



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:25 AM UTC

PDB ID : 8PV6 / pdb_00008pv6
EMDB ID : EMD-17955
Title : Chaetomium thermophilum pre-60S State 3 - post-5S rotation with Rix1 complex with Foot - composite structure
Authors : Thoms, M.; Cheng, J.; Denk, T.; Berninghausen, O.; Beckmann, R.
Deposited on : 2023-07-17
Resolution : 2.94 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

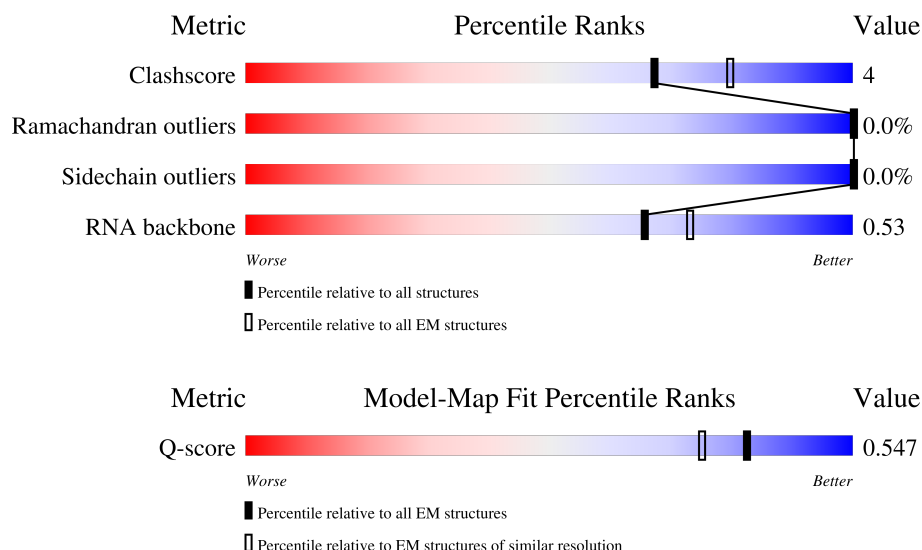
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.94 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.



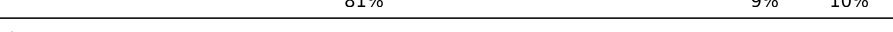
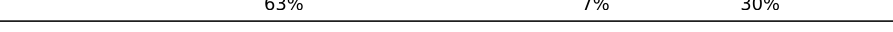
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13068 (2.44 - 3.44)

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	C1	3342	
2	C2	156	
3	C3	162	

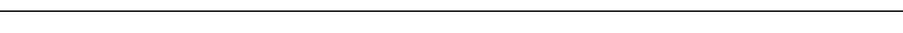
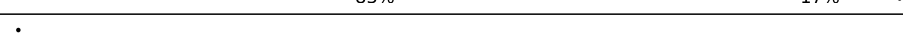
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Mol	Chain	Length	Quality of chain
4	C4	119	
5	CF	270	
6	CH	661	
7	CI	414	
8	CJ	679	
9	CK	261	
10	CL	558	
11	CM	249	
11	LF	249	
12	CN	246	
13	CO	120	
14	CQ	225	
15	CR	767	
16	CS	338	
17	CT	437	
17	CU	437	
18	CV	781	
18	CW	781	
19	Cb	117	
20	Cd	627	
21	Ce	443	
22	Ch	517	
23	Cz	123	
24	LA	254	
25	LB	392	

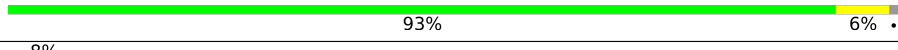
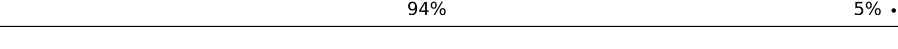
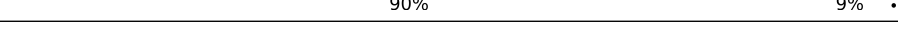
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Mol	Chain	Length	Quality of chain
26	LC	365	
27	LD	304	
28	LE	200	
29	LG	262	
30	LH	229	
31	LJ	173	
32	LK	165	
33	LL	213	
34	LM	142	
35	LN	203	
36	LO	204	
37	LP	187	
38	LQ	213	
39	LR	2898	
40	LS	174	
41	LT	160	
42	LU	127	
43	LV	139	
44	LX	156	
45	LY	138	
46	LZ	135	
47	La	149	
48	Lb	65	
49	Lc	108	
50	Ld	120	

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Mol	Chain	Length	Quality of chain
51	Le	131	
52	Lf	109	
53	Lg	119	
54	Lh	935	
55	Li	110	
56	Lj	95	
57	Lk	94	
58	Ll	51	
59	Lp	92	
60	Lq	147	
61	Lr	217	

2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 172014 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 26S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	3100	Total	C	N	O	P	0	0
			66359	29636	12012	21611	3100		

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C2	156	Total	C	N	O	P	0	0
			3319	1484	589	1090	156		

- Molecule 3 is a RNA chain called ITS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C3	3	Total	C	N	O	P	0	0
			60	27	7	23	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C4	115	Total	C	N	O	P	0	0
			2451	1093	438	805	115		

- Molecule 5 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	CF	245	Total	C	N	O	S	0	0
			1934	1215	350	360	9		

- Molecule 6 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	CH	627	Total	C	N	O	S	0	0
			5061	3180	924	938	19		

- Molecule 7 is a protein called Putative RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CI	93	Total	C	N	O	S	0	0
			729	472	132	122	3		

- Molecule 8 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CJ	382	Total	C	N	O	S	0	0
			3116	2008	548	550	10		

- Molecule 9 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CK	233	Total	C	N	O	S	0	0
			1878	1183	363	328	4		

- Molecule 10 is a protein called Putative GTP binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	CL	79	Total	C	N	O	0	0
			618	386	124	108		

- Molecule 11 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CM	217	Total	C	N	O	S	0	0
			1773	1144	329	297	3		
11	LF	248	Total	C	N	O	S	0	0
			2023	1297	377	346	3		

- Molecule 12 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	CN	246	Total	C	N	O	S	0	0
			1850	1154	322	368	6		

- Molecule 13 is a protein called DUF2423 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	CO	62	Total	C	N	O	S	0	0
			468	290	94	82	2		

- Molecule 14 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	CQ	183	Total	C	N	O	S	0	0
			1476	923	304	239	10		

- Molecule 15 is a protein called Protein SDA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	CR	516	Total	C	N	O	S	0	0
			3844	2445	683	703	13		

- Molecule 16 is a protein called Pre-rRNA-processing protein IPI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	CS	307	Total	C	N	O	S	0	0
			2391	1520	418	446	7		

- Molecule 17 is a protein called Pre-rRNA-processing protein IPI3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CT	393	Total	C	N	O	S	0	0
			2941	1865	492	566	18		
17	CU	393	Total	C	N	O	S	0	0
			2953	1873	494	568	18		

- Molecule 18 is a protein called Pre-rRNA-processing protein RIX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CV	550	Total	C	N	O	S	0	0
			4217	2691	735	777	14		
18	CW	550	Total	C	N	O	S	0	0
			4204	2685	729	776	14		

- Molecule 19 is a protein called Zinc finger domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Cb	101	Total	C	N	O	S	0	0
			830	517	161	148	4		

- Molecule 20 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Cd	451	Total	C	N	O	S	0	0
			3614	2301	660	642	11		

- Molecule 21 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Ce	302	Total	C	N	O	S	0	0
			2476	1541	471	460	4		

- Molecule 22 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Ch	389	Total	C	N	O	S	1	0
			3050	1916	568	557	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ch	117	ASP	GLU	engineered mutation	UNP G0SC29

- Molecule 23 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Cz	103	Total	C	N	O	S	0	0
			884	548	183	149	4		

- Molecule 24 is a protein called 60S ribosomal protein L2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LA	247	Total	C	N	O	S	0	0
			1878	1175	374	326	3		

- Molecule 25 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LB	388	Total	C	N	O	S	0	0
			3097	1969	578	537	13		

- Molecule 26 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LC	363	Total	C	N	O	S	0	0
			2745	1734	524	478	9		

- Molecule 27 is a protein called 60S ribosomal protein l5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LD	298	Total	C	N	O	S	0	0
			2366	1496	424	443	3		

- Molecule 28 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LE	191	Total	C	N	O	S	0	0
			1470	941	267	259	3		

- Molecule 29 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LG	235	Total	C	N	O	S	0	0
			1880	1204	348	323	5		

- Molecule 30 is a protein called 60S ribosomal protein l9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LH	190	Total	C	N	O	S	0	0
			1495	949	268	272	6		

- Molecule 31 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LJ	168	Total	C	N	O	S	0	0
			1367	854	266	241	6		

- Molecule 32 is a protein called 60S ribosomal protein L12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LK	158	Total	C	N	O	S	0	0
			1184	743	215	224	2		

- Molecule 33 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LL	203	Total	C	N	O	S	0	0
			1587	989	325	271	2		

- Molecule 34 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LM	141	Total	C	N	O	S	0	0
			1126	714	216	195	1		

- Molecule 35 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LN	202	Total	C	N	O	S	0	0
			1704	1062	360	278	4		

- Molecule 36 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LO	203	Total	C	N	O	S	0	0
			1611	1034	305	267	5		

- Molecule 37 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LP	171	Total	C	N	O	S	0	0
			1343	834	274	232	3		

- Molecule 38 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LQ	146	Total	C	N	O	S	0	0
			1156	730	228	196	2		

- Molecule 39 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LR	155	Total	C	N	O	S	0	0
			1241	772	262	203	4		

- Molecule 40 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LS	174	Total	C	N	O	S	0	0
			1430	920	267	238	5		

- Molecule 41 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LT	141	Total	C	N	O	S	0	0
			1124	712	215	195	2		

- Molecule 42 is a protein called 60S ribosomal protein L22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LU	105	Total	C	N	O	S	0	0
			838	542	144	151	1		

- Molecule 43 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LV	135	Total	C	N	O	S	0	0
			991	630	184	170	7		

- Molecule 44 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LX	145	Total	C	N	O	S	0	0
			1113	709	206	198			

- Molecule 45 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LY	133	Total	C	N	O	S	0	0
			1056	658	213	183	2		

- Molecule 46 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LZ	135	Total	C	N	O	S	0	0
			1102	707	203	188	4		

- Molecule 47 is a protein called 60S ribosomal protein L28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	La	108	Total	C	N	O	S	0	0
			872	556	168	147	1		

- Molecule 48 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	Lb	36	Total	C	N	O	0	0
			286	178	61	47		

- Molecule 49 is a protein called 60S ribosomal protein l30-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lc	95	Total	C	N	O	S	0	0
			705	449	122	129	5		

- Molecule 50 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Ld	110	Total	C	N	O	S	0	0
			875	555	171	148	1		

- Molecule 51 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Le	126	Total	C	N	O	S	0	0
			1017	640	208	163	6		

- Molecule 52 is a protein called 60S ribosomal protein l33-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Lf	108	Total	C	N	O	S	0	0
			862	546	171	144	1		

- Molecule 53 is a protein called Ribosomal protein l34-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Lg	118	Total	C	N	O	S	0	0
			901	561	184	152	4		

- Molecule 54 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	Lh	122	Total	C	N	O	0	0
			1003	637	198	168		

- Molecule 55 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Li	101	Total	C	N	O	S	0	0
			821	506	178	136	1		

- Molecule 56 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Lj	88	Total	C	N	O	S	0	0
			698	427	154	112	5		

- Molecule 57 is a protein called 60S ribosomal protein L38-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Lk	76	Total	C	N	O	S	0	0
			624	394	119	109	2		

- Molecule 58 is a protein called Ribosomal protein eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	Ll	50	Total	C	N	O	0	0
			436	275	97	64		

- Molecule 59 is a protein called 60S ribosomal protein L43-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Lp	91	Total	C	N	O	S	0	0
			694	428	138	122	6		

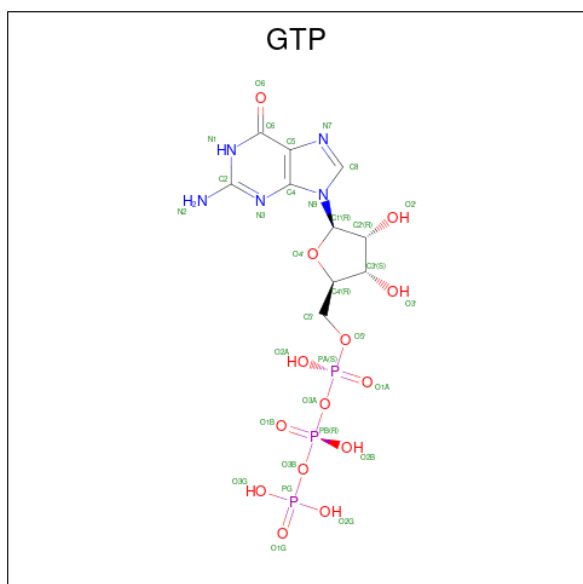
- Molecule 60 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	Lq	139	Total	C	N	O	0	0
			1061	666	207	188		

- Molecule 61 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Lr	214	Total	C	N	O	S	0	0
			1660	1056	296	300	8		

- Molecule 62 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
62	CH	1	Total	C	N	O	P	0
			32	10	5	14	3	
62	Cd	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 63 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
63	CH	1	Total	Mg	0
			1	1	
63	Cd	2	Total	Mg	0
			2	2	

- Molecule 64 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
64	CQ	1	Total	Zn	0
			1	1	
64	Cb	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
64	Lg	1	Total 1	Zn 1	0
64	Lj	1	Total 1	Zn 1	0
64	Lp	1	Total 1	Zn 1	0

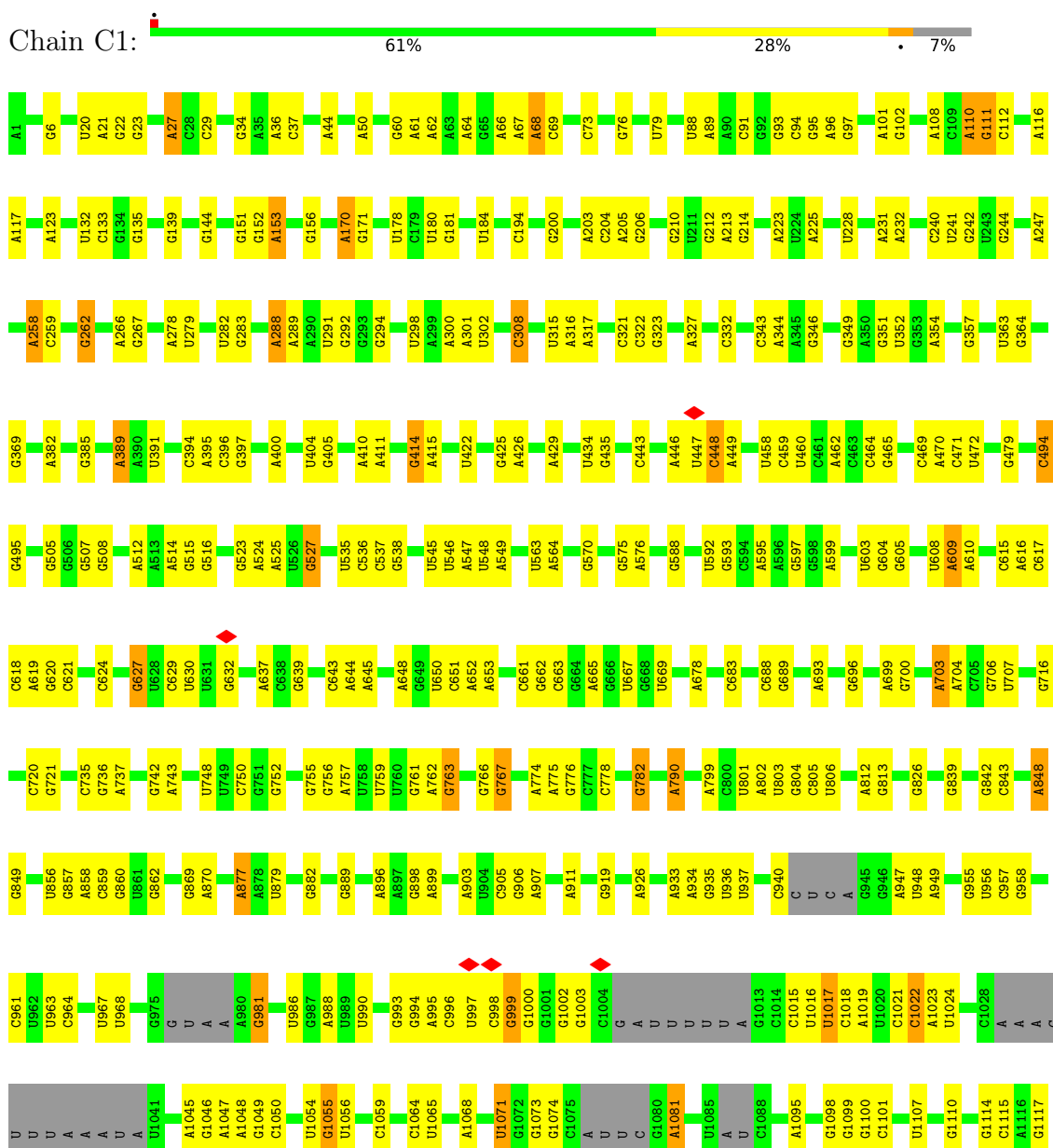
- Molecule 65 is water.

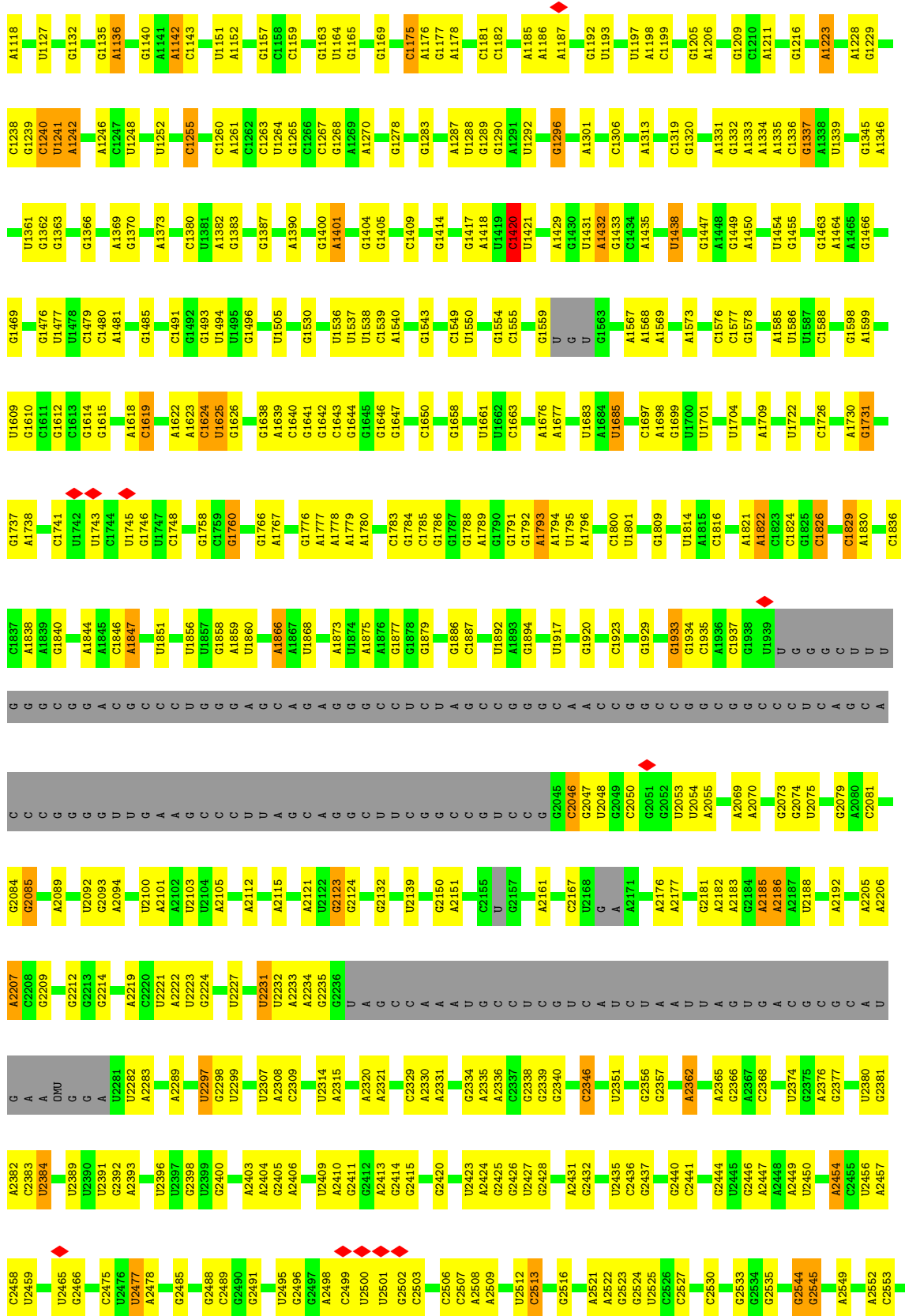
Mol	Chain	Residues	Atoms		AltConf
65	C1	1	Total 1	O 1	0
65	CH	1	Total 1	O 1	0
65	Cd	2	Total 2	O 2	0

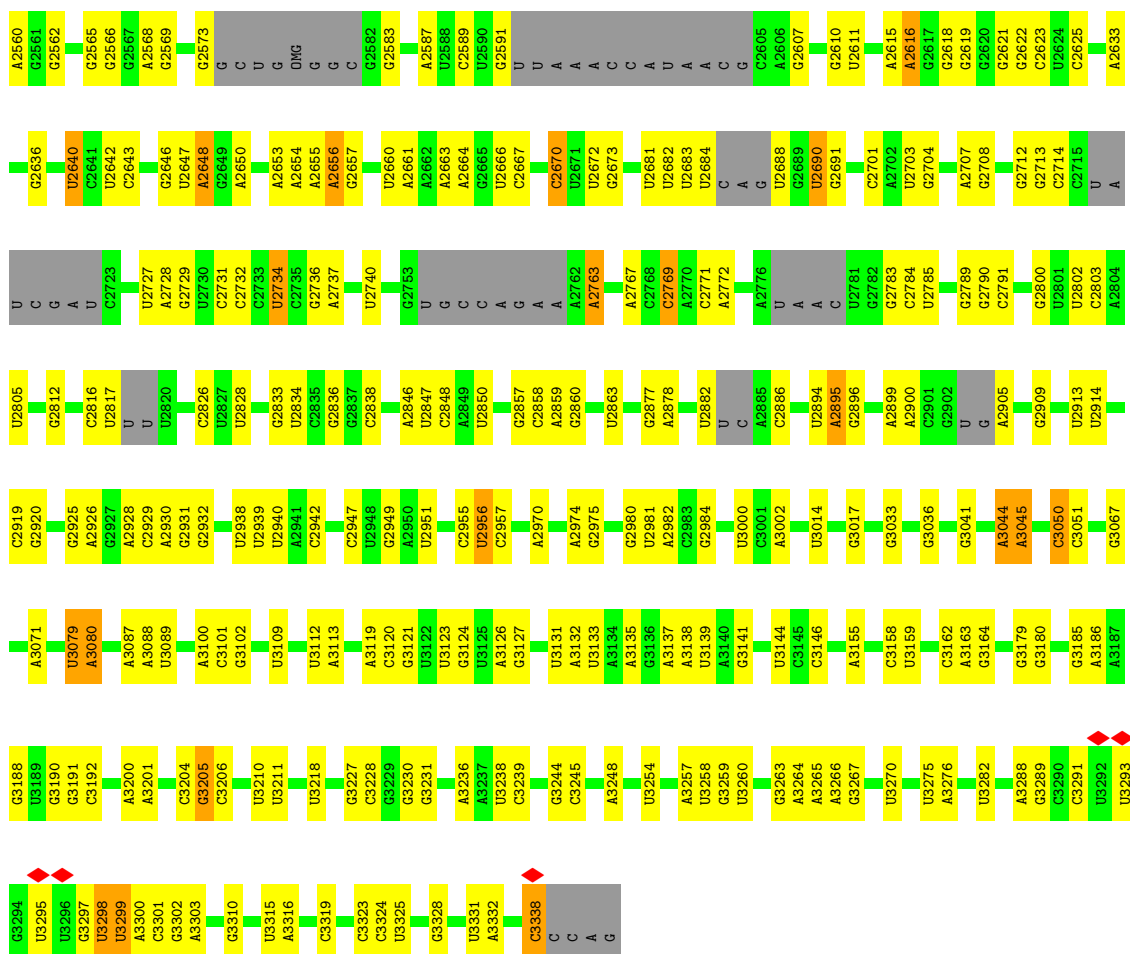
3 Residue-property plots

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

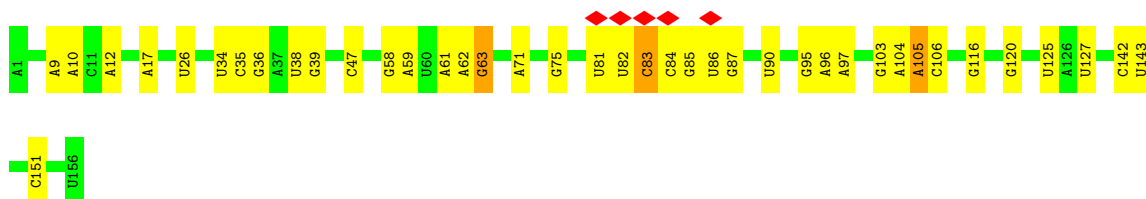
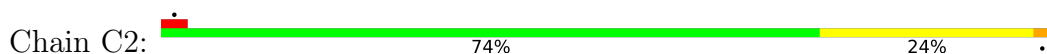
• Molecule 1: 26S rRNA



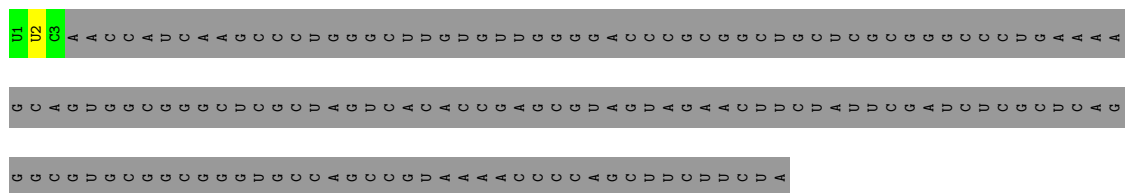




- Molecule 2: 5.8S rRNA



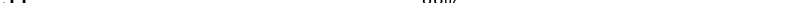
- Molecule 3: ITS2

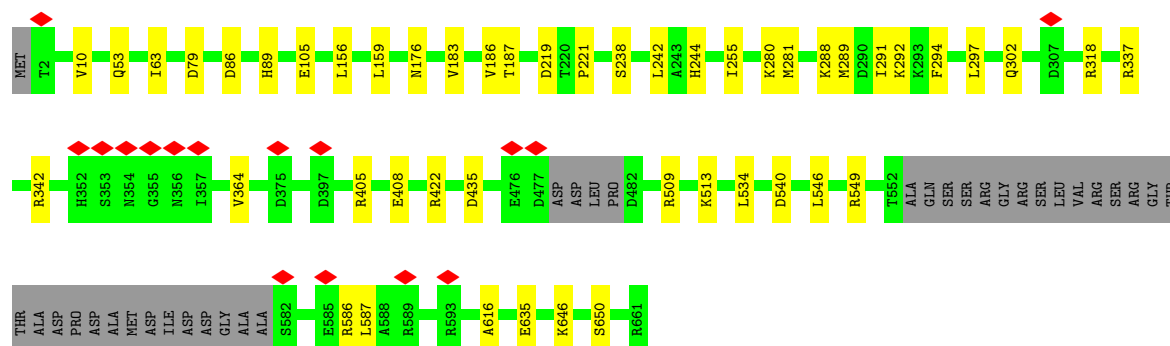


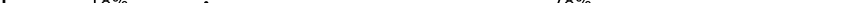
- Molecule 4: 5S rRNA

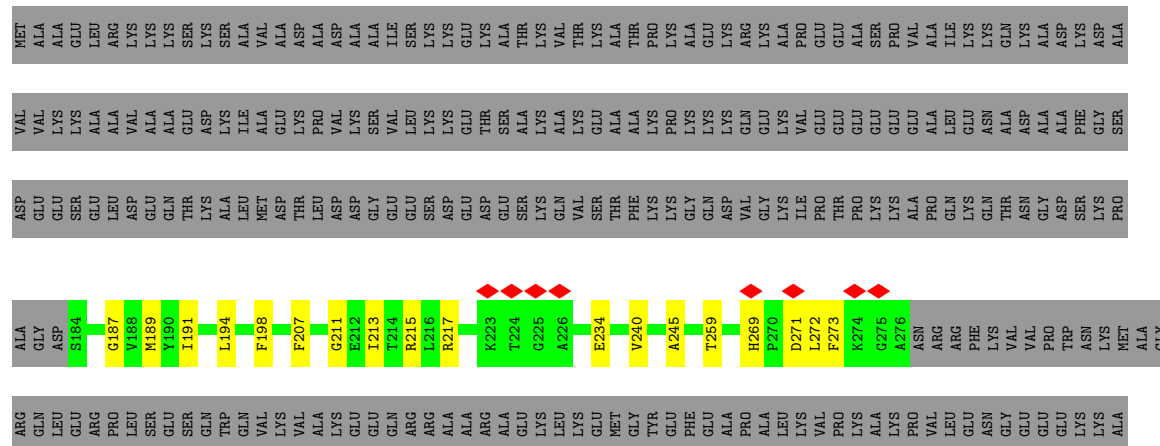
G114		A1	C6 G7 A8 C9	U12	G18	A23	C26	G29	G37 U38	G41	U45 G46 C47	U54 A55	A64 G65	C68	G72 U73 U74	A75 G76	G83 G84	G87 G88	U G A C	G93	G98 G99	G100 A101	G109 U110	G111
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- Chain CF: 

- Chain CH: 

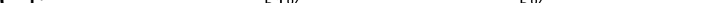


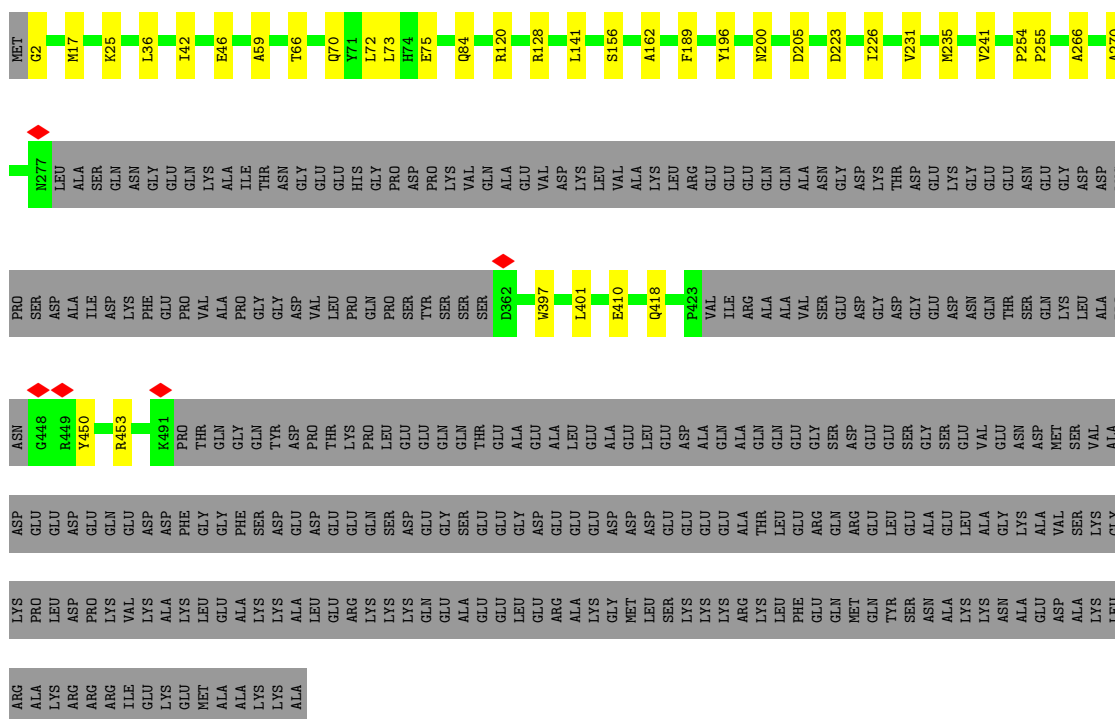
- Chain CI: 



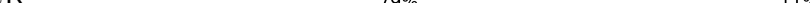
[illegible]

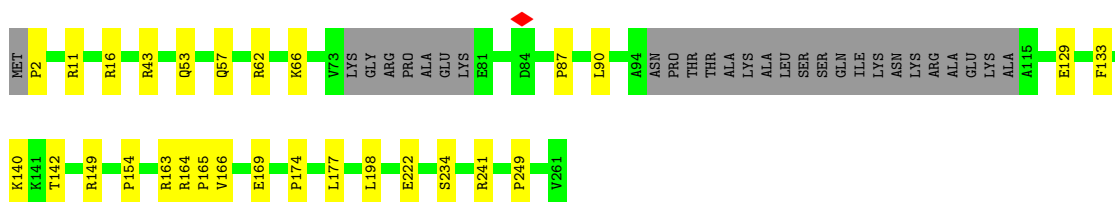
- Molecule 8: Pescadillo homolog

Chain CJ: 



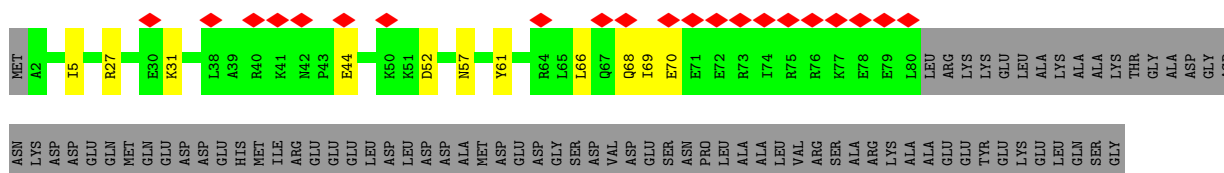
- Molecule 9: Ribosome biogenesis protein NSA2 homolog

Chain CK:  79% 11% 11%



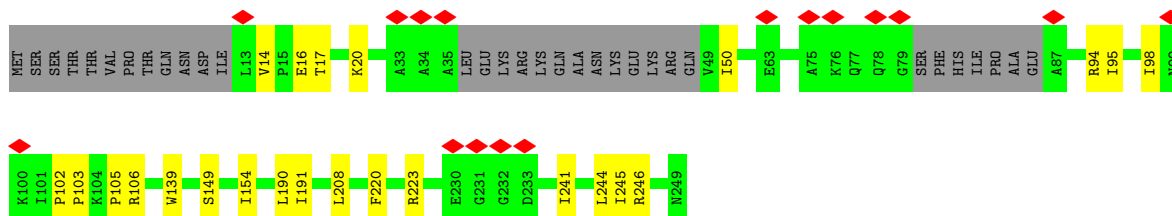
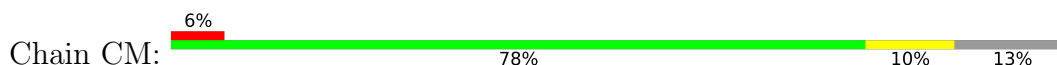
- Molecule 10: Putative GTP binding protein

Chain CL: 12% : 86%



ILE	LEU	HIS	GLY	ASN	GLU	SER
ALA	VAL	LEU	SER	ALA	THR	GLY
ASP	GLN	VAL	ALA	ARG	THR	THR
GLN	VAL	LEU	GLY	PHE	SER	ARG
VAL	ARG	ASN	GLY	SER	HIS	ASP
ALA	LYS	ALA	ARG	HIS	ASP	ASP
PRO	ARG	ILE	THR	ARG	VAL	GLU
ASP	GLY	PRO	PRO	ASP	GLU	ASP
GLN	ARG	PRO	CYS	ILE	GLN	ASP
LYS	LEU	LYS	PRO	THR	ALA	SER
ILE	GLY	GLN	ALA	VAL	VAL	ASP
ILE	ARG	ILE	GLY	GLN	MET	ASP
VAL	GLY	GLU	ALA	SER	ALA	SER
THR	GLY	ASP	GLU	THR	ALA	SER
GLU	VAL	PRO	ALA	SER	ALA	ASP
TRP	PRO	VAL	GLY	ALA	GLY	GLY
ALA	ASN	PRO	VAL	ALA	GLY	GLY
LYS	ILE	ALA	THR	LEU	GLN	GLY
GLU	GLN	VAL	THR	PHE	LYS	ASP
PHE	ALA	THR	ALA	ARG	ARG	ASP
LYS	ALA	LEU	ILE	ALA	LEU	GLY
LEU	ALA	LEU	ARG	LEU	MET	VAL
ALA	MET	LEU	ALA	LYS	LEU	ILE
GLY	THR	LYS	VAL	ALA	ILE	THR
LEU	VAL	ARG	LYS	TYR	LEU	GLU
TRP	VAL	LEU	ILE	ALA	ASN	VAL
GLY	THR	SER	ASP	ALA	LYS	HIS
ASP	ASP	ALA	SER	ALA	VAL	GLY
GLU	TRP	THR	LYS	ARG	ASP	GLY
GLU	GLN	PRO	LEU	ARG	VAL	GLY
GLN	ASP	GLU	THR	LEU	LEU	GLY
THR	GLY	GLU	LEU	LYS	PRO	THR
GLU	GLU	MET	LEU	ARG	PRO	ARG
GLY	ILE	ASP	ASP	ALA	PRO	LYS
ASP	GLN	ARG	SER	ILE	VAL	LYS
LYS	TRP	MET	GLY	GLY	LYS	TYR
MET	THR	GLN	ILE	GLY	GLY	LYS
GLU	GLU	VAL	VAL	VAL	TRP	VAL
ALA	PRO	TYR	PHE	ILE	LEU	PHE
	PRO	ASP	PRO	GLY	THR	LYS
	LYS	ILE	SER	TYR	TYR	GLN
	ILE	PRO	THR	PRO	LEU	VAL
	ALA	PRO	ALA	ASN	ARG	VAL
	VAL	LEU	SER	VAL	ARG	GLU
	GLY	LEU	SER	GLY	PHE	GLN
	VAL	LYS	GLN	LYS	PHE	ALA
	GLY	ASP	THR	SER	PRO	ASP
	LYS	PRO	PHE	SER	THR	VAL
	GLY	SER	ILE	VAL	LEU	ILE
	GLY	GLY	PRO	ILE	PRO	LEU
	ASN	GLY	LYS	ASN	LEU	TYR
	GLY	GLY	ASN	ALA	ARG	VAL
	GLY	ASP	PRO	LEU	ALA	ALA
	LYS	ALA	VAL	LEU	SER	ASP
	VAL	THR	GLU	SER	ASN	ALA
	VAL	MET	ALA	ARG	PRO	ARG
	ARG	ASP	HIS	LEU	ALA	ASP
	LYS	DUE	ALA	PRO	PRO	PRO

- Molecule 11: 60S ribosomal protein l7-like protein



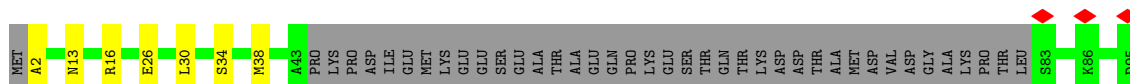
- Molecule 11: 60S ribosomal protein l7-like protein



- Molecule 12: Eukaryotic translation initiation factor 6

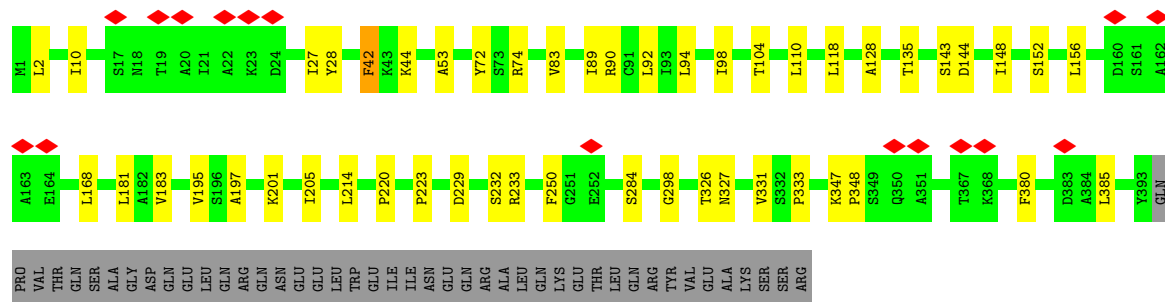
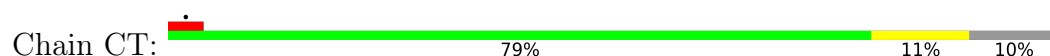


- Molecule 13: DUF2423 domain-containing protein

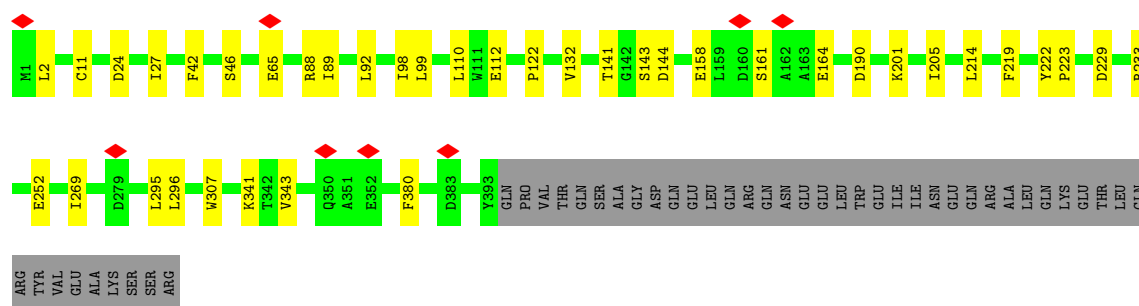
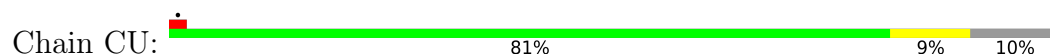




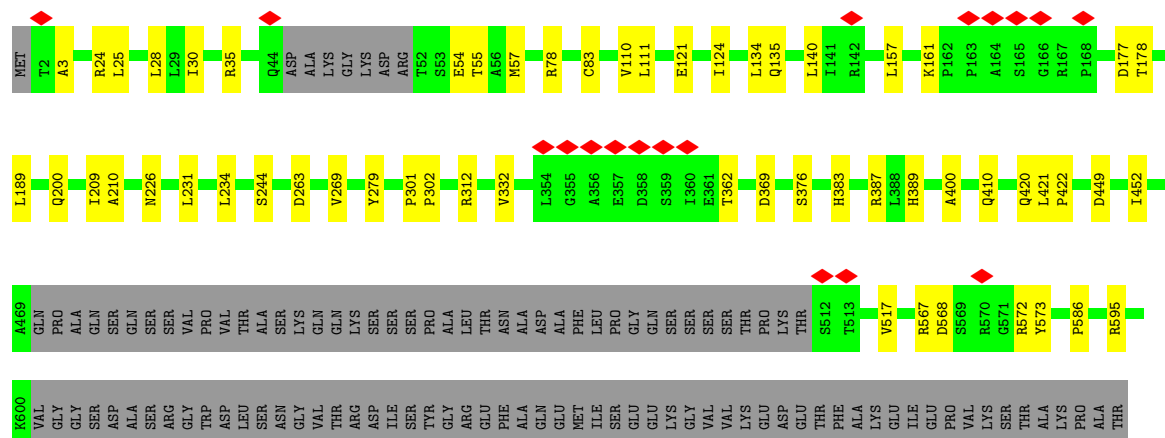
- Molecule 17: Pre-rRNA-processing protein IPI3



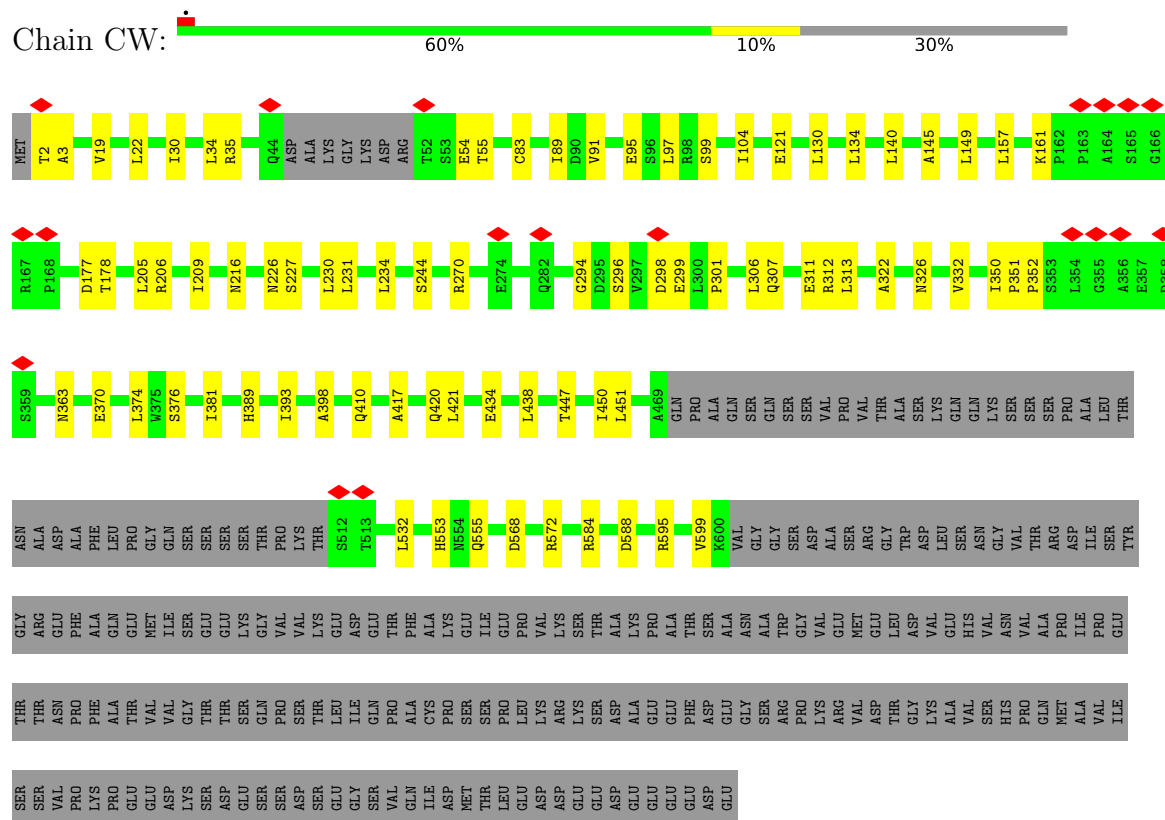
- Molecule 17: Pre-rRNA-processing protein IPI3



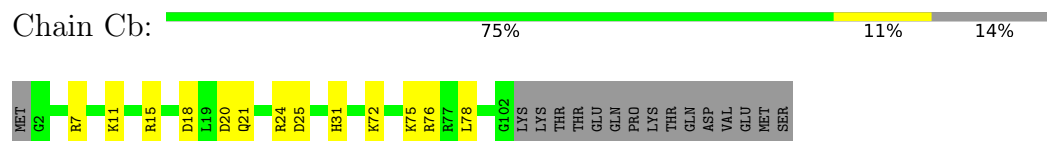
- Molecule 18: Pre-rRNA-processing protein RIX1



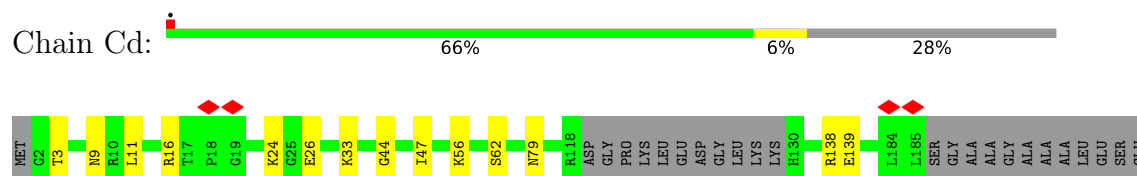
- Molecule 18: Pre-rRNA-processing protein RIX1



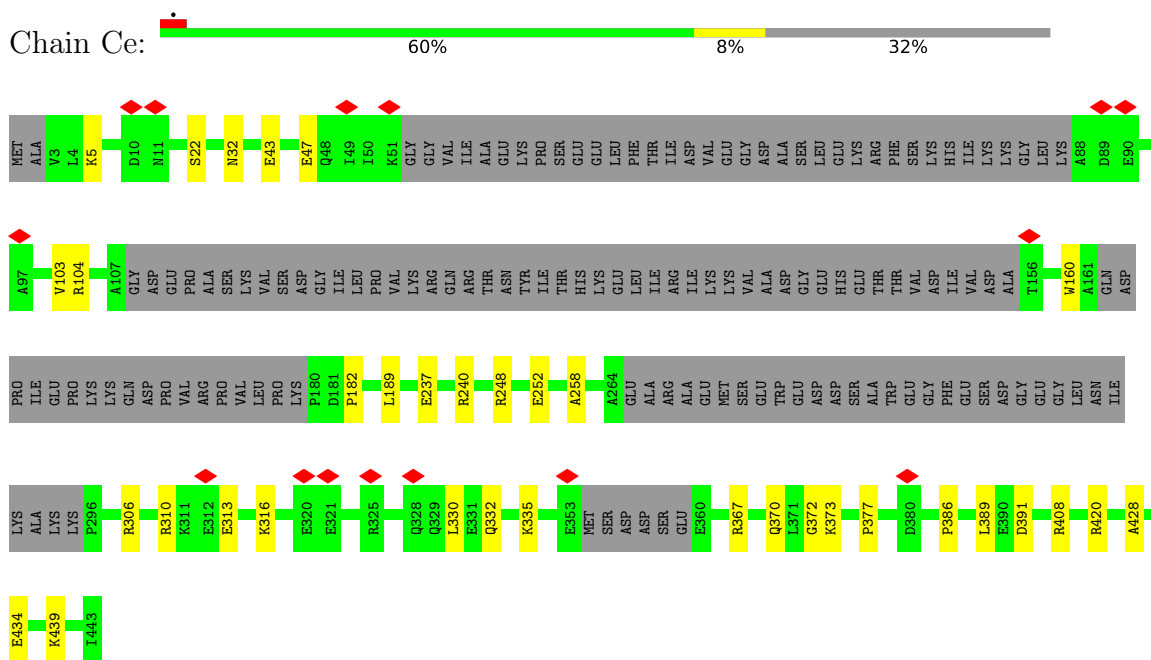
- Molecule 19: Zinc finger domain-containing protein



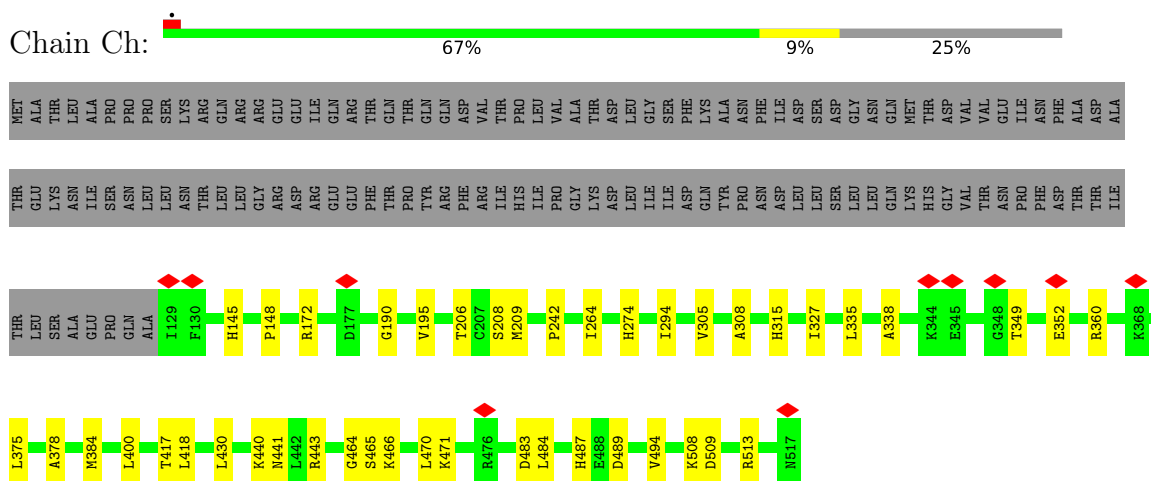
- Molecule 20: Nucleolar GTP-binding protein 2



- Molecule 21: Ribosome biogenesis protein NOP53



- Molecule 22: Ribosome assembly protein 4



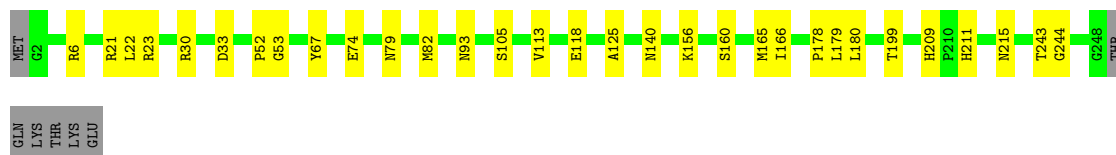
- Molecule 23: rRNA-processing protein

Chain Cz:  75% 9% 16%



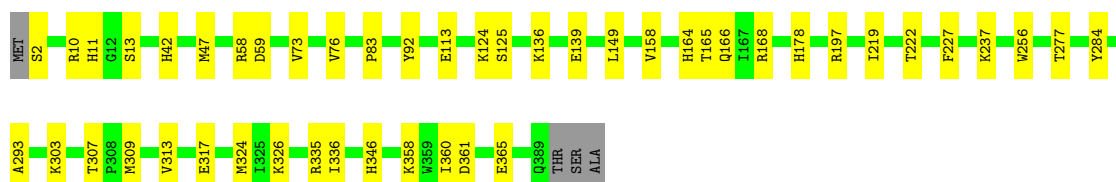
- Molecule 24: 60S ribosomal protein L2-like protein

Chain LA:  85% 12%



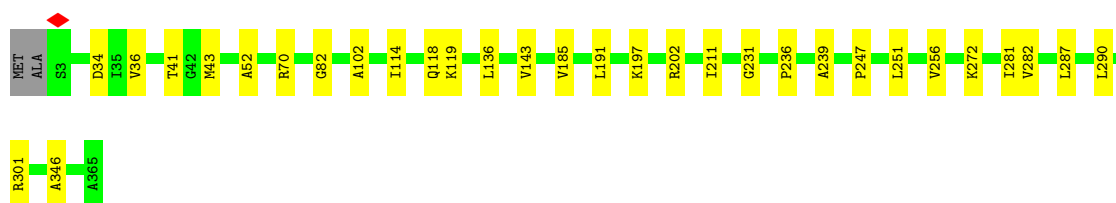
- Molecule 25: 60S ribosomal protein L3-like protein

Chain LB:  87% 12%



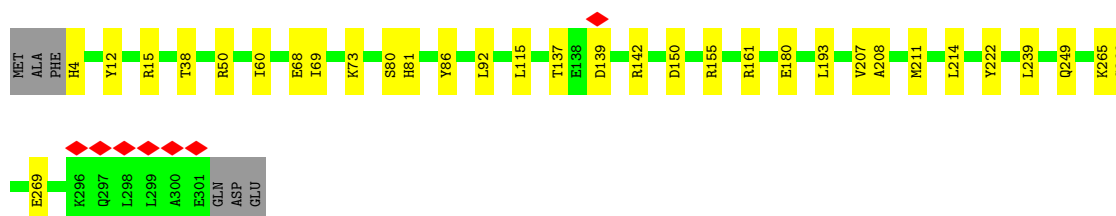
- Molecule 26: 60S ribosomal protein L4-like protein

Chain LC:  91% 8%



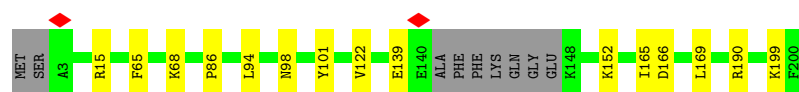
- Molecule 27: 60S ribosomal protein l5-like protein

Chain LD:  88% 11%



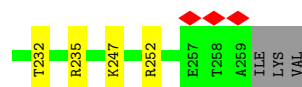
- Molecule 28: 60S ribosomal protein L6

Chain LE:  88% 8%



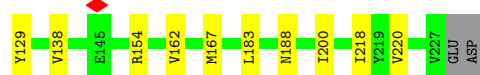
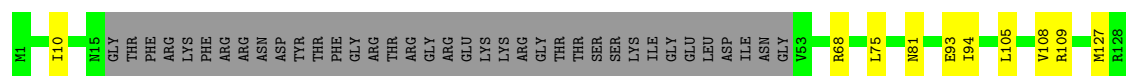
- Molecule 29: 60S ribosomal protein L8

Chain LG: 82% 8% 10%



- Molecule 30: 60S ribosomal protein l9-like protein

Chain LH: 74% 9% 17%



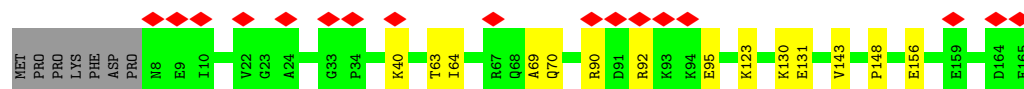
- Molecule 31: Putative ribosomal protein

Chain LJ: 85% 12% 3%



- Molecule 32: 60S ribosomal protein L12-like protein

Chain LK: 10% 87% 8% 5%



- Molecule 33: 60S ribosomal protein L13

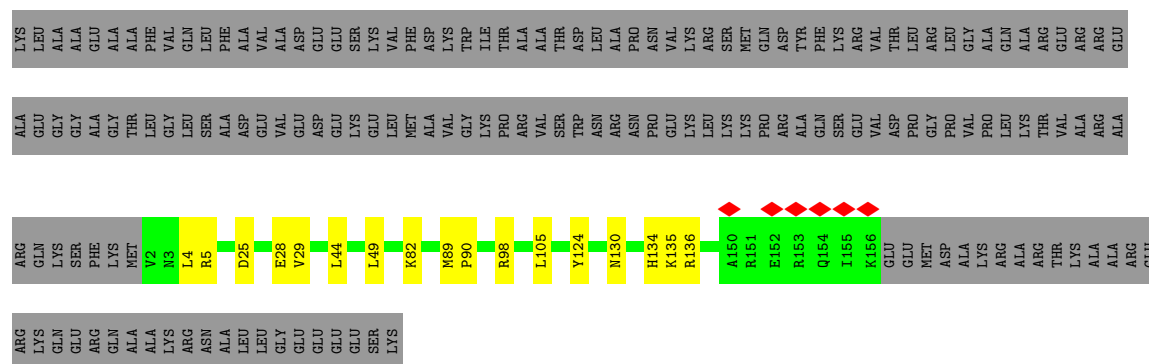
Chain LL: 87% 8% 5%



- Molecule 34: 60S ribosomal protein L14-like protein

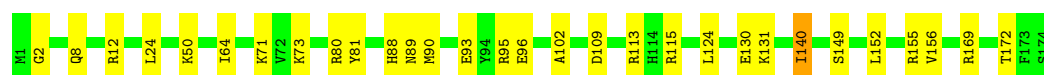






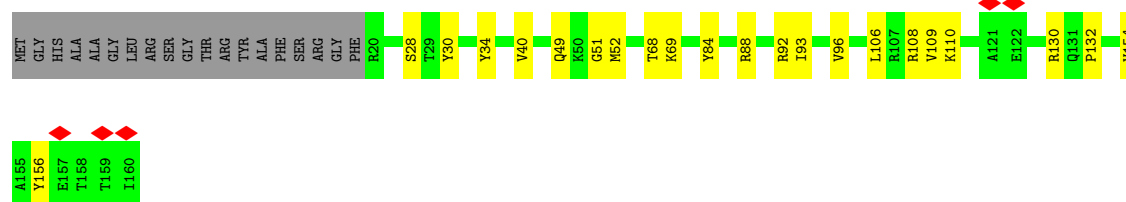
- Molecule 40: 60S ribosomal protein L20

Chain LS: 83% 17%



- Molecule 41: 60S ribosomal protein l21-like protein

Chain LT: 74% 14% 12%



- Molecule 42: 60S ribosomal protein L22-like protein

Chain LU: 69% 13% 17%



- Molecule 43: 60S ribosomal protein l23-like protein

Chain LV: 88% 9%

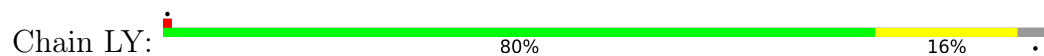


- Molecule 44: 60S ribosomal protein L25-like protein

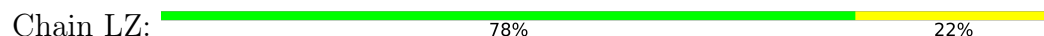
Chain LX: 85% 8% 7%



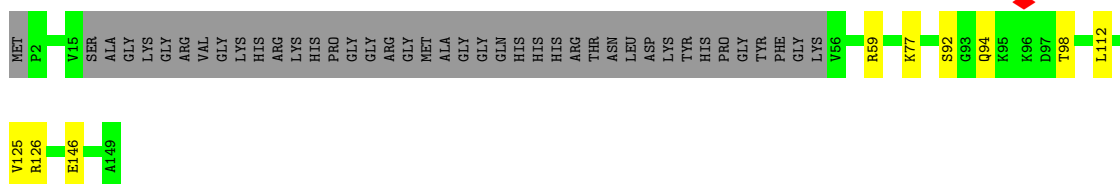
- Molecule 45: 60S ribosomal protein L26-like protein



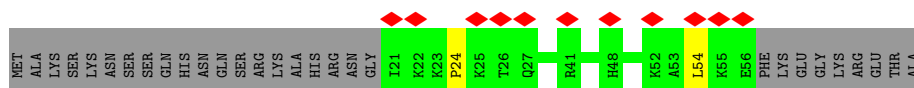
- Molecule 46: 60S ribosomal protein L27



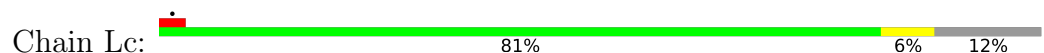
- Molecule 47: 60S ribosomal protein L28-like protein



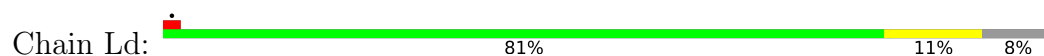
- Molecule 48: 60S ribosomal protein L29

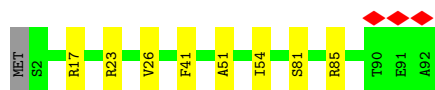


- Molecule 49: 60S ribosomal protein l30-like protein



- Molecule 50: Putative 60S ribosomal protein





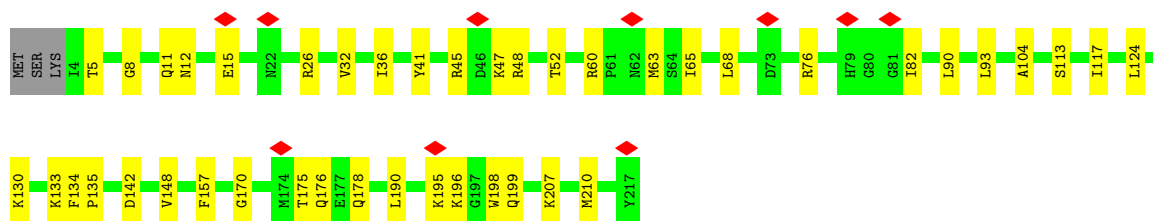
- Molecule 60: Putative 60S ribosomal protein

Chain Lq: 84% 10% 5%



- Molecule 61: Ribosomal protein

Chain Lr: 5% 79% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25753	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.708	Depositor
Minimum map value	0.000	Depositor
Average map value	0.018	Depositor
Map value standard deviation	0.134	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	522.5, 522.5, 522.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, ZN, OMG, OMC, MG, A2M, OMU

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	C1	0.17	2/73447 (0.0%)	0.31	0/114487
2	C2	0.15	0/3710	0.29	0/5778
3	C3	0.09	0/65	0.21	0/98
4	C4	0.16	0/2737	0.33	0/4262
5	CF	0.15	0/1972	0.39	0/2660
6	CH	0.17	0/5145	0.39	0/6923
7	CI	0.19	0/749	0.58	0/1013
8	CJ	0.16	0/3196	0.36	0/4319
9	CK	0.17	0/1913	0.40	0/2571
10	CL	0.23	0/627	0.61	1/839 (0.1%)
11	CM	0.17	0/1805	0.42	0/2417
11	LF	0.18	0/2061	0.43	0/2765
12	CN	0.18	0/1875	0.46	0/2552
13	CO	0.21	0/470	0.51	0/619
14	CQ	0.20	0/1500	0.46	0/1995
15	CR	0.18	0/3912	0.43	0/5320
16	CS	0.20	0/2442	0.41	0/3315
17	CT	0.19	0/3009	0.49	0/4113
17	CU	0.18	0/3021	0.47	0/4128
18	CV	0.20	0/4312	0.48	2/5897 (0.0%)
18	CW	0.21	0/4299	0.48	2/5882 (0.0%)
19	Cb	0.19	0/845	0.47	0/1128
20	Cd	0.16	0/3691	0.39	2/4975 (0.0%)
21	Ce	0.16	0/2506	0.40	0/3338
22	Ch	0.17	0/3137	0.47	0/4262
23	Cz	0.19	0/892	0.45	0/1167
24	LA	0.19	0/1917	0.42	0/2580
25	LB	0.17	0/3165	0.39	0/4250
26	LC	0.17	0/2802	0.36	0/3778
27	LD	0.16	0/2412	0.43	0/3247
28	LE	0.18	0/1497	0.41	0/2018
29	LG	0.18	0/1909	0.41	0/2556

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	LH	0.16	0/1515	0.41	0/2037
31	LJ	0.19	0/1389	0.49	0/1856
32	LK	0.18	0/1198	0.46	0/1611
33	LL	0.17	0/1614	0.38	0/2168
34	LM	0.16	0/1145	0.37	0/1539
35	LN	0.19	0/1741	0.41	0/2332
36	LO	0.16	0/1645	0.37	0/2205
37	LP	0.16	0/1364	0.40	0/1835
38	LQ	0.16	0/1170	0.37	0/1573
39	LR	0.16	0/1260	0.33	0/1683
40	LS	0.17	0/1465	0.42	1/1970 (0.1%)
41	LT	0.18	0/1146	0.45	0/1546
42	LU	0.18	0/851	0.45	0/1143
43	LV	0.17	0/1009	0.38	0/1357
44	LX	0.19	0/1131	0.45	0/1526
45	LY	0.20	0/1070	0.50	0/1432
46	LZ	0.20	0/1125	0.49	0/1508
47	La	0.16	0/892	0.37	0/1200
48	Lb	0.15	0/293	0.38	0/392
49	Lc	0.17	0/714	0.43	0/960
50	Ld	0.19	0/889	0.43	1/1192 (0.1%)
51	Le	0.21	0/1035	0.50	0/1379
52	Lf	0.18	0/883	0.39	0/1187
53	Lg	0.20	0/914	0.47	0/1228
54	Lh	0.18	0/1014	0.40	0/1349
55	Li	0.16	0/828	0.40	0/1092
56	Lj	0.17	0/712	0.43	0/944
57	Lk	0.21	0/632	0.48	1/842 (0.1%)
58	Ll	0.17	0/446	0.34	0/593
59	Lp	0.20	0/702	0.45	0/935
60	Lq	0.17	0/1079	0.40	0/1454
61	Lr	0.21	0/1684	0.53	1/2266 (0.0%)
All	All	0.17	2/181595 (0.0%)	0.38	11/261586 (0.0%)

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
17	CT	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1847	A2M	O3'-P	5.04	1.61	1.56
1	C1	848	A2M	O3'-P	5.03	1.61	1.56

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	CV	400	ALA	CA-C-N	6.47	124.32	120.24
18	CV	400	ALA	C-N-CA	6.47	124.32	120.24
20	Cd	410	TYR	CA-C-N	5.52	123.72	120.24
20	Cd	410	TYR	C-N-CA	5.52	123.72	120.24
18	CW	451	LEU	CA-C-N	5.47	123.68	120.24
18	CW	451	LEU	C-N-CA	5.47	123.68	120.24
50	Ld	49	GLN	CA-CB-CG	5.42	124.95	114.10
40	LS	140	ILE	N-CA-C	-5.29	108.34	113.53
61	Lr	15	GLU	N-CA-CB	5.05	118.63	110.40
57	Lk	13	GLU	N-CA-CB	5.04	117.53	110.12
10	CL	68	GLN	N-CA-CB	5.02	118.72	110.39

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	CT	42	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C1	66359	0	33489	431	0
2	C2	3319	0	1678	17	0
3	C3	60	0	32	0	0
4	C4	2451	0	1244	11	0
5	CF	1934	0	1945	19	0
6	CH	5061	0	5152	30	0
7	CI	729	0	707	9	0
8	CJ	3116	0	3122	25	0
9	CK	1878	0	1963	23	0
10	CL	618	0	630	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	CM	1773	0	1879	14	0
11	LF	2023	0	2132	12	0
12	CN	1850	0	1845	19	0
13	CO	468	0	503	5	0
14	CQ	1476	0	1519	13	0
15	CR	3844	0	3684	34	0
16	CS	2391	0	2411	18	0
17	CT	2941	0	2877	28	0
17	CU	2953	0	2906	25	0
18	CV	4217	0	4334	35	0
18	CW	4204	0	4309	48	0
19	Cb	830	0	838	10	0
20	Cd	3614	0	3741	24	0
21	Ce	2476	0	2584	28	0
22	Ch	3050	0	2974	25	0
23	Cz	884	0	967	10	0
24	LA	1878	0	1940	21	0
25	LB	3097	0	3214	30	0
26	LC	2745	0	2864	23	0
27	LD	2366	0	2315	22	0
28	LE	1470	0	1561	10	0
29	LG	1880	0	2018	15	0
30	LH	1495	0	1573	10	0
31	LJ	1367	0	1399	13	0
32	LK	1184	0	1249	11	0
33	LL	1587	0	1655	15	0
34	LM	1126	0	1198	16	0
35	LN	1704	0	1767	16	0
36	LO	1611	0	1702	13	0
37	LP	1343	0	1369	7	0
38	LQ	1156	0	1252	12	0
39	LR	1241	0	1298	12	0
40	LS	1430	0	1492	24	0
41	LT	1124	0	1170	16	0
42	LU	838	0	861	11	0
43	LV	991	0	1044	7	0
44	LX	1113	0	1184	9	0
45	LY	1056	0	1143	14	0
46	LZ	1102	0	1159	22	0
47	La	872	0	903	6	0
48	Lb	286	0	286	2	0
49	Lc	705	0	751	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	Ld	875	0	918	9	0
51	Le	1017	0	1092	9	0
52	Lf	862	0	891	5	0
53	Lg	901	0	941	5	0
54	Lh	1003	0	1116	7	0
55	Li	821	0	895	6	0
56	Lj	698	0	726	12	0
57	Lk	624	0	671	10	0
58	Ll	436	0	473	7	0
59	Lp	694	0	733	8	0
60	Lq	1061	0	1108	12	0
61	Lr	1660	0	1768	30	0
62	CH	32	0	12	1	0
62	Cd	32	0	12	0	0
63	CH	1	0	0	0	0
63	Cd	2	0	0	0	0
64	CQ	1	0	0	0	0
64	Cb	1	0	0	0	0
64	Lg	1	0	0	0	0
64	Lj	1	0	0	0	0
64	Lp	1	0	0	0	0
65	C1	1	0	0	0	0
65	CH	1	0	0	0	0
65	Cd	2	0	0	0	0
All	All	172014	0	139188	1144	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 (1144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1107:U:H3	1:C1:1117:G:H1	1.19	0.86
8:CJ:128:ARG:HH12	21:Ce:160:TRP:H	1.23	0.83
1:C1:1809:G:HO2'	8:CJ:2:GLY:N	1.79	0.81
1:C1:3289:G:H1	1:C1:3298:U:H3	1.27	0.81
40:LS:93:GLU:HG3	40:LS:140:ILE:HD12	1.66	0.75
21:Ce:306:ARG:HE	21:Ce:310:ARG:HH21	1.32	0.75
18:CV:383:HIS:HE1	18:CV:387:ARG:NH1	1.87	0.72
32:LK:90:ARG:HH21	32:LK:95:GLU:HG2	1.54	0.72
1:C1:1000:G:H1	1:C1:1017:U:H3	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:CN:100:ARG:HG3	14:CQ:26:GLY:HA3	1.70	0.71
18:CV:383:HIS:CE1	18:CV:387:ARG:NH1	2.59	0.70
9:CK:165:PRO:HG2	20:Cd:326:GLN:HE21	1.57	0.70
18:CV:30:ILE:HD11	18:CV:83:CYS:HB3	1.74	0.69
43:LV:67:GLY:H	43:LV:72:ARG:HH21	1.37	0.69
45:LY:47:ILE:HD13	45:LY:114:ARG:HH21	1.59	0.67
41:LT:49:GLN:HA	41:LT:52:MET:HE3	1.75	0.67
18:CV:78:ARG:HD2	18:CV:110:VAL:HG22	1.77	0.67
18:CW:145:ALA:O	18:CW:149:LEU:HB2	1.95	0.67
21:Ce:258:ALA:HB2	46:LZ:123:SER:HB2	1.77	0.67
20:Cd:406:HIS:CE1	20:Cd:409:GLN:HB3	2.29	0.67
31:LJ:54:THR:HG22	31:LJ:62:ARG:H	1.59	0.66
22:Ch:470:LEU:HB2	22:Ch:484:LEU:HB2	1.77	0.66
17:CT:232:SER:HB2	18:CW:595:ARG:HD3	1.77	0.66
31:LJ:93:ARG:HD3	31:LJ:95:ARG:H	1.60	0.66
24:LA:79:ASN:HB2	24:LA:82:MET:HE3	1.78	0.66
1:C1:2101:A:HO2'	56:Lj:2:THR:N	1.94	0.66
1:C1:806:U:H5''	24:LA:21:ARG:HD3	1.76	0.66
1:C1:2899:A:H2'	25:LB:256:TRP:HB3	1.78	0.65
1:C1:2928:A:N7	24:LA:215:ASN:ND2	2.43	0.65
1:C1:949:A:H62	1:C1:1098:G:H8	1.45	0.65
1:C1:1661:U:OP1	6:CH:509:ARG:NH1	2.30	0.65
61:Lr:11:GLN:NE2	61:Lr:12:ASN:OD1	2.30	0.65
21:Ce:434:GLU:HB3	21:Ce:439:LYS:HE3	1.79	0.64
18:CW:270:ARG:HH12	18:CW:363:ASN:HD22	1.46	0.64
20:Cd:429:LEU:HD21	20:Cd:441:MET:HG3	1.78	0.64
22:Ch:195:VAL:HG12	22:Ch:206:THR:HG22	1.80	0.64
46:LZ:96:ASN:OD1	46:LZ:97:ALA:N	2.31	0.64
61:Lr:5:THR:HG23	61:Lr:8:GLY:H	1.63	0.63
25:LB:293:ALA:HB2	25:LB:303:LYS:HG3	1.81	0.63
6:CH:53:GLN:HE21	6:CH:105:GLU:HG2	1.63	0.63
1:C1:3041:G:H4'	14:CQ:42:MET:HE1	1.81	0.63
1:C1:981:G:H1	1:C1:2656:A:H62	1.45	0.63
12:CN:106:ASN:ND2	43:LV:135:ALA:O	2.32	0.63
1:C1:2740:U:H4'	33:LL:200:LYS:HE3	1.80	0.62
12:CN:107:VAL:HG23	12:CN:108:ILE:HG13	1.81	0.62
40:LS:130:GLU:HG2	40:LS:131:LYS:HG3	1.81	0.62
17:CU:27:ILE:HB	17:CU:42:PHE:HB2	1.81	0.62
33:LL:17:HIS:HB3	33:LL:20:ARG:HH11	1.65	0.62
46:LZ:13:THR:HB	53:Lg:87:ARG:HG3	1.82	0.62
1:C1:1614:G:N7	46:LZ:16:ARG:NH1	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:CS:310:GLU:HA	59:Lp:85:ARG:HH12	1.65	0.61
51:Le:36:PRO:HB2	51:Le:44:ARG:HB2	1.83	0.61
61:Lr:196:LYS:HB3	61:Lr:199:GLN:HB2	1.81	0.61
1:C1:2850:U:HO2'	13:CO:2:ALA:N	1.99	0.61
15:CR:285:LYS:O	61:Lr:47:LYS:NZ	2.31	0.61
25:LB:136:LYS:HA	25:LB:139:GLU:HG2	1.82	0.61
18:CV:301:PRO:O	18:CV:312:ARG:NH2	2.34	0.61
51:Le:88:MET:HG3	60:Lq:36:THR:HA	1.83	0.61
56:Lj:54:LYS:O	56:Lj:58:VAL:HB	2.01	0.61
1:C1:2420:G:O2'	1:C1:2444:G:N2	2.34	0.60
12:CN:98:GLU:OE2	14:CQ:76:ASN:ND2	2.34	0.60
1:C1:2446:G:H22	1:C1:2449:A:H5'	1.67	0.60
18:CV:177:ASP:OD1	18:CV:226:ASN:ND2	2.34	0.60
37:LP:125:GLN:HB2	37:LP:141:SER:HB2	1.83	0.60
6:CH:289:MET:HE1	6:CH:318:ARG:HG2	1.82	0.60
46:LZ:88:LEU:HD21	46:LZ:120:ARG:HG3	1.83	0.60
1:C1:1211:A:H5''	5:CF:203:SER:HB3	1.83	0.60
1:C1:1264:U:H2'	1:C1:1265:G:H8	1.65	0.60
1:C1:1431:U:H2'	1:C1:1432:A2M:H8	1.84	0.60
1:C1:1875:A:OP2	19:Cb:7:ARG:NH2	2.31	0.60
17:CU:11:CYS:HG	17:CU:46:SER:HG	1.48	0.60
29:LG:165:LEU:HA	35:LN:7:LEU:HD11	1.84	0.59
1:C1:2478:A:N1	1:C1:2553:C:N4	2.50	0.59
24:LA:82:MET:HE1	24:LA:165:MET:HE2	1.84	0.59
1:C1:435:G:OP1	60:Lq:126:LYS:NZ	2.34	0.59
1:C1:2079:G:OP1	1:C1:2081:C:N4	2.36	0.59
2:C2:12:A:OP1	37:LP:3:ARG:NH1	2.36	0.59
2:C2:71:A:O2'	2:C2:83:C:N4	2.36	0.59
6:CH:183:VAL:HG21	6:CH:219:ASP:HB2	1.84	0.59
34:LM:32:GLU:OE2	40:LS:95:ARG:NH2	2.36	0.59
1:C1:44:A:H4'	35:LN:84:PRO:HD2	1.85	0.59
1:C1:2932:G:N7	9:CK:140:LYS:NZ	2.43	0.59
45:LY:86:ARG:HB3	45:LY:96:ILE:HD11	1.86	0.58
6:CH:186:VAL:HG23	6:CH:187:THR:HG23	1.85	0.58
1:C1:1045:A:N3	41:LT:130:ARG:NH2	2.51	0.58
24:LA:118:GLU:OE2	24:LA:156:LYS:NZ	2.37	0.58
47:La:92:SER:OG	47:La:94:GLN:NE2	2.31	0.58
1:C1:2214:G:OP1	15:CR:101:LYS:NZ	2.36	0.58
7:CI:215:ARG:HH21	7:CI:273:PHE:HD2	1.52	0.58
15:CR:297:HIS:CE1	61:Lr:48:ARG:HH12	2.22	0.58
61:Lr:90:LEU:HD22	61:Lr:124:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:CT:90:ARG:HG2	17:CT:104:THR:HG22	1.85	0.58
1:C1:2454:A:H1'	61:Lr:207:LYS:HE2	1.86	0.58
18:CV:586:PRO:O	18:CV:595:ARG:NH2	2.36	0.58
54:Lh:15:LYS:O	54:Lh:66:LYS:NZ	2.34	0.58
1:C1:1748:C:OP2	57:Lk:74:ARG:NH1	2.36	0.57
1:C1:1223:A2M:OP1	32:LK:92:ARG:NH2	2.37	0.57
2:C2:63:G:O2'	54:Lh:54:LYS:NZ	2.36	0.57
26:LC:185:VAL:HG11	26:LC:231:GLY:HA3	1.87	0.57
32:LK:130:LYS:NZ	32:LK:156:GLU:OE2	2.25	0.57
17:CT:195:VAL:HG22	17:CT:205:ILE:HG12	1.87	0.57
34:LM:54:ARG:NH2	34:LM:76:ALA:O	2.37	0.57
4:C4:75:A:N3	40:LS:50:LYS:NZ	2.51	0.57
18:CW:296:SER:OG	18:CW:299:GLU:OE1	2.22	0.57
35:LN:36:ILE:HG12	35:LN:64:VAL:HG23	1.87	0.57
1:C1:1685:U:O2	1:C1:1766:G:O2'	2.22	0.57
17:CT:380:PHE:HB2	17:CT:385:LEU:HD12	1.87	0.57
1:C1:767:G:O6	47:La:77:LYS:NZ	2.38	0.57
1:C1:1182:C:H5''	10:CL:31:LYS:HD3	1.86	0.57
15:CR:486:GLU:O	61:Lr:52:THR:OG1	2.22	0.57
18:CV:157:LEU:HD11	18:CV:200:GLN:HB2	1.87	0.57
36:LO:127:ARG:HG2	36:LO:131:LEU:HD13	1.87	0.57
6:CH:342:ARG:NH1	12:CN:243:GLU:OE2	2.38	0.57
16:CS:73:ASP:OD1	16:CS:76:ARG:NH2	2.36	0.57
21:Ce:248:ARG:NH2	21:Ce:252:GLU:OE2	2.37	0.57
22:Ch:264:ILE:HD12	22:Ch:274:HIS:HB2	1.86	0.57
23:Cz:117:ARG:NH2	31:LJ:54:THR:O	2.38	0.57
24:LA:105:SER:HB3	24:LA:160:SER:HB3	1.87	0.57
40:LS:12:ARG:HB3	40:LS:24:LEU:HD23	1.87	0.57
18:CW:301:PRO:O	18:CW:312:ARG:NH2	2.37	0.56
20:Cd:138:ARG:HG3	20:Cd:139:GLU:HG3	1.87	0.56
30:LH:68:ARG:NH1	30:LH:188:ASN:OD1	2.38	0.56
5:CF:32:GLU:O	5:CF:36:LYS:NZ	2.39	0.56
7:CI:269:HIS:ND1	7:CI:271:ASP:OD2	2.37	0.56
18:CW:205:LEU:HD11	18:CW:230:LEU:HD23	1.87	0.56
1:C1:1081:A:OP2	41:LT:108:ARG:NH1	2.39	0.56
15:CR:292:ASN:OD1	15:CR:297:HIS:NE2	2.34	0.56
1:C1:643:C:H2'	1:C1:644:A:H8	1.69	0.56
1:C1:2392:G:H2'	1:C1:2393:A:H8	1.70	0.56
17:CT:201:LYS:NZ	17:CT:220:PRO:O	2.38	0.56
25:LB:59:ASP:HB2	25:LB:358:LYS:HD2	1.87	0.56
14:CQ:17:LYS:NZ	25:LB:361:ASP:OD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CW:555:GLN:NE2	18:CW:588:ASP:OD2	2.36	0.56
61:Lr:65:ILE:HD12	61:Lr:148:VAL:HG13	1.86	0.56
1:C1:346:G:O6	56:Lj:55:ARG:NH2	2.39	0.56
1:C1:742:G:HO2'	1:C1:752:G:H22	1.54	0.56
36:LO:13:LYS:O	40:LS:169:ARG:NH2	2.39	0.56
12:CN:74:THR:HB	12:CN:98:GLU:HA	1.87	0.56
14:CQ:158:GLU:HA	14:CQ:161:ARG:HD2	1.88	0.56
18:CW:398:ALA:HA	18:CW:438:LEU:HD11	1.88	0.56
22:Ch:471:LYS:NZ	22:Ch:483:ASP:OD1	2.39	0.56
1:C1:1737:G:OP1	42:LU:101:ARG:NH2	2.35	0.55
12:CN:4:ARG:HB3	12:CN:208:LEU:HA	1.87	0.55
21:Ce:103:VAL:HG23	21:Ce:104:ARG:HG2	1.87	0.55
1:C1:1476:G:OP2	1:C1:1476:G:N2	2.36	0.55
15:CR:294:SER:OG	61:Lr:45:ARG:NH2	2.38	0.55
54:Lh:15:LYS:HD3	54:Lh:19:GLU:HG3	1.87	0.55
1:C1:1159:C:H4'	36:LO:91:PRO:HD3	1.89	0.55
6:CH:156:LEU:HD23	6:CH:159:LEU:HD12	1.88	0.55
33:LL:169:SER:OG	33:LL:172:GLU:OE1	2.23	0.55
1:C1:34:G:OP1	35:LN:73:ARG:NH1	2.39	0.55
1:C1:2161:A:H62	1:C1:2209:G:H21	1.55	0.55
18:CW:420:GLN:HG2	18:CW:421:LEU:HD12	1.88	0.55
32:LK:90:ARG:NH2	32:LK:95:GLU:O	2.39	0.55
1:C1:563:U:H2'	1:C1:564:A:H8	1.71	0.55
1:C1:1469:G:H21	53:Lg:7:THR:HG22	1.71	0.55
1:C1:2833:G:OP2	1:C1:2833:G:N2	2.36	0.55
23:Cz:76:ARG:NH1	23:Cz:77:GLN:OE1	2.39	0.55
60:Lq:9:ILE:HG22	60:Lq:47:VAL:HG22	1.89	0.55
6:CH:549:ARG:NH1	42:LU:31:ASP:OD2	2.35	0.55
29:LG:232:THR:HG22	29:LG:235:ARG:HH12	1.71	0.55
46:LZ:14:ARG:NH2	53:Lg:84:ASN:OD1	2.40	0.55
15:CR:410:ILE:HG23	15:CR:421:MET:HE1	1.89	0.55
17:CU:158:GLU:HB2	17:CU:161:SER:HB2	1.89	0.55
2:C2:75:G:OP2	45:LY:73:TYR:OH	2.23	0.55
5:CF:61:ASN:O	32:LK:123:LYS:NZ	2.40	0.55
8:CJ:70:GLN:HA	8:CJ:73:LEU:HD12	1.87	0.55
11:CM:103:PRO:HA	11:CM:106:ARG:HG2	1.89	0.55
17:CT:83:VAL:HG22	17:CT:347:LYS:HG2	1.89	0.55
29:LG:56:PRO:HD2	29:LG:59:ILE:HD12	1.87	0.55
57:Lk:14:ILE:HA	57:Lk:17:ARG:HD3	1.88	0.55
1:C1:2074:G:O6	19:Cb:72:LYS:NZ	2.39	0.55
1:C1:258:A:OP1	55:Li:38:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:742:G:O2'	1:C1:752:G:N2	2.38	0.55
1:C1:2362:A:OP1	26:LC:70:ARG:NH2	2.39	0.55
1:C1:262:G:H5''	35:LN:14:LYS:HE2	1.89	0.54
1:C1:1420:OMC:HM22	1:C1:1421:U:H5'	1.88	0.54
1:C1:2112:A:N6	1:C1:2150:G:O2'	2.35	0.54
6:CH:242:LEU:O	6:CH:280:LYS:NZ	2.35	0.54
46:LZ:49:PRO:HD3	46:LZ:67:ILE:HG12	1.90	0.54
1:C1:64:A:H5''	35:LN:174:LEU:HD13	1.88	0.54
1:C1:223:A:OP2	45:LY:4:ARG:NH1	2.40	0.54
1:C1:1438:U:OP1	1:C1:1859:A:N6	2.40	0.54
1:C1:3033:G:H1'	6:CH:513:LYS:HE3	1.88	0.54
20:Cd:3:THR:O	20:Cd:9:ASN:ND2	2.36	0.54
21:Ce:332:GLN:HB3	21:Ce:335:LYS:HE2	1.88	0.54
1:C1:69:C:OP2	1:C1:294:G:N2	2.39	0.54
1:C1:2425:G:O6	1:C1:2456:U:O2	2.25	0.54
1:C1:2475:C:H5''	29:LG:252:ARG:HH22	1.73	0.54
18:CW:393:ILE:HG21	18:CW:434:GLU:HB3	1.88	0.54
20:Cd:285:ILE:HD11	20:Cd:296:ALA:HB2	1.87	0.54
18:CW:30:ILE:HD11	18:CW:83:CYS:HB3	1.90	0.54
15:CR:283:ARG:O	15:CR:287:ALA:CB	2.56	0.54
39:LR:44:LEU:HD22	39:LR:49:LEU:HD22	1.89	0.54
1:C1:1135:G:O2'	1:C1:2334:G:N2	2.41	0.54
1:C1:1260:C:H2'	1:C1:1261:A:H8	1.72	0.54
5:CF:227:TRP:HB2	5:CF:234:VAL:HG22	1.89	0.54
9:CK:133:PHE:HB3	9:CK:149:ARG:HB3	1.89	0.54
22:Ch:417:THR:HG23	22:Ch:418:LEU:HG	1.89	0.54
39:LR:98:ARG:NH1	39:LR:130:ASN:OD1	2.38	0.54
1:C1:948:U:H2'	1:C1:949:A:H8	1.72	0.54
6:CH:422:ARG:NH1	6:CH:435:ASP:O	2.40	0.54
9:CK:129:GLU:HB2	20:Cd:62:SER:H	1.71	0.54
1:C1:64:A:N3	1:C1:79:U:O2'	2.37	0.54
8:CJ:36:LEU:HD11	8:CJ:75:GLU:HG2	1.89	0.54
15:CR:194:ARG:HD2	15:CR:229:PHE:HD1	1.73	0.54
18:CW:322:ALA:O	18:CW:326:ASN:ND2	2.41	0.54
22:Ch:441:ASN:HD22	22:Ch:443:ARG:HE	1.56	0.54
46:LZ:24:ILE:HA	46:LZ:42:VAL:HG12	1.89	0.54
1:C1:1641:G:H2'	1:C1:1642:G:C8	2.43	0.54
1:C1:2338:G:OP2	1:C1:2338:G:N2	2.33	0.54
1:C1:2544:G:OP1	21:Ce:439:LYS:NZ	2.31	0.54
21:Ce:103:VAL:HG12	55:Li:45:ARG:HD2	1.90	0.54
25:LB:76:VAL:HG12	25:LB:326:LYS:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LD:214:LEU:HB3	27:LD:222:TYR:HB2	1.88	0.54
1:C1:3002:A:H4'	25:LB:13:SER:HB2	1.89	0.54
2:C2:86:U:O2	56:Lj:87:ARG:NH1	2.41	0.54
9:CK:62:ARG:HH12	9:CK:66:LYS:HE2	1.71	0.54
26:LC:236:PRO:HG2	26:LC:239:ALA:HB3	1.89	0.54
29:LG:78:ILE:HG23	29:LG:163:ILE:HD13	1.90	0.54
1:C1:632:G:H5'	1:C1:1100:G:H1'	1.88	0.53
1:C1:1216:G:N2	32:LK:131:GLU:OE1	2.37	0.53
1:C1:2681:U:O2'	41:LT:88:ARG:O	2.23	0.53
1:C1:2860:G:O2'	1:C1:2982:A:N1	2.41	0.53
18:CV:135:GLN:HG2	18:CV:189:LEU:HD22	1.90	0.53
1:C1:1319:C:H2'	1:C1:1320:G:H8	1.73	0.53
1:C1:1373:A:N6	1:C1:1401:A:O2'	2.41	0.53
1:C1:2544:G:O6	29:LG:66:LYS:NZ	2.41	0.53
15:CR:412:GLU:OE1	15:CR:416:ARG:NH1	2.40	0.53
18:CV:383:HIS:HE1	18:CV:387:ARG:HH11	1.56	0.53
20:Cd:406:HIS:HE1	20:Cd:409:GLN:HB3	1.71	0.53
22:Ch:384:MET:HB2	22:Ch:400:LEU:HB2	1.91	0.53
30:LH:138:VAL:HG11	30:LH:183:LEU:HD11	1.90	0.53
60:Lq:11:GLU:OE2	60:Lq:14:ARG:NH1	2.41	0.53
16:CS:310:GLU:HA	59:Lp:85:ARG:NH1	2.24	0.53
18:CW:206:ARG:NH2	18:CW:294:GLY:O	2.41	0.53
34:LM:73:PRO:HG2	34:LM:76:ALA:HB2	1.90	0.53
36:LO:159:GLU:OE1	36:LO:162:ARG:NH1	2.42	0.53
1:C1:210:G:OP1	45:LY:15:ARG:NH1	2.40	0.53
1:C1:1136:A:OP1	1:C1:2335:A:N6	2.41	0.53
1:C1:1726:C:O2'	57:Lk:4:GLU:OE2	2.26	0.53
14:CQ:18:GLY:HA3	14:CQ:31:PHE:O	2.08	0.53
32:LK:63:THR:O	32:LK:69:ALA:HA	2.08	0.53
1:C1:813:G:O2'	1:C1:1844:A:N3	2.42	0.53
4:C4:6:C:O2'	27:LD:50:ARG:NH2	2.42	0.53
18:CV:121:GLU:HG3	18:CV:178:THR:HG21	1.89	0.53
18:CW:2:THR:N	18:CW:54:GLU:OE2	2.41	0.53
1:C1:2477:U:OP2	1:C1:2545:G:N2	2.31	0.53
1:C1:2919:C:H2'	1:C1:2920:G:H8	1.73	0.53
12:CN:99:GLU:OE2	12:CN:125:THR:OG1	2.16	0.53
18:CV:3:ALA:HA	18:CV:55:THR:HG22	1.91	0.53
46:LZ:22:VAL:HG12	46:LZ:44:GLY:HA3	1.90	0.53
50:Ld:14:ASP:HB3	50:Ld:97:LEU:HD11	1.90	0.53
1:C1:1241:U:O5'	5:CF:57:ARG:NH1	2.42	0.53
11:CM:102:PRO:HB2	11:CM:105:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:LS:109:ASP:OD2	40:LS:113:ARG:NH1	2.40	0.53
61:Lr:41:TYR:OH	61:Lr:47:LYS:O	2.26	0.53
1:C1:3299:U:H2'	1:C1:3300:A:H8	1.74	0.53
15:CR:418:PRO:O	15:CR:451:TYR:OH	2.25	0.53
18:CV:35:ARG:NH1	18:CW:376:SER:O	2.42	0.53
18:CW:104:ILE:HG12	18:CW:130:LEU:HD13	1.90	0.53
1:C1:1929:G:OP2	39:LR:135:LYS:NZ	2.41	0.53
1:C1:153:A:OP1	33:LL:87:ARG:NH2	2.38	0.53
1:C1:3044:A:H3'	1:C1:3045:A:H8	1.74	0.53
6:CH:10:VAL:HG22	6:CH:63:ILE:HD12	1.89	0.53
31:LJ:16:GLN:HB2	31:LJ:133:THR:HB	1.91	0.53
1:C1:1758:G:O2'	1:C1:1760:G:OP2	2.27	0.52
2:C2:26:U:O2'	26:LC:52:ALA:O	2.26	0.52
7:CI:187:GLY:O	7:CI:234:GLU:HA	2.08	0.52
42:LU:40:GLU:OE2	42:LU:44:ASN:ND2	2.43	0.52
43:LV:106:ASN:OD1	43:LV:110:GLU:N	2.42	0.52
61:Lr:26:ARG:NH2	61:Lr:210:MET:SD	2.75	0.52
2:C2:103:G:OP2	2:C2:105:A:O2'	2.23	0.52
15:CR:283:ARG:O	15:CR:287:ALA:HB2	2.08	0.52
15:CR:99:LEU:HD22	15:CR:103:LEU:HD23	1.91	0.52
17:CT:27:ILE:HB	17:CT:42:PHE:HB2	1.89	0.52
51:Le:88:MET:HE1	60:Lq:114:ARG:HA	1.91	0.52
1:C1:2767:A:N6	1:C1:2913:U:O2'	2.42	0.52
1:C1:3238:U:O4	25:LB:124:LYS:NZ	2.42	0.52
29:LG:101:ARG:NH2	29:LG:191:THR:O	2.42	0.52
30:LH:127:MET:HG2	30:LH:220:VAL:HA	1.91	0.52
1:C1:706:G:OP2	1:C1:706:G:N2	2.35	0.52
1:C1:1766:G:H2'	1:C1:1767:A:C8	2.45	0.52
1:C1:3270:U:H5''	25:LB:309:MET:HE2	1.91	0.52
12:CN:233:ILE:HA	12:CN:237:MET:HB2	1.92	0.52
18:CW:351:PRO:HG2	18:CW:417:ALA:HB1	1.91	0.52
1:C1:1242:A:N3	1:C1:1263:C:O2'	2.41	0.52
1:C1:1337:G:N2	1:C1:1339:U:O2'	2.35	0.52
1:C1:1658:G:O6	42:LU:81:ARG:NH2	2.43	0.52
5:CF:64:ARG:NH1	5:CF:65:ILE:O	2.43	0.52
17:CT:44:LYS:O	17:CT:72:TYR:OH	2.27	0.52
26:LC:36:VAL:HG21	26:LC:251:LEU:HD21	1.90	0.52
38:LQ:150:THR:OG1	38:LQ:152:ASP:OD1	2.25	0.52
61:Lr:60:ARG:HD3	61:Lr:63:MET:HE3	1.92	0.52
1:C1:2789:G:H2'	1:C1:2790:G:C8	2.44	0.52
17:CT:118:LEU:HB2	17:CT:348:PRO:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Cd:328:SER:HB3	20:Cd:376:ILE:HD11	1.92	0.52
31:LJ:94:ARG:HG2	31:LJ:157:ARG:HH21	1.74	0.52
15:CR:377:VAL:O	15:CR:417:GLN:NE2	2.42	0.52
21:Ce:386:PRO:HA	21:Ce:389:LEU:HD23	1.91	0.52
44:LX:149:ALA:HA	44:LX:153:LEU:HB2	1.92	0.52
46:LZ:16:ARG:NH2	46:LZ:17:TYR:OH	2.43	0.52
7:CI:207:PHE:HB2	7:CI:213:ILE:HD11	1.90	0.52
17:CT:135:THR:HG22	17:CT:183:VAL:HG11	1.92	0.52
39:LR:134:HIS:CE1	39:LR:136:ARG:HB3	2.45	0.52
1:C1:877:A:O2'	1:C1:879:U:OP2	2.27	0.52
1:C1:1816:C:O2'	1:C1:1822:A:N1	2.40	0.52
2:C2:63:G:H22	2:C2:97:A:H2	1.57	0.52
7:CI:217:ARG:NE	7:CI:272:LEU:O	2.43	0.52
1:C1:750:C:OP1	33:LL:201:ARG:NH1	2.42	0.51
6:CH:255:ILE:HB	6:CH:297:LEU:HD21	1.92	0.51
20:Cd:411:ILE:HG13	20:Cd:439:LEU:HD11	1.92	0.51
25:LB:219:ILE:HG12	25:LB:277:THR:HG23	1.92	0.51
1:C1:2621:G:O2'	27:LD:155:ARG:NH1	2.43	0.51
6:CH:534:LEU:HD12	6:CH:546:LEU:HD11	1.93	0.51
8:CJ:42:ILE:HG13	8:CJ:72:LEU:HD11	1.92	0.51
14:CQ:179:GLU:OE1	50:Ld:86:ARG:NH1	2.43	0.51
24:LA:30:ARG:HG2	24:LA:74:GLU:HG3	1.92	0.51
28:LE:94:LEU:HD23	28:LE:122:VAL:HG11	1.92	0.51
55:Li:60:ALA:HB3	55:Li:63:GLU:HG3	1.92	0.51
1:C1:462:A:OP1	60:Lq:92:LYS:NZ	2.43	0.51
1:C1:643:C:H2'	1:C1:644:A:C8	2.44	0.51
1:C1:2368:C:H4'	9:CK:142:THR:HG21	1.92	0.51
1:C1:2392:G:H2'	1:C1:2393:A:C8	2.45	0.51
1:C1:2734:U:OP1	33:LL:193:ARG:NH1	2.35	0.51
4:C4:23:A:N3	4:C4:119:U:O2'	2.42	0.51
15:CR:341:LYS:HD3	15:CR:376:LEU:HD13	1.92	0.51
11:LF:102:PRO:HB2	11:LF:105:PRO:HD2	1.93	0.51
1:C1:1624:C:H5'	1:C1:1625:U:H5''	1.92	0.51
17:CT:90:ARG:HG3	17:CT:128:ALA:HB1	1.92	0.51
18:CW:121:GLU:HG3	18:CW:178:THR:HG21	1.91	0.51
18:CW:350:ILE:HD11	18:CW:417:ALA:HB2	1.93	0.51
41:LT:68:THR:HG22	41:LT:69:LYS:H	1.75	0.51
1:C1:282:U:H2'	1:C1:283:G:H8	1.75	0.51
1:C1:1785:C:H2'	1:C1:1786:G:H8	1.75	0.51
4:C4:38:U:N3	4:C4:41:G:OP2	2.42	0.51
27:LD:137:THR:HG22	27:LD:139:ASP:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2346:C:OP2	36:LO:87:ARG:NH2	2.41	0.51
1:C1:2509:A:OP1	24:LA:93:ASN:ND2	2.43	0.51
1:C1:2984:G:H4'	9:CK:2:PRO:HG3	1.91	0.51
18:CV:376:SER:O	18:CW:35:ARG:NH1	2.42	0.51
22:Ch:327:ILE:HB	22:Ch:375:LEU:HD11	1.93	0.51
28:LE:94:LEU:HD21	28:LE:165:ILE:HD12	1.91	0.51
1:C1:448:C:H41	28:LE:15:ARG:HH21	1.59	0.51
1:C1:1480:C:H2'	1:C1:1481:A:H8	1.76	0.51
18:CW:389:HIS:NE2	18:CW:410:GLN:OE1	2.44	0.51
21:Ce:373:LYS:HD2	21:Ce:420:ARG:H	1.75	0.51
42:LU:47:ILE:HD12	42:LU:62:ILE:HD11	1.93	0.51
1:C1:344:A:N6	58:Ll:37:TYR:O	2.40	0.51
1:C1:405:G:OP1	37:LP:62:ARG:NH1	2.44	0.51
6:CH:281:MET:HE1	6:CH:337:ARG:HB3	1.92	0.51
11:CM:14:VAL:HB	11:CM:17:THR:HG22	1.91	0.51
1:C1:2073:G:O6	19:Cb:72:LYS:NZ	2.39	0.51
6:CH:292:LYS:HE2	6:CH:297:LEU:HD23	1.93	0.51
15:CR:297:HIS:CG	61:Lr:48:ARG:HH22	2.28	0.51
33:LL:192:ALA:HB2	55:Li:19:GLY:HA2	1.93	0.51
46:LZ:50:SER:HB2	46:LZ:64:ARG:HB3	1.93	0.51
61:Lr:157:PHE:HE1	61:Lr:190:LEU:HB2	1.76	0.51
1:C1:101:A:H3'	1:C1:102:G:H21	1.76	0.50
1:C1:609:A:H2	60:Lq:135:GLY:HA2	1.75	0.50
1:C1:958:G:H5''	38:LQ:168:ARG:HH12	1.76	0.50
1:C1:1361:U:H2'	1:C1:1362:G:H8	1.76	0.50
1:C1:1779:A:H2'	1:C1:1780:A:H8	1.76	0.50
1:C1:180:U:H1'	45:LY:128:VAL:HG11	1.93	0.50
1:C1:663:C:O2'	1:C1:667:U:OP1	2.27	0.50
1:C1:736:G:H2'	1:C1:737:A:H8	1.77	0.50
1:C1:2477:U:H5'	29:LG:71:ARG:HG3	1.93	0.50
12:CN:109:VAL:HB	12:CN:149:GLY:HA2	1.92	0.50
1:C1:2513:C:N4	49:Lc:60:GLU:OE2	2.45	0.50
1:C1:3109:U:H3	1:C1:3338:C:H42	1.59	0.50
17:CT:2:LEU:HD12	17:CT:333:PRO:HG3	1.94	0.50
18:CV:157:LEU:O	18:CV:161:LYS:HB2	2.12	0.50
18:CW:97:LEU:HD23	18:CW:134:LEU:HD23	1.94	0.50
30:LH:10:ILE:HG12	30:LH:109:ARG:HG2	1.94	0.50
34:LM:13:ARG:NH2	40:LS:149:SER:O	2.45	0.50
51:Le:97:ILE:HG21	51:Le:106:ARG:HG2	1.93	0.50
1:C1:1157:G:N2	36:LO:89:MET:SD	2.85	0.50
8:CJ:141:LEU:HD11	8:CJ:241:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:CM:98:ILE:HG12	11:CM:139:TRP:HE1	1.75	0.50
18:CV:210:ALA:O	18:CV:312:ARG:NH1	2.44	0.50
31:LJ:87:VAL:HG21	31:LJ:113:LEU:HD23	1.93	0.50
59:Lp:51:ALA:HB3	59:Lp:54:ILE:HD12	1.94	0.50
1:C1:1142:A:OP1	38:LQ:31:GLY:N	2.45	0.50
18:CW:34:LEU:HA	18:CW:91:VAL:HG21	1.92	0.50
28:LE:86:PRO:HB3	28:LE:166:ASP:HB2	1.93	0.50
30:LH:94:ILE:HG22	30:LH:105:LEU:HD11	1.93	0.50
1:C1:68:A:O2'	1:C1:308:C:O2	2.29	0.50
1:C1:3000:U:OP2	1:C1:3050:C:N4	2.44	0.50
2:C2:120:G:H5'	21:Ce:182:PRO:HB3	1.94	0.50
1:C1:29:C:O2'	1:C1:62:A:N3	2.38	0.50
1:C1:2100:U:OP2	1:C1:2105:A:N6	2.37	0.50
1:C1:2320:A:H2'	1:C1:2321:A:H8	1.76	0.50
1:C1:3265:A:OP1	50:Ld:27:ARG:NH1	2.45	0.50
21:Ce:330:LEU:HD12	57:Lk:49:LEU:HD22	1.93	0.50
38:LQ:174:ARG:HB2	38:LQ:177:VAL:HG23	1.94	0.50
57:Lk:29:PRO:O	57:Lk:32:GLN:NE2	2.45	0.50
1:C1:2314:U:H2'	1:C1:2315:A:H8	1.76	0.50
8:CJ:17:MET:HE3	8:CJ:66:THR:HA	1.94	0.50
13:CO:26:GLU:OE2	25:LB:346:HIS:ND1	2.44	0.50
22:Ch:208:SER:OG	22:Ch:209:MET:N	2.45	0.50
53:Lg:92:ARG:O	53:Lg:96:ILE:HG12	2.12	0.50
15:CR:27:PRO:O	15:CR:77:TYR:OH	2.27	0.50
17:CT:152:SER:HB2	17:CT:168:LEU:HD11	1.94	0.50
18:CV:134:LEU:HD22	18:CV:140:LEU:HB3	1.93	0.50
21:Ce:370:GLN:NE2	21:Ce:372:GLY:O	2.45	0.50
1:C1:967:U:H2'	1:C1:968:U:H6	1.76	0.49
1:C1:1206:A:N1	23:Cz:40:ARG:NH2	2.59	0.49
1:C1:1577:C:H5'	1:C1:1676:A:H1'	1.94	0.49
1:C1:2075:U:H1'	14:CQ:42:MET:HE2	1.94	0.49
1:C1:2900:A:N7	25:LB:2:SER:N	2.60	0.49
1:C1:3289:G:O6	1:C1:3298:U:O4	2.29	0.49
29:LG:83:TYR:OH	29:LG:235:ARG:NH2	2.45	0.49
1:C1:404:U:H2'	1:C1:405:G:H8	1.76	0.49
1:C1:1779:A:H2'	1:C1:1780:A:C8	2.47	0.49
1:C1:2376:A:H2'	1:C1:2377:G:H8	1.76	0.49
24:LA:113:VAL:HG12	24:LA:166:ILE:HD13	1.95	0.49
27:LD:50:ARG:NH1	27:LD:150:ASP:OD2	2.45	0.49
1:C1:1238:C:H2'	1:C1:1239:G:H8	1.77	0.49
5:CF:175:ILE:HD12	5:CF:180:CYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CH:616:ALA:HB1	58:Ll:25:GLN:HB3	1.94	0.49
13:CO:13:ASN:OD1	13:CO:16:ARG:NH1	2.46	0.49
33:LL:169:SER:HA	47:La:98:THR:HA	1.94	0.49
34:LM:14:VAL:HG23	34:LM:30:ILE:HD13	1.95	0.49
43:LV:41:VAL:HG12	43:LV:60:VAL:HG12	1.93	0.49
1:C1:2123:G:H2'	1:C1:2124:G:H8	1.76	0.49
22:Ch:148:PRO:HB3	22:Ch:508:LYS:HA	1.94	0.49
26:LC:301:ARG:HH21	38:LQ:69:GLU:HG2	1.77	0.49
11:LF:126:THR:HG21	41:LT:132:PRO:HG2	1.92	0.49
31:LJ:134:ARG:NH2	31:LJ:159:GLU:OE1	2.40	0.49
1:C1:1821:A:H1'	58:Ll:45:ARG:HH22	1.77	0.49
1:C1:2181:G:H2'	1:C1:2182:A:H8	1.78	0.49
23:Cz:84:LYS:HG2	23:Cz:88:LYS:HE3	1.94	0.49
52:Lf:22:ARG:HD3	52:Lf:23:ARG:HG3	1.93	0.49
1:C1:1559:G:OP2	1:C1:1559:G:N2	2.32	0.49
1:C1:2763:A:H5'	20:Cd:24:LYS:HG3	1.94	0.49
1:C1:2981:U:H2'	1:C1:2982:A:H8	1.78	0.49
12:CN:186:VAL:HG12	12:CN:218:ILE:HD11	1.95	0.49
17:CT:385:LEU:HD11	18:CV:30:ILE:HD12	1.95	0.49
26:LC:287:LEU:HA	26:LC:290:LEU:HD12	1.95	0.49
1:C1:3139:U:HO2'	40:LS:172:THR:HG1	1.61	0.49
17:CU:341:LYS:HD2	17:CU:343:VAL:HG22	1.95	0.49
31:LJ:33:ARG:HD2	31:LJ:121:ILE:HA	1.94	0.49
1:C1:604:G:H2'	1:C1:605:G:C8	2.48	0.49
1:C1:716:G:H5''	38:LQ:71:PRO:HB2	1.95	0.49
1:C1:1612:G:OP1	46:LZ:68:LYS:NZ	2.41	0.49
1:C1:2205:A:H5''	24:LA:244:GLY:HA3	1.94	0.49
4:C4:47:C:OP2	27:LD:161:ARG:NH1	2.43	0.49
17:CU:98:ILE:HD12	17:CU:110:LEU:HD23	1.94	0.49
18:CW:306:LEU:HD22	18:CW:370:GLU:HG3	1.94	0.49
32:LK:64:ILE:HG12	32:LK:69:ALA:HB2	1.95	0.49
1:C1:262:G:OP2	35:LN:44:ARG:NH1	2.37	0.49
1:C1:639:G:O2'	1:C1:1418:A:OP1	2.31	0.49
6:CH:79:ASP:OD2	6:CH:244:HIS:NE2	2.46	0.49
25:LB:10:ARG:NH1	25:LB:11:HIS:O	2.45	0.49
38:LQ:79:ARG:HA	38:LQ:82:MET:HE2	1.95	0.49
46:LZ:69:PRO:HG3	46:LZ:114:LYS:HB2	1.95	0.49
47:La:126:ARG:HG2	47:La:146:GLU:HB2	1.95	0.49
57:Lk:26:LYS:NZ	57:Lk:28:ASN:OD1	2.38	0.49
1:C1:2092:U:H2'	1:C1:2093:G:C8	2.48	0.49
2:C2:9:A:H2'	2:C2:10:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:CN:177:LEU:HD12	12:CN:181:LEU:HD11	1.95	0.49
16:CS:68:VAL:HG11	16:CS:104:LYS:HB3	1.95	0.49
18:CV:244:SER:HA	18:CV:332:VAL:HG12	1.94	0.49
1:C1:300:A:H2'	1:C1:301:A:C8	2.48	0.48
17:CU:205:ILE:O	17:CU:214:LEU:N	2.42	0.48
33:LL:23:ARG:NH1	33:LL:24:CYS:O	2.46	0.48
16:CS:293:ASP:OD1	16:CS:297:ARG:NH2	2.40	0.48
1:C1:911:A:O2'	56:Lj:49:TRP:O	2.32	0.48
1:C1:1278:G:O2'	40:LS:115:ARG:NH1	2.46	0.48
6:CH:86:ASP:HB3	6:CH:89:HIS:HB2	1.95	0.48
42:LU:120:ASP:N	42:LU:120:ASP:OD1	2.46	0.48
1:C1:735:C:H2'	1:C1:736:G:H8	1.77	0.48
1:C1:2525:U:H3	1:C1:2535:G:H1	1.61	0.48
29:LG:151:ALA:HA	29:LG:204:THR:HG22	1.95	0.48
30:LH:167:MET:HE1	30:LH:200:ILE:HD11	1.95	0.48
40:LS:80:ARG:HG3	40:LS:124:LEU:HD11	1.96	0.48
1:C1:170:A:H3'	1:C1:171:G:H8	1.78	0.48
1:C1:507:G:H5''	26:LC:346:ALA:HB2	1.96	0.48
13:CO:34:SER:O	13:CO:38:MET:HB2	2.13	0.48
15:CR:334:THR:HG22	15:CR:372:ALA:HB2	1.96	0.48
15:CR:415:MET:HG2	15:CR:450:LEU:HD13	1.96	0.48
18:CW:134:LEU:HD22	18:CW:140:LEU:HB3	1.96	0.48
40:LS:71:LYS:O	40:LS:73:LYS:NZ	2.40	0.48
40:LS:80:ARG:HE	40:LS:89:ASN:HD21	1.62	0.48
1:C1:300:A:H2'	1:C1:301:A:H8	1.79	0.48
1:C1:1387:G:N2	1:C1:1390:A:OP2	2.39	0.48
1:C1:2308:A:H5''	50:Ld:32:THR:HG23	1.95	0.48
25:LB:47:MET:HE3	25:LB:165:THR:HG23	1.96	0.48
30:LH:75:LEU:HD13	30:LH:108:VAL:HG13	1.96	0.48
45:LY:82:GLU:OE1	45:LY:83:ARG:NH1	2.47	0.48
9:CK:53:GLN:O	9:CK:57:GLN:HG3	2.14	0.48
15:CR:625:LEU:O	61:Lr:198:TRP:NE1	2.47	0.48
17:CU:24:ASP:OD1	17:CU:24:ASP:N	2.47	0.48
1:C1:1496:G:OP1	39:LR:5:ARG:NH2	2.47	0.48
1:C1:2176:A:N3	1:C1:2560:A:O2'	2.42	0.48
8:CJ:25:LYS:HE3	8:CJ:73:LEU:HD11	1.95	0.48
9:CK:174:PRO:HG2	9:CK:177:LEU:HD12	1.95	0.48
19:Cb:15:ARG:NH2	19:Cb:18:ASP:OD2	2.43	0.48
1:C1:1824:C:O2'	56:Lj:11:ARG:NH1	2.46	0.48
6:CH:288:LYS:HB3	6:CH:291:ILE:HD12	1.95	0.48
1:C1:27:A:N3	1:C1:321:C:O2'	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C2:83:C:OP1	2:C2:85:G:N2	2.46	0.48
9:CK:87:PRO:HD2	9:CK:90:LEU:HD12	1.95	0.48
26:LC:281:ILE:HG13	26:LC:282:VAL:HG23	1.96	0.48
1:C1:410:A:H2'	1:C1:411:A:C8	2.49	0.47
1:C1:1264:U:H5''	5:CF:69:LYS:HG3	1.96	0.47
10:CL:52:ASP:OD1	10:CL:52:ASP:N	2.43	0.47
10:CL:61:TYR:OH	40:LS:130:GLU:OE1	2.28	0.47
12:CN:85:ARG:NH2	12:CN:89:PRO:O	2.47	0.47
22:Ch:349:THR:HG23	22:Ch:352:GLU:H	1.78	0.47
1:C1:357:G:OP2	56:Lj:52:LYS:NZ	2.37	0.47
24:LA:178:PRO:HB2	24:LA:180:LEU:HD12	1.96	0.47
34:LM:59:LEU:HD13	40:LS:152:LEU:HD11	1.96	0.47
1:C1:206:G:OP2	45:LY:1:MET:N	2.39	0.47
1:C1:242:G:O6	33:LL:132:LYS:NZ	2.47	0.47
1:C1:703:A:N1	1:C1:763:G:O2'	2.39	0.47
1:C1:2523:G:H2'	1:C1:2524:G:H8	1.79	0.47
1:C1:2623:C:OP2	31:LJ:143:ARG:NH1	2.47	0.47
17:CT:229:ASP:OD1	17:CT:233:ARG:N	2.47	0.47
17:CU:295:LEU:HB3	17:CU:307:TRP:HB2	1.96	0.47
21:Ce:306:ARG:O	21:Ce:310:ARG:HG2	2.14	0.47
22:Ch:464:GLY:HA3	22:Ch:494:VAL:HG21	1.96	0.47
27:LD:60:ILE:HB	27:LD:80:SER:HB2	1.96	0.47
1:C1:363:U:H4'	1:C1:397:G:H5'	1.95	0.47
1:C1:464:C:H2'	1:C1:465:G:H8	1.78	0.47
5:CF:94:ARG:NH2	5:CF:95:TYR:OH	2.46	0.47
17:CT:74:ARG:HH22	17:CT:331:VAL:HG11	1.79	0.47
18:CV:269:VAL:HG12	18:CV:362:THR:HG22	1.97	0.47
24:LA:23:ARG:HH21	24:LA:53:GLY:HA3	1.79	0.47
1:C1:20:U:H2'	1:C1:21:A:C8	2.50	0.47
1:C1:95:G:H2'	1:C1:96:A:C8	2.49	0.47
1:C1:2046:C:P	21:Ce:310:ARG:HH22	2.37	0.47
1:C1:3179:G:H2'	1:C1:3180:G:H8	1.80	0.47
1:C1:869:G:H2'	1:C1:870:A:C8	2.50	0.47
1:C1:1193:U:H5	5:CF:3:LYS:HB2	1.78	0.47
1:C1:1559:G:N7	44:LX:46:HIS:NE2	2.61	0.47
7:CI:211:GLY:HA3	7:CI:240:VAL:HG11	1.97	0.47
36:LO:28:LEU:O	36:LO:103:ARG:NH1	2.47	0.47
49:Lc:41:LYS:HG3	49:Lc:96:LEU:HD22	1.97	0.47
1:C1:1135:G:OP2	1:C1:1135:G:N2	2.37	0.47
1:C1:3315:U:OP1	50:Ld:23:HIS:NE2	2.35	0.47
9:CK:166:VAL:HA	9:CK:169:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CV:24:ARG:NE	18:CW:216:ASN:OD1	2.40	0.47
20:Cd:16:ARG:NH1	20:Cd:26:GLU:OE2	2.48	0.47
25:LB:47:MET:HB3	25:LB:336:ILE:HD11	1.97	0.47
38:LQ:147:ARG:HE	38:LQ:149:LEU:HD21	1.80	0.47
42:LU:27:GLN:HG2	42:LU:28:PRO:HD3	1.95	0.47
1:C1:21:A:H2'	1:C1:22:G:C8	2.50	0.47
1:C1:1054:U:H2'	1:C1:1055:G:C8	2.50	0.47
1:C1:2046:C:O5'	21:Ce:310:ARG:NH2	2.47	0.47
8:CJ:200:ASN:ND2	8:CJ:205:ASP:OD1	2.43	0.47
8:CJ:450:TYR:HB2	8:CJ:453:ARG:HD3	1.97	0.47
1:C1:525:A:O2'	1:C1:527:G:OP2	2.32	0.47
1:C1:2769:C:OP2	1:C1:2914:U:O2'	2.33	0.47
20:Cd:47:ILE:HD12	20:Cd:56:LYS:HD3	1.97	0.47
11:LF:138:PRO:HA	11:LF:234:LEU:HD13	1.97	0.47
34:LM:59:LEU:O	40:LS:155:ARG:NH2	2.48	0.47
57:Lk:17:ARG:NH2	57:Lk:19:ASP:OD2	2.43	0.47
1:C1:111:G:OP2	33:LL:73:ARG:NH2	2.48	0.47
1:C1:1626:G:O2'	1:C1:1788:G:N2	2.39	0.47
1:C1:3079:U:H1'	1:C1:3080:A:H5''	1.97	0.47
17:CU:89:ILE:HG21	17:CU:92:LEU:HD23	1.97	0.47
11:LF:155:TYR:OH	11:LF:188:GLU:OE2	2.33	0.47
30:LH:154:ARG:HG2	30:LH:162:VAL:HG22	1.97	0.47
1:C1:848:A2M:HM'2	1:C1:849:G:H5'	1.97	0.46
22:Ch:489:ASP:HB3	22:Ch:508:LYS:HB3	1.96	0.46
1:C1:91:C:OP1	47:La:59:ARG:NH1	2.48	0.46
1:C1:1480:C:H2'	1:C1:1481:A:C8	2.50	0.46
1:C1:2640:U:OP2	31:LJ:52:ARG:NH1	2.48	0.46
1:C1:3120:C:H2'	1:C1:3121:G:H8	1.81	0.46
1:C1:3137:A:H2'	1:C1:3138:A:H8	1.79	0.46
4:C4:12:U:OP2	4:C4:68:C:O2'	2.34	0.46
6:CH:587:LEU:HD22	44:LX:146:LEU:HD13	1.97	0.46
8:CJ:397:TRP:HB2	8:CJ:401:LEU:HD12	1.97	0.46
26:LC:287:LEU:HD11	38:LQ:60:LEU:HB2	1.96	0.46
1:C1:775:A:H2'	1:C1:776:G:H8	1.81	0.46
1:C1:1920:G:H21	1:C1:3303:A:H8	1.63	0.46
1:C1:2681:U:H2'	1:C1:2682:U:C6	2.50	0.46
1:C1:3288:A:H2'	1:C1:3289:G:H8	1.80	0.46
4:C4:114:G:O2'	27:LD:73:LYS:NZ	2.49	0.46
7:CI:194:LEU:HD22	7:CI:198:PHE:HD2	1.80	0.46
11:CM:149:SER:HG	11:CM:246:ARG:HH12	1.59	0.46
15:CR:86:ASP:OD1	15:CR:90:GLN:NE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:Lr:113:SER:O	61:Lr:117:ILE:HB	2.15	0.46
1:C1:2974:A:H2'	1:C1:2975:G:H8	1.80	0.46
9:CK:154:PRO:HG2	9:CK:249:PRO:HB2	1.96	0.46
19:Cb:75:LYS:HA	19:Cb:78:LEU:HG	1.98	0.46
26:LC:34:ASP:OD1	26:LC:34:ASP:N	2.46	0.46
27:LD:86:TYR:O	27:LD:249:GLN:NE2	2.48	0.46
1:C1:2728:A:H2'	1:C1:2729:G:C8	2.51	0.46
25:LB:307:THR:HG21	25:LB:317:GLU:HG2	1.98	0.46
34:LM:21:LYS:HE2	34:LM:25:GLY:HA2	1.96	0.46
1:C1:76:G:H5'	33:LL:58:VAL:HB	1.97	0.46
1:C1:2384:OMU:HM23	1:C1:2384:OMU:H1'	1.64	0.46
1:C1:2488:G:N7	24:LA:67:TYR:OH	2.46	0.46
1:C1:2670:C:O2'	1:C1:2703:U:OP1	2.34	0.46
17:CU:229:ASP:OD1	17:CU:233:ARG:N	2.49	0.46
27:LD:38:THR:HG22	41:LT:30:TYR:HB3	1.97	0.46
31:LJ:156:THR:HB	31:LJ:159:GLU:HG3	1.96	0.46
49:Lc:78:ILE:HG12	49:Lc:89:ARG:HG2	1.97	0.46
60:Lq:10:TRP:O	60:Lq:14:ARG:HB3	2.16	0.46
1:C1:1192:G:H5''	5:CF:3:LYS:HB3	1.97	0.46
1:C1:2389:U:H3	1:C1:2562:G:H1	1.64	0.46
4:C4:83:G:H2'	4:C4:84:G:C8	2.51	0.46
16:CS:106:LEU:HD11	16:CS:139:ILE:HG12	1.97	0.46
18:CV:567:ARG:NH2	18:CV:573:TYR:OH	2.46	0.46
22:Ch:509:ASP:OD2	22:Ch:513:ARG:NH1	2.49	0.46
25:LB:58:ARG:NH1	25:LB:284:TYR:OH	2.48	0.46
1:C1:1463:G:O2'	1:C1:1851:U:O4	2.26	0.46
1:C1:2516:G:O2'	46:LZ:135:PHE:OXT	2.30	0.46
1:C1:2616:A:N6	15:CR:469:THR:OG1	2.48	0.46
11:LF:182:TYR:CZ	11:LF:203:GLN:HG2	2.51	0.46
61:Lr:104:ALA:O	61:Lr:133:LYS:NZ	2.48	0.46
1:C1:957:C:H2'	1:C1:958:G:C8	2.50	0.46
1:C1:2491:G:H4'	29:LG:247:LYS:HD2	1.98	0.46
20:Cd:238:HIS:HD1	20:Cd:332:ILE:HG13	1.81	0.46
21:Ce:237:GLU:HA	21:Ce:240:ARG:HG2	1.98	0.46
34:LM:72:LEU:HD12	34:LM:73:PRO:HD2	1.97	0.46
35:LN:8:GLU:HB2	35:LN:50:ARG:HH22	1.81	0.46
1:C1:494:C:H2'	1:C1:495:G:H8	1.81	0.46
1:C1:523:G:H2'	1:C1:524:A:C8	2.51	0.46
1:C1:3179:G:H2'	1:C1:3180:G:C8	2.51	0.46
12:CN:21:ASN:ND2	12:CN:112:ASP:OD2	2.43	0.46
28:LE:199:LYS:O	34:LM:117:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:652:A:H2'	1:C1:653:A:H8	1.81	0.45
1:C1:1252:U:H1'	1:C1:1255:C:H5	1.81	0.45
18:CW:95:GLU:OE2	18:CW:99:SER:OG	2.33	0.45
39:LR:89:MET:HE3	39:LR:90:PRO:HD2	1.98	0.45
1:C1:364:G:O2'	1:C1:389:A2M:N6	2.49	0.45
1:C1:651:C:H2'	1:C1:652:A:H8	1.81	0.45
1:C1:1151:U:H2'	1:C1:1152:A:H8	1.81	0.45
1:C1:1879:G:O2'	1:C1:2297:U:O4	2.29	0.45
12:CN:21:ASN:HB2	12:CN:67:ARG:HB3	1.97	0.45
16:CS:129:PRO:HB3	16:CS:168:VAL:HG13	1.97	0.45
21:Ce:377:PRO:O	21:Ce:408:ARG:NH1	2.49	0.45
45:LY:85:THR:HG22	45:LY:95:PRO:HA	1.99	0.45
52:Lf:16:LEU:HD11	52:Lf:33:LYS:HB2	1.98	0.45
52:Lf:44:ASN:HA	52:Lf:47:LEU:HG	1.97	0.45
1:C1:1646:G:H2'	1:C1:1647:G:H8	1.81	0.45
6:CH:405:ARG:HA	6:CH:408:GLU:HG2	1.98	0.45
11:CM:50:ILE:HD11	44:LX:31:VAL:HG21	1.99	0.45
22:Ch:338:ALA:O	22:Ch:360:ARG:NH1	2.47	0.45
33:LL:17:HIS:HB3	33:LL:20:ARG:NH1	2.29	0.45
1:C1:404:U:H2'	1:C1:405:G:C8	2.52	0.45
1:C1:575:G:H2'	1:C1:576:A:H8	1.81	0.45
1:C1:1555:C:H5''	21:Ce:428:ALA:HB2	1.98	0.45
1:C1:2647:U:OP1	27:LD:12:TYR:OH	2.33	0.45
5:CF:44:SER:OG	5:CF:222:SER:OG	2.32	0.45
21:Ce:43:GLU:O	21:Ce:47:GLU:HG2	2.16	0.45
27:LD:266:SER:HB3	27:LD:269:GLU:HG2	1.98	0.45
56:Lj:64:MET:HE3	56:Lj:67:LEU:HD23	1.99	0.45
1:C1:1791:G:H5''	8:CJ:59:ALA:HB2	1.99	0.45
1:C1:2427:U:H2'	1:C1:2428:G:C8	2.51	0.45
2:C2:47:C:H1'	2:C2:61:A:H2'	1.98	0.45
8:CJ:84:GLN:OE1	8:CJ:120:ARG:NH2	2.41	0.45
8:CJ:189:PHE:HB3	8:CJ:196:TYR:HB2	1.97	0.45
17:CT:110:LEU:HD11	17:CT:156:LEU:HD13	1.97	0.45
11:LF:92:VAL:O	11:LF:120:GLY:HA2	2.15	0.45
11:LF:156:LYS:NZ	11:LF:249:ASN:OXT	2.43	0.45
61:Lr:90:LEU:HA	61:Lr:93:LEU:HD12	1.98	0.45
1:C1:1345:G:H2'	1:C1:1346:A:C8	2.52	0.45
1:C1:1435:A:N3	1:C1:2309:C:O2'	2.47	0.45
1:C1:1741:C:O2'	1:C1:1743:U:OP2	2.29	0.45
1:C1:3275:U:H4'	1:C1:3276:A:H5'	1.99	0.45
8:CJ:418:GLN:OE1	8:CJ:453:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LG:188:ARG:O	29:LG:191:THR:OG1	2.34	0.45
56:Lj:20:ARG:NH1	56:Lj:39:TYR:OH	2.47	0.45
61:Lr:36:ILE:HG21	61:Lr:190:LEU:HD21	1.99	0.45
1:C1:203:A:H4'	1:C1:205:A:N7	2.32	0.45
1:C1:632:G:H1'	1:C1:1100:G:H21	1.82	0.45
7:CI:191:ILE:HA	7:CI:259:THR:O	2.16	0.45
16:CS:281:MET:HG2	16:CS:283:PRO:HD3	1.97	0.45
1:C1:262:G:N2	1:C1:288:A:OP2	2.36	0.45
1:C1:957:C:H2'	1:C1:958:G:H8	1.82	0.45
1:C1:1866:A:O2'	25:LB:227:PHE:O	2.31	0.45
1:C1:2420:G:N1	1:C1:2424:A:OP2	2.40	0.45
2:C2:58:G:O6	56:Lj:63:ARG:NH1	2.50	0.45
5:CF:8:ARG:HA	5:CF:8:ARG:HD3	1.72	0.45
27:LD:265:LYS:HB3	27:LD:269:GLU:HB2	1.99	0.45
28:LE:98:ASN:HB3	28:LE:101:TYR:HD1	1.80	0.45
42:LU:22:ILE:HB	42:LU:109:VAL:HG22	1.97	0.45
1:C1:1676:A:H2'	1:C1:1677:A:C8	2.52	0.45
1:C1:2495:U:H2'	1:C1:2496:G:C8	2.51	0.45
25:LB:313:VAL:HG23	25:LB:365:GLU:HG3	1.99	0.45
36:LO:129:LEU:HD22	40:LS:156:VAL:HG13	1.99	0.45
22:Ch:441:ASN:ND2	22:Ch:443:ARG:HE	2.14	0.45
23:Cz:77:GLN:HA	23:Cz:80:ILE:HG12	1.97	0.45
45:LY:54:GLU:HB2	45:LY:107:LYS:HB3	1.98	0.45
1:C1:332:C:OP1	1:C1:1363:G:O2'	2.36	0.44
1:C1:2329:C:H2'	1:C1:2330:A:H8	1.83	0.44
8:CJ:128:ARG:NH1	21:Ce:160:TRP:H	2.04	0.44
17:CT:197:ALA:HB1	17:CT:223:PRO:HB2	2.00	0.44
17:CT:205:ILE:O	17:CT:214:LEU:N	2.49	0.44
17:CU:143:SER:OG	17:CU:144:ASP:N	2.49	0.44
18:CV:369:ASP:OD1	18:CV:369:ASP:N	2.49	0.44
25:LB:92:TYR:HB2	25:LB:158:VAL:HB	1.99	0.44
34:LM:120:VAL:HG12	34:LM:124:LYS:HE2	1.99	0.44
35:LN:84:PRO:HA	35:LN:87:GLN:HB2	1.98	0.44
39:LR:25:ASP:HB3	39:LR:28:GLU:HB2	1.98	0.44
45:LY:39:ARG:HD2	45:LY:45:ARG:HD2	2.00	0.44
1:C1:661:C:H2'	1:C1:662:G:C8	2.53	0.44
1:C1:782:G:H22	26:LC:102:ALA:HA	1.82	0.44
1:C1:1186:A:H62	1:C1:1283:G:H21	1.64	0.44
1:C1:2427:U:H2'	1:C1:2428:G:H8	1.82	0.44
1:C1:2648:A:OP2	27:LD:15:ARG:NH2	2.50	0.44
4:C4:45:U:H2'	4:C4:46:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CH:294:PHE:O	6:CH:302:GLN:NE2	2.50	0.44
6:CH:586:ARG:HH21	44:LX:156:VAL:HG12	1.82	0.44
8:CJ:223:ASP:HB3	8:CJ:226:ILE:HG22	1.99	0.44
11:LF:154:ILE:HG22	11:LF:187:ILE:HD11	1.98	0.44
1:C1:652:A:H2'	1:C1:653:A:C8	2.52	0.44
1:C1:696:G:N2	1:C1:699:A:OP2	2.42	0.44
1:C1:774:A:H2'	1:C1:775:A:H8	1.82	0.44
8:CJ:156:SER:HB2	8:CJ:162:ALA:HB2	1.99	0.44
17:CT:143:SER:OG	17:CT:144:ASP:N	2.50	0.44
26:LC:43:MET:HE2	26:LC:119:LYS:HE2	1.98	0.44
27:LD:208:ALA:HB2	27:LD:239:LEU:HD12	1.98	0.44
60:Lq:66:LYS:O	60:Lq:103:TYR:OH	2.29	0.44
1:C1:990:U:H5''	9:CK:234:SER:HB3	1.98	0.44
1:C1:2625:C:OP2	1:C1:2646:G:N1	2.44	0.44
30:LH:81:ASN:HB3	30:LH:93:GLU:HG3	1.98	0.44
34:LM:18:ARG:HB3	34:LM:30:ILE:HD12	1.98	0.44
51:Le:120:VAL:HB	51:Le:123:ALA:HB2	1.99	0.44
1:C1:661:C:H2'	1:C1:662:G:H8	1.83	0.44
1:C1:1018:C:H2'	1:C1:1019:A:O4'	2.17	0.44
1:C1:2878:A:H61	1:C1:2886:C:H42	1.66	0.44
17:CT:98:ILE:HG21	17:CT:110:LEU:HD23	2.00	0.44
40:LS:124:LEU:HD22	41:LT:154:VAL:HG12	1.98	0.44
1:C1:88:U:H2'	1:C1:89:A:H8	1.83	0.44
1:C1:1447:G:N2	1:C1:1450:A:OP2	2.49	0.44
1:C1:2618:G:H2'	1:C1:2619:G:H8	1.82	0.44
1:C1:3120:C:H2'	1:C1:3121:G:C8	2.53	0.44
14:CQ:16:SER:HB3	25:LB:73:VAL:HG11	1.98	0.44
15:CR:427:GLN:OE1	31:LJ:63:ASN:ND2	2.48	0.44
17:CT:10:ILE:HD11	17:CT:28:TYR:HE2	1.82	0.44
1:C1:688:C:H2'	1:C1:689:G:H8	1.83	0.44
1:C1:2307:U:H2'	1:C1:2308:A:C8	2.52	0.44
1:C1:2320:A:H2'	1:C1:2321:A:C8	2.53	0.44
1:C1:2362:A:H5'	1:C1:2905:A:H61	1.82	0.44
16:CS:310:GLU:O	59:Lp:85:ARG:NH2	2.50	0.44
17:CU:65:GLU:HA	17:CU:88:ARG:HH22	1.82	0.44
18:CV:111:LEU:HD21	18:CV:124:ILE:HG13	2.00	0.44
59:Lp:23:ARG:HA	59:Lp:26:VAL:HG12	1.99	0.44
1:C1:414:G:O6	1:C1:2346:C:O2'	2.33	0.44
1:C1:1610:G:H1	1:C1:1793:A:H5''	1.83	0.44
1:C1:2859:A:C8	9:CK:2:PRO:HG2	2.53	0.44
24:LA:118:GLU:HG3	24:LA:125:ALA:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LC:136:LEU:HD23	26:LC:143:VAL:HG11	1.99	0.44
35:LN:62:TYR:HD2	35:LN:134:LEU:HD13	1.83	0.44
41:LT:93:ILE:HA	41:LT:96:VAL:HG22	2.00	0.44
1:C1:2069:A:H2'	1:C1:2070:A:C8	2.53	0.44
1:C1:2176:A:H2'	1:C1:2177:A:C8	2.53	0.44
18:CW:205:LEU:HD13	18:CW:227:SER:HA	2.00	0.44
23:Cz:104:HIS:CE1	23:Cz:108:LEU:HD11	2.53	0.44
11:LF:7:PRO:HD2	60:Lq:88:ARG:HB3	1.98	0.44
55:Li:15:GLY:HA3	55:Li:25:LYS:HZ2	1.83	0.44
1:C1:1022:C:H2'	1:C1:1023:A:H8	1.83	0.43
1:C1:1177:G:H2'	1:C1:1178:A:C8	2.53	0.43
1:C1:1206:A:H61	23:Cz:40:ARG:HH22	1.66	0.43
5:CF:87:ASP:O	5:CF:227:TRP:NE1	2.50	0.43
16:CS:143:ILE:O	16:CS:147:MET:CB	2.66	0.43
17:CU:92:LEU:HD13	17:CU:99:LEU:HD11	2.00	0.43
59:Lp:81:SER:O	59:Lp:85:ARG:HG2	2.18	0.43
1:C1:279:U:O2'	35:LN:179:ARG:O	2.35	0.43
1:C1:619:A:H2'	1:C1:620:G:C8	2.54	0.43
1:C1:801:U:H2'	1:C1:802:A:H8	1.84	0.43
1:C1:1289:G:OP1	36:LO:64:ARG:NH1	2.47	0.43
11:CM:241:ILE:O	11:CM:245:ILE:HG12	2.17	0.43
11:CM:241:ILE:HD12	11:CM:244:LEU:HD12	1.99	0.43
15:CR:303:GLN:HB2	15:CR:342:LEU:HD22	1.99	0.43
21:Ce:5:LYS:HE2	21:Ce:5:LYS:HB3	1.84	0.43
39:LR:4:LEU:HD11	39:LR:29:VAL:HG13	2.00	0.43
46:LZ:56:MET:HE1	46:LZ:64:ARG:HD3	1.99	0.43
1:C1:116:A:H2'	1:C1:258:A:H2'	1.99	0.43
1:C1:508:G:OP1	11:LF:73:ARG:NH2	2.42	0.43
1:C1:617:C:H2'	1:C1:618:C:H6	1.82	0.43
1:C1:651:C:H2'	1:C1:652:A:C8	2.53	0.43
1:C1:1643:C:H2'	1:C1:1644:G:H8	1.82	0.43
1:C1:2956:U:H2'	1:C1:2957:C:C6	2.53	0.43
9:CK:149:ARG:HH22	20:Cd:44:GLY:HA2	1.83	0.43
18:CV:25:LEU:HD22	18:CV:28:LEU:HD21	2.00	0.43
18:CW:19:VAL:HA	18:CW:22:LEU:HD12	1.98	0.43
18:CW:298:ASP:OD1	18:CW:298:ASP:N	2.50	0.43
22:Ch:465:SER:OG	22:Ch:466:LYS:N	2.49	0.43
1:C1:774:A:H2'	1:C1:775:A:C8	2.53	0.43
9:CK:164:ARG:HB2	9:CK:169:GLU:HB3	1.99	0.43
16:CS:143:ILE:O	16:CS:147:MET:HB2	2.18	0.43
18:CW:3:ALA:HA	18:CW:55:THR:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:CW:177:ASP:OD1	18:CW:226:ASN:ND2	2.36	0.43
18:CW:568:ASP:OD1	18:CW:572:ARG:N	2.52	0.43
33:LL:90:ALA:HB1	33:LL:95:ILE:HB	2.00	0.43
34:LM:112:LEU:HD22	34:LM:116:ASP:HB3	1.99	0.43
61:Lr:68:LEU:HD22	61:Lr:90:LEU:HD21	2.00	0.43
1:C1:352:U:OP1	56:Lj:11:ARG:NH2	2.47	0.43
1:C1:1476:G:H2'	58:Ll:13:LEU:HD22	1.99	0.43
1:C1:2074:G:C6	19:Cb:76:ARG:HD3	2.53	0.43
1:C1:2115:A:O2'	1:C1:2206:A:O2'	2.32	0.43
1:C1:2413:A:H2'	1:C1:2414:G:C8	2.54	0.43
1:C1:2704:G:N2	1:C1:2707:A:OP2	2.42	0.43
11:CM:94:ARG:NH1	11:CM:95:ILE:O	2.47	0.43
16:CS:205:GLY:O	24:LA:140:ASN:ND2	2.50	0.43
18:CW:350:ILE:HD12	18:CW:351:PRO:HD2	2.00	0.43
24:LA:6:ARG:HH12	24:LA:199:THR:H	1.66	0.43
42:LU:27:GLN:NE2	42:LU:111:GLU:OE2	2.46	0.43
1:C1:1002:G:H2'	1:C1:1003:G:C8	2.54	0.43
1:C1:1698:A:H2'	1:C1:1699:G:C8	2.54	0.43
1:C1:1709:A:N6	59:Lp:41:PHE:O	2.50	0.43
1:C1:1826:C:OP1	1:C1:1829:C:N4	2.44	0.43
5:CF:144:SER:OG	5:CF:154:ASP:OD1	2.34	0.43
20:Cd:33:LYS:HB3	20:Cd:33:LYS:HE3	1.88	0.43
49:Lc:59:LEU:HD13	49:Lc:92:THR:HG21	2.00	0.43
1:C1:1199:C:OP2	10:CL:57:ASN:ND2	2.52	0.43
1:C1:2727:U:H2'	1:C1:2728:A:H8	1.83	0.43
18:CW:89:ILE:HG21	18:CW:130:LEU:HD21	2.01	0.43
25:LB:222:THR:O	25:LB:335:ARG:NH1	2.51	0.43
28:LE:139:GLU:HG3	28:LE:152:LYS:HG2	1.99	0.43
34:LM:20:LEU:HD21	34:LM:30:ILE:HD11	2.00	0.43
61:Lr:176:GLN:HE21	61:Lr:176:GLN:HB3	1.72	0.43
1:C1:382:A:H5''	37:LP:16:ARG:HG3	2.01	0.43
1:C1:644:A:H2'	1:C1:645:A:C8	2.53	0.43
1:C1:1023:A:OP1	23:Cz:116:LYS:NZ	2.41	0.43
1:C1:1449:G:N2	1:C1:1493:G:H5''	2.33	0.43
1:C1:2621:G:H2'	1:C1:2622:G:H8	1.83	0.43
1:C1:2895:A:H2'	1:C1:2896:G:C8	2.54	0.43
12:CN:15:VAL:HA	12:CN:61:ARG:HG2	2.01	0.43
16:CS:270:LEU:HB3	17:CU:2:LEU:HD12	1.99	0.43
18:CV:263:ASP:OD2	18:CV:279:TYR:OH	2.37	0.43
18:CV:420:GLN:HG2	18:CV:421:LEU:HD22	2.00	0.43
18:CW:307:GLN:O	18:CW:311:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Ce:391:ASP:OD1	21:Ce:391:ASP:N	2.51	0.43
37:LP:115:LYS:HB2	37:LP:151:THR:HG22	2.00	0.43
46:LZ:88:LEU:HD23	46:LZ:88:LEU:HA	1.82	0.43
1:C1:2207:A:H5'	24:LA:243:THR:HB	2.00	0.43
5:CF:92:LEU:HD22	5:CF:227:TRP:HB3	1.99	0.43
12:CN:140:GLN:HG2	12:CN:173:LEU:HD21	2.01	0.43
17:CU:132:VAL:HG22	17:CU:141:THR:HG22	1.99	0.43
35:LN:96:ARG:NH2	35:LN:104:GLU:OE1	2.51	0.43
39:LR:105:LEU:HD22	39:LR:135:LYS:HG3	2.01	0.43
41:LT:106:LEU:HA	41:LT:109:VAL:HG12	2.01	0.43
50:Ld:89:ASP:OD1	50:Ld:89:ASP:N	2.50	0.43
57:Lk:24:ARG:HA	57:Lk:69:LYS:O	2.18	0.43
61:Lr:82:ILE:HD13	61:Lr:148:VAL:HG21	2.01	0.43
1:C1:302:U:OP1	55:Li:93:LYS:NZ	2.45	0.43
1:C1:804:G:H2'	1:C1:805:C:H6	1.84	0.43
4:C4:76:G:O2'	4:C4:100:G:O6	2.34	0.43
6:CH:635:GLU:OE2	58:Li:41:ARG:NH1	2.47	0.43
17:CU:219:PHE:HD1	17:CU:223:PRO:HG3	1.83	0.43
35:LN:56:LYS:NZ	35:LN:145:ASP:OD1	2.52	0.43
40:LS:81:TYR:CE1	40:LS:90:MET:HE3	2.54	0.43
46:LZ:45:ILE:HG23	46:LZ:67:ILE:HG23	2.01	0.43
60:Lq:10:TRP:HB2	60:Lq:47:VAL:HG11	2.00	0.43
1:C1:1454:U:H2'	1:C1:1455:G:C8	2.53	0.42
1:C1:1588:C:O2'	44:LX:92:GLN:NE2	2.51	0.42
6:CH:364:VAL:HG21	12:CN:246:TYR:HD1	1.84	0.42
15:CR:195:GLU:OE2	15:CR:199:ARG:NH2	2.43	0.42
40:LS:8:GLN:HB2	40:LS:64:ILE:HD11	2.01	0.42
1:C1:3158:C:O2	28:LE:190:ARG:NH2	2.43	0.42
2:C2:36:G:OP1	56:Lj:66:TYR:OH	2.31	0.42
14:CQ:137:LEU:HD11	14:CQ:163:GLU:HB3	2.01	0.42
15:CR:16:LEU:HD12	15:CR:65:ASP:HB3	2.01	0.42
18:CV:301:PRO:HA	18:CV:302:PRO:HD3	1.90	0.42
22:Ch:487:HIS:ND1	22:Ch:509:ASP:OD2	2.52	0.42
24:LA:209:HIS:HE1	24:LA:211:HIS:CD2	2.37	0.42
38:LQ:47:PRO:HG3	38:LQ:58:VAL:HG21	2.01	0.42
54:Lh:100:GLU:O	54:Lh:104:ARG:HG3	2.19	0.42
61:Lr:130:LYS:HE3	61:Lr:130:LYS:HB3	1.85	0.42
1:C1:464:C:H2'	1:C1:465:G:C8	2.54	0.42
1:C1:1576:C:H2'	1:C1:1577:C:C6	2.54	0.42
1:C1:1619:C:OP2	53:Lg:75:ARG:NH1	2.42	0.42
1:C1:2307:U:H2'	1:C1:2308:A:H8	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:3266:A:H2'	1:C1:3267:G:H8	1.85	0.42
7:CI:189:MET:HE2	7:CI:245:ALA:HB2	2.01	0.42
9:CK:198:LEU:HD12	9:CK:222:GLU:HG2	2.01	0.42
18:CW:313:LEU:HD23	18:CW:381:ILE:HD13	2.00	0.42
24:LA:22:LEU:HB3	24:LA:52:PRO:HG2	2.02	0.42
26:LC:114:ILE:HB	26:LC:119:LYS:HE3	2.00	0.42
27:LD:69:ILE:HG13	41:LT:28:SER:HB2	2.00	0.42
44:LX:89:ILE:HG12	44:LX:95:LEU:HD23	1.99	0.42
58:LI:13:LEU:O	58:LI:17:GLN:HG3	2.19	0.42
1:C1:410:A:H2'	1:C1:411:A:H8	1.84	0.42
1:C1:575:G:H2'	1:C1:576:A:C8	2.54	0.42
1:C1:683:C:OP1	26:LC:272:LYS:NZ	2.40	0.42
1:C1:1296:G:O2'	1:C1:1301:A:N1	2.41	0.42
1:C1:2800:G:O2'	10:CL:44:GLU:OE2	2.33	0.42
17:CU:222:TYR:HA	17:CU:223:PRO:HD3	1.92	0.42
18:CV:389:HIS:NE2	18:CV:410:GLN:OE1	2.52	0.42
18:CW:306:LEU:HD21	18:CW:374:LEU:HB2	2.02	0.42
1:C1:1933:G:N2	1:C1:2055:A:OP1	2.47	0.42
6:CH:221:PRO:O	6:CH:238:SER:OG	2.34	0.42
9:CK:11:ARG:HE	9:CK:16:ARG:HD3	1.84	0.42
9:CK:163:ARG:HH12	20:CD:228:LYS:HG3	1.83	0.42
11:CM:16:GLU:HG2	11:CM:20:LYS:HE3	2.01	0.42
43:LV:9:PRO:HB2	43:LV:127:LEU:HD13	2.02	0.42
43:LV:82:ARG:NH1	43:LV:119:PRO:O	2.42	0.42
1:C1:1240:C:O2	5:CF:54:LYS:NZ	2.50	0.42
1:C1:1638:G:H2'	1:C1:1639:A:C8	2.55	0.42
1:C1:2391:U:H2'	1:C1:2392:G:H8	1.84	0.42
8:CJ:141:LEU:HD23	8:CJ:141:LEU:HA	1.92	0.42
8:CJ:410:GLU:O	8:CJ:453:ARG:NH1	2.53	0.42
22:Ch:294:ILE:HG13	22:Ch:308:ALA:HB2	2.02	0.42
22:Ch:305:VAL:HB	22:Ch:315:HIS:HB2	2.01	0.42
25:LB:83:PRO:O	25:LB:166:GLN:NE2	2.52	0.42
32:LK:143:VAL:HG23	32:LK:148:PRO:HG3	2.00	0.42
37:LP:116:HIS:HB3	37:LP:149:ILE:HB	2.00	0.42
40:LS:81:TYR:CE1	40:LS:88:HIS:HB2	2.54	0.42
60:Lq:55:VAL:HG23	60:Lq:62:LYS:HB3	2.02	0.42
1:C1:289:A:N3	1:C1:292:G:O2'	2.50	0.42
1:C1:351:G:N2	1:C1:354:A:OP2	2.36	0.42
6:CH:540:ASP:OD1	6:CH:540:ASP:N	2.53	0.42
17:CU:219:PHE:HE2	17:CU:269:ILE:HD12	1.84	0.42
22:Ch:190:GLY:HA3	22:Ch:209:MET:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LB:149:LEU:HD13	25:LB:197:ARG:HH11	1.84	0.42
27:LD:81:HIS:HA	27:LD:92:LEU:HD13	2.02	0.42
27:LD:207:VAL:O	27:LD:211:MET:HG3	2.19	0.42
30:LH:129:TYR:HB3	30:LH:218:ILE:HG23	2.01	0.42
61:Lr:195:LYS:HD2	61:Lr:196:LYS:HG3	2.02	0.42
1:C1:37:C:H4'	1:C1:790:A:H2	1.84	0.42
1:C1:803:U:H2'	1:C1:804:G:H8	1.85	0.42
1:C1:859:C:N4	1:C1:860:G:O6	2.52	0.42
1:C1:999:G:H2'	1:C1:1000:G:C8	2.54	0.42
1:C1:1197:U:H2'	1:C1:1198:A:C8	2.55	0.42
1:C1:1306:C:H4'	40:LS:2:GLY:H	1.85	0.42
1:C1:1783:C:H2'	1:C1:1784:G:C8	2.54	0.42
1:C1:2516:G:N2	46:LZ:134:ARG:O	2.33	0.42
8:CJ:46:GLU:OE2	21:Ce:367:ARG:NH2	2.39	0.42
18:CW:209:ILE:HD11	18:CW:231:LEU:HD12	2.02	0.42
24:LA:33:ASP:OD1	24:LA:33:ASP:N	2.52	0.42
28:LE:65:PHE:HB3	28:LE:68:LYS:HG3	2.01	0.42
45:LY:62:HIS:HB3	45:LY:65:LYS:HD2	2.00	0.42
46:LZ:91:LEU:HD22	46:LZ:94:VAL:HG11	2.01	0.42
1:C1:1577:C:H2'	1:C1:1578:G:C8	2.55	0.42
1:C1:2112:A:H4'	24:LA:179:LEU:O	2.20	0.42
1:C1:3159:U:C4	34:LM:121:MET:HG3	2.55	0.42
10:CL:5:ILE:HD13	36:LO:49:PHE:HB2	2.02	0.42
17:CT:284:SER:N	17:CT:298:GLY:O	2.41	0.42
27:LD:68:GLU:HG3	27:LD:73:LYS:HE2	2.01	0.42
29:LG:81:PHE:HA	29:LG:182:ILE:HD13	2.01	0.42
50:Ld:45:LYS:O	50:Ld:48:ALA:N	2.52	0.42
1:C1:621:C:O2'	52:Lf:23:ARG:O	2.34	0.42
1:C1:1114:G:O3'	10:CL:27:ARG:NH1	2.52	0.42
1:C1:2618:G:H2'	1:C1:2619:G:C8	2.55	0.42
12:CN:118:HIS:HA	12:CN:119:PRO:HD3	1.92	0.42
15:CR:15:ASP:OD2	15:CR:18:ASN:ND2	2.53	0.42
18:CV:54:GLU:HA	18:CV:57:MET:HE2	2.02	0.42
20:Cd:274:ASP:OD1	20:Cd:274:ASP:N	2.50	0.42
25:LB:324:MET:HE1	25:LB:360:ILE:HD13	2.02	0.42
27:LD:180:GLU:HB2	27:LD:193:LEU:HD22	2.02	0.42
35:LN:68:ARG:NH1	35:LN:124:ASP:O	2.40	0.42
41:LT:84:TYR:HB2	48:Lb:24:PRO:HD3	2.01	0.42
52:Lf:47:LEU:HD11	52:Lf:76:PRO:HD3	2.00	0.42
1:C1:425:G:H2'	1:C1:426:A:C8	2.55	0.41
1:C1:627:OMG:OP1	51:Le:41:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:629:C:H2'	1:C1:630:U:C6	2.55	0.41
1:C1:1050:C:O3'	41:LT:110:LYS:NZ	2.53	0.41
1:C1:1701:U:OP2	39:LR:124:TYR:OH	2.31	0.41
1:C1:1877:G:OP2	19:Cb:11:LYS:NZ	2.38	0.41
1:C1:2069:A:H2'	1:C1:2070:A:H8	1.85	0.41
1:C1:2185:A:H2'	1:C1:2186:A:C8	2.54	0.41
1:C1:2568:A:H2'	1:C1:2569:G:C8	2.55	0.41
1:C1:2974:A:H2'	1:C1:2975:G:C8	2.54	0.41
1:C1:3204:C:H2'	1:C1:3205:G:C8	2.55	0.41
17:CT:53:ALA:HB1	17:CT:94:LEU:HB2	2.02	0.41
17:CU:190:ASP:OD1	17:CU:190:ASP:N	2.44	0.41
18:CV:209:ILE:HD11	18:CV:231:LEU:HD12	2.01	0.41
39:LR:105:LEU:HD13	39:LR:135:LYS:HD2	2.00	0.41
44:LX:106:ALA:O	44:LX:110:GLN:HG3	2.20	0.41
1:C1:231:A:H2'	1:C1:232:A:C8	2.55	0.41
1:C1:1814:U:OP2	58:Ll:10:LYS:NZ	2.47	0.41
1:C1:1892:U:N3	1:C1:2085:G:OP2	2.40	0.41
1:C1:2947:C:OP1	36:LO:66:ASN:ND2	2.52	0.41
14:CQ:137:LEU:HD23	14:CQ:137:LEU:HA	1.92	0.41
17:CU:98:ILE:HG22	17:CU:112:GLU:HG2	2.01	0.41
17:CU:122:PRO:HG2	17:CU:164:GLU:HB3	2.01	0.41
18:CV:568:ASP:OD1	18:CV:572:ARG:N	2.53	0.41
26:LC:197:LYS:HG2	26:LC:202:ARG:HG3	2.02	0.41
41:LT:51:GLY:HA3	41:LT:92:ARG:HG3	2.02	0.41
45:LY:110:LEU:HD23	45:LY:110:LEU:HA	1.89	0.41
61:Lr:32:VAL:N	61:Lr:170:GLY:O	2.53	0.41
61:Lr:175:THR:H	61:Lr:178:GLN:NE2	2.18	0.41
1:C1:110:A:N1	1:C1:315:U:O2'	2.52	0.41
1:C1:661:C:O2	26:LC:118:GLN:NE2	2.53	0.41
1:C1:1366:G:H4'	26:LC:247:PRO:HB2	2.03	0.41
1:C1:1615:G:N2	1:C1:1618:A:OP2	2.39	0.41
1:C1:2642:U:H2'	1:C1:2643:C:C6	2.55	0.41
5:CF:145:THR:HB	5:CF:148:GLU:HB2	2.02	0.41
9:CK:166:VAL:HG11	20:Cd:364:TRP:HH2	1.85	0.41
9:CK:241:ARG:NH2	20:Cd:79:ASN:OD1	2.50	0.41
22:Ch:242:PRO:HB3	22:Ch:335:LEU:HD22	2.01	0.41
29:LG:84:THR:HG22	29:LG:182:ILE:HG22	2.01	0.41
1:C1:108:A:O2'	1:C1:317:A:N3	2.43	0.41
10:CL:66:LEU:O	10:CL:70:GLU:HG2	2.20	0.41
14:CQ:173:SER:OG	50:Ld:19:GLU:OE1	2.37	0.41
15:CR:104:ARG:HD2	15:CR:141:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:CR:389:ILE:O	15:CR:393:PHE:HB2	2.21	0.41
16:CS:128:PRO:HA	16:CS:129:PRO:HD3	1.87	0.41
17:CU:380:PHE:HE2	18:CW:83:CYS:HA	1.86	0.41
18:CW:351:PRO:HA	18:CW:352:PRO:HD3	1.87	0.41
20:Cd:394:LEU:HD21	20:Cd:465:LEU:HD13	2.01	0.41
21:Ce:313:GLU:OE1	21:Ce:316:LYS:NZ	2.41	0.41
22:Ch:378:ALA:HA	22:Ch:384:MET:HG2	2.02	0.41
1:C1:882:G:H1'	1:C1:1569:A:N6	2.36	0.41
1:C1:2161:A:H62	1:C1:2209:G:N2	2.18	0.41
1:C1:3266:A:H2'	1:C1:3267:G:C8	2.56	0.41
16:CS:257:ARG:NH1	17:CU:252:GLU:OE2	2.50	0.41
17:CT:326:THR:OG1	17:CT:327:ASN:ND2	2.52	0.41
28:LE:169:LEU:HD23	28:LE:169:LEU:HA	1.93	0.41
1:C1:767:G:H1	38:LQ:117:ASP:HA	1.84	0.41
1:C1:1778:A:H2'	1:C1:1779:A:C8	2.56	0.41
1:C1:2925:G:H2'	1:C1:2926:A:C8	2.55	0.41
11:CM:190:LEU:HD21	11:CM:208:LEU:HD21	2.03	0.41
16:CS:187:PHE:HA	16:CS:190:MET:HE3	2.01	0.41
17:CT:148:ILE:HD13	17:CT:181:LEU:HD21	2.01	0.41
18:CW:447:THR:HA	18:CW:450:ILE:HG12	2.03	0.41
32:LK:63:THR:HB	32:LK:70:GLN:HG3	2.03	0.41
44:LX:63:SER:HB2	54:Lh:71:LEU:HD13	2.02	0.41
1:C1:349:G:O2'	26:LC:82:GLY:O	2.30	0.41
1:C1:400:A:H4'	1:C1:1380:C:H5'	2.03	0.41
1:C1:967:U:H2'	1:C1:968:U:C6	2.55	0.41
1:C1:1894:G:O2'	39:LR:82:LYS:O	2.34	0.41
1:C1:2383:C:H2'	1:C1:2384:OMU:H6	2.03	0.41
11:CM:220:PHE:HD2	11:CM:223:ARG:HG2	1.86	0.41
15:CR:181:ARG:NH1	15:CR:213:GLU:O	2.53	0.41
19:Cb:25:ASP:OD1	19:Cb:31:HIS:ND1	2.51	0.41
25:LB:113:GLU:OE2	25:LB:168:ARG:N	2.52	0.41
1:C1:1175:C:OP1	9:CK:43:ARG:NH2	2.51	0.41
1:C1:2231:U:H2'	16:CS:45:ASN:HD22	1.85	0.41
1:C1:2396:U:H1'	35:LN:125:SER:HB3	2.02	0.41
1:C1:2405:G:H2'	1:C1:2406:A:C8	2.56	0.41
1:C1:3263:G:H2'	1:C1:3264:A:C8	2.55	0.41
6:CH:176:ASN:N	62:CH:701:GTP:O2B	2.54	0.41
11:CM:154:ILE:HD12	11:CM:191:ILE:HG12	2.02	0.41
15:CR:373:THR:HG21	15:CR:413:VAL:HG13	2.03	0.41
18:CV:449:ASP:HA	18:CV:452:ILE:HD12	2.03	0.41
51:Le:75:PHE:CD2	51:Le:86:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:Lr:175:THR:OG1	61:Lr:178:GLN:NE2	2.54	0.41
1:C1:617:C:H2'	1:C1:618:C:C6	2.56	0.41
1:C1:1107:U:O2	1:C1:1117:G:N2	2.43	0.41
1:C1:1306:C:H4'	40:LS:2:GLY:N	2.36	0.41
1:C1:1598:G:H2'	1:C1:1599:A:C8	2.55	0.41
1:C1:1643:C:H2'	1:C1:1644:G:C8	2.56	0.41
1:C1:2391:U:H2'	1:C1:2392:G:C8	2.56	0.41
1:C1:2727:U:H2'	1:C1:2728:A:C8	2.56	0.41
1:C1:2771:C:H2'	1:C1:2772:A:C8	2.55	0.41
1:C1:2877:G:H2'	1:C1:2878:A:H8	1.85	0.41
8:CJ:266:ALA:HB3	8:CJ:270:ALA:HB2	2.01	0.41
9:CK:166:VAL:HG12	20:Cd:366:TYR:CE2	2.55	0.41
10:CL:69:ILE:HD11	41:LT:156:TYR:HB3	2.03	0.41
11:CM:102:PRO:HA	11:CM:103:PRO:HD3	1.98	0.41
14:CQ:56:ARG:NH1	14:CQ:62:GLU:OE2	2.52	0.41
17:CT:250:PHE:HB2	18:CW:599:VAL:HG12	2.03	0.41
18:CV:234:LEU:HD23	18:CV:234:LEU:HA	1.96	0.41
18:CV:422:PRO:HB3	18:CV:517:VAL:HG21	2.03	0.41
18:CW:234:LEU:HD23	18:CW:234:LEU:HA	1.96	0.41
19:Cb:20:ASP:OD1	19:Cb:21:GLN:N	2.53	0.41
20:Cd:323:ASP:OD1	20:Cd:323:ASP:N	2.54	0.41
21:Ce:22:SER:O	21:Ce:32:ASN:ND2	2.46	0.41
25:LB:237:LYS:HE3	43:LV:49:ASN:HD22	1.85	0.41
42:LU:19:LYS:NZ	42:LU:78:LEU:O	2.48	0.41
42:LU:91:LEU:HD11	42:LU:112:LEU:HD11	2.01	0.41
45:LY:2:LYS:NZ	45:LY:7:VAL:O	2.45	0.41
50:Ld:15:VAL:HA	50:Ld:85:ARG:O	2.20	0.41
1:C1:36:A:H2'	1:C1:37:C:H6	1.86	0.41
1:C1:615:C:H2'	1:C1:616:A:C8	2.56	0.41
1:C1:842:G:OP1	59:Lp:17:ARG:NH2	2.50	0.41
1:C1:1650:C:O2'	1:C1:1840:G:OP1	2.33	0.41
1:C1:2314:U:H2'	1:C1:2315:A:C8	2.56	0.41
8:CJ:254:PRO:HA	8:CJ:255:PRO:HD3	1.96	0.41
16:CS:283:PRO:O	16:CS:288:ARG:NH2	2.54	0.41
18:CW:157:LEU:O	18:CW:161:LYS:HB2	2.21	0.41
25:LB:164:HIS:HA	25:LB:178:HIS:O	2.20	0.41
26:LC:211:ILE:HG13	26:LC:256:VAL:HB	2.02	0.41
38:LQ:110:VAL:HG22	38:LQ:167:LEU:HB2	2.02	0.41
61:Lr:76:ARG:NH2	61:Lr:142:ASP:O	2.54	0.41
1:C1:1140:G:O2'	1:C1:1152:A:N3	2.48	0.40
1:C1:1387:G:O6	51:Le:17:ARG:NH1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1404:G:H2'	1:C1:1405:G:H8	1.86	0.40
1:C1:1450:A:N1	1:C1:1494:U:O2'	2.51	0.40
1:C1:1737:G:H2'	1:C1:1738:A:C8	2.56	0.40
1:C1:3123:U:H2'	1:C1:3124:G:C8	2.56	0.40
15:CR:193:THR:HG21	15:CR:211:MET:HE3	2.03	0.40
17:CT:89:ILE:HG21	17:CT:92:LEU:HD23	2.03	0.40
23:Cz:104:HIS:HB2	27:LD:4:HIS:HB2	2.04	0.40
27:LD:115:LEU:HD21	27:LD:142:ARG:HH21	1.85	0.40
11:LF:242:ASN:O	11:LF:246:ARG:HG2	2.21	0.40
31:LJ:49:SER:HB2	31:LJ:67:ALA:HB3	2.03	0.40
37:LP:122:ALA:HB3	37:LP:143:PRO:HG2	2.02	0.40
41:LT:34:TYR:HE1	41:LT:40:VAL:HG11	1.85	0.40
54:Lh:54:LYS:HA	54:Lh:54:LYS:HD3	1.89	0.40
57:Lk:34:ILE:HD13	57:Lk:55:ALA:HB1	2.03	0.40
1:C1:1071:U:H5''	48:Lb:54:LEU:HD11	2.03	0.40
1:C1:1073:G:H2'	1:C1:1074:G:C8	2.56	0.40
1:C1:2330:A:H2'	1:C1:2331:A:C8	2.56	0.40
1:C1:3191:G:H2'	1:C1:3192:C:C6	2.56	0.40
4:C4:37:G:N2	4:C4:41:G:N3	2.68	0.40
15:CR:106:LYS:HD2	15:CR:106:LYS:HA	1.83	0.40
18:CW:244:SER:HA	18:CW:332:VAL:HG12	2.03	0.40
22:Ch:145:HIS:CE1	22:Ch:172:ARG:HD2	2.56	0.40
23:Cz:33:LEU:HD23	23:Cz:33:LEU:HA	1.93	0.40
1:C1:1409:C:H4'	26:LC:41:THR:HG23	2.02	0.40
1:C1:2616:A:C6	15:CR:466:LYS:HA	2.56	0.40
1:C1:2666:U:H2'	1:C1:2667:C:C6	2.55	0.40
1:C1:2790:G:H2'	1:C1:2791:C:C6	2.56	0.40
1:C1:3236:A:OP1	25:LB:125:SER:OG	2.38	0.40
2:C2:142:C:H2'	2:C2:143:U:C6	2.57	0.40
18:CW:532:LEU:HD12	18:CW:532:LEU:HA	1.97	0.40
20:Cd:11:LEU:HD22	20:Cd:16:ARG:HD3	2.02	0.40
26:LC:191:LEU:HG	26:LC:197:LYS:HD3	2.04	0.40
29:LG:33:ARG:NH2	46:LZ:51:LYS:HD2	2.36	0.40
32:LK:40:LYS:HE2	32:LK:40:LYS:HB3	1.91	0.40
51:Le:87:LEU:HD13	51:Le:116:LEU:HD22	2.03	0.40
1:C1:266:A:H2'	1:C1:267:G:C8	2.57	0.40
1:C1:400:A:C2	2:C2:17:A:H1'	2.57	0.40
1:C1:449:A:H5'	11:LF:5:THR:HA	2.02	0.40
1:C1:603:U:H2'	1:C1:604:G:H8	1.87	0.40
1:C1:1530:G:OP1	35:LN:108:ARG:NH2	2.49	0.40
1:C1:1612:G:OP1	46:LZ:47:ARG:NH2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:3144:U:OP1	36:LO:170:TYR:OH	2.26	0.40
1:C1:3238:U:H2'	1:C1:3239:C:H6	1.85	0.40
2:C2:38:U:H5'	54:Lh:83:LEU:HD13	2.02	0.40
6:CH:646:LYS:O	6:CH:650:SER:HB3	2.22	0.40
8:CJ:42:ILE:HD13	21:Ce:189:LEU:HD21	2.04	0.40
8:CJ:231:VAL:O	8:CJ:235:MET:HG2	2.20	0.40
17:CU:201:LYS:HA	17:CU:222:TYR:HA	2.02	0.40
17:CU:296:LEU:HD23	17:CU:296:LEU:HA	1.97	0.40
33:LL:107:GLU:OE2	33:LL:107:GLU:N	2.53	0.40
36:LO:170:TYR:CE2	36:LO:174:LYS:HD2	2.57	0.40
40:LS:96:GLU:HG3	40:LS:102:ALA:HA	2.04	0.40
46:LZ:40:ALA:HB2	46:LZ:76:TYR:HE1	1.86	0.40
1:C1:515:G:H2'	1:C1:516:G:H8	1.86	0.40
1:C1:524:A:H2'	1:C1:525:A:C8	2.57	0.40
1:C1:1100:G:H2'	1:C1:1101:C:C6	2.56	0.40
1:C1:1264:U:H2'	1:C1:1265:G:C8	2.51	0.40
1:C1:1640:C:H2'	1:C1:1641:G:H8	1.86	0.40
1:C1:1731:G:H5'	57:Lk:26:LYS:HE2	2.03	0.40
1:C1:2181:G:H2'	1:C1:2182:A:C8	2.54	0.40
1:C1:2182:A:H2'	1:C1:2183:A:C8	2.57	0.40
5:CF:43:PHE:HB3	5:CF:223:LEU:HD23	2.02	0.40
13:CO:30:LEU:HD11	25:LB:42:HIS:CG	2.57	0.40
18:CW:553:HIS:CD2	18:CW:584:ARG:HE	2.39	0.40
19:Cb:24:ARG:HE	19:Cb:31:HIS:CD2	2.39	0.40
22:Ch:430:LEU:HD12	22:Ch:440:LYS:HG3	2.04	0.40
34:LM:93:LYS:O	34:LM:97:THR:HG23	2.21	0.40
47:La:112:LEU:HD22	47:La:125:VAL:HG11	2.04	0.40
61:Lr:134:PHE:HA	61:Lr:135:PRO:HD3	1.97	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	CF	243/270 (90%)	241 (99%)	2 (1%)	0	100	100
6	CH	621/661 (94%)	616 (99%)	5 (1%)	0	100	100
7	CI	91/414 (22%)	90 (99%)	1 (1%)	0	100	100
8	CJ	376/679 (55%)	374 (100%)	2 (0%)	0	100	100
9	CK	227/261 (87%)	223 (98%)	4 (2%)	0	100	100
10	CL	77/558 (14%)	76 (99%)	1 (1%)	0	100	100
11	CM	211/249 (85%)	206 (98%)	5 (2%)	0	100	100
11	LF	246/249 (99%)	241 (98%)	4 (2%)	1 (0%)	30	54
12	CN	244/246 (99%)	237 (97%)	7 (3%)	0	100	100
13	CO	56/120 (47%)	54 (96%)	2 (4%)	0	100	100
14	CQ	181/225 (80%)	178 (98%)	3 (2%)	0	100	100
15	CR	510/767 (66%)	504 (99%)	6 (1%)	0	100	100
16	CS	301/338 (89%)	298 (99%)	3 (1%)	0	100	100
17	CT	391/437 (90%)	384 (98%)	7 (2%)	0	100	100
17	CU	391/437 (90%)	380 (97%)	11 (3%)	0	100	100
18	CV	544/781 (70%)	535 (98%)	9 (2%)	0	100	100
18	CW	544/781 (70%)	536 (98%)	8 (2%)	0	100	100
19	Cb	99/117 (85%)	98 (99%)	1 (1%)	0	100	100
20	Cd	445/627 (71%)	437 (98%)	8 (2%)	0	100	100
21	Ce	290/443 (66%)	285 (98%)	5 (2%)	0	100	100
22	Ch	388/517 (75%)	375 (97%)	13 (3%)	0	100	100
23	Cz	101/123 (82%)	100 (99%)	1 (1%)	0	100	100
24	LA	245/254 (96%)	238 (97%)	7 (3%)	0	100	100
25	LB	386/392 (98%)	380 (98%)	6 (2%)	0	100	100
26	LC	361/365 (99%)	356 (99%)	5 (1%)	0	100	100
27	LD	296/304 (97%)	289 (98%)	7 (2%)	0	100	100
28	LE	187/200 (94%)	182 (97%)	5 (3%)	0	100	100
29	LG	233/262 (89%)	230 (99%)	3 (1%)	0	100	100
30	LH	188/229 (82%)	184 (98%)	4 (2%)	0	100	100
31	LJ	166/173 (96%)	163 (98%)	3 (2%)	0	100	100
32	LK	156/165 (94%)	156 (100%)	0	0	100	100
33	LL	201/213 (94%)	199 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	LM	139/142 (98%)	137 (99%)	2 (1%)	0	100	100
35	LN	200/203 (98%)	196 (98%)	4 (2%)	0	100	100
36	LO	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
37	LP	167/187 (89%)	164 (98%)	3 (2%)	0	100	100
38	LQ	142/213 (67%)	140 (99%)	2 (1%)	0	100	100
39	LR	153/2898 (5%)	152 (99%)	1 (1%)	0	100	100
40	LS	172/174 (99%)	169 (98%)	3 (2%)	0	100	100
41	LT	139/160 (87%)	136 (98%)	3 (2%)	0	100	100
42	LU	103/127 (81%)	100 (97%)	3 (3%)	0	100	100
43	LV	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
44	LX	143/156 (92%)	139 (97%)	4 (3%)	0	100	100
45	LY	131/138 (95%)	126 (96%)	5 (4%)	0	100	100
46	LZ	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
47	La	104/149 (70%)	101 (97%)	3 (3%)	0	100	100
48	Lb	34/65 (52%)	34 (100%)	0	0	100	100
49	Lc	93/108 (86%)	92 (99%)	1 (1%)	0	100	100
50	Ld	108/120 (90%)	108 (100%)	0	0	100	100
51	Le	124/131 (95%)	123 (99%)	1 (1%)	0	100	100
52	Lf	106/109 (97%)	103 (97%)	3 (3%)	0	100	100
53	Lg	116/119 (98%)	114 (98%)	2 (2%)	0	100	100
54	Lh	120/935 (13%)	116 (97%)	4 (3%)	0	100	100
55	Li	99/110 (90%)	99 (100%)	0	0	100	100
56	Lj	86/95 (90%)	86 (100%)	0	0	100	100
57	Lk	74/94 (79%)	74 (100%)	0	0	100	100
58	Ll	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
59	Lp	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
60	Lq	137/147 (93%)	134 (98%)	3 (2%)	0	100	100
61	Lr	212/217 (98%)	209 (99%)	3 (1%)	0	100	100
All	All	12502/19275 (65%)	12289 (98%)	212 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	LF	197	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CF	212/236 (90%)	212 (100%)	0	100	100
6	CH	548/575 (95%)	548 (100%)	0	100	100
7	CI	70/336 (21%)	70 (100%)	0	100	100
8	CJ	331/579 (57%)	331 (100%)	0	100	100
9	CK	203/225 (90%)	203 (100%)	0	100	100
10	CL	60/458 (13%)	60 (100%)	0	100	100
11	CM	185/215 (86%)	185 (100%)	0	100	100
11	LF	213/215 (99%)	213 (100%)	0	100	100
12	CN	204/206 (99%)	204 (100%)	0	100	100
13	CO	48/99 (48%)	48 (100%)	0	100	100
14	CQ	143/192 (74%)	143 (100%)	0	100	100
15	CR	374/663 (56%)	374 (100%)	0	100	100
16	CS	260/291 (89%)	260 (100%)	0	100	100
17	CT	323/376 (86%)	323 (100%)	0	100	100
17	CU	327/376 (87%)	327 (100%)	0	100	100
18	CV	472/675 (70%)	472 (100%)	0	100	100
18	CW	469/675 (70%)	469 (100%)	0	100	100
19	Cb	85/101 (84%)	85 (100%)	0	100	100
20	Cd	395/541 (73%)	395 (100%)	0	100	100
21	Ce	262/383 (68%)	262 (100%)	0	100	100
22	Ch	322/436 (74%)	322 (100%)	0	100	100
23	Cz	91/107 (85%)	91 (100%)	0	100	100
24	LA	190/198 (96%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	LB	328/331 (99%)	328 (100%)	0	100	100
26	LC	281/285 (99%)	281 (100%)	0	100	100
27	LD	233/253 (92%)	233 (100%)	0	100	100
28	LE	155/166 (93%)	155 (100%)	0	100	100
29	LG	197/222 (89%)	197 (100%)	0	100	100
30	LH	167/200 (84%)	167 (100%)	0	100	100
31	LJ	144/150 (96%)	143 (99%)	1 (1%)	76	86
32	LK	127/136 (93%)	127 (100%)	0	100	100
33	LL	158/176 (90%)	158 (100%)	0	100	100
34	LM	116/117 (99%)	116 (100%)	0	100	100
35	LN	179/180 (99%)	179 (100%)	0	100	100
36	LO	162/163 (99%)	162 (100%)	0	100	100
37	LP	133/152 (88%)	133 (100%)	0	100	100
38	LQ	124/178 (70%)	124 (100%)	0	100	100
39	LR	125/2396 (5%)	125 (100%)	0	100	100
40	LS	153/154 (99%)	153 (100%)	0	100	100
41	LT	120/135 (89%)	120 (100%)	0	100	100
42	LU	90/108 (83%)	90 (100%)	0	100	100
43	LV	98/102 (96%)	98 (100%)	0	100	100
44	LX	117/129 (91%)	117 (100%)	0	100	100
45	LY	116/119 (98%)	116 (100%)	0	100	100
46	LZ	119/121 (98%)	119 (100%)	0	100	100
47	La	93/122 (76%)	93 (100%)	0	100	100
48	Lb	28/55 (51%)	28 (100%)	0	100	100
49	Lc	76/88 (86%)	76 (100%)	0	100	100
50	Ld	90/105 (86%)	90 (100%)	0	100	100
51	Le	109/114 (96%)	109 (100%)	0	100	100
52	Lf	89/90 (99%)	89 (100%)	0	100	100
53	Lg	91/102 (89%)	91 (100%)	0	100	100
54	Lh	109/781 (14%)	109 (100%)	0	100	100
55	Li	84/93 (90%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	Lj	72/78 (92%)	72 (100%)	0	100	100
57	Lk	71/88 (81%)	71 (100%)	0	100	100
58	Ll	45/46 (98%)	45 (100%)	0	100	100
59	Lp	72/74 (97%)	72 (100%)	0	100	100
60	Lq	107/112 (96%)	107 (100%)	0	100	100
61	Lr	186/189 (98%)	186 (100%)	0	100	100
All	All	10551/16268 (65%)	10550 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	LJ	40	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
6	CH	14	GLN
6	CH	53	GLN
6	CH	77	HIS
6	CH	82	ASN
6	CH	418	ASN
8	CJ	173	HIS
9	CK	10	HIS
9	CK	14	HIS
9	CK	60	GLN
9	CK	143	HIS
11	CM	119	ASN
11	CM	178	ASN
11	CM	192	HIS
11	CM	203	GLN
16	CS	45	ASN
16	CS	223	GLN
17	CT	207	ASN
17	CT	360	GLN
17	CU	18	ASN
17	CU	127	GLN
17	CU	268	GLN
18	CV	200	GLN
18	CV	333	ASN

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Mol	Chain	Res	Type
18	CV	383	HIS
18	CV	553	HIS
18	CW	12	HIS
18	CW	382	HIS
18	CW	531	HIS
20	Cd	159	ASN
20	Cd	292	HIS
20	Cd	326	GLN
21	Ce	319	HIS
21	Ce	370	GLN
22	Ch	274	HIS
22	Ch	326	HIS
22	Ch	404	GLN
23	Cz	81	GLN
24	LA	140	ASN
24	LA	205	ASN
25	LB	183	GLN
26	LC	330	ASN
11	LF	77	GLN
11	LF	206	ASN
11	LF	242	ASN
30	LH	5	HIS
30	LH	95	HIS
30	LH	133	HIS
32	LK	14	HIS
32	LK	70	GLN
33	LL	131	ASN
35	LN	15	GLN
36	LO	32	GLN
37	LP	116	HIS
39	LR	99	GLN
41	LT	131	GLN
45	LY	56	GLN
46	LZ	126	ASN
47	La	11	HIS
47	La	62	HIS
47	La	94	GLN
51	Le	21	HIS
51	Le	72	HIS
54	Lh	33	GLN
54	Lh	37	GLN
54	Lh	67	GLN

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Mol	Chain	Res	Type
56	Lj	13	ASN
57	Lk	32	GLN
57	Lk	67	GLN
61	Lr	11	GLN
61	Lr	71	GLN
61	Lr	176	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	3079/3342 (92%)	557 (18%)	17 (0%)
2	C2	155/156 (99%)	21 (13%)	0
3	C3	2/162 (1%)	1 (50%)	0
4	C4	113/119 (94%)	21 (18%)	0
All	All	3349/3779 (88%)	600 (17%)	17 (0%)

All (600) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	6	G
1	C1	23	G
1	C1	27	A
1	C1	50	A
1	C1	60	G
1	C1	61	A
1	C1	66	A
1	C1	67	A
1	C1	68	A
1	C1	73	C
1	C1	93	G
1	C1	94	C
1	C1	97	G
1	C1	110	A
1	C1	111	G
1	C1	112	C
1	C1	117	A
1	C1	123	A
1	C1	132	U
1	C1	133	C
1	C1	135	G
1	C1	139	G

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Mol	Chain	Res	Type
1	C1	144	G
1	C1	151	G
1	C1	152	G
1	C1	153	A
1	C1	156	G
1	C1	170	A
1	C1	178	U
1	C1	181	G
1	C1	184	U
1	C1	194	C
1	C1	200	G
1	C1	204	C
1	C1	212	G
1	C1	213	A
1	C1	214	G
1	C1	225	A
1	C1	228	U
1	C1	240	C
1	C1	241	U
1	C1	244	G
1	C1	247	A
1	C1	258	A
1	C1	259	C
1	C1	262	G
1	C1	278	A
1	C1	288	A
1	C1	291	U
1	C1	298	U
1	C1	308	C
1	C1	316	A
1	C1	322	C
1	C1	323	G
1	C1	327	A
1	C1	343	C
1	C1	369	G
1	C1	385	OMG
1	C1	391	U
1	C1	394	C
1	C1	395	A
1	C1	396	C
1	C1	414	G
1	C1	415	A

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Mol	Chain	Res	Type
1	C1	422	U
1	C1	429	A
1	C1	434	U
1	C1	443	C
1	C1	446	A
1	C1	447	U
1	C1	448	C
1	C1	458	U
1	C1	459	C
1	C1	460	U
1	C1	469	C
1	C1	470	A
1	C1	471	C
1	C1	472	U
1	C1	479	G
1	C1	494	C
1	C1	505	G
1	C1	512	A
1	C1	514	A
1	C1	527	G
1	C1	535	U
1	C1	536	C
1	C1	537	C
1	C1	538	G
1	C1	545	U
1	C1	546	U
1	C1	547	A
1	C1	548	U
1	C1	549	A
1	C1	570	G
1	C1	588	G
1	C1	592	U
1	C1	593	G
1	C1	595	A
1	C1	597	G
1	C1	599	A
1	C1	608	U
1	C1	609	A
1	C1	610	A
1	C1	624	C
1	C1	627	OMG
1	C1	648	A

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Mol	Chain	Res	Type
1	C1	650	U
1	C1	665	A
1	C1	669	U
1	C1	678	A
1	C1	693	A
1	C1	700	G
1	C1	703	A
1	C1	704	A
1	C1	707	U
1	C1	720	C
1	C1	721	G
1	C1	743	A
1	C1	748	U
1	C1	755	G
1	C1	756	G
1	C1	757	A
1	C1	759	U
1	C1	761	G
1	C1	762	A
1	C1	763	G
1	C1	766	G
1	C1	767	G
1	C1	782	G
1	C1	790	A
1	C1	799	A
1	C1	812	A
1	C1	826	G
1	C1	839	G
1	C1	843	C
1	C1	856	U
1	C1	857	G
1	C1	862	G
1	C1	877	A
1	C1	889	G
1	C1	896	A
1	C1	898	G
1	C1	899	A
1	C1	903	A
1	C1	905	C
1	C1	906	G
1	C1	907	A
1	C1	919	G

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Mol	Chain	Res	Type
1	C1	926	A
1	C1	933	A
1	C1	934	A
1	C1	935	G
1	C1	936	U
1	C1	937	U
1	C1	940	C
1	C1	947	A
1	C1	955	G
1	C1	956	U
1	C1	961	C
1	C1	963	U
1	C1	964	C
1	C1	981	G
1	C1	986	U
1	C1	988	A
1	C1	993	G
1	C1	994	G
1	C1	995	A
1	C1	996	C
1	C1	997	U
1	C1	998	C
1	C1	999	G
1	C1	1015	C
1	C1	1016	U
1	C1	1017	U
1	C1	1021	C
1	C1	1022	C
1	C1	1024	U
1	C1	1046	G
1	C1	1047	A
1	C1	1048	A
1	C1	1049	G
1	C1	1055	G
1	C1	1056	U
1	C1	1059	C
1	C1	1064	C
1	C1	1065	U
1	C1	1068	A
1	C1	1071	U
1	C1	1081	A
1	C1	1095	A

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Mol	Chain	Res	Type
1	C1	1099	G
1	C1	1110	G
1	C1	1115	C
1	C1	1118	A
1	C1	1127	U
1	C1	1132	G
1	C1	1136	A
1	C1	1142	A
1	C1	1143	C
1	C1	1163	G
1	C1	1164	U
1	C1	1165	G
1	C1	1169	G
1	C1	1175	C
1	C1	1176	A
1	C1	1181	C
1	C1	1185	A
1	C1	1187	A
1	C1	1205	G
1	C1	1209	G
1	C1	1228	A
1	C1	1229	G
1	C1	1240	C
1	C1	1241	U
1	C1	1242	A
1	C1	1246	A
1	C1	1248	U
1	C1	1255	C
1	C1	1268	G
1	C1	1270	A
1	C1	1287	A
1	C1	1288	U
1	C1	1290	G
1	C1	1292	U
1	C1	1296	G
1	C1	1313	A
1	C1	1331	A
1	C1	1332	G
1	C1	1333	A
1	C1	1334	A
1	C1	1335	A
1	C1	1336	C

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Mol	Chain	Res	Type
1	C1	1337	G
1	C1	1369	A
1	C1	1370	G
1	C1	1382	A
1	C1	1383	G
1	C1	1400	G
1	C1	1401	A
1	C1	1414	G
1	C1	1417	G
1	C1	1420	OMC
1	C1	1429	A
1	C1	1433	OMG
1	C1	1438	U
1	C1	1464	A
1	C1	1466	G
1	C1	1477	U
1	C1	1479	C
1	C1	1485	G
1	C1	1491	OMC
1	C1	1505	U
1	C1	1536	U
1	C1	1538	U
1	C1	1539	C
1	C1	1540	A
1	C1	1543	G
1	C1	1549	C
1	C1	1550	U
1	C1	1554	G
1	C1	1567	A
1	C1	1568	A
1	C1	1573	A
1	C1	1585	A
1	C1	1586	U
1	C1	1609	U
1	C1	1619	C
1	C1	1622	A
1	C1	1623	A
1	C1	1624	C
1	C1	1625	U
1	C1	1663	C
1	C1	1683	U
1	C1	1685	U

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Mol	Chain	Res	Type
1	C1	1697	C
1	C1	1704	U
1	C1	1722	U
1	C1	1730	A
1	C1	1731	G
1	C1	1745	U
1	C1	1746	G
1	C1	1760	G
1	C1	1776	G
1	C1	1777	A
1	C1	1789	A
1	C1	1792	G
1	C1	1793	A
1	C1	1794	A
1	C1	1795	U
1	C1	1796	A
1	C1	1800	C
1	C1	1801	U
1	C1	1822	A
1	C1	1826	C
1	C1	1829	C
1	C1	1830	A
1	C1	1838	A
1	C1	1846	C
1	C1	1847	A2M
1	C1	1856	U
1	C1	1858	G
1	C1	1860	U
1	C1	1866	A
1	C1	1873	A
1	C1	1886	G
1	C1	1887	C
1	C1	1923	C
1	C1	1933	G
1	C1	1934	G
1	C1	1935	C
1	C1	1937	C
1	C1	2046	C
1	C1	2047	G
1	C1	2048	U
1	C1	2050	C
1	C1	2053	U

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Mol	Chain	Res	Type
1	C1	2054	U
1	C1	2084	G
1	C1	2085	G
1	C1	2089	A
1	C1	2094	A
1	C1	2103	U
1	C1	2121	A
1	C1	2123	G
1	C1	2132	G
1	C1	2139	U
1	C1	2151	A
1	C1	2167	C
1	C1	2185	A
1	C1	2186	A
1	C1	2188	U
1	C1	2192	A
1	C1	2207	A
1	C1	2212	G
1	C1	2219	A
1	C1	2221	U
1	C1	2222	A
1	C1	2223	U
1	C1	2224	G
1	C1	2227	U
1	C1	2231	U
1	C1	2232	U
1	C1	2233	A
1	C1	2235	G
1	C1	2283	A
1	C1	2297	U
1	C1	2298	G
1	C1	2299	U
1	C1	2336	A
1	C1	2339	G
1	C1	2340	G
1	C1	2346	C
1	C1	2351	U
1	C1	2356	G
1	C1	2357	G
1	C1	2362	A
1	C1	2365	A
1	C1	2366	G

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Mol	Chain	Res	Type
1	C1	2374	U
1	C1	2381	G
1	C1	2382	A
1	C1	2398	G
1	C1	2400	G
1	C1	2403	A
1	C1	2404	A
1	C1	2409	U
1	C1	2410	A
1	C1	2411	G
1	C1	2415	G
1	C1	2423	U
1	C1	2426	G
1	C1	2431	A
1	C1	2432	G
1	C1	2435	U
1	C1	2436	C
1	C1	2437	G
1	C1	2440	G
1	C1	2441	C
1	C1	2447	A
1	C1	2450	U
1	C1	2454	A
1	C1	2457	A
1	C1	2458	C
1	C1	2459	U
1	C1	2465	U
1	C1	2466	G
1	C1	2477	U
1	C1	2485	G
1	C1	2489	C
1	C1	2498	A
1	C1	2499	C
1	C1	2500	U
1	C1	2501	U
1	C1	2502	G
1	C1	2503	C
1	C1	2506	C
1	C1	2507	C
1	C1	2508	A
1	C1	2512	U
1	C1	2513	C

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Mol	Chain	Res	Type
1	C1	2521	A
1	C1	2522	A
1	C1	2527	C
1	C1	2530	C
1	C1	2533	G
1	C1	2544	G
1	C1	2545	G
1	C1	2549	A
1	C1	2552	A
1	C1	2565	G
1	C1	2566	G
1	C1	2573	G
1	C1	2583	G
1	C1	2587	A
1	C1	2589	C
1	C1	2591	G
1	C1	2607	G
1	C1	2610	G
1	C1	2611	U
1	C1	2615	A
1	C1	2616	A
1	C1	2633	A
1	C1	2636	G
1	C1	2640	U
1	C1	2648	A
1	C1	2650	A
1	C1	2653	A
1	C1	2654	A
1	C1	2655	A
1	C1	2656	A
1	C1	2657	G
1	C1	2660	U
1	C1	2661	A
1	C1	2663	A
1	C1	2664	A
1	C1	2670	C
1	C1	2672	U
1	C1	2673	G
1	C1	2684	U
1	C1	2690	OMU
1	C1	2691	G
1	C1	2701	C

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Mol	Chain	Res	Type
1	C1	2708	G
1	C1	2712	G
1	C1	2713	G
1	C1	2714	C
1	C1	2731	C
1	C1	2732	C
1	C1	2734	U
1	C1	2736	G
1	C1	2737	A
1	C1	2763	A
1	C1	2769	C
1	C1	2783	G
1	C1	2784	C
1	C1	2785	U
1	C1	2802	U
1	C1	2803	C
1	C1	2805	U
1	C1	2812	G
1	C1	2816	C
1	C1	2817	U
1	C1	2826	C
1	C1	2828	U
1	C1	2834	U
1	C1	2836	G
1	C1	2846	A
1	C1	2847	U
1	C1	2848	C
1	C1	2857	G
1	C1	2858	C
1	C1	2863	U
1	C1	2882	U
1	C1	2894	U
1	C1	2895	A
1	C1	2909	G
1	C1	2929	C
1	C1	2930	A
1	C1	2931	G
1	C1	2938	U
1	C1	2939	U
1	C1	2940	U
1	C1	2942	C
1	C1	2949	G

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Mol	Chain	Res	Type
1	C1	2951	U
1	C1	2955	C
1	C1	2956	U
1	C1	2970	A
1	C1	2980	G
1	C1	3014	U
1	C1	3017	G
1	C1	3036	G
1	C1	3044	A
1	C1	3045	A
1	C1	3050	C
1	C1	3051	C
1	C1	3067	G
1	C1	3071	A
1	C1	3080	A
1	C1	3087	A
1	C1	3088	A
1	C1	3089	U
1	C1	3100	A
1	C1	3101	C
1	C1	3102	G
1	C1	3112	U
1	C1	3113	A
1	C1	3119	A
1	C1	3126	A
1	C1	3127	G
1	C1	3131	U
1	C1	3133	U
1	C1	3135	A
1	C1	3141	G
1	C1	3146	C
1	C1	3155	A
1	C1	3162	C
1	C1	3163	A
1	C1	3164	G
1	C1	3185	G
1	C1	3186	A
1	C1	3188	G
1	C1	3190	G
1	C1	3200	A
1	C1	3201	A
1	C1	3206	C

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Mol	Chain	Res	Type
1	C1	3210	U
1	C1	3211	U
1	C1	3218	U
1	C1	3227	G
1	C1	3228	C
1	C1	3231	G
1	C1	3244	G
1	C1	3245	C
1	C1	3248	A
1	C1	3254	U
1	C1	3257	A
1	C1	3258	U
1	C1	3259	G
1	C1	3260	U
1	C1	3282	U
1	C1	3291	C
1	C1	3293	U
1	C1	3295	U
1	C1	3297	G
1	C1	3299	U
1	C1	3302	G
1	C1	3310	G
1	C1	3316	A
1	C1	3319	C
1	C1	3323	C
1	C1	3324	C
1	C1	3325	U
1	C1	3328	G
1	C1	3331	U
1	C1	3332	A
1	C1	3338	C
2	C2	34	U
2	C2	35	C
2	C2	39	G
2	C2	59	A
2	C2	62	A
2	C2	63	G
2	C2	81	U
2	C2	82	U
2	C2	83	C
2	C2	84	C
2	C2	87	G

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Mol	Chain	Res	Type
2	C2	90	U
2	C2	95	G
2	C2	96	A
2	C2	104	A
2	C2	105	A
2	C2	106	C
2	C2	116	G
2	C2	125	U
2	C2	127	U
2	C2	151	C
3	C3	2	U
4	C4	7	G
4	C4	8	A
4	C4	9	C
4	C4	18	G
4	C4	26	C
4	C4	29	G
4	C4	54	U
4	C4	55	A
4	C4	64	A
4	C4	65	G
4	C4	72	G
4	C4	73	U
4	C4	75	A
4	C4	76	G
4	C4	87	G
4	C4	88	G
4	C4	98	G
4	C4	101	A
4	C4	109	G
4	C4	110	U
4	C4	111	G

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	151	G
1	C1	1021	C
1	C1	1047	A
1	C1	1267	C
1	C1	1537	U
1	C1	2234	A

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Mol	Chain	Res	Type
1	C1	2282	U
1	C1	2409	U
1	C1	2712	G
1	C1	3079	U
1	C1	3132	A
1	C1	3205	G
1	C1	3210	U
1	C1	3230	G
1	C1	3258	U
1	C1	3298	U
1	C1	3301	C

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

32 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	$\# Z > 2$
1	OMC	C1	778	1	19,22,23	0.56	0	25,31,34	0.90	1 (4%)
1	A2M	C1	848	1	22,25,26	4.01	12 (54%)	30,36,39	3.44	15 (50%)
1	A2M	C1	2289	1	22,25,26	4.01	12 (54%)	30,36,39	3.32	14 (46%)
1	OMG	C1	646	1	23,26,27	0.48	0	32,38,41	0.49	0
1	OMC	C1	1812	1	19,22,23	0.55	0	25,31,34	0.76	0
1	OMC	C1	1836	1	19,22,23	0.59	0	25,31,34	0.97	1 (4%)
1	OMG	C1	2358	1	23,26,27	0.48	0	32,38,41	0.53	0
1	A2M	C1	389	1	22,25,26	3.98	11 (50%)	30,36,39	3.40	13 (43%)
1	A2M	C1	1223	1	22,25,26	3.98	11 (50%)	30,36,39	3.32	12 (40%)
1	OMG	C1	2881	1	23,26,27	0.47	0	32,38,41	0.45	0
1	OMG	C1	2876	1	23,26,27	0.48	0	32,38,41	0.48	0
1	A2M	C1	1847	1	22,25,26	3.98	12 (54%)	30,36,39	3.51	14 (46%)
1	OMU	C1	2683	1	19,22,23	3.11	6 (31%)	25,31,34	1.85	5 (20%)
1	A2M	C1	637	1	22,25,26	3.99	11 (50%)	30,36,39	3.38	13 (43%)
1	OMC	C1	1420	1	19,22,23	0.56	0	25,31,34	1.04	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	C1	627	1	23,26,27	0.53	0	32,38,41	0.48	0
1	OMU	C1	2688	1	19,22,23	3.17	6 (31%)	25,31,34	1.77	4 (16%)
1	OMG	C1	1433	1	23,26,27	0.48	0	32,38,41	0.50	0
1	OMU	C1	1917	1	19,22,23	3.14	6 (31%)	25,31,34	1.90	5 (20%)
1	A2M	C1	858	1	22,25,26	4.00	11 (50%)	30,36,39	3.43	13 (43%)
1	OMC	C1	2300	1	19,22,23	0.51	0	25,31,34	0.71	0
1	OMG	C1	385	1	23,26,27	0.47	0	32,38,41	0.58	0
1	OMC	C1	2918	1	19,22,23	0.55	0	25,31,34	0.78	0
1	OMU	C1	2380	1	19,22,23	3.05	6 (31%)	25,31,34	1.81	5 (20%)
1	OMC	C1	1491	1	19,22,23	0.54	0	25,31,34	0.76	0
1	A2M	C1	1432	1	22,25,26	3.99	12 (54%)	30,36,39	3.39	13 (43%)
1	OMU	C1	2384	1	19,22,23	3.09	6 (31%)	25,31,34	1.77	4 (16%)
1	OMG	C1	2774	1	23,26,27	0.47	0	32,38,41	0.46	0
1	OMG	C1	787	1	23,26,27	0.49	0	32,38,41	0.59	0
1	OMC	C1	2838	1	19,22,23	0.59	0	25,31,34	0.97	2 (8%)
1	OMU	C1	1868	1	19,22,23	3.09	6 (31%)	25,31,34	1.87	5 (20%)
1	OMU	C1	2690	1	19,22,23	3.24	6 (31%)	25,31,34	1.87	7 (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
1	OMC	C1	778	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	848	1	-	1/9/27/28	0/3/3/3
1	A2M	C1	2289	1	-	0/9/27/28	0/3/3/3
1	OMG	C1	646	1	-	0/9/27/28	0/3/3/3
1	OMC	C1	1812	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	1836	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	2358	1	-	0/9/27/28	0/3/3/3
1	A2M	C1	389	1	-	2/9/27/28	0/3/3/3
1	A2M	C1	1223	1	-	3/9/27/28	0/3/3/3
1	OMG	C1	2881	1	-	0/9/27/28	0/3/3/3
1	OMG	C1	2876	1	-	1/9/27/28	0/3/3/3
1	A2M	C1	1847	1	-	3/9/27/28	0/3/3/3
1	OMU	C1	2683	1	-	2/9/27/28	0/2/2/2
1	A2M	C1	637	1	-	1/9/27/28	0/3/3/3
1	OMC	C1	1420	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	C1	627	1	-	2/9/27/28	0/3/3/3
1	OMU	C1	2688	1	-	2/9/27/28	0/2/2/2
1	OMG	C1	1433	1	-	2/9/27/28	0/3/3/3
1	OMU	C1	1917	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	858	1	-	1/9/27/28	0/3/3/3
1	OMC	C1	2300	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	385	1	-	2/9/27/28	0/3/3/3
1	OMC	C1	2918	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	2380	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	1491	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	1432	1	-	0/9/27/28	0/3/3/3
1	OMU	C1	2384	1	-	1/9/27/28	0/2/2/2
1	OMG	C1	2774	1	-	0/9/27/28	0/3/3/3
1	OMG	C1	787	1	-	0/9/27/28	0/3/3/3
1	OMC	C1	2838	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	1868	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	2690	1	-	3/9/27/28	0/2/2/2

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2289	A2M	C3'-C2'	-13.09	1.24	1.53
1	C1	848	A2M	C3'-C2'	-13.04	1.24	1.53
1	C1	858	A2M	C3'-C2'	-13.03	1.24	1.53
1	C1	1223	A2M	C3'-C2'	-12.98	1.24	1.53
1	C1	637	A2M	C3'-C2'	-12.97	1.24	1.53
1	C1	1432	A2M	C3'-C2'	-12.97	1.24	1.53
1	C1	1847	A2M	C3'-C2'	-12.87	1.24	1.53
1	C1	389	A2M	C3'-C2'	-12.69	1.25	1.53
1	C1	2690	OMU	C2-N1	8.19	1.51	1.38
1	C1	1917	OMU	C2-N1	7.76	1.50	1.38
1	C1	2688	OMU	C2-N1	7.66	1.50	1.38
1	C1	2690	OMU	C2-N3	7.43	1.50	1.38
1	C1	2683	OMU	C2-N1	7.36	1.50	1.38
1	C1	1868	OMU	C2-N1	7.35	1.50	1.38
1	C1	2384	OMU	C2-N1	7.35	1.50	1.38
1	C1	2688	OMU	C2-N3	7.34	1.50	1.38
1	C1	2683	OMU	C2-N3	7.28	1.50	1.38
1	C1	2384	OMU	C2-N3	7.23	1.50	1.38
1	C1	1917	OMU	C2-N3	7.21	1.50	1.38
1	C1	1868	OMU	C2-N3	7.20	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2380	OMU	C2-N3	7.20	1.50	1.38
1	C1	2380	OMU	C2-N1	7.08	1.49	1.38
1	C1	389	A2M	O4'-C4'	-6.90	1.29	1.45
1	C1	1847	A2M	O4'-C4'	-6.61	1.30	1.45
1	C1	637	A2M	O4'-C4'	-6.56	1.30	1.45
1	C1	858	A2M	O4'-C4'	-6.55	1.30	1.45
1	C1	1432	A2M	O4'-C4'	-6.53	1.30	1.45
1	C1	848	A2M	O4'-C4'	-6.50	1.30	1.45
1	C1	1223	A2M	O4'-C4'	-6.45	1.30	1.45
1	C1	2289	A2M	O4'-C4'	-6.45	1.30	1.45
1	C1	2688	OMU	C6-C5	6.27	1.49	1.35
1	C1	2683	OMU	C6-C5	6.25	1.49	1.35
1	C1	2690	OMU	C6-C5	6.25	1.49	1.35
1	C1	1868	OMU	C6-C5	6.24	1.49	1.35
1	C1	2384	OMU	C6-C5	6.17	1.49	1.35
1	C1	1917	OMU	C6-C5	6.15	1.49	1.35
1	C1	2380	OMU	C6-C5	6.10	1.49	1.35
1	C1	2289	A2M	C3'-C4'	5.31	1.66	1.53
1	C1	1432	A2M	C3'-C4'	5.30	1.66	1.53
1	C1	1223	A2M	C3'-C4'	5.27	1.66	1.53
1	C1	858	A2M	C3'-C4'	5.24	1.66	1.53
1	C1	848	A2M	C3'-C4'	5.21	1.66	1.53
1	C1	637	A2M	C3'-C4'	5.16	1.66	1.53
1	C1	389	A2M	C3'-C4'	5.13	1.66	1.53
1	C1	1847	A2M	C3'-C4'	5.10	1.65	1.53
1	C1	848	A2M	C1'-N9	-4.56	1.33	1.46
1	C1	2289	A2M	O4'-C1'	4.48	1.52	1.42
1	C1	2688	OMU	C4-N3	4.47	1.46	1.38
1	C1	858	A2M	O4'-C1'	4.47	1.52	1.42
1	C1	1847	A2M	C1'-N9	-4.46	1.34	1.46
1	C1	1432	A2M	O4'-C1'	4.45	1.52	1.42
1	C1	2690	OMU	C4-N3	4.44	1.46	1.38
1	C1	1223	A2M	C6-N6	4.43	1.45	1.34
1	C1	858	A2M	C6-N6	4.42	1.45	1.34
1	C1	1847	A2M	O4'-C1'	4.42	1.52	1.42
1	C1	848	A2M	O4'-C1'	4.42	1.52	1.42
1	C1	389	A2M	C6-N6	4.42	1.45	1.34
1	C1	2289	A2M	C1'-N9	-4.41	1.34	1.46
1	C1	637	A2M	C6-N6	4.41	1.45	1.34
1	C1	1432	A2M	C6-N6	4.41	1.45	1.34
1	C1	1223	A2M	O4'-C1'	4.40	1.52	1.42
1	C1	2289	A2M	C6-N6	4.37	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	848	A2M	C6-N6	4.37	1.45	1.34
1	C1	2683	OMU	C4-N3	4.36	1.46	1.38
1	C1	1847	A2M	C6-N6	4.35	1.45	1.34
1	C1	637	A2M	O4'-C1'	4.35	1.52	1.42
1	C1	2380	OMU	C4-N3	4.34	1.46	1.38
1	C1	2384	OMU	C4-N3	4.33	1.46	1.38
1	C1	858	A2M	C1'-N9	-4.32	1.34	1.46
1	C1	1868	OMU	C4-N3	4.31	1.46	1.38
1	C1	1917	OMU	C4-N3	4.29	1.46	1.38
1	C1	389	A2M	O4'-C1'	4.27	1.51	1.42
1	C1	1223	A2M	C1'-N9	-4.26	1.34	1.46
1	C1	1432	A2M	C1'-N9	-4.25	1.34	1.46
1	C1	389	A2M	C1'-N9	-4.23	1.34	1.46
1	C1	637	A2M	C1'-N9	-4.22	1.34	1.46
1	C1	389	A2M	O2'-C2'	3.86	1.52	1.42
1	C1	637	A2M	O2'-C2'	3.68	1.51	1.42
1	C1	1223	A2M	O2'-C2'	3.59	1.51	1.42
1	C1	858	A2M	O2'-C2'	3.57	1.51	1.42
1	C1	1432	A2M	O2'-C2'	3.57	1.51	1.42
1	C1	848	A2M	O2'-C2'	3.55	1.51	1.42
1	C1	2289	A2M	O2'-C2'	3.50	1.51	1.42
1	C1	1847	A2M	O2'-C2'	3.48	1.51	1.42
1	C1	389	A2M	C2'-C1'	3.27	1.61	1.53
1	C1	848	A2M	C2'-C1'	3.10	1.60	1.53
1	C1	637	A2M	C2'-C1'	3.05	1.60	1.53
1	C1	1223	A2M	C2'-C1'	3.04	1.60	1.53
1	C1	1847	A2M	C2'-C1'	3.04	1.60	1.53
1	C1	1847	A2M	C5-C4	-3.02	1.33	1.39
1	C1	637	A2M	C5-C4	-3.01	1.33	1.39
1	C1	389	A2M	C5-C4	-3.01	1.33	1.39
1	C1	2289	A2M	C5-C4	-3.01	1.33	1.39
1	C1	1432	A2M	C5-C4	-2.99	1.33	1.39
1	C1	848	A2M	C5-C4	-2.98	1.33	1.39
1	C1	858	A2M	C5-C4	-2.97	1.33	1.39
1	C1	2289	A2M	C2'-C1'	2.97	1.60	1.53
1	C1	1432	A2M	C2'-C1'	2.93	1.60	1.53
1	C1	1223	A2M	C5-C4	-2.88	1.33	1.39
1	C1	858	A2M	C2'-C1'	2.84	1.60	1.53
1	C1	2690	OMU	C6-N1	2.81	1.44	1.38
1	C1	2688	OMU	C6-N1	2.81	1.44	1.38
1	C1	2683	OMU	C6-N1	2.70	1.44	1.38
1	C1	1432	A2M	C5-N7	-2.66	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1917	OMU	C6-N1	2.65	1.44	1.38
1	C1	1223	A2M	C5-N7	-2.64	1.34	1.39
1	C1	858	A2M	C5-N7	-2.64	1.34	1.39
1	C1	389	A2M	C5-N7	-2.64	1.34	1.39
1	C1	2380	OMU	C6-N1	2.64	1.44	1.38
1	C1	2384	OMU	C6-N1	2.63	1.44	1.38
1	C1	1868	OMU	C6-N1	2.62	1.44	1.38
1	C1	637	A2M	C5-N7	-2.60	1.34	1.39
1	C1	2289	A2M	C5-N7	-2.59	1.34	1.39
1	C1	1847	A2M	C5-N7	-2.54	1.34	1.39
1	C1	848	A2M	C5-N7	-2.45	1.34	1.39
1	C1	2688	OMU	C5-C4	2.36	1.48	1.43
1	C1	2683	OMU	C5-C4	2.32	1.48	1.43
1	C1	1868	OMU	C5-C4	2.28	1.48	1.43
1	C1	2380	OMU	C5-C4	2.26	1.48	1.43
1	C1	2384	OMU	C5-C4	2.22	1.48	1.43
1	C1	2690	OMU	C5-C4	2.22	1.48	1.43
1	C1	858	A2M	C8-N9	-2.22	1.33	1.37
1	C1	1847	A2M	C8-N9	-2.19	1.33	1.37
1	C1	1432	A2M	C8-N9	-2.17	1.33	1.37
1	C1	848	A2M	C8-N9	-2.15	1.33	1.37
1	C1	637	A2M	C8-N9	-2.14	1.33	1.37
1	C1	1917	OMU	C5-C4	2.14	1.48	1.43
1	C1	1847	A2M	O3'-C3'	2.13	1.48	1.43
1	C1	389	A2M	C8-N9	-2.09	1.34	1.37
1	C1	848	A2M	O3'-C3'	2.08	1.48	1.43
1	C1	1223	A2M	O3'-C3'	2.07	1.48	1.43
1	C1	1432	A2M	O3'-C3'	2.03	1.48	1.43
1	C1	2289	A2M	C8-N9	-2.01	1.34	1.37
1	C1	2289	A2M	O3'-C3'	2.00	1.47	1.43

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1847	A2M	C1'-N9-C8	-9.66	105.66	127.09
1	C1	858	A2M	C1'-N9-C8	-9.38	106.28	127.09
1	C1	1432	A2M	C1'-N9-C8	-9.28	106.49	127.09
1	C1	389	A2M	C1'-N9-C8	-9.22	106.63	127.09
1	C1	637	A2M	C1'-N9-C8	-9.18	106.72	127.09
1	C1	848	A2M	C1'-N9-C8	-9.12	106.84	127.09
1	C1	1223	A2M	C1'-N9-C8	-9.00	107.12	127.09
1	C1	2289	A2M	C1'-N9-C8	-8.70	107.79	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1847	A2M	C4-N9-C1'	8.20	145.81	126.63
1	C1	858	A2M	C4-N9-C1'	8.09	145.56	126.63
1	C1	1432	A2M	C4-N9-C1'	8.08	145.53	126.63
1	C1	389	A2M	C4-N9-C1'	7.94	145.20	126.63
1	C1	637	A2M	C4-N9-C1'	7.91	145.12	126.63
1	C1	1223	A2M	C4-N9-C1'	7.74	144.74	126.63
1	C1	848	A2M	C4-N9-C1'	7.61	144.42	126.63
1	C1	2289	A2M	C4-N9-C1'	7.36	143.84	126.63
1	C1	858	A2M	N3-C2-N1	-5.90	119.65	128.58
1	C1	1847	A2M	N3-C2-N1	-5.88	119.68	128.58
1	C1	848	A2M	N3-C2-N1	-5.84	119.74	128.58
1	C1	1868	OMU	C4-N3-C2	-5.79	119.43	126.61
1	C1	389	A2M	N3-C2-N1	-5.72	119.92	128.58
1	C1	2289	A2M	N3-C2-N1	-5.71	119.94	128.58
1	C1	1432	A2M	N3-C2-N1	-5.70	119.96	128.58
1	C1	637	A2M	N3-C2-N1	-5.69	119.98	128.58
1	C1	1223	A2M	N3-C2-N1	-5.67	120.00	128.58
1	C1	2380	OMU	C4-N3-C2	-5.66	119.58	126.61
1	C1	848	A2M	N6-C6-N1	-5.64	105.81	118.38
1	C1	858	A2M	N6-C6-N1	-5.64	105.81	118.38
1	C1	2683	OMU	C4-N3-C2	-5.63	119.63	126.61
1	C1	1847	A2M	N6-C6-N1	-5.60	105.92	118.38
1	C1	637	A2M	N6-C6-N1	-5.54	106.04	118.38
1	C1	1432	A2M	N6-C6-N1	-5.50	106.12	118.38
1	C1	2289	A2M	N6-C6-N1	-5.49	106.15	118.38
1	C1	389	A2M	N6-C6-N1	-5.47	106.19	118.38
1	C1	2688	OMU	C4-N3-C2	-5.44	119.86	126.61
1	C1	1223	A2M	N6-C6-N1	-5.42	106.31	118.38
1	C1	2384	OMU	C4-N3-C2	-5.39	119.92	126.61
1	C1	1917	OMU	C4-N3-C2	-5.23	120.12	126.61
1	C1	2690	OMU	C4-N3-C2	-5.00	120.41	126.61
1	C1	637	A2M	C5-C4-N3	-4.98	119.86	126.72
1	C1	1432	A2M	C5-C4-N3	-4.91	119.95	126.72
1	C1	1847	A2M	C5-C4-N3	-4.90	119.97	126.72
1	C1	858	A2M	C5-C4-N3	-4.85	120.04	126.72
1	C1	389	A2M	C5-C4-N3	-4.82	120.08	126.72
1	C1	1223	A2M	C5-C4-N3	-4.73	120.20	126.72
1	C1	848	A2M	C5-C4-N3	-4.63	120.34	126.72
1	C1	848	A2M	N9-C8-N7	-4.57	107.46	113.94
1	C1	2289	A2M	C5-C4-N3	-4.51	120.51	126.72
1	C1	1847	A2M	N9-C8-N7	-4.50	107.56	113.94
1	C1	858	A2M	C5-C6-N6	4.48	134.37	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2289	A2M	N9-C8-N7	-4.42	107.67	113.94
1	C1	848	A2M	C5-C6-N6	4.36	134.08	123.29
1	C1	1847	A2M	C5-C6-N6	4.32	133.98	123.29
1	C1	2289	A2M	C5-C6-N6	4.31	133.95	123.29
1	C1	1223	A2M	C5-C6-N6	4.27	133.87	123.29
1	C1	1432	A2M	C5-C6-N6	4.27	133.86	123.29
1	C1	389	A2M	C5-C6-N6	4.27	133.86	123.29
1	C1	389	A2M	N9-C8-N7	-4.27	107.88	113.94
1	C1	637	A2M	C5-C6-N6	4.27	133.85	123.29
1	C1	637	A2M	N9-C8-N7	-4.23	107.93	113.94
1	C1	858	A2M	N9-C8-N7	-4.17	108.02	113.94
1	C1	1223	A2M	N9-C8-N7	-4.16	108.04	113.94
1	C1	2683	OMU	N3-C2-N1	4.12	120.25	114.89
1	C1	2289	A2M	O4'-C1'-N9	4.10	115.95	108.09
1	C1	1432	A2M	N9-C8-N7	-4.06	108.17	113.94
1	C1	1917	OMU	N3-C2-N1	4.02	120.12	114.89
1	C1	2380	OMU	N3-C2-N1	3.92	119.99	114.89
1	C1	1868	OMU	N3-C2-N1	3.91	119.99	114.89
1	C1	2384	OMU	N3-C2-N1	3.91	119.98	114.89
1	C1	2690	OMU	N3-C2-N1	3.86	119.92	114.89
1	C1	848	A2M	O4'-C1'-N9	3.83	115.44	108.09
1	C1	858	A2M	O4'-C1'-N9	3.82	115.42	108.09
1	C1	1432	A2M	O4'-C1'-N9	3.78	115.35	108.09
1	C1	2688	OMU	N3-C2-N1	3.78	119.81	114.89
1	C1	637	A2M	O4'-C1'-N9	3.75	115.30	108.09
1	C1	1868	OMU	C5-C4-N3	3.73	120.03	114.80
1	C1	1223	A2M	O4'-C1'-N9	3.67	115.14	108.09
1	C1	2380	OMU	C5-C4-N3	3.66	119.93	114.80
1	C1	1917	OMU	C1'-N1-C2	3.62	124.10	117.59
1	C1	389	A2M	O4'-C1'-N9	3.58	114.97	108.09
1	C1	2688	OMU	C5-C4-N3	3.52	119.74	114.80
1	C1	1847	A2M	C2-N3-C4	3.50	120.38	111.83
1	C1	2683	OMU	C5-C4-N3	3.47	119.66	114.80
1	C1	2384	OMU	C5-C4-N3	3.45	119.63	114.80
1	C1	858	A2M	C2-N3-C4	3.42	120.18	111.83
1	C1	637	A2M	C2-N3-C4	3.41	120.16	111.83
1	C1	848	A2M	C2-N3-C4	3.40	120.13	111.83
1	C1	1432	A2M	C2-N3-C4	3.37	120.06	111.83
1	C1	389	A2M	C2-N3-C4	3.36	120.03	111.83
1	C1	1917	OMU	C5-C4-N3	3.32	119.45	114.80
1	C1	1223	A2M	C2-N3-C4	3.28	119.84	111.83
1	C1	2289	A2M	C2-N3-C4	3.27	119.82	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2690	OMU	C5-C4-N3	3.27	119.38	114.80
1	C1	848	A2M	C2'-C1'-N9	-3.22	108.45	113.75
1	C1	1847	A2M	O4'-C1'-N9	3.20	114.24	108.09
1	C1	2690	OMU	C1'-N1-C2	3.08	123.13	117.59
1	C1	637	A2M	N3-C4-N9	3.07	132.39	127.17
1	C1	1847	A2M	N3-C4-N9	3.06	132.37	127.17
1	C1	1847	A2M	C5-N7-C8	3.02	108.20	103.45
1	C1	848	A2M	C5-N7-C8	3.00	108.17	103.45
1	C1	1432	A2M	N3-C4-N9	2.99	132.25	127.17
1	C1	858	A2M	N3-C4-N9	2.97	132.21	127.17
1	C1	1420	OMC	C1'-N1-C2	2.96	124.97	118.44
1	C1	389	A2M	N3-C4-N9	2.95	132.18	127.17
1	C1	389	A2M	C5-N7-C8	2.94	108.06	103.45
1	C1	1223	A2M	N3-C4-N9	2.93	132.15	127.17
1	C1	2289	A2M	C5-N7-C8	2.92	108.04	103.45
1	C1	637	A2M	C5-N7-C8	2.91	108.02	103.45
1	C1	1868	OMU	O4-C4-C5	-2.91	120.15	125.16
1	C1	848	A2M	N3-C4-N9	2.89	132.09	127.17
1	C1	2380	OMU	O4-C4-C5	-2.89	120.19	125.16
1	C1	1847	A2M	C2'-C1'-N9	-2.88	109.00	113.75
1	C1	2683	OMU	O4-C4-C5	-2.88	120.20	125.16
1	C1	848	A2M	C4-N9-C8	2.85	108.73	105.74
1	C1	2688	OMU	O4-C4-C5	-2.85	120.25	125.16
1	C1	2690	OMU	O4-C4-C5	-2.85	120.25	125.16
1	C1	858	A2M	C5-N7-C8	2.83	107.90	103.45
1	C1	2384	OMU	O4-C4-C5	-2.83	120.28	125.16
1	C1	1917	OMU	O4-C4-C5	-2.79	120.34	125.16
1	C1	2838	OMC	C1'-N1-C2	2.79	124.61	118.44
1	C1	2289	A2M	C2'-C1'-N9	-2.78	109.17	113.75
1	C1	1223	A2M	C5-N7-C8	2.78	107.81	103.45
1	C1	1432	A2M	C5-N7-C8	2.76	107.79	103.45
1	C1	1836	OMC	C1'-N1-C2	2.74	124.50	118.44
1	C1	2289	A2M	N3-C4-N9	2.68	131.72	127.17
1	C1	1847	A2M	C4-N9-C8	2.66	108.53	105.74
1	C1	2289	A2M	C4-N9-C8	2.51	108.37	105.74
1	C1	778	OMC	C1'-N1-C2	2.50	123.96	118.44
1	C1	2683	OMU	O2-C2-N1	-2.38	119.69	122.80
1	C1	848	A2M	C4'-O4'-C1'	-2.35	104.28	109.47
1	C1	1868	OMU	O2-C2-N1	-2.33	119.76	122.80
1	C1	389	A2M	C4-N9-C8	2.31	108.17	105.74
1	C1	2380	OMU	O2-C2-N1	-2.30	119.81	122.80
1	C1	637	A2M	C4-N9-C8	2.29	108.15	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	858	A2M	C4-N9-C8	2.29	108.15	105.74
1	C1	1223	A2M	C4-N9-C8	2.28	108.13	105.74
1	C1	1847	A2M	C4-C5-N7	-2.21	108.06	110.58
1	C1	848	A2M	C4-C5-N7	-2.19	108.08	110.58
1	C1	2690	OMU	C6-N1-C2	-2.16	118.37	121.00
1	C1	389	A2M	C4-C5-N7	-2.13	108.14	110.58
1	C1	1432	A2M	C4-N9-C8	2.13	107.98	105.74
1	C1	2289	A2M	C4-C5-N7	-2.13	108.15	110.58
1	C1	637	A2M	C4-C5-N7	-2.13	108.15	110.58
1	C1	858	A2M	C4-C5-N7	-2.10	108.19	110.58
1	C1	1432	A2M	C4-C5-N7	-2.03	108.26	110.58
1	C1	2838	OMC	C1'-N1-C6	-2.00	116.50	120.78
1	C1	2690	OMU	C2'-C3'-C4'	2.00	106.30	101.99

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C1	389	A2M	C1'-C2'-O2'-CM'
1	C1	637	A2M	C1'-C2'-O2'-CM'
1	C1	1223	A2M	C1'-C2'-O2'-CM'
1	C1	1433	OMG	O4'-C4'-C5'-O5'
1	C1	2384	OMU	C1'-C2'-O2'-CM2
1	C1	2683	OMU	C1'-C2'-O2'-CM2
1	C1	2688	OMU	C3'-C4'-C5'-O5'
1	C1	2688	OMU	O4'-C4'-C5'-O5'
1	C1	385	OMG	C3'-C4'-C5'-O5'
1	C1	627	OMG	C3'-C4'-C5'-O5'
1	C1	1223	A2M	O4'-C4'-C5'-O5'
1	C1	1433	OMG	C3'-C4'-C5'-O5'
1	C1	1847	A2M	C3'-C4'-C5'-O5'
1	C1	389	A2M	O4'-C4'-C5'-O5'
1	C1	627	OMG	O4'-C4'-C5'-O5'
1	C1	1847	A2M	O4'-C4'-C5'-O5'
1	C1	2690	OMU	C4'-C5'-O5'-P
1	C1	385	OMG	O4'-C4'-C5'-O5'
1	C1	1223	A2M	C3'-C4'-C5'-O5'
1	C1	848	A2M	O4'-C4'-C5'-O5'
1	C1	2683	OMU	C3'-C2'-O2'-CM2
1	C1	1847	A2M	C4'-C5'-O5'-P
1	C1	858	A2M	O4'-C4'-C5'-O5'
1	C1	2690	OMU	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
1	C1	2876	OMG	C3'-C2'-O2'-CM2
1	C1	2690	OMU	C2'-C1'-N1-C2

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C1	848	A2M	1	0
1	C1	389	A2M	1	0
1	C1	1223	A2M	1	0
1	C1	1420	OMC	1	0
1	C1	627	OMG	1	0
1	C1	1432	A2M	1	0
1	C1	2384	OMU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	$\# Z > 2$
62	GTP	Cd	1000	63	33,34,34	0.96	1 (3%)	50,54,54	1.61	9 (18%)
62	GTP	CH	701	63	33,34,34	0.89	1 (3%)	50,54,54	1.57	9 (18%)

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
62	GTP	Cd	1000	63	-	3/22/38/38	0/3/3/3
62	GTP	CH	701	63	-	4/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	Cd	1000	GTP	C2-N3	2.19	1.38	1.33
62	CH	701	GTP	C2-N3	2.07	1.38	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	Cd	1000	GTP	C5-C4-N3	-5.09	120.29	128.39
62	CH	701	GTP	C5-C4-N3	-4.78	120.78	128.39
62	Cd	1000	GTP	C2-N3-C4	4.64	120.29	112.30
62	CH	701	GTP	C2-N3-C4	4.55	120.13	112.30
62	Cd	1000	GTP	N9-C4-N3	3.31	132.56	125.95
62	Cd	1000	GTP	C2-N1-C6	-2.99	119.70	125.11
62	CH	701	GTP	N9-C4-N3	2.95	131.86	125.95
62	CH	701	GTP	C2-N1-C6	-2.92	119.81	125.11
62	CH	701	GTP	N9-C8-N7	-2.74	108.32	113.40
62	Cd	1000	GTP	N9-C8-N7	-2.60	108.57	113.40
62	Cd	1000	GTP	C5-C6-N1	2.58	119.81	113.25
62	CH	701	GTP	C8-N7-C5	2.53	108.77	104.26
62	CH	701	GTP	C5-C6-N1	2.52	119.68	113.25
62	Cd	1000	GTP	O6-C6-C5	-2.46	120.03	126.53
62	Cd	1000	GTP	C8-N7-C5	2.46	108.64	104.26
62	CH	701	GTP	O6-C6-C5	-2.38	120.26	126.53
62	Cd	1000	GTP	C3'-C2'-C1'	2.13	105.50	101.46
62	CH	701	GTP	C3'-C2'-C1'	2.04	105.32	101.46

There are no chirality outliers.

All (7) torsion outliers are listed below:

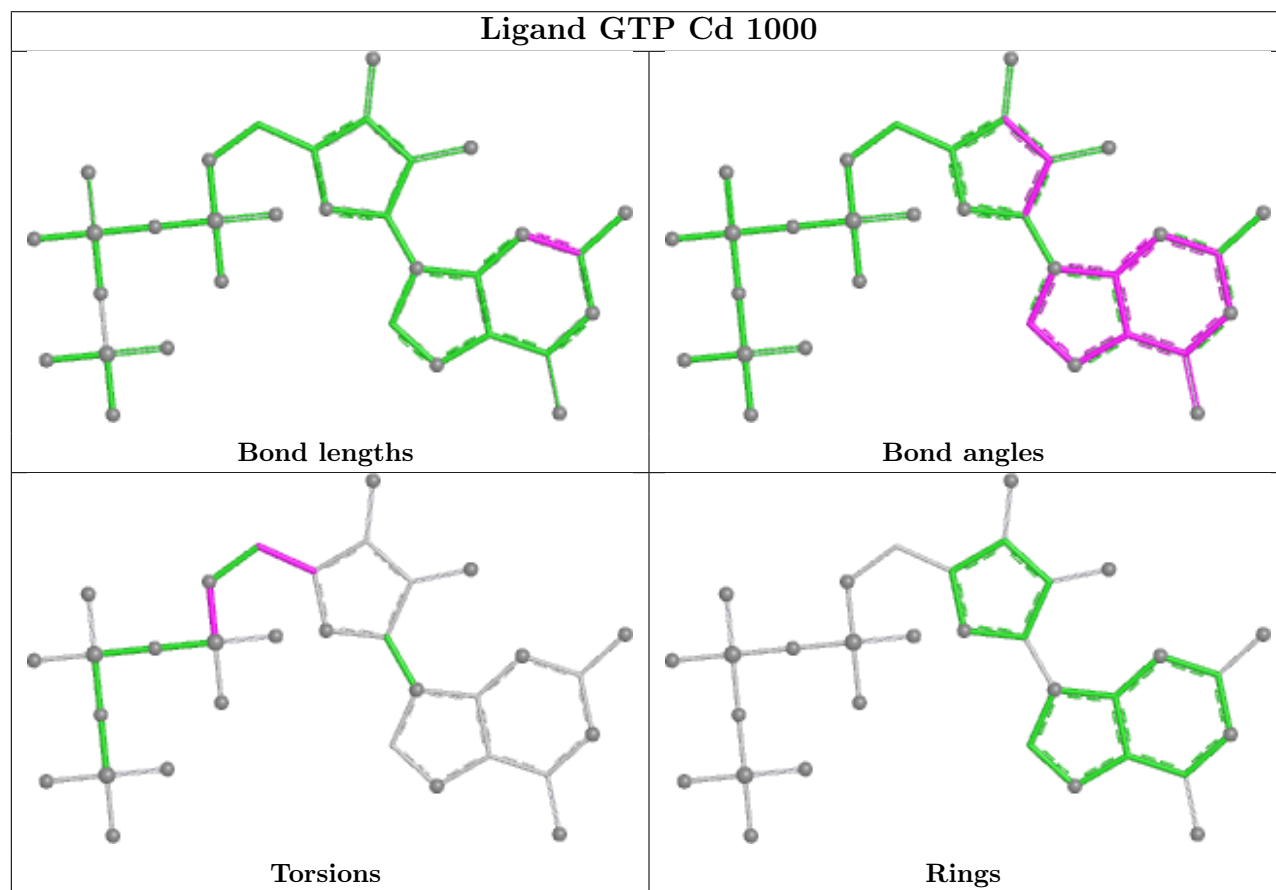
Mol	Chain	Res	Type	Atoms
62	CH	701	GTP	C5'-O5'-PA-O1A
62	CH	701	GTP	O4'-C4'-C5'-O5'
62	Cd	1000	GTP	C3'-C4'-C5'-O5'
62	Cd	1000	GTP	O4'-C4'-C5'-O5'
62	CH	701	GTP	PB-O3A-PA-O1A
62	Cd	1000	GTP	C5'-O5'-PA-O1A
62	CH	701	GTP	PB-O3A-PA-O2A

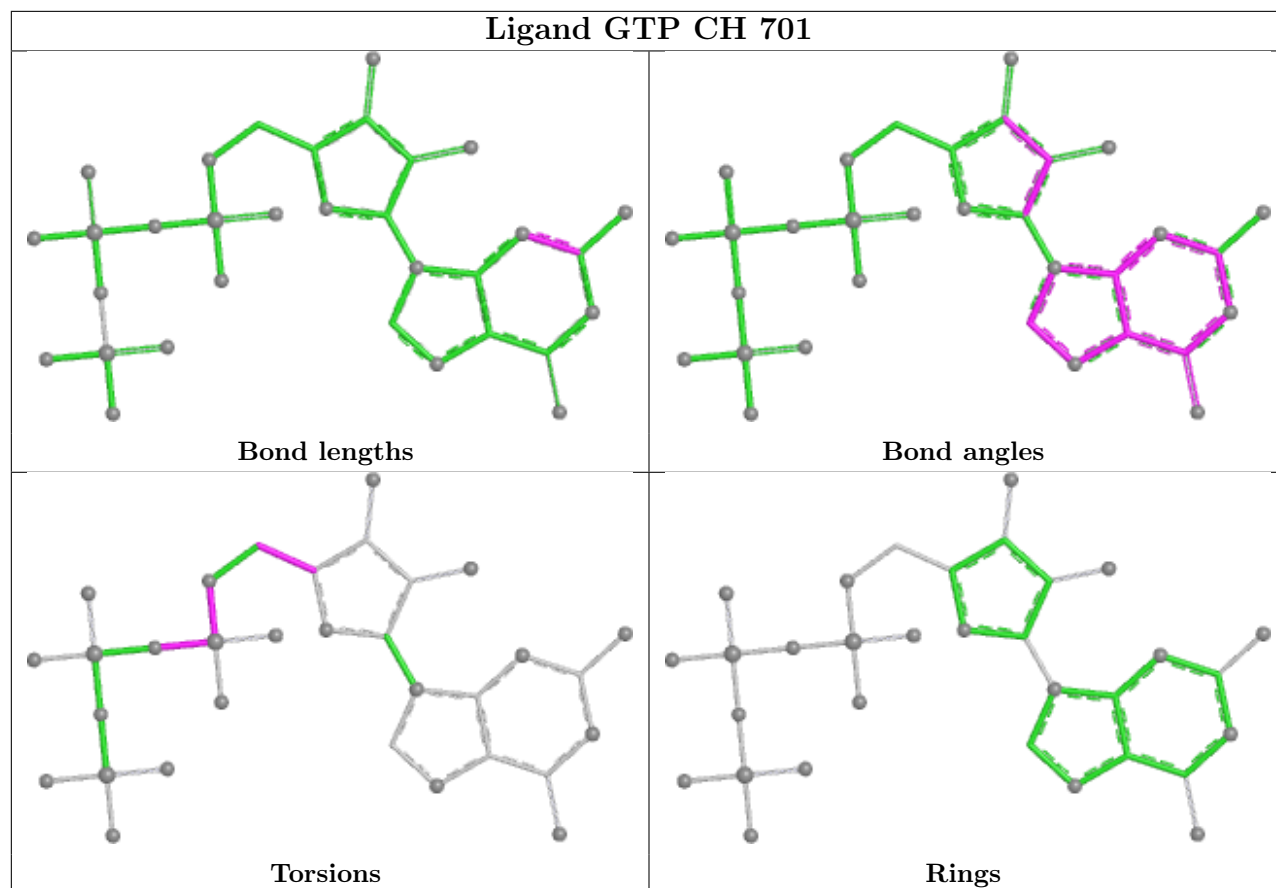
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	CH	701	GTP	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

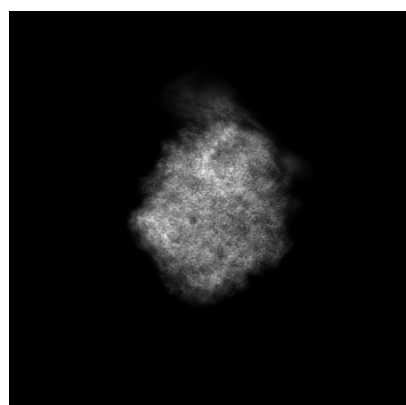
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17955. These allow visual inspection of the internal detail of the map and identification of artifacts.

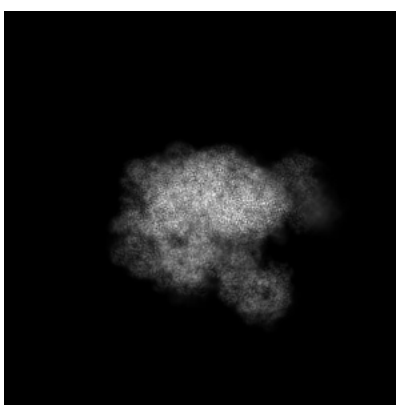
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

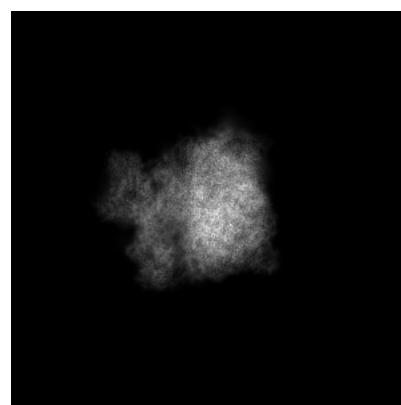
6.1.1 Primary map



X



Y

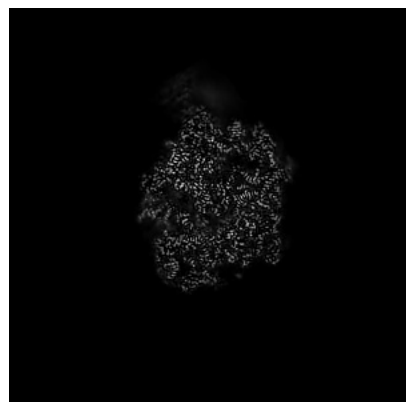


Z

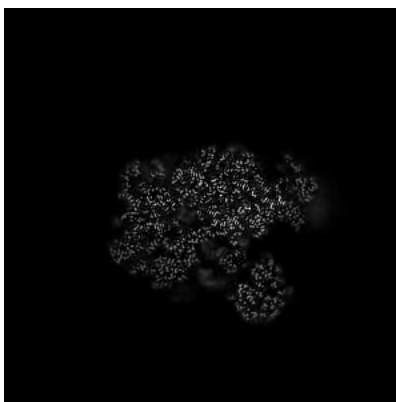
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

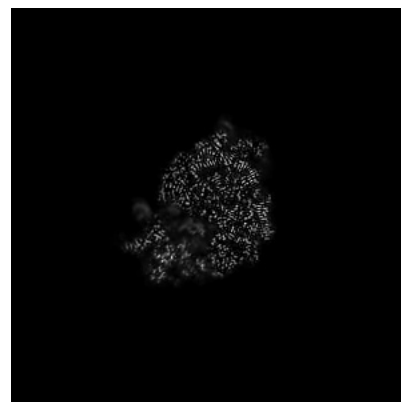
6.2.1 Primary map



X Index: 250



Y Index: 250

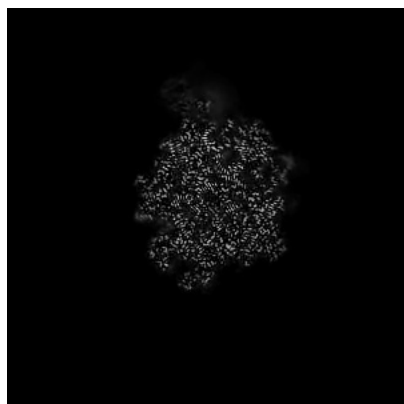


Z Index: 250

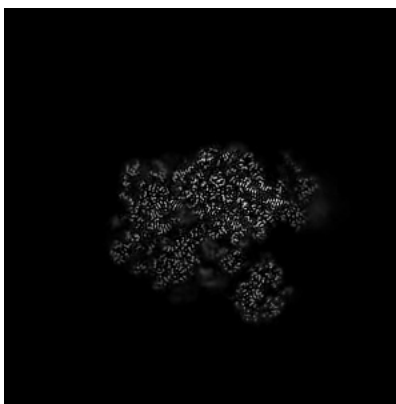
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

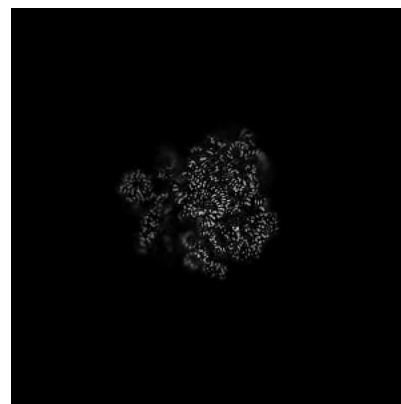
6.3.1 Primary map



X Index: 259



Y Index: 248

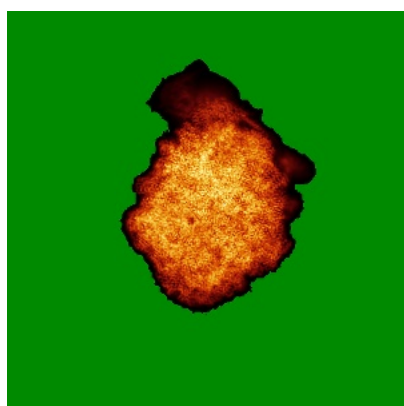


Z Index: 274

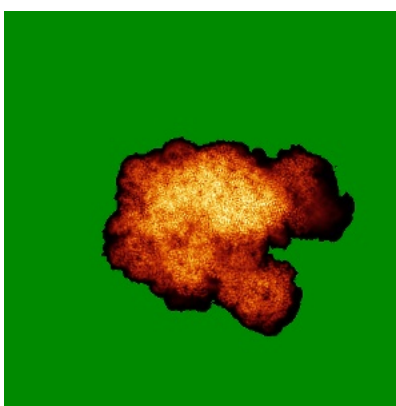
The images above show the largest variance slices of the map in three orthogonal directions.

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

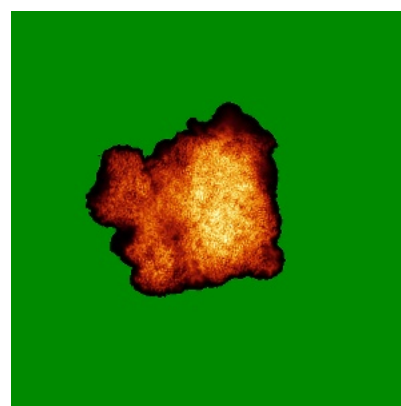
6.4.1 Primary map



X



Y



Z

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 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

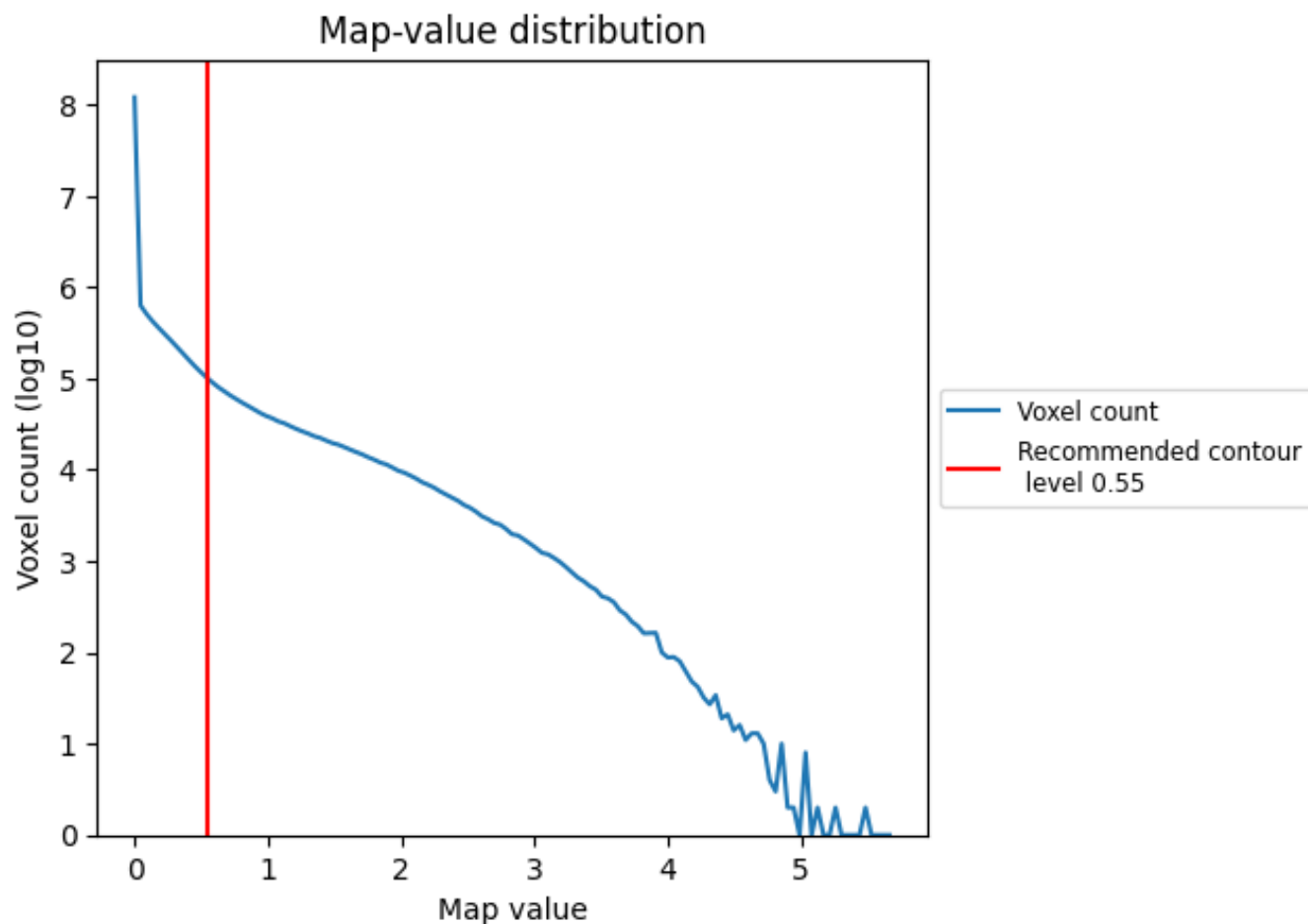
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

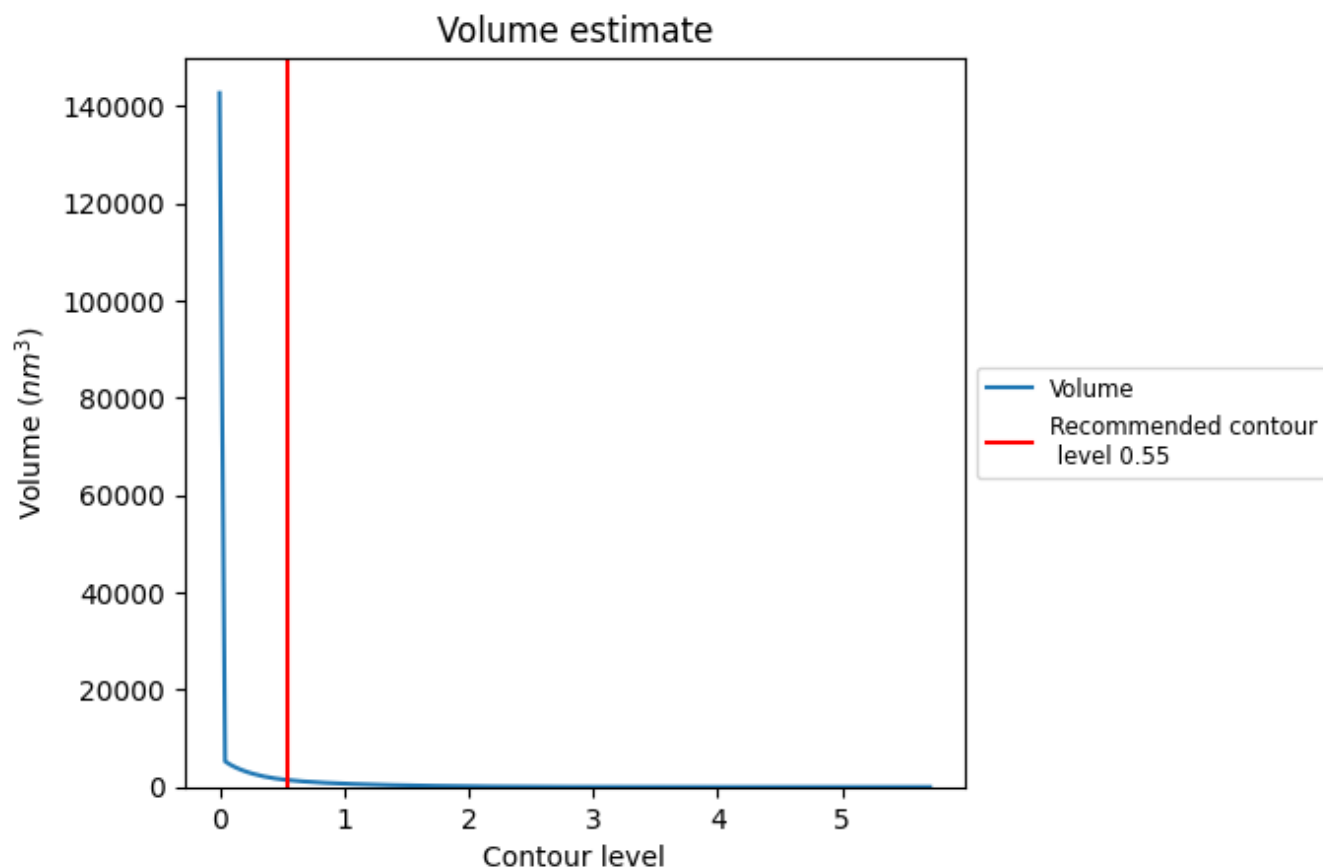
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

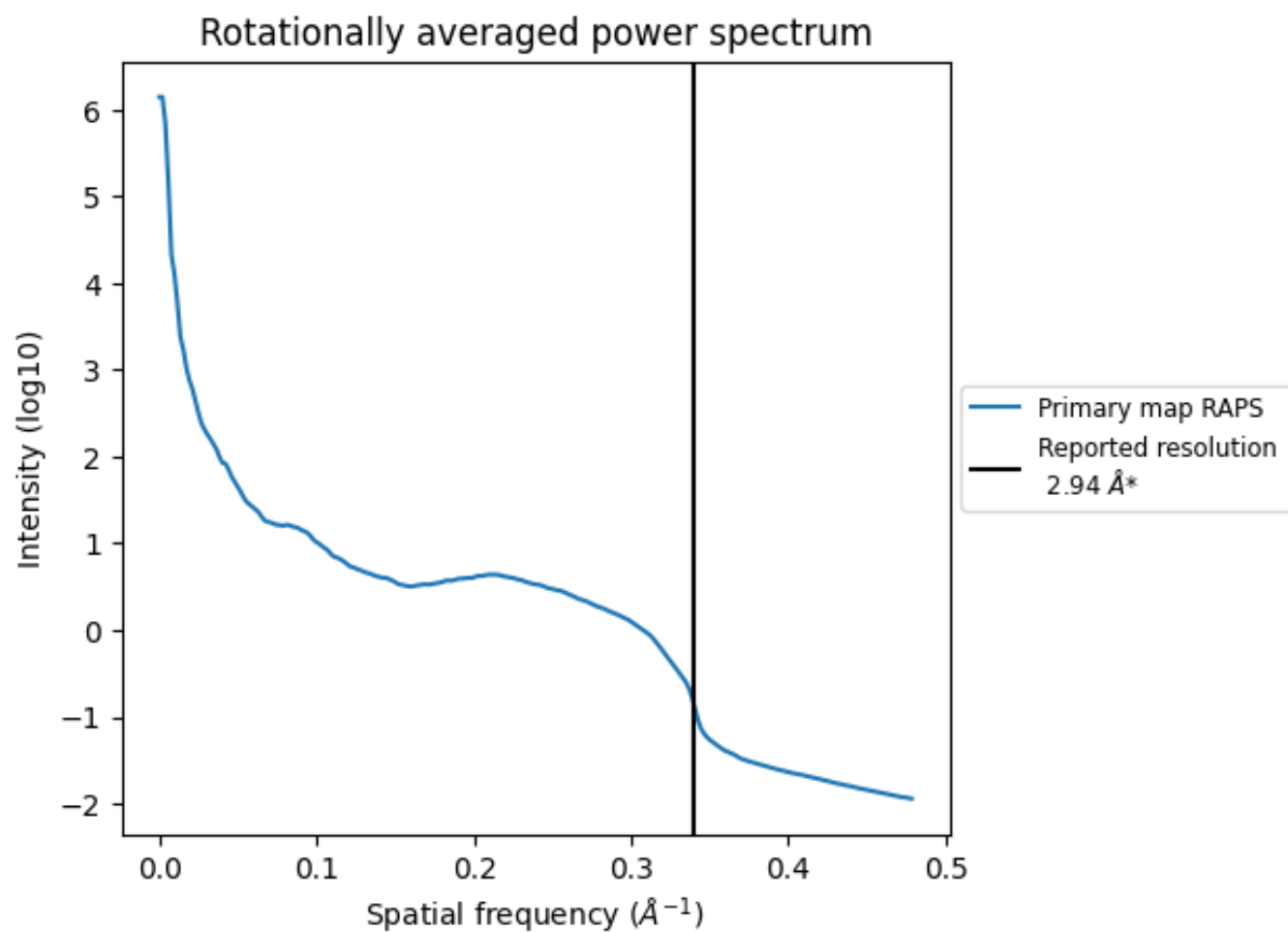
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1418 nm^3 ; this corresponds to an approximate mass of 1281 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 0.340 Å⁻¹

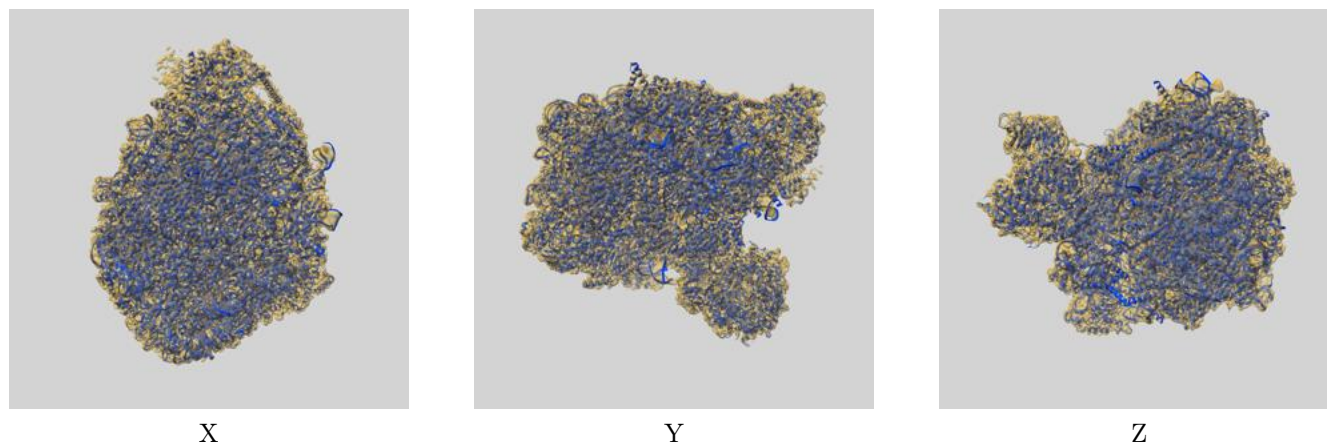
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

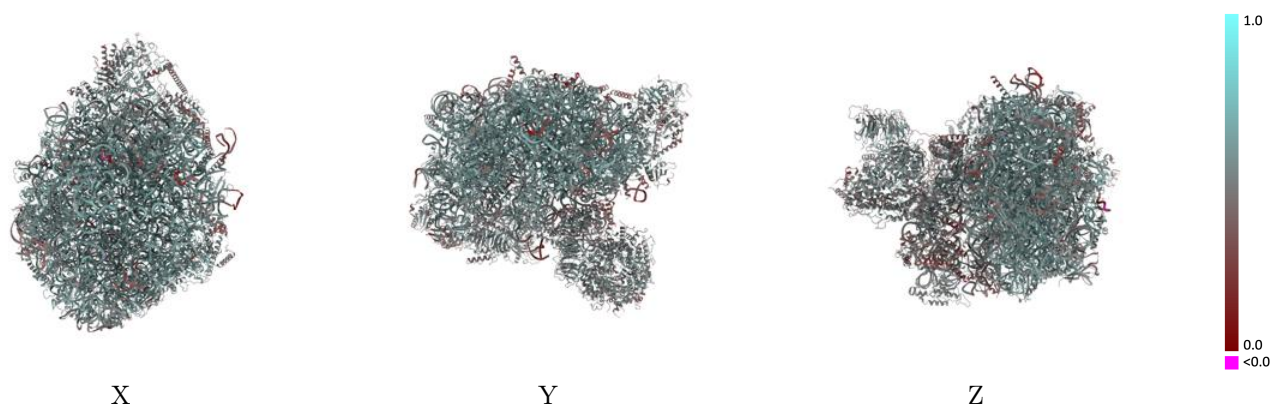
This section contains information regarding the fit between EMDB map EMD-17955 and PDB model 8PV6. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.55 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](#)

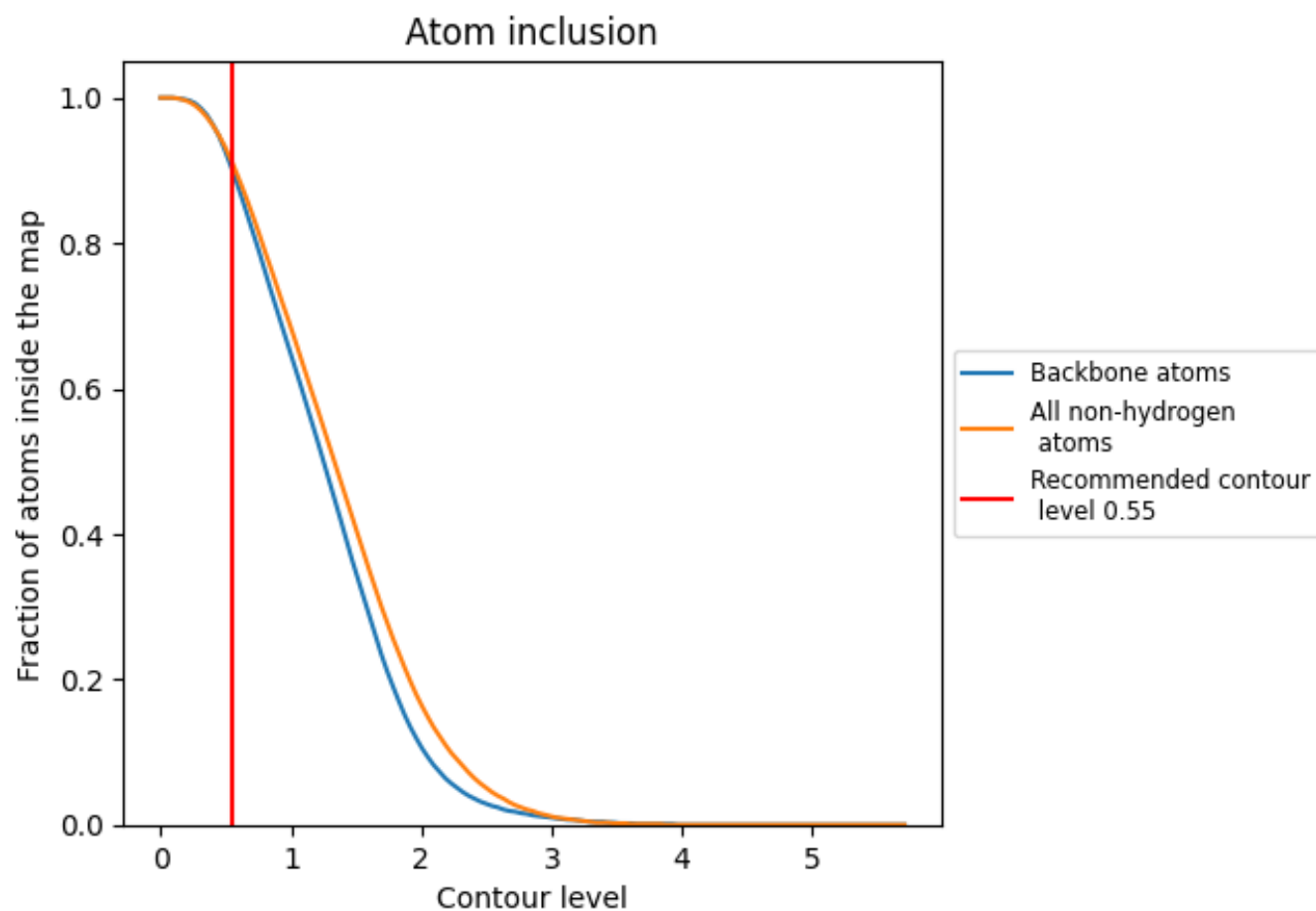


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9110	 0.5470
C1	 0.9730	 0.5650
C2	 0.9650	 0.5840
C3	 0.7830	 0.4850
C4	 0.9910	 0.5130
CF	 0.8150	 0.5010
CH	 0.8540	 0.5350
CI	 0.7360	 0.4770
CJ	 0.8890	 0.5370
CK	 0.9190	 0.5800
CL	 0.5890	 0.4240
CM	 0.7900	 0.4600
CN	 0.9200	 0.5660
CO	 0.8470	 0.5430
CQ	 0.8550	 0.5330
CR	 0.7820	 0.4910
CS	 0.6840	 0.4670
CT	 0.8430	 0.4930
CU	 0.8490	 0.5120
CV	 0.8310	 0.4910
CW	 0.8550	 0.4970
Cb	 0.9090	 0.5610
Cd	 0.8710	 0.5560
Ce	 0.7550	 0.4740
Ch	 0.8490	 0.5090
Cz	 0.7980	 0.4710
LA	 0.9700	 0.6120
LB	 0.9610	 0.6020
LC	 0.9410	 0.5920
LD	 0.8980	 0.4940
LE	 0.8840	 0.5500
LF	 0.9210	 0.5670
LG	 0.9160	 0.5630
LH	 0.8920	 0.5670
LJ	 0.9350	 0.5140



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Chain	Atom inclusion	Q-score
LK	 0.7190	 0.4370
LL	 0.9070	 0.5690
LM	 0.9040	 0.5690
LN	 0.9900	 0.6170
LO	 0.9480	 0.5970
LP	 0.9550	 0.5920
LQ	 0.9470	 0.5870
LR	 0.9320	 0.5800
LS	 0.9300	 0.5750
LT	 0.8690	 0.4840
LU	 0.8710	 0.5320
LV	 0.9550	 0.5910
LX	 0.9200	 0.5650
LY	 0.9140	 0.5690
LZ	 0.9310	 0.5550
La	 0.9280	 0.5810
Lb	 0.5310	 0.3630
Lc	 0.8850	 0.5530
Ld	 0.9190	 0.5820
Le	 0.9420	 0.5920
Lf	 0.9760	 0.6190
Lg	 0.9080	 0.5770
Lh	 0.8800	 0.5300
Li	 0.9350	 0.5590
Lj	 0.9780	 0.6190
Lk	 0.8410	 0.5310
Ll	 0.9810	 0.6210
Lp	 0.8880	 0.5630
Lq	 0.9410	 0.5790
Lr	 0.6770	 0.3720