



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:39 AM UTC

PDB ID : 8PVL / pdb\_00008pvl  
EMDB ID : EMD-17970  
Title : Chaetomium thermophilum pre-60S State 7 - pre-5S rotation lacking  
Utp30/ITS2 - composite structure  
Authors : Thoms, M.; Cheng, J.; Denk, T.; Berninghausen, O.; Beckmann, R.  
Deposited on : 2023-07-17  
Resolution : 2.19 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

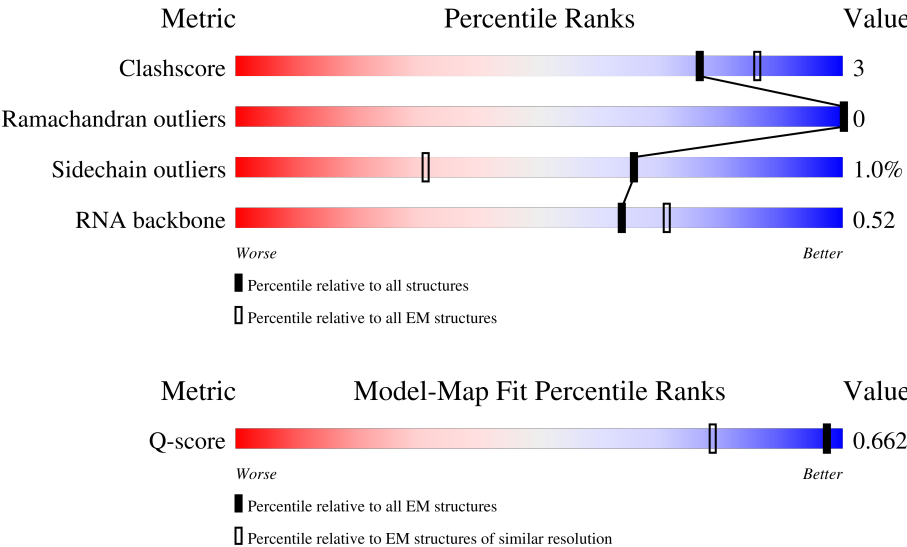
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

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

The reported resolution of this entry is 2.19 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.











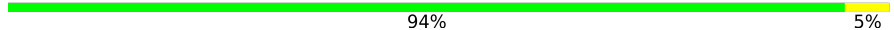


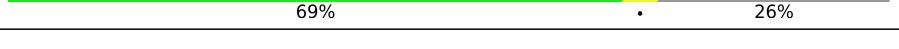


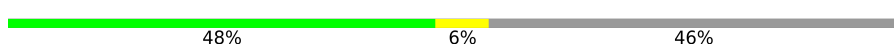





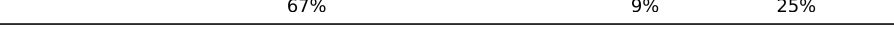
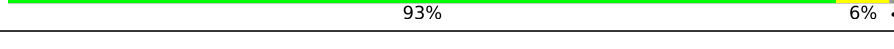
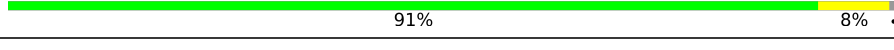
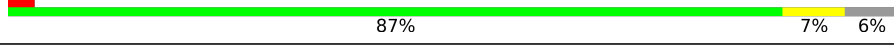

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2745 ( 1.70 - 2.69 )

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

Mol	Chain	Length	Quality of chain
1	C1	3342	<div> <div style="width: 64%; background-color: green;"></div> <div style="width: 25%; background-color: yellow;"></div> <div style="width: 8%; background-color: red;"></div> <div style="width: 3%; background-color: grey;"></div> </div>
2	C2	156	<div> <div style="width: 81%; background-color: green;"></div> <div style="width: 17%; background-color: yellow;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div>
3	C3	162	<div> <div style="width: 98%; background-color: grey;"></div> </div>

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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	Cb	117	
16	Cd	627	
17	Ce	443	
18	Cf	350	
19	Cg	202	
20	Ch	517	
21	Cz	123	
22	LA	254	
23	LB	392	
24	LC	365	
25	LD	304	
26	LE	200	
27	LG	262	






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Mol	Chain	Length	Quality of chain
28	LH	229	
29	LJ	173	
30	LK	165	
31	LL	213	
32	LM	142	
33	LN	203	
34	LO	204	
35	LP	187	
36	LQ	213	
37	LR	2898	
38	LS	174	
39	LT	160	
40	LU	127	
41	LV	139	
42	LX	156	
43	LY	138	
44	LZ	135	
45	La	149	
46	Lc	108	
47	Ld	120	
48	Le	131	
49	Lf	109	
50	Lg	119	
51	Lh	935	
52	Li	110	

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Mol	Chain	Length	Quality of chain
53	Lj	95	
54	Lk	94	
55	Ll	51	
56	Lp	92	
57	Lq	147	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	OMC	C1	1420	X	-	-	-
1	OMG	C1	1433	X	-	-	-
1	OMC	C1	1491	X	-	-	-
1	OMC	C1	1812	X	-	-	-
1	OMC	C1	1836	X	-	-	-
1	OMC	C1	2300	X	-	-	-
1	OMG	C1	2358	X	-	-	-
1	OMG	C1	2578	X	-	-	-
1	OMG	C1	2774	X	-	-	-
1	OMC	C1	2838	X	-	-	-
1	OMG	C1	2876	X	-	-	-
1	OMG	C1	2881	X	-	-	-
1	OMC	C1	2918	X	-	-	-
1	OMG	C1	385	X	-	-	-
1	OMG	C1	627	X	-	-	-
1	OMG	C1	646	X	-	-	-
1	OMC	C1	778	X	-	-	-
1	OMG	C1	787	X	-	-	-

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 152760 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	3078	Total	C	N	O	P	0	0
			65888	29429	11926	21455	3078		

- 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	119	Total	C	N	O	P	0	0
			2536	1131	453	833	119		

- 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
			5063	3181	924	939	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CI	91	Total	C	N	O	S	0	0
			720	467	130	120	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	237	Total	C	N	O	S	0	0
			1903	1198	368	333	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CL	79	Total	C	N	O	S	0	0
			622	389	125	108			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CM	216	Total	C	N	O	S	0	0
			1769	1142	328	296	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
			1853	1156	322	368	7		

- 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
			1480	925	304	241	10		

- Molecule 15 is a protein called Zinc finger domain-containing protein.

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

- Molecule 16 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Cd	462	Total	C	N	O	S	0	0
			3691	2350	671	659	11		

- Molecule 17 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Ce	239	Total	C	N	O	S	0	0
			1977	1231	378	364	4		

- Molecule 18 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Cf	285	Total	C	N	O	S	0	0
			2282	1443	417	401	21		

- Molecule 19 is a protein called Ribosome biogenesis regulatory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Cg	188	Total	C	N	O	S	0	0
			1478	924	283	270	1		

- Molecule 20 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Ch	485	Total	C	N	O	S	1	0
			3812	2396	696	710	10		

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 21 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Cz	101	Total	C	N	O	S	0	0
			869	541	180	144	4		

- Molecule 22 is a protein called 60S ribosomal protein L2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LA	191	Total	C	N	O	S	0	0
			1454	917	278	256	3		

- Molecule 23 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LB	389	Total	C	N	O	S	0	0
			3104	1973	579	539	13		

- Molecule 24 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LC	363	Total	C	N	O	S	0	0
			2751	1737	527	478	9		

- Molecule 25 is a protein called 60S ribosomal protein l5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LD	286	Total	C	N	O	S	0	0
			2266	1434	407	422	3		

- Molecule 26 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LE	191	Total	C	N	O	S	0	0
			1477	944	267	263	3		

- Molecule 27 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LG	235	Total	C	N	O	S	0	0
			1889	1210	350	324	5		

- Molecule 28 is a protein called 60S ribosomal protein l9-like protein.

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

- Molecule 29 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LJ	169	Total	C	N	O	S	0	0
			1357	850	266	235	6		

- Molecule 30 is a protein called 60S ribosomal protein L12-like protein.

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

- Molecule 31 is a protein called 60S ribosomal protein L13.

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

- Molecule 32 is a protein called 60S ribosomal protein L14-like protein.

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

- Molecule 33 is a protein called Ribosomal protein L15.

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

- Molecule 34 is a protein called 60S ribosomal protein L16-like protein.

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

- Molecule 35 is a protein called 60S ribosomal protein l17-like protein.

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

- Molecule 36 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LQ	150	Total	C	N	O	S	0	0
			1200	759	239	200	2		

- Molecule 37 is a protein called Ribosomal protein L19.

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

- Molecule 38 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LS	174	Total	C	N	O	S	0	0
			1426	917	266	238	5		

- Molecule 39 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LT	129	Total	C	N	O	S	0	0
			1027	651	195	179	2		

- Molecule 40 is a protein called 60S ribosomal protein L22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LU	105	Total	C	N	O	S	0	0
			846	548	146	151	1		

- Molecule 41 is a protein called 60S ribosomal protein l23-like protein.

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

- Molecule 42 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LX	145	Total	C	N	O	S	0	0
			1133	723	211	199			

- Molecule 43 is a protein called 60S ribosomal protein L26-like protein.

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

- Molecule 44 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LZ	135	Total	C	N	O	S	0	0
			1112	713	207	188	4		

- Molecule 45 is a protein called 60S ribosomal protein L28-like protein.

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

- Molecule 46 is a protein called 60S ribosomal protein l30-like protein.

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

- Molecule 47 is a protein called Putative 60S ribosomal protein.

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

- Molecule 48 is a protein called 60S ribosomal protein L32-like protein.

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

- Molecule 49 is a protein called 60S ribosomal protein l33-like protein.

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

- Molecule 50 is a protein called Ribosomal protein l34-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lg	118	Total	C	N	O	S	0	0
			914	567	186	157	4		

- Molecule 51 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

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

- Molecule 52 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Li	101	Total	C	N	O	S	0	0
			827	509	181	136	1		

- Molecule 53 is a protein called Ribosomal protein L37.

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

- Molecule 54 is a protein called 60S ribosomal protein L38-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Lk	76	Total	C	N	O	S	0	0
			632	400	121	109	2		

- Molecule 55 is a protein called Ribosomal protein eL39.

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

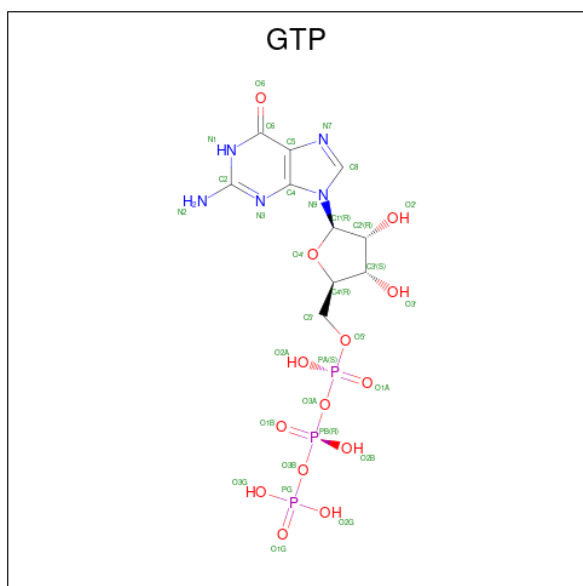
- Molecule 56 is a protein called 60S ribosomal protein L43-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Lp	91	Total	C	N	O	S	0	0
			698	430	138	124	6		

- Molecule 57 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	Lq	139	Total	C	N	O	0	0
			1073	672	213	188		

- Molecule 58 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	CQ	1	Total 1	Zn 1	0
60	Cb	1	Total 1	Zn 1	0
60	Lg	1	Total 1	Zn 1	0
60	Lj	1	Total 1	Zn 1	0
60	Lp	1	Total 1	Zn 1	0

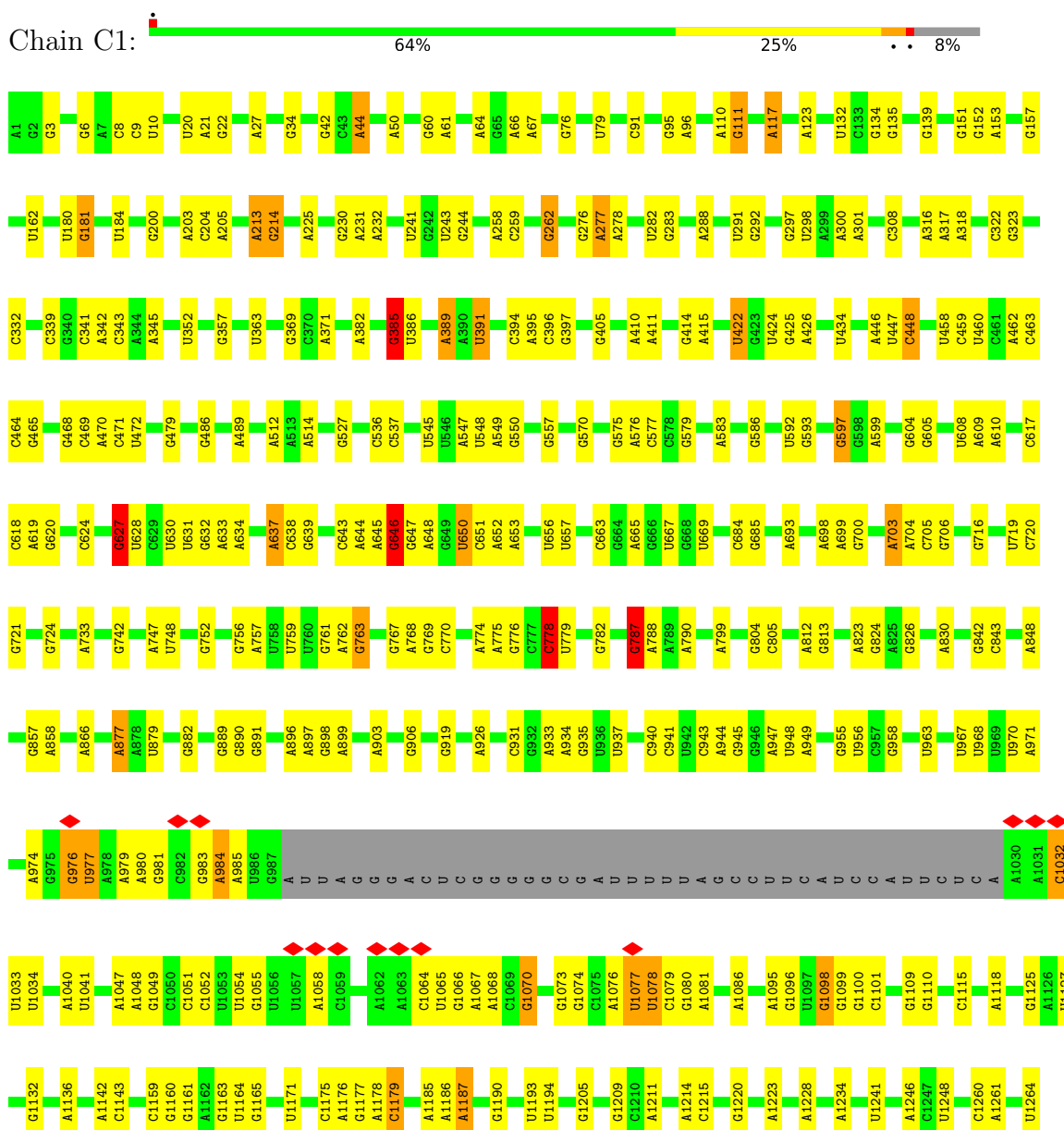
- Molecule 61 is water.

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

### 3 Residue-property plots

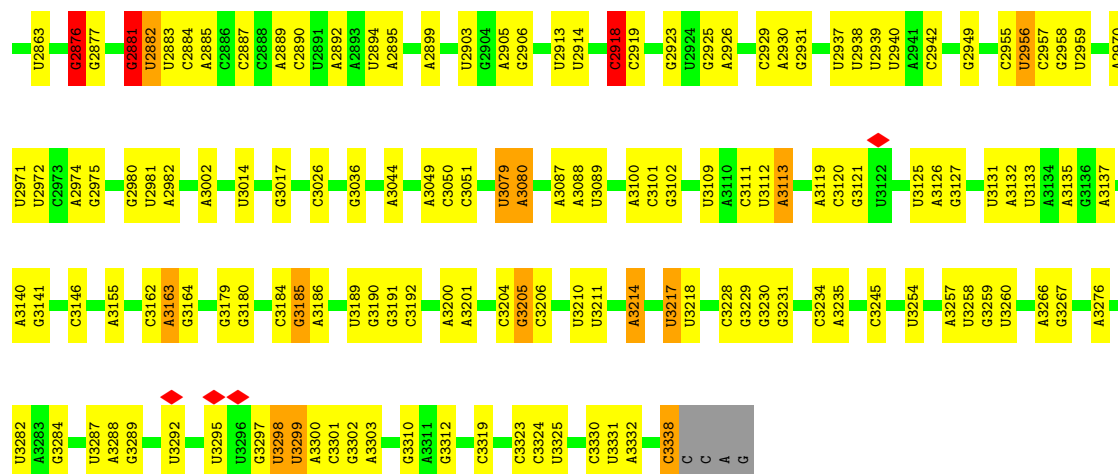
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

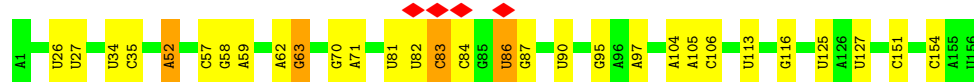
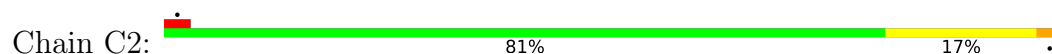




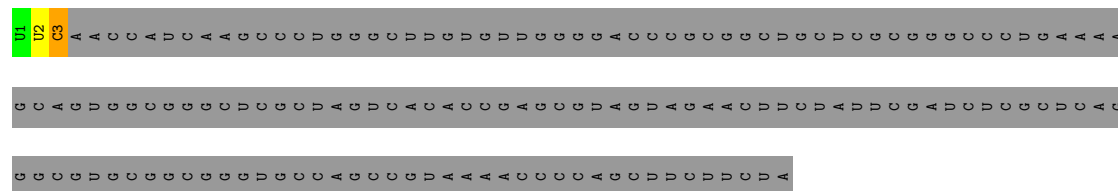




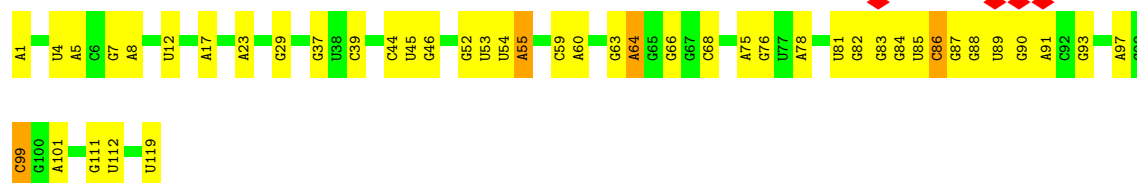
• Molecule 2: 5.8S rRNA



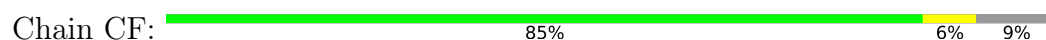
• Molecule 3: ITS2



• Molecule 4: 5S rRNA



• Molecule 5: Large ribosomal subunit protein uL10

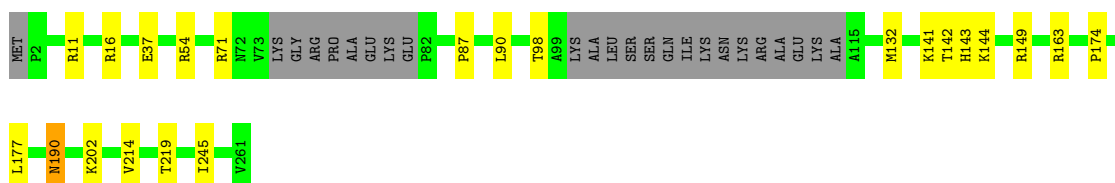


• Molecule 6: Nucleolar GTP-binding protein 1



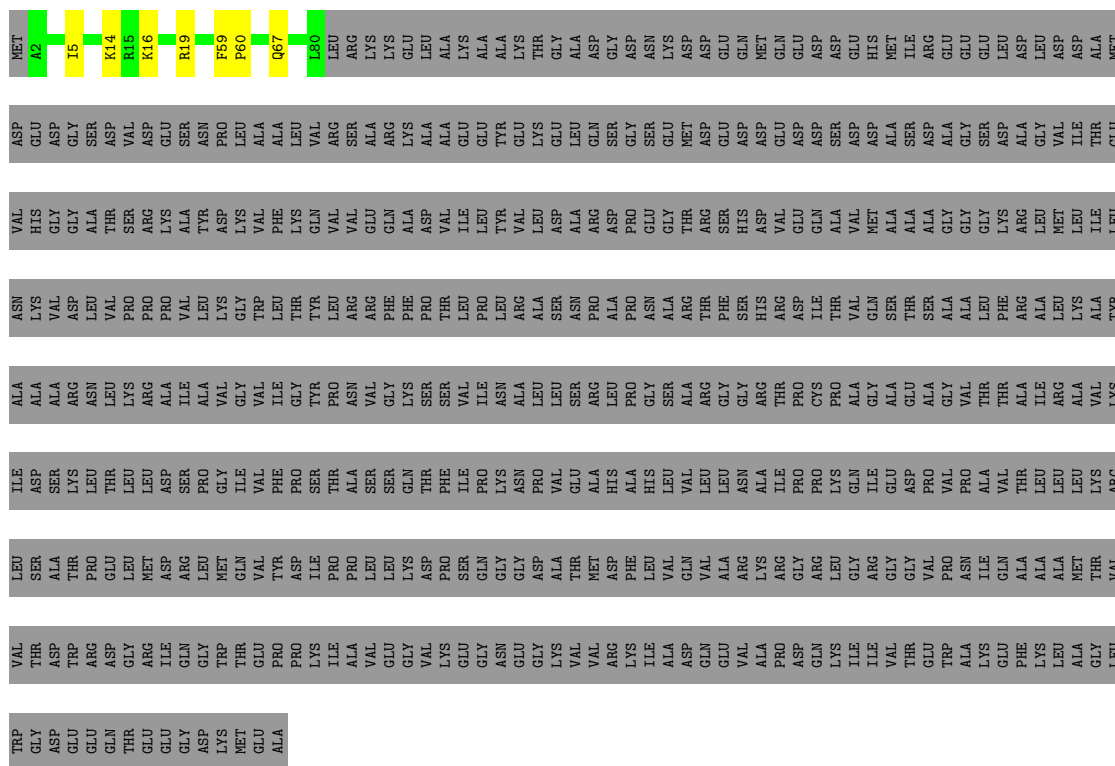
- Molecule 9: Ribosome biogenesis protein NSA2 homolog

Chain CK:  82% 8% 9%




- Molecule 10: Putative GTP binding protein

Chain CL:  13% . 86%



- Molecule 11: 60S ribosomal protein 17-like protein

Chain CM: 





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

Chain LF: 94% 5%



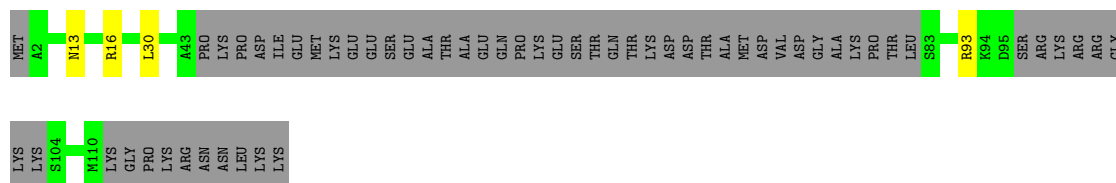
- Molecule 12: Eukaryotic translation initiation factor 6

Chain CN: 88% 12%



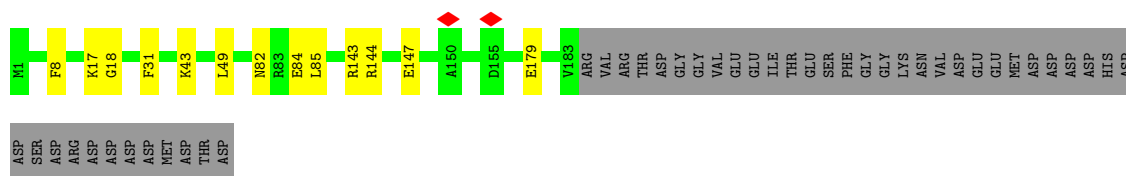
- Molecule 13: DUF2423 domain-containing protein

Chain CO: 48% . 48%



- Molecule 14: Ribosome biogenesis protein RLP24

Chain CQ: 76% 6% 19%



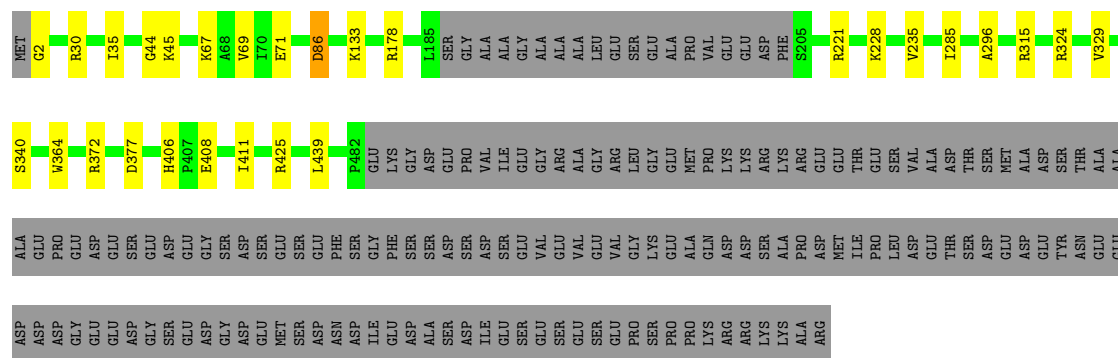
- Molecule 15: Zinc finger domain-containing protein

Chain Cb: 77% 9% . 14%



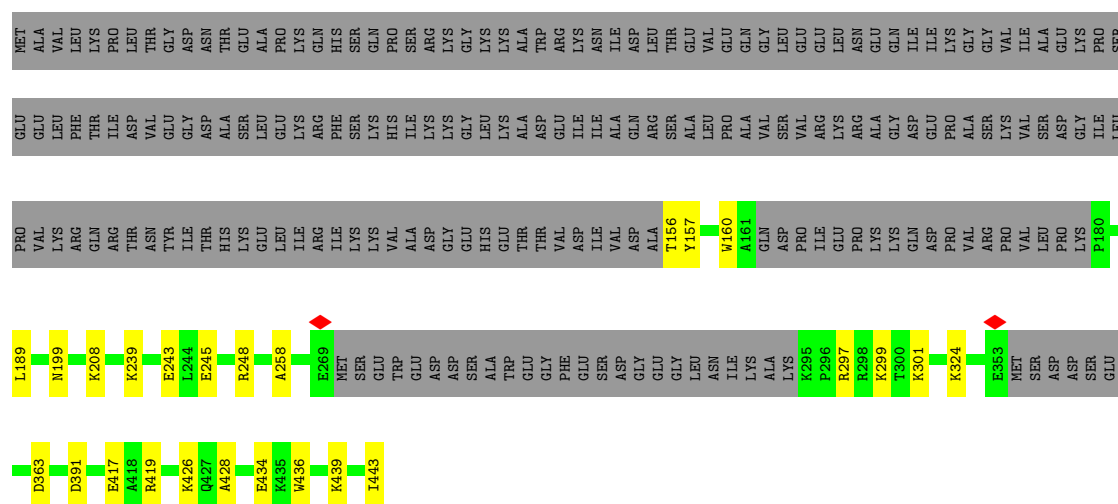
- Molecule 16: Nucleolar GTP-binding protein 2

Chain Cd: 69% . 26%



• Molecule 17: Ribosome biogenesis protein NOP53

Chain Ce: 48% 6% 46%



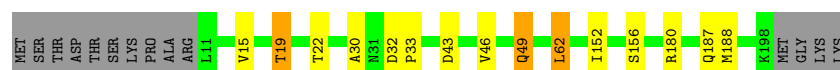
• Molecule 18: Ribosome production factor 2 homolog

Chain Cf: 72% 10% 19%



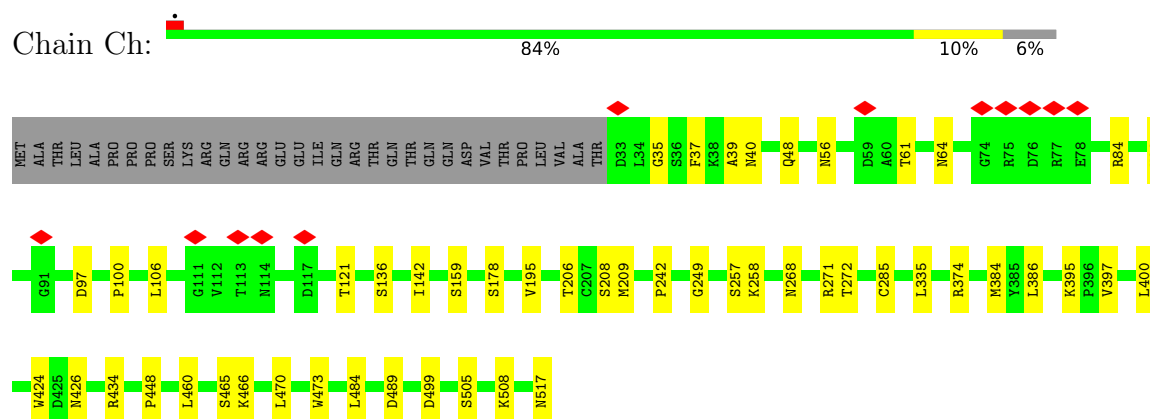
• Molecule 19: Ribosome biogenesis regulatory protein

Chain Cg: 86% 6% 7%



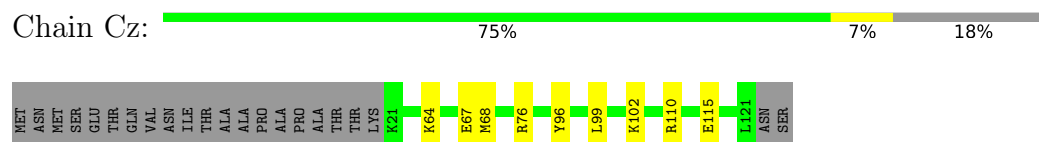
- Molecule 20: Ribosome assembly protein 4

Chain Ch:



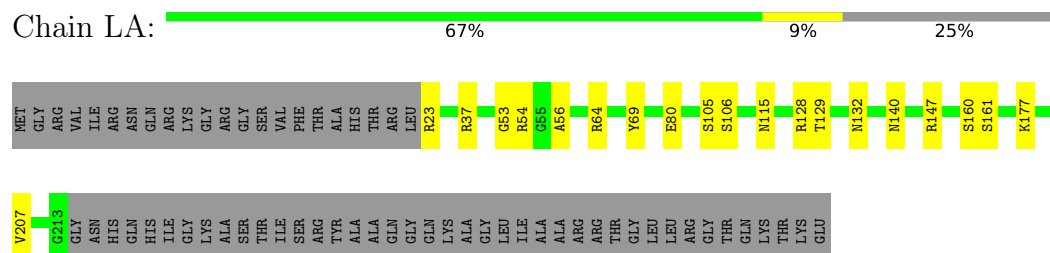
- Molecule 21: rRNA-processing protein

Chain Cz:



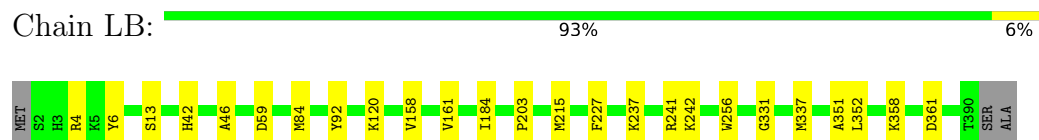
- Molecule 22: 60S ribosomal protein L2-like protein

Chain LA:



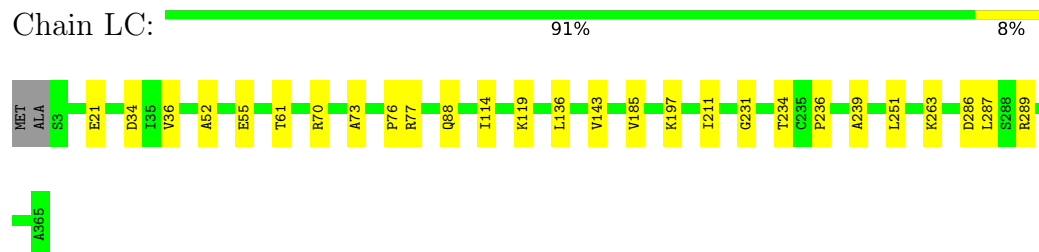
- Molecule 23: 60S ribosomal protein L3-like protein

Chain LB:



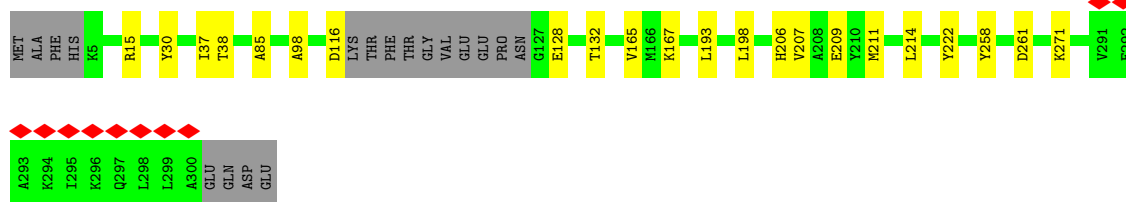
- Molecule 24: 60S ribosomal protein L4-like protein

Chain LC:




- Molecule 25: 60S ribosomal protein l5-like protein

Chain LD:  87% 7% 6%




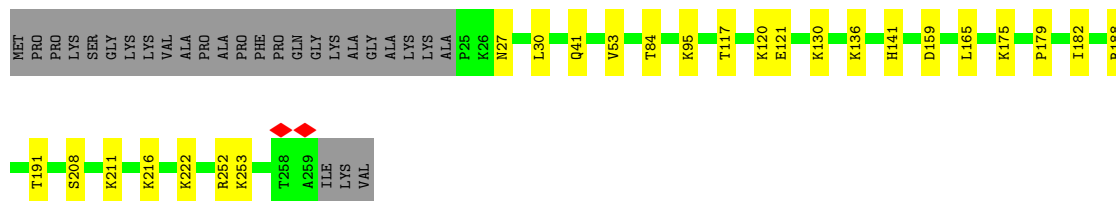
- Molecule 26: 60S ribosomal protein L6

Chain LE:  88% 8% .




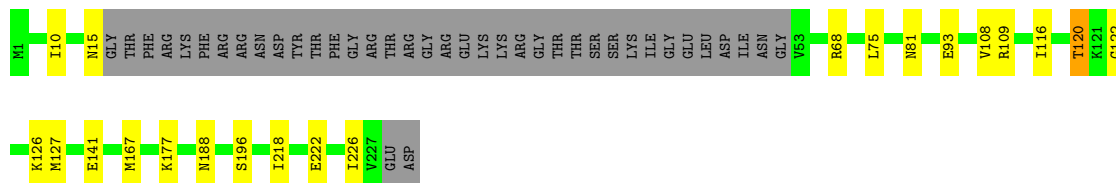
- Molecule 27: 60S ribosomal protein L8

Chain LG:  80% 10% 10%




- Molecule 28: 60S ribosomal protein 19-like protein

Chain LH:  74% 9% 17%



- Molecule 29: Putative ribosomal protein

Chain LJ:  84% 13% ..



- Molecule 30: 60S ribosomal protein L12-like protein

Chain LK:  88% 6% ..





95%

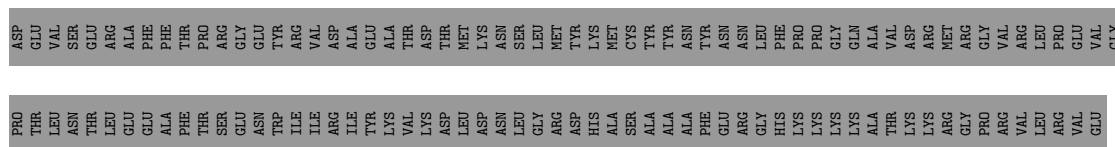




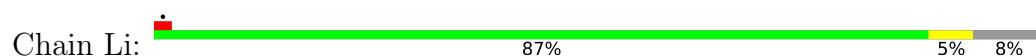


- MET V2 R17 P36 I39 M53 I56 V83 H89 I97 R106 V127 THR THR GLU VAL

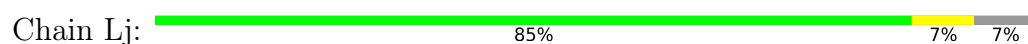




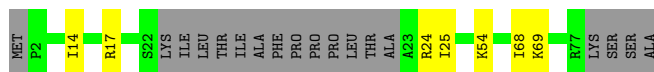
• Molecule 52: 60S ribosomal protein L36



• Molecule 53: Ribosomal protein L37



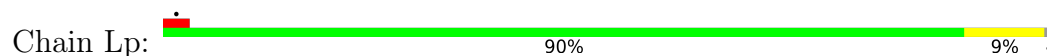
• Molecule 54: 60S ribosomal protein L38-like protein



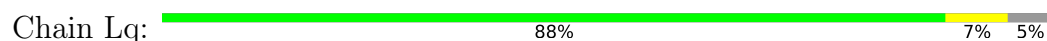
• Molecule 55: Ribosomal protein eL39



• Molecule 56: 60S ribosomal protein L43-like protein



• Molecule 57: Putative 60S ribosomal protein



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	276213	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 ( $e^-/\text{\AA}^2$ )	45.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	7.906	Depositor
Minimum map value	0.000	Depositor
Average map value	0.017	Depositor
Map value standard deviation	0.160	Depositor
Recommended contour level	0.5	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: OMG, ZN, OMC, GTP, A2M, OMU, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	C1	0.18	1/72882 (0.0%)	0.35	1/113631 (0.0%)
2	C2	0.17	0/3710	0.32	0/5778
3	C3	0.07	0/65	0.17	0/98
4	C4	0.17	0/2833	0.33	0/4414
5	CF	0.14	0/1972	0.32	0/2660
6	CH	0.18	0/5147	0.42	1/6926 (0.0%)
7	CI	0.17	0/740	0.49	0/1001
8	CJ	0.17	0/3196	0.34	0/4319
9	CK	0.16	0/1939	0.38	0/2608
10	CL	0.17	0/631	0.35	0/843
11	CM	0.20	0/1801	0.48	0/2412
11	LF	0.18	0/2061	0.39	0/2765
12	CN	0.17	0/1878	0.42	0/2555
13	CO	0.16	0/470	0.35	0/619
14	CQ	0.20	0/1504	0.42	0/2000
15	Cb	0.18	0/845	0.42	0/1128
16	Cd	0.15	0/3770	0.34	0/5082
17	Ce	0.17	0/2002	0.36	1/2662 (0.0%)
18	Cf	0.14	0/2326	0.33	0/3113
19	Cg	0.18	0/1508	0.44	1/2051 (0.0%)
20	Ch	0.17	0/3914	0.46	0/5319
21	Cz	0.23	0/877	0.47	0/1148
22	LA	0.15	0/1488	0.39	0/2009
23	LB	0.16	0/3172	0.41	0/4260
24	LC	0.15	0/2808	0.36	0/3785
25	LD	0.14	0/2308	0.33	0/3105
26	LE	0.16	0/1504	0.36	1/2027 (0.0%)
27	LG	0.16	0/1918	0.38	0/2565
28	LH	0.15	0/1515	0.38	0/2037
29	LJ	0.21	0/1379	0.54	4/1844 (0.2%)
30	LK	0.20	0/1198	0.47	0/1611
31	LL	0.16	0/1614	0.35	0/2168

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	LM	0.16	0/1145	0.35	0/1539
33	LN	0.16	0/1741	0.36	0/2332
34	LO	0.20	0/1645	0.44	1/2205 (0.0%)
35	LP	0.16	0/1364	0.39	0/1835
36	LQ	0.16	0/1218	0.39	0/1639
37	LR	0.15	0/1260	0.33	0/1683
38	LS	0.16	0/1461	0.37	0/1966
39	LT	0.21	0/1046	0.50	1/1409 (0.1%)
40	LU	0.18	0/859	0.42	0/1151
41	LV	0.14	0/1009	0.38	0/1357
42	LX	0.17	0/1151	0.43	0/1547
43	LY	0.16	0/1070	0.42	0/1432
44	LZ	0.17	0/1135	0.39	0/1519
45	La	0.14	0/892	0.32	0/1200
46	Lc	0.15	0/714	0.33	0/960
47	Ld	0.16	0/889	0.34	0/1192
48	Le	0.15	0/1035	0.37	0/1379
49	Lf	0.14	0/883	0.33	0/1187
50	Lg	0.17	0/927	0.38	0/1244
51	Lh	0.21	0/1014	0.44	0/1349
52	Li	0.15	0/834	0.36	0/1099
53	Lj	0.16	0/712	0.39	0/944
54	Lk	0.17	0/640	0.37	0/850
55	Ll	0.14	0/446	0.28	0/593
56	Lp	0.17	0/706	0.45	0/940
57	Lq	0.16	0/1091	0.39	0/1468
All	All	0.17	1/161862 (0.0%)	0.37	11/234562 (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
1	C1	36	0
6	CH	0	1
All	All	36	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	848	A2M	O3'-P	5.05	1.61	1.56

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	LO	197	GLU	CA-CB-CG	8.82	131.74	114.10
39	LT	125	PRO	CA-N-CD	-7.81	101.07	112.00
19	Cg	49	GLN	CA-CB-CG	7.78	129.65	114.10
29	LJ	40	GLN	CA-CB-CG	6.16	126.43	114.10
29	LJ	39	GLU	CA-C-N	-5.94	111.62	122.38
29	LJ	39	GLU	C-N-CA	-5.94	111.62	122.38
17	Ce	324	LYS	CB-CG-CD	5.55	124.06	111.30
1	C1	2160	C	C2'-C3'-O3'	5.19	117.29	109.50
26	LE	50	LYS	CB-CG-CD	5.15	123.14	111.30
29	LJ	166	GLN	CA-CB-CG	5.07	124.23	114.10
6	CH	298	ASP	N-CA-C	-5.05	101.95	109.42

All (36) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C1	385	OMG	C3',C4'
1	C1	627	OMG	C3',C4'
1	C1	646	OMG	C3',C4'
1	C1	778	OMC	C3',C4'
1	C1	787	OMG	C3',C4'
1	C1	1420	OMC	C3',C4'
1	C1	1433	OMG	C3',C4'
1	C1	1491	OMC	C3',C4'
1	C1	1812	OMC	C3',C4'
1	C1	1836	OMC	C3',C4'
1	C1	2300	OMC	C3',C4'
1	C1	2358	OMG	C3',C4'
1	C1	2578	OMG	C3',C4'
1	C1	2774	OMG	C3',C4'
1	C1	2838	OMC	C3',C4'
1	C1	2876	OMG	C3',C4'
1	C1	2881	OMG	C3',C4'
1	C1	2918	OMC	C3',C4'

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	CH	298	ASP	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C1	65888	0	33223	347	0
2	C2	3319	0	1678	12	0
3	C3	60	0	32	1	0
4	C4	2536	0	1286	20	0
5	CF	1934	0	1945	8	0
6	CH	5063	0	5157	47	0
7	CI	720	0	699	9	0
8	CJ	3116	0	3122	19	0
9	CK	1903	0	1990	16	0
10	CL	622	0	641	6	0
11	CM	1769	0	1876	10	0
11	LF	2023	0	2132	7	0
12	CN	1853	0	1852	17	0
13	CO	468	0	503	4	0
14	CQ	1480	0	1523	8	0
15	Cb	830	0	838	5	0
16	Cd	3691	0	3818	23	0
17	Ce	1977	0	2061	18	0
18	Cf	2282	0	2347	21	0
19	Cg	1478	0	1517	8	0
20	Ch	3812	0	3715	26	0
21	Cz	869	0	956	7	0
22	LA	1454	0	1490	14	0
23	LB	3104	0	3221	17	0
24	LC	2751	0	2875	19	0
25	LD	2266	0	2219	17	0
26	LE	1477	0	1567	8	0
27	LG	1889	0	2043	18	0
28	LH	1495	0	1573	12	0
29	LJ	1357	0	1385	15	0
30	LK	1184	0	1249	9	0
31	LL	1587	0	1655	11	0
32	LM	1126	0	1198	8	0
33	LN	1704	0	1767	11	0
34	LO	1611	0	1702	15	0
35	LP	1343	0	1369	11	0
36	LQ	1200	0	1296	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	LR	1241	0	1298	8	0
38	LS	1426	0	1481	14	0
39	LT	1027	0	1076	9	0
40	LU	846	0	883	8	0
41	LV	991	0	1044	7	0
42	LX	1133	0	1234	8	0
43	LY	1056	0	1143	14	0
44	LZ	1112	0	1181	13	0
45	La	872	0	903	4	0
46	Lc	705	0	751	6	0
47	Ld	875	0	918	6	0
48	Le	1017	0	1092	6	0
49	Lf	862	0	891	6	0
50	Lg	914	0	960	5	0
51	Lh	1003	0	1116	9	0
52	Li	827	0	906	4	0
53	Lj	698	0	726	7	0
54	Lk	632	0	693	4	0
55	Ll	436	0	473	3	0
56	Lp	698	0	737	4	0
57	Lq	1073	0	1130	6	0
58	CH	32	0	12	1	0
58	Cd	32	0	12	0	0
59	CH	1	0	0	0	0
59	Cd	2	0	0	0	0
60	CQ	1	0	0	0	0
60	Cb	1	0	0	0	0
60	Lg	1	0	0	0	0
60	Lj	1	0	0	0	0
60	Lp	1	0	0	0	0
61	CH	1	0	0	0	0
61	Cd	2	0	0	0	0
All	All	152760	0	120180	803	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 3.

All (803) 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:C1:2400:G:H1	1:C1:2473:U:H3	0.97	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:3289:G:H1	1:C1:3298:U:H3	1.19	0.90
30:LK:8:ASN:HD22	30:LK:8:ASN:N	1.73	0.86
1:C1:1054:U:H3	1:C1:1070:G:H1	0.89	0.83
44:LZ:81:PRO:HB2	46:Lc:65:MET:HE1	1.68	0.74
1:C1:2577:G:H4'	1:C1:2578:OMG:H5'	1.70	0.74
1:C1:1420:OMC:H5'	24:LC:73:ALA:HB2	1.68	0.73
9:CK:190:ASN:C	9:CK:190:ASN:HD22	1.97	0.72
1:C1:958:G:OP2	36:LQ:78:ARG:NH2	2.25	0.70
6:CH:549:ARG:NH2	40:LU:31:ASP:OD1	2.24	0.69
23:LB:331:GLY:HA3	23:LB:337:MET:HE1	1.74	0.69
1:C1:2648:A:OP1	25:LD:15:ARG:NH1	2.25	0.69
44:LZ:96:ASN:ND2	44:LZ:98:ASP:OD2	2.25	0.69
12:CN:118:HIS:HB3	12:CN:121:LEU:HD13	1.76	0.67
16:Cd:133:LYS:HE2	16:Cd:133:LYS:H	1.60	0.67
1:C1:557:G:OP2	24:LC:353:LYS:NZ	2.29	0.66
18:Cf:142:MET:HE1	18:Cf:165:ILE:HA	1.78	0.66
1:C1:949:A:H62	1:C1:1098:G:H8	1.44	0.65
16:Cd:285:ILE:HD11	16:Cd:296:ALA:HB2	1.78	0.65
20:Ch:489:ASP:HB3	20:Ch:508:LYS:HB3	1.78	0.65
4:C4:37:G:N7	21:Cz:110:ARG:NH2	2.45	0.64
57:Lq:31:ASP:HB3	57:Lq:34:ASN:HB2	1.80	0.64
44:LZ:49:PRO:HD3	44:LZ:67:ILE:HG12	1.80	0.63
1:C1:2899:A:H2'	23:LB:256:TRP:HB3	1.79	0.63
1:C1:2544:G:H5'	17:Ce:436:TRP:HE1	1.64	0.63
1:C1:1792:G:N7	44:LZ:63:LYS:NZ	2.41	0.63
1:C1:3109:U:H3	1:C1:3338:C:H42	1.46	0.63
1:C1:2164:G:H1	1:C1:2204:U:H3	1.47	0.63
43:LY:86:ARG:HB3	43:LY:96:ILE:HD11	1.80	0.62
41:LV:25:MET:HE1	41:LV:80:ILE:HG12	1.82	0.61
36:LQ:110:VAL:HG12	36:LQ:112:ALA:H	1.65	0.61
1:C1:643:C:H2'	1:C1:644:A:H8	1.66	0.61
1:C1:2197:G:HO2'	16:Cd:2:GLY:N	1.98	0.61
8:CJ:25:LYS:HE3	8:CJ:73:LEU:HD11	1.82	0.61
9:CK:163:ARG:HH22	16:Cd:228:LYS:HG2	1.65	0.61
1:C1:2474:A:O2'	27:LG:252:ARG:NH2	2.31	0.60
12:CN:109:VAL:HB	12:CN:149:GLY:HA2	1.82	0.60
1:C1:2789:G:H2'	1:C1:2790:G:C8	2.36	0.60
29:LJ:33:ARG:HD2	29:LJ:121:ILE:HA	1.82	0.60
1:C1:984:A:N1	1:C1:1033:U:O2'	2.35	0.60
1:C1:2221:U:H2'	1:C1:2222:A:H8	1.67	0.60
1:C1:2586:C:O2'	29:LJ:61:ARG:NH2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CH:242:LEU:O	6:CH:280:LYS:NZ	2.34	0.59
1:C1:259:C:OP1	33:LN:5:LYS:NZ	2.32	0.59
1:C1:2803:C:OP1	21:Cz:76:ARG:NH1	2.35	0.59
47:Ld:28:LEU:HD11	47:Ld:40:ALA:HB2	1.85	0.59
1:C1:2477:U:OP2	1:C1:2545:G:N2	2.33	0.59
51:Lh:15:LYS:O	51:Lh:66:LYS:NZ	2.35	0.59
1:C1:1619:C:OP2	50:Lg:75:ARG:NH1	2.29	0.59
20:Ch:470:LEU:HB2	20:Ch:484:LEU:HB2	1.84	0.59
24:LC:286:ASP:OD2	24:LC:289:ARG:NH2	2.36	0.59
1:C1:111:G:OP2	31:LL:73:ARG:NH2	2.35	0.58
1:C1:2838:OMC:H5	1:C1:2906:G:H1	1.50	0.58
4:C4:88:G:N2	4:C4:91:A:OP2	2.34	0.58
4:C4:99:C:H5'	18:Cf:96:ARG:HH12	1.66	0.58
44:LZ:14:ARG:NH2	50:Lg:84:ASN:OD1	2.36	0.58
1:C1:3284:G:H21	1:C1:3303:A:H2	1.51	0.58
20:Ch:61:THR:OG1	20:Ch:64:ASN:OD1	2.20	0.58
30:LK:8:ASN:N	30:LK:8:ASN:ND2	2.41	0.58
32:LM:59:LEU:O	38:LS:155:ARG:NH2	2.35	0.58
40:LU:77:ASP:OD1	40:LU:77:ASP:N	2.36	0.58
20:Ch:384:MET:HB2	20:Ch:400:LEU:HB2	1.85	0.58
22:LA:53:GLY:O	22:LA:192:LYS:NZ	2.37	0.58
22:LA:105:SER:HB3	22:LA:160:SER:HB3	1.86	0.58
1:C1:948:U:H2'	1:C1:949:A:H8	1.68	0.58
1:C1:1190:G:OP1	9:CK:54:ARG:NH2	2.37	0.57
1:C1:1491:OMC:OP1	35:LP:127:ARG:NH1	2.31	0.57
4:C4:39:C:H4'	29:LJ:45:THR:HG23	1.86	0.57
1:C1:1264:U:H2'	1:C1:1265:G:H8	1.69	0.57
1:C1:1737:G:OP1	40:LU:101:ARG:NH2	2.32	0.57
1:C1:64:A:H5''	33:LN:174:LEU:HD13	1.87	0.57
20:Ch:195:VAL:HG12	20:Ch:206:THR:HG22	1.86	0.57
17:Ce:417:GLU:OE2	17:Ce:419:ARG:NH1	2.37	0.57
20:Ch:35:GLY:O	20:Ch:56:ASN:ND2	2.38	0.57
1:C1:3:G:H1'	42:LX:36:LYS:HE3	1.87	0.57
23:LB:84:MET:O	23:LB:203:PRO:HA	2.04	0.57
28:LH:68:ARG:NH1	28:LH:188:ASN:OD1	2.38	0.57
34:LO:139:THR:HG22	34:LO:142:ARG:H	1.69	0.57
25:LD:37:ILE:HG13	25:LD:38:THR:HG23	1.88	0.56
4:C4:53:U:O2'	4:C4:55:A:N7	2.38	0.56
23:LB:92:TYR:HB2	23:LB:158:VAL:HB	1.87	0.56
18:Cf:142:MET:HE3	18:Cf:168:PHE:HB2	1.87	0.56
35:LP:125:GLN:HB3	35:LP:141:SER:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Lh:16:ASN:ND2	51:Lh:19:GLU:OE2	2.38	0.56
51:Lh:34:LEU:HB3	51:Lh:49:ILE:HG22	1.86	0.56
1:C1:1920:G:H21	1:C1:3303:A:H8	1.52	0.56
9:CK:202:LYS:NZ	16:Cd:71:GLU:OE1	2.39	0.56
16:Cd:364:TRP:HA	16:Cd:377:ASP:O	2.06	0.56
25:LD:214:LEU:HB3	25:LD:222:TYR:HB2	1.87	0.56
1:C1:2478:A:N1	1:C1:2553:C:N4	2.54	0.56
17:Ce:258:ALA:HB2	44:LZ:123:SER:HB2	1.88	0.56
29:LJ:112:ASP:OD1	29:LJ:112:ASP:N	2.37	0.56
1:C1:2796:A:O2'	1:C1:2810:A:N6	2.39	0.56
26:LE:86:PRO:HB3	26:LE:166:ASP:HB2	1.88	0.56
6:CH:540:ASP:OD1	14:CQ:143:ARG:NH1	2.39	0.55
18:Cf:113:MET:HB2	18:Cf:261:ARG:HB3	1.89	0.55
1:C1:1431:U:H2'	1:C1:1432:A2M:H8	1.87	0.55
6:CH:264:LYS:HE2	6:CH:264:LYS:H	1.71	0.55
17:Ce:245:GLU:OE1	17:Ce:248:ARG:NH1	2.39	0.55
1:C1:1812:OMC:OP1	42:LX:133:LYS:NZ	2.29	0.55
6:CH:582:SER:OG	6:CH:583:ALA:N	2.38	0.55
6:CH:357:ILE:HG23	6:CH:361:LEU:HD23	1.89	0.55
19:Cg:30:ALA:HB2	19:Cg:62:LEU:HG	1.89	0.55
19:Cg:43:ASP:HB3	19:Cg:46:VAL:HG12	1.88	0.55
40:LU:58:ASP:O	40:LU:61:LYS:NZ	2.40	0.55
56:Lp:51:ALA:HB3	56:Lp:54:ILE:HD12	1.89	0.54
7:CI:246:ARG:NH2	17:Ce:443:ILE:OXT	2.40	0.54
27:LG:208:SER:HA	27:LG:211:LYS:HG3	1.88	0.54
1:C1:1041:U:OP2	11:LF:104:LYS:NZ	2.40	0.54
12:CN:32:GLU:OE1	12:CN:50:ARG:NH1	2.41	0.54
32:LM:44:PRO:HG3	32:LM:81:VAL:HG12	1.90	0.54
2:C2:86:U:O2	53:Lj:87:ARG:NH1	2.40	0.54
6:CH:586:ARG:HE	42:LX:156:VAL:HB	1.71	0.54
1:C1:1403:C:OP2	24:LC:197:LYS:NZ	2.40	0.54
1:C1:277:A:N1	1:C1:2744:A:O2'	2.40	0.54
20:Ch:178:SER:O	25:LD:167:LYS:NZ	2.41	0.54
37:LR:98:ARG:NH1	37:LR:130:ASN:OD1	2.34	0.54
1:C1:34:G:OP1	33:LN:73:ARG:NE	2.41	0.54
1:C1:639:G:O2'	1:C1:1418:A:OP1	2.26	0.54
8:CJ:128:ARG:HD3	17:Ce:160:TRP:H	1.73	0.54
1:C1:716:G:H5''	36:LQ:71:PRO:HB2	1.90	0.53
1:C1:2860:G:O2'	1:C1:2982:A:N1	2.41	0.53
6:CH:628:ASN:O	35:LP:125:GLN:NE2	2.40	0.53
29:LJ:11:ARG:NH2	29:LJ:152:SER:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1779:A:H2'	1:C1:1780:A:C8	2.43	0.53
1:C1:643:C:H2'	1:C1:644:A:C8	2.43	0.53
1:C1:842:G:H8	22:LA:183:SER:HB3	1.72	0.53
1:C1:1095:A:H2'	1:C1:1096:G:C8	2.43	0.53
1:C1:1685:U:O2	1:C1:1766:G:O2'	2.27	0.53
16:Cd:324:ARG:O	16:Cd:372:ARG:NH2	2.40	0.53
1:C1:42:G:H21	1:C1:2571:U:H4'	1.73	0.53
6:CH:388:LYS:HE2	6:CH:388:LYS:H	1.73	0.53
18:Cf:30:CYS:HA	18:Cf:86:LEU:O	2.08	0.53
1:C1:976:G:H4'	1:C1:977:U:H5'	1.91	0.53
1:C1:2308:A:H5''	47:Ld:32:THR:HG23	1.91	0.53
1:C1:8:C:OP1	8:CJ:93:ARG:NH1	2.41	0.53
2:C2:26:U:O2'	24:LC:52:ALA:O	2.26	0.53
6:CH:223:ILE:HG23	6:CH:231:MET:HE1	1.91	0.53
1:C1:1879:G:O2'	1:C1:2297:U:O4	2.26	0.52
2:C2:83:C:N3	43:LY:50:ARG:NH2	2.50	0.52
30:LK:28:LEU:HD12	30:LK:31:LYS:HE3	1.91	0.52
1:C1:1054:U:O4	1:C1:1070:G:O6	2.27	0.52
1:C1:2510:C:O2'	27:LG:41:GLN:OE1	2.27	0.52
7:Cl:191:ILE:HA	7:Cl:259:THR:O	2.09	0.52
28:LH:126:LYS:HB2	28:LH:222:GLU:HB3	1.91	0.52
39:LT:52:MET:HE2	39:LT:55:LYS:HD3	1.90	0.52
44:LZ:69:PRO:HG3	44:LZ:114:LYS:HB2	1.91	0.52
1:C1:1599:A:OP2	8:CJ:52:LYS:NZ	2.40	0.52
1:C1:2892:A:OP2	41:LV:6:ARG:NH1	2.42	0.52
24:LC:236:PRO:HG2	24:LC:239:ALA:HB3	1.91	0.52
8:CJ:400:VAL:HG21	11:CM:192:HIS:HA	1.91	0.52
22:LA:177:LYS:HB2	56:Lp:29:GLN:HG2	1.92	0.52
1:C1:448:C:H41	26:LE:15:ARG:HH21	1.56	0.52
1:C1:277:A:N7	45:La:59:ARG:NH2	2.58	0.52
14:CQ:43:LYS:NZ	15:Cb:18:ASP:OD1	2.36	0.52
28:LH:167:MET:HE3	28:LH:196:SER:HB3	1.91	0.52
6:CH:72:ASP:OD1	16:Cd:178:ARG:NH2	2.42	0.52
9:CK:132:MET:HE1	9:CK:214:VAL:HG11	1.92	0.52
18:Cf:187:VAL:HG22	18:Cf:227:LEU:HD23	1.92	0.52
27:LG:27:ASN:HB3	27:LG:30:LEU:HG	1.91	0.52
35:LP:126:ARG:HA	35:LP:140:MET:HG2	1.92	0.52
1:C1:1758:G:O2'	1:C1:1760:G:OP2	2.26	0.52
6:CH:641:HIS:HB2	35:LP:136:ILE:HD12	1.92	0.52
57:Lq:9:ILE:HG22	57:Lq:47:VAL:HG22	1.90	0.52
1:C1:44:A:H5'	33:LN:83:LYS:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2092:U:H2'	1:C1:2093:G:C8	2.45	0.51
1:C1:1641:G:H2'	1:C1:1642:G:C8	2.46	0.51
1:C1:2112:A:N6	1:C1:2150:G:O2'	2.42	0.51
44:LZ:114:LYS:NZ	44:LZ:118:GLU:OE2	2.36	0.51
22:LA:115:ASN:OD1	22:LA:128:ARG:NH1	2.42	0.51
23:LB:161:VAL:HG13	23:LB:184:ILE:HD11	1.92	0.51
57:Lq:10:TRP:O	57:Lq:14:ARG:HB3	2.11	0.51
20:Ch:271:ARG:NH1	20:Ch:272:THR:O	2.44	0.51
48:Le:36:PRO:HD2	48:Le:53:MET:HE3	1.92	0.51
1:C1:2516:G:N1	50:Lg:97:GLU:OE1	2.41	0.51
7:CI:188:VAL:HG22	7:CI:234:GLU:HB2	1.91	0.51
39:LT:155:ALA:O	39:LT:158:THR:OG1	2.23	0.51
1:C1:2767:A:N6	1:C1:2913:U:O2'	2.39	0.51
32:LM:94:TRP:O	32:LM:97:THR:OG1	2.24	0.51
46:Lc:44:LEU:HD23	46:Lc:95:ILE:HD12	1.93	0.51
1:C1:300:A:H2'	1:C1:301:A:C8	2.46	0.50
1:C1:604:G:H2'	1:C1:605:G:C8	2.46	0.50
1:C1:1463:G:O2'	1:C1:1851:U:O4	2.27	0.50
1:C1:1186:A:H62	1:C1:1283:G:H21	1.59	0.50
5:CF:240:GLY:O	5:CF:245:LYS:NZ	2.40	0.50
17:Ce:434:GLU:HB3	17:Ce:439:LYS:HE3	1.93	0.50
22:LA:23:ARG:HH21	22:LA:53:GLY:HA3	1.76	0.50
32:LM:54:ARG:NH2	32:LM:76:ALA:O	2.38	0.50
1:C1:391:U:H5'	35:LP:3:ARG:HD3	1.92	0.50
1:C1:2320:A:H2'	1:C1:2321:A:H8	1.77	0.50
17:Ce:156:THR:OG1	17:Ce:157:TYR:N	2.41	0.50
23:LB:215:MET:HE2	23:LB:351:ALA:HB2	1.94	0.50
1:C1:352:U:OP1	53:Lj:11:ARG:NH2	2.45	0.50
5:CF:94:ARG:HD2	5:CF:245:LYS:HD3	1.93	0.50
11:LF:114:LEU:HD21	11:LF:121:VAL:HG22	1.93	0.50
1:C1:20:U:H2'	1:C1:21:A:C8	2.46	0.50
1:C1:1160:G:OP2	34:LO:96:ARG:NH2	2.44	0.50
1:C1:1676:A:H2'	1:C1:1677:A:C8	2.46	0.50
8:CJ:75:GLU:HG3	8:CJ:77:LEU:H	1.75	0.50
23:LB:4:ARG:NH1	23:LB:6:TYR:O	2.44	0.50
23:LB:46:ALA:HA	23:LB:84:MET:HE1	1.94	0.50
24:LC:36:VAL:HG21	24:LC:251:LEU:HD21	1.93	0.50
29:LJ:15:ILE:HD12	29:LJ:78:GLU:HG2	1.93	0.50
6:CH:183:VAL:HG21	6:CH:219:ASP:HB2	1.94	0.50
8:CJ:113:PRO:HB3	8:CJ:164:MET:HE3	1.93	0.50
1:C1:91:C:OP1	45:La:59:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:CM:14:VAL:HG12	11:CM:17:THR:H	1.77	0.50
18:Cf:165:ILE:O	18:Cf:169:ARG:HB2	2.11	0.50
1:C1:1842:U:OP1	37:LR:70:ARG:NH2	2.37	0.50
26:LE:94:LEU:HD22	26:LE:122:VAL:HG11	1.93	0.50
29:LJ:38:LEU:HD13	29:LJ:70:VAL:HG23	1.94	0.50
31:LL:115:ARG:NH2	31:LL:155:PHE:O	2.35	0.50
49:Lf:16:LEU:HD11	49:Lf:33:LYS:HB2	1.94	0.50
51:Lh:6:LYS:HG2	51:Lh:51:ASP:HB3	1.94	0.50
1:C1:967:U:H2'	1:C1:968:U:H6	1.76	0.49
1:C1:2327:G:H22	1:C1:2359:G:H1'	1.77	0.49
2:C2:71:A:O2'	2:C2:83:C:N4	2.44	0.49
27:LG:188:ARG:O	27:LG:191:THR:OG1	2.30	0.49
38:LS:100:VAL:O	38:LS:104:GLU:HG3	2.12	0.49
54:Lk:25:ILE:HG13	54:Lk:68:ILE:HD11	1.94	0.49
1:C1:2405:G:H1	1:C1:2468:U:H3	1.59	0.49
6:CH:455:ASP:N	6:CH:455:ASP:OD1	2.44	0.49
11:CM:102:PRO:HB2	11:CM:105:PRO:HD2	1.93	0.49
1:C1:1491:OMC:H5'	1:C1:2317:C:H1'	1.95	0.49
6:CH:186:VAL:HG23	6:CH:187:THR:HG23	1.94	0.49
36:LQ:126:MET:O	36:LQ:146:GLY:HA3	2.13	0.49
1:C1:813:G:O2'	1:C1:1844:A:N3	2.40	0.49
1:C1:1766:G:H2'	1:C1:1767:A:C8	2.47	0.49
8:CJ:36:LEU:HD11	8:CJ:75:GLU:HG2	1.95	0.49
18:Cf:145:ALA:HB3	18:Cf:188:THR:HG22	1.94	0.49
31:LL:191:ASP:OD1	31:LL:198:ARG:NH1	2.39	0.49
54:Lk:14:ILE:HA	54:Lk:17:ARG:HD3	1.94	0.49
9:CK:219:THR:HB	9:CK:245:ILE:HD12	1.95	0.49
27:LG:136:LYS:HD2	27:LG:141:HIS:HE1	1.78	0.49
28:LH:10:ILE:HG12	28:LH:109:ARG:HG2	1.95	0.49
1:C1:575:G:H2'	1:C1:576:A:H8	1.78	0.49
1:C1:768:A:H4'	1:C1:769:G:H5'	1.95	0.49
14:CQ:18:GLY:HA3	14:CQ:31:PHE:O	2.13	0.49
33:LN:159:ARG:HB3	33:LN:164:LEU:HB2	1.94	0.49
1:C1:1077:U:O2'	1:C1:1078:U:O2	2.27	0.49
1:C1:1638:G:H2'	1:C1:1639:A:C8	2.48	0.49
1:C1:2219:A:N6	1:C1:2221:U:OP1	2.46	0.49
6:CH:497:GLU:HA	47:Ld:107:LYS:HD2	1.95	0.49
1:C1:2330:A:H2'	1:C1:2331:A:C8	2.47	0.48
18:Cf:47:ASN:OD1	18:Cf:59:ARG:NH1	2.41	0.48
24:LC:211:ILE:HB	24:LC:234:THR:HG22	1.94	0.48
1:C1:162:U:O3'	31:LL:135:LYS:NZ	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CH:250:LEU:HD11	6:CH:334:VAL:HG11	1.95	0.48
12:CN:117:ILE:HB	12:CN:121:LEU:HD22	1.96	0.48
28:LH:15:ASN:OD1	28:LH:15:ASN:N	2.44	0.48
6:CH:395:LYS:H	6:CH:395:LYS:HZ3	1.61	0.48
7:CI:220:ARG:HG2	7:CI:227:SER:HA	1.96	0.48
18:Cf:179:GLU:OE1	25:LD:132:THR:OG1	2.28	0.48
41:LV:47:ARG:HH21	41:LV:48:LEU:HB3	1.78	0.48
44:LZ:22:VAL:HG12	44:LZ:44:GLY:HA3	1.96	0.48
1:C1:967:U:H2'	1:C1:968:U:C6	2.48	0.48
1:C1:2103:U:OP2	6:CH:657:LYS:NZ	2.42	0.48
1:C1:2176:A:H2'	1:C1:2177:A:C8	2.49	0.48
1:C1:2615:A:N6	1:C1:2672:U:O2'	2.45	0.48
20:Ch:465:SER:OG	20:Ch:466:LYS:N	2.46	0.48
26:LE:199:LYS:O	32:LM:117:ARG:NH2	2.46	0.48
38:LS:3:ARG:NH1	38:LS:3:ARG:HA	2.28	0.48
1:C1:489:A:O2'	1:C1:3214:A:N1	2.40	0.48
1:C1:1661:U:OP1	6:CH:509:ARG:NH1	2.47	0.48
1:C1:2489:C:OP1	22:LA:37:ARG:NH1	2.46	0.48
1:C1:3120:C:H2'	1:C1:3121:G:H8	1.78	0.48
4:C4:23:A:N3	4:C4:119:U:O2'	2.44	0.48
6:CH:361:LEU:O	6:CH:365:MET:HG2	2.13	0.48
1:C1:117:A:OP2	33:LN:2:GLY:N	2.47	0.48
1:C1:3026:C:OP2	37:LR:62:ARG:NH2	2.44	0.48
1:C1:3289:G:O6	1:C1:3298:U:O4	2.31	0.48
6:CH:587:LEU:HD22	42:LX:146:LEU:HD13	1.95	0.48
17:Ce:363:ASP:OD1	17:Ce:363:ASP:N	2.37	0.48
27:LG:159:ASP:OD1	27:LG:159:ASP:N	2.47	0.48
1:C1:652:A:H2'	1:C1:653:A:C8	2.48	0.48
1:C1:2802:U:O2'	1:C1:2805:U:O4	2.27	0.48
6:CH:534:LEU:HD12	6:CH:546:LEU:HD11	1.96	0.48
22:LA:129:THR:OG1	22:LA:132:ASN:ND2	2.43	0.48
25:LD:85:ALA:HB2	25:LD:258:TYR:HB2	1.95	0.48
7:CI:269:HIS:HB3	7:CI:272:LEU:HB2	1.95	0.48
14:CQ:17:LYS:NZ	23:LB:361:ASP:OD2	2.46	0.48
27:LG:179:PRO:HG3	27:LG:222:LYS:HE3	1.96	0.48
1:C1:2400:G:O6	1:C1:2473:U:O4	2.32	0.48
4:C4:45:U:H2'	4:C4:46:G:H8	1.77	0.48
6:CH:453:ASP:OD2	6:CH:457:LYS:NZ	2.46	0.48
8:CJ:397:TRP:HB2	8:CJ:401:LEU:HD12	1.95	0.48
12:CN:116:LEU:HD12	12:CN:152:MET:HE1	1.96	0.48
33:LN:60:VAL:HG22	33:LN:134:LEU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:278:A:H8	1:C1:297:G:H1'	1.79	0.48
1:C1:1179:C:O3'	10:CL:16:LYS:NZ	2.46	0.48
38:LS:3:ARG:HA	38:LS:3:ARG:HH11	1.79	0.48
1:C1:1611:C:OP2	44:LZ:47:ARG:NH2	2.37	0.47
6:CH:2:THR:OG1	6:CH:3:GLY:N	2.46	0.47
8:CJ:489:PHE:HB3	17:Ce:208:LYS:HD3	1.96	0.47
12:CN:232:ALA:O	12:CN:237:MET:N	2.41	0.47
18:Cf:98:HIS:CD2	18:Cf:120:PRO:HG3	2.49	0.47
18:Cf:143:VAL:HB	18:Cf:186:VAL:HG22	1.96	0.47
27:LG:165:LEU:HA	33:LN:7:LEU:HD11	1.95	0.47
28:LH:75:LEU:HD13	28:LH:108:VAL:HG13	1.96	0.47
1:C1:656:U:H2'	1:C1:657:U:C6	2.49	0.47
1:C1:2956:U:H2'	1:C1:2957:C:C6	2.49	0.47
1:C1:2314:U:H2'	1:C1:2315:A:H8	1.79	0.47
6:CH:391:LYS:O	12:CN:43:GLN:NE2	2.35	0.47
14:CQ:179:GLU:OE1	47:Ld:86:ARG:NH1	2.45	0.47
29:LJ:94:ARG:O	29:LJ:157:ARG:NH2	2.46	0.47
31:LL:141:ASP:OD1	31:LL:141:ASP:N	2.40	0.47
1:C1:3137:A:OP1	34:LO:38:ARG:NH2	2.46	0.47
1:C1:76:G:H5'	31:LL:58:VAL:HB	1.96	0.47
20:Ch:88:HIS:HB2	20:Ch:121:THR:HB	1.96	0.47
1:C1:804:G:H2'	1:C1:805:C:H6	1.79	0.47
1:C1:2628:G:H2'	1:C1:2629:G:H8	1.80	0.47
19:Cg:152:ILE:HD13	39:LT:57:TYR:HB2	1.95	0.47
29:LJ:94:ARG:HG2	29:LJ:172:VAL:HG12	1.96	0.47
46:Lc:17:LEU:O	46:Lc:21:ILE:HG12	2.15	0.47
1:C1:644:A:H2'	1:C1:645:A:C8	2.50	0.47
1:C1:705:C:OP1	1:C1:733:A:O2'	2.30	0.47
1:C1:1901:A:H2'	1:C1:1902:A:C8	2.50	0.47
1:C1:2320:A:H2'	1:C1:2321:A:C8	2.50	0.47
20:Ch:374:ARG:NH2	20:Ch:434:ARG:O	2.47	0.47
28:LH:116:ILE:O	28:LH:120:THR:OG1	2.28	0.47
37:LR:105:LEU:HD23	37:LR:138:LEU:HD23	1.97	0.47
48:Le:97:ILE:HG21	48:Le:106:ARG:HG2	1.97	0.47
1:C1:262:G:H5''	33:LN:14:LYS:HE2	1.96	0.47
1:C1:619:A:H2'	1:C1:620:G:C8	2.50	0.47
1:C1:1177:G:H2'	1:C1:1178:A:C8	2.50	0.47
15:Cb:6:LYS:HG3	15:Cb:9:MET:HE2	1.97	0.47
34:LO:170:TYR:CE2	34:LO:174:LYS:HD2	2.50	0.47
1:C1:1929:G:OP2	37:LR:135:LYS:NZ	2.38	0.47
1:C1:2231:U:O4	18:Cf:298:ARG:NH1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2581:C:OP1	19:Cg:180:ARG:NH1	2.48	0.47
6:CH:307:ASP:HA	6:CH:310:LYS:HB2	1.97	0.47
17:Ce:199:ASN:OD1	17:Ce:199:ASN:N	2.43	0.47
25:LD:116:ASP:N	25:LD:116:ASP:OD1	2.44	0.47
1:C1:341:C:O2	1:C1:345:A:O2'	2.32	0.47
1:C1:2376:A:H2'	1:C1:2377:G:H8	1.80	0.47
24:LC:185:VAL:HG11	24:LC:231:GLY:HA3	1.96	0.47
30:LK:117:ARG:HD2	30:LK:117:ARG:HA	1.73	0.47
56:Lp:78:ALA:O	56:Lp:82:THR:HG23	2.15	0.47
1:C1:448:C:H42	1:C1:468:G:H1'	1.80	0.46
1:C1:1264:U:H2'	1:C1:1265:G:C8	2.50	0.46
6:CH:365:MET:HA	6:CH:368:ILE:HG12	1.97	0.46
18:Cf:103:VAL:HG22	18:Cf:113:MET:HG2	1.97	0.46
30:LK:11:LYS:HE3	30:LK:11:LYS:HB3	1.77	0.46
52:Li:70:LEU:HD13	52:Li:100:GLN:HG2	1.97	0.46
1:C1:1373:A:N6	1:C1:1401:A:O2'	2.49	0.46
34:LO:13:LYS:O	38:LS:169:ARG:NH2	2.42	0.46
1:C1:2157:G:O6	16:Cd:315:ARG:NH2	2.45	0.46
1:C1:2974:A:H2'	1:C1:2975:G:H8	1.79	0.46
4:C4:63:G:H2'	4:C4:64:A:C8	2.51	0.46
1:C1:282:U:H2'	1:C1:283:G:H8	1.80	0.46
1:C1:300:A:H2'	1:C1:301:A:H8	1.80	0.46
1:C1:1826:C:OP1	1:C1:1829:C:N4	2.42	0.46
1:C1:2882:U:OP2	16:Cd:221:ARG:NE	2.37	0.46
39:LT:110:LYS:HB2	39:LT:110:LYS:HE2	1.75	0.46
42:LX:63:SER:HB2	51:Lh:71:LEU:HD13	1.96	0.46
8:CJ:42:ILE:HD13	17:Ce:189:LEU:HD21	1.98	0.46
1:C1:1305:U:O2'	38:LS:1:MET:SD	2.72	0.46
11:LF:93:ILE:HG21	11:LF:248:MET:HE1	1.98	0.46
32:LM:127:ARG:O	32:LM:131:GLU:HG3	2.16	0.46
1:C1:230:G:H2'	1:C1:231:A:C8	2.51	0.46
1:C1:586:G:H1	1:C1:597:G:H5''	1.80	0.46
1:C1:742:G:O2'	1:C1:752:G:N2	2.40	0.46
1:C1:877:A:O2'	1:C1:879:U:OP2	2.33	0.46
8:CJ:393:LYS:HE3	8:CJ:393:LYS:HB2	1.80	0.46
34:LO:3:SER:OG	34:LO:5:GLU:OE2	2.34	0.46
1:C1:405:G:OP1	35:LP:62:ARG:NH1	2.49	0.46
1:C1:464:C:H2'	1:C1:465:G:H8	1.81	0.46
1:C1:1345:G:H2'	1:C1:1346:A:C8	2.51	0.46
1:C1:2518:G:OP1	22:LA:69:TYR:OH	2.34	0.46
10:CL:5:ILE:HD13	34:LO:49:PHE:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LF:182:TYR:CZ	11:LF:203:GLN:HG2	2.51	0.46
47:Ld:15:VAL:HA	47:Ld:85:ARG:O	2.15	0.46
1:C1:2534:G:H5'	17:Ce:426:LYS:HG3	1.97	0.46
8:CJ:380:ARG:NH1	8:CJ:401:LEU:O	2.44	0.46
20:Ch:37:PHE:HE2	20:Ch:39:ALA:HB2	1.81	0.46
1:C1:410:A:H2'	1:C1:411:A:C8	2.51	0.45
1:C1:804:G:H2'	1:C1:805:C:C6	2.51	0.45
1:C1:1187:A:N6	1:C1:2810:A:O4'	2.50	0.45
1:C1:1698:A:H4'	37:LR:117:LYS:HD2	1.97	0.45
12:CN:158:GLY:HA2	12:CN:179:VAL:HB	1.99	0.45
16:Cd:86:ASP:OD1	16:Cd:86:ASP:N	2.48	0.45
11:LF:92:VAL:O	11:LF:120:GLY:HA2	2.15	0.45
1:C1:630:U:H2'	1:C1:631:U:C2	2.51	0.45
16:Cd:235:VAL:O	16:Cd:329:VAL:HA	2.16	0.45
19:Cg:19:THR:HB	19:Cg:33:PRO:HG2	1.98	0.45
1:C1:1193:U:H5	5:CF:3:LYS:HB2	1.81	0.45
1:C1:2164:G:N2	1:C1:2204:U:O2	2.44	0.45
1:C1:2925:G:H2'	1:C1:2926:A:C8	2.51	0.45
1:C1:3189:U:OP2	13:CO:93:ARG:NH1	2.41	0.45
11:CM:173:ALA:O	11:CM:177:GLU:HG2	2.16	0.45
34:LO:115:ASP:OD1	34:LO:115:ASP:N	2.50	0.45
37:LR:89:MET:HE3	37:LR:90:PRO:HD2	1.98	0.45
44:LZ:50:SER:HB2	44:LZ:64:ARG:HB3	1.98	0.45
1:C1:1304:G:O3'	38:LS:117:ARG:NH1	2.50	0.45
12:CN:14:GLY:O	12:CN:61:ARG:NH1	2.50	0.45
21:Cz:96:TYR:OH	21:Cz:115:GLU:OE1	2.28	0.45
34:LO:26:LYS:HA	34:LO:26:LYS:HD2	1.75	0.45
1:C1:180:U:H1'	43:LY:128:VAL:HG11	1.98	0.45
9:CK:149:ARG:HH22	16:Cd:44:GLY:HA2	1.82	0.45
16:Cd:340:SER:OG	16:Cd:377:ASP:OD2	2.34	0.45
20:Ch:395:LYS:HE3	20:Ch:395:LYS:HB3	1.84	0.45
33:LN:145:ASP:HB3	33:LN:148:ILE:HG22	1.98	0.45
54:Lk:24:ARG:HA	54:Lk:69:LYS:O	2.16	0.45
1:C1:1214:A:H5''	1:C1:1215:C:H5'	1.99	0.45
1:C1:1887:C:O2	23:LB:241:ARG:NH2	2.49	0.45
9:CK:190:ASN:O	9:CK:190:ASN:ND2	2.49	0.45
20:Ch:242:PRO:HB3	20:Ch:335:LEU:HD22	1.98	0.45
1:C1:1361:U:H2'	1:C1:1362:G:H8	1.82	0.45
1:C1:3179:G:H2'	1:C1:3180:G:C8	2.51	0.45
1:C1:3299:U:H2'	1:C1:3300:A:H8	1.81	0.45
51:Lh:46:LEU:O	51:Lh:49:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1576:C:H2'	1:C1:1577:C:C6	2.52	0.45
1:C1:1783:C:H2'	1:C1:1784:G:H8	1.81	0.45
1:C1:3079:U:H1'	1:C1:3080:A:H5''	1.98	0.45
1:C1:3179:G:H2'	1:C1:3180:G:H8	1.82	0.45
8:CJ:377:GLU:OE1	8:CJ:422:ARG:NH2	2.50	0.45
10:CL:67:GLN:HG3	21:Cz:64:LYS:NZ	2.31	0.45
11:LF:74:ILE:HD12	11:LF:74:ILE:HA	1.85	0.45
1:C1:1142:A:OP1	36:LQ:31:GLY:N	2.49	0.45
5:CF:61:ASN:OD1	5:CF:61:ASN:N	2.50	0.45
6:CH:228:LEU:HA	6:CH:231:MET:HG3	1.99	0.45
7:CI:200:GLU:CD	7:CI:200:GLU:H	2.24	0.45
11:CM:155:TYR:OH	11:CM:188:GLU:OE1	2.32	0.45
18:Cf:290:ASP:OD1	18:Cf:294:ASP:N	2.50	0.45
1:C1:698:A:H2'	1:C1:699:A:C8	2.52	0.44
1:C1:1476:G:H2'	55:Ll:13:LEU:HD22	1.99	0.44
1:C1:1491:OMC:H5'	1:C1:2317:C:C1'	2.47	0.44
1:C1:1661:U:H5''	6:CH:510:LYS:HD3	1.99	0.44
4:C4:44:C:OP2	29:LJ:138:ARG:NH2	2.49	0.44
6:CH:300:GLU:OE1	6:CH:300:GLU:N	2.49	0.44
12:CN:210:THR:HG23	12:CN:214:GLU:HG3	1.98	0.44
1:C1:775:A:H2'	1:C1:776:G:H8	1.82	0.44
1:C1:1783:C:H2'	1:C1:1784:G:C8	2.52	0.44
8:CJ:189:PHE:HB3	8:CJ:196:TYR:HB2	2.00	0.44
29:LJ:32:THR:O	29:LJ:36:LYS:HG3	2.17	0.44
1:C1:1588:C:O2'	42:LX:92:GLN:NE2	2.36	0.44
1:C1:1866:A:O2'	23:LB:227:PHE:O	2.33	0.44
1:C1:2790:G:H2'	1:C1:2791:C:C6	2.52	0.44
4:C4:8:A:OP2	25:LD:30:TYR:OH	2.33	0.44
6:CH:131:ALA:O	6:CH:135:MET:HG3	2.18	0.44
20:Ch:40:ASN:OD1	20:Ch:48:GLN:NE2	2.49	0.44
1:C1:970:U:H2'	1:C1:971:A:H8	1.82	0.44
1:C1:1067:A:H2'	1:C1:1068:A:H8	1.82	0.44
1:C1:1449:G:N2	1:C1:1493:G:H5''	2.32	0.44
1:C1:1623:A:H5''	1:C1:1624:C:C5	2.53	0.44
1:C1:1624:C:H5'	1:C1:1625:U:H5''	1.98	0.44
1:C1:2769:C:OP2	1:C1:2914:U:O2'	2.36	0.44
8:CJ:42:ILE:HG13	8:CJ:72:LEU:HD11	2.00	0.44
11:CM:107:LYS:O	11:CM:111:LEU:HD22	2.17	0.44
27:LG:117:THR:O	27:LG:121:GLU:HG3	2.17	0.44
31:LL:114:GLN:NE2	31:LL:118:ASP:OD1	2.51	0.44
47:Ld:39:ARG:O	47:Ld:43:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:231:A:H2'	1:C1:232:A:C8	2.53	0.44
1:C1:1698:A:H2'	1:C1:1699:G:C8	2.52	0.44
26:LE:38:LYS:HA	26:LE:38:LYS:HD3	1.87	0.44
26:LE:61:LEU:HD11	26:LE:103:ILE:HG13	1.99	0.44
35:LP:105:LYS:HB2	35:LP:105:LYS:HE2	1.80	0.44
41:LV:70:GLU:OE1	41:LV:70:GLU:N	2.50	0.44
4:C4:1:A:C8	25:LD:271:LYS:HG2	2.52	0.44
12:CN:101:LEU:HA	41:LV:137:VAL:HG22	1.99	0.44
15:Cb:41:ALA:HA	15:Cb:44:LEU:HD12	2.00	0.44
25:LD:193:LEU:HD21	25:LD:198:LEU:HD22	1.99	0.44
30:LK:164:ASP:OD1	30:LK:164:ASP:N	2.51	0.44
1:C1:980:A:H2'	1:C1:981:G:C8	2.53	0.44
1:C1:2335:A:OP1	10:CL:19:ARG:NH1	2.48	0.44
1:C1:2842:U:H2'	1:C1:2843:C:H6	1.83	0.44
1:C1:882:G:H1'	1:C1:1569:A:N6	2.33	0.44
1:C1:2160:C:H2'	1:C1:2161:A:C5	2.53	0.44
12:CN:61:ARG:HD3	41:LV:133:SER:HA	1.98	0.44
13:CO:13:ASN:OD1	13:CO:16:ARG:NH2	2.51	0.44
15:Cb:92:MET:HG3	15:Cb:97:TYR:HB3	2.00	0.44
21:Cz:99:LEU:HD23	21:Cz:99:LEU:HA	1.85	0.44
24:LC:34:ASP:OD1	24:LC:34:ASP:N	2.50	0.44
1:C1:2130:A:H2'	1:C1:2131:A:C8	2.53	0.44
1:C1:3185:G:OP1	34:LO:165:LYS:NZ	2.51	0.44
2:C2:83:C:O2	43:LY:109:HIS:NE2	2.47	0.44
20:Ch:159[B]:SER:OG	20:Ch:499:ASP:OD1	2.36	0.44
25:LD:271:LYS:HE2	25:LD:271:LYS:HB3	1.93	0.44
1:C1:371:A:H4'	43:LY:90:THR:HG22	2.00	0.43
1:C1:604:G:H2'	1:C1:605:G:H8	1.83	0.43
1:C1:787:OMG:C5'	24:LC:76:PRO:HD3	2.48	0.43
1:C1:1454:U:H2'	1:C1:1455:G:C8	2.53	0.43
1:C1:1770:U:OP1	56:Lp:48:ARG:NH2	2.46	0.43
11:CM:76:LYS:HB3	11:CM:76:LYS:HE3	1.62	0.43
12:CN:219:GLU:HA	12:CN:224:LEU:HD12	2.00	0.43
18:Cf:109:LYS:HB2	18:Cf:267:MET:HE1	2.00	0.43
43:LY:122:LYS:O	43:LY:126:GLU:HG3	2.18	0.43
51:Lh:6:LYS:HE3	51:Lh:6:LYS:HB3	1.84	0.43
1:C1:462:A:H2'	1:C1:463:C:C6	2.53	0.43
1:C1:1480:C:H2'	1:C1:1481:A:H8	1.82	0.43
1:C1:2666:U:H2'	1:C1:2667:C:C6	2.53	0.43
2:C2:26:U:H2'	2:C2:27:U:C6	2.53	0.43
6:CH:288:LYS:HB3	6:CH:291:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CH:483:GLU:N	6:CH:483:GLU:OE1	2.46	0.43
17:Ce:391:ASP:OD1	17:Ce:391:ASP:N	2.51	0.43
25:LD:207:VAL:O	25:LD:211:MET:HG3	2.17	0.43
1:C1:424:U:H2'	1:C1:425:G:C8	2.53	0.43
1:C1:1413:U:H2'	45:La:9:ARG:HH22	1.83	0.43
1:C1:1698:A:H2'	1:C1:1699:G:H8	1.83	0.43
1:C1:3111:C:C4	1:C1:3113:A:H1'	2.53	0.43
6:CH:128:LYS:HE3	6:CH:128:LYS:HB3	1.83	0.43
6:CH:168:THR:HA	6:CH:216:GLN:O	2.19	0.43
7:CI:216:LEU:HG	7:CI:233:ILE:HG12	2.00	0.43
27:LG:253:LYS:HA	27:LG:253:LYS:HD3	1.82	0.43
1:C1:2384:OMU:HM23	1:C1:2384:OMU:H1'	1.68	0.43
4:C4:4:U:H2'	4:C4:5:A:C8	2.53	0.43
21:Cz:68:MET:HE2	39:LT:160:ILE:HG12	2.00	0.43
30:LK:65:GLN:O	30:LK:68:GLN:NE2	2.51	0.43
30:LK:124:ASP:OD2	30:LK:124:ASP:N	2.50	0.43
1:C1:425:G:H2'	1:C1:426:A:C8	2.54	0.43
1:C1:617:C:H2'	1:C1:618:C:C6	2.53	0.43
1:C1:684:C:H2'	1:C1:685:G:C8	2.54	0.43
1:C1:1220:G:H22	1:C1:1234:A:H2	1.65	0.43
1:C1:2974:A:H2'	1:C1:2975:G:C8	2.52	0.43
9:CK:141:LYS:O	9:CK:144:LYS:NZ	2.40	0.43
1:C1:3120:C:H2'	1:C1:3121:G:C8	2.54	0.43
6:CH:341:GLU:O	6:CH:345:GLN:HG3	2.19	0.43
6:CH:453:ASP:OD1	6:CH:453:ASP:N	2.51	0.43
16:Cd:411:ILE:HG13	16:Cd:439:LEU:HD11	1.99	0.43
30:LK:54:LYS:HB3	30:LK:54:LYS:HE3	1.64	0.43
31:LL:189:ARG:HB2	52:Li:18:ARG:HD3	2.00	0.43
43:LY:79:ILE:HG23	43:LY:100:PRO:HG3	2.01	0.43
1:C1:1067:A:H2'	1:C1:1068:A:C8	2.54	0.43
12:CN:186:VAL:HG12	12:CN:218:ILE:HD11	1.99	0.43
20:Ch:208:SER:OG	20:Ch:209:MET:N	2.52	0.43
24:LC:114:ILE:HB	24:LC:119:LYS:HE3	2.00	0.43
1:C1:363:U:H4'	1:C1:397:G:H5'	2.01	0.43
1:C1:576:A:H2'	1:C1:577:C:C6	2.54	0.43
1:C1:769:G:H2'	1:C1:770:C:C6	2.53	0.43
1:C1:1704:U:H1'	1:C1:1705:C:C6	2.53	0.43
1:C1:1779:A:H2'	1:C1:1780:A:H8	1.82	0.43
2:C2:57:C:H4'	2:C2:63:G:N7	2.34	0.43
38:LS:68:HIS:O	38:LS:73:LYS:NZ	2.51	0.43
1:C1:774:A:H2'	1:C1:775:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2633:A:H5''	29:LJ:106:GLY:HA3	2.01	0.43
1:C1:2838:OMC:H2'	1:C1:2839:U:C6	2.53	0.43
2:C2:58:G:O6	53:Lj:63:ARG:NH1	2.48	0.43
16:Cd:30:ARG:HB3	16:Cd:35:ILE:HG12	2.00	0.43
16:Cd:67:LYS:HD3	16:Cd:67:LYS:HA	1.90	0.43
18:Cf:184:VAL:HB	18:Cf:232:ILE:HD11	2.01	0.43
26:LE:194:LYS:HB3	26:LE:196:HIS:CE1	2.54	0.43
28:LH:127:MET:HE2	28:LH:218:ILE:HG22	2.01	0.43
1:C1:21:A:H2'	1:C1:22:G:C8	2.54	0.43
1:C1:575:G:H2'	1:C1:576:A:C8	2.54	0.43
1:C1:651:C:H2'	1:C1:652:A:H8	1.81	0.43
1:C1:703:A:N1	1:C1:763:G:O2'	2.51	0.43
1:C1:2621:G:H2'	1:C1:2622:G:H8	1.84	0.43
1:C1:2627:U:H2'	1:C1:2628:G:H8	1.84	0.43
1:C1:2751:A:H2'	1:C1:2752:G:H8	1.84	0.43
1:C1:3234:C:H4'	1:C1:3235:A:H5'	2.01	0.43
2:C2:63:G:H22	2:C2:97:A:H2	1.66	0.43
5:CF:43:PHE:HB3	5:CF:223:LEU:HD23	2.01	0.43
23:LB:59:ASP:HB2	23:LB:358:LYS:HD3	2.01	0.43
40:LU:46:ARG:HA	40:LU:46:ARG:HD2	1.85	0.43
48:Le:89:HIS:NE2	57:Lq:36:THR:O	2.43	0.43
1:C1:203:A:H4'	1:C1:205:A:N7	2.34	0.42
1:C1:617:C:H2'	1:C1:618:C:H6	1.84	0.42
1:C1:1762:U:H2'	1:C1:1763:C:C6	2.54	0.42
1:C1:2318:G:OP1	35:LP:141:SER:OG	2.31	0.42
1:C1:2876:OMG:OP1	41:LV:49:ASN:N	2.46	0.42
1:C1:3191:G:H2'	1:C1:3192:C:C6	2.54	0.42
6:CH:589:ARG:HD3	6:CH:589:ARG:HA	1.85	0.42
9:CK:174:PRO:HG2	9:CK:177:LEU:HD12	1.99	0.42
10:CL:14:LYS:HB3	10:CL:14:LYS:HE2	1.65	0.42
34:LO:87:ARG:HG3	34:LO:101:LEU:HD11	2.01	0.42
43:LY:111:ASP:O	43:LY:115:GLU:HG2	2.19	0.42
48:Le:56:ILE:HD12	48:Le:56:ILE:HA	1.89	0.42
49:Lf:55:TYR:CZ	49:Lf:67:ARG:HB2	2.53	0.42
1:C1:650:U:H2'	1:C1:651:C:C6	2.53	0.42
1:C1:979:A:N6	1:C1:1033:U:O4	2.52	0.42
1:C1:1577:C:H2'	1:C1:1578:G:C8	2.54	0.42
1:C1:2391:U:H2'	1:C1:2392:G:H8	1.84	0.42
1:C1:2882:U:H2'	16:Cd:221:ARG:HD3	2.01	0.42
1:C1:2923:G:O2'	16:Cd:30:ARG:NH2	2.46	0.42
1:C1:2958:G:H2'	1:C1:2959:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:3163:A:N6	1:C1:3217:U:O2	2.39	0.42
12:CN:107:VAL:HG23	12:CN:108:ILE:HG13	2.01	0.42
36:LQ:90:VAL:HG13	36:LQ:94:ARG:HD2	2.01	0.42
43:LY:39:ARG:HD2	43:LY:45:ARG:HA	2.02	0.42
43:LY:49:ILE:HD11	43:LY:55:VAL:HG11	2.01	0.42
1:C1:1073:G:H2'	1:C1:1074:G:C8	2.53	0.42
1:C1:1517:A:H2'	1:C1:1518:A:C8	2.54	0.42
1:C1:2556:U:H2'	1:C1:2557:G:H8	1.84	0.42
1:C1:2628:G:H2'	1:C1:2629:G:C8	2.55	0.42
6:CH:288:LYS:HG2	58:CH:701:GTP:C6	2.54	0.42
22:LA:140:ASN:OD1	22:LA:147:ARG:NH1	2.53	0.42
31:LL:148:THR:HB	51:Lh:125:ALA:HB2	2.01	0.42
1:C1:2822:G:C2	6:CH:94:LEU:HD13	2.55	0.42
27:LG:216:LYS:HA	27:LG:216:LYS:HD3	1.64	0.42
34:LO:79:SER:HB2	34:LO:106:VAL:HB	2.02	0.42
1:C1:64:A:N3	1:C1:79:U:O2'	2.46	0.42
1:C1:866:A:C2	6:CH:661:ARG:HB3	2.54	0.42
1:C1:1260:C:H2'	1:C1:1261:A:H8	1.84	0.42
1:C1:2518:G:O2'	22:LA:64:ARG:NH2	2.52	0.42
1:C1:2858:C:O2'	1:C1:2860:G:OP2	2.31	0.42
7:CI:250:LYS:HA	7:CI:250:LYS:HD3	1.89	0.42
24:LC:350:LYS:HB3	24:LC:350:LYS:HE3	1.86	0.42
29:LJ:126:MET:HE2	29:LJ:126:MET:HB3	1.84	0.42
38:LS:162:LYS:HG3	49:Lf:38:ASP:HB3	2.02	0.42
40:LU:23:ILE:HD13	40:LU:110:TYR:HB2	2.02	0.42
54:Lk:54:LYS:HE3	54:Lk:54:LYS:HB3	1.77	0.42
1:C1:292:G:C8	52:Li:40:GLY:HA3	2.55	0.42
1:C1:1100:G:H2'	1:C1:1101:C:C6	2.54	0.42
1:C1:2101:A:C4	53:Lj:3:LYS:HB3	2.55	0.42
1:C1:2362:A:OP1	24:LC:70:ARG:NH1	2.45	0.42
1:C1:3002:A:H4'	23:LB:13:SER:HB2	2.00	0.42
1:C1:3287:U:H2'	1:C1:3288:A:C8	2.54	0.42
20:Ch:386:LEU:O	20:Ch:397:VAL:N	2.52	0.42
28:LH:122:GLY:HA3	28:LH:226:ILE:HD12	2.02	0.42
1:C1:382:A:H5''	35:LP:16:ARG:HG3	2.00	0.42
1:C1:652:A:H2'	1:C1:653:A:H8	1.84	0.42
1:C1:1454:U:H2'	1:C1:1455:G:H8	1.83	0.42
1:C1:2368:C:H4'	9:CK:142:THR:HG21	2.02	0.42
1:C1:2683:OMU:H1'	1:C1:2683:OMU:HM23	1.62	0.42
4:C4:45:U:H2'	4:C4:46:G:C8	2.54	0.42
13:CO:30:LEU:HD11	23:LB:42:HIS:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Cf:145:ALA:HA	19:Cg:32:ASP:HB3	2.01	0.42
20:Ch:84:ARG:NH1	20:Ch:97:ASP:OD1	2.51	0.42
25:LD:98:ALA:HB1	25:LD:165:VAL:HG23	2.01	0.42
25:LD:206:HIS:HA	25:LD:209:GLU:HG3	2.02	0.42
25:LD:261:ASP:OD1	25:LD:261:ASP:N	2.35	0.42
38:LS:12:ARG:HB3	38:LS:24:LEU:HD23	2.02	0.42
46:Lc:16:LYS:O	46:Lc:20:VAL:HG23	2.20	0.42
1:C1:985:A:N1	1:C1:1032:C:O2'	2.51	0.42
1:C1:1211:A:H5''	5:CF:203:SER:HB3	2.01	0.42
1:C1:1814:U:OP2	55:Ll:10:LYS:NZ	2.45	0.42
1:C1:2504:G:H2'	1:C1:2505:U:H6	1.85	0.42
1:C1:2574:G:O2'	1:C1:2575:C:O5'	2.31	0.42
1:C1:2771:C:H2'	1:C1:2772:A:C8	2.54	0.42
6:CH:348:LYS:HB2	6:CH:348:LYS:HE2	1.83	0.42
24:LC:55:GLU:H	24:LC:55:GLU:HG3	1.63	0.42
11:LF:214:SER:O	11:LF:248:MET:HG2	2.20	0.42
28:LH:177:LYS:HE2	28:LH:177:LYS:HB2	1.70	0.42
34:LO:129:LEU:HD11	38:LS:170:PRO:HG2	2.01	0.42
37:LR:44:LEU:HD22	37:LR:49:LEU:HD22	2.01	0.42
39:LT:93:ILE:H	39:LT:93:ILE:HG13	1.67	0.42
40:LU:60:ILE:HD13	40:LU:78:LEU:HD22	2.01	0.42
46:Lc:19:LEU:O	46:Lc:23:SER:OG	2.37	0.42
48:Le:39:ILE:HD12	48:Le:39:ILE:HA	1.91	0.42
1:C1:213:A:HO2'	1:C1:214:G:H21	1.68	0.42
1:C1:357:G:OP2	53:Lj:52:LYS:NZ	2.43	0.42
1:C1:637:A2M:H2'	1:C1:638:C:C6	2.55	0.42
1:C1:842:G:C8	22:LA:183:SER:HB3	2.54	0.42
1:C1:890:G:N2	33:LN:76:PRO:O	2.53	0.42
1:C1:1387:G:O6	48:Le:17:ARG:NH1	2.52	0.42
1:C1:1880:A:O2'	1:C1:1886:G:N7	2.48	0.42
1:C1:1893:A:N3	1:C1:2083:G:H2'	2.35	0.42
1:C1:1900:U:O2'	1:C1:1912:A:N7	2.51	0.42
1:C1:2079:G:OP1	1:C1:2081:C:N4	2.52	0.42
9:CK:11:ARG:NH1	9:CK:16:ARG:HD3	2.34	0.42
16:Cd:406:HIS:ND1	16:Cd:408:GLU:OE1	2.44	0.42
17:Ce:297:ARG:HH12	17:Ce:299:LYS:HG2	1.85	0.42
23:LB:237:LYS:HE2	23:LB:237:LYS:HB2	1.83	0.42
1:C1:424:U:O2'	49:Lf:58:GLN:OE1	2.37	0.42
1:C1:1171:U:OP1	1:C1:1193:U:O2'	2.26	0.42
1:C1:2236:G:N3	1:C1:2238:A:H1'	2.35	0.42
1:C1:2280:A:H5''	1:C1:2282:U:H5'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2376:A:H2'	1:C1:2377:G:C8	2.55	0.42
4:C4:59:C:H2'	4:C4:60:A:C8	2.55	0.42
20:Ch:136:SER:OG	20:Ch:517:ASN:OXT	2.38	0.42
50:Lg:2:ALA:HA	50:Lg:3:PRO:HD3	1.96	0.42
1:C1:2186:A:H2'	1:C1:2187:A:C8	2.55	0.41
1:C1:2632:A:OP1	29:LJ:96:ASN:ND2	2.50	0.41
1:C1:2718:U:OP2	19:Cg:187:GLN:NE2	2.53	0.41
1:C1:2728:A:H2'	1:C1:2729:G:C8	2.55	0.41
6:CH:297:LEU:HD13	6:CH:301:MET:HB3	2.02	0.41
20:Ch:100:PRO:HG3	20:Ch:106:LEU:HD22	2.02	0.41
24:LC:287:LEU:HD11	36:LQ:60:LEU:HB2	2.02	0.41
1:C1:422:U:O2'	49:Lf:90:PRO:O	2.32	0.41
1:C1:633:A:O5'	1:C1:1125:G:O2'	2.37	0.41
1:C1:651:C:H2'	1:C1:652:A:C8	2.55	0.41
1:C1:974:A:H5''	39:LT:43:LYS:HD2	2.01	0.41
1:C1:1871:A:OP2	23:LB:242:LYS:NZ	2.52	0.41
1:C1:2508:A:H2'	1:C1:2509:A:C8	2.55	0.41
1:C1:3184:C:O2	13:CO:93:ARG:NH2	2.40	0.41
2:C2:52:A:OP1	55:Ll:21:ARG:NH1	2.44	0.41
5:CF:59:GLU:OE1	5:CF:115:TYR:OH	2.33	0.41
9:CK:190:ASN:C	9:CK:190:ASN:ND2	2.72	0.41
23:LB:120:LYS:HA	23:LB:120:LYS:HD3	1.82	0.41
32:LM:20:LEU:HD21	32:LM:30:ILE:HD11	2.02	0.41
39:LT:110:LYS:O	39:LT:114:GLU:HG2	2.19	0.41
1:C1:9:C:H2'	1:C1:10:U:C6	2.56	0.41
1:C1:823:A:H2'	1:C1:824:G:H8	1.84	0.41
1:C1:2389:U:H3	1:C1:2562:G:H1	1.69	0.41
8:CJ:42:ILE:HD12	8:CJ:68:ASP:HB3	2.03	0.41
8:CJ:79:GLN:OE1	8:CJ:82:ARG:NH1	2.49	0.41
28:LH:81:ASN:HB3	28:LH:93:GLU:HG3	2.02	0.41
44:LZ:33:LYS:HB3	44:LZ:33:LYS:HE3	1.70	0.41
1:C1:970:U:H2'	1:C1:971:A:C8	2.55	0.41
1:C1:2841:U:H2'	1:C1:2842:U:C6	2.56	0.41
1:C1:3140:A:OP1	38:LS:154:HIS:ND1	2.49	0.41
4:C4:59:C:H2'	4:C4:60:A:H8	1.85	0.41
4:C4:63:G:H2'	4:C4:64:A:H8	1.84	0.41
5:CF:14:GLN:O	9:CK:71:ARG:NH2	2.53	0.41
14:CQ:82:ASN:HB3	14:CQ:85:LEU:HB3	2.03	0.41
27:LG:130:LYS:HD3	27:LG:130:LYS:HA	1.88	0.41
27:LG:175:LYS:HD3	52:Li:52:LEU:HD13	2.01	0.41
1:C1:2069:A:H2'	1:C1:2070:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2159:C:H2'	1:C1:2160:C:C6	2.55	0.41
1:C1:2182:A:H2'	1:C1:2183:A:C8	2.55	0.41
1:C1:410:A:H2'	1:C1:411:A:H8	1.84	0.41
1:C1:823:A:H2'	1:C1:824:G:C8	2.56	0.41
1:C1:1161:G:O6	49:Lf:22:ARG:HG2	2.19	0.41
1:C1:1638:G:H2'	1:C1:1639:A:H8	1.85	0.41
1:C1:2123:G:H2'	1:C1:2124:G:H8	1.85	0.41
1:C1:2771:C:H2'	1:C1:2772:A:H8	1.86	0.41
4:C4:17:A:OP1	29:LJ:154:ARG:NH2	2.49	0.41
6:CH:46:THR:HG23	6:CH:112:VAL:HG22	2.01	0.41
14:CQ:8:PHE:HE1	14:CQ:49:LEU:HD12	1.84	0.41
19:Cg:188:MET:HE3	19:Cg:188:MET:HB3	1.93	0.41
27:LG:84:THR:HG22	27:LG:182:ILE:HG22	2.02	0.41
39:LT:65:TYR:HD1	39:LT:75:ILE:HG13	1.85	0.41
1:C1:1159:C:H2'	1:C1:1160:G:N2	2.36	0.41
1:C1:1577:C:H5'	1:C1:1676:A:H1'	2.03	0.41
6:CH:585:GLU:CD	6:CH:585:GLU:H	2.29	0.41
10:CL:59:PHE:HA	10:CL:60:PRO:HD3	1.95	0.41
24:LC:136:LEU:HD23	24:LC:143:VAL:HG11	2.02	0.41
27:LG:95:LYS:HB2	27:LG:95:LYS:HE3	1.80	0.41
31:LL:55:ARG:HB2	31:LL:71:LEU:HD22	2.02	0.41
1:C1:462:A:OP1	57:Lq:92:LYS:NZ	2.49	0.41
1:C1:663:C:O2'	1:C1:667:U:OP1	2.31	0.41
1:C1:1290:G:O2'	1:C1:1291:A:N7	2.48	0.41
1:C1:1577:C:H2'	1:C1:1578:G:H8	1.86	0.41
1:C1:2307:U:H2'	1:C1:2308:A:C8	2.55	0.41
1:C1:2889:A:H2'	1:C1:2890:C:C6	2.55	0.41
1:C1:2981:U:H2'	1:C1:2982:A:H8	1.84	0.41
4:C4:4:U:H2'	4:C4:5:A:H8	1.86	0.41
12:CN:104:LEU:HA	12:CN:107:VAL:HG22	2.03	0.41
17:Ce:301:LYS:HA	17:Ce:301:LYS:HD2	1.74	0.41
26:LE:86:PRO:HD2	26:LE:89:ILE:HD12	2.03	0.41
38:LS:106:MET:HE3	38:LS:106:MET:HB3	1.82	0.41
1:C1:1778:A:H2'	1:C1:1779:A:C8	2.56	0.41
1:C1:2058:A:H2'	1:C1:2059:A:C8	2.56	0.41
1:C1:2393:A:H2'	1:C1:2394:C:C6	2.56	0.41
1:C1:2711:U:H2'	1:C1:2712:G:C8	2.56	0.41
2:C2:58:G:N7	53:Lj:63:ARG:NH2	2.46	0.41
4:C4:86:C:H2'	4:C4:87:G:C8	2.56	0.41
7:CI:198:PHE:HD1	7:CI:198:PHE:HA	1.67	0.41
12:CN:199:VAL:HG23	12:CN:204:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Cb:86:TYR:CE1	15:Cb:90:GLU:HG2	2.55	0.41
20:Ch:257:SER:OG	20:Ch:258:LYS:N	2.54	0.41
20:Ch:460:LEU:HA	20:Ch:473:TRP:O	2.21	0.41
21:Cz:102:LYS:HA	21:Cz:102:LYS:HD2	1.94	0.41
22:LA:54:ARG:HG2	22:LA:56:ALA:H	1.84	0.41
34:LO:194:LYS:HD3	34:LO:194:LYS:HA	1.76	0.41
40:LU:47:ILE:HD12	40:LU:62:ILE:HD11	2.02	0.41
43:LY:54:GLU:HG3	43:LY:107:LYS:HB3	2.01	0.41
1:C1:1447:G:N2	1:C1:1450:A:OP2	2.54	0.41
1:C1:1555:C:H5''	17:Ce:428:ALA:HB2	2.03	0.41
1:C1:1584:U:H4'	1:C1:1815:A:H4'	2.03	0.41
4:C4:12:U:OP2	4:C4:68:C:O2'	2.38	0.41
18:Cf:235:LYS:HG2	25:LD:128:GLU:HG2	2.03	0.41
53:Lj:43:LYS:HB2	53:Lj:43:LYS:HE3	1.86	0.41
1:C1:1584:U:H2'	1:C1:1585:A:O4'	2.20	0.40
1:C1:2495:U:H2'	1:C1:2496:G:C8	2.56	0.40
1:C1:2518:G:C6	22:LA:64:ARG:HD2	2.55	0.40
1:C1:2789:G:H2'	1:C1:2790:G:H8	1.81	0.40
1:C1:2971:U:H2'	1:C1:2972:U:C6	2.56	0.40
1:C1:3204:C:H2'	1:C1:3205:G:C8	2.56	0.40
6:CH:544:ILE:O	6:CH:549:ARG:NH1	2.54	0.40
20:Ch:470:LEU:HD11	20:Ch:505:SER:HB3	2.02	0.40
25:LD:214:LEU:HD13	25:LD:222:TYR:HA	2.04	0.40
43:LY:115:GLU:HG2	43:LY:115:GLU:H	1.71	0.40
1:C1:2615:A:H2'	1:C1:2616:A:C8	2.56	0.40
1:C1:2642:U:H2'	1:C1:2643:C:C6	2.55	0.40
1:C1:3266:A:H2'	1:C1:3267:G:H8	1.87	0.40
8:CJ:115:LYS:HE3	8:CJ:115:LYS:HB3	2.01	0.40
11:CM:127:LYS:HD3	11:CM:127:LYS:HA	1.84	0.40
18:Cf:169:ARG:HH12	18:Cf:172:PRO:HB3	1.86	0.40
20:Ch:424:TRP:HA	20:Ch:448:PRO:HB3	2.03	0.40
27:LG:53:VAL:HG22	42:LX:43:THR:HA	2.03	0.40
31:LL:124:ILE:HG23	31:LL:138:THR:HG21	2.03	0.40
35:LP:103:ASP:OD2	35:LP:109:THR:OG1	2.40	0.40
45:La:76:ASP:HB3	45:La:116:GLY:HA3	2.02	0.40
1:C1:706:G:OP2	1:C1:706:G:N2	2.41	0.40
1:C1:2149:U:H2'	1:C1:2150:G:O4'	2.21	0.40
1:C1:2562:G:O3'	16:Cd:2:GLY:N	2.55	0.40
14:CQ:144:ARG:HA	14:CQ:147:GLU:HG3	2.03	0.40
16:Cd:425:ARG:HD3	18:Cf:319:ARG:HA	2.03	0.40
46:Lc:77:ASN:OD1	46:Lc:77:ASN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:181:G:OP1	43:LY:125:ARG:NE	2.47	0.40
1:C1:317:A:H2'	1:C1:318:A:C8	2.57	0.40
1:C1:2117:U:H2'	1:C1:2118:G:H8	1.86	0.40
2:C2:70:G:OP1	43:LY:120:ARG:NH2	2.36	0.40
9:CK:87:PRO:HD2	9:CK:90:LEU:HD12	2.02	0.40
9:CK:143:HIS:CE1	16:CD:45:LYS:HE2	2.56	0.40
11:CM:241:ILE:HD12	11:CM:244:LEU:HD12	2.03	0.40
17:CE:239:LYS:O	17:CE:243:GLU:HG2	2.22	0.40
24:LC:21:GLU:OE1	24:LC:263:LYS:HG3	2.22	0.40
32:LM:128:ARG:HD3	32:LM:132:ARG:CZ	2.52	0.40
34:LO:35:VAL:HG22	34:LO:105:LYS:HB2	2.03	0.40
42:LX:78:HIS:HB2	51:Lh:39:ILE:HG12	2.02	0.40
44:LZ:13:THR:HB	50:Lg:87:ARG:HG3	2.04	0.40
1:C1:1051:C:H2'	1:C1:1052:C:H6	1.86	0.40
1:C1:1480:C:H2'	1:C1:1481:A:C8	2.57	0.40
1:C1:2790:G:H2'	1:C1:2791:C:H6	1.87	0.40
3:C3:3:C:H5''	11:CM:59:LYS:HD2	2.03	0.40
20:Ch:249:GLY:O	20:Ch:268:ASN:ND2	2.55	0.40
24:LC:77:ARG:HA	24:LC:88:GLN:O	2.21	0.40
27:LG:120:LYS:HE2	27:LG:120:LYS:HB3	1.87	0.40
28:LH:141:GLU:OE2	28:LH:141:GLU:N	2.54	0.40
38:LS:162:LYS:HA	38:LS:162:LYS:HD3	1.98	0.40
57:Lq:7:ASP:O	57:Lq:11:GLU:HG2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	CF	243/270 (90%)	240 (99%)	3 (1%)	0	100	100
6	CH	621/661 (94%)	616 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	CI	89/414 (22%)	87 (98%)	2 (2%)	0	100	100
8	CJ	376/679 (55%)	371 (99%)	5 (1%)	0	100	100
9	CK	231/261 (88%)	225 (97%)	6 (3%)	0	100	100
10	CL	77/558 (14%)	77 (100%)	0	0	100	100
11	CM	210/249 (84%)	206 (98%)	4 (2%)	0	100	100
11	LF	246/249 (99%)	239 (97%)	7 (3%)	0	100	100
12	CN	244/246 (99%)	239 (98%)	5 (2%)	0	100	100
13	CO	56/120 (47%)	56 (100%)	0	0	100	100
14	CQ	181/225 (80%)	179 (99%)	2 (1%)	0	100	100
15	Cb	99/117 (85%)	98 (99%)	1 (1%)	0	100	100
16	Cd	458/627 (73%)	449 (98%)	9 (2%)	0	100	100
17	Ce	231/443 (52%)	229 (99%)	2 (1%)	0	100	100
18	Cf	281/350 (80%)	280 (100%)	1 (0%)	0	100	100
19	Cg	186/202 (92%)	186 (100%)	0	0	100	100
20	Ch	484/517 (94%)	468 (97%)	16 (3%)	0	100	100
21	Cz	99/123 (80%)	98 (99%)	1 (1%)	0	100	100
22	LA	189/254 (74%)	186 (98%)	3 (2%)	0	100	100
23	LB	387/392 (99%)	380 (98%)	7 (2%)	0	100	100
24	LC	361/365 (99%)	355 (98%)	6 (2%)	0	100	100
25	LD	282/304 (93%)	280 (99%)	2 (1%)	0	100	100
26	LE	187/200 (94%)	183 (98%)	4 (2%)	0	100	100
27	LG	233/262 (89%)	229 (98%)	4 (2%)	0	100	100
28	LH	188/229 (82%)	185 (98%)	3 (2%)	0	100	100
29	LJ	167/173 (96%)	165 (99%)	2 (1%)	0	100	100
30	LK	156/165 (94%)	156 (100%)	0	0	100	100
31	LL	201/213 (94%)	200 (100%)	1 (0%)	0	100	100
32	LM	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
33	LN	200/203 (98%)	195 (98%)	5 (2%)	0	100	100
34	LO	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
35	LP	167/187 (89%)	164 (98%)	3 (2%)	0	100	100
36	LQ	148/213 (70%)	146 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	LR	153/2898 (5%)	152 (99%)	1 (1%)	0	100	100
38	LS	172/174 (99%)	170 (99%)	2 (1%)	0	100	100
39	LT	127/160 (79%)	125 (98%)	2 (2%)	0	100	100
40	LU	103/127 (81%)	100 (97%)	3 (3%)	0	100	100
41	LV	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
42	LX	143/156 (92%)	141 (99%)	2 (1%)	0	100	100
43	LY	131/138 (95%)	126 (96%)	5 (4%)	0	100	100
44	LZ	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
45	La	104/149 (70%)	104 (100%)	0	0	100	100
46	Lc	93/108 (86%)	93 (100%)	0	0	100	100
47	Ld	108/120 (90%)	107 (99%)	1 (1%)	0	100	100
48	Le	124/131 (95%)	123 (99%)	1 (1%)	0	100	100
49	Lf	106/109 (97%)	106 (100%)	0	0	100	100
50	Lg	116/119 (98%)	115 (99%)	1 (1%)	0	100	100
51	Lh	120/935 (13%)	118 (98%)	2 (2%)	0	100	100
52	Li	99/110 (90%)	98 (99%)	1 (1%)	0	100	100
53	Lj	86/95 (90%)	85 (99%)	1 (1%)	0	100	100
54	Lk	74/94 (79%)	74 (100%)	0	0	100	100
55	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
56	Lp	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
57	Lq	137/147 (93%)	133 (97%)	4 (3%)	0	100	100
All	All	10017/16004 (63%)	9867 (98%)	150 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CF	212/236 (90%)	207 (98%)	5 (2%)	43	58
6	CH	549/575 (96%)	541 (98%)	8 (2%)	57	73
7	CI	70/336 (21%)	68 (97%)	2 (3%)	37	51
8	CJ	331/579 (57%)	324 (98%)	7 (2%)	47	63
9	CK	206/225 (92%)	203 (98%)	3 (2%)	57	73
10	CL	61/458 (13%)	61 (100%)	0	100	100
11	CM	185/215 (86%)	183 (99%)	2 (1%)	65	79
11	LF	213/215 (99%)	211 (99%)	2 (1%)	70	84
12	CN	205/206 (100%)	202 (98%)	3 (2%)	57	73
13	CO	48/99 (48%)	48 (100%)	0	100	100
14	CQ	144/192 (75%)	143 (99%)	1 (1%)	76	87
15	Cb	85/101 (84%)	82 (96%)	3 (4%)	32	43
16	Cd	403/541 (74%)	401 (100%)	2 (0%)	81	90
17	Ce	206/383 (54%)	206 (100%)	0	100	100
18	Cf	250/310 (81%)	247 (99%)	3 (1%)	63	78
19	Cg	158/176 (90%)	152 (96%)	6 (4%)	29	40
20	Ch	408/436 (94%)	405 (99%)	3 (1%)	76	87
21	Cz	89/107 (83%)	88 (99%)	1 (1%)	65	79
22	LA	150/198 (76%)	146 (97%)	4 (3%)	39	53
23	LB	329/331 (99%)	328 (100%)	1 (0%)	86	93
24	LC	282/285 (99%)	280 (99%)	2 (1%)	76	87
25	LD	221/253 (87%)	221 (100%)	0	100	100
26	LE	157/166 (95%)	155 (99%)	2 (1%)	61	76
27	LG	200/222 (90%)	200 (100%)	0	100	100
28	LH	167/200 (84%)	166 (99%)	1 (1%)	78	89
29	LJ	140/150 (93%)	139 (99%)	1 (1%)	76	87
30	LK	127/136 (93%)	123 (97%)	4 (3%)	35	48
31	LL	158/176 (90%)	157 (99%)	1 (1%)	78	89
32	LM	116/117 (99%)	115 (99%)	1 (1%)	70	84
33	LN	179/180 (99%)	178 (99%)	1 (1%)	78	89
34	LO	162/163 (99%)	161 (99%)	1 (1%)	78	89
35	LP	133/152 (88%)	133 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	LQ	128/178 (72%)	127 (99%)	1 (1%)	73	85
37	LR	125/2396 (5%)	125 (100%)	0	100	100
38	LS	152/154 (99%)	151 (99%)	1 (1%)	76	87
39	LT	110/135 (82%)	109 (99%)	1 (1%)	70	84
40	LU	92/108 (85%)	91 (99%)	1 (1%)	65	79
41	LV	98/102 (96%)	97 (99%)	1 (1%)	68	81
42	LX	122/129 (95%)	121 (99%)	1 (1%)	73	85
43	LY	116/119 (98%)	115 (99%)	1 (1%)	70	84
44	LZ	121/121 (100%)	119 (98%)	2 (2%)	53	69
45	La	93/122 (76%)	92 (99%)	1 (1%)	65	79
46	Lc	76/88 (86%)	74 (97%)	2 (3%)	40	55
47	Ld	90/105 (86%)	90 (100%)	0	100	100
48	Le	109/114 (96%)	108 (99%)	1 (1%)	70	84
49	Lf	89/90 (99%)	86 (97%)	3 (3%)	32	44
50	Lg	95/102 (93%)	95 (100%)	0	100	100
51	Lh	109/781 (14%)	109 (100%)	0	100	100
52	Li	85/93 (91%)	85 (100%)	0	100	100
53	Lj	72/78 (92%)	71 (99%)	1 (1%)	59	75
54	Lk	73/88 (83%)	73 (100%)	0	100	100
55	Ll	45/46 (98%)	45 (100%)	0	100	100
56	Lp	73/74 (99%)	71 (97%)	2 (3%)	39	53
57	Lq	109/112 (97%)	109 (100%)	0	100	100
All	All	8526/13454 (63%)	8437 (99%)	89 (1%)	65	81

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	CF	97	THR
5	CF	122	VAL
5	CF	149	VAL
5	CF	178	LYS
5	CF	242	THR
6	CH	79	ASP
6	CH	85	TYR

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Mol	Chain	Res	Type
6	CH	168	THR
6	CH	191	THR
6	CH	549	ARG
6	CH	585	GLU
6	CH	608	GLN
6	CH	655	ILE
7	CI	198	PHE
7	CI	214	THR
8	CJ	101	SER
8	CJ	140	ASP
8	CJ	381	GLN
8	CJ	400	VAL
8	CJ	407	THR
8	CJ	456	VAL
8	CJ	465	ILE
9	CK	37	GLU
9	CK	98	THR
9	CK	190	ASN
11	CM	49	VAL
11	CM	162	VAL
12	CN	51	THR
12	CN	114	THR
12	CN	121	LEU
14	CQ	84	GLU
15	Cb	9	MET
15	Cb	28	SER
15	Cb	68	HIS
16	Cd	69	VAL
16	Cd	86	ASP
18	Cf	87	MET
18	Cf	91	SER
18	Cf	260	MET
19	Cg	15	VAL
19	Cg	19	THR
19	Cg	22	THR
19	Cg	49	GLN
19	Cg	62	LEU
19	Cg	156	SER
20	Ch	142	ILE
20	Ch	285	CYS
20	Ch	426	ASN
21	Cz	67	GLU

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Mol	Chain	Res	Type
22	LA	80	GLU
22	LA	106	SER
22	LA	161	SER
22	LA	207	VAL
23	LB	352	LEU
24	LC	61	THR
24	LC	354	VAL
26	LE	6	THR
26	LE	155	SER
11	LF	80	SER
11	LF	90	VAL
28	LH	120	THR
29	LJ	45	THR
30	LK	8	ASN
30	LK	22	VAL
30	LK	104	VAL
30	LK	164	ASP
31	LL	141	ASP
32	LM	14	VAL
33	LN	60	VAL
34	LO	139	THR
36	LQ	148	THR
38	LS	79	LEU
39	LT	143	ILE
40	LU	118	VAL
41	LV	114	SER
42	LX	37	THR
43	LY	78	VAL
44	LZ	5	LYS
44	LZ	34	SER
45	La	75	ILE
46	Lc	23	SER
46	Lc	27	VAL
48	Le	83	VAL
49	Lf	51	VAL
49	Lf	58	GLN
49	Lf	72	LYS
53	Lj	64	MET
56	Lp	21	SER
56	Lp	28	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
5	CF	85	GLN
6	CH	14	GLN
6	CH	77	HIS
6	CH	306	ASN
6	CH	499	HIS
7	CI	267	GLN
8	CJ	200	ASN
8	CJ	215	ASN
9	CK	10	HIS
9	CK	95	ASN
11	CM	25	GLN
12	CN	6	GLN
12	CN	11	ASN
12	CN	140	GLN
14	CQ	39	ASN
14	CQ	82	ASN
14	CQ	130	ASN
16	Cd	9	ASN
16	Cd	271	ASN
16	Cd	409	GLN
19	Cg	37	ASN
19	Cg	192	GLN
20	Ch	56	ASN
20	Ch	98	GLN
20	Ch	101	ASN
20	Ch	110	HIS
20	Ch	133	HIS
20	Ch	274	HIS
20	Ch	432	ASN
24	LC	60	GLN
24	LC	111	HIS
24	LC	292	ASN
24	LC	330	ASN
11	LF	9	GLN
11	LF	200	ASN
28	LH	133	HIS
28	LH	179	GLN
29	LJ	69	HIS
29	LJ	96	ASN
31	LL	103	ASN
32	LM	103	GLN
33	LN	91	GLN
33	LN	95	GLN

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Mol	Chain	Res	Type
33	LN	153	ASN
36	LQ	86	ASN
36	LQ	98	ASN
36	LQ	163	ASN
37	LR	143	HIS
39	LT	131	GLN
42	LX	124	ASN
44	LZ	77	ASN
44	LZ	105	GLN
46	Lc	71	HIS
47	Ld	29	HIS
47	Ld	62	GLN
47	Ld	64	ASN
47	Ld	88	ASN
48	Le	21	HIS
51	Lh	16	ASN
51	Lh	37	GLN
51	Lh	64	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	3069/3342 (91%)	550 (17%)	43 (1%)
2	C2	155/156 (99%)	23 (14%)	0
3	C3	2/162 (1%)	2 (100%)	0
4	C4	118/119 (99%)	24 (20%)	0
All	All	3344/3779 (88%)	599 (17%)	43 (1%)

All (599) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	6	G
1	C1	27	A
1	C1	44	A
1	C1	50	A
1	C1	60	G
1	C1	61	A
1	C1	66	A
1	C1	67	A
1	C1	95	G
1	C1	96	A

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Mol	Chain	Res	Type
1	C1	110	A
1	C1	111	G
1	C1	117	A
1	C1	123	A
1	C1	132	U
1	C1	134	G
1	C1	135	G
1	C1	139	G
1	C1	152	G
1	C1	153	A
1	C1	157	G
1	C1	181	G
1	C1	184	U
1	C1	200	G
1	C1	204	C
1	C1	213	A
1	C1	214	G
1	C1	225	A
1	C1	241	U
1	C1	244	G
1	C1	258	A
1	C1	262	G
1	C1	276	G
1	C1	277	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	332	C
1	C1	339	C
1	C1	342	A
1	C1	343	C
1	C1	369	G
1	C1	385	OMG
1	C1	386	U
1	C1	389	A2M
1	C1	391	U
1	C1	394	C
1	C1	395	A

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Mol	Chain	Res	Type
1	C1	396	C
1	C1	414	G
1	C1	415	A
1	C1	422	U
1	C1	434	U
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	486	G
1	C1	512	A
1	C1	514	A
1	C1	527	G
1	C1	536	C
1	C1	537	C
1	C1	545	U
1	C1	547	A
1	C1	548	U
1	C1	549	A
1	C1	550	G
1	C1	570	G
1	C1	583	A
1	C1	592	U
1	C1	593	G
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	628	U
1	C1	632	G
1	C1	634	A
1	C1	646	OMG

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Mol	Chain	Res	Type
1	C1	647	G
1	C1	648	A
1	C1	650	U
1	C1	665	A
1	C1	669	U
1	C1	693	A
1	C1	700	G
1	C1	703	A
1	C1	704	A
1	C1	719	U
1	C1	720	C
1	C1	721	G
1	C1	724	G
1	C1	747	A
1	C1	748	U
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	767	G
1	C1	778	OMC
1	C1	779	U
1	C1	782	G
1	C1	787	OMG
1	C1	788	A
1	C1	790	A
1	C1	799	A
1	C1	812	A
1	C1	826	G
1	C1	830	A
1	C1	843	C
1	C1	857	G
1	C1	877	A
1	C1	889	G
1	C1	891	G
1	C1	896	A
1	C1	897	A
1	C1	898	G
1	C1	899	A
1	C1	903	A

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Mol	Chain	Res	Type
1	C1	906	G
1	C1	919	G
1	C1	926	A
1	C1	931	C
1	C1	933	A
1	C1	934	A
1	C1	935	G
1	C1	937	U
1	C1	940	C
1	C1	941	C
1	C1	943	C
1	C1	944	A
1	C1	945	G
1	C1	947	A
1	C1	955	G
1	C1	956	U
1	C1	963	U
1	C1	976	G
1	C1	977	U
1	C1	983	G
1	C1	984	A
1	C1	1032	C
1	C1	1034	U
1	C1	1040	A
1	C1	1047	A
1	C1	1048	A
1	C1	1049	G
1	C1	1055	G
1	C1	1058	A
1	C1	1064	C
1	C1	1065	U
1	C1	1066	G
1	C1	1070	G
1	C1	1076	A
1	C1	1077	U
1	C1	1078	U
1	C1	1079	C
1	C1	1080	G
1	C1	1081	A
1	C1	1086	A
1	C1	1098	G
1	C1	1099	G

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Mol	Chain	Res	Type
1	C1	1109	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	1143	C
1	C1	1163	G
1	C1	1164	U
1	C1	1165	G
1	C1	1175	C
1	C1	1176	A
1	C1	1179	C
1	C1	1185	A
1	C1	1187	A
1	C1	1194	U
1	C1	1205	G
1	C1	1209	G
1	C1	1228	A
1	C1	1241	U
1	C1	1246	A
1	C1	1248	U
1	C1	1268	G
1	C1	1269	A
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
1	C1	1337	G
1	C1	1370	G
1	C1	1382	A
1	C1	1383	G

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Mol	Chain	Res	Type
1	C1	1401	A
1	C1	1417	G
1	C1	1420	OMC
1	C1	1421	U
1	C1	1429	A
1	C1	1433	OMG
1	C1	1434	C
1	C1	1458	G
1	C1	1464	A
1	C1	1485	G
1	C1	1491	OMC
1	C1	1492	G
1	C1	1505	U
1	C1	1536	U
1	C1	1538	U
1	C1	1539	C
1	C1	1540	A
1	C1	1542	A
1	C1	1543	G
1	C1	1549	C
1	C1	1550	U
1	C1	1554	G
1	C1	1560	U
1	C1	1563	G
1	C1	1567	A
1	C1	1568	A
1	C1	1569	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	1679	G
1	C1	1683	U
1	C1	1685	U
1	C1	1697	C
1	C1	1704	U
1	C1	1710	G
1	C1	1722	U

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Mol	Chain	Res	Type
1	C1	1730	A
1	C1	1731	G
1	C1	1743	U
1	C1	1745	U
1	C1	1746	G
1	C1	1758	G
1	C1	1760	G
1	C1	1776	G
1	C1	1777	A
1	C1	1792	G
1	C1	1793	A
1	C1	1794	A
1	C1	1795	U
1	C1	1796	A
1	C1	1799	U
1	C1	1800	C
1	C1	1801	U
1	C1	1812	OMC
1	C1	1813	G
1	C1	1822	A
1	C1	1826	C
1	C1	1829	C
1	C1	1836	OMC
1	C1	1837	C
1	C1	1846	C
1	C1	1847	A2M
1	C1	1856	U
1	C1	1858	G
1	C1	1859	A
1	C1	1860	U
1	C1	1866	A
1	C1	1873	A
1	C1	1886	G
1	C1	1887	C
1	C1	1917	OMU
1	C1	1934	G
1	C1	1935	C
1	C1	2046	C
1	C1	2047	G
1	C1	2048	U
1	C1	2050	C
1	C1	2052	G

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Mol	Chain	Res	Type
1	C1	2054	U
1	C1	2056	A
1	C1	2075	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	2126	C
1	C1	2132	G
1	C1	2139	U
1	C1	2151	A
1	C1	2156	U
1	C1	2157	G
1	C1	2158	C
1	C1	2161	A
1	C1	2167	C
1	C1	2169	G
1	C1	2171	A
1	C1	2172	U
1	C1	2173	G
1	C1	2186	A
1	C1	2188	U
1	C1	2192	A
1	C1	2203	G
1	C1	2205	A
1	C1	2206	A
1	C1	2212	G
1	C1	2216	G
1	C1	2217	U
1	C1	2218	A
1	C1	2219	A
1	C1	2220	C
1	C1	2221	U
1	C1	2222	A
1	C1	2223	U
1	C1	2224	G
1	C1	2225	A
1	C1	2226	C
1	C1	2229	U
1	C1	2230	C

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Mol	Chain	Res	Type
1	C1	2231	U
1	C1	2237	U
1	C1	2279	G
1	C1	2281	U
1	C1	2282	U
1	C1	2297	U
1	C1	2298	G
1	C1	2299	U
1	C1	2300	OMC
1	C1	2301	C
1	C1	2326	A
1	C1	2340	G
1	C1	2348	A
1	C1	2356	G
1	C1	2358	OMG
1	C1	2359	G
1	C1	2362	A
1	C1	2364	A
1	C1	2373	U
1	C1	2374	U
1	C1	2381	G
1	C1	2382	A
1	C1	2406	A
1	C1	2473	U
1	C1	2474	A
1	C1	2477	U
1	C1	2489	C
1	C1	2499	C
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	2515	G
1	C1	2516	G
1	C1	2521	A
1	C1	2526	C
1	C1	2527	C
1	C1	2533	G
1	C1	2544	G
1	C1	2545	G

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Mol	Chain	Res	Type
1	C1	2552	A
1	C1	2565	G
1	C1	2566	G
1	C1	2573	G
1	C1	2575	C
1	C1	2576	U
1	C1	2577	G
1	C1	2578	OMG
1	C1	2579	G
1	C1	2582	G
1	C1	2584	C
1	C1	2585	A
1	C1	2589	C
1	C1	2592	U
1	C1	2613	C
1	C1	2615	A
1	C1	2633	A
1	C1	2635	A
1	C1	2636	G
1	C1	2647	U
1	C1	2651	A
1	C1	2656	A
1	C1	2663	A
1	C1	2664	A
1	C1	2667	C
1	C1	2671	U
1	C1	2672	U
1	C1	2673	G
1	C1	2674	A
1	C1	2675	U
1	C1	2680	A
1	C1	2691	G
1	C1	2713	G
1	C1	2717	A
1	C1	2723	C
1	C1	2731	C
1	C1	2732	C
1	C1	2736	G
1	C1	2737	A
1	C1	2750	G
1	C1	2754	U
1	C1	2755	G

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Mol	Chain	Res	Type
1	C1	2757	C
1	C1	2758	A
1	C1	2761	A
1	C1	2762	A
1	C1	2763	A
1	C1	2769	C
1	C1	2774	OMG
1	C1	2775	G
1	C1	2783	G
1	C1	2785	U
1	C1	2802	U
1	C1	2803	C
1	C1	2804	A
1	C1	2805	U
1	C1	2806	A
1	C1	2812	G
1	C1	2815	G
1	C1	2816	C
1	C1	2817	U
1	C1	2826	C
1	C1	2828	U
1	C1	2836	G
1	C1	2838	OMC
1	C1	2839	U
1	C1	2846	A
1	C1	2857	G
1	C1	2858	C
1	C1	2863	U
1	C1	2876	OMG
1	C1	2877	G
1	C1	2881	OMG
1	C1	2882	U
1	C1	2883	U
1	C1	2884	C
1	C1	2885	A
1	C1	2887	C
1	C1	2894	U
1	C1	2895	A
1	C1	2903	U
1	C1	2905	A
1	C1	2918	OMC
1	C1	2919	C

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Mol	Chain	Res	Type
1	C1	2929	C
1	C1	2930	A
1	C1	2931	G
1	C1	2937	U
1	C1	2938	U
1	C1	2939	U
1	C1	2940	U
1	C1	2942	C
1	C1	2949	G
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	3049	A
1	C1	3050	C
1	C1	3051	C
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	3125	U
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

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Mol	Chain	Res	Type
1	C1	3185	G
1	C1	3186	A
1	C1	3190	G
1	C1	3200	A
1	C1	3201	A
1	C1	3206	C
1	C1	3210	U
1	C1	3211	U
1	C1	3214	A
1	C1	3217	U
1	C1	3218	U
1	C1	3228	C
1	C1	3229	G
1	C1	3231	G
1	C1	3245	C
1	C1	3254	U
1	C1	3257	A
1	C1	3258	U
1	C1	3259	G
1	C1	3260	U
1	C1	3276	A
1	C1	3282	U
1	C1	3292	U
1	C1	3295	U
1	C1	3297	G
1	C1	3299	U
1	C1	3302	G
1	C1	3310	G
1	C1	3312	G
1	C1	3319	C
1	C1	3323	C
1	C1	3324	C
1	C1	3325	U
1	C1	3331	U
1	C1	3332	A
1	C1	3338	C
2	C2	34	U
2	C2	35	C
2	C2	52	A
2	C2	59	A
2	C2	62	A
2	C2	63	G

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Mol	Chain	Res	Type
2	C2	81	U
2	C2	82	U
2	C2	83	C
2	C2	84	C
2	C2	86	U
2	C2	87	G
2	C2	90	U
2	C2	95	G
2	C2	104	A
2	C2	105	A
2	C2	106	C
2	C2	113	U
2	C2	116	G
2	C2	125	U
2	C2	127	U
2	C2	151	C
2	C2	154	C
3	C3	2	U
3	C3	3	C
4	C4	7	G
4	C4	29	G
4	C4	52	G
4	C4	54	U
4	C4	55	A
4	C4	64	A
4	C4	66	G
4	C4	75	A
4	C4	76	G
4	C4	78	A
4	C4	81	U
4	C4	82	G
4	C4	83	G
4	C4	84	G
4	C4	85	U
4	C4	86	C
4	C4	89	U
4	C4	90	G
4	C4	93	G
4	C4	97	A
4	C4	99	C
4	C4	101	A
4	C4	111	G

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Mol	Chain	Res	Type
4	C4	112	U

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	151	G
1	C1	243	U
1	C1	385	OMG
1	C1	579	G
1	C1	627	OMG
1	C1	646	OMG
1	C1	778	OMC
1	C1	787	OMG
1	C1	898	G
1	C1	1047	A
1	C1	1064	C
1	C1	1077	U
1	C1	1267	C
1	C1	1420	OMC
1	C1	1433	OMG
1	C1	1491	OMC
1	C1	1537	U
1	C1	1812	OMC
1	C1	1836	OMC
1	C1	2157	G
1	C1	2160	C
1	C1	2225	A
1	C1	2280	A
1	C1	2300	OMC
1	C1	2358	OMG
1	C1	2575	C
1	C1	2578	OMG
1	C1	2774	OMG
1	C1	2838	OMC
1	C1	2876	OMG
1	C1	2881	OMG
1	C1	2883	U
1	C1	2918	OMC
1	C1	3079	U
1	C1	3132	A
1	C1	3205	G
1	C1	3210	U

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Mol	Chain	Res	Type
1	C1	3230	G
1	C1	3258	U
1	C1	3298	U
1	C1	3301	C
1	C1	3324	C
1	C1	3330	C

## 5.4 Non-standard residues in protein, DNA, RNA chains

34 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	2300	1	19,22,23	3.02	8 (42%)	25,31,34	2.76	9 (36%)
1	OMG	C1	627	1	23,26,27	2.51	8 (34%)	32,38,41	2.80	18 (56%)
1	OMC	C1	1420	1	19,22,23	3.00	8 (42%)	25,31,34	2.55	9 (36%)
1	OMC	C1	1836	1	19,22,23	3.04	8 (42%)	25,31,34	2.74	11 (44%)
1	OMG	C1	2358	1	23,26,27	2.53	9 (39%)	32,38,41	2.79	18 (56%)
1	OMG	C1	385	1	23,26,27	2.51	9 (39%)	32,38,41	2.91	19 (59%)
1	A2M	C1	1432	1	22,25,26	4.00	12 (54%)	30,36,39	3.34	12 (40%)
1	A2M	C1	389	1	22,25,26	3.95	11 (50%)	30,36,39	3.34	11 (36%)
1	OMG	C1	2881	1	23,26,27	2.47	8 (34%)	32,38,41	2.86	17 (53%)
1	A2M	C1	637	1	22,25,26	3.96	12 (54%)	30,36,39	3.42	14 (46%)
1	OMU	C1	2380	1	19,22,23	3.08	6 (31%)	25,31,34	1.80	5 (20%)
1	OMU	C1	2384	1	19,22,23	3.12	6 (31%)	25,31,34	1.77	4 (16%)
1	OMG	C1	646	1	23,26,27	2.50	8 (34%)	32,38,41	2.86	17 (53%)
1	OMU	C1	1917	1	19,22,23	3.15	6 (31%)	25,31,34	1.83	5 (20%)
1	OMG	C1	2578	1	23,26,27	2.51	9 (39%)	32,38,41	2.84	18 (56%)
1	A2M	C1	858	1	22,25,26	4.01	12 (54%)	30,36,39	3.38	12 (40%)
1	A2M	C1	1223	1	22,25,26	3.97	10 (45%)	30,36,39	3.30	12 (40%)
1	OMC	C1	2838	1	19,22,23	3.08	8 (42%)	25,31,34	2.63	9 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMU	C1	2277	1	19,22,23	3.12	6 (31%)	25,31,34	1.76	5 (20%)
1	A2M	C1	2289	1	22,25,26	4.00	11 (50%)	30,36,39	3.29	14 (46%)
1	OMU	C1	2690	1	19,22,23	3.10	6 (31%)	25,31,34	1.80	5 (20%)
1	A2M	C1	848	1	22,25,26	3.99	11 (50%)	30,36,39	3.39	14 (46%)
1	OMG	C1	787	1	23,26,27	2.46	9 (39%)	32,38,41	2.90	16 (50%)
1	OMC	C1	778	1	19,22,23	3.10	8 (42%)	25,31,34	2.62	9 (36%)
1	OMC	C1	1812	1	19,22,23	3.05	8 (42%)	25,31,34	2.60	11 (44%)
1	OMC	C1	2918	1	19,22,23	3.11	8 (42%)	25,31,34	2.71	9 (36%)
1	OMC	C1	1491	1	19,22,23	2.92	8 (42%)	25,31,34	2.75	11 (44%)
1	OMU	C1	2683	1	19,22,23	3.07	6 (31%)	25,31,34	1.68	5 (20%)
1	OMG	C1	2876	1	23,26,27	2.53	8 (34%)	32,38,41	3.17	16 (50%)
1	A2M	C1	1847	1	22,25,26	3.98	12 (54%)	30,36,39	3.46	13 (43%)
1	OMU	C1	2688	1	19,22,23	3.13	6 (31%)	25,31,34	1.79	5 (20%)
1	OMG	C1	1433	1	23,26,27	2.48	9 (39%)	32,38,41	2.83	18 (56%)
1	OMU	C1	1868	1	19,22,23	3.12	6 (31%)	25,31,34	1.89	5 (20%)
1	OMG	C1	2774	1	23,26,27	2.50	9 (39%)	32,38,41	2.82	17 (53%)

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	2300	1	2/2/5/5	5/9/27/28	0/2/2/2
1	OMG	C1	627	1	2/2/5/5	2/9/27/28	0/3/3/3
1	OMC	C1	1420	1	2/2/5/5	5/9/27/28	0/2/2/2
1	OMC	C1	1836	1	2/2/5/5	4/9/27/28	0/2/2/2
1	OMG	C1	2358	1	2/2/5/5	4/9/27/28	0/3/3/3
1	OMG	C1	385	1	2/2/5/5	5/9/27/28	0/3/3/3
1	A2M	C1	1432	1	-	0/9/27/28	0/3/3/3
1	A2M	C1	389	1	-	3/9/27/28	0/3/3/3
1	OMG	C1	2881	1	2/2/5/5	4/9/27/28	0/3/3/3
1	A2M	C1	637	1	-	0/9/27/28	0/3/3/3
1	OMU	C1	2380	1	-	1/9/27/28	0/2/2/2
1	OMU	C1	2384	1	-	1/9/27/28	0/2/2/2
1	OMG	C1	646	1	2/2/5/5	3/9/27/28	0/3/3/3
1	OMU	C1	1917	1	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	C1	2578	1	2/2/5/5	3/9/27/28	0/3/3/3
1	OMC	C1	2838	1	2/2/5/5	5/9/27/28	0/2/2/2
1	A2M	C1	858	1	-	1/9/27/28	0/3/3/3
1	A2M	C1	1223	1	-	1/9/27/28	0/3/3/3
1	OMU	C1	2277	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	2289	1	-	0/9/27/28	0/3/3/3
1	OMU	C1	2690	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	848	1	-	1/9/27/28	0/3/3/3
1	OMG	C1	787	1	2/2/5/5	4/9/27/28	0/3/3/3
1	OMC	C1	778	1	2/2/5/5	4/9/27/28	0/2/2/2
1	OMC	C1	1812	1	2/2/5/5	4/9/27/28	0/2/2/2
1	OMC	C1	2918	1	2/2/5/5	4/9/27/28	0/2/2/2
1	OMG	C1	2876	1	2/2/5/5	4/9/27/28	0/3/3/3
1	OMC	C1	1491	1	2/2/5/5	6/9/27/28	0/2/2/2
1	OMU	C1	2683	1	-	1/9/27/28	0/2/2/2
1	A2M	C1	1847	1	-	3/9/27/28	0/3/3/3
1	OMU	C1	2688	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	1433	1	2/2/5/5	3/9/27/28	0/3/3/3
1	OMU	C1	1868	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	2774	1	2/2/5/5	4/9/27/28	0/3/3/3

All (289) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	858	A2M	C3'-C2'	-13.16	1.24	1.53
1	C1	2289	A2M	C3'-C2'	-13.03	1.24	1.53
1	C1	1432	A2M	C3'-C2'	-13.00	1.24	1.53
1	C1	848	A2M	C3'-C2'	-12.98	1.24	1.53
1	C1	1847	A2M	C3'-C2'	-12.96	1.24	1.53
1	C1	637	A2M	C3'-C2'	-12.95	1.24	1.53
1	C1	1223	A2M	C3'-C2'	-12.95	1.24	1.53
1	C1	389	A2M	C3'-C2'	-12.66	1.25	1.53
1	C1	1917	OMU	C2-N1	7.68	1.50	1.38
1	C1	2384	OMU	C2-N1	7.55	1.50	1.38
1	C1	1868	OMU	C2-N1	7.51	1.50	1.38
1	C1	2277	OMU	C2-N1	7.49	1.50	1.38
1	C1	2688	OMU	C2-N1	7.48	1.50	1.38
1	C1	2690	OMU	C2-N1	7.42	1.50	1.38
1	C1	2688	OMU	C2-N3	7.36	1.50	1.38
1	C1	2683	OMU	C2-N1	7.35	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2380	OMU	C2-N1	7.29	1.49	1.38
1	C1	2277	OMU	C2-N3	7.29	1.50	1.38
1	C1	1868	OMU	C2-N3	7.27	1.50	1.38
1	C1	2384	OMU	C2-N3	7.26	1.50	1.38
1	C1	1917	OMU	C2-N3	7.25	1.50	1.38
1	C1	2380	OMU	C2-N3	7.21	1.50	1.38
1	C1	2683	OMU	C2-N3	7.19	1.50	1.38
1	C1	2690	OMU	C2-N3	7.15	1.50	1.38
1	C1	2578	OMG	C4-N3	6.73	1.49	1.34
1	C1	2358	OMG	C4-N3	6.68	1.49	1.34
1	C1	385	OMG	C4-N3	6.66	1.49	1.34
1	C1	2876	OMG	C4-N3	6.66	1.49	1.34
1	C1	2774	OMG	C4-N3	6.63	1.49	1.34
1	C1	2881	OMG	C4-N3	6.61	1.49	1.34
1	C1	646	OMG	C4-N3	6.61	1.49	1.34
1	C1	637	A2M	O4'-C4'	-6.56	1.30	1.45
1	C1	389	A2M	O4'-C4'	-6.53	1.30	1.45
1	C1	1223	A2M	O4'-C4'	-6.53	1.30	1.45
1	C1	627	OMG	C4-N3	6.52	1.49	1.34
1	C1	1847	A2M	O4'-C4'	-6.50	1.30	1.45
1	C1	787	OMG	C4-N3	6.50	1.49	1.34
1	C1	1433	OMG	C4-N3	6.44	1.49	1.34
1	C1	858	A2M	O4'-C4'	-6.42	1.30	1.45
1	C1	1432	A2M	O4'-C4'	-6.40	1.30	1.45
1	C1	848	A2M	O4'-C4'	-6.38	1.30	1.45
1	C1	2289	A2M	O4'-C4'	-6.33	1.30	1.45
1	C1	1917	OMU	C6-C5	6.23	1.49	1.35
1	C1	1868	OMU	C6-C5	6.22	1.49	1.35
1	C1	2690	OMU	C6-C5	6.21	1.49	1.35
1	C1	2277	OMU	C6-C5	6.19	1.49	1.35
1	C1	2380	OMU	C6-C5	6.18	1.49	1.35
1	C1	2384	OMU	C6-C5	6.17	1.49	1.35
1	C1	2688	OMU	C6-C5	6.17	1.49	1.35
1	C1	2683	OMU	C6-C5	6.16	1.49	1.35
1	C1	2918	OMC	C4-N4	6.02	1.48	1.33
1	C1	778	OMC	C4-N4	5.99	1.48	1.33
1	C1	778	OMC	C2-N3	5.96	1.48	1.36
1	C1	1836	OMC	C2-N3	5.93	1.48	1.36
1	C1	2918	OMC	C2-N3	5.93	1.48	1.36
1	C1	2300	OMC	C4-N4	5.93	1.48	1.33
1	C1	1812	OMC	C2-N3	5.87	1.48	1.36
1	C1	1836	OMC	C4-N4	5.85	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2838	OMC	C4-N4	5.78	1.47	1.33
1	C1	1812	OMC	C4-N4	5.70	1.47	1.33
1	C1	1420	OMC	C4-N4	5.69	1.47	1.33
1	C1	2300	OMC	C2-N3	5.68	1.47	1.36
1	C1	2838	OMC	C2-N1	5.61	1.51	1.40
1	C1	1491	OMC	C2-N3	5.51	1.47	1.36
1	C1	1432	A2M	C3'-C4'	5.46	1.66	1.53
1	C1	2838	OMC	C6-C5	5.43	1.47	1.35
1	C1	2876	OMG	C2-N3	5.42	1.46	1.33
1	C1	1420	OMC	C2-N3	5.35	1.47	1.36
1	C1	646	OMG	C2-N3	5.34	1.46	1.33
1	C1	848	A2M	C3'-C4'	5.34	1.66	1.53
1	C1	1491	OMC	C4-N4	5.33	1.46	1.33
1	C1	2289	A2M	C3'-C4'	5.33	1.66	1.53
1	C1	858	A2M	C3'-C4'	5.29	1.66	1.53
1	C1	1223	A2M	C3'-C4'	5.25	1.66	1.53
1	C1	2838	OMC	C2-N3	5.22	1.46	1.36
1	C1	2774	OMG	C2-N3	5.22	1.45	1.33
1	C1	627	OMG	C2-N3	5.21	1.45	1.33
1	C1	787	OMG	C2-N3	5.21	1.45	1.33
1	C1	2578	OMG	C2-N3	5.18	1.45	1.33
1	C1	2774	OMG	C2-N2	5.17	1.46	1.34
1	C1	2578	OMG	C2-N2	5.15	1.46	1.34
1	C1	389	A2M	C3'-C4'	5.14	1.66	1.53
1	C1	2876	OMG	C2-N2	5.14	1.46	1.34
1	C1	385	OMG	C2-N3	5.13	1.45	1.33
1	C1	2918	OMC	C2-N1	5.13	1.50	1.40
1	C1	385	OMG	C2-N2	5.13	1.46	1.34
1	C1	2881	OMG	C2-N2	5.13	1.46	1.34
1	C1	2358	OMG	C2-N2	5.12	1.46	1.34
1	C1	627	OMG	C2-N2	5.12	1.46	1.34
1	C1	2881	OMG	C2-N3	5.11	1.45	1.33
1	C1	2358	OMG	C2-N3	5.11	1.45	1.33
1	C1	2918	OMC	C6-C5	5.10	1.46	1.35
1	C1	1433	OMG	C2-N3	5.09	1.45	1.33
1	C1	1812	OMC	C2-N1	5.07	1.50	1.40
1	C1	2300	OMC	C2-N1	5.05	1.50	1.40
1	C1	1433	OMG	C2-N2	5.04	1.46	1.34
1	C1	778	OMC	C2-N1	5.04	1.50	1.40
1	C1	1491	OMC	C2-N1	5.04	1.50	1.40
1	C1	637	A2M	C3'-C4'	5.03	1.65	1.53
1	C1	1847	A2M	C3'-C4'	5.02	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1420	OMC	C6-C5	4.98	1.46	1.35
1	C1	778	OMC	C6-C5	4.97	1.46	1.35
1	C1	787	OMG	C2-N2	4.94	1.45	1.34
1	C1	646	OMG	C2-N2	4.93	1.45	1.34
1	C1	1836	OMC	C2-N1	4.90	1.50	1.40
1	C1	1420	OMC	C2-N1	4.89	1.50	1.40
1	C1	1812	OMC	C4-N3	4.86	1.44	1.34
1	C1	778	OMC	C4-N3	4.84	1.44	1.34
1	C1	1836	OMC	C4-N3	4.79	1.44	1.34
1	C1	1836	OMC	C6-C5	4.76	1.46	1.35
1	C1	1812	OMC	C6-C5	4.73	1.46	1.35
1	C1	2918	OMC	C4-N3	4.70	1.43	1.34
1	C1	2300	OMC	C6-C5	4.66	1.45	1.35
1	C1	2300	OMC	C4-N3	4.63	1.43	1.34
1	C1	1491	OMC	C6-C5	4.58	1.45	1.35
1	C1	1847	A2M	O4'-C1'	4.55	1.52	1.42
1	C1	1420	OMC	C4-N3	4.53	1.43	1.34
1	C1	848	A2M	O4'-C1'	4.47	1.52	1.42
1	C1	2289	A2M	C1'-N9	-4.44	1.34	1.46
1	C1	2289	A2M	O4'-C1'	4.43	1.52	1.42
1	C1	848	A2M	C1'-N9	-4.43	1.34	1.46
1	C1	858	A2M	O4'-C1'	4.43	1.52	1.42
1	C1	637	A2M	C6-N6	4.42	1.45	1.34
1	C1	2688	OMU	C4-N3	4.42	1.46	1.38
1	C1	1491	OMC	C4-N3	4.41	1.43	1.34
1	C1	1432	A2M	O4'-C1'	4.39	1.52	1.42
1	C1	2277	OMU	C4-N3	4.38	1.46	1.38
1	C1	848	A2M	C6-N6	4.37	1.45	1.34
1	C1	389	A2M	C6-N6	4.37	1.45	1.34
1	C1	858	A2M	C6-N6	4.37	1.45	1.34
1	C1	637	A2M	O4'-C1'	4.37	1.52	1.42
1	C1	2384	OMU	C4-N3	4.36	1.46	1.38
1	C1	1223	A2M	C6-N6	4.36	1.45	1.34
1	C1	2289	A2M	C6-N6	4.36	1.45	1.34
1	C1	1432	A2M	C6-N6	4.36	1.45	1.34
1	C1	389	A2M	O4'-C1'	4.35	1.52	1.42
1	C1	1847	A2M	C6-N6	4.34	1.45	1.34
1	C1	1917	OMU	C4-N3	4.32	1.46	1.38
1	C1	2838	OMC	O2-C2	-4.30	1.15	1.23
1	C1	2300	OMC	O2-C2	-4.29	1.15	1.23
1	C1	858	A2M	C1'-N9	-4.29	1.34	1.46
1	C1	2690	OMU	C4-N3	4.28	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1223	A2M	C1'-N9	-4.28	1.34	1.46
1	C1	1847	A2M	C1'-N9	-4.28	1.34	1.46
1	C1	1420	OMC	O2-C2	-4.25	1.15	1.23
1	C1	1223	A2M	O4'-C1'	4.25	1.51	1.42
1	C1	1868	OMU	C4-N3	4.25	1.45	1.38
1	C1	2380	OMU	C4-N3	4.23	1.45	1.38
1	C1	1491	OMC	O2-C2	-4.23	1.15	1.23
1	C1	1836	OMC	O2-C2	-4.17	1.16	1.23
1	C1	2683	OMU	C4-N3	4.17	1.45	1.38
1	C1	1432	A2M	C1'-N9	-4.14	1.34	1.46
1	C1	778	OMC	O2-C2	-4.14	1.16	1.23
1	C1	2918	OMC	O2-C2	-4.13	1.16	1.23
1	C1	1812	OMC	O2-C2	-4.08	1.16	1.23
1	C1	389	A2M	C1'-N9	-4.07	1.35	1.46
1	C1	637	A2M	C1'-N9	-4.04	1.35	1.46
1	C1	2838	OMC	C4-N3	3.96	1.42	1.34
1	C1	389	A2M	O2'-C2'	3.94	1.52	1.42
1	C1	1432	A2M	O2'-C2'	3.64	1.51	1.42
1	C1	2289	A2M	O2'-C2'	3.63	1.51	1.42
1	C1	858	A2M	O2'-C2'	3.62	1.51	1.42
1	C1	848	A2M	O2'-C2'	3.61	1.51	1.42
1	C1	1223	A2M	O2'-C2'	3.59	1.51	1.42
1	C1	637	A2M	O2'-C2'	3.58	1.51	1.42
1	C1	1847	A2M	O2'-C2'	3.56	1.51	1.42
1	C1	389	A2M	C2'-C1'	3.40	1.61	1.53
1	C1	2876	OMG	C5-N7	-3.25	1.32	1.39
1	C1	627	OMG	C5-N7	-3.16	1.32	1.39
1	C1	2838	OMC	C5-C4	3.13	1.50	1.42
1	C1	848	A2M	C2'-C1'	3.08	1.60	1.53
1	C1	1847	A2M	C2'-C1'	3.08	1.60	1.53
1	C1	637	A2M	C2'-C1'	3.07	1.60	1.53
1	C1	646	OMG	O6-C6	-3.05	1.17	1.23
1	C1	646	OMG	C5-N7	-3.04	1.33	1.39
1	C1	1432	A2M	C2'-C1'	3.03	1.60	1.53
1	C1	787	OMG	C5-N7	-3.03	1.33	1.39
1	C1	2289	A2M	C5-C4	-3.00	1.33	1.39
1	C1	2876	OMG	O6-C6	-3.00	1.17	1.23
1	C1	2881	OMG	O6-C6	-3.00	1.17	1.23
1	C1	1223	A2M	C5-C4	-2.99	1.33	1.39
1	C1	2289	A2M	C2'-C1'	2.97	1.60	1.53
1	C1	2358	OMG	C5-N7	-2.97	1.33	1.39
1	C1	858	A2M	C5-C4	-2.94	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1432	A2M	C5-C4	-2.94	1.33	1.39
1	C1	848	A2M	C5-C4	-2.92	1.33	1.39
1	C1	2881	OMG	C5-N7	-2.91	1.33	1.39
1	C1	858	A2M	C2'-C1'	2.91	1.60	1.53
1	C1	2838	OMC	C6-N1	2.90	1.45	1.38
1	C1	1223	A2M	C2'-C1'	2.90	1.60	1.53
1	C1	2358	OMG	O6-C6	-2.90	1.18	1.23
1	C1	389	A2M	C5-C4	-2.88	1.33	1.39
1	C1	627	OMG	O6-C6	-2.87	1.18	1.23
1	C1	1433	OMG	O6-C6	-2.86	1.18	1.23
1	C1	1847	A2M	C5-C4	-2.86	1.34	1.39
1	C1	2774	OMG	C5-N7	-2.85	1.33	1.39
1	C1	787	OMG	O6-C6	-2.82	1.18	1.23
1	C1	2918	OMC	C5-C4	2.81	1.49	1.42
1	C1	637	A2M	C5-C4	-2.80	1.34	1.39
1	C1	778	OMC	C5-C4	2.80	1.49	1.42
1	C1	2578	OMG	C5-N7	-2.80	1.33	1.39
1	C1	2578	OMG	O6-C6	-2.79	1.18	1.23
1	C1	1433	OMG	C5-N7	-2.77	1.33	1.39
1	C1	1917	OMU	C6-N1	2.77	1.44	1.38
1	C1	385	OMG	O6-C6	-2.77	1.18	1.23
1	C1	2774	OMG	O6-C6	-2.77	1.18	1.23
1	C1	1420	OMC	C6-N1	2.76	1.44	1.38
1	C1	2918	OMC	C6-N1	2.74	1.44	1.38
1	C1	2690	OMU	C6-N1	2.73	1.44	1.38
1	C1	385	OMG	C2-N1	2.72	1.44	1.37
1	C1	385	OMG	C5-N7	-2.72	1.33	1.39
1	C1	2688	OMU	C6-N1	2.72	1.44	1.38
1	C1	389	A2M	C5-N7	-2.71	1.34	1.39
1	C1	1420	OMC	C5-C4	2.70	1.49	1.42
1	C1	2876	OMG	C2-N1	2.70	1.44	1.37
1	C1	2277	OMU	C6-N1	2.69	1.44	1.38
1	C1	1432	A2M	C5-N7	-2.68	1.34	1.39
1	C1	1223	A2M	C5-N7	-2.68	1.34	1.39
1	C1	637	A2M	C5-N7	-2.67	1.34	1.39
1	C1	1433	OMG	C2-N1	2.67	1.44	1.37
1	C1	2380	OMU	C6-N1	2.66	1.44	1.38
1	C1	778	OMC	C6-N1	2.66	1.44	1.38
1	C1	2683	OMU	C6-N1	2.65	1.44	1.38
1	C1	1868	OMU	C6-N1	2.64	1.44	1.38
1	C1	858	A2M	C5-N7	-2.63	1.34	1.39
1	C1	2384	OMU	C6-N1	2.63	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1812	OMC	C5-C4	2.63	1.49	1.42
1	C1	1847	A2M	C5-N7	-2.62	1.34	1.39
1	C1	2289	A2M	C5-N7	-2.59	1.34	1.39
1	C1	627	OMG	C4-N9	-2.59	1.31	1.38
1	C1	385	OMG	C5-C6	2.57	1.54	1.44
1	C1	1836	OMC	C5-C4	2.56	1.48	1.42
1	C1	2300	OMC	C5-C4	2.55	1.48	1.42
1	C1	1491	OMC	C5-C4	2.55	1.48	1.42
1	C1	1433	OMG	C6-N1	2.54	1.43	1.38
1	C1	2578	OMG	C2-N1	2.53	1.43	1.37
1	C1	385	OMG	C6-N1	2.52	1.43	1.38
1	C1	848	A2M	C5-N7	-2.52	1.34	1.39
1	C1	2774	OMG	C2-N1	2.51	1.43	1.37
1	C1	1836	OMC	C6-N1	2.51	1.44	1.38
1	C1	2358	OMG	C2-N1	2.50	1.43	1.37
1	C1	1812	OMC	C6-N1	2.49	1.44	1.38
1	C1	2300	OMC	C6-N1	2.48	1.44	1.38
1	C1	787	OMG	C4-N9	-2.48	1.31	1.38
1	C1	646	OMG	C4-N9	-2.46	1.31	1.38
1	C1	2881	OMG	C4-N9	-2.46	1.31	1.38
1	C1	2774	OMG	C6-N1	2.46	1.43	1.38
1	C1	646	OMG	C2-N1	2.45	1.43	1.37
1	C1	787	OMG	C2-N1	2.45	1.43	1.37
1	C1	627	OMG	C2-N1	2.44	1.43	1.37
1	C1	1491	OMC	C6-N1	2.43	1.43	1.38
1	C1	2876	OMG	C4-N9	-2.43	1.31	1.38
1	C1	1432	A2M	O3'-C3'	2.41	1.48	1.43
1	C1	2358	OMG	C4-N9	-2.40	1.31	1.38
1	C1	2881	OMG	C2-N1	2.40	1.43	1.37
1	C1	1433	OMG	C4-N9	-2.39	1.32	1.38
1	C1	2774	OMG	C4-N9	-2.38	1.32	1.38
1	C1	1868	OMU	C5-C4	2.38	1.48	1.43
1	C1	2358	OMG	C6-N1	2.37	1.43	1.38
1	C1	2876	OMG	C6-N1	2.36	1.43	1.38
1	C1	1433	OMG	C5-C6	2.35	1.53	1.44
1	C1	2690	OMU	C5-C4	2.33	1.48	1.43
1	C1	2578	OMG	C5-C6	2.32	1.53	1.44
1	C1	2578	OMG	C6-N1	2.29	1.43	1.38
1	C1	2774	OMG	C5-C6	2.26	1.52	1.44
1	C1	2380	OMU	C5-C4	2.24	1.48	1.43
1	C1	2688	OMU	C5-C4	2.23	1.48	1.43
1	C1	627	OMG	C6-N1	2.23	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2881	OMG	C5-C6	2.22	1.52	1.44
1	C1	2683	OMU	C5-C4	2.22	1.48	1.43
1	C1	2384	OMU	C5-C4	2.22	1.48	1.43
1	C1	2358	OMG	C5-C6	2.21	1.52	1.44
1	C1	1917	OMU	C5-C4	2.21	1.48	1.43
1	C1	2277	OMU	C5-C4	2.20	1.48	1.43
1	C1	1847	A2M	C8-N9	-2.18	1.33	1.37
1	C1	787	OMG	C6-N1	2.16	1.42	1.38
1	C1	2578	OMG	C4-N9	-2.15	1.32	1.38
1	C1	787	OMG	C5-C6	2.13	1.52	1.44
1	C1	637	A2M	C8-N9	-2.09	1.34	1.37
1	C1	848	A2M	O3'-C3'	2.08	1.48	1.43
1	C1	385	OMG	C4-N9	-2.05	1.32	1.38
1	C1	858	A2M	O3'-C3'	2.05	1.48	1.43
1	C1	1432	A2M	C8-N9	-2.03	1.34	1.37
1	C1	389	A2M	O3'-C3'	2.02	1.48	1.43
1	C1	646	OMG	C5-C6	2.02	1.52	1.44
1	C1	858	A2M	C8-N9	-2.02	1.34	1.37
1	C1	2289	A2M	O3'-C3'	2.02	1.47	1.43
1	C1	1847	A2M	O3'-C3'	2.01	1.47	1.43
1	C1	637	A2M	O3'-C3'	2.00	1.47	1.43

All (393) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1847	A2M	C1'-N9-C8	-9.48	106.06	127.09
1	C1	637	A2M	C1'-N9-C8	-9.32	106.41	127.09
1	C1	858	A2M	C1'-N9-C8	-9.05	107.00	127.09
1	C1	1432	A2M	C1'-N9-C8	-8.90	107.33	127.09
1	C1	389	A2M	C1'-N9-C8	-8.88	107.39	127.09
1	C1	1223	A2M	C1'-N9-C8	-8.80	107.56	127.09
1	C1	848	A2M	C1'-N9-C8	-8.75	107.68	127.09
1	C1	2289	A2M	C1'-N9-C8	-8.26	108.77	127.09
1	C1	1847	A2M	C4-N9-C1'	8.20	145.82	126.63
1	C1	637	A2M	C4-N9-C1'	8.20	145.81	126.63
1	C1	1432	A2M	C4-N9-C1'	7.81	144.90	126.63
1	C1	389	A2M	C4-N9-C1'	7.78	144.84	126.63
1	C1	858	A2M	C4-N9-C1'	7.77	144.81	126.63
1	C1	1223	A2M	C4-N9-C1'	7.56	144.31	126.63
1	C1	2876	OMG	C1'-N9-C8	-7.51	105.39	126.73
1	C1	848	A2M	C4-N9-C1'	7.38	143.89	126.63
1	C1	2289	A2M	C4-N9-C1'	6.97	142.94	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2918	OMC	C2'-C1'-N1	6.30	126.19	114.24
1	C1	2918	OMC	O2'-C2'-C1'	6.27	120.89	108.99
1	C1	2300	OMC	O2'-C2'-C1'	6.24	120.85	108.99
1	C1	778	OMC	O2'-C2'-C1'	6.18	120.72	108.99
1	C1	2289	A2M	N3-C2-N1	-6.14	119.29	128.58
1	C1	1491	OMC	O2'-C2'-C1'	6.10	120.56	108.99
1	C1	858	A2M	N3-C2-N1	-6.09	119.36	128.58
1	C1	1836	OMC	O2'-C2'-C1'	6.08	120.53	108.99
1	C1	2838	OMC	O2'-C2'-C1'	6.07	120.52	108.99
1	C1	1420	OMC	O2'-C2'-C1'	6.07	120.51	108.99
1	C1	787	OMG	C1'-N9-C8	-6.02	109.62	126.73
1	C1	2876	OMG	C1'-N9-C4	5.97	144.13	126.49
1	C1	646	OMG	C1'-N9-C8	-5.96	109.80	126.73
1	C1	1847	A2M	N3-C2-N1	-5.92	119.63	128.58
1	C1	1868	OMU	C4-N3-C2	-5.86	119.33	126.61
1	C1	1223	A2M	N3-C2-N1	-5.83	119.76	128.58
1	C1	389	A2M	N3-C2-N1	-5.83	119.76	128.58
1	C1	627	OMG	O2'-C2'-C1'	5.83	120.05	108.99
1	C1	2881	OMG	O2'-C2'-C1'	5.82	120.03	108.99
1	C1	848	A2M	N3-C2-N1	-5.81	119.78	128.58
1	C1	385	OMG	O2'-C2'-C1'	5.80	120.01	108.99
1	C1	2876	OMG	O2'-C2'-C1'	5.77	119.96	108.99
1	C1	778	OMC	C2'-C1'-N1	5.77	125.19	114.24
1	C1	787	OMG	O2'-C2'-C1'	5.73	119.86	108.99
1	C1	1812	OMC	O2'-C2'-C1'	5.72	119.86	108.99
1	C1	2578	OMG	O2'-C2'-C1'	5.69	119.80	108.99
1	C1	1432	A2M	N3-C2-N1	-5.69	119.97	128.58
1	C1	858	A2M	N6-C6-N1	-5.68	105.72	118.38
1	C1	2289	A2M	N6-C6-N1	-5.65	105.80	118.38
1	C1	1847	A2M	N6-C6-N1	-5.64	105.81	118.38
1	C1	637	A2M	N6-C6-N1	-5.64	105.81	118.38
1	C1	2690	OMU	C4-N3-C2	-5.61	119.64	126.61
1	C1	637	A2M	N3-C2-N1	-5.61	120.09	128.58
1	C1	2300	OMC	C2'-C1'-N1	5.60	124.87	114.24
1	C1	1223	A2M	N6-C6-N1	-5.60	105.91	118.38
1	C1	2774	OMG	O2'-C2'-C1'	5.58	119.59	108.99
1	C1	848	A2M	N6-C6-N1	-5.57	105.98	118.38
1	C1	2380	OMU	C4-N3-C2	-5.54	119.73	126.61
1	C1	1432	A2M	N6-C6-N1	-5.53	106.07	118.38
1	C1	2358	OMG	O2'-C2'-C1'	5.51	119.46	108.99
1	C1	2688	OMU	C4-N3-C2	-5.49	119.80	126.61
1	C1	389	A2M	N6-C6-N1	-5.48	106.16	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1433	OMG	O2'-C2'-C1'	5.45	119.33	108.99
1	C1	1836	OMC	C2'-C1'-N1	5.44	124.57	114.24
1	C1	646	OMG	O2'-C2'-C1'	5.42	119.28	108.99
1	C1	627	OMG	C1'-N9-C8	-5.41	111.37	126.73
1	C1	2384	OMU	C4-N3-C2	-5.39	119.92	126.61
1	C1	2277	OMU	C4-N3-C2	-5.35	119.97	126.61
1	C1	1917	OMU	C4-N3-C2	-5.30	120.03	126.61
1	C1	2838	OMC	C2'-C1'-N1	5.22	124.15	114.24
1	C1	1491	OMC	C2'-C1'-N1	5.22	124.14	114.24
1	C1	385	OMG	C5-C4-N3	-5.18	120.14	128.39
1	C1	637	A2M	C5-C4-N3	-5.12	119.66	126.72
1	C1	2683	OMU	C4-N3-C2	-5.04	120.36	126.61
1	C1	2881	OMG	C1'-N9-C8	-5.02	112.48	126.73
1	C1	2578	OMG	C5-C4-N3	-4.94	120.52	128.39
1	C1	1847	A2M	C5-C4-N3	-4.92	119.94	126.72
1	C1	385	OMG	C2-N3-C4	4.92	120.78	112.30
1	C1	1432	A2M	C5-C4-N3	-4.90	119.97	126.72
1	C1	1420	OMC	C2'-C1'-N1	4.87	123.48	114.24
1	C1	2838	OMC	O4'-C1'-N1	4.86	119.37	108.36
1	C1	2358	OMG	C1'-N9-C8	-4.86	112.93	126.73
1	C1	2876	OMG	C2'-C1'-N9	4.86	123.46	114.24
1	C1	389	A2M	C5-C4-N3	-4.82	120.08	126.72
1	C1	2774	OMG	C1'-N9-C8	-4.80	113.11	126.73
1	C1	2876	OMG	C5-C4-N3	-4.73	120.86	128.39
1	C1	787	OMG	C1'-N9-C4	4.68	140.32	126.49
1	C1	2578	OMG	C2-N3-C4	4.68	120.36	112.30
1	C1	858	A2M	C5-C4-N3	-4.66	120.30	126.72
1	C1	848	A2M	C5-C4-N3	-4.65	120.31	126.72
1	C1	1433	OMG	O4'-C1'-N9	4.64	118.87	108.36
1	C1	385	OMG	O4'-C1'-N9	4.63	118.84	108.36
1	C1	646	OMG	C5-C4-N3	-4.61	121.05	128.39
1	C1	2578	OMG	C1'-N9-C8	-4.61	113.63	126.73
1	C1	2289	A2M	C5-C6-N6	4.58	134.63	123.29
1	C1	2881	OMG	C2'-C1'-N9	4.57	122.91	114.24
1	C1	1223	A2M	C5-C4-N3	-4.55	120.45	126.72
1	C1	2578	OMG	O4'-C1'-N9	4.53	118.63	108.36
1	C1	646	OMG	O3'-C3'-C4'	4.52	124.06	111.08
1	C1	2358	OMG	C5-C4-N3	-4.50	121.23	128.39
1	C1	1433	OMG	C5-C4-N3	-4.48	121.25	128.39
1	C1	858	A2M	C5-C6-N6	4.47	134.37	123.29
1	C1	2358	OMG	C2-N3-C4	4.47	120.00	112.30
1	C1	2876	OMG	C5'-C4'-C3'	4.46	131.28	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	848	A2M	N9-C8-N7	-4.45	107.62	113.94
1	C1	2358	OMG	O3'-C3'-C4'	4.44	123.84	111.08
1	C1	2300	OMC	C1'-N1-C6	-4.44	111.29	120.78
1	C1	2578	OMG	O3'-C3'-C4'	4.43	123.81	111.08
1	C1	2774	OMG	O4'-C1'-N9	4.43	118.39	108.36
1	C1	1223	A2M	C5-C6-N6	4.43	134.24	123.29
1	C1	637	A2M	C5-C6-N6	4.42	134.22	123.29
1	C1	1491	OMC	C1'-N1-C6	-4.42	111.34	120.78
1	C1	2774	OMG	C5-C4-N3	-4.41	121.37	128.39
1	C1	1847	A2M	C5-C6-N6	4.40	134.19	123.29
1	C1	2358	OMG	O4'-C1'-N9	4.38	118.29	108.36
1	C1	2289	A2M	N9-C8-N7	-4.37	107.73	113.94
1	C1	787	OMG	C5-C4-N3	-4.35	121.46	128.39
1	C1	1433	OMG	C2-N3-C4	4.35	119.79	112.30
1	C1	1433	OMG	O3'-C3'-C4'	4.34	123.56	111.08
1	C1	2881	OMG	O3'-C3'-C2'	4.34	123.32	111.19
1	C1	2881	OMG	C5-C4-N3	-4.32	121.51	128.39
1	C1	848	A2M	C5-C6-N6	4.32	133.97	123.29
1	C1	1812	OMC	C1'-N1-C6	-4.32	111.56	120.78
1	C1	1432	A2M	C5-C6-N6	4.31	133.97	123.29
1	C1	2300	OMC	C1'-N1-C2	4.31	127.96	118.44
1	C1	627	OMG	O3'-C3'-C4'	4.31	123.46	111.08
1	C1	389	A2M	C5-C6-N6	4.31	133.95	123.29
1	C1	787	OMG	O4'-C1'-N9	4.30	118.09	108.36
1	C1	1836	OMC	C1'-N1-C6	-4.27	111.65	120.78
1	C1	2289	A2M	O4'-C1'-N9	4.24	116.24	108.09
1	C1	385	OMG	C1'-N9-C8	-4.24	114.68	126.73
1	C1	1836	OMC	C1'-N1-C2	4.23	127.78	118.44
1	C1	1223	A2M	N9-C8-N7	-4.22	107.95	113.94
1	C1	858	A2M	N9-C8-N7	-4.20	107.98	113.94
1	C1	1433	OMG	C1'-N9-C8	-4.20	114.81	126.73
1	C1	848	A2M	O4'-C1'-N9	4.18	116.12	108.09
1	C1	1812	OMC	O3'-C3'-C4'	4.17	123.05	111.08
1	C1	2774	OMG	C2-N3-C4	4.16	119.47	112.30
1	C1	627	OMG	C5-C4-N3	-4.14	121.80	128.39
1	C1	2876	OMG	O3'-C3'-C2'	4.14	122.78	111.19
1	C1	2774	OMG	C2'-C1'-N9	4.13	122.09	114.24
1	C1	2289	A2M	C5-C4-N3	-4.13	121.02	126.72
1	C1	2774	OMG	O3'-C3'-C4'	4.13	122.95	111.08
1	C1	1847	A2M	N9-C8-N7	-4.12	108.09	113.94
1	C1	1432	A2M	O4'-C1'-N9	4.12	116.00	108.09
1	C1	646	OMG	O4'-C1'-N9	4.11	117.68	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2918	OMC	O3'-C3'-C2'	4.11	122.70	111.19
1	C1	787	OMG	O3'-C3'-C2'	4.11	122.69	111.19
1	C1	1812	OMC	C2'-C1'-N1	4.09	122.00	114.24
1	C1	2380	OMU	N3-C2-N1	4.08	120.21	114.89
1	C1	2881	OMG	O4'-C1'-N9	4.08	117.61	108.36
1	C1	2881	OMG	O3'-C3'-C4'	4.07	122.77	111.08
1	C1	2881	OMG	C2-N3-C4	4.05	119.27	112.30
1	C1	1432	A2M	N9-C8-N7	-4.04	108.20	113.94
1	C1	1491	OMC	O3'-C3'-C4'	4.03	122.66	111.08
1	C1	1868	OMU	N3-C2-N1	4.03	120.13	114.89
1	C1	385	OMG	O3'-C3'-C4'	4.02	122.64	111.08
1	C1	1836	OMC	O3'-C3'-C4'	4.01	122.60	111.08
1	C1	2918	OMC	O4'-C1'-N1	4.01	117.44	108.36
1	C1	858	A2M	O4'-C1'-N9	4.01	115.78	108.09
1	C1	2300	OMC	O3'-C3'-C4'	4.01	122.59	111.08
1	C1	2690	OMU	N3-C2-N1	4.00	120.10	114.89
1	C1	787	OMG	O3'-C3'-C4'	4.00	122.57	111.08
1	C1	2876	OMG	O3'-C3'-C4'	4.00	122.56	111.08
1	C1	389	A2M	N9-C8-N7	-4.00	108.27	113.94
1	C1	637	A2M	N9-C8-N7	-3.99	108.27	113.94
1	C1	1917	OMU	N3-C2-N1	3.97	120.06	114.89
1	C1	646	OMG	C1'-N9-C4	3.97	138.22	126.49
1	C1	1433	OMG	C2'-C1'-N9	3.95	121.74	114.24
1	C1	627	OMG	C5'-C4'-C3'	3.95	129.44	115.21
1	C1	1420	OMC	O3'-C3'-C4'	3.95	122.42	111.08
1	C1	787	OMG	C2'-C1'-N9	3.94	121.72	114.24
1	C1	2876	OMG	N9-C4-N3	3.94	133.83	125.95
1	C1	1420	OMC	O3'-C3'-C2'	3.94	122.21	111.19
1	C1	627	OMG	C2-N3-C4	3.93	119.07	112.30
1	C1	778	OMC	O3'-C3'-C4'	3.92	122.34	111.08
1	C1	778	OMC	O4'-C1'-N1	3.92	117.24	108.36
1	C1	1812	OMC	O4'-C1'-N1	3.91	117.23	108.36
1	C1	627	OMG	O4'-C1'-N9	3.88	117.15	108.36
1	C1	1223	A2M	O4'-C1'-N9	3.88	115.53	108.09
1	C1	1491	OMC	C1'-N1-C2	3.87	126.99	118.44
1	C1	1812	OMC	C1'-N1-C2	3.87	126.99	118.44
1	C1	2838	OMC	O3'-C3'-C2'	3.86	122.00	111.19
1	C1	646	OMG	C5'-C4'-C3'	3.86	129.09	115.21
1	C1	1836	OMC	C5'-C4'-C3'	3.85	129.09	115.21
1	C1	646	OMG	C2-N3-C4	3.84	118.92	112.30
1	C1	2384	OMU	N3-C2-N1	3.82	119.87	114.89
1	C1	385	OMG	O3'-C3'-C2'	3.82	121.88	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2838	OMC	O3'-C3'-C4'	3.82	122.04	111.08
1	C1	2876	OMG	C2-N3-C4	3.81	118.87	112.30
1	C1	2838	OMC	O2-C2-N3	-3.80	116.34	122.33
1	C1	1491	OMC	C5'-C4'-C3'	3.80	128.88	115.21
1	C1	2300	OMC	C5'-C4'-C3'	3.79	128.86	115.21
1	C1	2683	OMU	N3-C2-N1	3.77	119.81	114.89
1	C1	2774	OMG	O3'-C3'-C2'	3.76	121.72	111.19
1	C1	2277	OMU	N3-C2-N1	3.75	119.78	114.89
1	C1	2688	OMU	N3-C2-N1	3.75	119.77	114.89
1	C1	2881	OMG	C1'-N9-C4	3.74	137.55	126.49
1	C1	2358	OMG	C5'-C4'-C3'	3.74	128.67	115.21
1	C1	1420	OMC	O4'-C1'-N1	3.73	116.82	108.36
1	C1	385	OMG	O4'-C4'-C5'	3.73	121.30	109.33
1	C1	778	OMC	C5'-C4'-C3'	3.73	128.64	115.21
1	C1	1491	OMC	O3'-C3'-C2'	3.72	121.61	111.19
1	C1	2918	OMC	O3'-C3'-C4'	3.72	121.78	111.08
1	C1	778	OMC	O3'-C3'-C2'	3.72	121.59	111.19
1	C1	1433	OMG	O3'-C3'-C2'	3.72	121.59	111.19
1	C1	2774	OMG	C5'-C4'-C3'	3.71	128.57	115.21
1	C1	1812	OMC	C5'-C4'-C3'	3.70	128.52	115.21
1	C1	1433	OMG	C5'-C4'-C3'	3.70	128.51	115.21
1	C1	2881	OMG	C5'-C4'-C3'	3.69	128.50	115.21
1	C1	1836	OMC	O3'-C3'-C2'	3.69	121.52	111.19
1	C1	2578	OMG	C5'-C4'-C3'	3.69	128.49	115.21
1	C1	2918	OMC	C5'-C4'-C3'	3.69	128.48	115.21
1	C1	385	OMG	C2'-C1'-N9	3.68	121.23	114.24
1	C1	2838	OMC	C5'-C4'-C3'	3.68	128.46	115.21
1	C1	1847	A2M	O4'-C1'-N9	3.68	115.16	108.09
1	C1	637	A2M	O4'-C1'-N9	3.66	115.12	108.09
1	C1	787	OMG	C2-N3-C4	3.65	118.59	112.30
1	C1	389	A2M	O4'-C1'-N9	3.65	115.11	108.09
1	C1	787	OMG	C5'-C4'-C3'	3.65	128.36	115.21
1	C1	1868	OMU	C5-C4-N3	3.64	119.89	114.80
1	C1	1491	OMC	O4'-C1'-N1	3.63	116.59	108.36
1	C1	2300	OMC	O3'-C3'-C2'	3.61	121.28	111.19
1	C1	2688	OMU	C5-C4-N3	3.61	119.85	114.80
1	C1	646	OMG	N9-C4-N3	3.60	133.15	125.95
1	C1	2690	OMU	C5-C4-N3	3.58	119.81	114.80
1	C1	2876	OMG	O6-C6-C5	-3.57	117.11	126.53
1	C1	787	OMG	O4'-C4'-C5'	3.56	120.75	109.33
1	C1	2578	OMG	O3'-C3'-C2'	3.56	121.14	111.19
1	C1	627	OMG	O3'-C3'-C2'	3.55	121.14	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	627	OMG	C1'-N9-C4	3.55	136.98	126.49
1	C1	2358	OMG	N9-C8-N7	-3.55	106.82	113.40
1	C1	2578	OMG	O4'-C4'-C5'	3.55	120.69	109.33
1	C1	627	OMG	N9-C8-N7	-3.53	106.86	113.40
1	C1	848	A2M	C2'-C1'-N9	-3.51	107.97	113.75
1	C1	1847	A2M	C2-N3-C4	3.51	120.40	111.83
1	C1	646	OMG	N9-C8-N7	-3.51	106.89	113.40
1	C1	1420	OMC	C5'-C4'-C3'	3.51	127.84	115.21
1	C1	2881	OMG	O4'-C4'-C5'	3.50	120.56	109.33
1	C1	2277	OMU	C5-C4-N3	3.50	119.70	114.80
1	C1	2384	OMU	C5-C4-N3	3.50	119.70	114.80
1	C1	1836	OMC	O4'-C1'-N1	3.50	116.28	108.36
1	C1	2380	OMU	C5-C4-N3	3.49	119.69	114.80
1	C1	2774	OMG	C1'-N9-C4	3.49	136.80	126.49
1	C1	1433	OMG	N9-C8-N7	-3.49	106.93	113.40
1	C1	646	OMG	O3'-C3'-C2'	3.48	120.94	111.19
1	C1	858	A2M	C2-N3-C4	3.48	120.33	111.83
1	C1	1491	OMC	O4'-C4'-C5'	3.47	120.44	109.33
1	C1	385	OMG	C5'-C4'-C3'	3.45	127.63	115.21
1	C1	2774	OMG	O4'-C4'-C5'	3.44	120.35	109.33
1	C1	637	A2M	C2-N3-C4	3.43	120.22	111.83
1	C1	1917	OMU	C5-C4-N3	3.43	119.60	114.80
1	C1	1432	A2M	C2-N3-C4	3.43	120.20	111.83
1	C1	2300	OMC	O4'-C1'-N1	3.41	116.09	108.36
1	C1	2774	OMG	N9-C8-N7	-3.40	107.09	113.40
1	C1	389	A2M	C2-N3-C4	3.39	120.11	111.83
1	C1	2918	OMC	O4'-C4'-C5'	3.37	120.14	109.33
1	C1	2838	OMC	O4'-C4'-C5'	3.37	120.14	109.33
1	C1	2881	OMG	N9-C8-N7	-3.36	107.16	113.40
1	C1	848	A2M	C2-N3-C4	3.36	120.04	111.83
1	C1	2358	OMG	O4'-C4'-C5'	3.35	120.08	109.33
1	C1	1433	OMG	O4'-C4'-C5'	3.35	120.07	109.33
1	C1	2578	OMG	N9-C8-N7	-3.34	107.21	113.40
1	C1	1420	OMC	O4'-C4'-C5'	3.33	120.02	109.33
1	C1	2358	OMG	O3'-C3'-C2'	3.32	120.48	111.19
1	C1	385	OMG	N9-C8-N7	-3.31	107.26	113.40
1	C1	1223	A2M	C2-N3-C4	3.30	119.89	111.83
1	C1	1812	OMC	O3'-C3'-C2'	3.30	120.41	111.19
1	C1	2289	A2M	C2'-C1'-N9	-3.29	108.34	113.75
1	C1	778	OMC	O4'-C4'-C5'	3.26	119.76	109.33
1	C1	627	OMG	C2'-C1'-N9	3.25	120.40	114.24
1	C1	1836	OMC	O4'-C4'-C5'	3.25	119.73	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1812	OMC	O4'-C4'-C5'	3.24	119.73	109.33
1	C1	627	OMG	O4'-C4'-C5'	3.24	119.72	109.33
1	C1	2683	OMU	C5-C4-N3	3.23	119.33	114.80
1	C1	2918	OMC	C1'-N1-C2	3.23	125.57	118.44
1	C1	2289	A2M	C2-N3-C4	3.23	119.71	111.83
1	C1	1420	OMC	C1'-N1-C6	-3.20	113.94	120.78
1	C1	646	OMG	O4'-C4'-C5'	3.20	119.59	109.33
1	C1	787	OMG	N9-C4-N3	3.19	132.33	125.95
1	C1	787	OMG	N9-C8-N7	-3.18	107.50	113.40
1	C1	385	OMG	C1'-N9-C4	3.18	135.88	126.49
1	C1	2578	OMG	C1'-N9-C4	3.15	135.79	126.49
1	C1	2358	OMG	C1'-N9-C4	3.15	135.78	126.49
1	C1	778	OMC	C1'-N1-C2	3.12	125.33	118.44
1	C1	1420	OMC	C1'-N1-C2	3.11	125.31	118.44
1	C1	2300	OMC	O4'-C4'-C5'	3.11	119.29	109.33
1	C1	1433	OMG	C1'-N9-C4	3.09	135.62	126.49
1	C1	2578	OMG	N9-C4-N3	3.07	132.09	125.95
1	C1	1847	A2M	N3-C4-N9	3.07	132.39	127.17
1	C1	778	OMC	C1'-N1-C6	-3.07	114.22	120.78
1	C1	637	A2M	N3-C4-N9	3.05	132.36	127.17
1	C1	2688	OMU	O4-C4-C5	-3.03	119.93	125.16
1	C1	2358	OMG	N9-C4-N3	3.03	132.00	125.95
1	C1	848	A2M	C5-N7-C8	3.02	108.20	103.45
1	C1	385	OMG	N9-C4-N3	2.99	131.93	125.95
1	C1	627	OMG	N9-C4-N3	2.98	131.91	125.95
1	C1	2358	OMG	C2'-C1'-N9	2.94	119.83	114.24
1	C1	1917	OMU	C1'-N1-C2	2.94	122.88	117.59
1	C1	389	A2M	N3-C4-N9	2.92	132.13	127.17
1	C1	2774	OMG	N9-C4-N3	2.90	131.75	125.95
1	C1	858	A2M	N3-C4-N9	2.88	132.06	127.17
1	C1	637	A2M	C5-N7-C8	2.88	107.97	103.45
1	C1	2876	OMG	O4'-C4'-C5'	2.88	118.55	109.33
1	C1	385	OMG	C2-N1-C6	-2.88	119.90	125.11
1	C1	1433	OMG	C2-N1-C6	-2.87	119.90	125.11
1	C1	1432	A2M	N3-C4-N9	2.87	132.05	127.17
1	C1	1432	A2M	C5-N7-C8	2.87	107.96	103.45
1	C1	2384	OMU	O4-C4-C5	-2.86	120.23	125.16
1	C1	646	OMG	O6-C6-C5	-2.85	119.02	126.53
1	C1	1847	A2M	C5-N7-C8	2.84	107.92	103.45
1	C1	1868	OMU	O4-C4-C5	-2.83	120.27	125.16
1	C1	2918	OMC	C1'-N1-C6	-2.83	114.72	120.78
1	C1	2876	OMG	O4'-C1'-N9	2.83	114.77	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	389	A2M	C5-N7-C8	2.82	107.88	103.45
1	C1	2881	OMG	N9-C4-N3	2.81	131.58	125.95
1	C1	1223	A2M	C5-N7-C8	2.81	107.86	103.45
1	C1	2289	A2M	C5-N7-C8	2.81	107.86	103.45
1	C1	646	OMG	C2'-C1'-N9	2.80	119.56	114.24
1	C1	848	A2M	N3-C4-N9	2.80	131.93	127.17
1	C1	2277	OMU	O4-C4-C5	-2.80	120.33	125.16
1	C1	858	A2M	C5-N7-C8	2.79	107.83	103.45
1	C1	2380	OMU	O4-C4-C5	-2.77	120.39	125.16
1	C1	2578	OMG	C2'-C1'-N9	2.76	119.47	114.24
1	C1	1917	OMU	O4-C4-C5	-2.75	120.42	125.16
1	C1	2876	OMG	N9-C8-N7	-2.75	108.30	113.40
1	C1	1223	A2M	N3-C4-N9	2.75	131.84	127.17
1	C1	627	OMG	O6-C6-C5	-2.74	119.31	126.53
1	C1	2690	OMU	O4-C4-C5	-2.68	120.54	125.16
1	C1	1433	OMG	N9-C4-N3	2.66	131.27	125.95
1	C1	2578	OMG	C5-C6-N1	2.66	120.01	113.25
1	C1	2876	OMG	C2-N1-C6	-2.65	120.30	125.11
1	C1	385	OMG	C5-C6-N1	2.64	119.97	113.25
1	C1	2683	OMU	O4-C4-C5	-2.63	120.62	125.16
1	C1	1433	OMG	C5-C6-N1	2.63	119.94	113.25
1	C1	1433	OMG	O6-C6-C5	-2.62	119.61	126.53
1	C1	2578	OMG	C2-N1-C6	-2.62	120.36	125.11
1	C1	848	A2M	C4-N9-C8	2.55	108.41	105.74
1	C1	646	OMG	C2-N1-C6	-2.55	120.49	125.11
1	C1	2358	OMG	O6-C6-C5	-2.54	119.82	126.53
1	C1	1836	OMC	N4-C4-N3	2.54	122.45	117.91
1	C1	2774	OMG	O6-C6-C5	-2.50	119.93	126.53
1	C1	2358	OMG	C5-C6-N1	2.49	119.59	113.25
1	C1	2578	OMG	O6-C6-C5	-2.47	120.01	126.53
1	C1	646	OMG	C5-C6-N1	2.47	119.53	113.25
1	C1	787	OMG	O6-C6-C5	-2.45	120.06	126.53
1	C1	2876	OMG	C5-C6-N1	2.43	119.44	113.25
1	C1	2289	A2M	C4-N9-C8	2.43	108.29	105.74
1	C1	2358	OMG	N1-C2-N3	-2.41	118.90	123.32
1	C1	385	OMG	O6-C6-C5	-2.37	120.29	126.53
1	C1	1812	OMC	N4-C4-N3	2.36	122.12	117.91
1	C1	2380	OMU	O2-C2-N1	-2.34	119.75	122.80
1	C1	2774	OMG	C5-C6-N1	2.34	119.21	113.25
1	C1	858	A2M	C4-N9-C8	2.33	108.19	105.74
1	C1	2881	OMG	C5-C6-N1	2.32	119.15	113.25
1	C1	2289	A2M	N3-C4-N9	2.31	131.10	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	787	OMG	C2-N1-C6	-2.31	120.93	125.11
1	C1	627	OMG	N1-C2-N3	-2.30	119.11	123.32
1	C1	627	OMG	C5-C6-N1	2.28	119.07	113.25
1	C1	1223	A2M	C4-N9-C8	2.28	108.13	105.74
1	C1	1847	A2M	C4-N9-C8	2.27	108.12	105.74
1	C1	2774	OMG	C2-N1-C6	-2.27	121.00	125.11
1	C1	385	OMG	C8-N7-C5	2.26	108.28	104.26
1	C1	1433	OMG	N2-C2-N1	2.26	121.53	116.76
1	C1	848	A2M	C4-C5-N7	-2.25	108.01	110.58
1	C1	2358	OMG	C2-N1-C6	-2.24	121.05	125.11
1	C1	2838	OMC	O2-C2-N1	2.23	123.28	118.90
1	C1	637	A2M	C4-C5-N7	-2.22	108.04	110.58
1	C1	2578	OMG	N1-C2-N3	-2.22	119.27	123.32
1	C1	646	OMG	C8-N9-C4	2.20	110.16	106.03
1	C1	787	OMG	C5-C6-N1	2.20	118.86	113.25
1	C1	2881	OMG	N1-C2-N3	-2.18	119.33	123.32
1	C1	1432	A2M	C4-C5-N7	-2.18	108.09	110.58
1	C1	1812	OMC	C5-C4-N4	-2.18	116.82	120.63
1	C1	637	A2M	O4'-C1'-C2'	-2.14	102.91	106.59
1	C1	1433	OMG	C8-N7-C5	2.13	108.06	104.26
1	C1	2881	OMG	O6-C6-C5	-2.12	120.93	126.53
1	C1	1836	OMC	C5-C4-N4	-2.12	116.92	120.63
1	C1	1491	OMC	O2-C2-N1	2.12	123.05	118.90
1	C1	2774	OMG	N1-C2-N3	-2.12	119.45	123.32
1	C1	1868	OMU	O2-C2-N1	-2.09	120.07	122.80
1	C1	385	OMG	N2-C2-N1	2.09	121.16	116.76
1	C1	2688	OMU	O2-C2-N1	-2.09	120.08	122.80
1	C1	1847	A2M	C4-C5-N7	-2.08	108.20	110.58
1	C1	385	OMG	N1-C2-N3	-2.07	119.53	123.32
1	C1	1491	OMC	C5-C4-N4	-2.07	117.01	120.63
1	C1	627	OMG	C8-N9-C4	2.07	109.91	106.03
1	C1	2578	OMG	C8-N7-C5	2.06	107.93	104.26
1	C1	2690	OMU	O2-C2-N1	-2.06	120.12	122.80
1	C1	2289	A2M	C4-C5-N7	-2.05	108.23	110.58
1	C1	2277	OMU	O2-C2-N1	-2.03	120.16	122.80
1	C1	2683	OMU	O2-C2-N1	-2.03	120.16	122.80
1	C1	637	A2M	C6-C5-C4	2.01	119.92	117.18
1	C1	2358	OMG	C8-N7-C5	2.01	107.84	104.26
1	C1	627	OMG	C2-N1-C6	-2.01	121.47	125.11
1	C1	2881	OMG	C2-N1-C6	-2.00	121.48	125.11

All (36) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C1	385	OMG	C3'
1	C1	385	OMG	C4'
1	C1	627	OMG	C3'
1	C1	627	OMG	C4'
1	C1	646	OMG	C3'
1	C1	646	OMG	C4'
1	C1	778	OMC	C3'
1	C1	778	OMC	C4'
1	C1	787	OMG	C3'
1	C1	787	OMG	C4'
1	C1	1420	OMC	C3'
1	C1	1420	OMC	C4'
1	C1	1433	OMG	C3'
1	C1	1433	OMG	C4'
1	C1	1491	OMC	C3'
1	C1	1491	OMC	C4'
1	C1	1812	OMC	C3'
1	C1	1812	OMC	C4'
1	C1	1836	OMC	C3'
1	C1	1836	OMC	C4'
1	C1	2300	OMC	C3'
1	C1	2300	OMC	C4'
1	C1	2358	OMG	C3'
1	C1	2358	OMG	C4'
1	C1	2578	OMG	C3'
1	C1	2578	OMG	C4'
1	C1	2774	OMG	C3'
1	C1	2774	OMG	C4'
1	C1	2838	OMC	C3'
1	C1	2838	OMC	C4'
1	C1	2876	OMG	C3'
1	C1	2876	OMG	C4'
1	C1	2881	OMG	C3'
1	C1	2881	OMG	C4'
1	C1	2918	OMC	C3'
1	C1	2918	OMC	C4'

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C1	385	OMG	O4'-C4'-C5'-O5'
1	C1	385	OMG	C3'-C4'-C5'-O5'
1	C1	385	OMG	C3'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
1	C1	389	A2M	C1'-C2'-O2'-CM'
1	C1	627	OMG	C3'-C2'-O2'-CM2
1	C1	646	OMG	C4'-C5'-O5'-P
1	C1	646	OMG	C3'-C2'-O2'-CM2
1	C1	778	OMC	C3'-C2'-O2'-CM2
1	C1	787	OMG	C3'-C2'-O2'-CM2
1	C1	1420	OMC	C3'-C2'-O2'-CM2
1	C1	1420	OMC	O4'-C4'-C5'-O5'
1	C1	1433	OMG	C3'-C2'-O2'-CM2
1	C1	1491	OMC	C3'-C2'-O2'-CM2
1	C1	1812	OMC	C3'-C2'-O2'-CM2
1	C1	1812	OMC	C4'-C5'-O5'-P
1	C1	1836	OMC	C3'-C2'-O2'-CM2
1	C1	1836	OMC	C3'-C4'-C5'-O5'
1	C1	1836	OMC	C4'-C5'-O5'-P
1	C1	1917	OMU	O4'-C4'-C5'-O5'
1	C1	2300	OMC	C3'-C2'-O2'-CM2
1	C1	2358	OMG	C4'-C5'-O5'-P
1	C1	2358	OMG	C3'-C2'-O2'-CM2
1	C1	2380	OMU	C1'-C2'-O2'-CM2
1	C1	2384	OMU	C1'-C2'-O2'-CM2
1	C1	2578	OMG	C3'-C2'-O2'-CM2
1	C1	2683	OMU	C1'-C2'-O2'-CM2
1	C1	2774	OMG	C4'-C5'-O5'-P
1	C1	2774	OMG	C3'-C2'-O2'-CM2
1	C1	2838	OMC	O4'-C1'-N1-C2
1	C1	2838	OMC	O4'-C1'-N1-C6
1	C1	2838	OMC	C3'-C2'-O2'-CM2
1	C1	2876	OMG	C3'-C2'-O2'-CM2
1	C1	2881	OMG	C4'-C5'-O5'-P
1	C1	2881	OMG	C3'-C2'-O2'-CM2
1	C1	2918	OMC	C3'-C2'-O2'-CM2
1	C1	389	A2M	O4'-C4'-C5'-O5'
1	C1	646	OMG	C3'-C4'-C5'-O5'
1	C1	778	OMC	C3'-C4'-C5'-O5'
1	C1	787	OMG	C3'-C4'-C5'-O5'
1	C1	1812	OMC	C3'-C4'-C5'-O5'
1	C1	1847	A2M	O4'-C4'-C5'-O5'
1	C1	1847	A2M	C3'-C4'-C5'-O5'
1	C1	1917	OMU	C3'-C4'-C5'-O5'
1	C1	2300	OMC	C3'-C4'-C5'-O5'
1	C1	2358	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	C1	2578	OMG	O4'-C4'-C5'-O5'
1	C1	2774	OMG	C3'-C4'-C5'-O5'
1	C1	2838	OMC	C3'-C4'-C5'-O5'
1	C1	2881	OMG	C3'-C4'-C5'-O5'
1	C1	2918	OMC	C3'-C4'-C5'-O5'
1	C1	2300	OMC	C4'-C5'-O5'-P
1	C1	1433	OMG	C3'-C4'-C5'-O5'
1	C1	1491	OMC	O4'-C4'-C5'-O5'
1	C1	778	OMC	C4'-C5'-O5'-P
1	C1	1433	OMG	C4'-C5'-O5'-P
1	C1	1491	OMC	C4'-C5'-O5'-P
1	C1	2838	OMC	C4'-C5'-O5'-P
1	C1	627	OMG	C3'-C4'-C5'-O5'
1	C1	1491	OMC	C3'-C4'-C5'-O5'
1	C1	2918	OMC	C4'-C5'-O5'-P
1	C1	1420	OMC	C3'-C4'-C5'-O5'
1	C1	787	OMG	C4'-C5'-O5'-P
1	C1	1223	A2M	O4'-C4'-C5'-O5'
1	C1	848	A2M	O4'-C4'-C5'-O5'
1	C1	385	OMG	C4'-C5'-O5'-P
1	C1	787	OMG	O4'-C4'-C5'-O5'
1	C1	2300	OMC	C2'-C1'-N1-C2
1	C1	2876	OMG	C3'-C4'-C5'-O5'
1	C1	1420	OMC	C4'-C5'-O5'-P
1	C1	2578	OMG	C4'-C5'-O5'-P
1	C1	1847	A2M	C4'-C5'-O5'-P
1	C1	1491	OMC	C2'-C1'-N1-C2
1	C1	2300	OMC	C2'-C1'-N1-C6
1	C1	2876	OMG	O4'-C4'-C5'-O5'
1	C1	1491	OMC	C2'-C1'-N1-C6
1	C1	2918	OMC	C2'-C1'-N1-C6
1	C1	2774	OMG	C2'-C1'-N9-C4
1	C1	2358	OMG	C2'-C1'-N9-C4
1	C1	2876	OMG	C2'-C1'-N9-C4
1	C1	389	A2M	C3'-C4'-C5'-O5'
1	C1	778	OMC	C2'-C1'-N1-C2
1	C1	1420	OMC	C2'-C1'-N1-C2
1	C1	1812	OMC	C2'-C1'-N1-C2
1	C1	1836	OMC	C2'-C1'-N1-C2
1	C1	385	OMG	C2'-C1'-N9-C4
1	C1	2881	OMG	C2'-C1'-N9-C4
1	C1	858	A2M	O4'-C4'-C5'-O5'

There are no ring outliers.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C1	1420	OMC	1	0
1	C1	1432	A2M	1	0
1	C1	637	A2M	1	0
1	C1	2384	OMU	1	0
1	C1	2578	OMG	1	0
1	C1	2838	OMC	2	0
1	C1	787	OMG	1	0
1	C1	1812	OMC	1	0
1	C1	1491	OMC	3	0
1	C1	2683	OMU	1	0
1	C1	2876	OMG	1	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	$\# Z  > 2$
58	GTP	CH	701	59	33,34,34	0.88	1 (3%)	50,54,54	1.58	9 (18%)
58	GTP	Cd	703	59	33,34,34	0.91	0	50,54,54	1.60	8 (16%)

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
58	GTP	CH	701	59	-	6/22/38/38	0/3/3/3
58	GTP	Cd	703	59	-	3/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	CH	701	GTP	C2-N3	2.11	1.38	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	CH	701	GTP	C5-C4-N3	-4.96	120.50	128.39
58	Cd	703	GTP	C5-C4-N3	-4.81	120.73	128.39
58	Cd	703	GTP	C2-N3-C4	4.58	120.19	112.30
58	CH	701	GTP	C2-N3-C4	4.55	120.13	112.30
58	CH	701	GTP	N9-C4-N3	3.14	132.24	125.95
58	Cd	703	GTP	N9-C4-N3	2.92	131.80	125.95
58	CH	701	GTP	C2-N1-C6	-2.91	119.83	125.11
58	Cd	703	GTP	C2-N1-C6	-2.88	119.90	125.11
58	Cd	703	GTP	N9-C8-N7	-2.71	108.37	113.40
58	CH	701	GTP	N9-C8-N7	-2.64	108.51	113.40
58	Cd	703	GTP	C8-N7-C5	2.50	108.72	104.26
58	CH	701	GTP	C5-C6-N1	2.49	119.59	113.25
58	Cd	703	GTP	C5-C6-N1	2.49	119.59	113.25
58	CH	701	GTP	C8-N7-C5	2.46	108.64	104.26
58	Cd	703	GTP	O6-C6-C5	-2.41	120.18	126.53
58	CH	701	GTP	O6-C6-C5	-2.37	120.26	126.53
58	CH	701	GTP	C3'-C2'-C1'	2.13	105.49	101.46

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	CH	701	GTP	C5'-O5'-PA-O3A
58	CH	701	GTP	C5'-O5'-PA-O1A
58	CH	701	GTP	C5'-O5'-PA-O2A
58	Cd	703	GTP	C5'-O5'-PA-O1A
58	CH	701	GTP	O4'-C4'-C5'-O5'
58	CH	701	GTP	C3'-C4'-C5'-O5'
58	Cd	703	GTP	O4'-C4'-C5'-O5'
58	Cd	703	GTP	C3'-C4'-C5'-O5'
58	CH	701	GTP	PB-O3A-PA-O2A

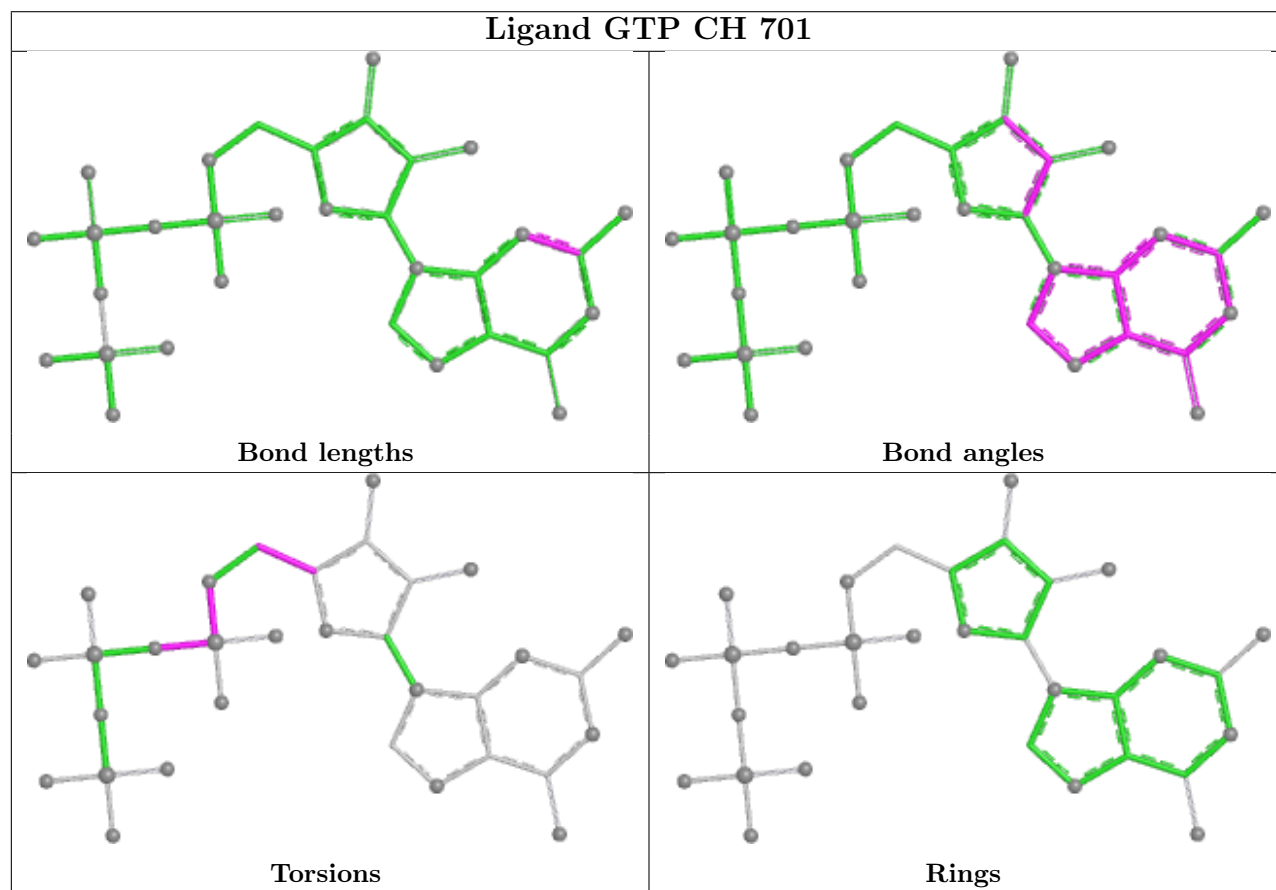


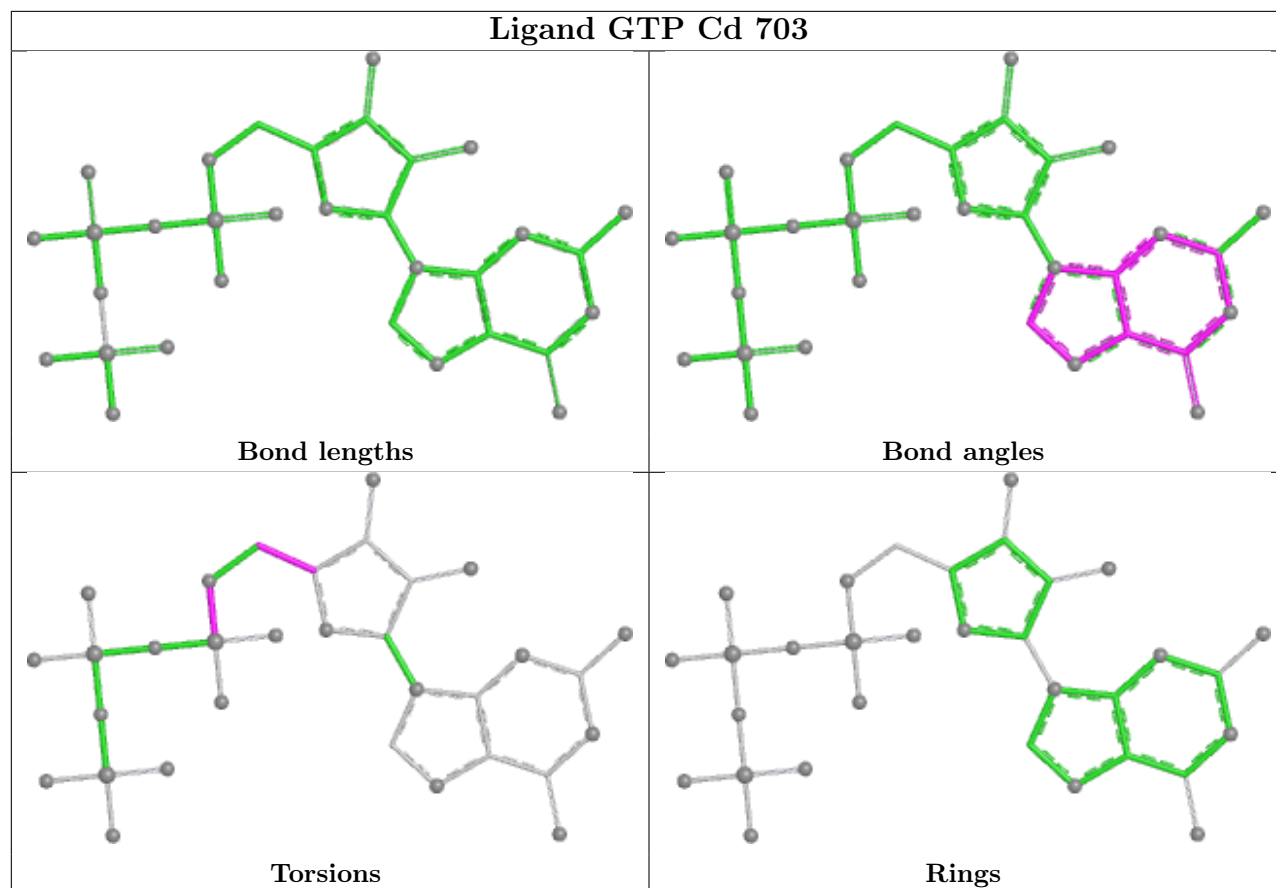
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	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.

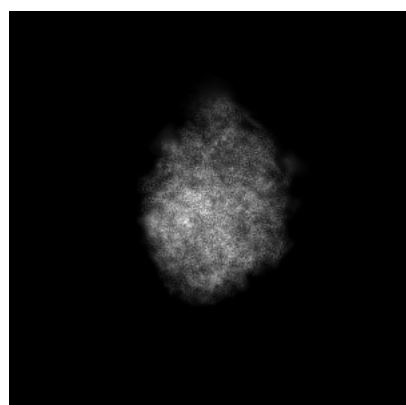
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17970. These allow visual inspection of the internal detail of the map and identification of artifacts.

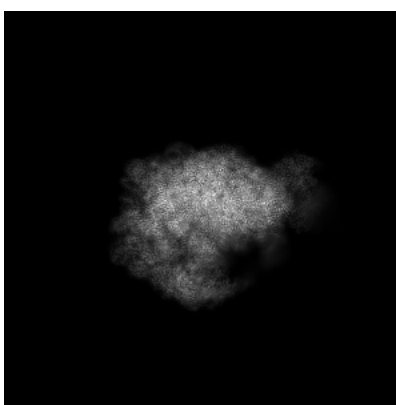
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

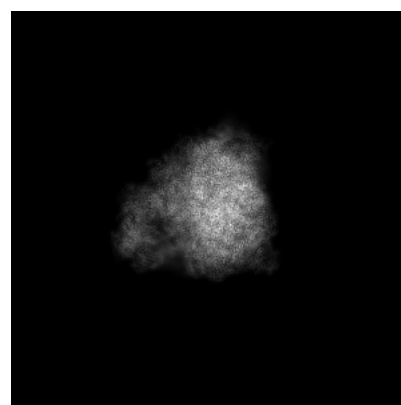
#### 6.1.1 Primary map



X



Y

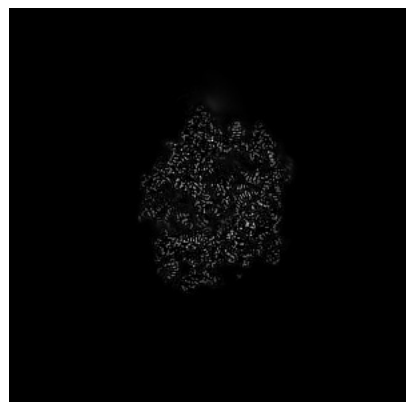


Z

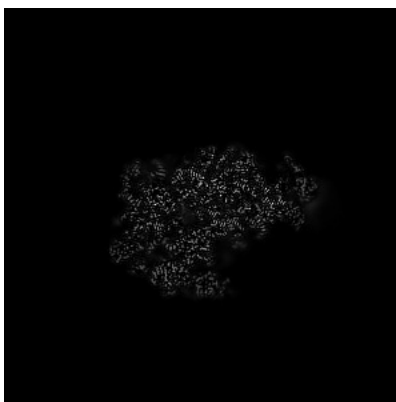
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

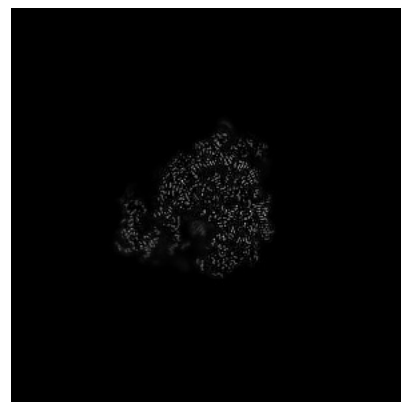
#### 6.2.1 Primary map



X Index: 250



Y Index: 250

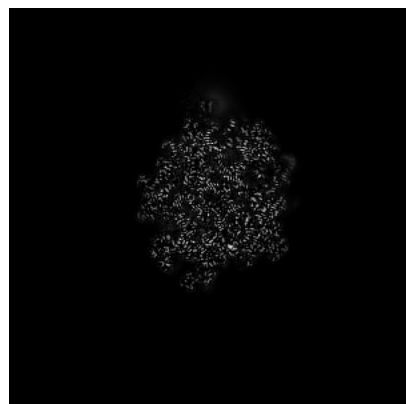


Z Index: 250

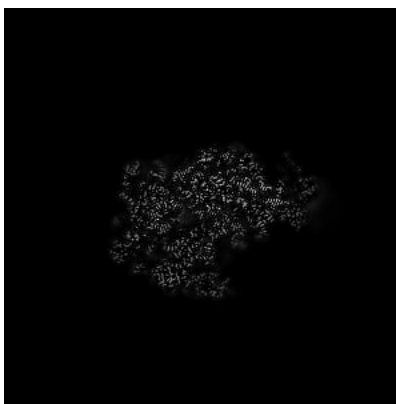
The images above show central slices of the map in three orthogonal directions.

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

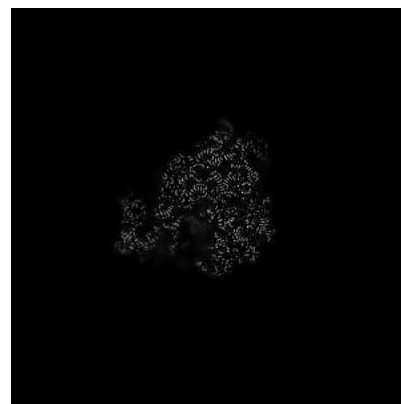
### 6.3.1 Primary map



X Index: 259



Y Index: 248

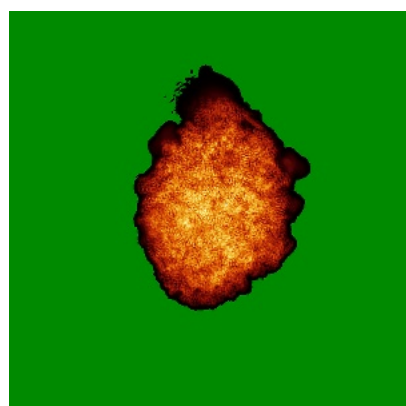


Z Index: 252

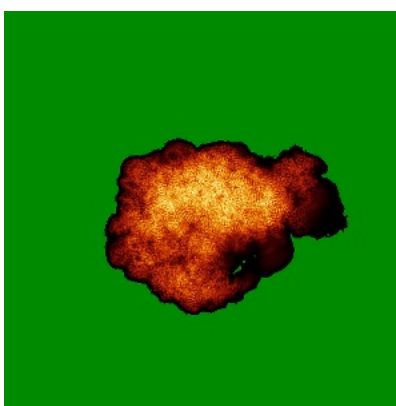
The images above show the largest variance slices of the map in three orthogonal directions.

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

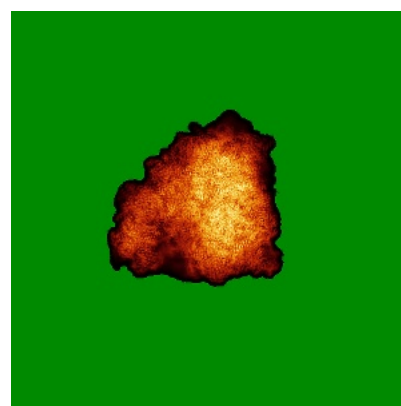
### 6.4.1 Primary map



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

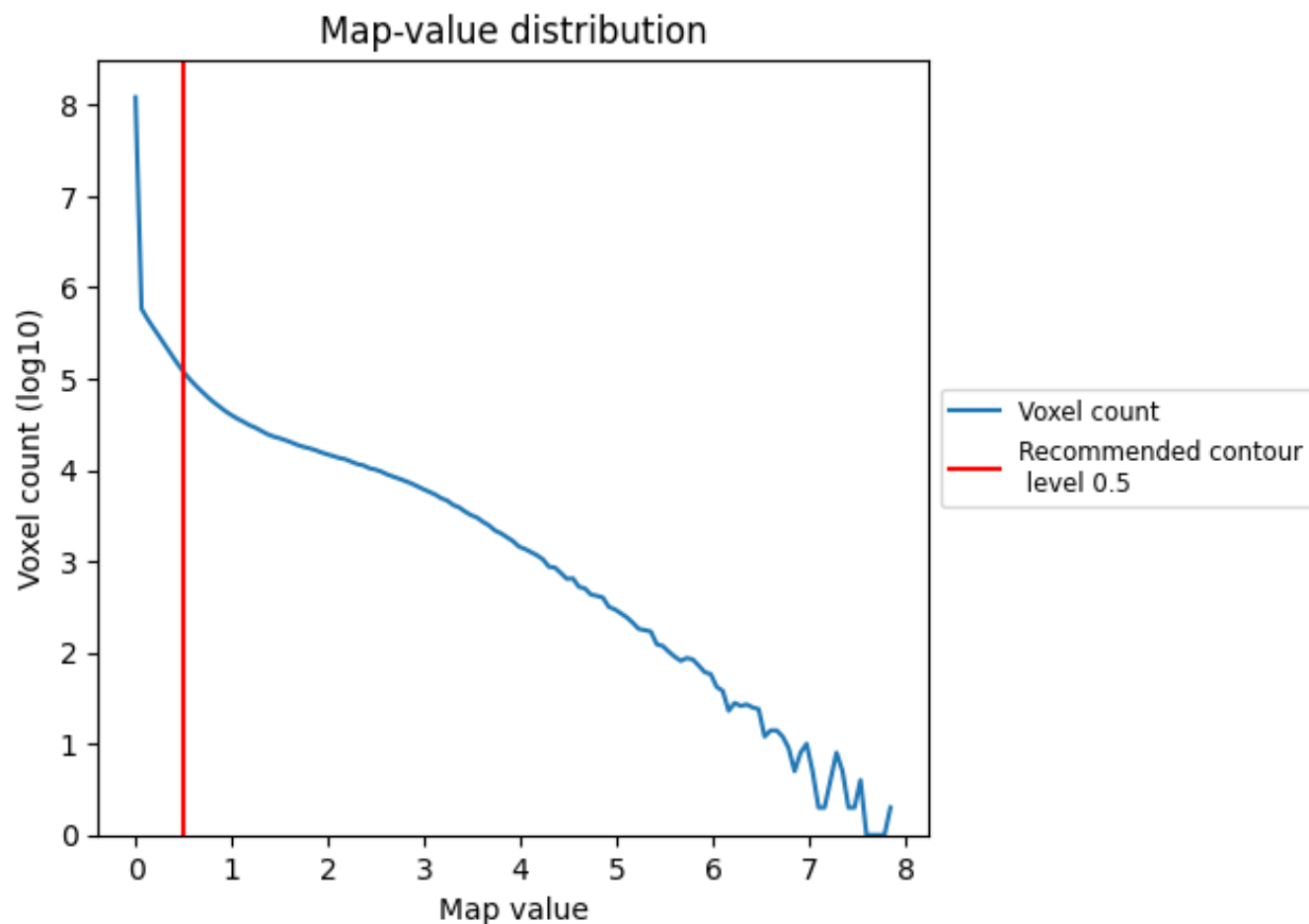
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

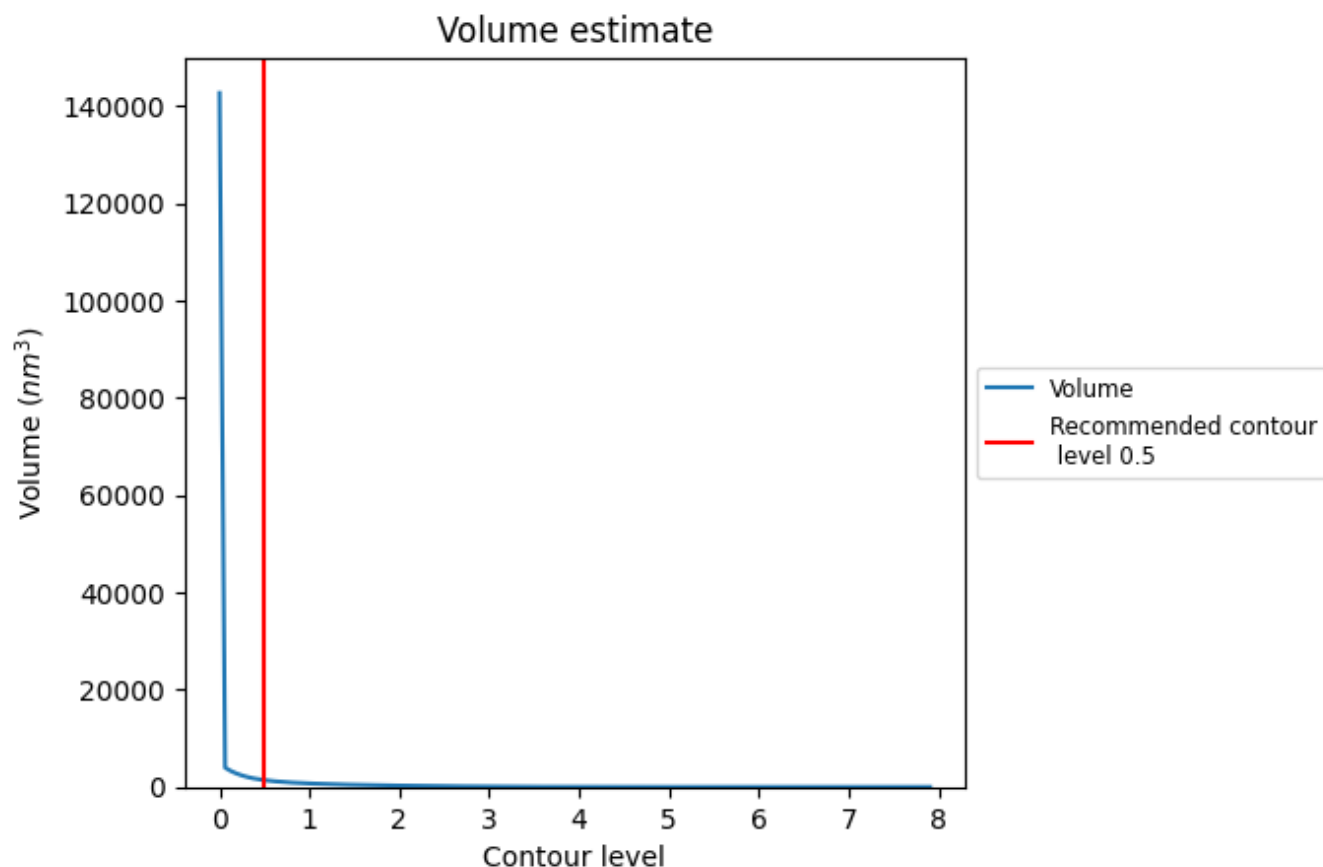
This section contains the results of statistical analysis of the map.

### 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.

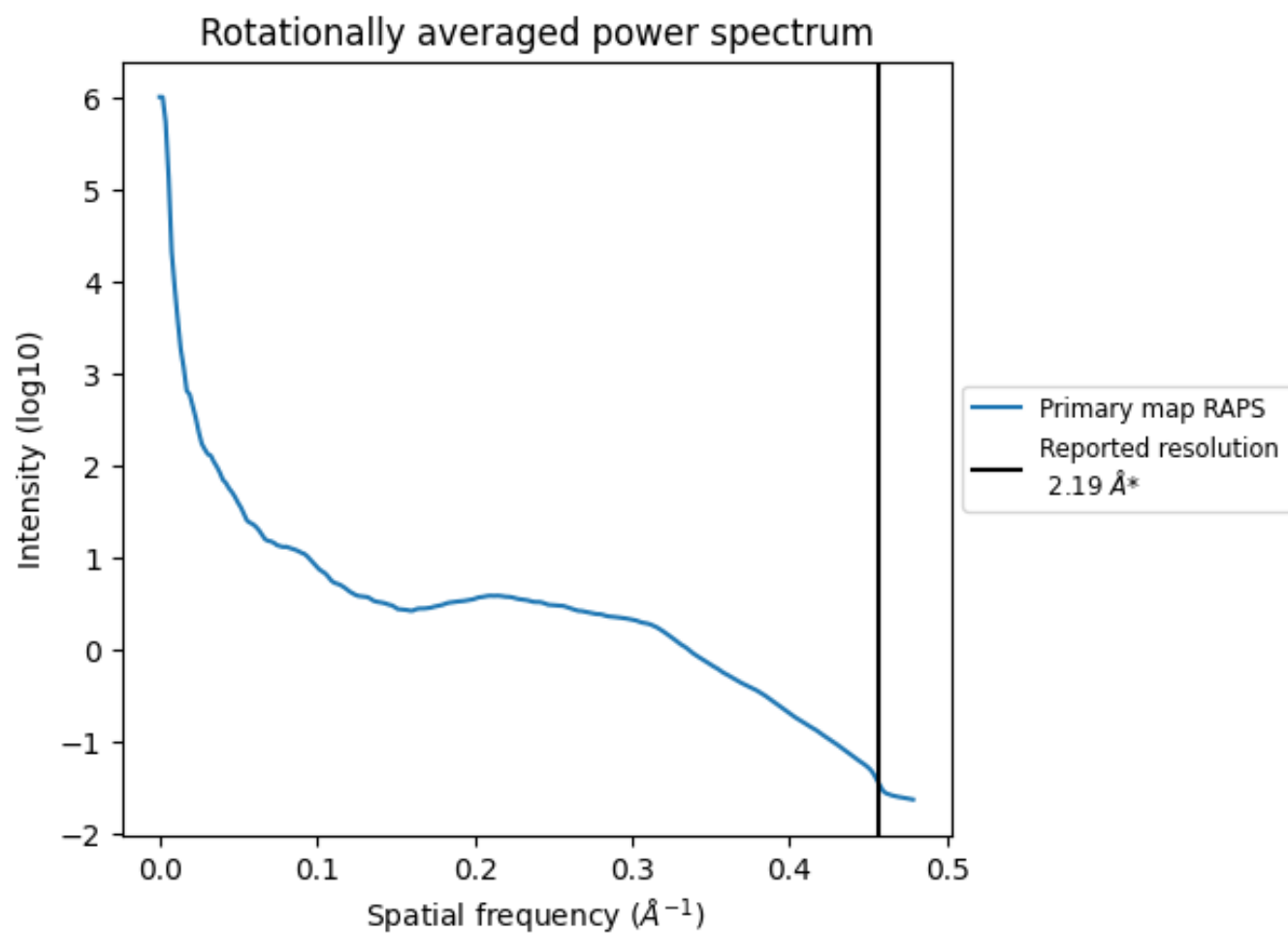
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1395  $\text{nm}^3$ ; this corresponds to an approximate mass of 1260 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 0.457  $\text{\AA}^{-1}$



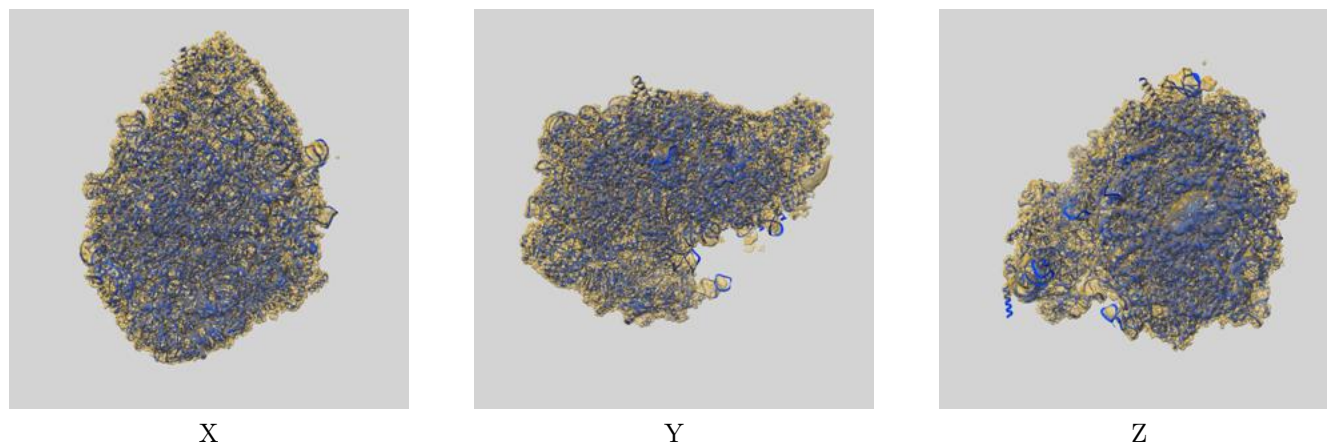
## 8 Fourier-Shell correlation

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

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

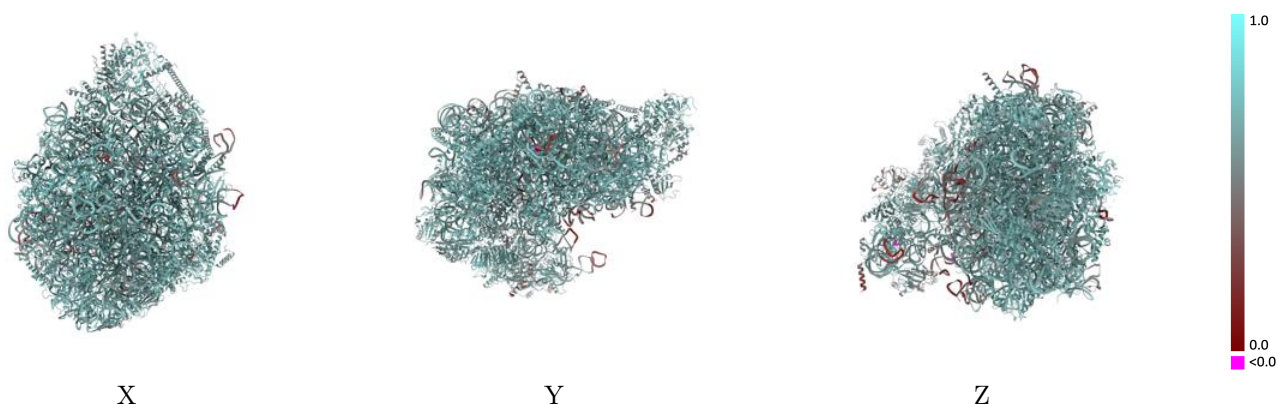
This section contains information regarding the fit between EMDB map EMD-17970 and PDB model 8PVL. Per-residue inclusion information can be found in section 3 on page 16.

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



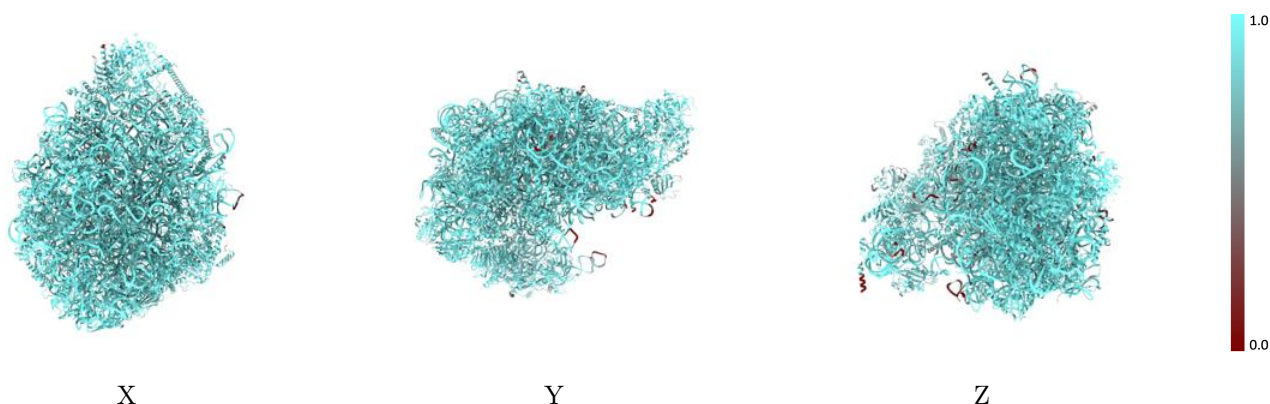
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



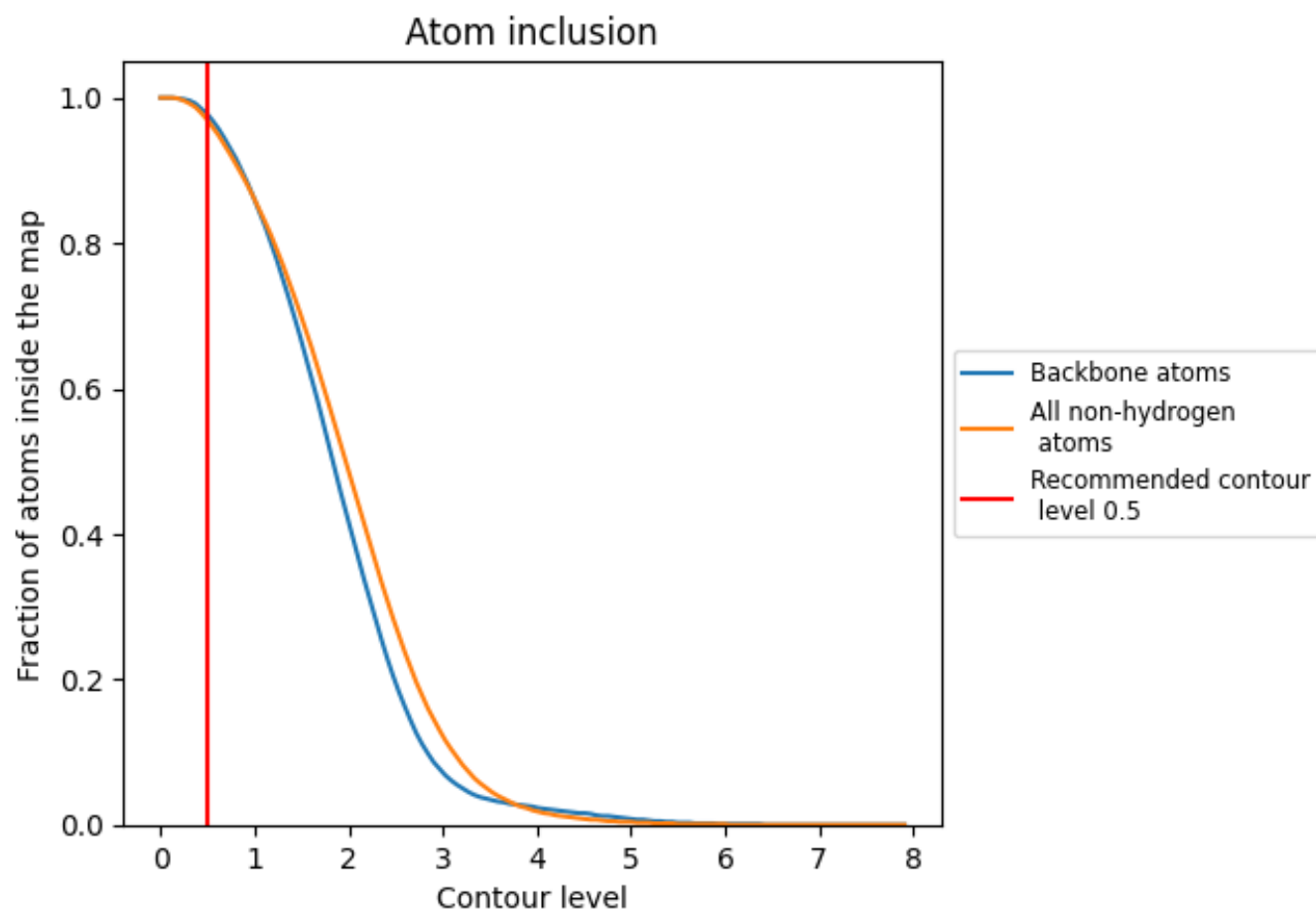
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9690	 0.6620
C1	 0.9800	 0.6510
C2	 0.9780	 0.6760
C3	 0.8670	 0.5710
C4	 0.9330	 0.5790
CF	 0.9470	 0.6370
CH	 0.9490	 0.6660
CI	 0.8830	 0.6030
CJ	 0.9790	 0.6670
CK	 0.9850	 0.7000
CL	 0.9520	 0.6360
CM	 0.9040	 0.6030
CN	 0.9740	 0.6950
CO	 0.9560	 0.6790
CQ	 0.9370	 0.6650
Cb	 0.9850	 0.6930
Cd	 0.9740	 0.6850
Ce	 0.8950	 0.6110
Cf	 0.9650	 0.6480
Cg	 0.9620	 0.6320
Ch	 0.9340	 0.6380
Cz	 0.8850	 0.5770
LA	 0.9890	 0.7000
LB	 0.9890	 0.7190
LC	 0.9860	 0.7170
LD	 0.9390	 0.6360
LE	 0.9590	 0.6730
LF	 0.9740	 0.7010
LG	 0.9700	 0.6730
LH	 0.9690	 0.6870
LJ	 0.9360	 0.5660
LK	 0.9290	 0.6040
LL	 0.9620	 0.6900
LM	 0.9730	 0.6900
LN	 0.9970	 0.7180



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Chain	Atom inclusion	Q-score
LO	 0.9890	 0.7170
LP	 0.9940	 0.7130
LQ	 0.9780	 0.6950
LR	 0.9750	 0.7060
LS	 0.9830	 0.6900
LT	 0.9310	 0.5880
LU	 0.9580	 0.6480
LV	 0.9960	 0.7150
LX	 0.9690	 0.6770
LY	 0.9800	 0.6990
LZ	 0.9740	 0.6880
La	 0.9700	 0.6960
Lc	 0.9610	 0.6770
Ld	 0.9740	 0.7070
Le	 0.9920	 0.7240
Lf	 0.9960	 0.7330
Lg	 0.9430	 0.6850
Lh	 0.9560	 0.6460
Li	 0.9540	 0.6590
Lj	 0.9930	 0.7280
Lk	 0.9370	 0.6590
Ll	 1.0000	 0.7330
Lp	 0.9500	 0.6840
Lq	 0.9720	 0.6880