.41
2:1:876:A2M:HM'3	2:1:876:A2M:H1'	1.88	0.41
2:1:887:G:H2'	2:1:888:A:C8	2.56	0.41
2:1:897:U:H2'	2:1:898:OMU:H6	2.02	0.41
2:1:1472:U:H5'	25:R:4:LEU:HB2	2.02	0.41
2:1:2103:U:H2'	2:1:2104:A:H8	1.86	0.41
2:1:2568:C:O2'	2:1:2569:A:O4'	2.34	0.41
2:1:2899:C:O2'	2:1:2901:G:OP2	2.38	0.41
2:1:3231:U:H2'	2:1:3232:G:H8	1.85	0.41
61:1:3401:B3P:H32	61:1:3401:B3P:H62	1.88	0.41
24:Q:65:SER:HB3	24:Q:93:ILE:HG21	2.02	0.41
34:a:91:LEU:HD23	34:a:121:VAL:HG21	2.02	0.41
50:q:232:LYS:O	50:q:235:SER:OG	2.37	0.41
51:r:239:TRP:HZ2	57:x:3:THR:HG21	1.85	0.41
53:t:139:PRO:HA	53:t:179:LEU:O	2.21	0.41
55:v:90:MET:HE2	55:v:90:MET:HB2	1.91	0.41
57:x:115:ASP:OD1	57:x:115:ASP:N	2.53	0.41
60:4:325:SER:HB3	60:4:499:PRO:HG2	2.01	0.41
2:1:2413:A:H2'	2:1:2415:C:C6	2.55	0.41
2:1:2669:G:H2'	2:1:2670:G:H8	1.85	0.41
7:8:124:THR:O	7:8:127:SER:OG	2.26	0.41
18:K:80:LEU:HD13	18:K:281:ILE:CD1	2.50	0.41
50:q:237:LEU:HD12	50:q:240:LYS:HD2	2.02	0.41
52:s:71:ASP:OD1	52:s:75:ARG:HG3	2.20	0.41
2:1:411:U:H2'	2:1:412:G:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:436:A:H2'	2:1:437:G:C8	2.56	0.41
2:1:563:U:H2'	2:1:564:G:C8	2.56	0.41
2:1:980:A:H2'	2:1:981:U:O4'	2.21	0.41
2:1:1138:U:H2'	2:1:1139:G:H8	1.86	0.41
2:1:1149:G:OP1	39:f:20:LYS:NZ	2.53	0.41
2:1:1438:U:H2'	2:1:1439:U:C6	2.55	0.41
2:1:1567:U:H1'	50:q:437:LYS:HA	2.02	0.41
2:1:1740:U:H1'	2:1:1741:A:H2	1.86	0.41
2:1:2108:C:H1'	2:1:3344:A:H8	1.86	0.41
2:1:2275:A:C4	46:m:266:PRO:HG3	2.56	0.41
2:1:2683:U:H2'	2:1:2684:C:C6	2.54	0.41
4:3:106:U:H2'	4:3:107:C:H6	1.85	0.41
11:D:68:THR:HG22	55:v:132:THR:OG1	2.21	0.41
27:T:90:ASN:OD1	56:w:177:ARG:NH1	2.52	0.41
47:n:441:LEU:HD12	47:n:441:LEU:HA	1.92	0.41
55:v:103:ILE:HG23	55:v:113:MET:HG2	2.02	0.41
57:x:454:SER:OG	57:x:496:VAL:O	2.25	0.41
58:y:118:HIS:HB3	58:y:121:ILE:HG23	2.03	0.41
60:4:206:LYS:NZ	60:4:565:PHE:O	2.49	0.41
2:1:1184:A:H2'	2:1:1185:C:C6	2.56	0.41
2:1:1209:G:H5'	30:W:4:SER:HB2	2.03	0.41
2:1:3193:C:H2'	2:1:3194:C:C6	2.56	0.41
4:3:59:U:H2'	4:3:60:G:H8	1.85	0.41
6:6:22:G:N7	18:K:96:LYS:NZ	2.66	0.41
13:F:110:ARG:CZ	24:Q:3:ILE:HG21	2.50	0.41
18:K:80:LEU:HD12	18:K:281:ILE:HD13	2.02	0.41
24:Q:64:VAL:HG21	24:Q:113:LYS:HD3	2.03	0.41
40:g:19:LYS:HA	40:g:19:LYS:HD3	1.90	0.41
57:x:214:ASP:HA	57:x:215:PRO:HD3	1.94	0.41
1:A:204:MET:HB3	1:A:208:ASP:HB2	2.03	0.40
2:1:1688:U:H2'	2:1:1689:U:C6	2.56	0.40
2:1:2863:G:C2	35:b:95:LEU:HD13	2.55	0.40
2:1:3162:C:H2'	2:1:3163:A:C8	2.56	0.40
13:F:148:VAL:HG12	13:F:181:ILE:HD11	2.03	0.40
16:I:87:GLN:OE1	54:u:7:HIS:ND1	2.36	0.40
18:K:39:LYS:HB2	18:K:39:LYS:HE3	1.82	0.40
26:S:125:LYS:HE2	26:S:125:LYS:HB2	1.90	0.40
27:T:91:LEU:HD12	27:T:96:ILE:HG21	2.03	0.40
46:m:431:LEU:HD23	46:m:453:ILE:HD11	2.03	0.40
60:4:336:THR:OG1	60:4:337:LEU:N	2.54	0.40
60:4:405:ASN:HB3	60:4:407:GLU:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:619:A:OP1	23:P:167:ARG:NH1	2.53	0.40
2:1:663:OMC:HM23	2:1:663:OMC:H1'	1.81	0.40
2:1:1471:U:H2'	2:1:1472:U:C6	2.56	0.40
2:1:1486:G:H21	40:g:6:THR:HG22	1.86	0.40
2:1:1571:A:C6	47:n:149:ASN:HB2	2.56	0.40
2:1:3393:U:H2'	2:1:3394:U:C6	2.56	0.40
37:d:55:LEU:HB2	37:d:95:PRO:HD3	2.04	0.40
40:g:106:LYS:HD3	40:g:106:LYS:HA	1.94	0.40
53:t:39:LYS:HB2	53:t:39:LYS:HE2	1.88	0.40
57:x:234:SER:OG	57:x:254:SER:OG	2.28	0.40
60:4:442:TRP:HB2	60:4:498:LEU:HD11	2.04	0.40
2:1:731:U:H2'	2:1:732:C:C6	2.56	0.40
2:1:1237:G:H22	2:1:1251:A:H2	1.69	0.40
2:1:2438:A:H2'	2:1:2439:A:H8	1.86	0.40
2:1:3006:A:H2'	2:1:3007:U:O4'	2.21	0.40
4:3:19:C:H2'	4:3:20:A:H8	1.86	0.40
18:K:46:LYS:HE3	18:K:46:LYS:HB3	1.91	0.40
27:T:65:TYR:CZ	27:T:88:ARG:HD2	2.57	0.40
60:4:38:ALA:O	60:4:42:VAL:HG13	2.21	0.40
2:1:1222:G:OP1	30:W:23:LYS:NZ	2.34	0.40
2:1:2526:C:H2'	2:1:2527:G:H8	1.85	0.40
2:1:2662:G:H2'	2:1:2663:G:C8	2.57	0.40
9:B:46:PHE:HE2	9:B:81:THR:HB	1.87	0.40
9:B:106:TRP:O	9:B:137:TYR:OH	2.34	0.40
14:G:72:PRO:HA	14:G:73:PRO:HD3	1.97	0.40
24:Q:65:SER:HB3	24:Q:93:ILE:CG2	2.51	0.40
55:v:83:ASP:OD1	55:v:108:TYR:OH	2.29	0.40
2:1:371:G:H4'	2:1:396:A:N1	2.37	0.40
2:1:1624:G:O2'	2:1:1643:A:N1	2.46	0.40
2:1:2565:U:H3	2:1:2576:G:H1	1.70	0.40
2:1:2684:C:H2'	2:1:2685:C:H6	1.86	0.40
2:1:2979:U:H1'	2:1:2980:U:C5	2.57	0.40
2:1:3112:G:O6	2:1:3120:C:H5''	2.21	0.40
4:3:11:A:N1	4:3:67:G:O2'	2.52	0.40
18:K:254:LEU:HB2	18:K:259:PHE:CE2	2.57	0.40
36:c:32:LYS:HE2	36:c:32:LYS:HB3	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	211/254 (83%)	202 (96%)	9 (4%)	0	100	100
5	5	71/120 (59%)	71 (100%)	0	0	100	100
7	8	156/165 (94%)	150 (96%)	6 (4%)	0	100	100
8	9	110/175 (63%)	108 (98%)	2 (2%)	0	100	100
9	B	384/387 (99%)	379 (99%)	5 (1%)	0	100	100
10	C	359/362 (99%)	348 (97%)	11 (3%)	0	100	100
11	D	266/297 (90%)	261 (98%)	5 (2%)	0	100	100
12	E	151/176 (86%)	149 (99%)	2 (1%)	0	100	100
13	F	217/244 (89%)	211 (97%)	6 (3%)	0	100	100
14	G	220/256 (86%)	216 (98%)	4 (2%)	0	100	100
15	H	189/191 (99%)	184 (97%)	5 (3%)	0	100	100
16	I	129/166 (78%)	125 (97%)	4 (3%)	0	100	100
17	J	169/174 (97%)	166 (98%)	3 (2%)	0	100	100
18	K	262/376 (70%)	256 (98%)	6 (2%)	0	100	100
19	L	178/199 (89%)	174 (98%)	4 (2%)	0	100	100
20	M	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
21	N	185/204 (91%)	178 (96%)	7 (4%)	0	100	100
22	O	195/199 (98%)	194 (100%)	1 (0%)	0	100	100
23	P	171/184 (93%)	164 (96%)	7 (4%)	0	100	100
24	Q	145/186 (78%)	144 (99%)	1 (1%)	0	100	100
25	R	154/189 (82%)	151 (98%)	3 (2%)	0	100	100
26	S	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
27	T	110/160 (69%)	107 (97%)	3 (3%)	0	100	100
28	U	104/121 (86%)	100 (96%)	4 (4%)	0	100	100
29	V	134/137 (98%)	131 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	W	232/236 (98%)	230 (99%)	2 (1%)	0	100	100
31	X	137/142 (96%)	133 (97%)	4 (3%)	0	100	100
32	Y	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
33	Z	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
34	a	90/149 (60%)	86 (96%)	4 (4%)	0	100	100
35	b	638/647 (99%)	617 (97%)	21 (3%)	0	100	100
36	c	95/105 (90%)	95 (100%)	0	0	100	100
37	d	105/113 (93%)	104 (99%)	1 (1%)	0	100	100
38	e	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
39	f	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
40	g	110/121 (91%)	108 (98%)	2 (2%)	0	100	100
41	h	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
42	i	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
43	j	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
44	k	75/78 (96%)	75 (100%)	0	0	100	100
45	l	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
46	m	462/486 (95%)	452 (98%)	10 (2%)	0	100	100
47	n	363/605 (60%)	353 (97%)	10 (3%)	0	100	100
48	o	131/220 (60%)	129 (98%)	2 (2%)	0	100	100
49	p	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
50	q	152/455 (33%)	144 (95%)	8 (5%)	0	100	100
51	r	224/261 (86%)	220 (98%)	4 (2%)	0	100	100
52	s	68/77 (88%)	67 (98%)	1 (2%)	0	100	100
53	t	283/322 (88%)	280 (99%)	3 (1%)	0	100	100
54	u	148/199 (74%)	146 (99%)	2 (1%)	0	100	100
55	v	291/344 (85%)	283 (97%)	8 (3%)	0	100	100
56	w	192/201 (96%)	190 (99%)	2 (1%)	0	100	100
57	x	500/514 (97%)	488 (98%)	12 (2%)	0	100	100
58	y	242/245 (99%)	232 (96%)	10 (4%)	0	100	100
59	z	83/106 (78%)	83 (100%)	0	0	100	100
60	4	534/593 (90%)	527 (99%)	7 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	10648/12402 (86%)	10401 (98%)	247 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	A	166/196 (85%)	166 (100%)	0	100	100
5	5	67/106 (63%)	67 (100%)	0	100	100
7	8	129/136 (95%)	128 (99%)	1 (1%)	73	81
8	9	106/153 (69%)	106 (100%)	0	100	100
9	B	322/323 (100%)	321 (100%)	1 (0%)	86	91
10	C	288/289 (100%)	286 (99%)	2 (1%)	76	83
11	D	226/245 (92%)	226 (100%)	0	100	100
12	E	133/153 (87%)	132 (99%)	1 (1%)	73	81
13	F	184/205 (90%)	184 (100%)	0	100	100
14	G	185/208 (89%)	185 (100%)	0	100	100
15	H	171/171 (100%)	169 (99%)	2 (1%)	63	74
16	I	117/141 (83%)	117 (100%)	0	100	100
17	J	148/150 (99%)	148 (100%)	0	100	100
18	K	247/346 (71%)	247 (100%)	0	100	100
19	L	142/159 (89%)	141 (99%)	1 (1%)	76	83
20	M	108/109 (99%)	108 (100%)	0	100	100
21	N	165/176 (94%)	165 (100%)	0	100	100
22	O	160/162 (99%)	159 (99%)	1 (1%)	78	85
23	P	141/146 (97%)	140 (99%)	1 (1%)	76	83
24	Q	121/151 (80%)	121 (100%)	0	100	100
25	R	129/154 (84%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	S	155/156 (99%)	155 (100%)	0	100	100
27	T	98/137 (72%)	98 (100%)	0	100	100
28	U	93/107 (87%)	93 (100%)	0	100	100
29	V	104/105 (99%)	104 (100%)	0	100	100
30	W	211/213 (99%)	210 (100%)	1 (0%)	81	87
31	X	116/118 (98%)	114 (98%)	2 (2%)	53	66
32	Y	109/110 (99%)	108 (99%)	1 (1%)	70	80
33	Z	115/116 (99%)	115 (100%)	0	100	100
34	a	76/119 (64%)	76 (100%)	0	100	100
35	b	568/573 (99%)	564 (99%)	4 (1%)	76	83
36	c	81/88 (92%)	81 (100%)	0	100	100
37	d	94/97 (97%)	94 (100%)	0	100	100
38	e	109/111 (98%)	108 (99%)	1 (1%)	70	80
39	f	90/91 (99%)	90 (100%)	0	100	100
40	g	95/103 (92%)	95 (100%)	0	100	100
41	h	104/105 (99%)	104 (100%)	0	100	100
42	i	81/82 (99%)	81 (100%)	0	100	100
43	j	69/71 (97%)	69 (100%)	0	100	100
44	k	68/69 (99%)	68 (100%)	0	100	100
45	l	45/46 (98%)	45 (100%)	0	100	100
46	m	411/428 (96%)	408 (99%)	3 (1%)	76	83
47	n	332/548 (61%)	332 (100%)	0	100	100
48	o	118/199 (59%)	117 (99%)	1 (1%)	73	81
49	p	71/72 (99%)	70 (99%)	1 (1%)	59	70
50	q	145/420 (34%)	144 (99%)	1 (1%)	76	83
51	r	203/229 (89%)	202 (100%)	1 (0%)	81	87
52	s	65/70 (93%)	65 (100%)	0	100	100
53	t	256/287 (89%)	255 (100%)	1 (0%)	84	89
54	u	133/180 (74%)	133 (100%)	0	100	100
55	v	264/309 (85%)	263 (100%)	1 (0%)	84	89
56	w	172/178 (97%)	171 (99%)	1 (1%)	78	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	x	442/450 (98%)	435 (98%)	7 (2%)	55	68
58	y	210/211 (100%)	210 (100%)	0	100	100
59	z	77/95 (81%)	77 (100%)	0	100	100
60	4	471/520 (91%)	467 (99%)	4 (1%)	73	81
All	All	9306/10692 (87%)	9266 (100%)	40 (0%)	81	89

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	8	124	THR
9	B	335	ILE
10	C	138	ARG
10	C	177	ASP
12	E	91	VAL
15	H	132	VAL
15	H	157	ASN
19	L	46	ILE
22	O	84	LEU
23	P	36	ILE
30	W	228	VAL
31	X	24	LEU
31	X	134	ASP
32	Y	126	LEU
35	b	230	GLU
35	b	315	VAL
35	b	573	LEU
35	b	574	THR
38	e	31	ASN
46	m	388	VAL
46	m	417	GLU
46	m	440	LYS
48	o	102	PHE
49	p	26	VAL
50	q	203	ARG
51	r	194	PHE
53	t	274	ASN
55	v	267	ILE
56	w	166	VAL
57	x	75	VAL
57	x	115	ASP
57	x	146	ILE

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Mol	Chain	Res	Type
57	x	159	MET
57	x	208	ASN
57	x	418	VAL
57	x	450	VAL
60	4	143	LEU
60	4	191	MET
60	4	255	ASN
60	4	370	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
7	8	115	GLN
7	8	156	ASN
9	B	182	GLN
10	C	48	GLN
10	C	59	GLN
10	C	196	ASN
11	D	151	GLN
12	E	97	ASN
14	G	24	ASN
14	G	28	HIS
14	G	243	GLN
15	H	96	HIS
15	H	102	ASN
18	K	225	ASN
18	K	250	ASN
18	K	269	GLN
18	K	330	ASN
19	L	99	HIS
19	L	106	GLN
19	L	114	GLN
19	L	120	GLN
20	M	11	ASN
20	M	56	GLN
21	N	95	GLN
22	O	182	ASN
25	R	141	HIS
25	R	156	ASN
26	S	74	ASN
26	S	122	HIS
27	T	54	HIS

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Mol	Chain	Res	Type
27	T	95	HIS
28	U	40	HIS
30	W	22	ASN
33	Z	106	GLN
33	Z	122	HIS
35	b	120	GLN
35	b	333	ASN
35	b	394	ASN
35	b	415	ASN
35	b	429	ASN
35	b	540	HIS
35	b	546	GLN
35	b	619	GLN
35	b	626	ASN
36	c	75	ASN
37	d	43	HIS
38	e	13	HIS
38	e	49	ASN
38	e	71	HIS
39	f	17	GLN
39	f	24	ASN
40	g	3	GLN
40	g	69	HIS
40	g	98	GLN
41	h	59	ASN
41	h	99	GLN
42	i	12	ASN
42	i	35	ASN
42	i	63	ASN
43	j	48	ASN
45	l	4	GLN
45	l	33	ASN
46	m	80	ASN
47	n	157	ASN
47	n	160	GLN
47	n	165	GLN
47	n	230	HIS
48	o	100	HIS
51	r	13	GLN
51	r	49	GLN
51	r	68	HIS
51	r	179	GLN

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Mol	Chain	Res	Type
52	s	26	HIS
55	v	151	HIS
55	v	187	GLN
55	v	238	HIS
56	w	8	ASN
57	x	12	GLN
57	x	44	ASN
57	x	241	HIS
58	y	145	ASN
59	z	10	HIS
60	4	33	GLN
60	4	112	GLN
60	4	188	HIS
60	4	398	ASN
60	4	403	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	1	2976/3396 (87%)	512 (17%)	6 (0%)
3	2	157/158 (99%)	26 (16%)	0
4	3	120/121 (99%)	26 (21%)	0
6	6	54/74 (72%)	20 (37%)	0
All	All	3307/3749 (88%)	584 (17%)	6 (0%)

All (584) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	1	2	U
2	1	5	G
2	1	14	U
2	1	26	A
2	1	42	C
2	1	43	A
2	1	49	A
2	1	59	G
2	1	60	A
2	1	65	A
2	1	66	A
2	1	67	A
2	1	72	C

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Mol	Chain	Res	Type
2	1	92	G
2	1	109	A
2	1	110	G
2	1	111	C
2	1	117	U
2	1	121	A
2	1	122	A
2	1	135	C
2	1	136	G
2	1	155	G
2	1	156	G
2	1	157	A
2	1	166	C
2	1	172	G
2	1	182	U
2	1	187	A
2	1	190	U
2	1	191	U
2	1	200	C
2	1	206	G
2	1	210	U
2	1	218	G
2	1	219	A
2	1	220	G
2	1	238	A
2	1	244	G
2	1	249	U
2	1	250	U
2	1	251	G
2	1	252	U
2	1	253	A
2	1	262	U
2	1	263	C
2	1	269	G
2	1	284	A
2	1	286	U
2	1	295	A
2	1	305	U
2	1	306	A
2	1	311	C
2	1	323	A
2	1	329	U

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Mol	Chain	Res	Type
2	1	339	C
2	1	349	A
2	1	375	A
2	1	376	G
2	1	398	A
2	1	399	A
2	1	401	U
2	1	402	A
2	1	403	C
2	1	421	G
2	1	422	A
2	1	439	C
2	1	495	G
2	1	516	A
2	1	517	G
2	1	520	U
2	1	521	A
2	1	535	G
2	1	543	C
2	1	547	G
2	1	548	G
2	1	555	U
2	1	557	A
2	1	559	A
2	1	579	G
2	1	589	A
2	1	592	A
2	1	604	G
2	1	609	G
2	1	611	A
2	1	620	U
2	1	621	A
2	1	629	U
2	1	637	C
2	1	643	U
2	1	644	G
2	1	645	A
2	1	646	A
2	1	648	C
2	1	649	A2M
2	1	660	A
2	1	677	A

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Mol	Chain	Res	Type
2	1	681	U
2	1	691	A
2	1	705	A
2	1	712	G
2	1	715	A
2	1	719	U
2	1	720	A
2	1	750	G
2	1	758	C
2	1	761	A
2	1	764	U
2	1	765	C
2	1	766	U
2	1	767	U
2	1	776	PSU
2	1	777	U
2	1	781	G
2	1	785	G
2	1	806	A
2	1	808	A
2	1	817	A2M
2	1	818	C
2	1	830	A
2	1	837	A
2	1	861	C
2	1	874	U
2	1	875	G
2	1	896	A
2	1	907	G
2	1	914	A
2	1	916	G
2	1	917	A
2	1	921	A
2	1	923	C
2	1	926	A
2	1	936	A
2	1	937	G
2	1	938	C
2	1	944	C
2	1	954	U
2	1	957	C
2	1	960	PSU

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Mol	Chain	Res	Type
2	1	973	A
2	1	974	G
2	1	975	C
2	1	976	U
2	1	979	U
2	1	980	A
2	1	991	G
2	1	1064	A
2	1	1066	G
2	1	1072	G
2	1	1086	C
2	1	1094	U
2	1	1095	U
2	1	1096	U
2	1	1097	G
2	1	1098	A
2	1	1103	A
2	1	1105	A
2	1	1108	U
2	1	1109	U
2	1	1115	G
2	1	1116	G
2	1	1117	G
2	1	1132	C
2	1	1140	G
2	1	1143	A
2	1	1153	A
2	1	1155	C
2	1	1159	A
2	1	1160	C
2	1	1180	A
2	1	1181	U
2	1	1189	C
2	1	1191	U
2	1	1192	C
2	1	1193	A
2	1	1198	C
2	1	1204	A
2	1	1217	A
2	1	1221	A
2	1	1222	G
2	1	1224	C

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Mol	Chain	Res	Type
2	1	1244	A
2	1	1245	A
2	1	1250	G
2	1	1252	A
2	1	1254	C
2	1	1259	A
2	1	1263	A
2	1	1265	U
2	1	1271	A
2	1	1272	C
2	1	1277	C
2	1	1278	A
2	1	1287	A
2	1	1307	G
2	1	1308	A
2	1	1313	G
2	1	1348	U
2	1	1355	A
2	1	1356	U
2	1	1386	A
2	1	1391	C
2	1	1399	A
2	1	1404	G
2	1	1419	A
2	1	1421	G
2	1	1434	G
2	1	1436	U
2	1	1437	OMC
2	1	1446	A
2	1	1455	U
2	1	1481	A
2	1	1503	A
2	1	1508	C
2	1	1536	G
2	1	1539	A
2	1	1555	U
2	1	1557	A
2	1	1560	G
2	1	1561	G
2	1	1567	U
2	1	1568	U
2	1	1569	U

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Mol	Chain	Res	Type
2	1	1573	G
2	1	1575	A
2	1	1581	C
2	1	1582	C
2	1	1583	A
2	1	1587	A
2	1	1589	A
2	1	1628	C
2	1	1629	U
2	1	1639	C
2	1	1642	A
2	1	1643	A
2	1	1657	C
2	1	1705	U
2	1	1715	A
2	1	1724	U
2	1	1725	C
2	1	1741	A
2	1	1750	A
2	1	1751	G
2	1	1763	U
2	1	1770	G
2	1	1780	G
2	1	1797	A
2	1	1798	A
2	1	1813	A
2	1	1816	A
2	1	1817	G
2	1	1820	U
2	1	1821	U
2	1	1839	A
2	1	1842	A
2	1	1849	C
2	1	1866	C
2	1	1879	A
2	1	1880	U
2	1	1893	A
2	1	1906	G
2	1	1953	G
2	1	2094	C
2	1	2112	U
2	1	2121	G

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Mol	Chain	Res	Type
2	1	2122	G
2	1	2131	A
2	1	2140	U
2	1	2142	1MA
2	1	2158	A
2	1	2169	G
2	1	2193	U
2	1	2194	G
2	1	2197	OMC
2	1	2205	U
2	1	2209	U
2	1	2219	A
2	1	2220	A2M
2	1	2221	G
2	1	2222	A
2	1	2223	A
2	1	2225	U
2	1	2244	A
2	1	2249	G
2	1	2250	G
2	1	2268	U
2	1	2269	U
2	1	2272	G
2	1	2274	U
2	1	2276	G
2	1	2277	C
2	1	2316	G
2	1	2317	A
2	1	2334	U
2	1	2335	G
2	1	2336	U
2	1	2340	PSU
2	1	2371	G
2	1	2373	A
2	1	2374	C
2	1	2375	G
2	1	2388	U
2	1	2393	G
2	1	2397	A
2	1	2398	A
2	1	2401	A
2	1	2402	A

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Mol	Chain	Res	Type
2	1	2414	G
2	1	2416	PSU
2	1	2417	OMU
2	1	2418	G
2	1	2419	A
2	1	2422	C
2	1	2435	G
2	1	2445	A
2	1	2502	A
2	1	2504	U
2	1	2505	U
2	1	2514	U
2	1	2515	A
2	1	2523	A
2	1	2524	A
2	1	2530	G
2	1	2531	C
2	1	2532	U
2	1	2547	A
2	1	2549	G
2	1	2550	U
2	1	2552	C
2	1	2555	G
2	1	2561	A
2	1	2569	A
2	1	2570	U
2	1	2571	U
2	1	2572	C
2	1	2573	G
2	1	2586	G
2	1	2593	A
2	1	2595	A
2	1	2606	G
2	1	2607	G
2	1	2618	G
2	1	2619	G
2	1	2623	G
2	1	2624	G
2	1	2627	C
2	1	2655	U
2	1	2656	A
2	1	2659	G

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Mol	Chain	Res	Type
2	1	2672	G
2	1	2674	A
2	1	2676	A
2	1	2677	G
2	1	2678	A
2	1	2691	A
2	1	2693	C
2	1	2697	A
2	1	2698	G
2	1	2699	G
2	1	2704	A
2	1	2712	U
2	1	2715	A
2	1	2718	U
2	1	2719	U
2	1	2721	A
2	1	2730	G
2	1	2731	U
2	1	2749	G
2	1	2750	U
2	1	2754	G
2	1	2756	C
2	1	2758	A
2	1	2759	U
2	1	2760	C
2	1	2761	G
2	1	2762	A
2	1	2763	U
2	1	2766	U
2	1	2767	U
2	1	2771	U
2	1	2772	C
2	1	2777	G
2	1	2791	OMG
2	1	2792	A
2	1	2794	G
2	1	2797	C
2	1	2798	C
2	1	2799	A
2	1	2800	G
2	1	2801	A
2	1	2802	A

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Mol	Chain	Res	Type
2	1	2804	A
2	1	2810	C
2	1	2811	A
2	1	2817	A
2	1	2818	U
2	1	2819	A
2	1	2821	C
2	1	2822	U
2	1	2824	G
2	1	2834	G
2	1	2847	A
2	1	2849	C
2	1	2861	U
2	1	2864	A
2	1	2871	G
2	1	2872	A
2	1	2873	U
2	1	2876	C
2	1	2878	G
2	1	2887	A
2	1	2889	C
2	1	2898	G
2	1	2899	C
2	1	2923	PSU
2	1	2924	U
2	1	2925	C
2	1	2926	A
2	1	2935	U
2	1	2936	A
2	1	2941	A
2	1	2948	OMC
2	1	2953	U
2	1	2954	U
2	1	2955	U
2	1	2956	A
2	1	2970	C
2	1	2971	A
2	1	2978	U
2	1	2979	U
2	1	2980	U
2	1	2981	U
2	1	2983	C

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Mol	Chain	Res	Type
2	1	2990	G
2	1	2996	U
2	1	2997	G
2	1	3012	A
2	1	3022	G
2	1	3023	U
2	1	3032	A
2	1	3055	U
2	1	3056	U
2	1	3058	U
2	1	3078	U
2	1	3079	U
2	1	3080	G
2	1	3086	A
2	1	3092	C
2	1	3093	C
2	1	3100	U
2	1	3102	G
2	1	3104	U
2	1	3109	G
2	1	3122	A
2	1	3127	A
2	1	3129	A
2	1	3130	A
2	1	3131	U
2	1	3142	A
2	1	3151	U
2	1	3154	C
2	1	3155	U
2	1	3156	U
2	1	3157	U
2	1	3161	C
2	1	3163	A
2	1	3165	A
2	1	3167	A
2	1	3168	A
2	1	3171	U
2	1	3172	A
2	1	3173	G
2	1	3174	A
2	1	3176	G
2	1	3179	U

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Mol	Chain	Res	Type
2	1	3180	A
2	1	3181	C
2	1	3187	A
2	1	3196	U
2	1	3207	U
2	1	3210	A
2	1	3217	C
2	1	3218	A
2	1	3219	G
2	1	3224	G
2	1	3243	A
2	1	3244	A
2	1	3245	A
2	1	3247	G
2	1	3259	U
2	1	3263	G
2	1	3273	A
2	1	3276	G
2	1	3280	U
2	1	3282	U
2	1	3283	U
2	1	3284	G
2	1	3285	C
2	1	3286	G
2	1	3288	G
2	1	3294	A
2	1	3295	A
2	1	3304	U
2	1	3316	A
2	1	3319	U
2	1	3341	U
2	1	3345	G
2	1	3369	G
2	1	3375	A
2	1	3378	C
2	1	3389	U
2	1	3396	U
3	2	23	U
3	2	34	U
3	2	35	C
3	2	39	G
3	2	52	A

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Mol	Chain	Res	Type
3	2	59	A
3	2	62	C
3	2	63	G
3	2	75	G
3	2	80	A
3	2	82	U
3	2	83	C
3	2	84	C
3	2	85	G
3	2	86	U
3	2	87	G
3	2	88	A
3	2	90	U
3	2	95	G
3	2	104	A
3	2	106	C
3	2	111	A
3	2	113	U
3	2	125	U
3	2	126	A
3	2	151	C
4	3	11	A
4	3	14	U
4	3	18	C
4	3	22	A
4	3	33	U
4	3	49	G
4	3	50	PSU
4	3	51	A
4	3	54	U
4	3	65	G
4	3	72	A
4	3	73	C
4	3	74	C
4	3	76	A
4	3	83	U
4	3	85	G
4	3	86	U
4	3	87	G
4	3	93	C
4	3	95	A
4	3	99	G

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Mol	Chain	Res	Type
4	3	102	A
4	3	109	G
4	3	112	G
4	3	114	U
4	3	121	U
6	6	4	U
6	6	5	C
6	6	6	U
6	6	7	C
6	6	17	G
6	6	23	U
6	6	24	A
6	6	33	U
6	6	43	A
6	6	47	A
6	6	48	A
6	6	49	C
6	6	52	G
6	6	54	A
6	6	56	U
6	6	58	G
6	6	59	C
6	6	228	U
6	6	229	U
6	6	231	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	1	374	A
2	1	588	G
2	1	1355	A
2	1	1568	U
2	1	3121	U
2	1	3283	U

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

57 non-standard protein/DNA/RNA residues are modelled in this entry.

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
2	OMC	1	663	2	19,22,23	0.53	0	25,31,34	0.70	0
2	OMC	1	1437	2,62	19,22,23	0.57	0	25,31,34	1.01	1 (4%)
2	PSU	1	2133	2	18,21,22	1.04	1 (5%)	21,30,33	1.62	4 (19%)
2	5MC	1	2278	2	19,22,23	1.66	3 (15%)	26,32,35	1.11	3 (11%)
2	PSU	1	2266	2	18,21,22	1.20	2 (11%)	21,30,33	1.54	5 (23%)
2	PSU	1	2314	2	18,21,22	1.14	1 (5%)	21,30,33	1.54	4 (19%)
2	OMU	1	2729	2	19,22,23	0.76	1 (5%)	25,31,34	0.93	2 (8%)
2	OMG	1	867	2	23,26,27	1.11	4 (17%)	32,38,41	0.88	1 (3%)
2	PSU	1	2264	2	18,21,22	1.21	2 (11%)	21,30,33	1.56	4 (19%)
2	PSU	1	1110	2	18,21,22	1.22	2 (11%)	21,30,33	1.54	5 (23%)
2	PSU	1	2129	2	18,21,22	1.13	1 (5%)	21,30,33	1.52	4 (19%)
2	OMU	1	2724	2	19,22,23	0.83	1 (5%)	25,31,34	0.85	1 (4%)
2	OMU	1	2347	2	19,22,23	0.83	1 (5%)	25,31,34	0.82	1 (4%)
2	A2M	1	1133	2	22,25,26	1.37	2 (9%)	30,36,39	1.02	2 (6%)
3	PSU	2	73	3	18,21,22	1.10	1 (5%)	21,30,33	1.56	4 (19%)
2	OMC	1	2197	2	19,22,23	0.48	0	25,31,34	0.66	0
2	PSU	1	960	2	18,21,22	1.17	2 (11%)	21,30,33	1.49	4 (19%)
2	OMG	1	908	2	23,26,27	1.17	4 (17%)	32,38,41	0.89	1 (3%)
2	OMG	1	1450	2	23,26,27	1.10	4 (17%)	32,38,41	0.81	0
2	OMC	1	650	2	19,22,23	0.52	0	25,31,34	0.65	0
2	OMU	1	2921	2	19,22,23	0.90	1 (5%)	25,31,34	0.93	2 (8%)
4	PSU	3	50	4	18,21,22	1.23	2 (11%)	21,30,33	1.60	4 (19%)
2	OMG	1	2815	2	23,26,27	1.16	4 (17%)	32,38,41	0.88	1 (3%)
2	OMC	1	2948	2	19,22,23	0.52	0	25,31,34	0.88	1 (4%)
2	PSU	1	1124	2	18,21,22	1.18	1 (5%)	21,30,33	1.57	4 (19%)
2	OMU	1	2417	2	19,22,23	0.81	1 (5%)	25,31,34	0.91	2 (8%)
2	OMG	1	2791	2	23,26,27	1.20	4 (17%)	32,38,41	0.89	1 (3%)
2	A2M	1	1449	2,62	22,25,26	1.30	2 (9%)	30,36,39	0.94	2 (6%)
2	1MA	1	2142	2,62	21,25,26	0.50	0	30,37,40	0.81	1 (3%)
2	PSU	1	990	2	18,21,22	1.16	1 (5%)	21,30,33	1.51	4 (19%)
2	OMG	1	2793	2	23,26,27	1.21	4 (17%)	32,38,41	0.98	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	1	2865	2	18,21,22	1.21	2 (11%)	21,30,33	1.55	4 (19%)
2	PSU	1	776	2	18,21,22	1.23	3 (16%)	21,30,33	1.58	4 (19%)
2	OMC	1	2959	2	19,22,23	0.54	0	25,31,34	0.81	1 (4%)
2	PSU	1	2191	2	18,21,22	1.15	1 (5%)	21,30,33	1.59	4 (19%)
2	A2M	1	817	2,62	22,25,26	1.33	2 (9%)	30,36,39	0.97	2 (6%)
2	PSU	1	2340	2	18,21,22	1.13	1 (5%)	21,30,33	1.57	4 (19%)
2	PSU	1	2923	2	18,21,22	1.25	3 (16%)	21,30,33	1.30	5 (23%)
2	PSU	1	2826	2,62	18,21,22	1.12	1 (5%)	21,30,33	1.64	4 (19%)
2	A2M	1	649	2	22,25,26	1.35	3 (13%)	30,36,39	0.99	2 (6%)
2	OMU	1	1888	2	19,22,23	1.17	1 (5%)	25,31,34	1.34	4 (16%)
2	5MC	1	2870	2	19,22,23	1.57	3 (15%)	26,32,35	1.15	2 (7%)
2	PSU	1	966	2	18,21,22	1.24	3 (16%)	21,30,33	1.57	4 (19%)
2	OMU	1	898	2	19,22,23	0.76	1 (5%)	25,31,34	0.93	2 (8%)
2	A2M	1	876	2	22,25,26	1.35	2 (9%)	30,36,39	0.92	1 (3%)
2	OMU	1	2421	2	19,22,23	0.83	1 (5%)	25,31,34	0.91	2 (8%)
2	A2M	1	2220	2	22,25,26	1.50	4 (18%)	30,36,39	1.08	3 (10%)
2	PSU	1	2880	2	18,21,22	1.19	1 (5%)	21,30,33	1.52	4 (19%)
2	OMG	1	805	2	23,26,27	1.14	4 (17%)	32,38,41	0.93	1 (3%)
2	A2M	1	807	2	22,25,26	1.39	3 (13%)	30,36,39	0.96	2 (6%)
2	PSU	1	2735	2	18,21,22	1.15	1 (5%)	21,30,33	1.57	4 (19%)
2	OMC	1	2337	2	19,22,23	0.50	0	25,31,34	0.69	0
2	PSU	1	2351	2	18,21,22	1.16	1 (5%)	21,30,33	1.58	4 (19%)
2	PSU	1	2416	2	18,21,22	1.18	1 (5%)	21,30,33	1.62	4 (19%)
2	PSU	1	986	2	18,21,22	1.15	2 (11%)	21,30,33	1.46	4 (19%)
2	PSU	1	2975	2	18,21,22	1.14	1 (5%)	21,30,33	1.67	4 (19%)
2	PSU	1	2349	2,62	18,21,22	1.10	1 (5%)	21,30,33	1.49	6 (28%)

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
2	OMC	1	663	2	-	1/9/27/28	0/2/2/2
2	OMC	1	1437	2,62	-	4/9/27/28	0/2/2/2
2	PSU	1	2133	2	-	0/7/25/26	0/2/2/2
2	5MC	1	2278	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	1	2266	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2314	2	-	0/7/25/26	0/2/2/2
2	OMU	1	2729	2	-	0/9/27/28	0/2/2/2
2	OMG	1	867	2	-	0/9/27/28	0/3/3/3
2	PSU	1	2264	2	-	0/7/25/26	0/2/2/2
2	PSU	1	1110	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2129	2	-	0/7/25/26	0/2/2/2
2	OMU	1	2724	2	-	0/9/27/28	0/2/2/2
2	OMU	1	2347	2	-	0/9/27/28	0/2/2/2
2	A2M	1	1133	2	-	0/9/27/28	0/3/3/3
3	PSU	2	73	3	-	0/7/25/26	0/2/2/2
2	OMC	1	2197	2	-	2/9/27/28	0/2/2/2
2	PSU	1	960	2	-	2/7/25/26	0/2/2/2
2	OMG	1	908	2	-	0/9/27/28	0/3/3/3
2	OMG	1	1450	2	-	2/9/27/28	0/3/3/3
2	OMC	1	650	2	-	0/9/27/28	0/2/2/2
2	OMU	1	2921	2	-	7/9/27/28	0/2/2/2
4	PSU	3	50	4	-	2/7/25/26	0/2/2/2
2	OMG	1	2815	2	-	0/9/27/28	0/3/3/3
2	OMC	1	2948	2	-	2/9/27/28	0/2/2/2
2	PSU	1	1124	2	-	0/7/25/26	0/2/2/2
2	OMU	1	2417	2	-	2/9/27/28	0/2/2/2
2	OMG	1	2791	2	-	3/9/27/28	0/3/3/3
2	A2M	1	1449	2,62	-	0/9/27/28	0/3/3/3
2	1MA	1	2142	2,62	-	2/7/25/26	0/3/3/3
2	PSU	1	990	2	-	0/7/25/26	0/2/2/2
2	OMG	1	2793	2	-	0/9/27/28	0/3/3/3
2	PSU	1	2865	2	-	2/7/25/26	0/2/2/2
2	PSU	1	776	2	-	2/7/25/26	0/2/2/2
2	OMC	1	2959	2	-	0/9/27/28	0/2/2/2
2	PSU	1	2191	2	-	0/7/25/26	0/2/2/2
2	A2M	1	817	2,62	-	2/9/27/28	0/3/3/3
2	PSU	1	2340	2	-	3/7/25/26	0/2/2/2
2	PSU	1	2923	2	-	3/7/25/26	0/2/2/2
2	PSU	1	2826	2,62	-	1/7/25/26	0/2/2/2
2	A2M	1	649	2	-	3/9/27/28	0/3/3/3
2	OMU	1	1888	2	-	2/9/27/28	0/2/2/2
2	5MC	1	2870	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	1	966	2	-	0/7/25/26	0/2/2/2
2	OMU	1	898	2	-	0/9/27/28	0/2/2/2
2	A2M	1	876	2	-	0/9/27/28	0/3/3/3
2	OMU	1	2421	2	-	2/9/27/28	0/2/2/2
2	A2M	1	2220	2	-	2/9/27/28	0/3/3/3
2	PSU	1	2880	2	-	0/7/25/26	0/2/2/2
2	OMG	1	805	2	-	1/9/27/28	0/3/3/3
2	A2M	1	807	2	-	0/9/27/28	0/3/3/3
2	PSU	1	2735	2	-	0/7/25/26	0/2/2/2
2	OMC	1	2337	2	-	0/9/27/28	0/2/2/2
2	PSU	1	2351	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2416	2	-	3/7/25/26	0/2/2/2
2	PSU	1	986	2	-	1/7/25/26	0/2/2/2
2	PSU	1	2975	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2349	2,62	-	0/7/25/26	0/2/2/2

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	2278	5MC	C5-C4	6.02	1.48	1.44
2	1	2870	5MC	C5-C4	5.65	1.48	1.44
2	1	1888	OMU	C2-N1	4.53	1.45	1.38
2	1	876	A2M	O5'-C5'	-3.67	1.33	1.44
2	1	1449	A2M	O5'-C5'	-3.64	1.33	1.44
2	1	2220	A2M	O5'-C5'	-3.64	1.33	1.44
2	1	807	A2M	O5'-C5'	-3.58	1.33	1.44
2	1	817	A2M	O5'-C5'	-3.55	1.33	1.44
2	1	1133	A2M	O5'-C5'	-3.54	1.33	1.44
4	3	50	PSU	C2-N1	3.38	1.41	1.36
2	1	2865	PSU	C2-N1	3.37	1.41	1.36
2	1	649	A2M	O5'-C5'	-3.36	1.34	1.44
2	1	1110	PSU	C2-N1	3.33	1.41	1.36
2	1	776	PSU	C2-N1	3.31	1.41	1.36
2	1	2975	PSU	C2-N1	3.30	1.41	1.36
2	1	2340	PSU	C2-N1	3.30	1.41	1.36
2	1	2264	PSU	C2-N1	3.29	1.41	1.36
2	1	966	PSU	C2-N1	3.27	1.40	1.36
2	1	2880	PSU	C2-N1	3.26	1.40	1.36
2	1	2351	PSU	C2-N1	3.24	1.40	1.36
2	1	1124	PSU	C2-N1	3.23	1.40	1.36
2	1	2191	PSU	C2-N1	3.23	1.40	1.36
2	1	2266	PSU	C2-N1	3.18	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	2735	PSU	C2-N1	3.13	1.40	1.36
2	1	2133	PSU	C2-N1	3.10	1.40	1.36
2	1	2416	PSU	C2-N1	3.10	1.40	1.36
2	1	2826	PSU	C2-N1	3.08	1.40	1.36
2	1	2793	OMG	C6-N1	3.06	1.44	1.38
2	1	2129	PSU	C2-N1	3.01	1.40	1.36
2	1	986	PSU	C2-N1	2.98	1.40	1.36
2	1	2314	PSU	C2-N1	2.96	1.40	1.36
2	1	908	OMG	C6-N1	2.96	1.44	1.38
2	1	960	PSU	C2-N1	2.96	1.40	1.36
3	2	73	PSU	C2-N1	2.95	1.40	1.36
2	1	990	PSU	C2-N1	2.94	1.40	1.36
2	1	2791	OMG	C6-N1	2.92	1.44	1.38
2	1	2923	PSU	C2-N1	2.92	1.40	1.36
2	1	2815	OMG	C6-N1	2.84	1.44	1.38
2	1	2349	PSU	C2-N1	2.84	1.40	1.36
2	1	867	OMG	C6-N1	2.82	1.44	1.38
2	1	805	OMG	C6-N1	2.81	1.44	1.38
2	1	2921	OMU	C2-N1	2.79	1.42	1.38
2	1	2278	5MC	C6-C5	2.78	1.39	1.34
2	1	2815	OMG	C2-N2	2.69	1.40	1.34
2	1	2791	OMG	C2-N2	2.68	1.40	1.34
2	1	1450	OMG	C6-N1	2.68	1.43	1.38
2	1	2347	OMU	C2-N1	2.68	1.42	1.38
2	1	2220	A2M	C5-C4	2.61	1.43	1.39
2	1	908	OMG	C2-N2	2.59	1.40	1.34
2	1	2724	OMU	C2-N1	2.58	1.42	1.38
2	1	1450	OMG	C2-N2	2.57	1.40	1.34
2	1	805	OMG	C2-N2	2.56	1.40	1.34
2	1	2793	OMG	C2-N2	2.55	1.40	1.34
2	1	867	OMG	C2-N2	2.52	1.40	1.34
2	1	898	OMU	C2-N1	2.43	1.42	1.38
2	1	2870	5MC	C6-C5	2.43	1.38	1.34
2	1	2421	OMU	C2-N1	2.42	1.42	1.38
2	1	2417	OMU	C2-N1	2.41	1.42	1.38
2	1	2793	OMG	C4-N3	2.40	1.39	1.34
2	1	2791	OMG	C4-N3	2.40	1.39	1.34
2	1	805	OMG	C4-N3	2.38	1.39	1.34
2	1	2815	OMG	C4-N3	2.38	1.39	1.34
2	1	2870	5MC	C6-N1	-2.35	1.34	1.38
2	1	1133	A2M	C5-C4	2.34	1.43	1.39
2	1	908	OMG	C4-N3	2.31	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	2793	OMG	C8-N9	2.31	1.42	1.37
2	1	876	A2M	C5-C4	2.29	1.43	1.39
2	1	1450	OMG	C4-N3	2.25	1.39	1.34
2	1	2791	OMG	C8-N9	2.25	1.42	1.37
2	1	867	OMG	C4-N3	2.24	1.39	1.34
2	1	2220	A2M	C4-N3	2.24	1.38	1.34
2	1	649	A2M	C5-C4	2.22	1.43	1.39
2	1	807	A2M	C5-C4	2.21	1.43	1.39
2	1	2278	5MC	C6-N1	-2.20	1.34	1.38
2	1	817	A2M	C5-C4	2.19	1.43	1.39
2	1	908	OMG	C8-N9	2.18	1.42	1.37
2	1	966	PSU	C6-N1	2.16	1.39	1.36
2	1	1449	A2M	C5-C4	2.16	1.42	1.39
4	3	50	PSU	C6-N1	2.16	1.39	1.36
2	1	2264	PSU	C6-N1	2.14	1.39	1.36
2	1	2220	A2M	C8-N9	2.13	1.41	1.37
2	1	2815	OMG	C8-N9	2.13	1.42	1.37
2	1	807	A2M	C8-N9	2.12	1.41	1.37
2	1	2729	OMU	C2-N1	2.12	1.41	1.38
2	1	960	PSU	C4-N3	2.10	1.42	1.38
2	1	805	OMG	C8-N9	2.08	1.42	1.37
2	1	1450	OMG	C8-N9	2.07	1.42	1.37
2	1	966	PSU	C4-N3	2.06	1.42	1.38
2	1	776	PSU	C6-N1	2.06	1.39	1.36
2	1	2923	PSU	C4-N3	2.05	1.42	1.38
2	1	776	PSU	C4-N3	2.04	1.42	1.38
2	1	649	A2M	O4'-C4'	-2.04	1.40	1.45
2	1	2266	PSU	C4-N3	2.04	1.42	1.38
2	1	2865	PSU	C4-N3	2.04	1.42	1.38
2	1	867	OMG	C8-N9	2.03	1.42	1.37
2	1	2923	PSU	C2-N3	2.03	1.40	1.37
2	1	986	PSU	C4-N3	2.03	1.42	1.38
2	1	1110	PSU	C6-N1	2.01	1.39	1.36

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	2975	PSU	C6-C5-C4	4.69	121.34	118.17
2	1	2865	PSU	C6-C5-C4	4.69	121.34	118.17
4	3	50	PSU	C6-C5-C4	4.62	121.29	118.17
2	1	2826	PSU	C6-C5-C4	4.56	121.25	118.17
2	1	2416	PSU	C6-C5-C4	4.52	121.23	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	2191	PSU	C6-C5-C4	4.45	121.18	118.17
2	1	776	PSU	C6-C5-C4	4.43	121.16	118.17
2	1	2735	PSU	C6-C5-C4	4.40	121.14	118.17
2	1	1124	PSU	C6-C5-C4	4.34	121.10	118.17
2	1	2351	PSU	C6-C5-C4	4.32	121.09	118.17
2	1	2264	PSU	C6-C5-C4	4.31	121.08	118.17
2	1	966	PSU	C6-C5-C4	4.26	121.05	118.17
2	1	2314	PSU	C6-C5-C4	4.16	120.98	118.17
3	2	73	PSU	C6-C5-C4	4.12	120.96	118.17
2	1	2340	PSU	C6-C5-C4	4.09	120.93	118.17
2	1	2129	PSU	C6-C5-C4	4.03	120.89	118.17
2	1	2266	PSU	C6-C5-C4	4.00	120.88	118.17
2	1	1110	PSU	C6-C5-C4	3.99	120.86	118.17
2	1	990	PSU	C6-C5-C4	3.98	120.86	118.17
2	1	2880	PSU	C6-C5-C4	3.94	120.83	118.17
2	1	2133	PSU	C6-C5-C4	3.84	120.77	118.17
2	1	960	PSU	C6-C5-C4	3.56	120.58	118.17
2	1	2870	5MC	C5-C6-N1	-3.40	119.62	123.31
2	1	986	PSU	C6-C5-C4	3.37	120.45	118.17
2	1	2349	PSU	C6-C5-C4	3.29	120.39	118.17
2	1	2923	PSU	O4-C4-N3	-3.28	113.95	120.11
2	1	2975	PSU	C4-N3-C2	-3.21	121.95	126.37
2	1	2133	PSU	O4-C4-N3	-3.20	114.09	120.11
2	1	2416	PSU	C4-N3-C2	-3.16	122.02	126.37
2	1	2826	PSU	C4-N3-C2	-3.16	122.02	126.37
2	1	2351	PSU	C4-N3-C2	-3.15	122.03	126.37
3	2	73	PSU	C4-N3-C2	-3.13	122.06	126.37
2	1	2129	PSU	C4-N3-C2	-3.11	122.08	126.37
2	1	966	PSU	C4-N3-C2	-3.10	122.09	126.37
2	1	2865	PSU	C4-N3-C2	-3.10	122.09	126.37
2	1	2349	PSU	O4-C4-N3	-3.09	114.30	120.11
2	1	2278	5MC	C5-C6-N1	-3.08	119.96	123.31
2	1	776	PSU	C4-N3-C2	-3.07	122.14	126.37
2	1	1124	PSU	C4-N3-C2	-3.02	122.21	126.37
2	1	2266	PSU	C4-N3-C2	-3.02	122.22	126.37
2	1	2880	PSU	C4-N3-C2	-3.01	122.22	126.37
2	1	986	PSU	O4-C4-N3	-3.01	114.45	120.11
2	1	990	PSU	C4-N3-C2	-3.00	122.23	126.37
2	1	2191	PSU	C4-N3-C2	-3.00	122.24	126.37
2	1	1110	PSU	C4-N3-C2	-2.98	122.26	126.37
4	3	50	PSU	C4-N3-C2	-2.98	122.27	126.37
2	1	2133	PSU	C4-N3-C2	-2.97	122.27	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	2735	PSU	C4-N3-C2	-2.97	122.28	126.37
2	1	2264	PSU	C4-N3-C2	-2.96	122.29	126.37
2	1	960	PSU	C4-N3-C2	-2.96	122.29	126.37
2	1	2314	PSU	C4-N3-C2	-2.95	122.31	126.37
2	1	2340	PSU	C4-N3-C2	-2.95	122.31	126.37
2	1	986	PSU	C4-N3-C2	-2.85	122.44	126.37
2	1	2278	5MC	C5-C4-N3	-2.77	118.91	121.75
2	1	2340	PSU	O4-C4-N3	-2.76	114.93	120.11
2	1	2349	PSU	C4-N3-C2	-2.74	122.60	126.37
2	1	1437	OMC	C1'-N1-C2	2.74	124.48	118.44
2	1	2220	A2M	N3-C4-N9	2.72	131.80	127.17
2	1	960	PSU	O4-C4-N3	-2.69	115.05	120.11
2	1	1110	PSU	O4-C4-N3	-2.68	115.07	120.11
2	1	2142	1MA	N1-C6-N6	2.68	126.44	119.71
2	1	2923	PSU	C4-N3-C2	-2.66	122.70	126.37
2	1	2191	PSU	O4-C4-N3	-2.64	115.15	120.11
2	1	1888	OMU	C1'-N1-C2	2.64	122.33	117.59
2	1	2880	PSU	O4-C4-N3	-2.63	115.16	120.11
2	1	2351	PSU	O4-C4-N3	-2.62	115.18	120.11
2	1	2266	PSU	O4-C4-N3	-2.58	115.26	120.11
2	1	2133	PSU	N1-C2-N3	2.56	117.87	115.17
2	1	1888	OMU	O2-C2-N1	2.56	126.13	122.80
2	1	966	PSU	O4-C4-N3	-2.55	115.31	120.11
3	2	73	PSU	O4-C4-N3	-2.55	115.31	120.11
2	1	2735	PSU	O4-C4-N3	-2.55	115.32	120.11
4	3	50	PSU	O4-C4-N3	-2.54	115.33	120.11
2	1	2264	PSU	O4-C4-N3	-2.54	115.34	120.11
2	1	990	PSU	O4-C4-N3	-2.53	115.36	120.11
2	1	1124	PSU	O4-C4-N3	-2.53	115.37	120.11
2	1	2975	PSU	O4-C4-N3	-2.52	115.38	120.11
2	1	2948	OMC	C1'-N1-C2	2.50	123.95	118.44
2	1	2129	PSU	O4-C4-N3	-2.49	115.42	120.11
2	1	776	PSU	O4-C4-N3	-2.48	115.44	120.11
2	1	2729	OMU	C4-N3-C2	-2.47	123.54	126.61
2	1	2416	PSU	O4-C4-N3	-2.46	115.49	120.11
2	1	2826	PSU	O4-C4-N3	-2.46	115.49	120.11
2	1	2314	PSU	O4-C4-N3	-2.45	115.50	120.11
2	1	2921	OMU	CM2-O2'-C2'	-2.44	108.20	114.47
2	1	2421	OMU	CM2-O2'-C2'	-2.40	108.31	114.47
2	1	2826	PSU	N1-C2-N3	2.39	117.69	115.17
2	1	2729	OMU	CM2-O2'-C2'	-2.39	108.33	114.47
2	1	2417	OMU	CM2-O2'-C2'	-2.39	108.33	114.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	2421	OMU	C4-N3-C2	-2.39	123.65	126.61
2	1	2417	OMU	C4-N3-C2	-2.38	123.66	126.61
2	1	2921	OMU	C4-N3-C2	-2.38	123.66	126.61
2	1	2865	PSU	O4-C4-N3	-2.38	115.65	120.11
2	1	898	OMU	C4-N3-C2	-2.32	123.73	126.61
2	1	2314	PSU	N1-C2-N3	2.32	117.62	115.17
2	1	2870	5MC	C5-C4-N3	-2.32	119.38	121.75
2	1	2975	PSU	N1-C2-N3	2.32	117.61	115.17
2	1	2340	PSU	N1-C2-N3	2.31	117.61	115.17
2	1	2724	OMU	C4-N3-C2	-2.31	123.75	126.61
2	1	817	A2M	C3'-C2'-C1'	-2.30	98.39	102.81
2	1	2220	A2M	C5-C4-N3	-2.30	123.55	126.72
3	2	73	PSU	N1-C2-N3	2.29	117.58	115.17
2	1	898	OMU	CM2-O2'-C2'	-2.28	108.63	114.47
2	1	776	PSU	N1-C2-N3	2.26	117.55	115.17
2	1	2735	PSU	N1-C2-N3	2.25	117.53	115.17
2	1	1888	OMU	CM2-O2'-C2'	-2.25	108.71	114.47
2	1	1133	A2M	N3-C4-N9	2.23	130.96	127.17
2	1	649	A2M	N3-C4-N9	2.23	130.96	127.17
2	1	990	PSU	N1-C2-N3	2.23	117.52	115.17
2	1	2347	OMU	C4-N3-C2	-2.22	123.86	126.61
2	1	2264	PSU	N1-C2-N3	2.21	117.50	115.17
2	1	2865	PSU	N1-C2-N3	2.21	117.50	115.17
2	1	960	PSU	N1-C2-N3	2.21	117.50	115.17
2	1	2349	PSU	N1-C2-N3	2.21	117.50	115.17
2	1	1124	PSU	N1-C2-N3	2.19	117.47	115.17
2	1	2416	PSU	N1-C2-N3	2.19	117.47	115.17
2	1	876	A2M	N3-C4-N9	2.19	130.88	127.17
2	1	966	PSU	N1-C2-N3	2.19	117.47	115.17
2	1	2191	PSU	N1-C2-N3	2.18	117.47	115.17
2	1	2351	PSU	N1-C2-N3	2.18	117.47	115.17
2	1	1133	A2M	C2'-C1'-N9	-2.17	110.18	113.75
2	1	2923	PSU	C6-C5-C4	2.17	119.64	118.17
2	1	2880	PSU	N1-C2-N3	2.17	117.45	115.17
2	1	1888	OMU	O2-C2-N3	-2.16	117.51	121.49
2	1	2266	PSU	N1-C2-N3	2.16	117.44	115.17
2	1	2791	OMG	O6-C6-N1	-2.16	116.06	120.11
2	1	2815	OMG	O6-C6-N1	-2.16	116.06	120.11
2	1	1110	PSU	N1-C2-N3	2.16	117.44	115.17
4	3	50	PSU	N1-C2-N3	2.16	117.44	115.17
2	1	2129	PSU	N1-C2-N3	2.14	117.43	115.17
2	1	2278	5MC	O2-C2-N3	-2.14	118.96	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	805	OMG	O6-C6-N1	-2.13	116.11	120.11
2	1	986	PSU	N1-C2-N3	2.12	117.41	115.17
2	1	2923	PSU	O4-C4-C5	2.12	129.28	124.01
2	1	867	OMG	O6-C6-N1	-2.11	116.14	120.11
2	1	1110	PSU	O4'-C1'-C2'	2.10	108.06	105.15
2	1	2220	A2M	C2-N1-C6	-2.10	115.29	118.73
2	1	2959	OMC	C1'-N1-C2	2.10	123.07	118.44
2	1	2793	OMG	O6-C6-N1	-2.09	116.18	120.11
2	1	1449	A2M	C2-N1-C6	-2.08	115.32	118.73
2	1	2923	PSU	N1-C2-N3	2.07	117.35	115.17
2	1	2266	PSU	O4'-C1'-C2'	2.06	108.00	105.15
2	1	807	A2M	C2-N1-C6	-2.06	115.34	118.73
2	1	817	A2M	C2-N1-C6	-2.06	115.35	118.73
2	1	2349	PSU	O4-C4-C5	2.05	129.10	124.01
2	1	1449	A2M	N3-C4-N9	2.05	130.65	127.17
2	1	649	A2M	C2-N1-C6	-2.04	115.38	118.73
2	1	807	A2M	N3-C4-N9	2.03	130.62	127.17
2	1	908	OMG	O6-C6-N1	-2.03	116.30	120.11
2	1	2349	PSU	O4'-C1'-C2'	2.01	107.93	105.15

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1	776	PSU	C3'-C4'-C5'-O5'
2	1	776	PSU	O4'-C4'-C5'-O5'
2	1	960	PSU	O4'-C4'-C5'-O5'
2	1	1437	OMC	C1'-C2'-O2'-CM2
2	1	1450	OMG	O4'-C4'-C5'-O5'
2	1	1888	OMU	O4'-C1'-N1-C2
2	1	1888	OMU	O4'-C1'-N1-C6
2	1	2142	1MA	O4'-C4'-C5'-O5'
2	1	2197	OMC	C3'-C4'-C5'-O5'
2	1	2197	OMC	O4'-C4'-C5'-O5'
2	1	2340	PSU	O4'-C4'-C5'-O5'
2	1	2791	OMG	O4'-C4'-C5'-O5'
2	1	2921	OMU	C2'-C1'-N1-C2
2	1	2921	OMU	C2'-C1'-N1-C6
2	1	2923	PSU	O4'-C1'-C5-C4
2	1	2923	PSU	O4'-C1'-C5-C6
2	1	2948	OMC	O4'-C4'-C5'-O5'
4	3	50	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	1	960	PSU	C3'-C4'-C5'-O5'
2	1	2220	A2M	O4'-C4'-C5'-O5'
2	1	2220	A2M	C3'-C4'-C5'-O5'
2	1	2417	OMU	C3'-C4'-C5'-O5'
2	1	2417	OMU	O4'-C4'-C5'-O5'
2	1	2421	OMU	O4'-C4'-C5'-O5'
2	1	2948	OMC	C3'-C4'-C5'-O5'
4	3	50	PSU	C3'-C4'-C5'-O5'
2	1	1437	OMC	O4'-C4'-C5'-O5'
2	1	2142	1MA	C3'-C4'-C5'-O5'
2	1	2416	PSU	C3'-C4'-C5'-O5'
2	1	2421	OMU	C3'-C4'-C5'-O5'
2	1	2340	PSU	C3'-C4'-C5'-O5'
2	1	1450	OMG	C3'-C4'-C5'-O5'
2	1	2791	OMG	C3'-C4'-C5'-O5'
2	1	2416	PSU	O4'-C4'-C5'-O5'
2	1	2865	PSU	O4'-C4'-C5'-O5'
2	1	1437	OMC	C3'-C4'-C5'-O5'
2	1	2921	OMU	O4'-C4'-C5'-O5'
2	1	649	A2M	C4'-C5'-O5'-P
2	1	663	OMC	C1'-C2'-O2'-CM2
2	1	649	A2M	C3'-C4'-C5'-O5'
2	1	2921	OMU	C3'-C4'-C5'-O5'
2	1	2921	OMU	O4'-C1'-N1-C6
2	1	2921	OMU	O4'-C1'-N1-C2
2	1	2865	PSU	C3'-C4'-C5'-O5'
2	1	817	A2M	C4'-C5'-O5'-P
2	1	2340	PSU	C4'-C5'-O5'-P
2	1	2826	PSU	O4'-C1'-C5-C4
2	1	986	PSU	O4'-C4'-C5'-O5'
2	1	2416	PSU	C4'-C5'-O5'-P
2	1	2791	OMG	C4'-C5'-O5'-P
2	1	2923	PSU	C4'-C5'-O5'-P
2	1	649	A2M	O4'-C4'-C5'-O5'
2	1	2921	OMU	C4'-C5'-O5'-P
2	1	817	A2M	O4'-C4'-C5'-O5'
2	1	1437	OMC	C2'-C1'-N1-C2
2	1	805	OMG	C3'-C2'-O2'-CM2

There are no ring outliers.

19 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1	663	OMC	2	0
2	1	1437	OMC	2	0
2	1	2314	PSU	1	0
2	1	2724	OMU	2	0
2	1	2347	OMU	1	0
2	1	1133	A2M	1	0
2	1	908	OMG	1	0
2	1	1450	OMG	1	0
2	1	2417	OMU	1	0
2	1	1449	A2M	1	0
2	1	2793	OMG	2	0
2	1	2959	OMC	2	0
2	1	2191	PSU	1	0
2	1	898	OMU	2	0
2	1	876	A2M	1	0
2	1	2220	A2M	2	0
2	1	2880	PSU	1	0
2	1	807	A2M	1	0
2	1	986	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 93 ligands modelled in this entry, 87 are monoatomic - leaving 6 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	$\# Z > 2$
61	B3P	1	3401	62	18,18,18	1.50	2 (11%)	23,23,23	1.87	6 (26%)
64	GDP	m	801	66,62	29,30,30	1.17	3 (10%)	45,47,47	1.73	6 (13%)
64	GDP	b	801	62	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)
65	ALF	m	802	-	4,4,4	1.45	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	B3P	1	3402	-	18,18,18	1.52	2 (11%)	23,23,23	1.92	6 (26%)
61	B3P	1	3403	-	18,18,18	1.58	2 (11%)	23,23,23	1.88	6 (26%)

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
61	B3P	1	3401	62	-	4/28/28/28	-
64	GDP	m	801	66,62	-	3/16/32/32	0/3/3/3
64	GDP	b	801	62	-	3/16/32/32	0/3/3/3
61	B3P	1	3402	-	-	11/28/28/28	-
61	B3P	1	3403	-	-	8/28/28/28	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	1	3403	B3P	C6-C4	5.36	1.59	1.53
61	1	3402	B3P	C6-C4	5.04	1.59	1.53
61	1	3401	B3P	C6-C4	5.02	1.59	1.53
64	b	801	GDP	C5-C4	3.07	1.47	1.38
64	m	801	GDP	C5-C4	3.05	1.47	1.38
64	m	801	GDP	C6-N1	-2.45	1.34	1.38
61	1	3402	B3P	C7-C4	2.43	1.56	1.53
61	1	3403	B3P	C7-C4	2.43	1.56	1.53
61	1	3401	B3P	C7-C4	2.40	1.56	1.53
64	b	801	GDP	C6-N1	-2.38	1.34	1.38
64	m	801	GDP	C5-N7	-2.09	1.34	1.39
64	b	801	GDP	C5-N7	-2.05	1.35	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	b	801	GDP	C5-C4-N3	-6.00	118.84	128.39
64	m	801	GDP	C5-C4-N3	-5.83	119.10	128.39
61	1	3403	B3P	O5-C6-C4	5.06	121.98	111.68
61	1	3402	B3P	O5-C6-C4	5.02	121.88	111.68
64	b	801	GDP	C2-N3-C4	4.97	120.86	112.30
64	m	801	GDP	C2-N3-C4	4.93	120.78	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	1	3401	B3P	O5-C6-C4	4.88	121.60	111.68
64	b	801	GDP	N9-C4-N3	4.41	134.77	125.95
64	m	801	GDP	N9-C4-N3	4.32	134.59	125.95
61	1	3402	B3P	C3-N1-C4	-4.02	110.28	116.17
61	1	3401	B3P	C2-N2-C8	-3.75	110.68	116.17
61	1	3403	B3P	C3-N1-C4	-3.69	110.76	116.17
61	1	3403	B3P	C2-N2-C8	-3.60	110.89	116.17
61	1	3402	B3P	C2-N2-C8	-3.57	110.94	116.17
61	1	3401	B3P	C3-N1-C4	-3.55	110.97	116.17
64	m	801	GDP	C6-C5-N7	3.37	136.42	130.29
64	b	801	GDP	C6-C5-N7	3.29	136.28	130.29
61	1	3401	B3P	O3-C11-C8	-2.79	106.00	111.68
61	1	3402	B3P	O6-C7-C4	-2.76	106.06	111.68
61	1	3401	B3P	O6-C7-C4	-2.76	106.07	111.68
61	1	3402	B3P	O4-C5-C4	-2.69	106.21	111.68
61	1	3403	B3P	O6-C7-C4	-2.66	106.27	111.68
61	1	3401	B3P	O4-C5-C4	-2.66	106.28	111.68
61	1	3402	B3P	O3-C11-C8	-2.63	106.34	111.68
64	b	801	GDP	C4-C5-N7	-2.59	106.56	110.67
64	m	801	GDP	C4-C5-N7	-2.57	106.60	110.67
61	1	3403	B3P	O3-C11-C8	-2.53	106.54	111.68
61	1	3403	B3P	O4-C5-C4	-2.20	107.21	111.68
64	m	801	GDP	O6-C6-C5	-2.13	120.90	126.53
64	b	801	GDP	O6-C6-C5	-2.07	121.08	126.53

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	1	3401	B3P	N1-C4-C6-O5
61	1	3401	B3P	C5-C4-C6-O5
61	1	3401	B3P	C7-C4-C6-O5
61	1	3402	B3P	N1-C4-C5-O4
61	1	3402	B3P	C6-C4-C5-O4
61	1	3402	B3P	C7-C4-C5-O4
61	1	3402	B3P	N1-C4-C6-O5
61	1	3402	B3P	C5-C4-C6-O5
61	1	3402	B3P	C7-C4-C6-O5
61	1	3403	B3P	N1-C4-C5-O4
61	1	3403	B3P	C6-C4-C5-O4
61	1	3403	B3P	C7-C4-C5-O4
61	1	3403	B3P	N1-C4-C6-O5

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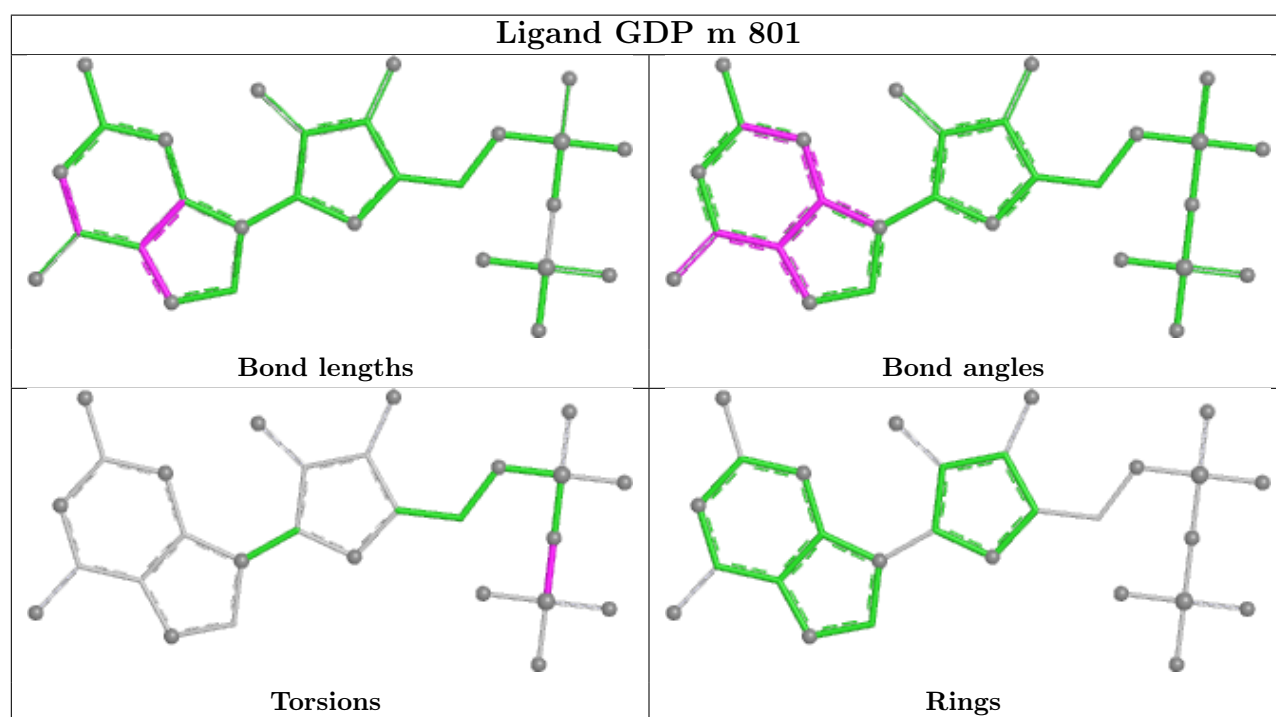
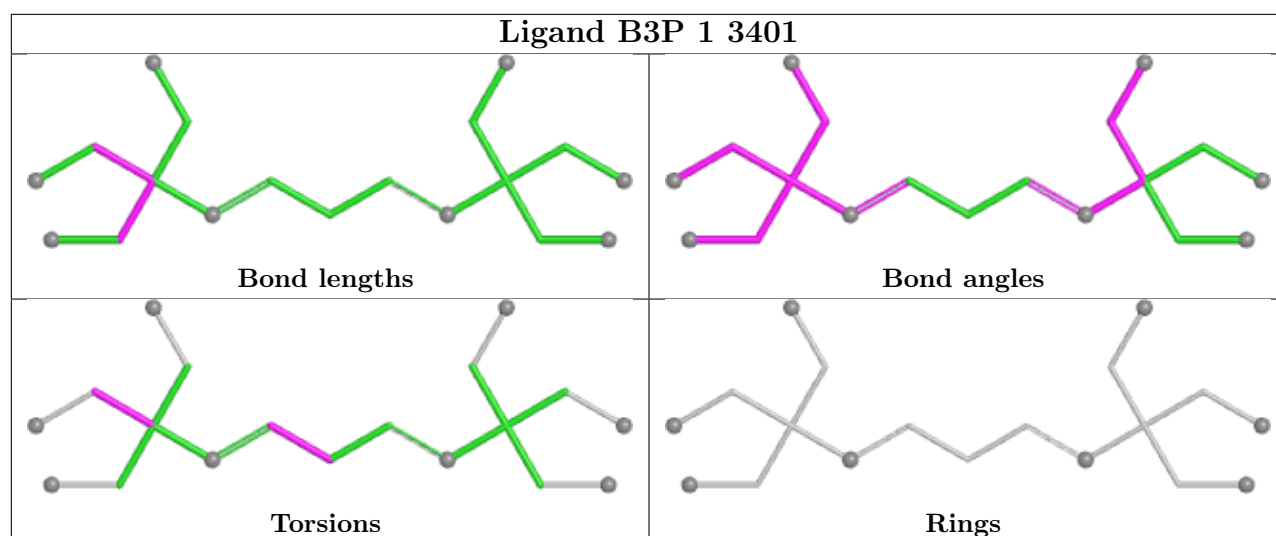
Mol	Chain	Res	Type	Atoms
61	1	3403	B3P	C5-C4-C6-O5
61	1	3403	B3P	C7-C4-C6-O5
64	b	801	GDP	C5'-O5'-PA-O3A
64	b	801	GDP	C5'-O5'-PA-O1A
64	m	801	GDP	PA-O3A-PB-O2B
64	m	801	GDP	PA-O3A-PB-O3B
61	1	3403	B3P	C2-C1-C3-N1
61	1	3401	B3P	C2-C1-C3-N1
61	1	3402	B3P	O3-C11-C8-N2
61	1	3402	B3P	C11-C8-N2-C2
61	1	3402	B3P	C1-C2-N2-C8
61	1	3402	B3P	C10-C8-N2-C2
61	1	3402	B3P	O3-C11-C8-C10
64	b	801	GDP	C5'-O5'-PA-O2A
61	1	3403	B3P	C5-C4-C7-O6
64	m	801	GDP	PA-O3A-PB-O1B

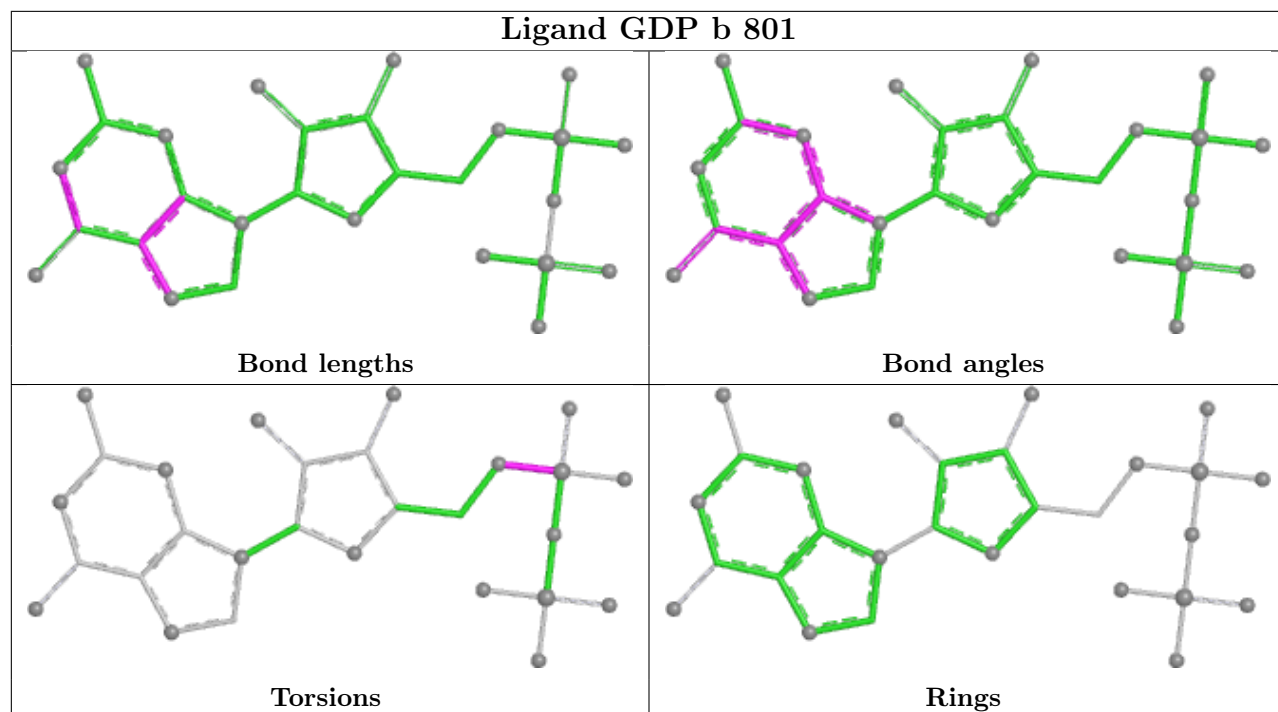
There are no ring outliers.

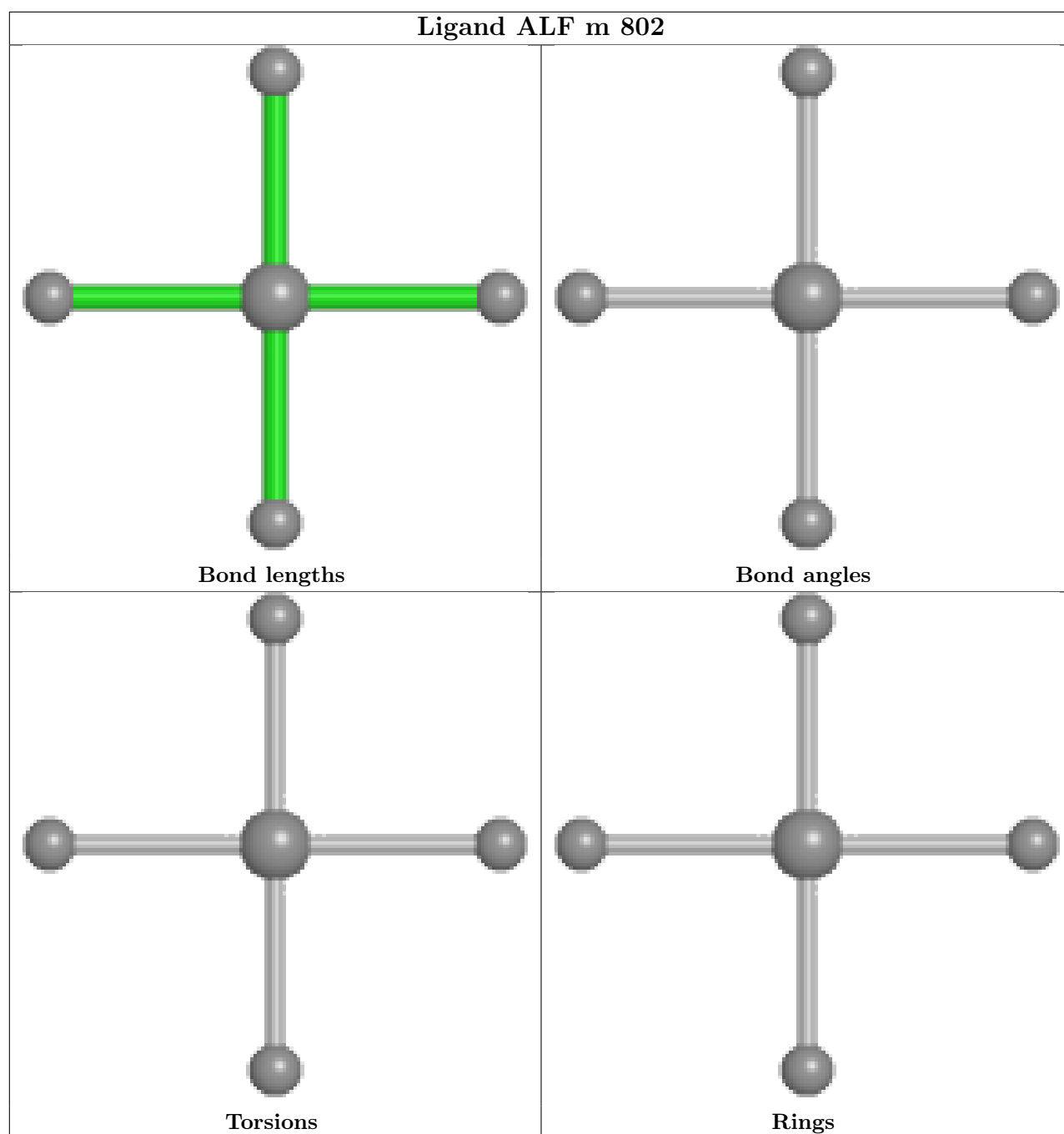
4 monomers are involved in 7 short contacts:

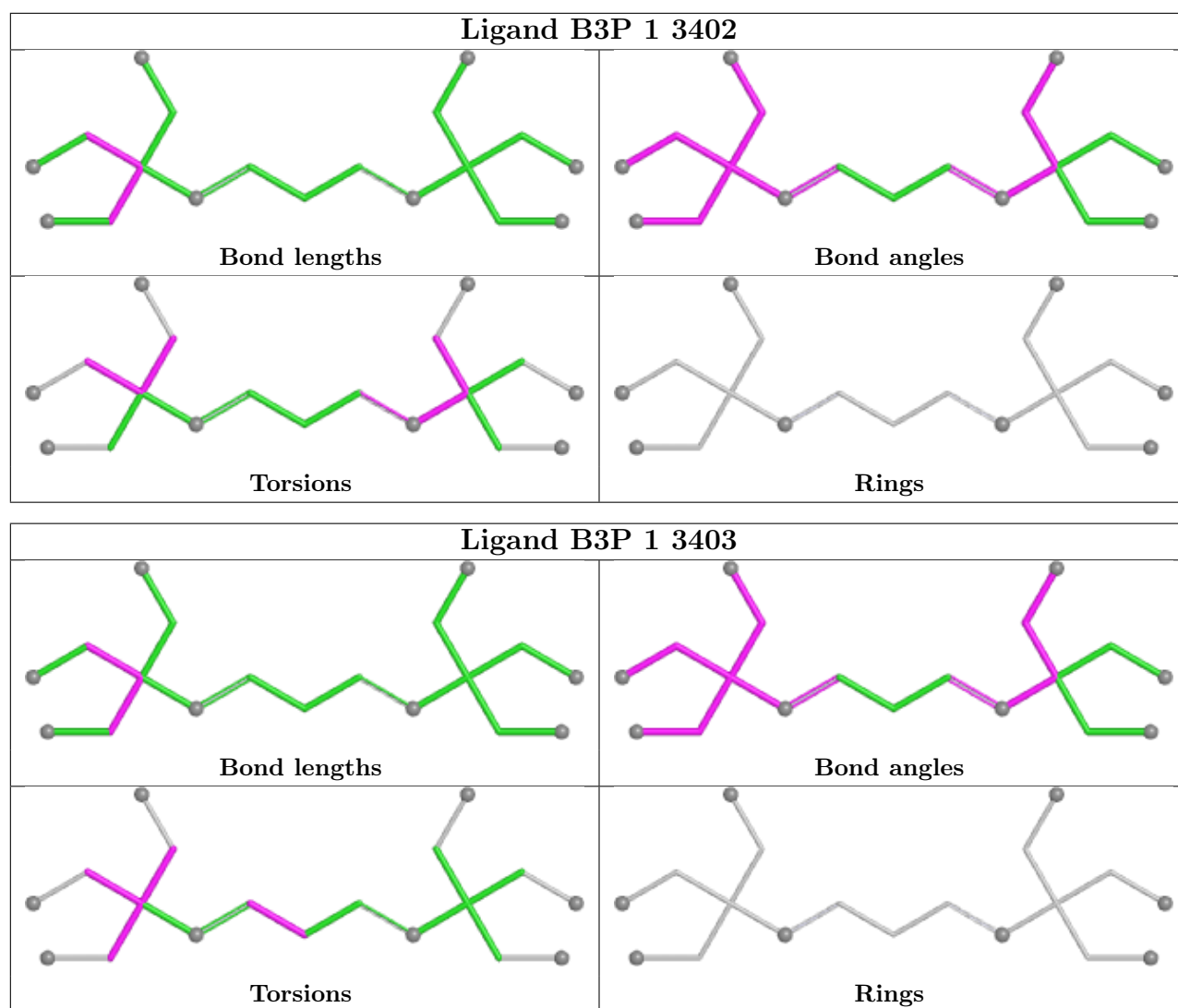
Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	1	3401	B3P	3	0
64	b	801	GDP	1	0
65	m	802	ALF	1	0
61	1	3403	B3P	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

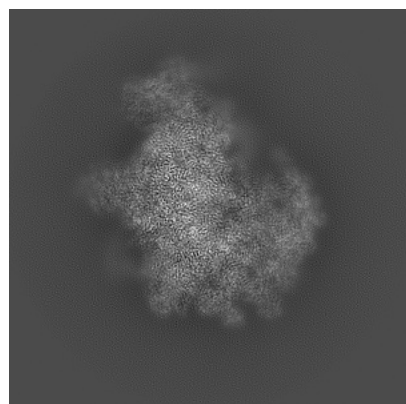
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26686. These allow visual inspection of the internal detail of the map and identification of artifacts.

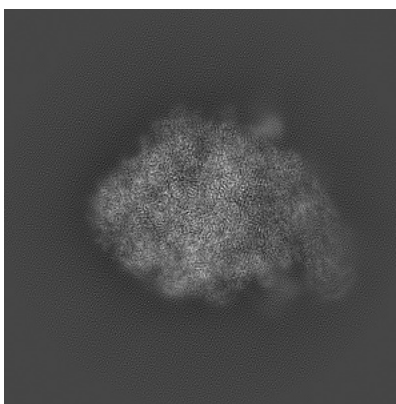
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

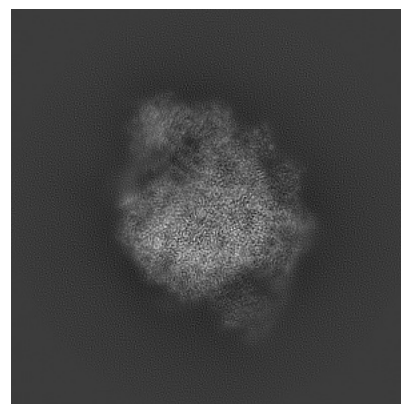
6.1.1 Primary map



X

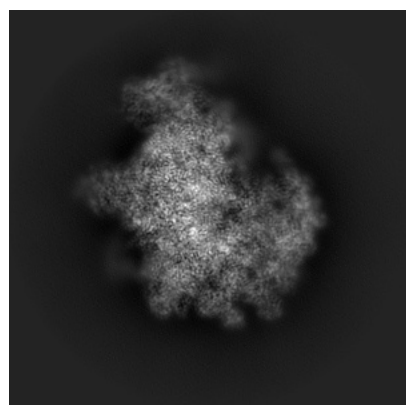


Y

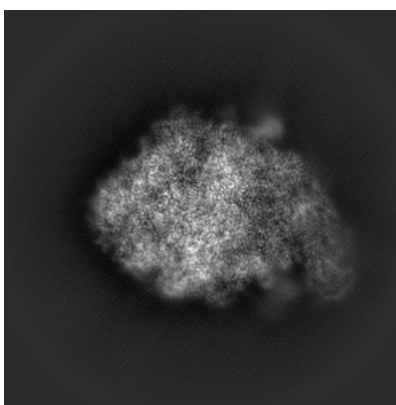


Z

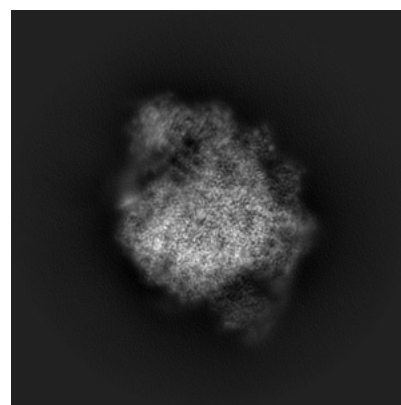
6.1.2 Raw map



X



Y

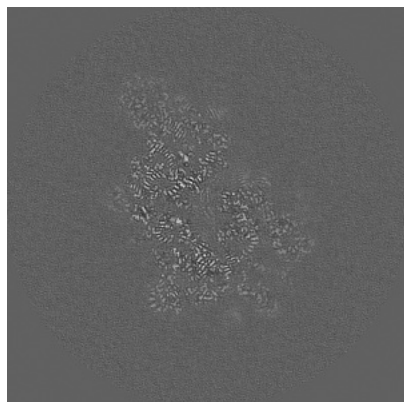


Z

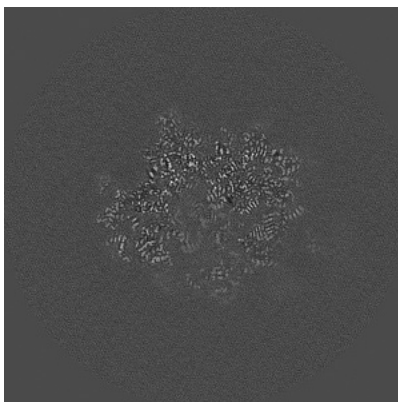
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

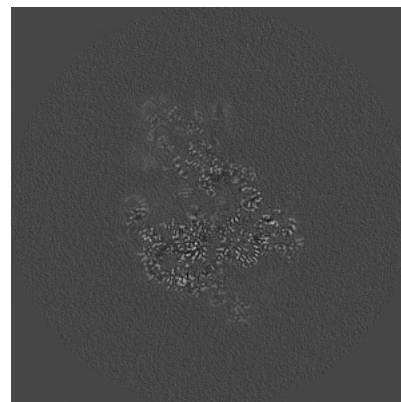
6.2.1 Primary map



X Index: 200

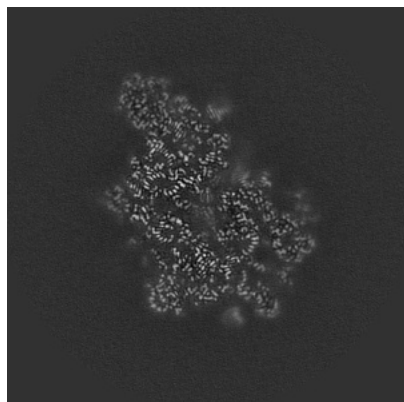


Y Index: 200

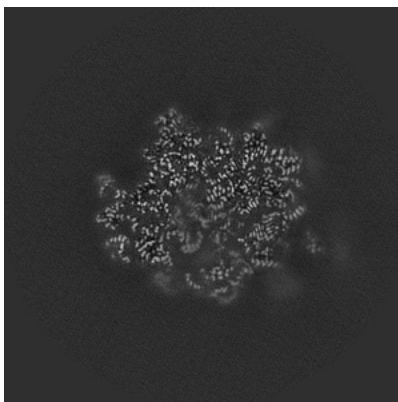


Z Index: 200

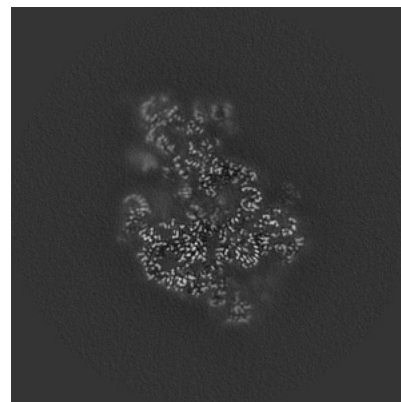
6.2.2 Raw map



X Index: 200



Y Index: 200

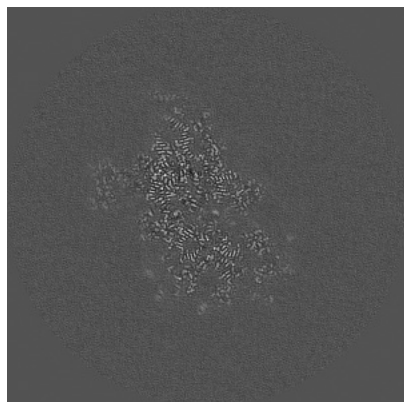


Z Index: 200

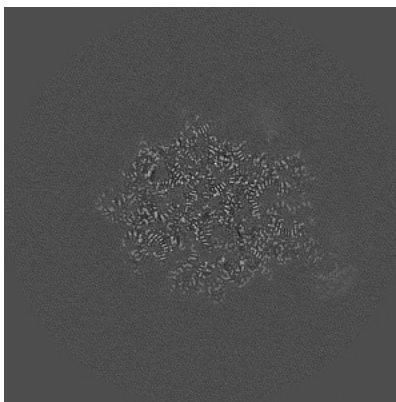
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

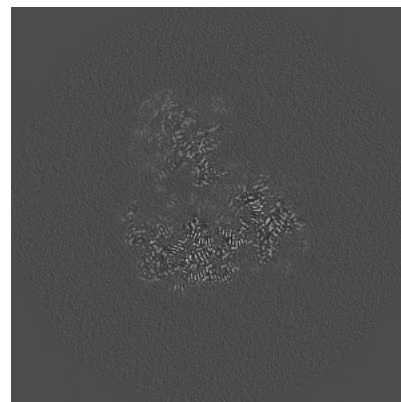
6.3.1 Primary map



X Index: 224

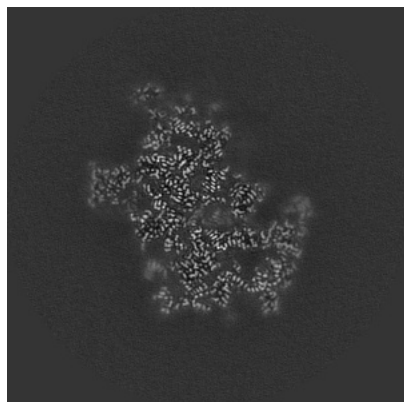


Y Index: 174

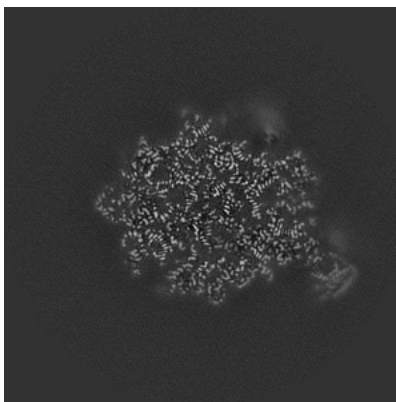


Z Index: 189

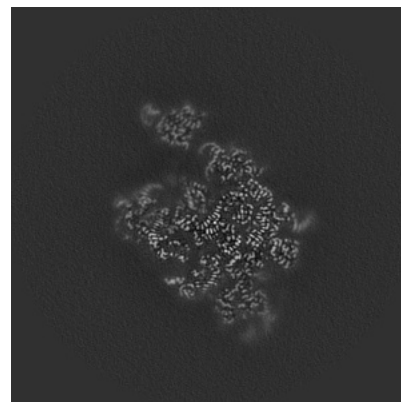
6.3.2 Raw map



X Index: 216



Y Index: 174

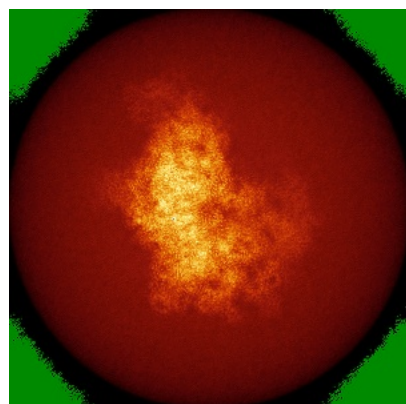


Z Index: 221

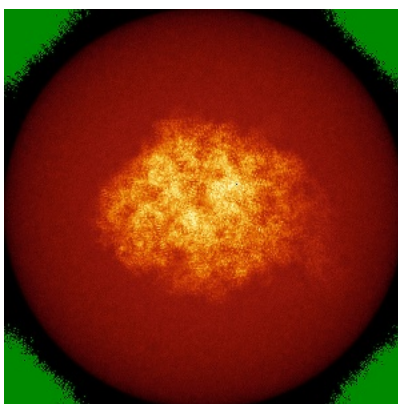
The images above show the largest variance slices of the map in three orthogonal directions.

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

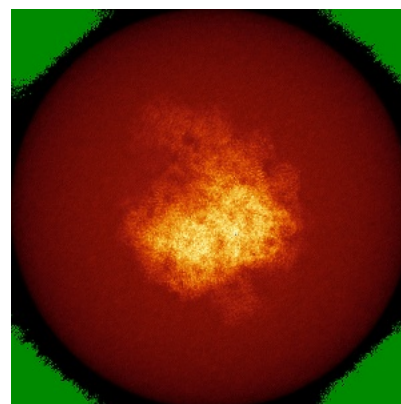
6.4.1 Primary map



X

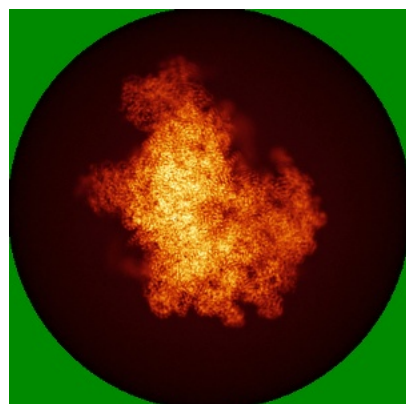


Y



Z

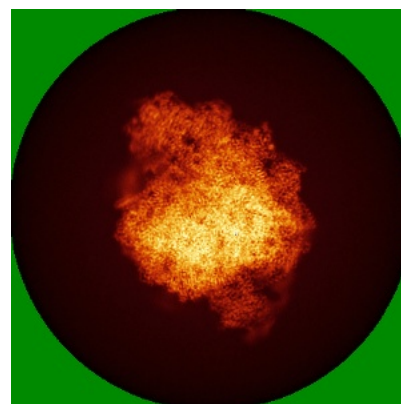
6.4.2 Raw map



X



Y

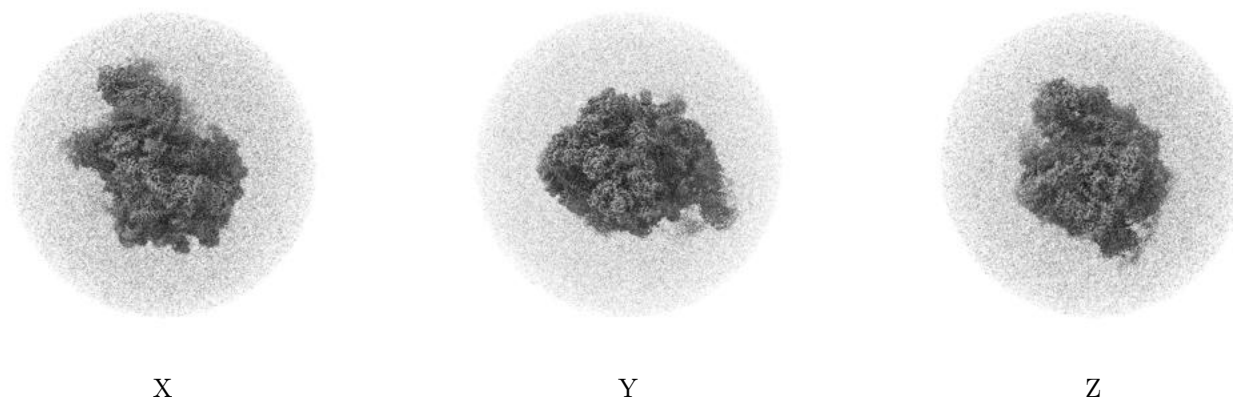


Z

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.

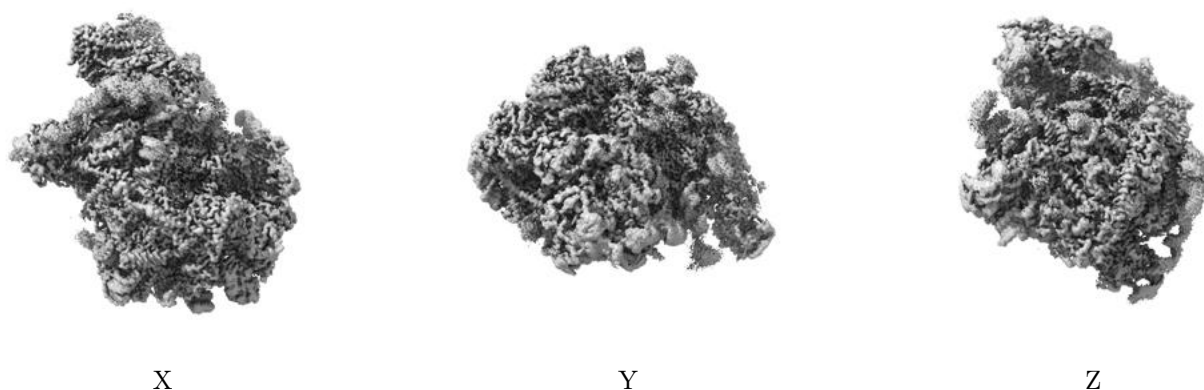
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. 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.

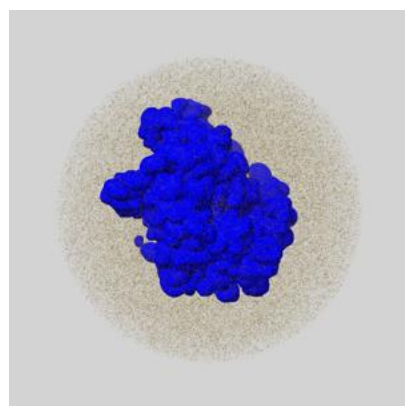
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

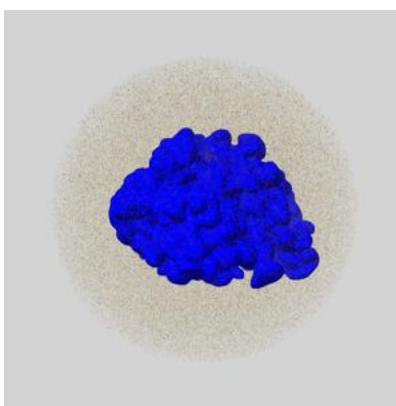
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

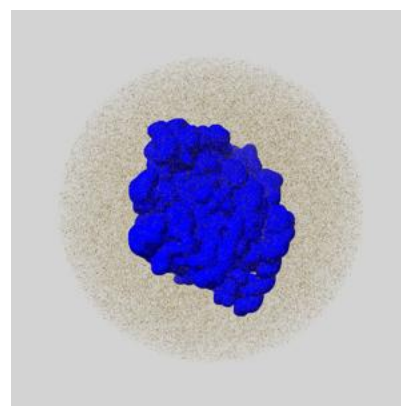
6.6.1 emd_26686_msk_1.map [i](#)



X



Y

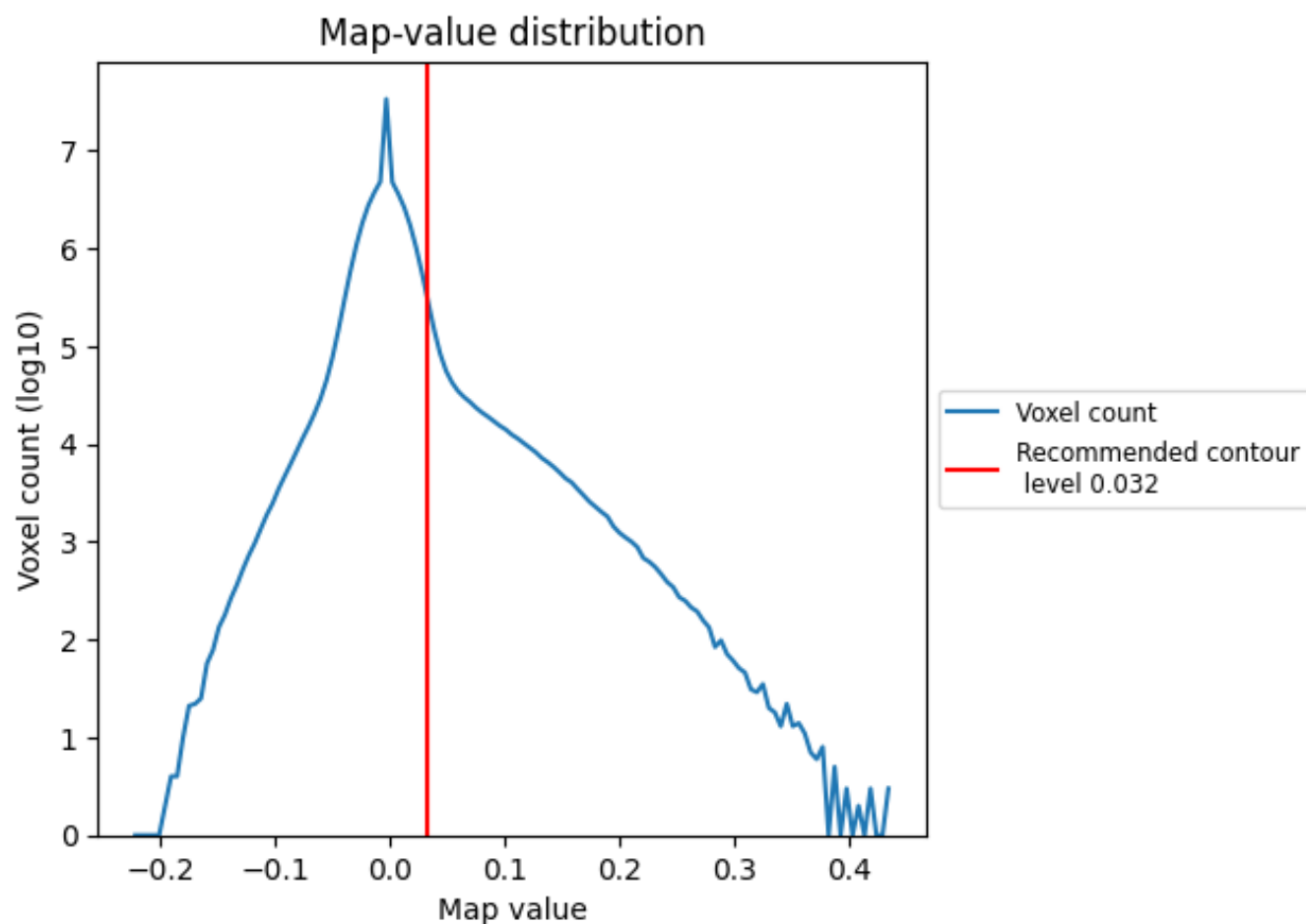


Z

7 Map analysis [i](#)

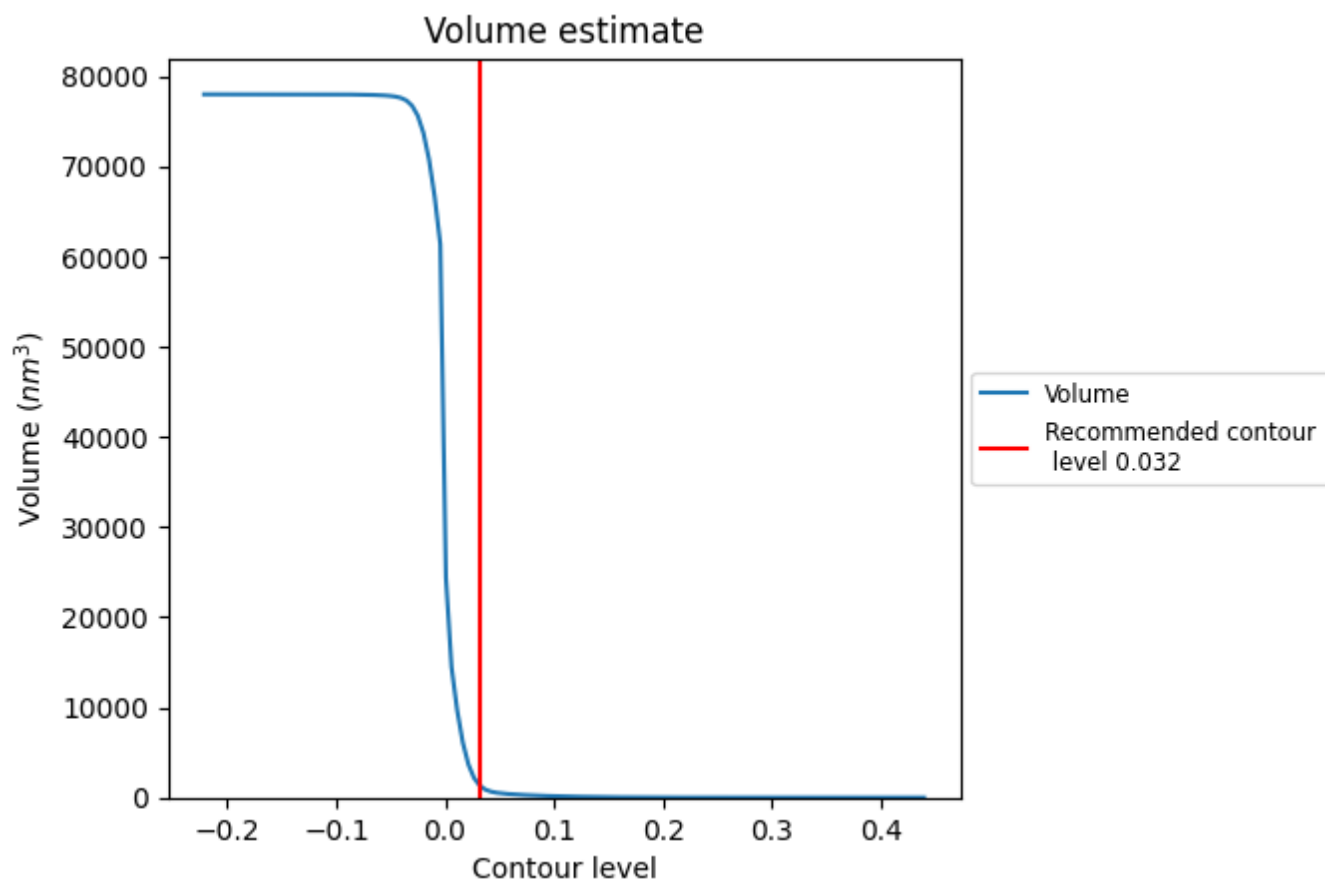
This section contains the results of statistical analysis of the map.

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.

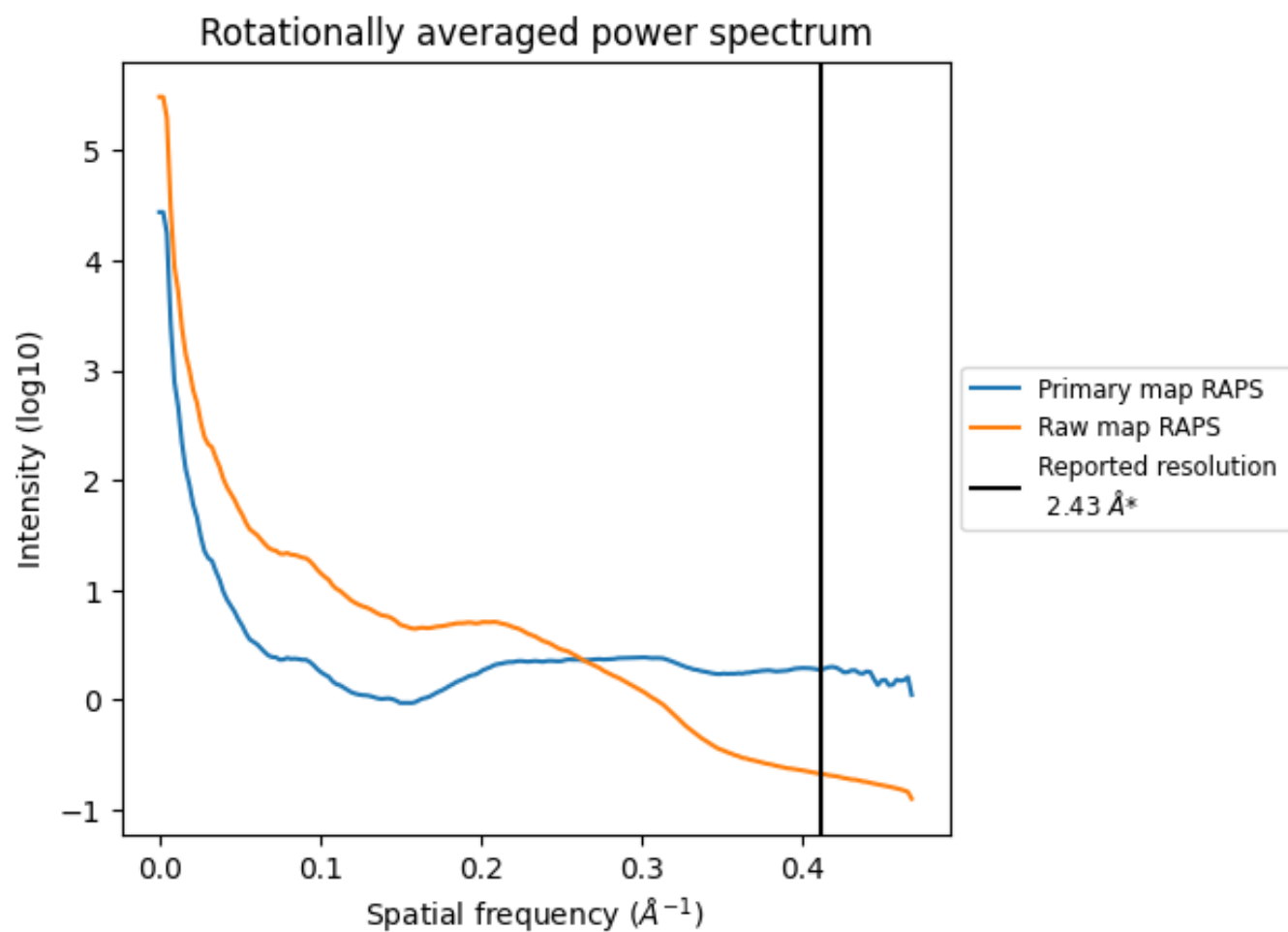
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1308 nm^3 ; this corresponds to an approximate mass of 1181 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

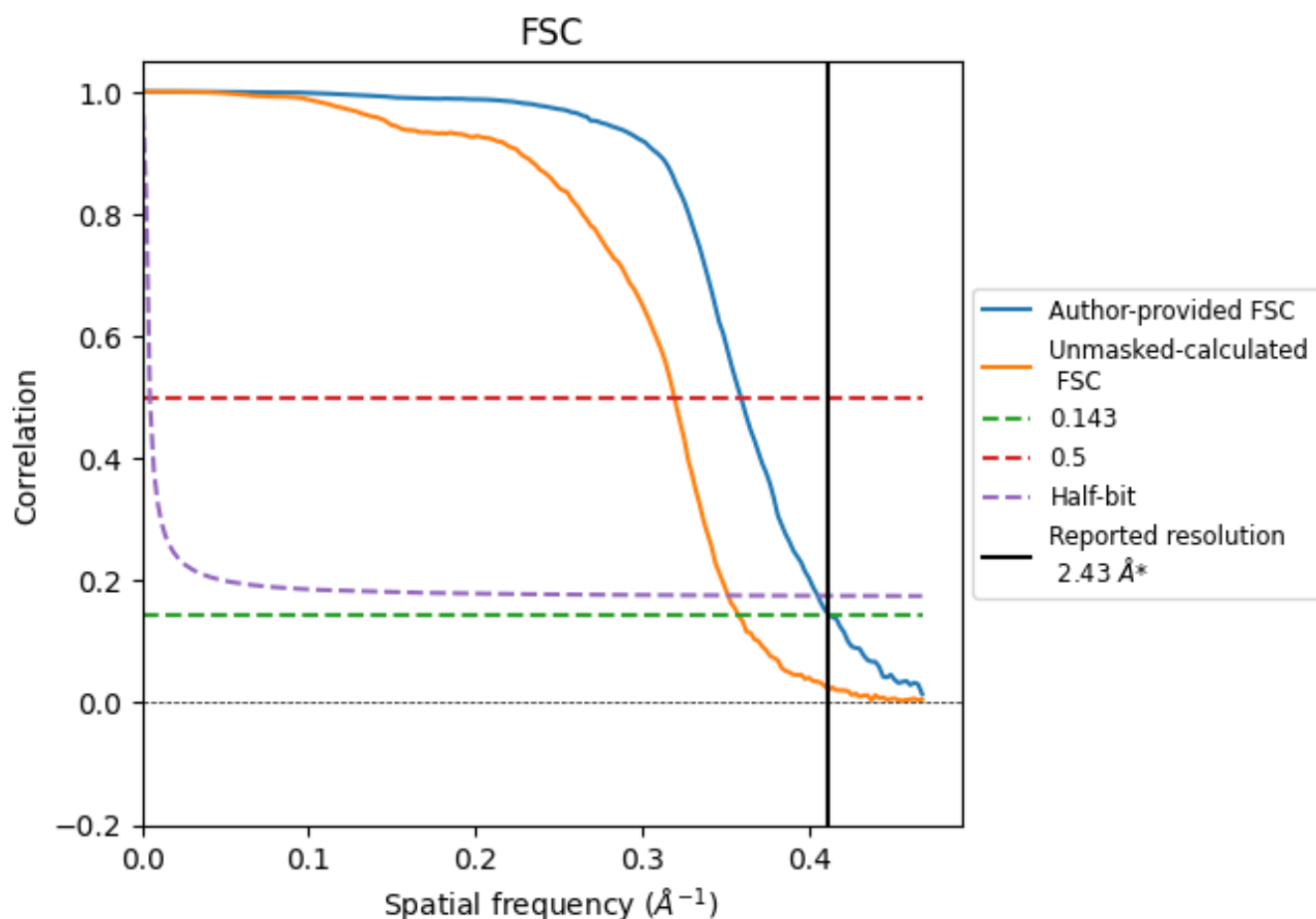


*Reported resolution corresponds to spatial frequency of 0.412 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.412 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

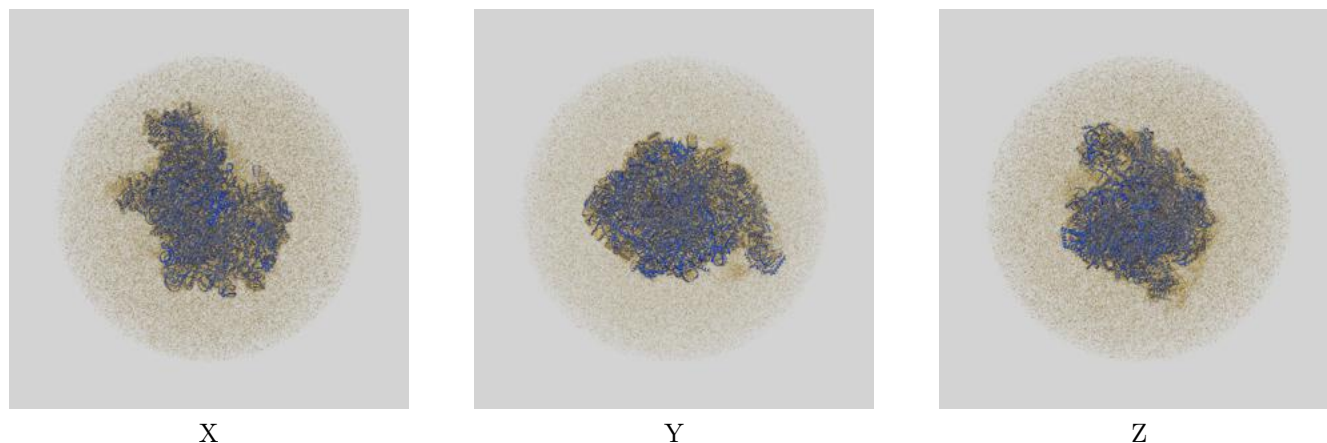
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.43	-	-
Author-provided FSC curve	2.42	2.78	2.47
Unmasked-calculated*	2.79	3.13	2.84

*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 2.79 differs from the reported value 2.43 by more than 10 %

9 Map-model fit [i](#)

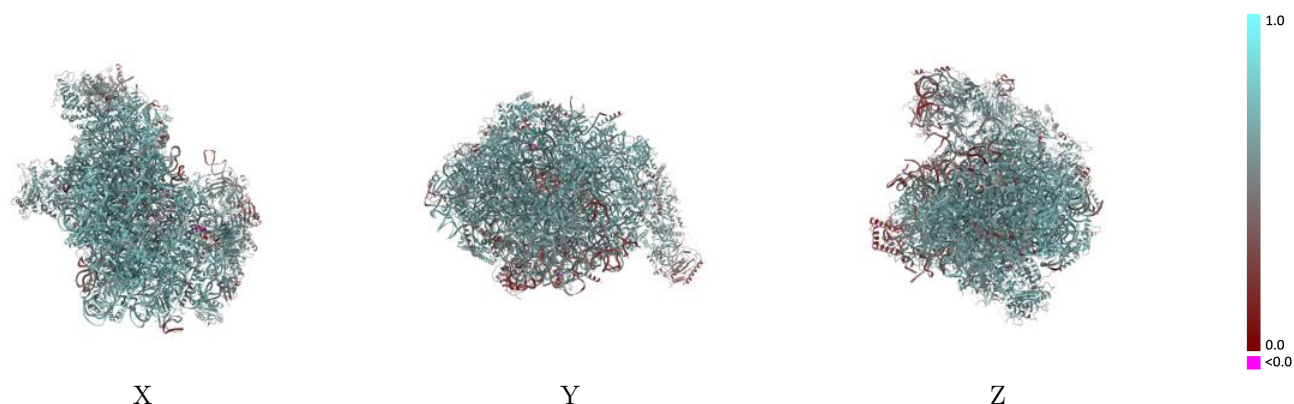
This section contains information regarding the fit between EMDB map EMD-26686 and PDB model 7UQB. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



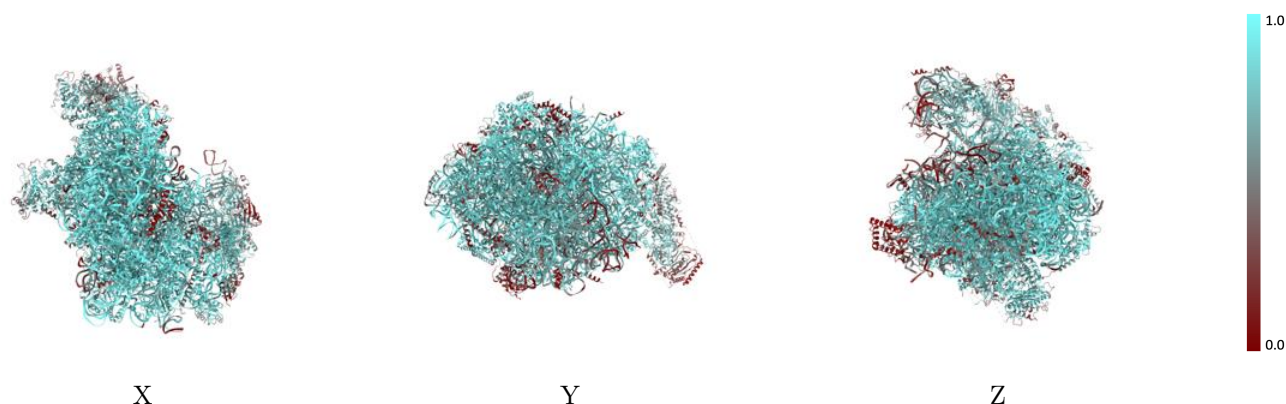
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



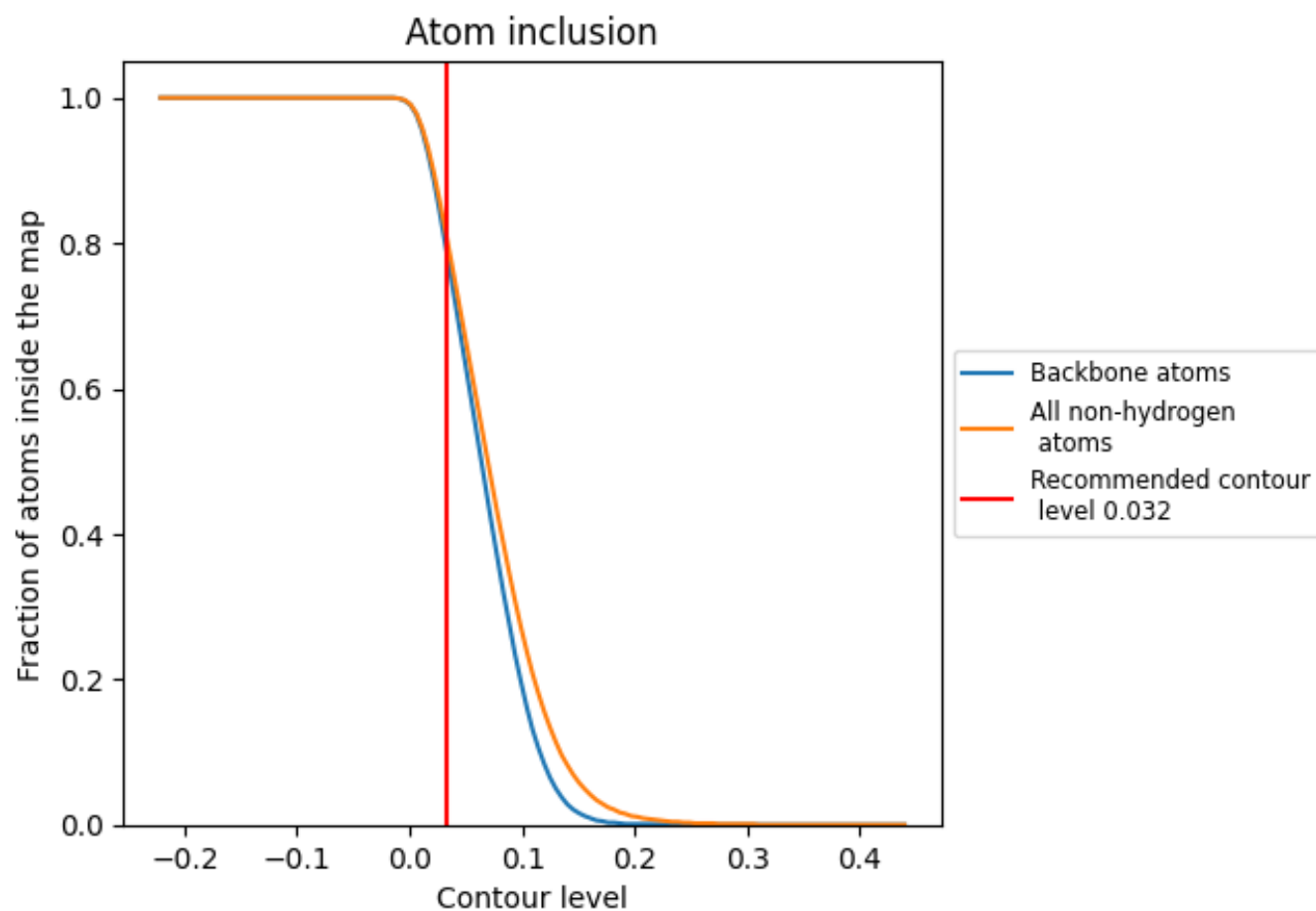
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 82% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8160	 0.6210
1	 0.8720	 0.6290
2	 0.9540	 0.6800
3	 0.5990	 0.4310
4	 0.7440	 0.6080
5	 0.2570	 0.3740
6	 0.6030	 0.4860
8	 0.3960	 0.4670
9	 0.7670	 0.6320
A	 0.9180	 0.7000
B	 0.9610	 0.7140
C	 0.9270	 0.6900
D	 0.6470	 0.5310
E	 0.8630	 0.6550
F	 0.9240	 0.6830
G	 0.8640	 0.6470
H	 0.8800	 0.6620
I	 0.1450	 0.4980
J	 0.2870	 0.3590
K	 0.3370	 0.4190
L	 0.8160	 0.6290
M	 0.9150	 0.6790
N	 0.9480	 0.6940
O	 0.9500	 0.7090
P	 0.9310	 0.6970
Q	 0.8540	 0.6410
R	 0.8990	 0.6770
S	 0.8510	 0.6460
T	 0.6730	 0.5630
U	 0.8470	 0.6440
V	 0.9210	 0.6900
W	 0.7370	 0.5850
X	 0.9310	 0.6890
Y	 0.9110	 0.6810
Z	 0.8690	 0.6480



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Chain	Atom inclusion	Q-score
a	 0.8140	 0.6220
b	 0.8150	 0.6310
c	 0.8540	 0.6340
d	 0.8830	 0.6770
e	 0.9280	 0.6980
f	 0.9700	 0.7170
g	 0.8910	 0.6720
h	 0.9110	 0.6830
i	 0.7560	 0.5950
j	 0.9750	 0.7210
k	 0.7530	 0.6110
l	 0.9780	 0.7270
m	 0.8290	 0.6430
n	 0.7380	 0.6000
o	 0.5210	 0.4940
p	 0.9000	 0.6800
q	 0.6300	 0.5600
r	 0.8970	 0.6810
s	 0.6630	 0.5620
t	 0.5740	 0.5400
u	 0.8720	 0.6640
v	 0.6990	 0.5710
w	 0.6670	 0.5720
x	 0.7100	 0.5680
y	 0.8790	 0.6620
z	 0.8250	 0.6400