



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:38 PM UTC

PDB ID : 9E6Q / pdb_00009e6q
EMDB ID : EMD-47578
Title : Cryo-EM structure of the Pyrobaculum calidifontis 50S ribosomal subunit in complex with Dri
Authors : Nissley, A.J.; Cate, J.H.D.
Deposited on : 2024-10-30
Resolution : 1.95 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

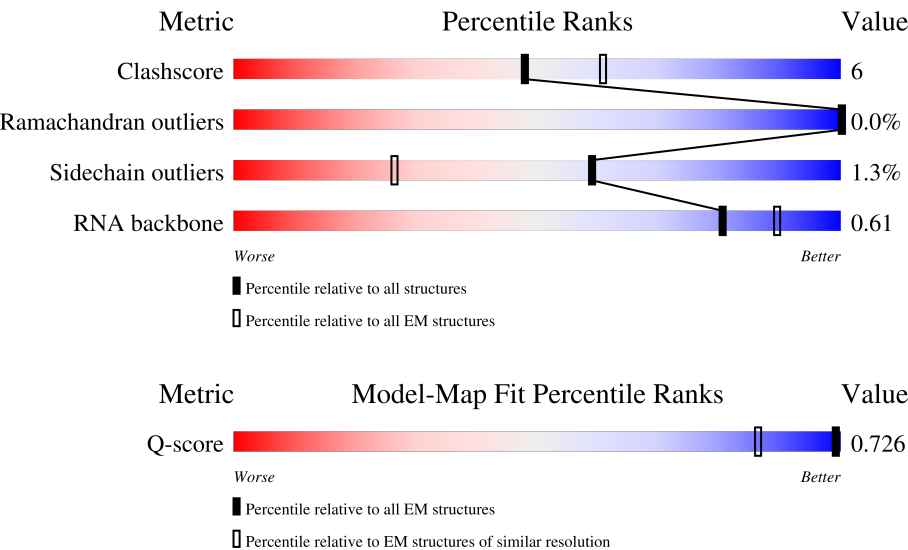
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 1.95 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.



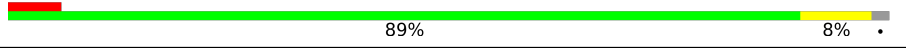
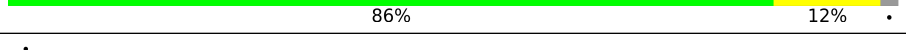
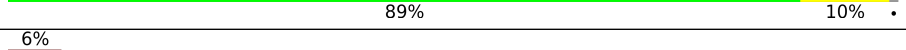
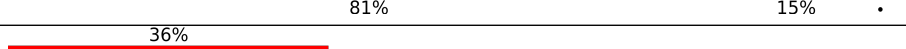
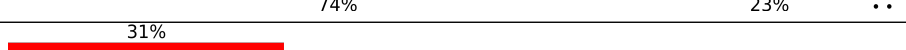
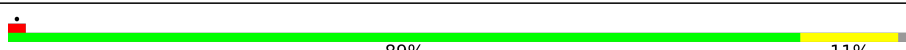
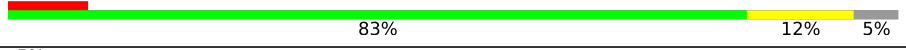
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	1316 (1.45 - 2.45)

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

Mol	Chain	Length	Quality of chain
1	1	3024	10% 66% 24% 6%
2	2	129	5% 69% 26% 5%
3	3	655	5% 38% 6% 56%

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Mol	Chain	Length	Quality of chain
4	AA	244	
5	AB	338	
6	AC	285	
7	AD	178	
8	AE	196	
9	AF	149	
10	AG	186	
11	AH	157	
12	AI	144	
13	AJ	103	
13	AK	103	
14	AL	156	
15	AM	189	
16	AN	178	
17	AO	205	
18	AP	122	
19	AQ	147	
20	AR	78	
21	AS	99	
22	AT	184	
23	AU	81	
24	AV	128	
25	AW	62	
26	AX	79	
27	AY	179	

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Mol	Chain	Length	Quality of chain
28	AZ	101	
29	Aa	91	
30	Ab	153	
31	Ac	84	
32	Ad	52	
33	Ae	67	
34	Af	51	
35	Ag	53	
36	Ah	91	
37	Ai	102	
38	Aj	184	
39	Ak	93	

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 114588 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2842	Total	C	N	O	P	0	0
			61237	27268	11426	19701	2842		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	129	Total	C	N	O	P	0	0
			2769	1231	512	897	129		

- Molecule 3 is a protein called Putative signal-transduction protein with CBS domains.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	290	Total	C	N	O	S	0	0
			2272	1470	400	399	3		

- Molecule 4 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AA	239	Total	C	N	O	S	0	0
			1803	1136	354	308	5		

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AB	336	Total	C	N	O	S	0	0
			2611	1681	476	450	4		

- Molecule 6 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AC	278	Total	C	N	O	S	0	0
			2178	1406	395	371	6		

- Molecule 7 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AD	178	Total	C	N	O	S	0	0
			1412	894	273	238	7		

- Molecule 8 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AE	195	Total	C	N	O	S	0	0
			1520	990	254	272	4		

- Molecule 9 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AF	145	Total	C	N	O	S	0	0
			1095	705	187	202	1		

- Molecule 10 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AG	183	Total	C	N	O	S	0	0
			1510	979	278	246	7		

- Molecule 11 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AH	155	Total	C	N	O	S	0	0
			1244	785	249	209	1		

- Molecule 12 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AI	138	Total	C	N	O	S	0	0
			1068	682	202	181	3		

- Molecule 13 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AJ	101	Total	C	N	O	S	0	0
			788	500	143	144	1		
13	AK	90	Total	C	N	O	S	0	0
			700	441	130	128	1		

- Molecule 14 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AL	152	Total	C	N	O	S	0	0
			1198	761	232	202	3		

- Molecule 15 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AM	184	Total	C	N	O	S	0	0
			1558	992	315	245	6		

- Molecule 16 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AN	169	Total	C	N	O	S	0	0
			1336	847	254	227	8		

- Molecule 17 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AO	200	Total	C	N	O	S	0	0
			1615	1027	309	278	1		

- Molecule 18 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AP	121	Total	C	N	O	S	0	0
			920	583	181	155	1		

- Molecule 19 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AQ	146	Total	C	N	O	S	0	0
			1214	759	244	208	3		

- Molecule 20 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AR	76	Total	C	N	O	S	0	0
			603	382	109	109	3		

- Molecule 21 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AS	98	Total	C	N	O	S	0	0
			788	503	150	134	1		

- Molecule 22 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AT	183	Total	C	N	O	S	0	0
			1496	978	268	247	3		

- Molecule 23 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AU	81	Total	C	N	O	S	0	0
			651	417	115	117	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AV	121	Total	C	N	O	S	0	0
			976	619	194	161	2		

- Molecule 25 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AW	56	Total	C	N	O	S	0	0
			449	287	86	70	6		

- Molecule 26 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AX	67	Total	C	N	O	S	0	0
			554	343	117	92	2		

- Molecule 27 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AY	172	Total	C	N	O	S	0	0
			1374	888	245	235	6		

- Molecule 28 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AZ	98	Total	C	N	O	S	0	0
			742	481	128	132	1		

- Molecule 29 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Aa	88	Total	C	N	O		0	0
			726	460	146	120			

- Molecule 30 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ab	140	Total	C	N	O	S	0	0
			1183	757	239	186	1		

- Molecule 31 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ac	83	Total	C	N	O	S	0	0
			649	407	138	102	2		

- Molecule 32 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ad	52	Total	C	N	O	S	0	0
			429	265	93	65	6		

- Molecule 33 is a protein called LSU ribosomal protein L38E.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Ae	66	Total	C	N	O	0	0
			552	363	93	96		

- Molecule 34 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	Af	50	Total	C	N	O	0	0
			415	260	96	59		

- Molecule 35 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ag	50	Total	C	N	O	S	0	0
			417	259	88	66	4		

- Molecule 36 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ah	91	Total	C	N	O	S	0	0
			739	467	142	123	7		

- Molecule 37 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ai	99	Total	C	N	O	S	0	0
			769	489	148	127	5		

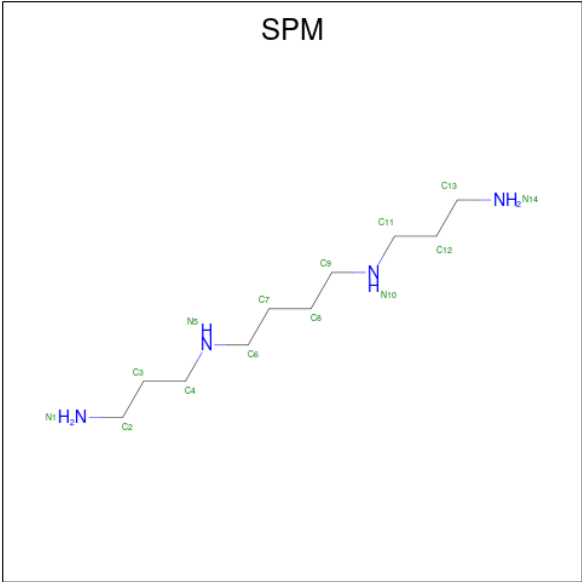
- Molecule 38 is a protein called DJ-1/PfpI domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Aj	183	Total	C	N	O	S	0	0
			1469	954	248	265	2		

- Molecule 39 is a protein called PaREP1 domain containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ak	90	Total	C	N	O	S	0	0
			743	478	127	136	2		

- Molecule 40 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms			AltConf
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	

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Mol	Chain	Residues	Atoms			AltConf
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	1	1	Total	C	N	0
			14	10	4	
40	AL	1	Total	C	N	0
			14	10	4	
40	AM	1	Total	C	N	0
			14	10	4	

- Molecule 41 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
41	1	168	Total	Mg	0
			168	168	
41	AA	1	Total	Mg	0
			1	1	
41	AL	2	Total	Mg	0
			2	2	
41	AN	1	Total	Mg	0
			1	1	
41	AT	1	Total	Mg	0
			1	1	

- Molecule 42 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
42	AW	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
42	Ad	1	Total 1	Zn 1	0
42	Ag	1	Total 1	Zn 1	0
42	Ah	1	Total 1	Zn 1	0
42	Ai	1	Total 1	Zn 1	0

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		AltConf
43	1	6534	Total 6534	O 6534	0
43	2	147	Total 147	O 147	0
43	3	58	Total 58	O 58	0
43	AA	83	Total 83	O 83	0
43	AB	85	Total 85	O 85	0
43	AC	83	Total 83	O 83	0
43	AD	16	Total 16	O 16	0
43	AE	22	Total 22	O 22	0
43	AF	19	Total 19	O 19	0
43	AG	50	Total 50	O 50	0
43	AH	49	Total 49	O 49	0
43	AI	30	Total 30	O 30	0
43	AJ	13	Total 13	O 13	0
43	AK	15	Total 15	O 15	0
43	AL	49	Total 49	O 49	0

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Mol	Chain	Residues	Atoms		AltConf
43	AM	66	Total 66	O 66	0
43	AN	51	Total 51	O 51	0
43	AO	32	Total 32	O 32	0
43	AP	28	Total 28	O 28	0
43	AQ	45	Total 45	O 45	0
43	AR	13	Total 13	O 13	0
43	AS	37	Total 37	O 37	0
43	AT	46	Total 46	O 46	0
43	AU	22	Total 22	O 22	0
43	AV	30	Total 30	O 30	0
43	AW	13	Total 13	O 13	0
43	AX	32	Total 32	O 32	0
43	AY	38	Total 38	O 38	0
43	AZ	18	Total 18	O 18	0
43	Aa	22	Total 22	O 22	0
43	Ab	42	Total 42	O 42	0
43	Ac	21	Total 21	O 21	0
43	Ad	26	Total 26	O 26	0
43	Ae	17	Total 17	O 17	0
43	Af	18	Total 18	O 18	0
43	Ag	11	Total 11	O 11	0

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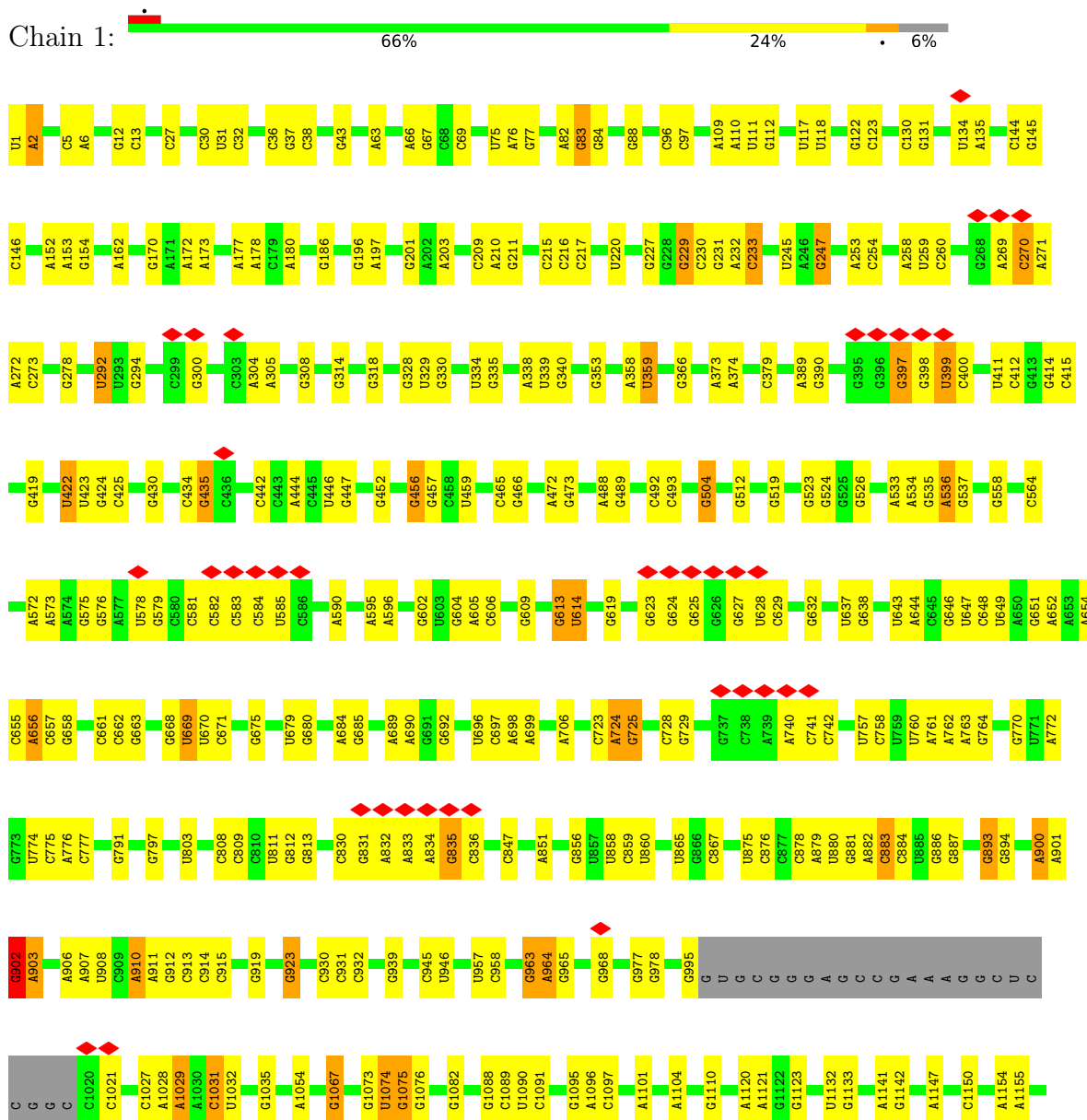
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Mol	Chain	Residues	Atoms		AltConf
43	Ah	26	Total 26	O 26	0
43	Ai	34	Total 34	O 34	0
43	Aj	41	Total 41	O 41	0
43	Ak	12	Total 12	O 12	0

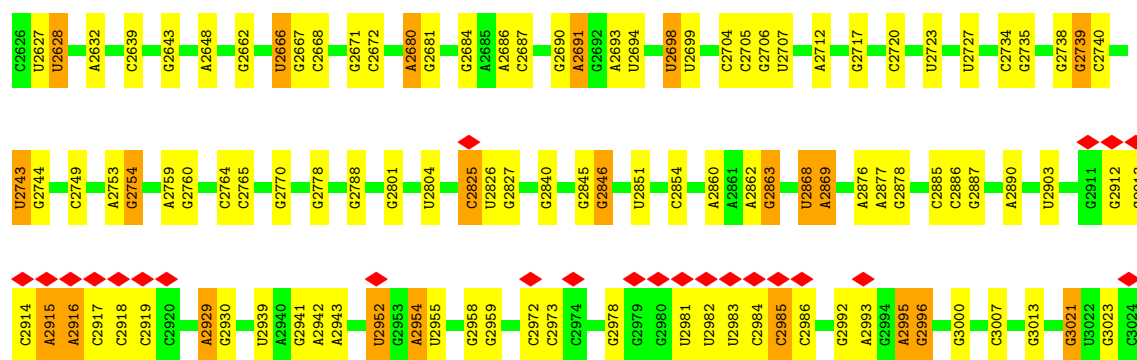
3 Residue-property plots

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.

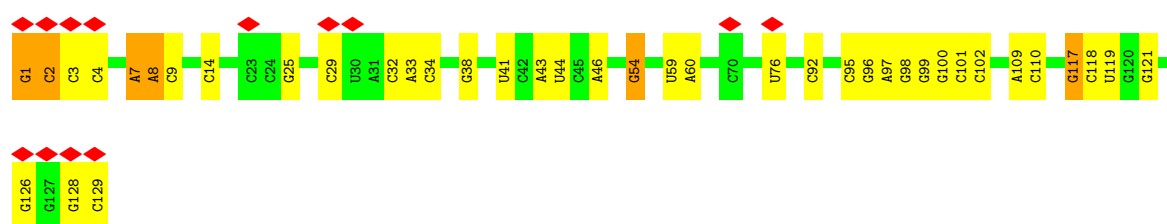
• Molecule 1: 23S rRNA



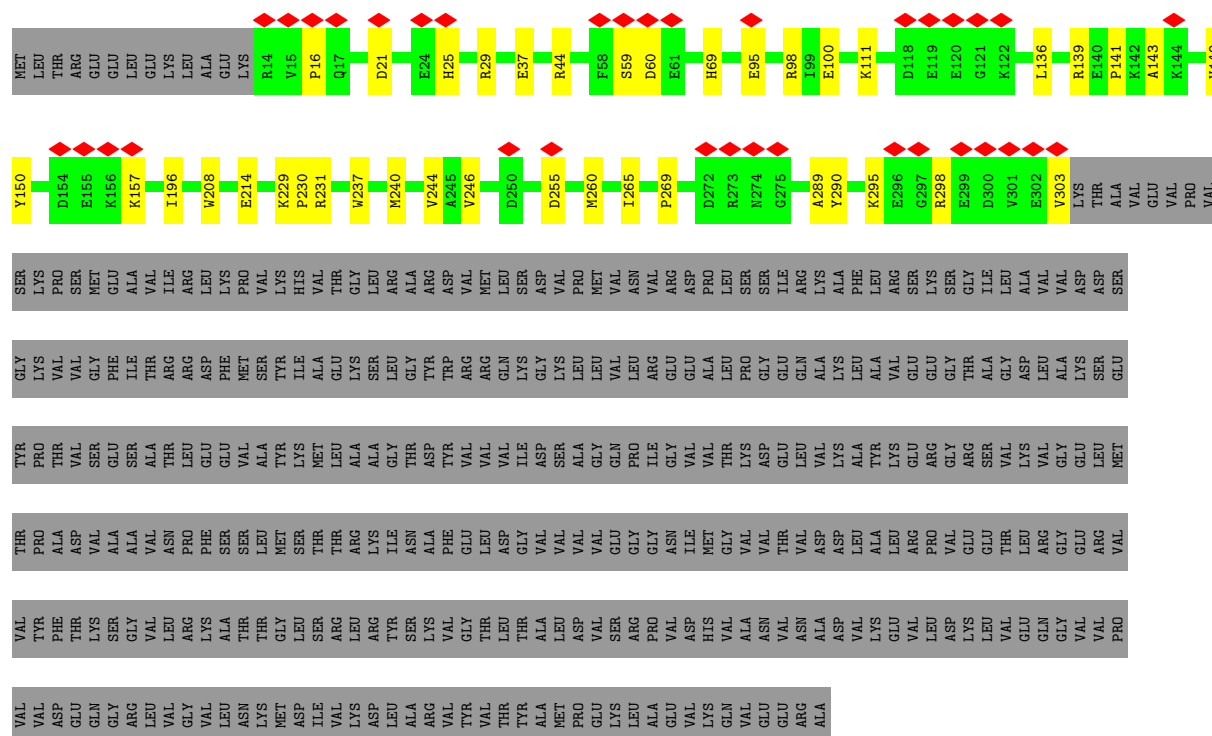
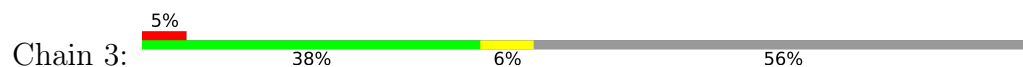




• Molecule 2: 5S rRNA

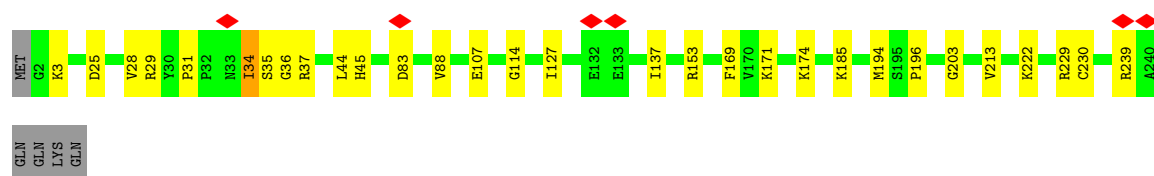


• Molecule 3: Putative signal-transduction protein with CBS domains



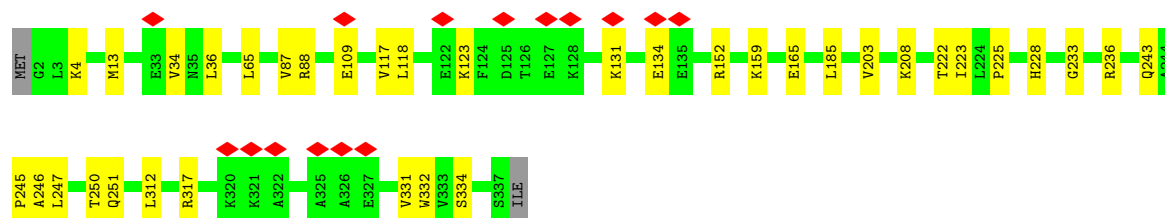
• Molecule 4: Large ribosomal subunit protein uL2

Chain AA: 

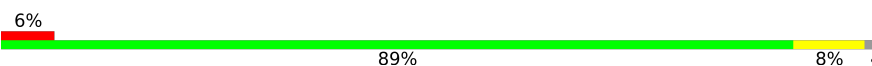


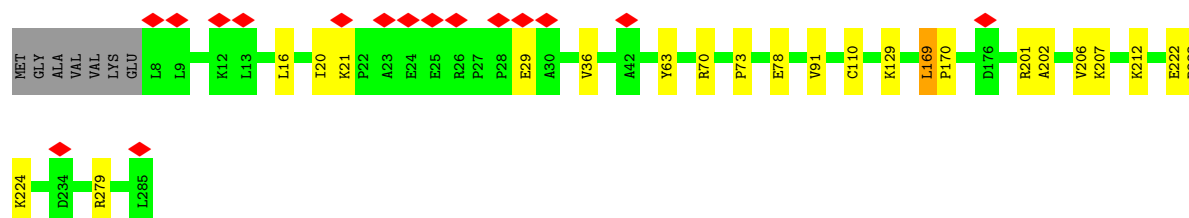
- Molecule 5: Large ribosomal subunit protein uL3

Chain AB: 



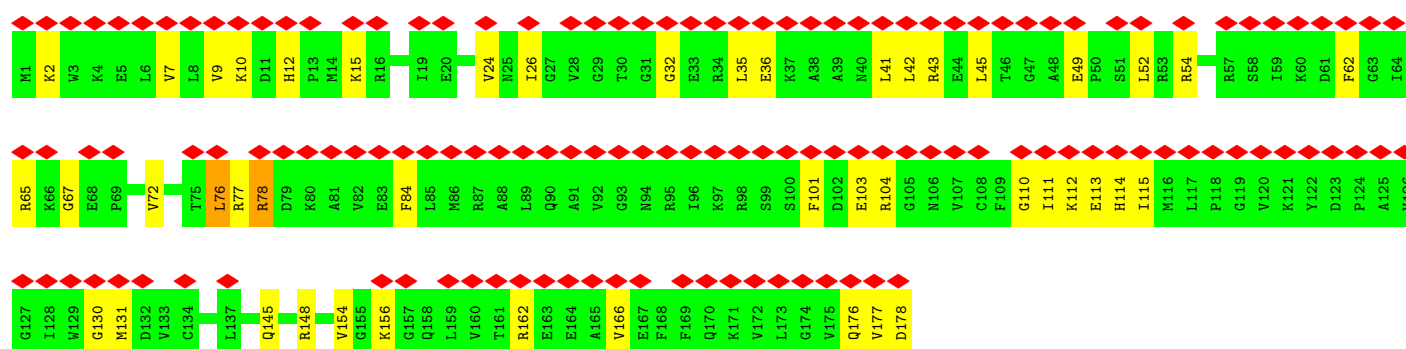
- Molecule 6: Large ribosomal subunit protein uL4

Chain AC: 



- Molecule 7: Large ribosomal subunit protein uL5

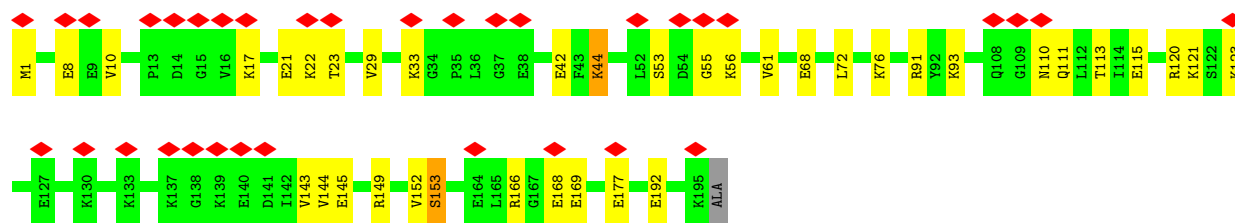
Chain AD: 



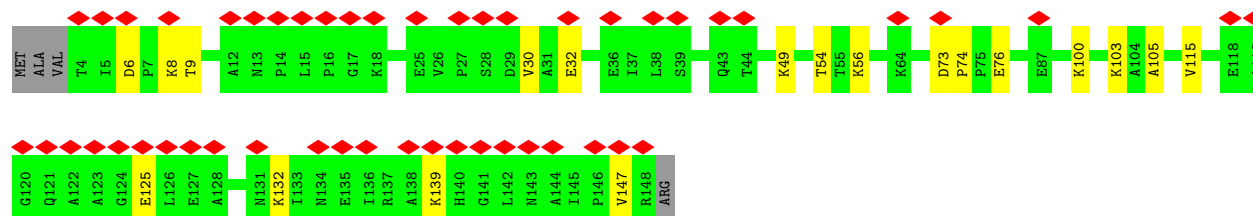
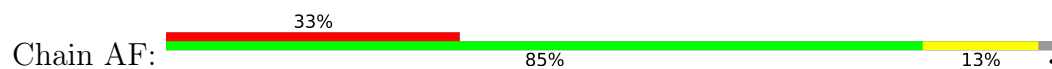
- Molecule 8: Large ribosomal subunit protein uL6

Chain AE: 

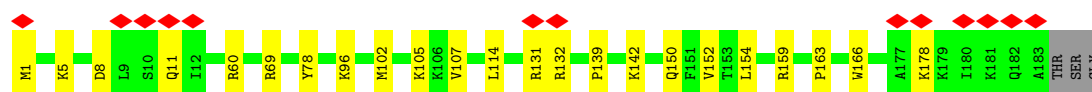
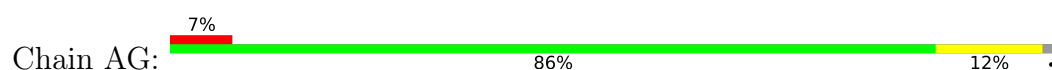




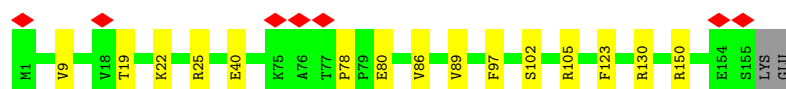
• Molecule 9: Large ribosomal subunit protein eL8



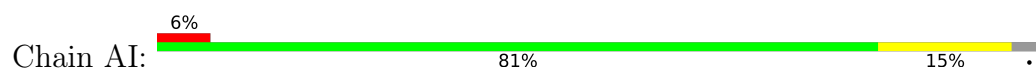
• Molecule 10: Large ribosomal subunit protein uL13



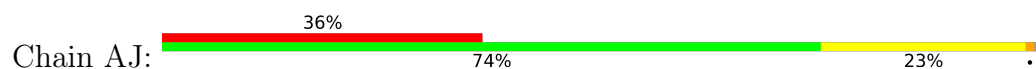
• Molecule 11: Large ribosomal subunit protein eL13

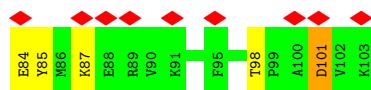


• Molecule 12: Large ribosomal subunit protein uL14

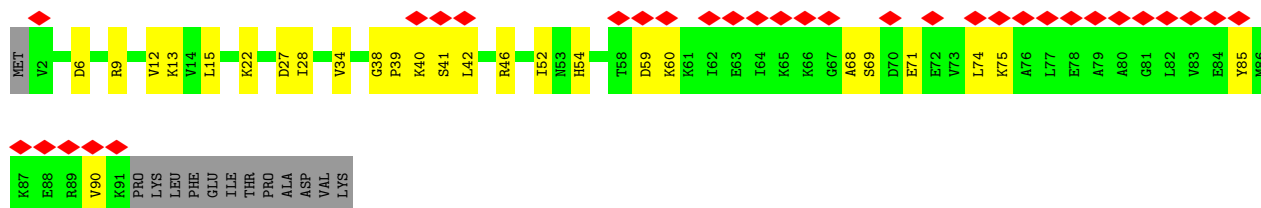


• Molecule 13: eL14

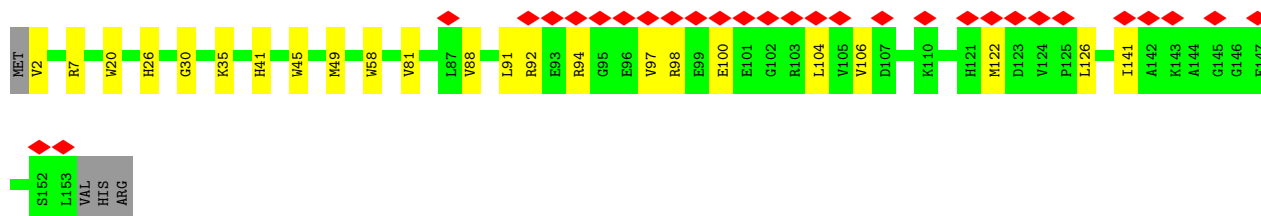
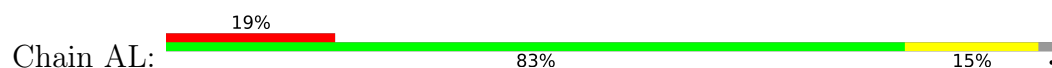




- Molecule 13: eL14



- Molecule 14: Large ribosomal subunit protein uL15



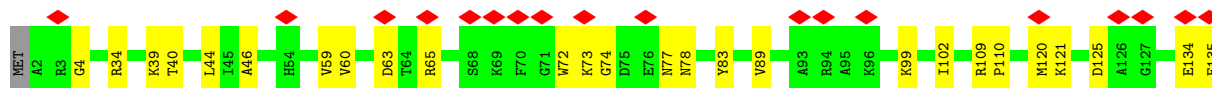
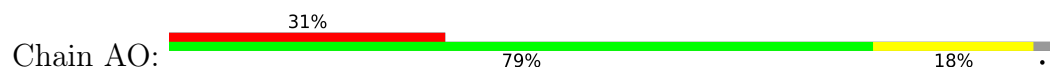
- Molecule 15: 50S ribosomal protein L15e

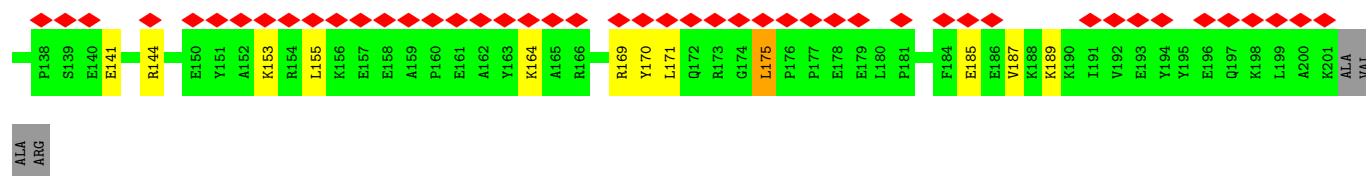


- Molecule 16: Large ribosomal subunit protein uL16



- Molecule 17: Large ribosomal subunit protein uL18

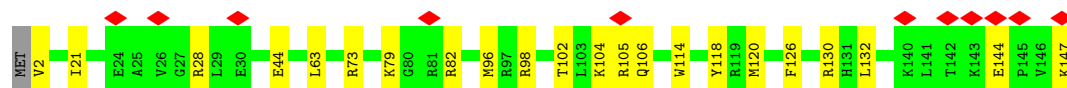
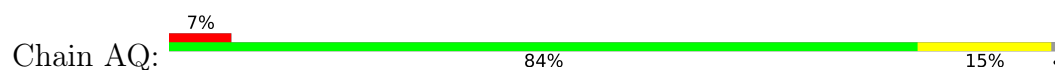




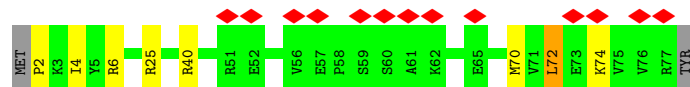
- Molecule 18: Large ribosomal subunit protein eL18



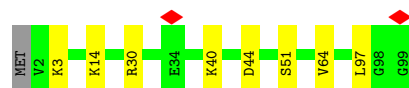
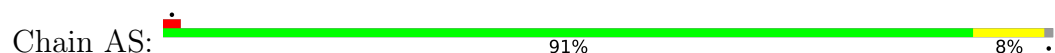
- Molecule 19: Large ribosomal subunit protein eL19



- Molecule 20: Large ribosomal subunit protein eL20



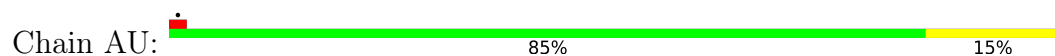
- Molecule 21: Large ribosomal subunit protein eL21



- Molecule 22: Large ribosomal subunit protein uL22

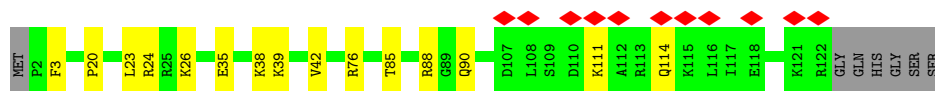
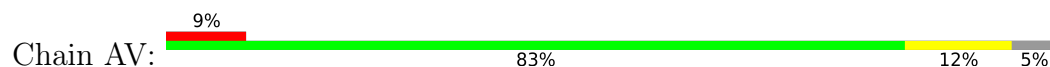


- Molecule 23: Large ribosomal subunit protein uL23

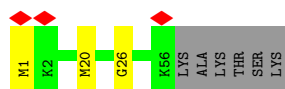




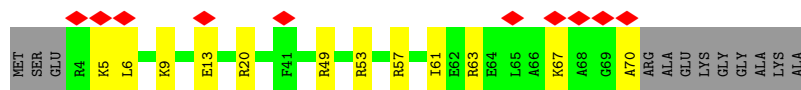
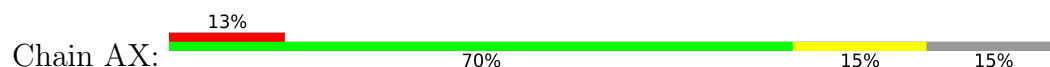
- Molecule 24: Large ribosomal subunit protein uL24



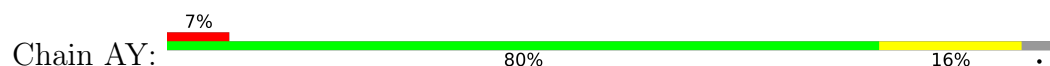
- Molecule 25: Large ribosomal subunit protein eL24



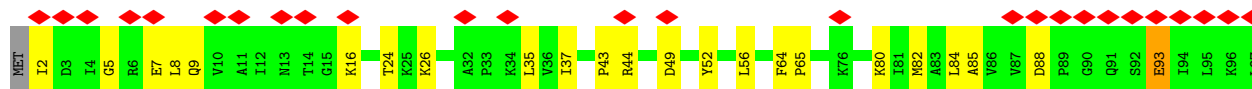
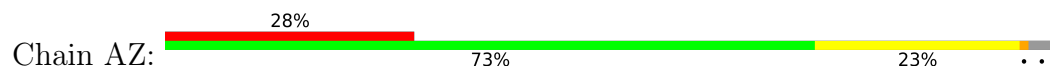
- Molecule 26: Large ribosomal subunit protein uL29



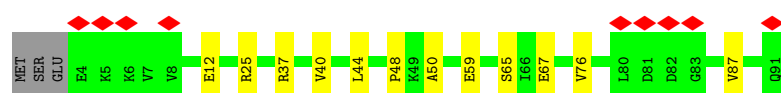
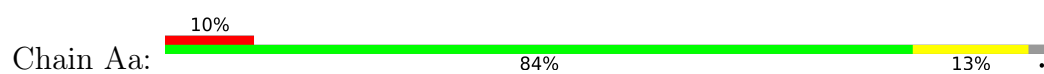
- Molecule 27: Large ribosomal subunit protein uL30



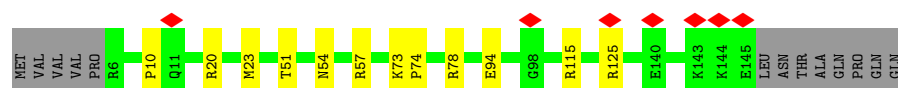
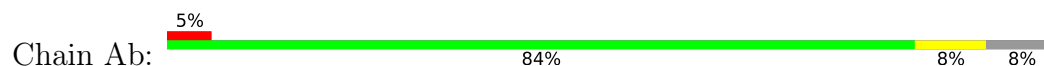
- Molecule 28: Large ribosomal subunit protein eL30



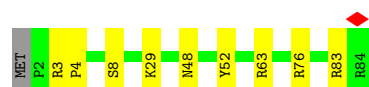
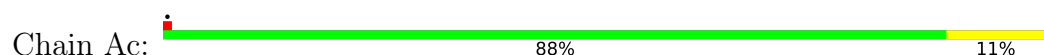
- Molecule 29: Large ribosomal subunit protein eL31



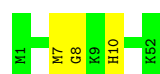
- Molecule 30: Large ribosomal subunit protein eL32



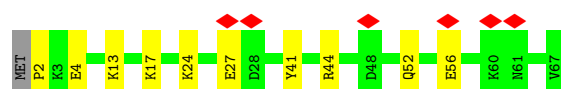
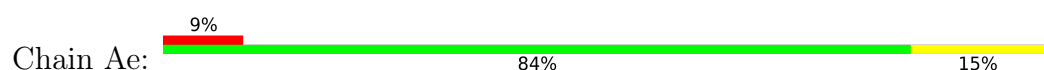
- Molecule 31: Large ribosomal subunit protein eL34



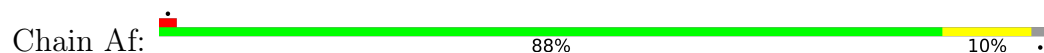
- Molecule 32: Large ribosomal subunit protein eL37



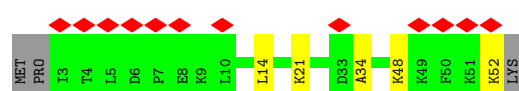
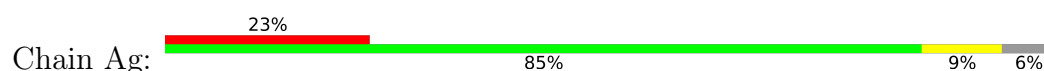
- Molecule 33: LSU ribosomal protein L38E



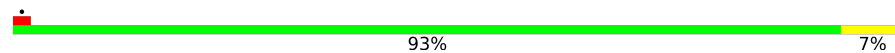
- Molecule 34: Large ribosomal subunit protein eL39

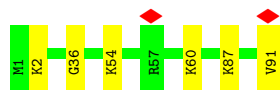


- Molecule 35: Large ribosomal subunit protein eL40



- Molecule 36: eL42

Chain Ah:  93% 7%



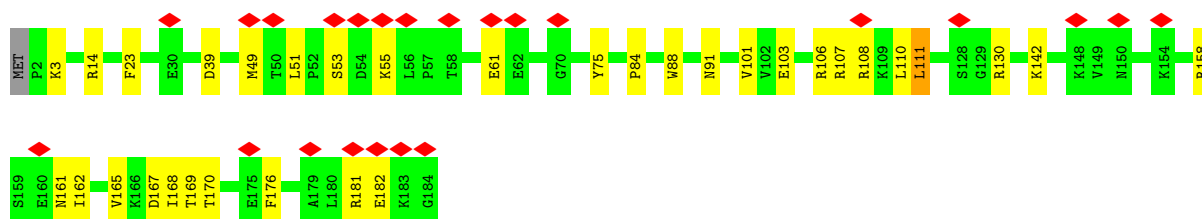
- Molecule 37: Large ribosomal subunit protein eL43

Chain Ai:  23% 83% 14%



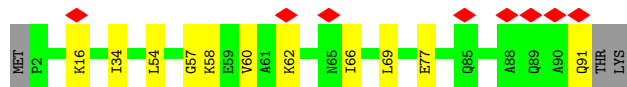
- Molecule 38: DJ-1/PfpI domain-containing protein

Chain Aj:  12% 82% 17%



- Molecule 39: PaREP1 domain containing protein

Chain Ak:  9% 85% 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	183467	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.352	Depositor
Minimum map value	-0.518	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.152	Depositor
Map size ($\text{\AA}$)	504.2144, 504.2144, 504.2144	wwPDB
Map dimensions	608, 608, 608	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8293, 0.8293, 0.8293	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5MC, UR3, 4AC, ZN, OMC, OMG, OMU, G7M, SPM, B8T, A2M, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.42	5/66967 (0.0%)	0.41	14/104542 (0.0%)
2	2	0.33	0/3096	0.36	1/4830 (0.0%)
3	3	0.28	0/2323	0.34	0/3153
4	AA	0.33	0/1847	0.44	0/2489
5	AB	0.33	0/2678	0.39	0/3643
6	AC	0.32	0/2234	0.42	0/3024
7	AD	0.24	0/1431	0.38	0/1913
8	AE	0.27	0/1548	0.36	0/2087
9	AF	0.24	0/1114	0.34	0/1513
10	AG	0.30	0/1542	0.32	0/2076
11	AH	0.29	0/1265	0.34	0/1692
12	AI	0.29	0/1093	0.40	0/1487
13	AJ	0.24	0/795	0.35	0/1068
13	AK	0.31	0/704	0.39	0/944
14	AL	0.29	0/1225	0.40	0/1639
15	AM	0.30	0/1594	0.34	0/2138
16	AN	0.30	0/1365	0.37	0/1841
17	AO	0.24	0/1647	0.34	0/2212
18	AP	0.28	0/933	0.34	0/1263
19	AQ	0.28	0/1233	0.33	0/1645
20	AR	0.29	0/610	0.30	0/817
21	AS	0.34	0/805	0.44	0/1081
22	AT	0.31	0/1536	0.37	0/2075
23	AU	0.29	0/655	0.33	0/877
24	AV	0.29	0/990	0.34	0/1325
25	AW	0.29	0/460	0.32	0/613
26	AX	0.26	0/557	0.27	0/738
27	AY	0.32	0/1407	0.38	0/1905
28	AZ	0.24	0/754	0.35	0/1021
29	Aa	0.30	0/735	0.35	0/986
30	Ab	0.30	0/1209	0.35	0/1621
31	Ac	0.32	0/663	0.38	0/889

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ad	0.35	0/442	0.36	0/587
33	Ae	0.28	0/562	0.28	0/753
34	Af	0.32	0/423	0.38	0/566
35	Ag	0.27	0/424	0.36	0/564
36	Ah	0.30	0/753	0.32	0/1001
37	Ai	0.31	0/788	0.43	0/1057
38	Aj	0.26	0/1497	0.35	0/2029
39	Ak	0.27	0/754	0.31	0/1005
All	All	0.38	5/112658 (0.0%)	0.39	15/166709 (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
7	AD	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2011	A2M	O3'-P	5.19	1.61	1.56
1	1	1990	A2M	O3'-P	5.15	1.61	1.56
1	1	2059	A2M	O3'-P	5.11	1.61	1.56
1	1	908	OMU	O3'-P	5.05	1.61	1.56
1	1	2691	A2M	O3'-P	5.02	1.61	1.56

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2030	G	P-O3'-C3'	-9.57	105.85	120.20
1	1	2041	C	P-O3'-C3'	-8.84	106.94	120.20
1	1	1677	G	P-O3'-C3'	-8.49	107.46	120.20
1	1	2903	U	P-O3'-C3'	-8.18	107.93	120.20
1	1	1678	G	P-O3'-C3'	-7.53	108.91	120.20
1	1	1987	PSU	P-O3'-C3'	-7.48	108.98	120.20
1	1	1603	G	P-O3'-C3'	-7.14	109.49	120.20
1	1	2952	U	P-O3'-C3'	-6.77	110.04	120.20
2	2	1	G	P-O3'-C3'	-6.45	110.53	120.20
1	1	2399	A	P-O3'-C3'	-5.65	111.73	120.20
1	1	1911	PSU	P-O3'-C3'	-5.50	111.96	120.20
1	1	397	G	P-O3'-C3'	-5.40	112.11	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1564	G	P-O3'-C3'	-5.39	112.12	120.20
1	1	1602	U	P-O3'-C3'	-5.31	112.24	120.20
1	1	2143	OMC	P-O3'-C3'	-5.19	112.41	120.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	AD	77	ARG	Sidechain
7	AD	78	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	61237	0	30991	517	0
2	2	2769	0	1405	28	0
3	3	2272	0	2350	32	0
4	AA	1803	0	1849	20	0
5	AB	2611	0	2737	26	0
6	AC	2178	0	2263	19	0
7	AD	1412	0	1511	38	0
8	AE	1520	0	1607	30	0
9	AF	1095	0	1156	18	0
10	AG	1510	0	1627	22	0
11	AH	1244	0	1346	13	0
12	AI	1068	0	1110	16	0
13	AJ	788	0	853	18	0
13	AK	700	0	760	23	0
14	AL	1198	0	1233	16	0
15	AM	1558	0	1641	19	0
16	AN	1336	0	1378	10	0
17	AO	1615	0	1688	29	0
18	AP	920	0	1010	9	0
19	AQ	1214	0	1272	26	0
20	AR	603	0	647	7	0
21	AS	788	0	832	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AT	1496	0	1575	13	0
23	AU	651	0	720	11	0
24	AV	976	0	1073	13	0
25	AW	449	0	465	3	0
26	AX	554	0	613	11	0
27	AY	1374	0	1422	23	0
28	AZ	742	0	796	18	0
29	Aa	726	0	794	8	0
30	Ab	1183	0	1270	11	0
31	Ac	649	0	698	10	0
32	Ad	429	0	430	3	0
33	Ae	552	0	592	9	0
34	Af	415	0	464	8	0
35	Ag	417	0	440	3	0
36	Ah	739	0	782	5	0
37	Ai	769	0	792	13	0
38	Aj	1469	0	1535	24	0
39	Ak	743	0	775	6	0
40	1	616	0	1144	103	0
40	AL	14	0	26	0	0
40	AM	14	0	26	5	0
41	1	168	0	0	0	0
41	AA	1	0	0	0	0
41	AL	2	0	0	0	0
41	AN	1	0	0	0	0
41	AT	1	0	0	0	0
42	AW	1	0	0	0	0
42	Ad	1	0	0	0	0
42	Ag	1	0	0	0	0
42	Ah	1	0	0	0	0
42	Ai	1	0	0	0	0
43	1	6534	0	0	177	0
43	2	147	0	0	9	0
43	3	58	0	0	6	0
43	AA	83	0	0	5	0
43	AB	85	0	0	3	0
43	AC	83	0	0	2	0
43	AD	16	0	0	4	0
43	AE	22	0	0	5	0
43	AF	19	0	0	5	0
43	AG	50	0	0	4	0
43	AH	49	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	AI	30	0	0	2	0
43	AJ	13	0	0	1	0
43	AK	15	0	0	5	0
43	AL	49	0	0	2	0
43	AM	66	0	0	2	0
43	AN	51	0	0	2	0
43	AO	32	0	0	7	0
43	AP	28	0	0	1	0
43	AQ	45	0	0	7	0
43	AR	13	0	0	1	0
43	AS	37	0	0	1	0
43	AT	46	0	0	1	0
43	AU	22	0	0	5	0
43	AV	30	0	0	1	0
43	AW	13	0	0	0	0
43	AX	32	0	0	6	0
43	AY	38	0	0	6	0
43	AZ	18	0	0	4	0
43	Aa	22	0	0	3	0
43	Ab	42	0	0	3	0
43	Ac	21	0	0	1	0
43	Ad	26	0	0	0	0
43	Ae	17	0	0	2	0
43	Af	18	0	0	2	0
43	Ag	11	0	0	1	0
43	Ah	26	0	0	0	0
43	Ai	34	0	0	4	0
43	Aj	41	0	0	7	0
43	Ak	12	0	0	1	0
All	All	114588	0	77698	1076	0

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

All (1076) 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)
27:AY:41:LYS:HE2	43:AY:232:HOH:O	1.25	1.34
1:1:1377:G:H5'	43:1:4031:HOH:O	1.36	1.21
40:1:3128:SPM:H92	43:1:6884:HOH:O	1.40	1.17
2:2:126:G:H5'	43:2:303:HOH:O	1.41	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AO:169:ARG:HD2	43:AO:316:HOH:O	1.41	1.16
1:1:1:U:H4'	43:1:4500:HOH:O	1.43	1.16
43:1:5498:HOH:O	19:AQ:73:ARG:HD2	1.49	1.12
43:1:8228:HOH:O	3:3:157:LYS:HD2	1.48	1.12
13:AJ:3:LYS:HB3	43:AZ:205:HOH:O	1.49	1.10
43:1:6673:HOH:O	24:AV:26:LYS:HE2	1.51	1.09
1:1:1172:A:H2'	43:1:7813:HOH:O	1.52	1.08
1:1:583:C:H5''	43:1:4094:HOH:O	1.54	1.07
40:1:3143:SPM:H81	43:1:5111:HOH:O	1.54	1.07
1:1:399:U:H5''	43:1:8274:HOH:O	1.58	1.02
9:AF:32:GLU:HB3	43:AF:205:HOH:O	1.59	1.01
1:1:6:A:H8	43:1:8712:HOH:O	1.45	0.99
1:1:1635:U:H6	43:1:8331:HOH:O	1.46	0.97
11:AH:150:ARG:HD3	43:AH:207:HOH:O	1.64	0.96
27:AY:121:LYS:HG3	43:AY:235:HOH:O	1.66	0.94
1:1:1:U:H5''	43:1:3625:HOH:O	1.66	0.94
40:1:3115:SPM:H32	43:1:7204:HOH:O	1.68	0.93
1:1:270:C:H1'	43:1:3475:HOH:O	1.69	0.93
7:AD:114:HIS:CD2	43:AD:212:HOH:O	2.20	0.92
40:1:3108:SPM:H112	43:1:9215:HOH:O	1.70	0.92
1:1:697:C:H4'	43:1:5239:HOH:O	1.69	0.91
1:1:2743:U:C4	43:1:3625:HOH:O	2.25	0.90
1:1:1260:C:H6	43:1:9062:HOH:O	1.56	0.89
40:1:3135:SPM:H71	43:1:9084:HOH:O	1.70	0.89
10:AG:139:PRO:HG2	43:AG:235:HOH:O	1.74	0.88
1:1:995:G:H2'	43:1:3899:HOH:O	1.73	0.88
40:1:3140:SPM:C3	43:1:3703:HOH:O	2.22	0.87
40:1:3140:SPM:H32	43:1:3703:HOH:O	1.73	0.87
1:1:2992:G:H1'	43:1:4719:HOH:O	1.74	0.86
7:AD:45:LEU:HD11	43:AD:212:HOH:O	1.75	0.86
16:AN:71:GLN:HG3	43:AN:305:HOH:O	1.75	0.85
10:AG:159:ARG:HD3	43:AG:227:HOH:O	1.74	0.85
40:1:3137:SPM:H71	43:1:9629:HOH:O	1.75	0.85
40:1:3125:SPM:H22	43:1:7614:HOH:O	1.76	0.84
1:1:2417:U:H5'	7:AD:110:GLY:HA3	1.59	0.84
38:Aj:181:ARG:HB2	43:Aj:8732:HOH:O	1.79	0.83
1:1:1635:U:C6	43:1:8331:HOH:O	2.24	0.82
19:AQ:82:ARG:HG2	43:AQ:201:HOH:O	1.78	0.82
38:Aj:142:LYS:HE2	43:Aj:8721:HOH:O	1.78	0.81
19:AQ:82:ARG:CD	43:AQ:201:HOH:O	2.27	0.81
43:1:4008:HOH:O	11:AH:105:ARG:HD3	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AG:131:ARG:H	10:AG:131:ARG:HE	1.26	0.81
1:1:1514:A:H3'	43:1:5101:HOH:O	1.81	0.80
2:2:2:C:H2'	2:2:3:C:C6	2.16	0.80
1:1:679:U:HO2'	14:AL:2:VAL:N	1.80	0.79
27:AY:25:THR:HG21	43:AY:221:HOH:O	1.82	0.79
23:AU:13:ARG:HD2	43:AU:101:HOH:O	1.82	0.79
2:2:129:C:C5	43:2:342:HOH:O	2.33	0.79
8:AE:168:GLU:HG3	43:AE:211:HOH:O	1.82	0.79
1:1:1869:U:H5'	43:1:6814:HOH:O	1.83	0.79
1:1:88:G:H3'	43:1:3849:HOH:O	1.82	0.78
43:1:6696:HOH:O	16:AN:75:LYS:HD3	1.83	0.78
7:AD:41:LEU:HD11	43:AD:212:HOH:O	1.83	0.77
13:AJ:47:ARG:NH2	13:AJ:68:ALA:O	2.16	0.77
18:AP:21:ARG:HD3	43:AP:217:HOH:O	1.84	0.77
40:1:3143:SPM:HN5	5:AB:223:ILE:HB	1.49	0.77
1:1:2914:C:C5'	43:1:3714:HOH:O	2.33	0.76
7:AD:84:PHE:HZ	7:AD:131:MET:HE1	1.48	0.76
1:1:2913:G:C8	43:1:3499:HOH:O	2.39	0.76
2:2:41:U:H5''	43:2:232:HOH:O	1.85	0.76
1:1:2914:C:H5'	43:1:3714:HOH:O	1.85	0.76
3:3:150:TYR:H	3:3:298:ARG:HH12	1.32	0.76
17:AO:135:GLU:OE2	17:AO:135:GLU:N	2.18	0.76
27:AY:17:ILE:HG12	27:AY:44:MET:HG3	1.66	0.76
1:1:706:A:H5'	43:1:9189:HOH:O	1.85	0.75
15:AM:41:GLU:OE2	15:AM:41:GLU:N	2.18	0.75
9:AF:125:GLU:CG	43:AF:206:HOH:O	2.35	0.75
1:1:901:A:H2'	1:1:903:A:OP1	1.86	0.74
13:AJ:3:LYS:HE2	43:AZ:205:HOH:O	1.87	0.74
19:AQ:82:ARG:CG	43:AQ:201:HOH:O	2.34	0.74
26:AX:20:ARG:HB3	43:AX:110:HOH:O	1.86	0.74
39:AK:58:LYS:NZ	39:AK:77:GLU:OE2	2.20	0.74
1:1:1:U:H2'	1:1:2:A:C8	2.22	0.74
40:1:3142:SPM:H31	4:AA:45:HIS:H	1.52	0.73
17:AO:155:LEU:HD12	43:AO:310:HOH:O	1.88	0.73
14:AL:92:ARG:HD3	14:AL:104:LEU:HD21	1.70	0.73
1:1:834:A:H5''	43:1:6549:HOH:O	1.89	0.73
2:2:2:C:H2'	2:2:3:C:H6	1.54	0.73
1:1:422:U:H5'	43:1:3736:HOH:O	1.89	0.72
1:1:1635:U:H2'	43:1:8331:HOH:O	1.89	0.72
40:1:3133:SPM:H32	43:1:4557:HOH:O	1.90	0.72
1:1:397:G:H5''	43:1:3433:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AT:77:LYS:NZ	43:AT:301:HOH:O	2.23	0.71
13:AK:59:ASP:HA	43:AK:206:HOH:O	1.89	0.71
1:1:761:A:C4	43:1:3570:HOH:O	2.43	0.71
6:AC:201:ARG:NH2	6:AC:224:LYS:O	2.23	0.71
1:1:699:A:N1	43:1:3426:HOH:O	2.24	0.71
8:AE:1:MET:SD	43:AE:222:HOH:O	2.48	0.71
13:AK:68:ALA:HA	43:AK:201:HOH:O	1.89	0.71
1:1:447:G:H1'	43:1:7322:HOH:O	1.90	0.70
1:1:697:C:C5'	43:1:5239:HOH:O	2.39	0.70
1:1:2313:C:H5''	43:1:7731:HOH:O	1.90	0.70
1:1:112:G:OP2	40:1:3117:SPM:N1	2.23	0.70
23:AU:3:LYS:NZ	23:AU:58:GLU:OE1	2.21	0.70
1:1:697:C:H5''	43:1:5239:HOH:O	1.91	0.70
1:1:1031:C:H5''	16:AN:19:ARG:HH12	1.57	0.70
40:1:3126:SPM:H42	43:1:4420:HOH:O	1.92	0.70
26:AX:67:LYS:NZ	43:AX:101:HOH:O	2.25	0.69
1:1:2:A:H2	1:1:3021:G:H1	1.39	0.69
1:1:422:U:C5'	43:1:3736:HOH:O	2.41	0.69
2:2:121:G:N7	43:2:204:HOH:O	2.24	0.69
3:3:25:HIS:CE1	43:3:712:HOH:O	2.44	0.69
39:AK:16:LYS:HD2	43:AK:109:HOH:O	1.93	0.69
1:1:2215:G:P	43:1:3546:HOH:O	2.50	0.68
17:AO:34:ARG:HD3	43:AO:324:HOH:O	1.92	0.68
1:1:1603:G:H2'	1:1:1604:C:C6	2.28	0.68
30:Ab:125:ARG:HB2	43:Ab:206:HOH:O	1.93	0.68
1:1:2913:G:H3'	43:1:3499:HOH:O	1.94	0.68
40:1:3133:SPM:N14	43:1:3431:HOH:O	2.25	0.68
43:1:8205:HOH:O	24:AV:26:LYS:HE3	1.93	0.68
1:1:1435:C:H4'	31:Ac:3:ARG:HB2	1.76	0.68
40:1:3115:SPM:C3	43:1:7204:HOH:O	2.33	0.67
1:1:2739:G:H5'	22:AT:92:GLY:HA2	1.75	0.67
43:1:8205:HOH:O	24:AV:26:LYS:CE	2.41	0.67
40:1:3125:SPM:H42	43:1:7614:HOH:O	1.95	0.67
1:1:1029:A:H4'	40:1:3106:SPM:H72	1.75	0.67
1:1:2825:C:N4	43:1:3403:HOH:O	2.20	0.67
43:1:4326:HOH:O	15:AM:163:ARG:HD2	1.95	0.67
1:1:867:C:OP2	40:1:3116:SPM:N14	2.25	0.67
14:AL:91:LEU:HD23	14:AL:94:ARG:HH12	1.59	0.67
1:1:1032:U:O4	40:1:3106:SPM:H122	1.94	0.67
1:1:813:G:H5'	31:Ac:8:SER:HA	1.77	0.67
1:1:338:A:O2'	1:1:339:U:H2'	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1492:U:OP1	40:AM:201:SPM:H121	1.95	0.66
7:AD:145:GLN:HG3	7:AD:154:VAL:HG23	1.77	0.66
23:AU:13:ARG:CD	43:AU:101:HOH:O	2.41	0.66
26:AX:63:ARG:NH2	43:AX:103:HOH:O	2.29	0.66
37:AI:84:GLU:HG3	43:AI:314:HOH:O	1.94	0.66
5:AB:117:VAL:HG23	5:AB:118:LEU:HG	1.78	0.65
8:AE:29:VAL:HG22	8:AE:42:GLU:HG2	1.78	0.65
1:1:1901:G:N3	43:1:3486:HOH:O	2.30	0.65
15:AM:166:GLU:OE2	15:AM:170:LYS:NZ	2.28	0.65
1:1:1870:A:H4'	19:AQ:98:ARG:HD2	1.78	0.65
1:1:1171:A:N6	43:1:3456:HOH:O	2.28	0.65
1:1:596:A:N3	43:1:3464:HOH:O	2.28	0.65
3:3:149:VAL:HG21	3:3:289:ALA:HB2	1.78	0.65
40:1:3120:SPM:N14	43:1:3489:HOH:O	2.30	0.64
1:1:995:G:C2'	43:1:3899:HOH:O	2.36	0.64
1:1:1110:G:C8	27:AY:23:PRO:HG3	2.32	0.64
1:1:2118:G:OP2	40:1:3143:SPM:H32	1.96	0.64
4:AA:185:LYS:HG2	43:AA:464:HOH:O	1.97	0.64
22:AT:170:LYS:O	22:AT:175:LYS:NZ	2.31	0.64
38:AJ:181:ARG:CB	43:AJ:8732:HOH:O	2.42	0.64
13:AK:59:ASP:CA	43:AK:206:HOH:O	2.45	0.64
24:AV:35:GLU:OE2	24:AV:35:GLU:N	2.27	0.64
1:1:963:G:H1'	1:1:1054:A:N6	2.12	0.64
5:AB:208:LYS:HG2	43:AB:408:HOH:O	1.97	0.64
8:AE:120:ARG:NH2	8:AE:169:GLU:OE1	2.31	0.64
9:AF:125:GLU:HG2	43:AF:206:HOH:O	1.94	0.63
17:AO:59:VAL:HG12	17:AO:60:VAL:HG23	1.80	0.63
13:AJ:58:THR:HG22	13:AJ:60:LYS:H	1.62	0.63
1:1:215:C:H2'	1:1:216:C:C6	2.33	0.63
7:AD:101:PHE:O	7:AD:162:ARG:NH2	2.28	0.63
13:AJ:23:ALA:HA	13:AJ:38:GLY:HA3	1.79	0.63
13:AJ:84:GLU:OE1	13:AJ:87:LYS:NZ	2.30	0.63
1:1:1514:A:OP2	31:Ac:29:LYS:NZ	2.31	0.63
10:AG:131:ARG:H	10:AG:131:ARG:NE	1.97	0.63
18:AP:51:VAL:HG12	18:AP:76:LEU:HB2	1.79	0.63
8:AE:144:VAL:HG12	8:AE:152:VAL:HG13	1.80	0.63
1:1:2743:U:C5	43:1:3625:HOH:O	2.48	0.63
1:1:797:G:H4'	43:1:8626:HOH:O	1.98	0.63
26:AX:70:ALA:C	43:AX:124:HOH:O	2.41	0.62
1:1:1260:C:C6	43:1:9062:HOH:O	2.40	0.62
15:AM:68:ILE:O	40:AM:201:SPM:N14	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AD:42:LEU:HD12	7:AD:72:VAL:HG12	1.81	0.62
13:AJ:72:GLU:HA	13:AJ:75:LYS:HD3	1.81	0.62
40:1:3143:SPM:N1	5:AB:222:THR:OG1	2.32	0.62
13:AK:71:GLU:CD	13:AK:71:GLU:H	2.07	0.62
6:AC:70:ARG:HD2	43:AC:378:HOH:O	2.00	0.62
34:Af:37:ARG:CZ	43:Af:101:HOH:O	2.47	0.61
1:1:1927:A:H4'	4:AA:169:PHE:O	1.99	0.61
1:1:2958:G:N7	40:1:3113:SPM:H72	2.15	0.61
9:AF:73:ASP:HB3	9:AF:74:PRO:HD3	1.82	0.61
1:1:1770:G:N7	40:1:3138:SPM:H111	2.16	0.61
1:1:145:G:H2'	1:1:146:C:C6	2.36	0.61
1:1:2184:C:H2'	1:1:2185:C:C6	2.36	0.61
9:AF:49:LYS:HD3	9:AF:105:ALA:HB1	1.83	0.61
1:1:1300:G:N1	6:AC:21:LYS:O	2.32	0.61
1:1:1684:C:H1'	43:1:3561:HOH:O	2.01	0.61
1:1:1734:C:OP1	33:Ae:41:TYR:OH	2.17	0.61
1:1:697:C:C4'	43:1:5239:HOH:O	2.34	0.61
34:Af:37:ARG:NH2	43:Af:101:HOH:O	2.33	0.61
1:1:259:U:H2'	1:1:260:C:C6	2.36	0.60
1:1:1456:A:N3	43:1:3503:HOH:O	2.31	0.60
43:1:7098:HOH:O	18:AP:44:ARG:HG3	2.00	0.60
1:1:1790:C:H5'	1:1:1791:U:H5''	1.84	0.60
1:1:1559:C:OP2	31:Ac:63:ARG:NH1	2.34	0.60
1:1:2993:A:H4'	43:1:8580:HOH:O	2.02	0.60
2:2:1:G:C2'	2:2:2:C:H5'	2.31	0.60
17:AO:109:ARG:HG3	17:AO:110:PRO:HD2	1.82	0.60
40:1:3140:SPM:H112	43:1:4978:HOH:O	2.02	0.60
5:AB:247:LEU:HA	43:AB:438:HOH:O	2.02	0.60
8:AE:113:THR:HB	8:AE:123:LYS:NZ	2.17	0.60
1:1:2102:A:O2'	1:1:2103:OMG:OP1	2.14	0.60
40:1:3129:SPM:H111	43:1:7904:HOH:O	2.01	0.60
27:AY:121:LYS:CG	43:AY:235:HOH:O	2.35	0.60
27:AY:123:ASP:C	43:AY:203:HOH:O	2.43	0.60
1:1:83:G:C5	34:Af:32:LYS:HD2	2.37	0.60
2:2:44:U:O2'	2:2:46:A:N7	2.25	0.60
23:AU:13:ARG:NE	43:AU:101:HOH:O	2.33	0.60
1:1:1898:A:O2'	40:1:3123:SPM:H22	2.02	0.59
1:1:692:G:N7	43:1:3500:HOH:O	2.31	0.59
14:AL:97:VAL:HG11	14:AL:104:LEU:HD23	1.83	0.59
40:1:3125:SPM:C4	43:1:7614:HOH:O	2.48	0.59
1:1:1493:A:OP2	40:AM:201:SPM:H122	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:84:G:N7	34:Af:30:LYS:HD2	2.18	0.59
1:1:2440:A:H2'	1:1:2441:G:C8	2.38	0.59
3:3:95:GLU:N	3:3:95:GLU:OE2	2.36	0.59
7:AD:65:ARG:HB2	7:AD:65:ARG:NH1	2.17	0.59
19:AQ:82:ARG:NE	43:AQ:201:HOH:O	2.33	0.59
8:AE:53:SER:OG	8:AE:56:LYS:NZ	2.34	0.59
40:1:3142:SPM:HN12	37:Ai:52:LEU:HB3	1.66	0.59
1:1:259:U:H2'	1:1:260:C:H6	1.67	0.59
1:1:1299:C:H2'	1:1:1300:G:H5''	1.85	0.59
1:1:2403:U:OP1	1:1:2495:C:O2'	2.20	0.59
1:1:902:OMG:H4'	1:1:903:A:OP1	2.02	0.58
7:AD:111:ILE:HB	7:AD:131:MET:HB2	1.85	0.58
15:AM:97:TRP:CH2	40:AM:201:SPM:H132	2.37	0.58
28:AZ:16:LYS:H	28:AZ:88:ASP:HB3	1.68	0.58
1:1:465:C:H2'	1:1:466:G:C8	2.39	0.58
1:1:1859:U:P	19:AQ:130:ARG:HH21	2.26	0.58
1:1:624:G:H2'	1:1:625:G:C8	2.39	0.58
1:1:762:A:H2'	1:1:763:A:C8	2.39	0.58
1:1:1635:U:H4'	43:1:7125:HOH:O	2.03	0.58
11:AH:86:VAL:HG12	15:AM:157:ARG:HG3	1.86	0.58
29:Aa:40:VAL:HG21	29:Aa:87:VAL:HG21	1.85	0.58
33:Ae:52:GLN:HB2	43:Ae:110:HOH:O	2.04	0.57
1:1:1260:C:H5'	43:1:9062:HOH:O	2.03	0.57
3:3:29:ARG:NH2	3:3:59:SER:O	2.36	0.57
28:AZ:44:ARG:HG2	28:AZ:44:ARG:HH11	1.68	0.57
28:AZ:65:PRO:O	37:Ai:93:LYS:HG3	2.04	0.57
1:1:646:G:H5''	30:Ab:51:THR:HG21	1.86	0.57
4:AA:88:VAL:HG21	37:Ai:81:ILE:O	2.05	0.57
1:1:1904:A:N3	43:1:3526:HOH:O	2.32	0.57
19:AQ:82:ARG:HD2	43:AQ:209:HOH:O	2.04	0.57
38:Aj:3:LYS:NZ	38:Aj:3:LYS:HB3	2.20	0.57
1:1:761:A:N3	43:1:3570:HOH:O	2.34	0.57
1:1:1154:A:H2'	1:1:1155:A:C8	2.39	0.57
43:1:3438:HOH:O	19:AQ:79:LYS:HD3	2.04	0.57
1:1:583:C:C5'	43:1:4094:HOH:O	2.30	0.57
1:1:1578:G:H2'	1:1:1579:C:C6	2.40	0.57
1:1:2329:G:H2'	1:1:2330:G:H8	1.69	0.57
40:1:3125:SPM:C2	43:1:7614:HOH:O	2.42	0.57
8:AE:10:VAL:HG22	8:AE:76:LYS:HG3	1.87	0.57
1:1:444:A:H1'	1:1:2001:A:C2	2.39	0.57
19:AQ:144:GLU:N	19:AQ:144:GLU:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:227:G:OP2	40:1:3115:SPM:H41	2.05	0.56
1:1:830:C:H2'	1:1:831:G:O4'	2.05	0.56
1:1:2662:G:N7	40:1:3130:SPM:N1	2.53	0.56
8:AE:93:LYS:NZ	8:AE:192:GLU:OE1	2.35	0.56
1:1:831:G:H2'	43:1:3483:HOH:O	2.05	0.56
1:1:1292:C:H2'	1:1:1293:G:C8	2.40	0.56
17:AO:144:ARG:NH1	17:AO:185:GLU:OE2	2.38	0.56
7:AD:176:GLN:NE2	7:AD:178:ASP:OD2	2.38	0.56
36:Ah:2:LYS:HD2	36:Ah:91:VAL:HG21	1.86	0.56
1:1:122:G:H2'	1:1:123:C:C6	2.41	0.56
1:1:1901:G:N7	43:1:3521:HOH:O	2.32	0.56
37:Ai:84:GLU:CG	43:Ai:314:HOH:O	2.53	0.56
38:Aj:108:ARG:HG3	38:Aj:108:ARG:HH11	1.71	0.56
1:1:2622:G:OP2	40:1:3128:SPM:H81	2.05	0.56
2:2:129:C:C3'	43:2:220:HOH:O	2.53	0.56
14:AL:45:TRP:CZ2	14:AL:49:MET:HE3	2.40	0.56
1:1:2164:C:H5'	43:1:6277:HOH:O	2.06	0.56
6:AC:202:ALA:HA	6:AC:223:PRO:HG2	1.87	0.56
1:1:2029:G:H2'	1:1:2030:G:O4'	2.05	0.56
3:3:246:VAL:HG12	3:3:269:PRO:HG2	1.88	0.56
7:AD:166:VAL:HG23	7:AD:177:VAL:HG11	1.88	0.56
18:AP:62:ASP:OD2	18:AP:119:LYS:NZ	2.39	0.56
1:1:1899:G:O4'	40:1:3123:SPM:N1	2.39	0.55
1:1:2194:U:H2'	1:1:2195:U:C6	2.40	0.55
22:AT:8:LEU:HD12	22:AT:12:GLN:HB2	1.88	0.55
43:1:8228:HOH:O	3:3:157:LYS:CD	2.28	0.55
13:AJ:13:LYS:NZ	43:AJ:202:HOH:O	2.39	0.55
24:AV:20:PRO:HD2	24:AV:23:LEU:HD12	1.88	0.55
1:1:1578:G:H2'	1:1:1579:C:H6	1.70	0.55
29:Aa:12:GLU:HG2	29:Aa:76:VAL:HG22	1.88	0.55
1:1:2914:C:O2'	1:1:2915:A:H8	1.89	0.55
32:Ad:7:MET:HA	32:Ad:10:HIS:HD2	1.71	0.55
1:1:906:A:O2'	40:1:3114:SPM:H131	2.07	0.55
7:AD:148:ARG:NH1	17:AO:109:ARG:HH21	2.04	0.55
10:AG:159:ARG:HG3	10:AG:166:TRP:CD2	2.41	0.55
12:AI:100:VAL:HG22	25:AW:20:MET:HE3	1.88	0.55
43:1:8228:HOH:O	3:3:157:LYS:HE3	2.06	0.55
1:1:2469:G:H3'	43:1:6485:HOH:O	2.06	0.55
1:1:2743:U:N3	43:1:3625:HOH:O	2.37	0.55
17:AO:73:LYS:HB2	17:AO:175:LEU:HD12	1.88	0.55
1:1:526:G:N7	40:1:3141:SPM:H121	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2532:G:H2'	1:1:2533:C:C6	2.42	0.55
19:AQ:105:ARG:HH11	19:AQ:105:ARG:HG3	1.72	0.54
1:1:456:G:OP1	15:AM:48:ARG:NH2	2.34	0.54
10:AG:150:GLN:NE2	43:AG:205:HOH:O	2.40	0.54
1:1:419:G:O2'	1:1:422:U:O2'	2.24	0.54
1:1:2048:A:H2'	1:1:2049:A:C8	2.43	0.54
1:1:2356:C:H5'	1:1:2357:G:H5''	1.89	0.54
27:AY:25:THR:HG23	27:AY:30:ALA:HB2	1.89	0.54
1:1:2540:U:OP2	36:Ah:60:LYS:HG2	2.08	0.54
1:1:30:C:H2'	1:1:31:U:C6	2.43	0.54
1:1:2476:A:O2'	1:1:2506:G:H4'	2.07	0.54
1:1:247:G:OP2	11:AH:25:ARG:NH2	2.33	0.54
10:AG:60:ARG:HG3	10:AG:152:VAL:HG11	1.89	0.54
1:1:741:C:H2'	1:1:742:C:H6	1.73	0.54
40:1:3127:SPM:H32	43:1:3621:HOH:O	2.07	0.54
40:1:3130:SPM:H22	43:1:5978:HOH:O	2.08	0.54
13:AK:59:ASP:OD1	13:AK:59:ASP:N	2.38	0.54
1:1:2985:C:H2'	1:1:2986:C:H6	1.72	0.54
1:1:178:A:OP2	40:1:3121:SPM:N1	2.41	0.54
1:1:919:G:H4'	40:1:3134:SPM:H21	1.89	0.54
8:AE:8:GLU:HG3	8:AE:72:LEU:HB3	1.89	0.54
17:AO:134:GLU:HB3	43:AO:322:HOH:O	2.07	0.54
1:1:231:G:H2'	1:1:232:A:C8	2.43	0.53
1:1:2185:C:H2'	1:1:2186:U:C6	2.43	0.53
38:Aj:14:ARG:NH2	43:Aj:8702:HOH:O	2.39	0.53
1:1:1035:G:N2	40:1:3106:SPM:HN42	2.06	0.53
12:AI:8:ARG:NH2	12:AI:115:ASP:OD2	2.41	0.53
1:1:422:U:O4	40:1:3115:SPM:N14	2.40	0.53
1:1:2417:U:H2'	1:1:2418:C:C6	2.43	0.53
3:3:196:ILE:HD11	3:3:269:PRO:HD3	1.90	0.53
12:AI:68:VAL:HG22	12:AI:80:ILE:HG12	1.90	0.53
1:1:1321:G:OP2	40:1:3112:SPM:N14	2.41	0.53
1:1:657:C:C5	40:1:3110:SPM:H42	2.44	0.53
3:3:237:TRP:HA	3:3:240:MET:HG2	1.90	0.53
5:AB:65:LEU:HD11	12:AI:95:PRO:HB2	1.90	0.53
1:1:82:A:H1'	34:Af:30:LYS:HE2	1.89	0.53
1:1:270:C:C1'	43:1:3475:HOH:O	2.43	0.53
23:AU:9:GLU:CD	23:AU:9:GLU:H	2.17	0.53
1:1:1299:C:OP2	18:AP:22:LYS:HE2	2.09	0.53
1:1:1318:G:O6	40:1:3112:SPM:N1	2.42	0.53
1:1:2116:OMC:OP2	40:1:3143:SPM:H31	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:196:ILE:HG12	3:3:244:VAL:HG21	1.90	0.53
11:AH:80:GLU:HA	11:AH:80:GLU:OE1	2.08	0.53
15:AM:97:TRP:CZ3	40:AM:201:SPM:H132	2.44	0.53
20:AR:6:ARG:NH1	43:AR:103:HOH:O	2.42	0.53
1:1:1801:C:H5''	5:AB:233:GLY:HA3	1.91	0.53
1:1:6:A:H2'	43:1:3556:HOH:O	2.09	0.53
1:1:957:U:H2'	1:1:958:C:C6	2.43	0.52
1:1:1557:A:OP2	13:AJ:48:ARG:NH2	2.40	0.52
1:1:2694:U:H4'	43:1:8356:HOH:O	2.09	0.52
13:AK:34:VAL:HG13	13:AK:52:ILE:HD11	1.90	0.52
38:Aj:3:LYS:HB3	38:Aj:3:LYS:HZ2	1.73	0.52
7:AD:54:ARG:HD2	7:AD:67:GLY:O	2.09	0.52
27:AY:117:THR:HG23	27:AY:134:CYS:HB3	1.90	0.52
30:Ab:57:ARG:HD3	43:Ab:224:HOH:O	2.09	0.52
1:1:1789:G:O2'	40:1:3135:SPM:H132	2.09	0.52
1:1:2627:U:H2'	1:1:2628:OMU:H6	1.91	0.52
40:1:3140:SPM:H61	43:1:3523:HOH:O	2.09	0.52
1:1:1907:U:H2'	1:1:1908:G:C8	2.45	0.52
1:1:2185:C:H2'	1:1:2186:U:H6	1.74	0.52
1:1:2959:G:N7	40:1:3113:SPM:H121	2.24	0.52
3:3:44:ARG:HD3	43:3:716:HOH:O	2.08	0.52
10:AG:131:ARG:HD2	10:AG:132:ARG:H	1.75	0.52
11:AH:19:THR:HA	43:AH:241:HOH:O	2.10	0.52
19:AQ:28:ARG:NH1	19:AQ:44:GLU:OE1	2.42	0.52
40:1:3140:SPM:C4	43:1:3703:HOH:O	2.55	0.52
40:1:3112:SPM:H112	43:1:6691:HOH:O	2.10	0.52
4:AA:196:PRO:HD3	4:AA:203:GLY:HA2	1.92	0.52
11:AH:40:GLU:HA	11:AH:40:GLU:OE1	2.09	0.52
13:AJ:101:ASP:OD1	13:AJ:101:ASP:N	2.43	0.52
1:1:2918:C:H2'	1:1:2919:C:C6	2.44	0.52
1:1:1930:U:H2'	1:1:1931:C:C6	2.45	0.52
2:2:96:G:H2'	2:2:97:A:C8	2.44	0.52
7:AD:104:ARG:HG3	7:AD:104:ARG:HH11	1.74	0.52
33:Ae:27:GLU:CD	33:Ae:27:GLU:H	2.16	0.52
3:3:229:LYS:HG2	43:3:746:HOH:O	2.10	0.52
1:1:1356:U:H2'	1:1:1357:C:C6	2.44	0.52
40:1:3126:SPM:C4	43:1:4420:HOH:O	2.56	0.52
4:AA:37:ARG:N	43:AA:404:HOH:O	2.43	0.52
1:1:887:G:O6	40:1:3137:SPM:H81	2.10	0.51
1:1:1514:A:H2'	1:1:1515:A:C8	2.45	0.51
27:AY:125:LYS:HE3	27:AY:125:LYS:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:584:C:H2'	1:1:585:U:C6	2.45	0.51
1:1:584:C:H2'	1:1:585:U:H6	1.75	0.51
1:1:2439:A:H2'	1:1:2440:A:C8	2.44	0.51
5:AB:152:ARG:CZ	5:AB:159:LYS:HG2	2.40	0.51
23:AU:72:MET:HE1	23:AU:81:LEU:HD11	1.92	0.51
28:AZ:43:PRO:HD2	28:AZ:82:MET:SD	2.51	0.51
37:AI:84:GLU:CD	43:AI:314:HOH:O	2.53	0.51
1:1:2995:A:O2'	1:1:2996:G:OP1	2.28	0.51
43:1:8205:HOH:O	24:AV:26:LYS:HE2	2.05	0.51
8:AE:55:GLY:N	43:AE:202:HOH:O	2.40	0.51
1:1:1612:C:HO2'	1:1:1688:U:HO2'	1.58	0.51
1:1:1310:G:OP1	27:AY:139:LYS:NZ	2.39	0.51
1:1:1570:U:H2'	1:1:1571:C:C6	2.45	0.51
1:1:1922:A:H1'	1:1:2059:A2M:N6	2.26	0.51
1:1:2868:U:H1'	1:1:2869:A:H5''	1.92	0.51
1:1:2913:G:N9	43:1:3499:HOH:O	2.43	0.51
1:1:229:G:H5'	1:1:230:C:H5''	1.93	0.51
1:1:1635:U:H5''	43:1:8331:HOH:O	2.11	0.51
43:1:8228:HOH:O	3:3:157:LYS:CE	2.56	0.51
7:AD:32:GLY:O	7:AD:36:GLU:N	2.40	0.51
1:1:1569:G:H2'	1:1:1570:U:C6	2.46	0.51
1:1:2001:A:H2'	1:1:2002:A:O4'	2.11	0.51
5:AB:88:ARG:NH1	5:AB:165:GLU:OE2	2.43	0.51
7:AD:12:HIS:HB3	7:AD:15:LYS:HG3	1.92	0.51
10:AG:1:MET:SD	10:AG:1:MET:N	2.76	0.51
1:1:145:G:O6	40:1:3117:SPM:H72	2.11	0.51
1:1:1120:A:H2'	1:1:1121:A:C8	2.45	0.51
1:1:1299:C:OP2	18:AP:18:ARG:NH2	2.39	0.51
1:1:2041:C:H2'	1:1:2042:C:C6	2.45	0.51
2:2:43:A:H2'	2:2:44:U:C6	2.46	0.51
8:AE:68:GLU:OE1	8:AE:68:GLU:N	2.43	0.51
38:Aj:167:ASP:OD1	38:Aj:169:THR:OG1	2.29	0.51
1:1:459:U:H5'	11:AH:89:VAL:HG22	1.92	0.50
1:1:791:G:OP1	40:1:3134:SPM:H31	2.11	0.50
1:1:910:A:H5''	1:1:911:A:H5'	1.93	0.50
1:1:1317:A:OP2	40:1:3112:SPM:H21	2.09	0.50
1:1:1615:A:H2'	1:1:1616:A:C8	2.46	0.50
1:1:2712:A:H5''	4:AA:203:GLY:HA3	1.92	0.50
1:1:2913:G:H21	1:1:2916:A:H62	1.59	0.50
40:1:3134:SPM:H92	43:1:6203:HOH:O	2.10	0.50
12:AI:25:ASN:OD1	12:AI:40:ARG:NH1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:724:A:H1'	1:1:725:G:OP2	2.11	0.50
9:AF:125:GLU:CD	43:AF:206:HOH:O	2.52	0.50
28:AZ:8:LEU:HD21	28:AZ:84:LEU:HD21	1.94	0.50
1:1:152:A:H2'	1:1:153:A:C8	2.46	0.50
1:1:2680:A:H5'	43:1:8085:HOH:O	2.11	0.50
9:AF:6:ASP:OD1	9:AF:8:LYS:HG3	2.11	0.50
1:1:1949:OMG:OP2	40:1:3119:SPM:H61	2.12	0.50
1:1:2193:C:OP1	4:AA:3:LYS:HD2	2.11	0.50
4:AA:174:LYS:HG2	43:AA:482:HOH:O	2.11	0.50
1:1:623:G:N2	43:1:3721:HOH:O	2.41	0.50
1:1:741:C:H2'	1:1:742:C:C6	2.47	0.50
1:1:977:G:N3	1:1:2380:A:H2'	2.26	0.50
1:1:1090:U:H2'	1:1:1091:C:C6	2.46	0.50
1:1:1640:U:OP2	19:AQ:118:TYR:OH	2.28	0.50
1:1:2605:U:H5'	1:1:2684:G:H5''	1.93	0.50
13:AJ:27:ASP:HB3	13:AJ:35:VAL:HB	1.92	0.50
1:1:145:G:OP2	40:1:3117:SPM:H21	2.12	0.50
1:1:808:C:H2'	1:1:809:C:H6	1.77	0.50
8:AE:149:ARG:O	8:AE:153:SER:OG	2.23	0.50
16:AN:50:VAL:HG23	16:AN:171:LYS:HG2	1.93	0.50
1:1:774:U:H2'	1:1:775:C:C6	2.46	0.50
1:1:876:C:H5''	43:1:8012:HOH:O	2.11	0.50
1:1:1028:A:H2'	1:1:1031:C:C5	2.46	0.50
1:1:2705:C:H2'	1:1:2706:G:C8	2.46	0.50
43:1:8671:HOH:O	5:AB:236:ARG:HD2	2.11	0.50
13:AJ:10:VAL:HG22	13:AJ:24:VAL:HG22	1.92	0.50
21:AS:14:LYS:NZ	43:AS:103:HOH:O	2.42	0.50
1:1:1517:C:H2'	1:1:1518:G:C8	2.47	0.50
10:AG:8:ASP:HB3	10:AG:11:GLN:HB2	1.93	0.50
1:1:1930:U:H2'	1:1:1931:C:H6	1.76	0.50
31:Ac:3:ARG:HB3	31:Ac:4:PRO:HD3	1.93	0.50
1:1:1171:A:H5''	1:1:1172:A:H4'	1.94	0.49
1:1:1430:A:H5'	1:1:1431:A:OP2	2.12	0.49
1:1:2398:A:H4'	1:1:2399:A:O4'	2.12	0.49
1:1:2917:C:H2'	1:1:2918:C:C6	2.47	0.49
2:2:1:G:H2'	2:2:2:C:H5'	1.93	0.49
13:AK:27:ASP:OD1	13:AK:28:ILE:N	2.45	0.49
1:1:658:G:OP2	40:1:3110:SPM:H81	2.12	0.49
1:1:2995:A:H2'	1:1:2996:G:C8	2.47	0.49
1:1:624:G:H2'	1:1:625:G:H8	1.76	0.49
1:1:654:A:H5'	40:1:3110:SPM:HN12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1909:A:H5'	43:1:5373:HOH:O	2.12	0.49
12:AI:77:ARG:HG2	12:AI:77:ARG:HH11	1.78	0.49
13:AK:69:SER:N	43:AK:201:HOH:O	2.39	0.49
28:AZ:7:GLU:OE2	28:AZ:93:GLU:HG2	2.12	0.49
1:1:254:C:OP2	9:AF:56:LYS:NZ	2.35	0.49
9:AF:6:ASP:OD1	9:AF:9:THR:HG23	2.12	0.49
9:AF:8:LYS:HB3	15:AM:18:GLU:CG	2.43	0.49
14:AL:91:LEU:HB3	14:AL:97:VAL:HG23	1.94	0.49
30:Ab:94:GLU:OE1	30:Ab:94:GLU:N	2.38	0.49
1:1:1175:C:H2'	1:1:1176:A:H5'	1.95	0.49
1:1:1420:C:H5'	19:AQ:21:ILE:O	2.13	0.49
43:1:3623:HOH:O	24:AV:88:ARG:NH1	2.45	0.49
3:3:98:ARG:HG2	43:3:703:HOH:O	2.12	0.49
3:3:150:TYR:O	3:3:298:ARG:NH2	2.39	0.49
38:Aj:167:ASP:HB3	38:Aj:170:THR:OG1	2.12	0.49
1:1:6:A:C2'	43:1:3556:HOH:O	2.61	0.49
1:1:1770:G:H3'	40:1:3138:SPM:HN42	1.76	0.49
1:1:1909:A:N6	37:Ai:19:TYR:HA	2.28	0.49
4:AA:127:ILE:HB	4:AA:137:ILE:HG22	1.95	0.49
1:1:1481:A:H2'	1:1:1482:A:C8	2.47	0.49
43:1:5965:HOH:O	37:Ai:11:PRO:HG3	2.13	0.49
5:AB:203:VAL:HG12	5:AB:312:LEU:HD22	1.94	0.49
19:AQ:96:MET:HG2	19:AQ:132:LEU:HD22	1.95	0.49
1:1:12:G:H2'	1:1:13:C:C6	2.48	0.49
1:1:144:C:OP2	40:1:3117:SPM:H22	2.13	0.49
3:3:16:PRO:HB3	3:3:21:ASP:HB2	1.93	0.49
16:AN:114:GLU:CD	16:AN:114:GLU:H	2.21	0.49
12:AI:54:ARG:NH2	43:AI:202:HOH:O	2.37	0.49
13:AK:59:ASP:CB	43:AK:206:HOH:O	2.60	0.49
29:Aa:25:ARG:NH2	29:Aa:67:GLU:OE1	2.44	0.49
2:2:7:A:O2'	2:2:8:A:OP1	2.30	0.48
4:AA:153:ARG:HD3	43:AA:442:HOH:O	2.13	0.48
13:AK:15:LEU:HD12	13:AK:54:HIS:CD2	2.47	0.48
33:Ae:4:GLU:OE2	33:Ae:44:ARG:NH1	2.46	0.48
1:1:1259:A:O4'	10:AG:69:ARG:NH2	2.46	0.48
1:1:1035:G:H22	40:1:3106:SPM:HN42	1.61	0.48
1:1:2022:A:O2'	1:1:2023:G:OP1	2.26	0.48
1:1:2690:G:O2'	1:1:2693:A:OP2	2.32	0.48
4:AA:213:VAL:HG21	4:AA:222:LYS:HA	1.95	0.48
10:AG:139:PRO:HA	10:AG:142:LYS:HG3	1.95	0.48
14:AL:98:ARG:HE	14:AL:100:GLU:CD	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AU:1:MET:HE1	43:AU:106:HOH:O	2.12	0.48
1:1:1330:C:HO2'	6:AC:63:TYR:HH	1.54	0.48
1:1:2504:G:H4'	1:1:2505:A:C5	2.48	0.48
40:1:3137:SPM:H121	43:1:6323:HOH:O	2.12	0.48
17:AO:4:GLY:HA3	43:AO:325:HOH:O	2.13	0.48
23:AU:69:TYR:HA	43:AU:117:HOH:O	2.12	0.48
30:Ab:115:ARG:HG2	30:Ab:115:ARG:HH11	1.79	0.48
1:1:1075:G:C8	1:1:1075:G:H5''	2.48	0.48
1:1:1175:C:C2'	1:1:1176:A:H5'	2.42	0.48
1:1:2913:G:N2	1:1:2916:A:H62	2.12	0.48
43:1:5498:HOH:O	19:AQ:73:ARG:CD	2.30	0.48
1:1:2135:A:H2'	1:1:2136:C:H6	1.77	0.48
8:AE:110:ASN:OD1	8:AE:111:GLN:NE2	2.44	0.48
9:AF:30:VAL:HG22	9:AF:132:LYS:HE3	1.94	0.48
9:AF:54:THR:HG23	9:AF:115:VAL:HB	1.94	0.48
13:AJ:12:VAL:HG22	13:AJ:22:LYS:HG3	1.94	0.48
13:AJ:72:GLU:O	13:AJ:75:LYS:HG2	2.14	0.48
19:AQ:104:LYS:HD3	19:AQ:114:TRP:CG	2.48	0.48
28:AZ:44:ARG:HG2	28:AZ:44:ARG:NH1	2.27	0.48
1:1:414:G:H2'	1:1:415:C:C6	2.48	0.48
1:1:1663:C:H2'	1:1:1664:G:C8	2.49	0.48
1:1:2914:C:C3'	43:1:3714:HOH:O	2.61	0.48
9:AF:103:LYS:HB3	9:AF:103:LYS:HE3	1.69	0.48
14:AL:88:VAL:HG11	14:AL:126:LEU:HD11	1.96	0.48
22:AT:118:LYS:HE3	22:AT:118:LYS:HB2	1.66	0.48
23:AU:7:ILE:O	23:AU:7:ILE:HG22	2.13	0.48
39:Ak:62:LYS:HE3	39:Ak:62:LYS:HB2	1.56	0.48
1:1:1401:G:H1'	1:1:2825:C:N4	2.28	0.48
1:1:1428:G:OP2	40:1:3138:SPM:H112	2.13	0.48
13:AK:38:GLY:HA3	13:AK:39:PRO:C	2.39	0.48
1:1:2845:G:H2'	1:1:2846:G:C8	2.48	0.48
1:1:2915:A:O2'	1:1:2916:A:O4'	2.19	0.48
8:AE:91:ARG:HG3	8:AE:143:VAL:HG13	1.96	0.48
8:AE:113:THR:HB	8:AE:123:LYS:HZ1	1.79	0.48
14:AL:35:LYS:HE3	14:AL:35:LYS:HB3	1.61	0.48
1:1:670:U:H2'	1:1:671:C:C6	2.49	0.48
1:1:1687:G:H2'	1:1:1688:U:O4'	2.14	0.48
1:1:2992:G:C1'	43:1:4719:HOH:O	2.45	0.48
37:Ai:31:GLU:HA	37:Ai:34:GLN:HB3	1.96	0.48
1:1:504:G:H5''	43:1:7787:HOH:O	2.13	0.47
1:1:651:G:H2'	1:1:2150:C:C5	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1252:A:H4'	1:1:1253:A:H5''	1.96	0.47
1:1:1264:G:N3	10:AG:102:MET:HE2	2.29	0.47
13:AJ:28:ILE:HG13	13:AJ:34:VAL:HG12	1.95	0.47
27:AY:59:ARG:HA	27:AY:59:ARG:HH11	1.79	0.47
1:1:1696:A:O2'	43:1:3404:HOH:O	2.20	0.47
1:1:1770:G:OP2	40:1:3138:SPM:H121	2.14	0.47
1:1:1819:C:O2	5:AB:228:HIS:NE2	2.38	0.47
1:1:2140:C:H2'	1:1:2141:C:O4'	2.13	0.47
1:1:2918:C:H2'	1:1:2919:C:H6	1.79	0.47
6:AC:129:LYS:HE3	6:AC:129:LYS:HB3	1.64	0.47
14:AL:94:ARG:HG3	14:AL:94:ARG:HH11	1.79	0.47
38:Aj:130:ARG:HH22	38:Aj:162:ILE:HD12	1.79	0.47
1:1:215:C:H2'	1:1:216:C:H6	1.76	0.47
1:1:446:U:OP2	43:1:3401:HOH:O	2.20	0.47
1:1:763:A:H2'	1:1:764:G:O4'	2.14	0.47
1:1:811:U:O4	40:1:3137:SPM:H41	2.14	0.47
1:1:1350:G:H5''	30:Ab:78:ARG:HG2	1.95	0.47
1:1:1495:U:O2'	1:1:1496:A:H2'	2.15	0.47
1:1:2400:A:H1'	43:1:7372:HOH:O	2.14	0.47
1:1:2918:C:H3'	43:1:3562:HOH:O	2.13	0.47
1:1:465:C:H5'	43:1:8227:HOH:O	2.15	0.47
1:1:656:A:H2'	1:1:657:C:C6	2.49	0.47
1:1:2131:G:OP1	43:1:3402:HOH:O	2.20	0.47
7:AD:103:GLU:N	7:AD:103:GLU:OE1	2.46	0.47
1:1:2011:A2M:O5'	1:1:2011:A2M:H8	2.14	0.47
5:AB:13:MET:SD	5:AB:250:THR:HA	2.55	0.47
9:AF:76:GLU:HG2	15:AM:11:TRP:CD1	2.49	0.47
19:AQ:98:ARG:O	19:AQ:102:THR:OG1	2.27	0.47
1:1:253:A:H8	1:1:254:C:C5	2.32	0.47
1:1:627:G:H2'	1:1:628:U:C6	2.50	0.47
1:1:728:C:H2'	1:1:729:G:O4'	2.14	0.47
1:1:1097:C:OP2	40:1:3132:SPM:H112	2.14	0.47
1:1:1241:G:P	43:1:3509:HOH:O	2.72	0.47
1:1:2417:U:O2	7:AD:130:GLY:HA3	2.14	0.47
1:1:2749:C:O2'	5:AB:165:GLU:OE2	2.28	0.47
2:2:117:G:H2'	2:2:118:C:C6	2.49	0.47
3:3:141:PRO:HB2	3:3:143:ALA:O	2.15	0.47
15:AM:148:SER:OG	43:AM:301:HOH:O	2.20	0.47
28:AZ:80:LYS:HG3	43:AZ:211:HOH:O	2.14	0.47
39:Ak:66:ILE:HG22	39:Ak:69:LEU:H	1.78	0.47
1:1:178:A:N7	40:1:3121:SPM:H21	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:602:G:N2	1:1:605:A:OP2	2.42	0.47
1:1:675:G:N7	43:1:3579:HOH:O	2.35	0.47
1:1:1926:U:H2'	1:1:1927:A:C5	2.49	0.47
1:1:314:G:N7	43:1:3596:HOH:O	2.36	0.47
1:1:536:A:C8	1:1:536:A:H5''	2.49	0.47
1:1:776:A:H2'	1:1:777:C:C6	2.50	0.47
1:1:2329:G:H2'	1:1:2330:G:C8	2.48	0.47
1:1:1234:C:C6	43:1:8475:HOH:O	2.56	0.47
1:1:2403:U:H2'	1:1:2404:C:C6	2.50	0.47
1:1:2512:U:H2'	1:1:2513:C:C6	2.50	0.47
12:AI:132:ARG:HG3	43:AI:222:HOH:O	2.15	0.47
14:AL:7:ARG:HG2	43:AL:309:HOH:O	2.14	0.47
24:AV:111:LYS:HG3	43:AV:229:HOH:O	2.14	0.47
1:1:430:G:H4'	43:1:9219:HOH:O	2.15	0.46
1:1:832:A:N3	1:1:832:A:H3'	2.30	0.46
1:1:1292:C:H2'	1:1:1293:G:H8	1.80	0.46
2:2:102:C:OP1	43:2:201:HOH:O	2.21	0.46
5:AB:331:VAL:HG11	25:AW:1:MET:HG2	1.96	0.46
20:AR:72:LEU:HD12	20:AR:72:LEU:HA	1.81	0.46
26:AX:63:ARG:CZ	43:AX:103:HOH:O	2.62	0.46
1:1:300:G:H4'	43:1:6916:HOH:O	2.14	0.46
1:1:340:G:H5'	1:1:359:U:O2'	2.14	0.46
1:1:761:A:N1	1:1:2484:A:O2'	2.44	0.46
1:1:912:G:H2'	1:1:913:C:C6	2.49	0.46
1:1:2929:A:H2'	1:1:2930:G:O4'	2.15	0.46
1:1:2985:C:H2'	1:1:2986:C:C6	2.50	0.46
3:3:295:LYS:HB2	3:3:298:ARG:HG3	1.96	0.46
21:AS:30:ARG:HH22	21:AS:44:ASP:HB3	1.80	0.46
22:AT:73:PRO:HB2	22:AT:96:ALA:HB1	1.96	0.46
1:1:632:G:O2'	1:1:1347:G:OP1	2.32	0.46
1:1:1754:C:O2	32:Ad:8:GLY:HA2	2.16	0.46
1:1:170:G:OP2	40:1:3102:SPM:N1	2.48	0.46
2:2:100:G:H2'	2:2:101:C:C6	2.51	0.46
2:2:109:A:H2'	2:2:110:C:O4'	2.15	0.46
9:AF:76:GLU:HG2	15:AM:11:TRP:CG	2.50	0.46
29:Aa:65:SER:HB3	43:Aa:107:HOH:O	2.16	0.46
35:Ag:48:LYS:HD2	43:Ag:202:HOH:O	2.16	0.46
1:1:398:G:H1'	43:1:6368:HOH:O	2.14	0.46
1:1:833:A:H2'	1:1:834:A:O4'	2.16	0.46
1:1:963:G:O2'	1:1:964:A:O5'	2.31	0.46
1:1:2417:U:C2	7:AD:130:GLY:HA3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:118:C:H2'	2:2:119:U:O4'	2.15	0.46
3:3:100:GLU:H	3:3:100:GLU:CD	2.23	0.46
12:AI:113:GLU:OE1	12:AI:113:GLU:N	2.46	0.46
16:AN:20:GLU:CD	16:AN:20:GLU:H	2.24	0.46
17:AO:83:TYR:OH	17:AO:125:ASP:OD2	2.22	0.46
1:1:5:C:N4	43:1:3976:HOH:O	2.49	0.46
1:1:2354:U:H2'	1:1:2355:U:C6	2.50	0.46
40:1:3117:SPM:H111	43:1:5364:HOH:O	2.15	0.46
7:AD:43:ARG:HD3	7:AD:49:GLU:OE1	2.15	0.46
14:AL:7:ARG:CZ	43:AL:309:HOH:O	2.63	0.46
22:AT:58:LYS:HE3	22:AT:125:GLU:HA	1.97	0.46
1:1:397:G:H2'	1:1:398:G:O4'	2.15	0.46
4:AA:28:VAL:C	4:AA:29:ARG:HG2	2.41	0.46
22:AT:126:ARG:HD3	22:AT:170:LYS:HB3	1.98	0.46
1:1:1253:A:O2'	1:1:1254:G:H5''	2.15	0.46
1:1:2623:OMU:OP1	5:AB:4:LYS:HE3	2.16	0.46
17:AO:141:GLU:OE1	17:AO:141:GLU:N	2.34	0.46
27:AY:77:VAL:HG22	27:AY:179:LEU:HD21	1.96	0.46
30:Ab:51:THR:OG1	30:Ab:54:ASN:HB2	2.16	0.46
1:1:2734:C:H5'	43:1:4273:HOH:O	2.15	0.46
1:1:2992:G:H2'	1:1:2993:A:C8	2.51	0.46
6:AC:36:VAL:HG22	43:AC:348:HOH:O	2.16	0.46
7:AD:112:LYS:HG3	7:AD:113:GLU:OE1	2.15	0.46
27:AY:20:ARG:HB2	27:AY:63:TRP:CD1	2.51	0.46
1:1:637:U:H2'	1:1:638:G:H8	1.80	0.45
1:1:757:U:H2'	1:1:758:C:C6	2.51	0.45
1:1:1713:A:H2'	1:1:1714:A:C8	2.51	0.45
1:1:2163:C:H2'	1:1:2164:C:C6	2.51	0.45
40:1:3116:SPM:H22	43:1:7540:HOH:O	2.16	0.45
5:AB:332:TRP:CH2	5:AB:334:SER:HA	2.51	0.45
8:AE:53:SER:OG	8:AE:53:SER:O	2.32	0.45
9:AF:100:LYS:HA	9:AF:100:LYS:HD3	1.79	0.45
10:AG:1:MET:N	10:AG:131:ARG:O	2.48	0.45
1:1:424:G:H2'	1:1:425:C:O4'	2.16	0.45
1:1:662:C:H2'	1:1:663:G:C8	2.51	0.45
1:1:1469:U:C4	23:AU:55:PRO:HG3	2.51	0.45
1:1:1872:C:H5''	43:1:7418:HOH:O	2.15	0.45
1:1:2340:C:H2'	1:1:2341:G:C8	2.51	0.45
1:1:2886:C:H2'	1:1:2887:G:O4'	2.15	0.45
7:AD:115:ILE:H	7:AD:115:ILE:HG13	1.63	0.45
28:AZ:80:LYS:NZ	43:AZ:202:HOH:O	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Aj:130:ARG:NH2	38:Aj:162:ILE:HD12	2.31	0.45
1:1:680:G:OP2	18:AP:46:ARG:NH2	2.44	0.45
1:1:1075:G:N3	1:1:1075:G:H2'	2.31	0.45
1:1:1858:G:O3'	19:AQ:130:ARG:NH2	2.44	0.45
21:AS:14:LYS:HD3	21:AS:14:LYS:HA	1.59	0.45
33:Ae:52:GLN:O	33:Ae:56:GLU:HG3	2.17	0.45
1:1:2184:C:H2'	1:1:2185:C:H6	1.80	0.45
1:1:2622:G:N7	40:1:3128:SPM:H122	2.31	0.45
3:3:230:PRO:O	3:3:231:ARG:HD3	2.16	0.45
10:AG:163:PRO:HG3	43:AG:201:HOH:O	2.15	0.45
27:AY:123:ASP:CG	43:AY:203:HOH:O	2.60	0.45
1:1:1172:A:C8	43:1:7813:HOH:O	2.56	0.45
1:1:1620:U:H2'	1:1:1621:C:C6	2.52	0.45
1:1:2739:G:H2'	1:1:2740:C:C6	2.51	0.45
1:1:2764:C:H2'	1:1:2765:C:H6	1.81	0.45
8:AE:91:ARG:HB2	8:AE:145:GLU:OE2	2.17	0.45
15:AM:30:LYS:O	15:AM:33:LYS:HG2	2.16	0.45
22:AT:58:LYS:H	22:AT:58:LYS:CE	2.30	0.45
27:AY:169:PRO:HG3	38:Aj:75:TYR:CZ	2.50	0.45
38:Aj:101:VAL:HG13	38:Aj:111:LEU:HD21	1.98	0.45
1:1:32:C:H4'	6:AC:73:PRO:HG2	1.97	0.45
1:1:808:C:H2'	1:1:809:C:C6	2.52	0.45
1:1:2671:G:H2'	1:1:2672:C:C6	2.52	0.45
43:1:5548:HOH:O	34:Af:47:GLN:HG2	2.17	0.45
8:AE:123:LYS:NZ	8:AE:123:LYS:HB3	2.30	0.45
1:1:903:A:H5'	43:1:3800:HOH:O	2.17	0.45
1:1:1807:C:O2'	1:1:2801:G:H4'	2.17	0.45
1:1:1834:A:H2'	1:1:1835:C:O4'	2.17	0.45
1:1:2360:U:H3'	1:1:2361:G:H5''	1.99	0.45
17:AO:164:LYS:HB2	17:AO:164:LYS:HE2	1.62	0.45
37:Ai:83:PRO:HB2	37:Ai:86:LEU:HD12	1.99	0.45
1:1:524:G:O6	40:1:3141:SPM:H71	2.17	0.45
1:1:536:A:H3'	34:Af:33:ARG:NH1	2.31	0.45
1:1:923:G:H5'	14:AL:30:GLY:HA3	1.99	0.45
1:1:1337:C:H5''	1:1:1339:G:O4'	2.17	0.45
1:1:2157:C:H2'	1:1:2158:U:C6	2.52	0.45
1:1:2845:G:O2'	1:1:2846:G:O4'	2.24	0.45
40:1:3140:SPM:H42	43:1:3703:HOH:O	2.15	0.45
2:2:129:C:H3'	43:2:220:HOH:O	2.14	0.45
1:1:1174:A:OP2	1:1:1174:A:H8	2.00	0.45
5:AB:109:GLU:OE1	5:AB:123:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AC:78:GLU:CD	6:AC:78:GLU:H	2.23	0.45
17:AO:171:LEU:HD12	43:AO:328:HOH:O	2.17	0.45
39:Ak:34:ILE:HD13	39:Ak:57:GLY:HA2	1.99	0.45
1:1:637:U:H2'	1:1:638:G:C8	2.52	0.45
1:1:851:A:H5''	43:1:3782:HOH:O	2.17	0.45
1:1:1173:G:N3	1:1:1173:G:H2'	2.32	0.45
1:1:1619:G:H2'	1:1:1620:U:C6	2.52	0.45
1:1:2135:A:H2'	1:1:2136:C:C6	2.52	0.45
17:AO:99:LYS:HA	17:AO:99:LYS:HD3	1.69	0.45
38:Aj:51:LEU:HD21	38:Aj:55:LYS:HB3	1.98	0.45
1:1:36:C:H2'	1:1:37:G:C8	2.52	0.44
1:1:2006:G:H4'	43:1:6363:HOH:O	2.17	0.44
33:Ae:13:LYS:O	33:Ae:17:LYS:HE2	2.16	0.44
1:1:572:A:H2'	1:1:573:A:C8	2.52	0.44
1:1:647:U:H2'	1:1:648:C:C6	2.53	0.44
1:1:724:A:H62	1:1:770:G:H2'	1.81	0.44
1:1:957:U:H2'	1:1:958:C:H6	1.83	0.44
1:1:2077:OMU:HM22	1:1:2078:C:H5'	1.99	0.44
1:1:2181:G:N7	1:1:2615:A:H1'	2.32	0.44
40:1:3142:SPM:H112	4:AA:25:ASP:OD2	2.18	0.44
3:3:111:LYS:HD2	3:3:111:LYS:HA	1.84	0.44
6:AC:206:VAL:HG22	6:AC:222:GLU:HG3	2.00	0.44
7:AD:10:LYS:HD3	7:AD:10:LYS:HA	1.70	0.44
17:AO:44:LEU:HG	17:AO:77:ASN:HB2	1.99	0.44
19:AQ:102:THR:O	19:AQ:106:GLN:HG3	2.17	0.44
20:AR:2:PRO:O	20:AR:70:MET:HE1	2.18	0.44
26:AX:9:LYS:O	26:AX:13:GLU:HG3	2.17	0.44
30:Ab:10:PRO:HD3	43:Ab:203:HOH:O	2.16	0.44
1:1:519:G:O6	40:1:3141:SPM:H41	2.16	0.44
1:1:2753:A:OP2	43:1:3405:HOH:O	2.21	0.44
15:AM:18:GLU:CD	15:AM:18:GLU:H	2.24	0.44
27:AY:26:PRO:HG2	27:AY:29:ILE:HD12	1.99	0.44
1:1:1164:C:OP2	43:1:3407:HOH:O	2.21	0.44
4:AA:229:ARG:NH2	4:AA:239:ARG:HG3	2.32	0.44
17:AO:153:LYS:HB2	17:AO:153:LYS:HE2	1.85	0.44
24:AV:35:GLU:H	24:AV:35:GLU:CD	2.23	0.44
24:AV:85:THR:HA	24:AV:90:GLN:O	2.17	0.44
29:Aa:67:GLU:HB2	43:Aa:107:HOH:O	2.17	0.44
1:1:434:C:H1'	43:1:4112:HOH:O	2.16	0.44
1:1:669:U:H2'	1:1:670:U:C6	2.53	0.44
1:1:1990:A2M:O5'	1:1:1990:A2M:H8	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2492:A:H2'	1:1:2493:A:C8	2.52	0.44
1:1:2532:G:H2'	1:1:2533:C:H6	1.82	0.44
3:3:260:MET:HG2	3:3:265:ILE:O	2.18	0.44
8:AE:61:VAL:HG22	8:AE:72:LEU:HD11	1.98	0.44
20:AR:25:ARG:HD3	43:Aj:8729:HOH:O	2.17	0.44
38:Aj:110:LEU:HD12	38:Aj:161:ASN:O	2.17	0.44
1:1:2216:G:H4'	43:1:7911:HOH:O	2.17	0.44
1:1:2349:G:N3	1:1:2349:G:H2'	2.33	0.44
1:1:2559:G:OP2	43:1:3408:HOH:O	2.21	0.44
1:1:2691:A2M:HM'3	1:1:2691:A2M:H1'	1.87	0.44
43:1:7665:HOH:O	6:AC:91:VAL:HG22	2.17	0.44
8:AE:44:LYS:HB2	8:AE:44:LYS:HE3	1.45	0.44
28:AZ:24:THR:HG23	28:AZ:85:ALA:HB2	2.00	0.44
1:1:582:C:H2'	1:1:583:C:C6	2.52	0.44
1:1:2104:OMG:OP2	40:1:3136:SPM:H42	2.18	0.44
6:AC:212:LYS:HB2	6:AC:212:LYS:HE2	1.75	0.44
12:AI:73:LYS:HE3	12:AI:75:GLU:OE2	2.17	0.44
38:Aj:103:GLU:O	38:Aj:107:ARG:HG3	2.17	0.44
1:1:172:A:H2'	1:1:173:A:C8	2.53	0.44
1:1:435:G:OP2	43:1:3406:HOH:O	2.21	0.44
1:1:662:C:H2'	1:1:663:G:H8	1.83	0.44
1:1:2340:C:H2'	1:1:2341:G:H8	1.81	0.44
1:1:2753:A:H2'	1:1:2754:G:O4'	2.17	0.44
2:2:54:G:OP2	17:AO:78:ASN:HB3	2.18	0.44
3:3:214:GLU:OE2	43:3:701:HOH:O	2.21	0.44
8:AE:22:LYS:NZ	43:AE:205:HOH:O	2.51	0.44
28:AZ:5:GLY:O	28:AZ:9:GLN:HG3	2.17	0.44
28:AZ:49:ASP:CG	31:Ac:83:ARG:HH22	2.26	0.44
38:Aj:142:LYS:CG	43:Aj:8721:HOH:O	2.66	0.44
1:1:318:G:P	43:1:4028:HOH:O	2.75	0.44
1:1:1150:C:N4	43:1:3645:HOH:O	2.38	0.44
1:1:1416:G:H5''	43:1:7732:HOH:O	2.18	0.44
1:1:2510:G:O3'	36:Ah:36:GLY:HA3	2.18	0.44
40:1:3114:SPM:H92	32:Ad:7:MET:SD	2.58	0.44
43:1:7830:HOH:O	20:AR:40:ARG:HG2	2.16	0.44
43:1:8270:HOH:O	7:AD:62:PHE:HE1	2.00	0.44
2:2:38:G:N7	43:2:209:HOH:O	2.36	0.44
1:1:1154:A:H2'	1:1:1155:A:H8	1.83	0.43
1:1:2954:A:N3	40:1:3113:SPM:H21	2.32	0.43
7:AD:84:PHE:CD1	7:AD:84:PHE:C	2.96	0.43
26:AX:49:ARG:O	26:AX:53:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:233:C:OP1	43:1:3411:HOH:O	2.21	0.43
6:AC:169:LEU:HD12	6:AC:169:LEU:HA	1.86	0.43
8:AE:115:GLU:HG2	8:AE:123:LYS:HG2	2.00	0.43
13:AK:40:LYS:HE3	13:AK:46:ARG:HG2	2.00	0.43
20:AR:4:ILE:HD11	20:AR:70:MET:HG3	2.00	0.43
1:1:334:U:H2'	1:1:335:G:O4'	2.19	0.43
1:1:1569:G:H2'	1:1:1570:U:H6	1.83	0.43
1:1:1612:C:OP2	43:1:3409:HOH:O	2.21	0.43
1:1:2203:G:H2'	1:1:2204:C:C6	2.53	0.43
40:1:3106:SPM:H31	43:1:3680:HOH:O	2.18	0.43
2:2:9:C:H4'	2:2:32:C:H4'	2.00	0.43
7:AD:26:ILE:HD12	7:AD:42:LEU:HG	2.01	0.43
8:AE:113:THR:HB	8:AE:123:LYS:HZ3	1.83	0.43
11:AH:97:PHE:CD1	15:AM:103:GLU:HG2	2.53	0.43
12:AI:77:ARG:HG2	12:AI:77:ARG:NH1	2.33	0.43
1:1:122:G:H2'	1:1:123:C:H6	1.80	0.43
1:1:230:C:OP2	1:1:2509:C:O2'	2.29	0.43
1:1:271:A:H2'	1:1:272:A:C8	2.53	0.43
1:1:379:C:H5	43:1:9497:HOH:O	2.01	0.43
1:1:411:U:H2'	1:1:412:C:C6	2.54	0.43
1:1:1572:C:H2'	1:1:1573:C:C6	2.54	0.43
1:1:2326:C:H5''	43:1:7473:HOH:O	2.17	0.43
1:1:609:G:H5'	43:1:7340:HOH:O	2.17	0.43
1:1:689:A:H2'	1:1:690:A:C8	2.54	0.43
1:1:1496:A:O2'	43:1:3410:HOH:O	2.21	0.43
1:1:2022:A:HO2'	1:1:2023:G:P	2.38	0.43
7:AD:10:LYS:HD3	43:AD:216:HOH:O	2.17	0.43
7:AD:24:VAL:HG13	7:AD:131:MET:HE3	1.99	0.43
17:AO:72:TRP:HE3	17:AO:187:VAL:HG21	1.83	0.43
24:AV:38:LYS:HD2	24:AV:39:LYS:N	2.34	0.43
1:1:186:G:OP1	11:AH:130:ARG:NH2	2.43	0.43
1:1:914:C:H2'	1:1:915:C:C6	2.52	0.43
1:1:1945:A:H2'	1:1:1946:A:C8	2.53	0.43
1:1:2582:G:OP1	16:AN:154:ARG:NH2	2.47	0.43
2:2:3:C:H2'	2:2:4:C:C6	2.54	0.43
4:AA:107:GLU:HG2	4:AA:114:GLY:N	2.34	0.43
9:AF:139:LYS:HB2	9:AF:139:LYS:HE2	1.83	0.43
26:AX:20:ARG:CD	43:AX:110:HOH:O	2.67	0.43
1:1:30:C:H2'	1:1:31:U:H6	1.82	0.43
1:1:1537:G:H2'	1:1:1538:C:C6	2.54	0.43
43:1:3613:HOH:O	10:AG:105:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AQ:82:ARG:HD3	43:AQ:201:HOH:O	2.07	0.43
1:1:613:G:H1'	1:1:614:U:OP2	2.19	0.43
1:1:1772:G:N7	40:1:3138:SPM:H72	2.34	0.43
1:1:2045:C:H2'	1:1:2046:U:C6	2.53	0.43
10:AG:96:LYS:HE3	10:AG:114:LEU:HG	2.00	0.43
21:AS:3:LYS:HB2	21:AS:3:LYS:HE2	1.85	0.43
1:1:216:C:H2'	1:1:217:C:C6	2.54	0.43
1:1:1839:G:OP2	37:AI:7:LYS:HE2	2.18	0.43
1:1:2764:C:H2'	1:1:2765:C:C6	2.54	0.43
40:1:3108:SPM:H21	43:1:7024:HOH:O	2.18	0.43
40:1:3129:SPM:H71	43:1:5123:HOH:O	2.18	0.43
8:AE:177:GLU:OE1	35:AG:52:LYS:NZ	2.37	0.43
17:AO:83:TYR:HE2	17:AO:121:LYS:HG3	1.84	0.43
17:AO:189:LYS:HB3	17:AO:189:LYS:HE2	1.63	0.43
22:AT:178:LYS:O	22:AT:184:ARG:NH1	2.52	0.43
1:1:292:U:O2	1:1:292:U:H2'	2.19	0.43
1:1:1096:A:N6	1:1:1110:G:H1'	2.34	0.43
1:1:2104:OMG:OP1	40:1:3136:SPM:H92	2.18	0.43
2:2:8:A:H5''	2:2:9:C:OP2	2.18	0.43
7:AD:42:LEU:HA	7:AD:42:LEU:HD23	1.75	0.43
27:AY:22:ILE:O	27:AY:25:THR:HG22	2.19	0.43
28:AZ:37:ILE:HD12	28:AZ:84:LEU:HD11	2.01	0.43
1:1:886:G:H1'	1:1:1510:A:N6	2.34	0.42
1:1:893:G:H5''	43:1:7140:HOH:O	2.19	0.42
1:1:1088:G:H2'	1:1:1089:C:C6	2.54	0.42
1:1:1665:G:N2	33:Ae:2:PRO:HG2	2.34	0.42
43:1:8628:HOH:O	6:AC:207:LYS:HE3	2.18	0.42
6:AC:16:LEU:HD13	6:AC:20:ILE:HD12	2.00	0.42
1:1:353:G:OP2	40:1:3108:SPM:H111	2.18	0.42
1:1:878:C:H2'	1:1:879:A:O4'	2.19	0.42
1:1:1429:A:O2'	1:1:1431:A:OP2	2.34	0.42
13:AK:15:LEU:HD23	13:AK:15:LEU:HA	1.88	0.42
1:1:69:C:OP1	26:AX:57:ARG:HD3	2.20	0.42
1:1:812:G:O6	40:1:3137:SPM:H42	2.18	0.42
1:1:1833:A:H2'	1:1:1834:A:C8	2.54	0.42
1:1:2213:G:N2	1:1:2317:U:O4	2.28	0.42
1:1:2478:G:O6	40:1:3140:SPM:H91	2.20	0.42
2:2:33:A:H2'	2:2:34:C:C6	2.53	0.42
13:AK:71:GLU:O	13:AK:75:LYS:HD3	2.19	0.42
36:Ah:87:LYS:HE2	36:Ah:87:LYS:HB3	1.74	0.42
1:1:186:G:H5''	11:AH:123:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:995:G:C8	43:1:3899:HOH:O	2.70	0.42
1:1:1536:C:H2'	1:1:1537:G:C8	2.54	0.42
1:1:2098:A:H5'	43:1:5515:HOH:O	2.19	0.42
1:1:2639:C:OP1	8:AE:166:ARG:NH1	2.52	0.42
1:1:2686:A:OP1	5:AB:243:GLN:HB2	2.19	0.42
40:1:3131:SPM:H31	43:1:9229:HOH:O	2.19	0.42
3:3:208:TRP:CD1	3:3:208:TRP:H	2.38	0.42
7:AD:103:GLU:HG3	7:AD:162:ARG:NH1	2.34	0.42
8:AE:17:LYS:HD3	8:AE:33:LYS:HE2	2.01	0.42
13:AK:60:LYS:HD3	13:AK:85:TYR:CE2	2.55	0.42
21:AS:30:ARG:NH2	21:AS:44:ASP:HB3	2.34	0.42
22:AT:142:ASN:HB3	22:AT:154:PHE:O	2.20	0.42
24:AV:20:PRO:O	24:AV:24:ARG:HG3	2.20	0.42
27:AY:122:LYS:H	27:AY:122:LYS:HG2	1.65	0.42
1:1:1647:G:N3	1:1:1647:G:H5'	2.35	0.42
1:1:2187:A:O2'	1:1:2189:G:H5''	2.20	0.42
1:1:2335:G:H4'	1:1:2337:C:C2	2.55	0.42
1:1:2551:U:OP1	3:3:231:ARG:HD2	2.19	0.42
43:1:7103:HOH:O	5:AB:225:PRO:HB2	2.20	0.42
5:AB:251:GLN:HB2	43:AB:436:HOH:O	2.18	0.42
9:AF:125:GLU:CB	43:AF:206:HOH:O	2.62	0.42
1:1:231:G:OP1	40:1:3121:SPM:N14	2.53	0.42
1:1:564:C:OP1	43:1:3412:HOH:O	2.22	0.42
1:1:1516:A:O2'	1:1:1527:U:O2	2.36	0.42
1:1:2336:A:H4'	1:1:2337:C:O5'	2.19	0.42
3:3:100:GLU:OE2	3:3:139:ARG:NH1	2.43	0.42
4:AA:169:PHE:O	4:AA:171:LYS:N	2.52	0.42
7:AD:112:LYS:HA	7:AD:112:LYS:HE2	2.01	0.42
13:AK:71:GLU:CD	13:AK:71:GLU:N	2.76	0.42
17:AO:63:ASP:OD1	17:AO:65:ARG:HB2	2.18	0.42
38:Aj:84:PRO:HD2	38:Aj:88:TRP:CE3	2.54	0.42
38:Aj:103:GLU:OE1	38:Aj:106:ARG:NH2	2.46	0.42
1:1:83:G:C6	34:Af:32:LYS:HD2	2.55	0.42
1:1:581:C:H2'	1:1:582:C:C6	2.55	0.42
1:1:883:C:H2'	1:1:884:C:C6	2.55	0.42
1:1:1174:A:OP1	1:1:1236:G:N2	2.39	0.42
1:1:1715:A:H2'	1:1:1716:G:O4'	2.20	0.42
7:AD:7:VAL:HG12	7:AD:9:VAL:HG23	2.01	0.42
27:AY:179:LEU:HA	27:AY:179:LEU:HD23	1.74	0.42
1:1:1073:G:H5''	1:1:1074:U:OP2	2.20	0.42
1:1:2105:U:OP2	40:1:3136:SPM:H41	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2358:G:H2'	1:1:2359:C:H6	1.85	0.42
1:1:2406:G:H2'	1:1:2407:C:O4'	2.19	0.42
5:AB:87:VAL:HG23	5:AB:185:LEU:HD13	2.00	0.42
5:AB:131:LYS:HE3	5:AB:131:LYS:HB2	1.65	0.42
17:AO:109:ARG:NH2	43:AO:301:HOH:O	2.30	0.42
28:AZ:64:PHE:CD1	28:AZ:65:PRO:HD2	2.54	0.42
38:Aj:142:LYS:CE	43:Aj:8721:HOH:O	2.54	0.42
1:1:1028:A:H2'	1:1:1031:C:H5	1.84	0.42
1:1:1256:U:C2	5:AB:245:PRO:HG3	2.54	0.42
1:1:1635:U:C4'	43:1:7125:HOH:O	2.64	0.42
1:1:1872:C:H1'	19:AQ:147:LYS:HE3	2.02	0.42
1:1:1957:OMG:HM22	1:1:1958:G:O4'	2.20	0.42
1:1:2845:G:C2	5:AB:317:ARG:HG2	2.55	0.42
1:1:2914:C:O2'	1:1:2915:A:O5'	2.37	0.42
17:AO:120:MET:HB3	17:AO:120:MET:HE2	1.75	0.42
19:AQ:120:MET:HE2	19:AQ:126:PHE:CZ	2.55	0.42
29:Aa:50:ALA:HA	43:Aa:101:HOH:O	2.19	0.42
30:Ab:115:ARG:HG2	30:Ab:115:ARG:NH1	2.34	0.42
37:Ai:27:VAL:O	37:Ai:31:GLU:HG3	2.19	0.42
1:1:835:G:H2'	1:1:836:C:C6	2.55	0.42
1:1:856:G:OP2	40:1:3139:SPM:H112	2.20	0.42
40:1:3112:SPM:H112	40:1:3112:SPM:H72	2.01	0.42
43:1:4123:HOH:O	26:AX:5:LYS:HB2	2.18	0.42
2:2:1:G:O2'	2:2:2:C:H5'	2.20	0.42
17:AO:39:LYS:HB2	17:AO:39:LYS:HE2	1.80	0.42
1:1:272:A:H2'	1:1:273:C:O4'	2.20	0.41
1:1:2072:U:H4'	43:1:4819:HOH:O	2.20	0.41
1:1:2621:C:H2'	1:1:2622:G:O4'	2.20	0.41
2:2:14:C:H5''	43:2:208:HOH:O	2.19	0.41
4:AA:36:GLY:HA3	43:AA:404:HOH:O	2.19	0.41
13:AJ:52:ILE:HD11	28:AZ:26:LYS:HG3	2.02	0.41
37:Ai:78:GLY:O	43:Ai:301:HOH:O	2.22	0.41
1:1:740:A:H2'	1:1:741:C:O4'	2.20	0.41
1:1:900:A:C6	4:AA:194:MET:HE2	2.55	0.41
1:1:2840:G:H4'	12:AI:99:TRP:HH2	1.85	0.41
7:AD:112:LYS:HD3	7:AD:112:LYS:O	2.19	0.41
11:AH:78:PRO:HG3	15:AM:172:ILE:HD11	2.02	0.41
13:AK:40:LYS:C	13:AK:42:LEU:N	2.79	0.41
27:AY:98:TRP:CD2	27:AY:136:PRO:HG2	2.55	0.41
28:AZ:37:ILE:HB	28:AZ:84:LEU:HD12	2.01	0.41
35:Ag:21:LYS:NZ	35:Ag:34:ALA:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:813:G:C5'	31:Ac:8:SER:HA	2.48	0.41
1:1:1358:C:H2'	1:1:1359:G:C8	2.55	0.41
3:3:136:LEU:HD22	3:3:290:TYR:HB3	2.01	0.41
6:AC:78:GLU:OE1	6:AC:78:GLU:N	2.46	0.41
8:AE:177:GLU:OE2	8:AE:177:GLU:O	2.38	0.41
12:AI:117:LYS:HE3	12:AI:117:LYS:HB3	1.66	0.41
13:AK:9:ARG:HE	13:AK:9:ARG:HB2	1.65	0.41
1:1:130:C:H2'	1:1:131:G:O4'	2.20	0.41
1:1:172:A:H2'	1:1:173:A:H8	1.85	0.41
1:1:209:C:H4'	1:1:210:A:C8	2.55	0.41
1:1:1448:G:O2'	1:1:1449:C:H5'	2.20	0.41
1:1:2312:C:H2'	1:1:2313:C:C6	2.55	0.41
1:1:2494:C:H2'	1:1:2495:C:C6	2.55	0.41
8:AE:21:GLU:HG2	8:AE:23:THR:HG23	2.01	0.41
13:AK:60:LYS:HD3	13:AK:85:TYR:CZ	2.56	0.41
31:Ac:29:LYS:HE3	31:Ac:52:TYR:O	2.20	0.41
38:Aj:158:ARG:HD3	38:Aj:182:GLU:HB3	2.03	0.41
1:1:96:C:H2'	1:1:97:C:C6	2.56	0.41
1:1:648:C:H2'	1:1:649:U:O4'	2.21	0.41
1:1:657:C:O5'	40:1:3110:SPM:H82	2.20	0.41
1:1:1518:G:H5'	1:1:1615:A:H1'	2.02	0.41
1:1:1669:U:OP1	33:Ae:24:LYS:NZ	2.51	0.41
4:AA:31:PRO:HG2	4:AA:34:ILE:HG23	2.01	0.41
12:AI:52:VAL:HG22	12:AI:53:HIS:H	1.86	0.41
13:AJ:27:ASP:OD1	13:AJ:28:ILE:N	2.52	0.41
18:AP:17:ILE:HD13	18:AP:40:GLU:HG3	2.03	0.41
18:AP:51:VAL:HG23	18:AP:71:LEU:O	2.21	0.41
24:AV:76:ARG:HD3	24:AV:76:ARG:HA	1.83	0.41
28:AZ:35:LEU:HD13	28:AZ:98:VAL:HG22	2.02	0.41
36:Ah:54:LYS:HE3	36:Ah:54:LYS:HB3	1.85	0.41
1:1:278:G:O2'	43:1:3413:HOH:O	2.22	0.41
1:1:582:C:H2'	1:1:583:C:H6	1.85	0.41
1:1:1264:G:C2	10:AG:102:MET:HE2	2.56	0.41
1:1:1393:G:N7	22:AT:41:SER:OG	2.49	0.41
1:1:1485:C:H2'	1:1:1486:G:H8	1.84	0.41
1:1:1570:U:H2'	1:1:1571:C:H6	1.82	0.41
1:1:2192:G:H2'	1:1:2193:C:C6	2.56	0.41
1:1:2912:G:C6	1:1:2913:G:C6	3.09	0.41
6:AC:169:LEU:HA	6:AC:170:PRO:C	2.46	0.41
14:AL:122:MET:HG2	14:AL:141:ILE:HD13	2.02	0.41
16:AN:71:GLN:NE2	43:AN:305:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AO:63:ASP:OD1	17:AO:63:ASP:C	2.63	0.41
1:1:1825:G:N3	1:1:1898:A:H2'	2.36	0.41
3:3:303:VAL:HG23	43:3:755:HOH:O	2.20	0.41
7:AD:35:LEU:HD21	7:AD:52:LEU:HG	2.03	0.41
13:AK:40:LYS:CE	13:AK:46:ARG:HG2	2.51	0.41
15:AM:46:LEU:HB2	43:AM:312:HOH:O	2.21	0.41
17:AO:46:ALA:HB3	17:AO:89:VAL:HG21	2.03	0.41
27:AY:50:SER:O	27:AY:54:MET:HG2	2.21	0.41
30:Ab:20:ARG:HG3	30:Ab:73:LYS:HD3	2.03	0.41
1:1:399:U:H3'	43:1:8495:HOH:O	2.21	0.41
1:1:536:A:H5''	1:1:536:A:H8	1.86	0.41
1:1:595:A:H2'	1:1:596:A:C8	2.56	0.41
1:1:760:U:O2'	43:1:3415:HOH:O	2.22	0.41
1:1:931:C:H2'	1:1:932:C:C6	2.55	0.41
1:1:1422:C:H4'	29:Aa:59:GLU:HG2	2.01	0.41
1:1:1948:G:N7	40:1:3119:SPM:H91	2.36	0.41
1:1:2627:U:H2'	1:1:2628:OMU:C6	2.51	0.41
1:1:2955:U:C4	40:1:3113:SPM:H22	2.56	0.41
1:1:2972:C:H2'	1:1:2973:C:H6	1.86	0.41
7:AD:156:LYS:HA	7:AD:156:LYS:HD3	1.76	0.41
10:AG:154:LEU:HD23	10:AG:154:LEU:HA	1.89	0.41
13:AJ:22:LYS:HE2	13:AJ:85:TYR:CZ	2.56	0.41
14:AL:20:TRP:CG	14:AL:26:HIS:HB2	2.55	0.41
15:AM:123:ASP:OD2	15:AM:124:GLY:N	2.54	0.41
1:1:832:A:C2	1:1:833:A:N7	2.89	0.41
1:1:858:U:H2'	1:1:859:C:C6	2.56	0.41
1:1:1571:C:H2'	1:1:1572:C:C6	2.56	0.41
1:1:1588:A:H2'	1:1:1589:G:O4'	2.21	0.41
1:1:2358:G:H2'	1:1:2359:C:C6	2.56	0.41
1:1:2698:UR3:H2'	1:1:2699:U:C6	2.56	0.41
1:1:2972:C:H2'	1:1:2973:C:C6	2.56	0.41
2:2:95:C:H2'	2:2:96:G:O4'	2.21	0.41
5:AB:246:ALA:HB3	10:AG:78:TYR:HE2	1.86	0.41
6:AC:29:GLU:H	6:AC:29:GLU:CD	2.28	0.41
6:AC:279:ARG:HE	6:AC:279:ARG:HB3	1.47	0.41
7:AD:76:LEU:HD13	7:AD:76:LEU:HA	1.94	0.41
8:AE:121:LYS:O	43:AE:201:HOH:O	2.20	0.41
10:AG:5:LYS:NZ	10:AG:5:LYS:HB3	2.36	0.41
12:AI:89:ARG:HH11	12:AI:104:ASP:HA	1.86	0.41
19:AQ:63:LEU:HD12	19:AQ:63:LEU:HA	1.80	0.41
21:AS:40:LYS:HD3	21:AS:64:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AU:26:GLU:H	23:AU:26:GLU:HG2	1.74	0.41
26:AX:6:LEU:HA	26:AX:6:LEU:HD23	1.83	0.41
27:AY:80:LYS:HE2	27:AY:179:LEU:HD13	2.03	0.41
30:Ab:23:MET:SD	30:Ab:74:PRO:HD3	2.60	0.41
31:Ac:48:ASN:OD1	31:Ac:48:ASN:N	2.49	0.41
33:Ae:52:GLN:NE2	43:Ae:102:HOH:O	2.54	0.41
39:Ak:54:LEU:HD13	39:Ak:77:GLU:HG3	2.03	0.41
1:1:1563:G:OP1	1:1:1731:G:O2'	2.25	0.41
1:1:1714:A:H2'	1:1:1715:A:C8	2.55	0.41
1:1:2941:G:O2'	1:1:2943:A:OP2	2.27	0.41
11:AH:9:VAL:HG22	11:AH:22:LYS:HD3	2.01	0.41
12:AI:124:PRO:HG3	25:AW:26:GLY:HA2	2.03	0.41
29:Aa:37:ARG:HD3	29:Aa:48:PRO:O	2.20	0.41
1:1:201:G:N7	40:1:3129:SPM:H31	2.36	0.40
1:1:590:A:OP1	40:1:3131:SPM:H81	2.21	0.40
1:1:2062:C:O2'	3:3:37:GLU:OE1	2.36	0.40
1:1:2738:G:H2'	1:1:2739:G:O4'	2.21	0.40
1:1:2862:A:H4'	1:1:2863:G:OP2	2.20	0.40
40:1:3109:SPM:H122	43:1:3774:HOH:O	2.21	0.40
7:AD:2:LYS:HE3	7:AD:2:LYS:HB3	1.77	0.40
14:AL:88:VAL:HG12	14:AL:106:VAL:HG11	2.01	0.40
1:1:2468:U:H3	40:1:3140:SPM:H31	1.86	0.40
10:AG:178:LYS:H	10:AG:178:LYS:CD	2.32	0.40
16:AN:101:ASN:OD1	16:AN:111:ARG:NH2	2.53	0.40
31:Ac:76:ARG:NE	43:Ac:101:HOH:O	2.44	0.40
38:Aj:168:ILE:HD12	38:Aj:168:ILE:HA	1.82	0.40
1:1:604:G:OP1	13:AK:13:LYS:NZ	2.38	0.40
1:1:1402:A:P	40:1:3135:SPM:H41	2.61	0.40
1:1:1706:C:OP1	43:1:3414:HOH:O	2.22	0.40
1:1:2410:A:H2'	1:1:2411:G:O4'	2.22	0.40
1:1:2666:OMU:HM23	1:1:2668:C:C6	2.57	0.40
13:AK:6:ASP:HB3	20:AR:74:LYS:HB3	2.04	0.40
19:AQ:28:ARG:HE	19:AQ:28:ARG:HB3	1.72	0.40
38:Aj:23:PHE:HB3	38:Aj:176:PHE:CD2	2.57	0.40
38:Aj:39:ASP:OD1	38:Aj:91:ASN:ND2	2.40	0.40
1:1:472:A:O2'	1:1:473:G:H5'	2.22	0.40
1:1:939:G:H2'	1:1:1067:G:H5''	2.02	0.40
1:1:2132:C:H2'	1:1:2133:G:O4'	2.22	0.40
3:3:69:HIS:CG	16:AN:106:MET:HG3	2.56	0.40
15:AM:24:MET:HE2	15:AM:121:ALA:HB2	2.03	0.40
17:AO:74:GLY:HA2	17:AO:170:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AQ:82:ARG:CD	43:AQ:209:HOH:O	2.66	0.40
28:AZ:52:TYR:CZ	28:AZ:56:LEU:HD11	2.56	0.40
1:1:6:A:N6	22:AT:183:LYS:HE2	2.37	0.40
1:1:661:C:H2'	1:1:662:C:C6	2.56	0.40
1:1:1027:C:O2'	1:1:1028:A:H5'	2.22	0.40
13:AK:12:VAL:HG11	13:AK:90:VAL:HG21	2.04	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	
3	3	288/655 (44%)	282 (98%)	6 (2%)	0	100	100
4	AA	237/244 (97%)	229 (97%)	8 (3%)	0	100	100
5	AB	334/338 (99%)	327 (98%)	7 (2%)	0	100	100
6	AC	276/285 (97%)	267 (97%)	9 (3%)	0	100	100
7	AD	176/178 (99%)	168 (96%)	8 (4%)	0	100	100
8	AE	193/196 (98%)	190 (98%)	3 (2%)	0	100	100
9	AF	143/149 (96%)	141 (99%)	2 (1%)	0	100	100
10	AG	181/186 (97%)	180 (99%)	1 (1%)	0	100	100
11	AH	153/157 (98%)	152 (99%)	1 (1%)	0	100	100
12	AI	136/144 (94%)	134 (98%)	2 (2%)	0	100	100
13	AJ	99/103 (96%)	97 (98%)	2 (2%)	0	100	100
13	AK	88/103 (85%)	84 (96%)	3 (3%)	1 (1%)	11	4
14	AL	150/156 (96%)	144 (96%)	6 (4%)	0	100	100
15	AM	182/189 (96%)	179 (98%)	3 (2%)	0	100	100
16	AN	167/178 (94%)	165 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AO	198/205 (97%)	197 (100%)	1 (0%)	0	100	100
18	AP	119/122 (98%)	118 (99%)	1 (1%)	0	100	100
19	AQ	144/147 (98%)	144 (100%)	0	0	100	100
20	AR	74/78 (95%)	73 (99%)	1 (1%)	0	100	100
21	AS	96/99 (97%)	91 (95%)	5 (5%)	0	100	100
22	AT	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
23	AU	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
24	AV	119/128 (93%)	117 (98%)	1 (1%)	1 (1%)	16	8
25	AW	54/62 (87%)	54 (100%)	0	0	100	100
26	AX	65/79 (82%)	65 (100%)	0	0	100	100
27	AY	170/179 (95%)	165 (97%)	5 (3%)	0	100	100
28	AZ	96/101 (95%)	92 (96%)	4 (4%)	0	100	100
29	Aa	86/91 (94%)	85 (99%)	1 (1%)	0	100	100
30	Ab	138/153 (90%)	137 (99%)	1 (1%)	0	100	100
31	Ac	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
32	Ad	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
33	Ae	64/67 (96%)	64 (100%)	0	0	100	100
34	Af	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
35	Ag	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
36	Ah	89/91 (98%)	89 (100%)	0	0	100	100
37	Ai	97/102 (95%)	91 (94%)	6 (6%)	0	100	100
38	Aj	181/184 (98%)	172 (95%)	9 (5%)	0	100	100
39	Ak	88/93 (95%)	88 (100%)	0	0	100	100
All	All	5168/5747 (90%)	5051 (98%)	115 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	AK	41	SER
24	AV	3	PHE

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	
3	3	243/552 (44%)	241 (99%)	2 (1%)	73	74
4	AA	181/186 (97%)	176 (97%)	5 (3%)	38	30
5	AB	280/282 (99%)	277 (99%)	3 (1%)	65	64
6	AC	226/231 (98%)	224 (99%)	2 (1%)	70	70
7	AD	149/149 (100%)	147 (99%)	2 (1%)	61	58
8	AE	165/165 (100%)	163 (99%)	2 (1%)	63	61
9	AF	115/118 (98%)	114 (99%)	1 (1%)	70	70
10	AG	163/165 (99%)	162 (99%)	1 (1%)	78	79
11	AH	133/135 (98%)	132 (99%)	1 (1%)	73	74
12	AI	115/118 (98%)	115 (100%)	0	100	100
13	AJ	87/89 (98%)	85 (98%)	2 (2%)	44	38
13	AK	77/89 (86%)	75 (97%)	2 (3%)	40	33
14	AL	121/125 (97%)	118 (98%)	3 (2%)	42	34
15	AM	161/165 (98%)	161 (100%)	0	100	100
16	AN	134/140 (96%)	132 (98%)	2 (2%)	57	54
17	AO	166/169 (98%)	163 (98%)	3 (2%)	51	47
18	AP	99/100 (99%)	98 (99%)	1 (1%)	68	67
19	AQ	127/128 (99%)	126 (99%)	1 (1%)	73	74
20	AR	69/71 (97%)	68 (99%)	1 (1%)	59	56
21	AS	84/85 (99%)	82 (98%)	2 (2%)	43	36
22	AT	157/158 (99%)	153 (98%)	4 (2%)	42	34
23	AU	71/71 (100%)	70 (99%)	1 (1%)	59	56
24	AV	107/112 (96%)	105 (98%)	2 (2%)	50	45
25	AW	48/53 (91%)	48 (100%)	0	100	100
26	AX	58/65 (89%)	57 (98%)	1 (2%)	53	49
27	AY	147/152 (97%)	145 (99%)	2 (1%)	59	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	AZ	77/79 (98%)	75 (97%)	2 (3%)	40	33
29	Aa	78/81 (96%)	77 (99%)	1 (1%)	61	58
30	Ab	125/137 (91%)	125 (100%)	0	100	100
31	Ac	67/68 (98%)	67 (100%)	0	100	100
32	Ad	44/44 (100%)	44 (100%)	0	100	100
33	Ae	60/61 (98%)	60 (100%)	0	100	100
34	Af	42/43 (98%)	42 (100%)	0	100	100
35	Ag	46/49 (94%)	45 (98%)	1 (2%)	45	40
36	Ah	82/82 (100%)	82 (100%)	0	100	100
37	Ai	77/80 (96%)	76 (99%)	1 (1%)	61	58
38	Aj	161/162 (99%)	156 (97%)	5 (3%)	35	26
39	Ak	79/82 (96%)	77 (98%)	2 (2%)	42	34
All	All	4421/4841 (91%)	4363 (99%)	58 (1%)	59	58

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	60	ASP
3	3	255	ASP
4	AA	34	ILE
4	AA	35	SER
4	AA	44	LEU
4	AA	83	ASP
4	AA	230	CYS
5	AB	34	VAL
5	AB	36	LEU
5	AB	134	GLU
6	AC	110	CYS
6	AC	169	LEU
7	AD	76	LEU
7	AD	78	ARG
8	AE	44	LYS
8	AE	153	SER
9	AF	147	VAL
10	AG	107	VAL
11	AH	102	SER
13	AJ	98	THR
13	AJ	101	ASP

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Mol	Chain	Res	Type
13	AK	22	LYS
13	AK	74	LEU
14	AL	41	HIS
14	AL	58	TRP
14	AL	81	VAL
16	AN	50	VAL
16	AN	106	MET
17	AO	40	THR
17	AO	102	ILE
17	AO	175	LEU
18	AP	37	GLU
19	AQ	2	VAL
20	AR	72	LEU
21	AS	51	SER
21	AS	97	LEU
22	AT	8	LEU
22	AT	12	GLN
22	AT	16	LEU
22	AT	138	ILE
23	AU	18	GLU
24	AV	42	VAL
24	AV	114	GLN
26	AX	61	ILE
27	AY	9	THR
27	AY	148	ARG
28	AZ	2	ILE
28	AZ	93	GLU
29	Aa	44	LEU
35	Ag	14	LEU
37	Ai	45	SER
38	Aj	49	MET
38	Aj	53	SER
38	Aj	61	GLU
38	Aj	111	LEU
38	Aj	165	VAL
39	Ak	60	VAL
39	Ak	91	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
3	3	88	ASN

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Mol	Chain	Res	Type
5	AB	6	ASN
5	AB	243	GLN
5	AB	299	GLN
6	AC	37	ASN
6	AC	39	GLN
6	AC	84	HIS
7	AD	145	GLN
11	AH	8	GLN
15	AM	138	GLN
15	AM	174	HIS
16	AN	60	GLN
18	AP	4	ASN
27	AY	101	ASN
30	Ab	49	GLN
38	Aj	147	ASN
39	Ak	65	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2837/3024 (93%)	343 (12%)	32 (1%)
2	2	128/129 (99%)	13 (10%)	1 (0%)
All	All	2965/3153 (94%)	356 (12%)	33 (1%)

All (356) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	A
1	1	27	C
1	1	43	G
1	1	63	A
1	1	66	A
1	1	67	G
1	1	75	U
1	1	76	A
1	1	77	G
1	1	83	G
1	1	109	A
1	1	110	A
1	1	111	U
1	1	118	U

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Mol	Chain	Res	Type
1	1	134	U
1	1	135	A
1	1	154	G
1	1	162	A
1	1	177	A
1	1	196	G
1	1	197	A
1	1	203	A
1	1	211	G
1	1	220	U
1	1	229	G
1	1	233	C
1	1	245	U
1	1	247	G
1	1	258	A
1	1	269	A
1	1	270	C
1	1	292	U
1	1	294	G
1	1	304	A
1	1	305	A
1	1	308	G
1	1	328	G
1	1	329	U
1	1	330	G
1	1	358	A
1	1	359	U
1	1	366	G
1	1	373	A
1	1	374	A
1	1	389	A
1	1	390	G
1	1	399	U
1	1	400	C
1	1	422	U
1	1	423	U
1	1	435	G
1	1	442	C
1	1	452	G
1	1	457	G
1	1	488	A
1	1	489	G

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Mol	Chain	Res	Type
1	1	504	G
1	1	512	G
1	1	523	G
1	1	534	A
1	1	535	G
1	1	536	A
1	1	537	G
1	1	558	G
1	1	575	G
1	1	576	G
1	1	578	U
1	1	579	G
1	1	606	C
1	1	613	G
1	1	614	U
1	1	619	G
1	1	629	C
1	1	643	U
1	1	644	A
1	1	652	A
1	1	655	C
1	1	656	A
1	1	668	G
1	1	669	U
1	1	684	A
1	1	685	G
1	1	696	U
1	1	698	A
1	1	723	C
1	1	724	A
1	1	725	G
1	1	772	A
1	1	803	U
1	1	835	G
1	1	847	C
1	1	860	U
1	1	865	U
1	1	881	G
1	1	882	A
1	1	883	C
1	1	893	G
1	1	894	G

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Mol	Chain	Res	Type
1	1	900	A
1	1	902	OMG
1	1	903	A
1	1	907	A
1	1	910	A
1	1	923	G
1	1	930	C
1	1	945	C
1	1	946	U
1	1	964	A
1	1	965	G
1	1	968	G
1	1	978	G
1	1	1021	C
1	1	1029	A
1	1	1031	C
1	1	1067	G
1	1	1074	U
1	1	1075	G
1	1	1076	G
1	1	1082	G
1	1	1095	G
1	1	1101	A
1	1	1104	A
1	1	1123	G
1	1	1132	U
1	1	1133	G
1	1	1141	A
1	1	1142	G
1	1	1147	A
1	1	1160	G
1	1	1171	A
1	1	1172	A
1	1	1173	G
1	1	1174	A
1	1	1176	A
1	1	1177	G
1	1	1237	A
1	1	1238	G
1	1	1254	G
1	1	1255	A
1	1	1256	U

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Mol	Chain	Res	Type
1	1	1259	A
1	1	1260	C
1	1	1265	A
1	1	1268	A
1	1	1300	G
1	1	1301	U
1	1	1302	U
1	1	1303	G
1	1	1312	G
1	1	1315	G
1	1	1322	G
1	1	1323	G
1	1	1338	A
1	1	1354	G
1	1	1365	C
1	1	1383	C
1	1	1393	G
1	1	1424	G
1	1	1429	A
1	1	1430	A
1	1	1431	A
1	1	1473	C
1	1	1474	C
1	1	1483	G
1	1	1500	A
1	1	1508	A
1	1	1510	A
1	1	1514	A
1	1	1515	A
1	1	1526	A
1	1	1527	U
1	1	1549	U
1	1	1550	C
1	1	1551	U
1	1	1559	C
1	1	1562	A
1	1	1564	G
1	1	1577	C
1	1	1602	U
1	1	1603	G
1	1	1632	G
1	1	1633	A

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Mol	Chain	Res	Type
1	1	1635	U
1	1	1636	G
1	1	1644	G
1	1	1655	G
1	1	1668	A
1	1	1669	U
1	1	1680	U
1	1	1681	U
1	1	1711	G
1	1	1712	A
1	1	1728	C
1	1	1732	C
1	1	1752	A
1	1	1757	C
1	1	1764	G
1	1	1765	C
1	1	1766	U
1	1	1777	A
1	1	1786	G
1	1	1789	G
1	1	1790	C
1	1	1792	C
1	1	1818	G
1	1	1840	G
1	1	1867	U
1	1	1868	A
1	1	1869	U
1	1	1870	A
1	1	1900	G
1	1	1909	A
1	1	1916	A
1	1	1918	C
1	1	1920	A
1	1	1936	C
1	1	1947	OMG
1	1	1999	A
1	1	2022	A
1	1	2023	G
1	1	2024	G
1	1	2031	G
1	1	2048	A
1	1	2051	G

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Mol	Chain	Res	Type
1	1	2054	G
1	1	2057	A
1	1	2058	A
1	1	2061	G
1	1	2065	U
1	1	2076	U
1	1	2084	U
1	1	2085	G
1	1	2086	C
1	1	2088	OMU
1	1	2092	U
1	1	2093	G
1	1	2103	OMG
1	1	2112	U
1	1	2113	G
1	1	2114	U
1	1	2118	G
1	1	2141	C
1	1	2142	U
1	1	2143	OMC
1	1	2151	A
1	1	2152	C
1	1	2153	A
1	1	2175	C
1	1	2180	A
1	1	2181	G
1	1	2182	U
1	1	2189	G
1	1	2215	G
1	1	2317	U
1	1	2318	A
1	1	2329	G
1	1	2336	A
1	1	2337	C
1	1	2357	G
1	1	2361	G
1	1	2362	OMG
1	1	2395	C
1	1	2399	A
1	1	2417	U
1	1	2420	G
1	1	2421	A

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Mol	Chain	Res	Type
1	1	2424	U
1	1	2432	A
1	1	2434	A
1	1	2446	A
1	1	2447	A
1	1	2448	A
1	1	2457	G
1	1	2498	G
1	1	2500	C
1	1	2518	C
1	1	2540	U
1	1	2541	G
1	1	2546	A
1	1	2547	A
1	1	2555	OMC
1	1	2559	G
1	1	2561	A
1	1	2562	A
1	1	2590	C
1	1	2594	C
1	1	2595	G
1	1	2605	U
1	1	2608	OMG
1	1	2615	A
1	1	2616	G
1	1	2617	A
1	1	2632	A
1	1	2643	G
1	1	2648	A
1	1	2680	A
1	1	2681	G
1	1	2687	C
1	1	2717	G
1	1	2723	U
1	1	2727	U
1	1	2735	G
1	1	2739	G
1	1	2743	U
1	1	2744	G
1	1	2754	G
1	1	2759	A
1	1	2760	G

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Mol	Chain	Res	Type
1	1	2770	G
1	1	2778	G
1	1	2788	G
1	1	2804	U
1	1	2825	C
1	1	2826	U
1	1	2827	G
1	1	2846	G
1	1	2854	C
1	1	2860	A
1	1	2863	G
1	1	2869	A
1	1	2876	A
1	1	2877	A
1	1	2878	G
1	1	2890	A
1	1	2915	A
1	1	2916	A
1	1	2929	A
1	1	2939	U
1	1	2942	A
1	1	2952	U
1	1	2954	A
1	1	2978	G
1	1	2981	U
1	1	2982	U
1	1	2983	U
1	1	2984	C
1	1	2985	C
1	1	2995	A
1	1	2996	G
1	1	3000	G
1	1	3007	C
1	1	3013	G
1	1	3021	G
2	2	2	C
2	2	8	A
2	2	25	G
2	2	29	C
2	2	54	G
2	2	59	U
2	2	60	A

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Mol	Chain	Res	Type
2	2	76	U
2	2	92	C
2	2	98	G
2	2	99	G
2	2	117	G
2	2	128	G

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	117	U
1	1	134	U
1	1	180	A
1	1	456	G
1	1	533	A
1	1	536	A
1	1	575	G
1	1	613	G
1	1	668	G
1	1	724	A
1	1	880	U
1	1	882	A
1	1	902	OMG
1	1	963	G
1	1	1075	G
1	1	1253	A
1	1	1337	C
1	1	1473	C
1	1	1514	A
1	1	1526	A
1	1	1868	A
1	1	2022	A
1	1	2065	U
1	1	2102	A
1	1	2336	A
1	1	2361	G
1	1	2420	G
1	1	2431	U
1	1	2615	A
1	1	2868	U
1	1	2984	C
1	1	2995	A

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Mol	Chain	Res	Type
2	2	7	A

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

65 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	OMG	1	2066	1	23,26,27	1.24	4 (17%)	32,38,41	1.96	6 (18%)
1	OMG	1	2103	1	23,26,27	1.22	4 (17%)	32,38,41	2.04	6 (18%)
1	OMC	1	2885	1	19,22,23	0.80	0	25,31,34	0.78	1 (4%)
1	OMU	1	2574	1	19,22,23	1.34	3 (15%)	25,31,34	1.81	4 (16%)
1	OMG	1	2362	1	23,26,27	1.25	3 (13%)	32,38,41	2.11	7 (21%)
1	PSU	1	1987	1	18,21,22	0.92	1 (5%)	21,30,33	0.72	0
1	OMG	1	2608	1	23,26,27	0.30	0	32,38,41	0.44	0
1	5MC	1	38	1	19,22,23	1.42	3 (15%)	26,32,35	1.31	3 (11%)
1	PSU	1	2610	1	18,21,22	0.91	1 (5%)	21,30,33	0.83	1 (4%)
1	OMG	1	1957	1	23,26,27	1.24	3 (13%)	32,38,41	1.97	6 (18%)
1	G7M	1	3023	1	23,26,27	1.83	2 (8%)	34,39,42	1.03	1 (2%)
1	A2M	1	2011	1	22,25,26	0.20	0	30,36,39	0.45	0
1	OMU	1	908	41,1	19,22,23	1.35	4 (21%)	25,31,34	2.02	8 (32%)
1	OMC	1	2538	1	19,22,23	0.78	0	25,31,34	0.75	0
1	OMU	1	2851	1	19,22,23	1.33	3 (15%)	25,31,34	1.81	4 (16%)
1	OMU	1	2155	1	19,22,23	1.39	3 (15%)	25,31,34	2.03	5 (20%)
1	B8T	1	79	1	19,22,23	0.43	0	25,31,34	0.35	0
1	PSU	1	1911	1	18,21,22	0.93	1 (5%)	21,30,33	0.77	0
1	OMC	1	2116	1	19,22,23	0.79	0	25,31,34	0.74	0
1	OMU	1	2707	1	19,22,23	1.36	4 (21%)	25,31,34	1.84	5 (20%)
1	OMC	1	1976	1	19,22,23	0.82	1 (5%)	25,31,34	0.98	1 (4%)
1	OMU	1	2408	1	19,22,23	1.31	4 (21%)	25,31,34	1.91	5 (20%)
1	4AC	1	2016	1	21,24,25	0.37	0	28,34,37	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	1	2059	41,1	22,25,26	0.25	0	30,36,39	0.61	0
1	OMG	1	2388	1	23,26,27	1.21	4 (17%)	32,38,41	2.13	8 (25%)
1	PSU	1	2571	1	18,21,22	0.93	1 (5%)	21,30,33	0.68	0
1	OMC	1	673	1	19,22,23	0.80	0	25,31,34	0.87	0
1	OMC	1	2018	1	19,22,23	0.80	1 (5%)	25,31,34	0.81	0
1	OMC	1	872	1	19,22,23	0.79	0	25,31,34	0.80	0
1	OMC	1	2555	1	19,22,23	0.79	0	25,31,34	0.88	1 (4%)
1	OMG	1	2667	1	23,26,27	1.24	4 (17%)	32,38,41	1.99	6 (18%)
1	OMC	1	1816	1	19,22,23	0.76	0	25,31,34	0.77	0
1	OMC	1	2624	1	19,22,23	0.29	0	25,31,34	0.31	0
1	PSU	1	2044	1	18,21,22	0.88	1 (5%)	21,30,33	0.68	0
1	UR3	1	2698	1	19,22,23	0.94	1 (5%)	26,32,35	1.77	4 (15%)
1	OMU	1	2088	1	19,22,23	1.37	3 (15%)	25,31,34	1.84	5 (20%)
1	A2M	1	1990	1	22,25,26	0.21	0	30,36,39	0.57	0
1	OMG	1	2017	1	23,26,27	1.19	4 (17%)	32,38,41	1.99	6 (18%)
1	PSU	1	2625	1	18,21,22	0.92	1 (5%)	21,30,33	0.78	0
1	OMU	1	2666	1	19,22,23	1.29	3 (15%)	25,31,34	1.99	5 (20%)
1	OMC	1	2704	1	19,22,23	0.82	1 (5%)	25,31,34	0.85	0
1	OMU	1	2623	1	19,22,23	1.34	4 (21%)	25,31,34	1.94	4 (16%)
1	B8T	1	2937	1	19,22,23	0.42	0	25,31,34	0.33	0
1	OMG	1	2071	1	23,26,27	1.25	4 (17%)	32,38,41	1.97	7 (21%)
1	OMU	1	2077	1	19,22,23	1.34	3 (15%)	25,31,34	1.86	4 (16%)
1	OMG	1	2104	1	23,26,27	1.24	4 (17%)	32,38,41	2.05	7 (21%)
1	OMC	1	492	1	19,22,23	0.80	1 (5%)	25,31,34	0.88	1 (4%)
1	OMC	1	2115	1	19,22,23	0.81	0	25,31,34	0.76	0
1	OMG	1	1949	1	23,26,27	1.26	4 (17%)	32,38,41	2.03	7 (21%)
1	OMC	1	493	1	19,22,23	0.82	1 (5%)	25,31,34	0.79	0
1	OMG	1	2366	1	23,26,27	1.22	4 (17%)	32,38,41	2.01	6 (18%)
1	PSU	1	2607	1	18,21,22	0.95	1 (5%)	21,30,33	0.72	0
1	5MC	1	2056	41,1	19,22,23	1.41	3 (15%)	26,32,35	1.13	3 (11%)
1	OMC	1	2143	1	19,22,23	0.29	0	25,31,34	0.38	0
1	OMC	1	2884	1	19,22,23	0.80	0	25,31,34	0.77	0
1	OMG	1	2537	1	23,26,27	1.22	3 (13%)	32,38,41	2.01	6 (18%)
1	OMU	1	2628	1	19,22,23	1.36	3 (15%)	25,31,34	1.89	5 (20%)
1	A2M	1	2691	41,1	22,25,26	0.20	0	30,36,39	0.41	0
1	OMG	1	2601	41,1	23,26,27	1.23	4 (17%)	32,38,41	1.97	6 (18%)
1	OMG	1	1971	1	23,26,27	1.24	3 (13%)	32,38,41	1.94	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	1	875	1	19,22,23	1.28	3 (15%)	25,31,34	1.87	5 (20%)
1	OMG	1	2176	41,1	23,26,27	1.21	4 (17%)	32,38,41	2.02	7 (21%)
1	OMG	1	902	41,1	23,26,27	1.22	4 (17%)	32,38,41	2.06	7 (21%)
1	OMC	1	2720	1	19,22,23	0.78	0	25,31,34	0.94	1 (4%)
1	OMG	1	1947	1	23,26,27	1.21	4 (17%)	32,38,41	2.02	7 (21%)

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	OMG	1	2066	1	-	0/9/27/28	0/3/3/3
1	OMG	1	2103	1	-	0/9/27/28	0/3/3/3
1	OMC	1	2885	1	-	0/9/27/28	0/2/2/2
1	OMU	1	2574	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2362	1	-	0/9/27/28	0/3/3/3
1	PSU	1	1987	1	-	0/7/25/26	0/2/2/2
1	OMG	1	2608	1	-	2/9/27/28	0/3/3/3
1	5MC	1	38	1	-	1/7/25/26	0/2/2/2
1	PSU	1	2610	1	-	0/7/25/26	0/2/2/2
1	OMG	1	1957	1	-	0/9/27/28	0/3/3/3
1	G7M	1	3023	1	-	0/7/25/26	0/3/3/3
1	A2M	1	2011	1	-	0/9/27/28	0/3/3/3
1	OMU	1	908	41,1	-	5/9/27/28	0/2/2/2
1	OMC	1	2538	1	-	0/9/27/28	0/2/2/2
1	OMU	1	2851	1	-	1/9/27/28	0/2/2/2
1	OMU	1	2155	1	-	3/9/27/28	0/2/2/2
1	B8T	1	79	1	-	0/7/27/28	0/2/2/2
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
1	OMC	1	2116	1	-	0/9/27/28	0/2/2/2
1	OMU	1	2707	1	-	0/9/27/28	0/2/2/2
1	OMC	1	1976	1	-	0/9/27/28	0/2/2/2
1	OMU	1	2408	1	-	0/9/27/28	0/2/2/2
1	4AC	1	2016	1	-	0/11/29/30	0/2/2/2
1	A2M	1	2059	41,1	-	2/9/27/28	0/3/3/3
1	OMG	1	2388	1	-	1/9/27/28	0/3/3/3
1	PSU	1	2571	1	-	0/7/25/26	0/2/2/2
1	OMC	1	673	1	-	0/9/27/28	0/2/2/2
1	OMC	1	2018	1	-	0/9/27/28	0/2/2/2
1	OMC	1	872	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	1	2555	1	-	1/9/27/28	0/2/2/2
1	OMG	1	2667	1	-	0/9/27/28	0/3/3/3
1	OMC	1	1816	1	-	0/9/27/28	0/2/2/2
1	OMC	1	2624	1	-	0/9/27/28	0/2/2/2
1	PSU	1	2044	1	-	0/7/25/26	0/2/2/2
1	UR3	1	2698	1	-	0/7/25/26	0/2/2/2
1	OMU	1	2088	1	-	0/9/27/28	0/2/2/2
1	A2M	1	1990	1	-	1/9/27/28	0/3/3/3
1	OMG	1	2017	1	-	0/9/27/28	0/3/3/3
1	PSU	1	2625	1	-	0/7/25/26	0/2/2/2
1	OMU	1	2666	1	-	0/9/27/28	0/2/2/2
1	OMC	1	2704	1	-	0/9/27/28	0/2/2/2
1	OMU	1	2623	1	-	0/9/27/28	0/2/2/2
1	B8T	1	2937	1	-	2/7/27/28	0/2/2/2
1	OMG	1	2071	1	-	0/9/27/28	0/3/3/3
1	OMU	1	2077	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2104	1	-	0/9/27/28	0/3/3/3
1	OMC	1	492	1	-	0/9/27/28	0/2/2/2
1	OMC	1	2115	1	-	0/9/27/28	0/2/2/2
1	OMG	1	1949	1	-	0/9/27/28	0/3/3/3
1	OMC	1	493	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2366	1	-	0/9/27/28	0/3/3/3
1	PSU	1	2607	1	-	0/7/25/26	0/2/2/2
1	5MC	1	2056	41,1	-	0/7/25/26	0/2/2/2
1	OMC	1	2143	1	-	2/9/27/28	0/2/2/2
1	OMC	1	2884	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2537	1	-	1/9/27/28	0/3/3/3
1	OMU	1	2628	1	-	0/9/27/28	0/2/2/2
1	A2M	1	2691	41,1	-	0/9/27/28	0/3/3/3
1	OMG	1	2601	41,1	-	1/9/27/28	0/3/3/3
1	OMG	1	1971	1	-	1/9/27/28	0/3/3/3
1	OMU	1	875	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2176	41,1	-	0/9/27/28	0/3/3/3
1	OMG	1	902	41,1	-	0/9/27/28	0/3/3/3
1	OMC	1	2720	1	-	0/9/27/28	0/2/2/2
1	OMG	1	1947	1	-	2/9/27/28	0/3/3/3

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	3023	G7M	C8-N7	7.54	1.45	1.33
1	1	2056	5MC	C5-C4	4.75	1.47	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	38	5MC	C5-C4	4.75	1.47	1.44
1	1	3023	G7M	C8-N9	4.02	1.46	1.35
1	1	2571	PSU	C6-C5	3.61	1.39	1.35
1	1	2607	PSU	C6-C5	3.59	1.39	1.35
1	1	2610	PSU	C6-C5	3.59	1.39	1.35
1	1	2625	PSU	C6-C5	3.57	1.39	1.35
1	1	1911	PSU	C6-C5	3.56	1.39	1.35
1	1	2088	OMU	C4-N3	-3.46	1.32	1.38
1	1	1987	PSU	C6-C5	3.46	1.39	1.35
1	1	2707	OMU	C4-N3	-3.42	1.32	1.38
1	1	2628	OMU	C4-N3	-3.41	1.32	1.38
1	1	2155	OMU	C4-N3	-3.41	1.32	1.38
1	1	2044	PSU	C6-C5	3.39	1.39	1.35
1	1	2574	OMU	C4-N3	-3.30	1.33	1.38
1	1	2623	OMU	C4-N3	-3.26	1.33	1.38
1	1	2851	OMU	C4-N3	-3.23	1.33	1.38
1	1	2408	OMU	C4-N3	-3.20	1.33	1.38
1	1	2666	OMU	C4-N3	-3.20	1.33	1.38
1	1	2077	OMU	C4-N3	-3.14	1.33	1.38
1	1	2362	OMG	C6-N1	-3.13	1.33	1.38
1	1	875	OMU	C4-N3	-3.12	1.33	1.38
1	1	2071	OMG	C6-N1	-3.08	1.33	1.38
1	1	908	OMU	C4-N3	-3.06	1.33	1.38
1	1	2104	OMG	C6-N1	-3.02	1.33	1.38
1	1	1949	OMG	C6-N1	-3.02	1.33	1.38
1	1	2155	OMU	C2-N3	-3.01	1.32	1.38
1	1	2366	OMG	C6-N1	-3.00	1.33	1.38
1	1	1971	OMG	C6-N1	-3.00	1.33	1.38
1	1	902	OMG	C6-N1	-2.98	1.33	1.38
1	1	2066	OMG	C6-N1	-2.96	1.33	1.38
1	1	1957	OMG	C6-N1	-2.96	1.33	1.38
1	1	38	5MC	C6-N1	-2.95	1.33	1.38
1	1	1957	OMG	C5-C4	2.95	1.46	1.38
1	1	2707	OMU	C2-N3	-2.93	1.32	1.38
1	1	2537	OMG	C6-N1	-2.89	1.33	1.38
1	1	2601	OMG	C6-N1	-2.88	1.33	1.38
1	1	1947	OMG	C6-N1	-2.85	1.33	1.38
1	1	2077	OMU	C2-N3	-2.85	1.33	1.38
1	1	2103	OMG	C6-N1	-2.85	1.33	1.38
1	1	2623	OMU	C2-N3	-2.85	1.33	1.38
1	1	2667	OMG	C6-N1	-2.85	1.33	1.38
1	1	2088	OMU	C2-N3	-2.84	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1971	OMG	C5-C4	2.83	1.46	1.38
1	1	2362	OMG	C5-C4	2.82	1.46	1.38
1	1	2066	OMG	C5-C4	2.81	1.46	1.38
1	1	2176	OMG	C6-N1	-2.81	1.33	1.38
1	1	2537	OMG	C5-C4	2.80	1.46	1.38
1	1	2388	OMG	C6-N1	-2.80	1.33	1.38
1	1	2408	OMU	C2-N3	-2.80	1.33	1.38
1	1	2667	OMG	C5-C4	2.79	1.46	1.38
1	1	2601	OMG	C5-C4	2.78	1.46	1.38
1	1	2103	OMG	C5-C4	2.77	1.46	1.38
1	1	2574	OMU	C2-N3	-2.76	1.33	1.38
1	1	2628	OMU	C2-N3	-2.75	1.33	1.38
1	1	2666	OMU	C2-N3	-2.73	1.33	1.38
1	1	2017	OMG	C6-N1	-2.73	1.33	1.38
1	1	2851	OMU	C2-N3	-2.72	1.33	1.38
1	1	2017	OMG	C5-C4	2.72	1.46	1.38
1	1	1949	OMG	C5-C4	2.70	1.46	1.38
1	1	2366	OMG	C5-C4	2.69	1.46	1.38
1	1	902	OMG	C5-C4	2.67	1.46	1.38
1	1	875	OMU	C2-N3	-2.67	1.33	1.38
1	1	908	OMU	C2-N3	-2.66	1.33	1.38
1	1	2071	OMG	C5-C4	2.66	1.46	1.38
1	1	2601	OMG	C5-N7	-2.65	1.33	1.39
1	1	2176	OMG	C5-C4	2.64	1.46	1.38
1	1	2388	OMG	C5-C4	2.64	1.46	1.38
1	1	1971	OMG	C5-N7	-2.62	1.33	1.39
1	1	2056	5MC	C6-N1	-2.58	1.33	1.38
1	1	2104	OMG	C5-C4	2.55	1.45	1.38
1	1	1947	OMG	C5-C4	2.52	1.45	1.38
1	1	1949	OMG	C5-N7	-2.52	1.34	1.39
1	1	2103	OMG	C5-N7	-2.51	1.34	1.39
1	1	2667	OMG	C5-N7	-2.49	1.34	1.39
1	1	1957	OMG	C5-N7	-2.49	1.34	1.39
1	1	1947	OMG	C5-N7	-2.49	1.34	1.39
1	1	2362	OMG	C5-N7	-2.49	1.34	1.39
1	1	2066	OMG	C5-N7	-2.48	1.34	1.39
1	1	2104	OMG	C5-N7	-2.48	1.34	1.39
1	1	2366	OMG	C5-N7	-2.46	1.34	1.39
1	1	2071	OMG	C5-N7	-2.44	1.34	1.39
1	1	2707	OMU	C5-C4	-2.44	1.38	1.43
1	1	902	OMG	C5-N7	-2.43	1.34	1.39
1	1	908	OMU	C5-C4	-2.41	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2176	OMG	C5-N7	-2.40	1.34	1.39
1	1	2628	OMU	C5-C4	-2.40	1.38	1.43
1	1	875	OMU	C5-C4	-2.38	1.38	1.43
1	1	2077	OMU	C5-C4	-2.37	1.38	1.43
1	1	2088	OMU	C5-C4	-2.36	1.38	1.43
1	1	2537	OMG	C5-N7	-2.36	1.34	1.39
1	1	2574	OMU	C5-C4	-2.36	1.38	1.43
1	1	2056	5MC	C6-C5	2.34	1.38	1.34
1	1	2388	OMG	C5-N7	-2.34	1.34	1.39
1	1	2623	OMU	C5-C4	-2.34	1.38	1.43
1	1	2851	OMU	C5-C4	-2.31	1.38	1.43
1	1	2017	OMG	C5-N7	-2.31	1.34	1.39
1	1	2408	OMU	C5-C4	-2.28	1.38	1.43
1	1	2155	OMU	C5-C4	-2.28	1.38	1.43
1	1	2104	OMG	C4-N9	-2.26	1.32	1.38
1	1	2176	OMG	C4-N9	-2.26	1.32	1.38
1	1	2071	OMG	C4-N9	-2.25	1.32	1.38
1	1	2666	OMU	C5-C4	-2.22	1.38	1.43
1	1	1949	OMG	C4-N9	-2.19	1.32	1.38
1	1	2698	UR3	C5-C4	-2.16	1.38	1.43
1	1	2388	OMG	C4-N9	-2.15	1.32	1.38
1	1	1947	OMG	C4-N9	-2.14	1.32	1.38
1	1	2066	OMG	C4-N9	-2.14	1.32	1.38
1	1	38	5MC	C6-C5	2.14	1.38	1.34
1	1	908	OMU	C2-N1	2.13	1.41	1.38
1	1	2667	OMG	C4-N9	-2.12	1.32	1.38
1	1	1976	OMC	C6-N1	-2.12	1.33	1.38
1	1	2017	OMG	C4-N9	-2.11	1.32	1.38
1	1	2601	OMG	C4-N9	-2.07	1.32	1.38
1	1	2018	OMC	C6-N1	-2.06	1.33	1.38
1	1	902	OMG	C4-N9	-2.06	1.32	1.38
1	1	2103	OMG	C4-N9	-2.05	1.32	1.38
1	1	2366	OMG	C4-N9	-2.04	1.32	1.38
1	1	493	OMC	C6-N1	-2.04	1.33	1.38
1	1	2704	OMC	C6-N1	-2.03	1.33	1.38
1	1	2408	OMU	C6-N1	-2.03	1.33	1.38
1	1	2623	OMU	C6-N1	-2.02	1.33	1.38
1	1	2707	OMU	C6-N1	-2.02	1.33	1.38
1	1	492	OMC	C6-N1	-2.01	1.33	1.38

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2698	UR3	C4-N3-C2	-6.86	119.06	124.58
1	1	2362	OMG	C5-C4-N3	-6.69	117.74	128.39
1	1	2537	OMG	C5-C4-N3	-6.32	118.33	128.39
1	1	1949	OMG	C5-C4-N3	-6.28	118.39	128.39
1	1	2103	OMG	C5-C4-N3	-6.20	118.52	128.39
1	1	2366	OMG	C5-C4-N3	-6.20	118.53	128.39
1	1	1971	OMG	C5-C4-N3	-6.12	118.66	128.39
1	1	1957	OMG	C5-C4-N3	-6.11	118.66	128.39
1	1	2601	OMG	C5-C4-N3	-6.05	118.75	128.39
1	1	2066	OMG	C5-C4-N3	-6.02	118.81	128.39
1	1	2667	OMG	C5-C4-N3	-6.01	118.82	128.39
1	1	2388	OMG	C5-C4-N3	-6.00	118.84	128.39
1	1	902	OMG	C5-C4-N3	-5.95	118.91	128.39
1	1	2017	OMG	C5-C4-N3	-5.95	118.92	128.39
1	1	2176	OMG	C5-C4-N3	-5.88	119.02	128.39
1	1	2071	OMG	C5-C4-N3	-5.77	119.21	128.39
1	1	1947	OMG	C5-C4-N3	-5.76	119.22	128.39
1	1	2104	OMG	C5-C4-N3	-5.73	119.27	128.39
1	1	2388	OMG	C2-N3-C4	5.48	121.73	112.30
1	1	2666	OMU	C4-N3-C2	-5.44	119.85	126.61
1	1	2362	OMG	C2-N3-C4	5.41	121.61	112.30
1	1	2155	OMU	C4-N3-C2	-5.41	119.90	126.61
1	1	2103	OMG	C2-N3-C4	5.26	121.37	112.30
1	1	2176	OMG	C2-N3-C4	5.23	121.30	112.30
1	1	2366	OMG	C2-N3-C4	5.22	121.30	112.30
1	1	902	OMG	C2-N3-C4	5.20	121.26	112.30
1	1	2408	OMU	C4-N3-C2	-5.18	120.18	126.61
1	1	2623	OMU	C4-N3-C2	-5.17	120.19	126.61
1	1	1949	OMG	C2-N3-C4	5.14	121.16	112.30
1	1	2017	OMG	C2-N3-C4	5.07	121.03	112.30
1	1	2667	OMG	C2-N3-C4	5.07	121.03	112.30
1	1	2601	OMG	C2-N3-C4	5.05	120.99	112.30
1	1	1947	OMG	C2-N3-C4	5.02	120.95	112.30
1	1	1957	OMG	C2-N3-C4	5.02	120.94	112.30
1	1	2537	OMG	C2-N3-C4	5.01	120.94	112.30
1	1	2104	OMG	C2-N3-C4	5.00	120.91	112.30
1	1	2362	OMG	N9-C4-N3	4.97	135.90	125.95
1	1	1971	OMG	C2-N3-C4	4.97	120.86	112.30
1	1	2707	OMU	C4-N3-C2	-4.95	120.47	126.61
1	1	2066	OMG	C2-N3-C4	4.94	120.81	112.30
1	1	875	OMU	C4-N3-C2	-4.91	120.52	126.61
1	1	2071	OMG	C2-N3-C4	4.90	120.74	112.30
1	1	2077	OMU	C4-N3-C2	-4.84	120.60	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2851	OMU	C4-N3-C2	-4.83	120.61	126.61
1	1	908	OMU	C1'-N1-C2	4.83	126.27	117.59
1	1	2628	OMU	C4-N3-C2	-4.83	120.62	126.61
1	1	2574	OMU	C4-N3-C2	-4.80	120.65	126.61
1	1	2088	OMU	C4-N3-C2	-4.72	120.75	126.61
1	1	2155	OMU	N3-C2-N1	4.70	121.01	114.89
1	1	2628	OMU	N3-C2-N1	4.65	120.94	114.89
1	1	2066	OMG	N9-C4-N3	4.63	135.22	125.95
1	1	2537	OMG	N9-C4-N3	4.63	135.21	125.95
1	1	1971	OMG	N9-C4-N3	4.61	135.18	125.95
1	1	2666	OMU	N3-C2-N1	4.61	120.89	114.89
1	1	2176	OMG	N9-C4-N3	4.59	135.13	125.95
1	1	2623	OMU	N3-C2-N1	4.52	120.77	114.89
1	1	1949	OMG	N9-C4-N3	4.50	134.95	125.95
1	1	1957	OMG	N9-C4-N3	4.50	134.95	125.95
1	1	2408	OMU	N3-C2-N1	4.46	120.70	114.89
1	1	2601	OMG	N9-C4-N3	4.46	134.87	125.95
1	1	2017	OMG	N9-C4-N3	4.40	134.75	125.95
1	1	2667	OMG	N9-C4-N3	4.38	134.70	125.95
1	1	2366	OMG	N9-C4-N3	4.37	134.69	125.95
1	1	2666	OMU	C5-C4-N3	4.35	120.90	114.80
1	1	2574	OMU	N3-C2-N1	4.35	120.55	114.89
1	1	875	OMU	N3-C2-N1	4.35	120.55	114.89
1	1	2707	OMU	N3-C2-N1	4.34	120.55	114.89
1	1	902	OMG	N9-C4-N3	4.34	134.63	125.95
1	1	2155	OMU	C5-C4-N3	4.29	120.80	114.80
1	1	2103	OMG	N9-C4-N3	4.27	134.49	125.95
1	1	2088	OMU	N3-C2-N1	4.26	120.44	114.89
1	1	2077	OMU	N3-C2-N1	4.25	120.42	114.89
1	1	3023	G7M	N9-C8-N7	-4.25	102.17	112.48
1	1	908	OMU	C4-N3-C2	-4.23	121.37	126.61
1	1	2071	OMG	N9-C4-N3	4.21	134.37	125.95
1	1	2623	OMU	C5-C4-N3	4.20	120.69	114.80
1	1	1947	OMG	N9-C4-N3	4.19	134.33	125.95
1	1	2388	OMG	N9-C4-N3	4.15	134.26	125.95
1	1	2851	OMU	C5-C4-N3	4.12	120.57	114.80
1	1	2077	OMU	C5-C4-N3	4.11	120.55	114.80
1	1	2408	OMU	C5-C4-N3	4.09	120.53	114.80
1	1	2707	OMU	C5-C4-N3	4.09	120.53	114.80
1	1	2388	OMG	C6-C5-N7	4.09	137.72	130.29
1	1	2088	OMU	C5-C4-N3	4.08	120.51	114.80
1	1	2574	OMU	C5-C4-N3	4.07	120.50	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	875	OMU	C5-C4-N3	4.03	120.45	114.80
1	1	2104	OMG	N9-C4-N3	4.01	133.97	125.95
1	1	908	OMU	N3-C2-N1	3.98	120.08	114.89
1	1	2851	OMU	N3-C2-N1	3.98	120.08	114.89
1	1	2628	OMU	C5-C4-N3	3.97	120.36	114.80
1	1	908	OMU	C5-C4-N3	3.86	120.21	114.80
1	1	902	OMG	C6-C5-N7	3.76	137.13	130.29
1	1	2104	OMG	C6-C5-N7	3.73	137.08	130.29
1	1	2103	OMG	C6-C5-N7	3.59	136.82	130.29
1	1	38	5MC	C5-C6-N1	-3.52	119.49	123.31
1	1	2698	UR3	C5-C4-N3	3.47	119.61	115.04
1	1	2366	OMG	C6-C5-N7	3.44	136.55	130.29
1	1	1949	OMG	C6-C5-N7	3.44	136.55	130.29
1	1	1947	OMG	C6-C5-N7	3.42	136.52	130.29
1	1	2071	OMG	C6-C5-N7	3.42	136.51	130.29
1	1	2017	OMG	C6-C5-N7	3.37	136.43	130.29
1	1	2667	OMG	C6-C5-N7	3.37	136.42	130.29
1	1	2176	OMG	C6-C5-N7	3.35	136.39	130.29
1	1	1957	OMG	C6-C5-N7	3.33	136.35	130.29
1	1	2537	OMG	C6-C5-N7	3.29	136.28	130.29
1	1	2623	OMU	O4-C4-C5	-3.27	119.53	125.16
1	1	2601	OMG	C6-C5-N7	3.26	136.22	130.29
1	1	875	OMU	O4-C4-C5	-3.23	119.60	125.16
1	1	2362	OMG	C6-C5-N7	3.23	136.16	130.29
1	1	2056	5MC	C5-C6-N1	-3.22	119.81	123.31
1	1	2666	OMU	O4-C4-C5	-3.14	119.75	125.16
1	1	2066	OMG	C6-C5-N7	3.12	135.97	130.29
1	1	38	5MC	C5-C4-N3	-3.12	118.56	121.75
1	1	1971	OMG	C6-C5-N7	3.08	135.90	130.29
1	1	2851	OMU	O4-C4-C5	-3.07	119.88	125.16
1	1	2077	OMU	O4-C4-C5	-3.05	119.89	125.16
1	1	2408	OMU	O4-C4-C5	-3.05	119.90	125.16
1	1	2155	OMU	O4-C4-C5	-2.99	120.00	125.16
1	1	908	OMU	O4-C4-C5	-2.99	120.01	125.16
1	1	2707	OMU	O4-C4-C5	-2.97	120.04	125.16
1	1	2103	OMG	C4-C5-N7	-2.96	105.97	110.67
1	1	2088	OMU	O4-C4-C5	-2.95	120.07	125.16
1	1	2388	OMG	C4-C5-N7	-2.92	106.04	110.67
1	1	875	OMU	O2-C2-N1	-2.86	119.08	122.80
1	1	2628	OMU	O4-C4-C5	-2.84	120.26	125.16
1	1	2056	5MC	C5-C4-N3	-2.83	118.85	121.75
1	1	1976	OMC	O2-C2-N3	-2.83	117.87	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2574	OMU	O4-C4-C5	-2.76	120.40	125.16
1	1	2104	OMG	C4-C5-N7	-2.75	106.31	110.67
1	1	2666	OMU	O2-C2-N1	-2.72	119.25	122.80
1	1	2537	OMG	C4-C5-N7	-2.71	106.37	110.67
1	1	2362	OMG	C4-C5-N7	-2.70	106.39	110.67
1	1	1949	OMG	C4-C5-N7	-2.69	106.41	110.67
1	1	38	5MC	O2-C2-N3	-2.68	118.10	122.33
1	1	2366	OMG	C4-C5-N7	-2.68	106.43	110.67
1	1	2155	OMU	O2'-C2'-C1'	2.67	114.05	108.99
1	1	902	OMG	C4-C5-N7	-2.66	106.46	110.67
1	1	908	OMU	C1'-N1-C6	-2.62	115.18	120.78
1	1	2667	OMG	C4-C5-N7	-2.58	106.58	110.67
1	1	2408	OMU	O2-C2-N1	-2.56	119.47	122.80
1	1	1957	OMG	C4-C5-N7	-2.55	106.62	110.67
1	1	2017	OMG	C4-C5-N7	-2.53	106.67	110.67
1	1	2071	OMG	C4-C5-N7	-2.49	106.73	110.67
1	1	1947	OMG	C2'-C1'-N9	-2.46	109.58	114.24
1	1	1947	OMG	C4-C5-N7	-2.44	106.80	110.67
1	1	2601	OMG	C4-C5-N7	-2.42	106.84	110.67
1	1	2610	PSU	C3'-C2'-C1'	2.42	104.54	101.69
1	1	2104	OMG	C2'-C1'-N9	-2.41	109.67	114.24
1	1	2601	OMG	O6-C6-C5	-2.40	120.19	126.53
1	1	1971	OMG	C4-C5-N7	-2.40	106.87	110.67
1	1	2176	OMG	O6-C6-C5	-2.39	120.21	126.53
1	1	2555	OMC	O2-C2-N3	-2.37	118.59	122.33
1	1	2017	OMG	O6-C6-C5	-2.37	120.28	126.53
1	1	2628	OMU	C1'-N1-C2	2.36	121.83	117.59
1	1	2066	OMG	C4-C5-N7	-2.35	106.95	110.67
1	1	2088	OMU	C1'-N1-C2	2.34	121.79	117.59
1	1	2056	5MC	O2-C2-N3	-2.31	118.68	122.33
1	1	2698	UR3	C3U-N3-C4	2.31	121.07	117.87
1	1	1947	OMG	O6-C6-C5	-2.29	120.48	126.53
1	1	2066	OMG	O6-C6-C5	-2.28	120.50	126.53
1	1	2104	OMG	O6-C6-C5	-2.27	120.53	126.53
1	1	2176	OMG	C4-C5-N7	-2.25	107.10	110.67
1	1	492	OMC	O2-C2-N3	-2.23	118.81	122.33
1	1	2071	OMG	O6-C6-C5	-2.17	120.79	126.53
1	1	2667	OMG	O6-C6-C5	-2.16	120.82	126.53
1	1	2366	OMG	O6-C6-C5	-2.16	120.84	126.53
1	1	2707	OMU	O2-C2-N1	-2.15	119.99	122.80
1	1	902	OMG	C5-C6-N1	2.15	118.73	113.25
1	1	2388	OMG	C5-C6-N1	2.14	118.69	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	908	OMU	O2-C2-N3	-2.13	117.56	121.49
1	1	2720	OMC	O2-C2-N3	-2.11	119.00	122.33
1	1	2362	OMG	O6-C6-C5	-2.11	120.97	126.53
1	1	1949	OMG	O6-C6-C5	-2.10	121.00	126.53
1	1	1971	OMG	O6-C6-C5	-2.08	121.03	126.53
1	1	2537	OMG	O6-C6-C5	-2.08	121.04	126.53
1	1	2071	OMG	C2'-C1'-N9	-2.07	110.32	114.24
1	1	1957	OMG	O6-C6-C5	-2.06	121.09	126.53
1	1	2176	OMG	C5-C6-N1	2.06	118.49	113.25
1	1	902	OMG	O6-C6-C5	-2.05	121.11	126.53
1	1	2388	OMG	C2'-C1'-N9	-2.04	110.36	114.24
1	1	2362	OMG	C5-C6-N1	2.04	118.44	113.25
1	1	1949	OMG	C5-C6-N1	2.04	118.44	113.25
1	1	2885	OMC	O2-C2-N3	-2.04	119.12	122.33
1	1	2388	OMG	O6-C6-C5	-2.03	121.17	126.53
1	1	908	OMU	C6-N1-C2	-2.03	118.53	121.00
1	1	2698	UR3	C6-N1-C2	-2.03	120.14	121.80
1	1	2103	OMG	O6-C6-C5	-2.00	121.25	126.53

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	1947	OMG	O4'-C4'-C5'-O5'
1	1	1990	A2M	C1'-C2'-O2'-CM'
1	1	2155	OMU	C1'-C2'-O2'-CM2
1	1	2608	OMG	O4'-C4'-C5'-O5'
1	1	1947	OMG	C3'-C4'-C5'-O5'
1	1	2143	OMC	C3'-C4'-C5'-O5'
1	1	2143	OMC	O4'-C4'-C5'-O5'
1	1	2937	B8T	C3'-C4'-C5'-O5'
1	1	38	5MC	C4'-C5'-O5'-P
1	1	2608	OMG	C3'-C4'-C5'-O5'
1	1	2937	B8T	O4'-C4'-C5'-O5'
1	1	2388	OMG	C4'-C5'-O5'-P
1	1	2555	OMC	C4'-C5'-O5'-P
1	1	2851	OMU	C3'-C4'-C5'-O5'
1	1	908	OMU	C2'-C1'-N1-C6
1	1	2155	OMU	C2'-C1'-N1-C6
1	1	908	OMU	C2'-C1'-N1-C2
1	1	2537	OMG	O4'-C4'-C5'-O5'
1	1	908	OMU	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
1	1	908	OMU	O4'-C1'-N1-C2
1	1	2059	A2M	O4'-C4'-C5'-O5'
1	1	908	OMU	C3'-C2'-O2'-CM2
1	1	2155	OMU	O4'-C1'-N1-C6
1	1	2601	OMG	C3'-C4'-C5'-O5'
1	1	1971	OMG	C3'-C2'-O2'-CM2
1	1	2059	A2M	C2'-C1'-N9-C8

There are no ring outliers.

15 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	2103	OMG	1	0
1	1	1957	OMG	1	0
1	1	2011	A2M	1	0
1	1	2116	OMC	1	0
1	1	2059	A2M	1	0
1	1	2698	UR3	1	0
1	1	1990	A2M	1	0
1	1	2666	OMU	1	0
1	1	2623	OMU	1	0
1	1	2077	OMU	1	0
1	1	2104	OMG	2	0
1	1	1949	OMG	1	0
1	1	2628	OMU	2	0
1	1	2691	A2M	1	0
1	1	902	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 224 ligands modelled in this entry, 178 are monoatomic - leaving 46 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	$\# Z > 2$
40	SPM	1	3121	-	13,13,13	0.24	0	12,12,12	0.24	0
40	SPM	1	3112	-	13,13,13	0.19	0	12,12,12	0.40	0
40	SPM	1	3124	-	13,13,13	0.16	0	12,12,12	0.34	0
40	SPM	1	3111	-	13,13,13	0.14	0	12,12,12	0.19	0
40	SPM	1	3138	-	13,13,13	0.16	0	12,12,12	0.18	0
40	SPM	AM	201	-	13,13,13	0.18	0	12,12,12	0.28	0
40	SPM	1	3139	-	13,13,13	0.18	0	12,12,12	0.14	0
40	SPM	1	3120	-	13,13,13	0.17	0	12,12,12	0.23	0
40	SPM	1	3131	-	13,13,13	0.15	0	12,12,12	0.25	0
40	SPM	1	3122	-	13,13,13	0.17	0	12,12,12	0.20	0
40	SPM	1	3142	-	13,13,13	0.17	0	12,12,12	0.37	0
40	SPM	1	3141	-	13,13,13	0.16	0	12,12,12	0.17	0
40	SPM	1	3135	-	13,13,13	0.15	0	12,12,12	0.33	0
40	SPM	1	3109	-	13,13,13	0.17	0	12,12,12	0.26	0
40	SPM	1	3114	-	13,13,13	0.20	0	12,12,12	0.31	0
40	SPM	1	3129	-	13,13,13	0.18	0	12,12,12	0.31	0
40	SPM	1	3104	-	13,13,13	0.16	0	12,12,12	0.40	0
40	SPM	1	3134	-	13,13,13	0.17	0	12,12,12	0.29	0
40	SPM	AL	201	-	13,13,13	0.16	0	12,12,12	0.20	0
40	SPM	1	3125	-	13,13,13	0.14	0	12,12,12	0.28	0
40	SPM	1	3113	-	13,13,13	0.16	0	12,12,12	0.21	0
40	SPM	1	3102	-	13,13,13	0.17	0	12,12,12	0.43	0
40	SPM	1	3126	-	13,13,13	0.14	0	12,12,12	0.42	0
40	SPM	1	3137	-	13,13,13	0.17	0	12,12,12	0.27	0
40	SPM	1	3132	-	13,13,13	0.17	0	12,12,12	0.19	0
40	SPM	1	3117	-	13,13,13	0.20	0	12,12,12	0.32	0
40	SPM	1	3144	-	13,13,13	0.19	0	12,12,12	0.24	0
40	SPM	1	3108	-	13,13,13	0.18	0	12,12,12	0.35	0
40	SPM	1	3118	-	13,13,13	0.16	0	12,12,12	0.26	0
40	SPM	1	3128	-	13,13,13	0.19	0	12,12,12	0.32	0
40	SPM	1	3105	-	13,13,13	0.17	0	12,12,12	0.18	0
40	SPM	1	3107	-	13,13,13	0.16	0	12,12,12	0.18	0
40	SPM	1	3133	-	13,13,13	0.16	0	12,12,12	0.29	0
40	SPM	1	3143	-	13,13,13	0.19	0	12,12,12	0.44	0
40	SPM	1	3103	-	13,13,13	0.16	0	12,12,12	0.34	0
40	SPM	1	3106	-	13,13,13	0.20	0	12,12,12	0.24	0
40	SPM	1	3123	-	13,13,13	0.18	0	12,12,12	0.33	0
40	SPM	1	3116	-	13,13,13	0.21	0	12,12,12	0.29	0
40	SPM	1	3130	-	13,13,13	0.15	0	12,12,12	0.22	0
40	SPM	1	3110	-	13,13,13	0.14	0	12,12,12	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	SPM	1	3127	-	13,13,13	0.16	0	12,12,12	0.22	0
40	SPM	1	3101	-	13,13,13	0.18	0	12,12,12	0.27	0
40	SPM	1	3140	-	13,13,13	0.15	0	12,12,12	0.26	0
40	SPM	1	3119	-	13,13,13	0.20	0	12,12,12	0.21	0
40	SPM	1	3136	-	13,13,13	0.18	0	12,12,12	0.37	0
40	SPM	1	3115	-	13,13,13	0.18	0	12,12,12	0.26	0

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
40	SPM	1	3121	-	-	1/11/11/11	-
40	SPM	1	3112	-	-	1/11/11/11	-
40	SPM	1	3124	-	-	0/11/11/11	-
40	SPM	1	3111	-	-	8/11/11/11	-
40	SPM	1	3138	-	-	8/11/11/11	-
40	SPM	AM	201	-	-	0/11/11/11	-
40	SPM	1	3139	-	-	2/11/11/11	-
40	SPM	1	3120	-	-	1/11/11/11	-
40	SPM	1	3131	-	-	1/11/11/11	-
40	SPM	1	3122	-	-	9/11/11/11	-
40	SPM	1	3142	-	-	1/11/11/11	-
40	SPM	1	3141	-	-	7/11/11/11	-
40	SPM	1	3135	-	-	1/11/11/11	-
40	SPM	1	3109	-	-	1/11/11/11	-
40	SPM	1	3114	-	-	3/11/11/11	-
40	SPM	1	3129	-	-	2/11/11/11	-
40	SPM	1	3104	-	-	2/11/11/11	-
40	SPM	1	3134	-	-	1/11/11/11	-
40	SPM	AL	201	-	-	3/11/11/11	-
40	SPM	1	3125	-	-	1/11/11/11	-
40	SPM	1	3113	-	-	9/11/11/11	-
40	SPM	1	3102	-	-	1/11/11/11	-
40	SPM	1	3126	-	-	1/11/11/11	-
40	SPM	1	3137	-	-	2/11/11/11	-
40	SPM	1	3132	-	-	9/11/11/11	-
40	SPM	1	3117	-	-	1/11/11/11	-
40	SPM	1	3144	-	-	2/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	SPM	1	3108	-	-	4/11/11/11	-
40	SPM	1	3118	-	-	0/11/11/11	-
40	SPM	1	3128	-	-	1/11/11/11	-
40	SPM	1	3105	-	-	1/11/11/11	-
40	SPM	1	3107	-	-	3/11/11/11	-
40	SPM	1	3133	-	-	2/11/11/11	-
40	SPM	1	3143	-	-	4/11/11/11	-
40	SPM	1	3103	-	-	0/11/11/11	-
40	SPM	1	3106	-	-	7/11/11/11	-
40	SPM	1	3123	-	-	3/11/11/11	-
40	SPM	1	3116	-	-	3/11/11/11	-
40	SPM	1	3130	-	-	0/11/11/11	-
40	SPM	1	3110	-	-	4/11/11/11	-
40	SPM	1	3127	-	-	0/11/11/11	-
40	SPM	1	3101	-	-	4/11/11/11	-
40	SPM	1	3140	-	-	1/11/11/11	-
40	SPM	1	3119	-	-	2/11/11/11	-
40	SPM	1	3136	-	-	0/11/11/11	-
40	SPM	1	3115	-	-	1/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	1	3106	SPM	C12-C11-N10-C9
40	1	3113	SPM	C12-C11-N10-C9
40	1	3122	SPM	C12-C11-N10-C9
40	1	3138	SPM	C3-C4-N5-C6
40	1	3134	SPM	N5-C6-C7-C8
40	1	3122	SPM	N10-C11-C12-C13
40	1	3132	SPM	C7-C8-C9-N10
40	1	3106	SPM	C7-C8-C9-N10
40	1	3122	SPM	C7-C8-C9-N10
40	1	3141	SPM	N5-C6-C7-C8
40	1	3106	SPM	C2-C3-C4-N5
40	1	3106	SPM	N10-C11-C12-C13
40	1	3113	SPM	C2-C3-C4-N5

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Mol	Chain	Res	Type	Atoms
40	1	3101	SPM	C7-C8-C9-N10
40	1	3102	SPM	C3-C4-N5-C6
40	1	3110	SPM	C2-C3-C4-N5
40	1	3113	SPM	N10-C11-C12-C13
40	1	3141	SPM	C2-C3-C4-N5
40	1	3138	SPM	C7-C8-C9-N10
40	1	3106	SPM	C8-C9-N10-C11
40	1	3122	SPM	C8-C9-N10-C11
40	1	3132	SPM	C3-C4-N5-C6
40	1	3137	SPM	C7-C8-C9-N10
40	1	3113	SPM	C8-C9-N10-C11
40	1	3132	SPM	C7-C6-N5-C4
40	1	3138	SPM	C2-C3-C4-N5
40	1	3143	SPM	C2-C3-C4-N5
40	1	3142	SPM	N5-C6-C7-C8
40	1	3101	SPM	C12-C11-N10-C9
40	1	3119	SPM	C8-C9-N10-C11
40	1	3132	SPM	C11-C12-C13-N14
40	1	3138	SPM	C8-C9-N10-C11
40	1	3141	SPM	N1-C2-C3-C4
40	1	3132	SPM	C6-C7-C8-C9
40	1	3144	SPM	C6-C7-C8-C9
40	1	3132	SPM	C2-C3-C4-N5
40	1	3108	SPM	C7-C8-C9-N10
40	1	3117	SPM	C8-C9-N10-C11
40	1	3129	SPM	C8-C9-N10-C11
40	1	3114	SPM	C6-C7-C8-C9
40	1	3123	SPM	C6-C7-C8-C9
40	1	3111	SPM	N10-C11-C12-C13
40	1	3113	SPM	C6-C7-C8-C9
40	1	3101	SPM	C8-C9-N10-C11
40	1	3110	SPM	C3-C4-N5-C6
40	1	3113	SPM	C11-C12-C13-N14
40	1	3114	SPM	C11-C12-C13-N14
40	1	3138	SPM	C11-C12-C13-N14
40	1	3139	SPM	C8-C9-N10-C11
40	1	3141	SPM	C11-C12-C13-N14
40	1	3143	SPM	C3-C4-N5-C6
40	1	3111	SPM	C6-C7-C8-C9
40	1	3114	SPM	C2-C3-C4-N5
40	1	3132	SPM	N5-C6-C7-C8
40	1	3111	SPM	C3-C4-N5-C6

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Mol	Chain	Res	Type	Atoms
40	1	3113	SPM	C7-C6-N5-C4
40	1	3141	SPM	C7-C6-N5-C4
40	1	3128	SPM	C6-C7-C8-C9
40	1	3108	SPM	N5-C6-C7-C8
40	1	3133	SPM	C6-C7-C8-C9
40	1	3113	SPM	C3-C4-N5-C6
40	1	3105	SPM	C6-C7-C8-C9
40	1	3125	SPM	C6-C7-C8-C9
40	1	3116	SPM	N5-C6-C7-C8
40	1	3107	SPM	C6-C7-C8-C9
40	1	3138	SPM	C7-C6-N5-C4
40	1	3107	SPM	C2-C3-C4-N5
40	1	3112	SPM	C7-C8-C9-N10
40	1	3111	SPM	N1-C2-C3-C4
40	1	3122	SPM	N1-C2-C3-C4
40	1	3122	SPM	C11-C12-C13-N14
40	1	3132	SPM	N1-C2-C3-C4
40	1	3132	SPM	C8-C9-N10-C11
40	1	3138	SPM	N1-C2-C3-C4
40	1	3140	SPM	C3-C4-N5-C6
40	1	3143	SPM	C6-C7-C8-C9
40	1	3101	SPM	C7-C6-N5-C4
40	1	3104	SPM	C8-C9-N10-C11
40	1	3126	SPM	C7-C6-N5-C4
40	1	3113	SPM	C7-C8-C9-N10
40	1	3115	SPM	C12-C11-N10-C9
40	1	3123	SPM	C8-C9-N10-C11
40	1	3122	SPM	N5-C6-C7-C8
40	1	3110	SPM	N10-C11-C12-C13
40	1	3111	SPM	N5-C6-C7-C8
40	1	3121	SPM	C7-C6-N5-C4
40	1	3120	SPM	C7-C6-N5-C4
40	1	3129	SPM	C12-C11-N10-C9
40	1	3144	SPM	C7-C6-N5-C4
40	1	3133	SPM	N5-C6-C7-C8
40	1	3143	SPM	C7-C8-C9-N10
40	1	3111	SPM	C2-C3-C4-N5
40	1	3116	SPM	C12-C11-N10-C9
40	AL	201	SPM	C7-C6-N5-C4
40	1	3104	SPM	C2-C3-C4-N5
40	1	3111	SPM	C12-C11-N10-C9
40	1	3122	SPM	C3-C4-N5-C6

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Mol	Chain	Res	Type	Atoms
40	1	3141	SPM	C12-C11-N10-C9
40	1	3135	SPM	N10-C11-C12-C13
40	1	3108	SPM	C8-C9-N10-C11
40	1	3110	SPM	N5-C6-C7-C8
40	1	3139	SPM	C6-C7-C8-C9
40	1	3122	SPM	C6-C7-C8-C9
40	1	3138	SPM	C6-C7-C8-C9
40	1	3106	SPM	C7-C6-N5-C4
40	1	3111	SPM	C8-C9-N10-C11
40	1	3137	SPM	C12-C11-N10-C9
40	1	3141	SPM	C3-C4-N5-C6
40	1	3116	SPM	C6-C7-C8-C9
40	1	3108	SPM	C7-C6-N5-C4
40	1	3123	SPM	C3-C4-N5-C6
40	AL	201	SPM	C6-C7-C8-C9
40	1	3131	SPM	C6-C7-C8-C9
40	1	3109	SPM	C12-C11-N10-C9
40	1	3107	SPM	C7-C8-C9-N10
40	1	3106	SPM	C3-C4-N5-C6
40	1	3119	SPM	C7-C6-N5-C4
40	AL	201	SPM	C12-C11-N10-C9

There are no ring outliers.

35 monomers are involved in 108 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	1	3121	SPM	3	0
40	1	3112	SPM	5	0
40	1	3138	SPM	5	0
40	AM	201	SPM	5	0
40	1	3139	SPM	1	0
40	1	3120	SPM	1	0
40	1	3131	SPM	2	0
40	1	3142	SPM	3	0
40	1	3141	SPM	3	0
40	1	3135	SPM	3	0
40	1	3109	SPM	1	0
40	1	3114	SPM	2	0
40	1	3129	SPM	3	0
40	1	3134	SPM	3	0
40	1	3125	SPM	4	0
40	1	3113	SPM	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	1	3102	SPM	1	0
40	1	3126	SPM	2	0
40	1	3137	SPM	5	0
40	1	3132	SPM	1	0
40	1	3117	SPM	5	0
40	1	3108	SPM	3	0
40	1	3128	SPM	3	0
40	1	3133	SPM	2	0
40	1	3143	SPM	5	0
40	1	3106	SPM	5	0
40	1	3123	SPM	2	0
40	1	3116	SPM	2	0
40	1	3130	SPM	2	0
40	1	3110	SPM	4	0
40	1	3127	SPM	1	0
40	1	3140	SPM	8	0
40	1	3119	SPM	2	0
40	1	3136	SPM	3	0
40	1	3115	SPM	4	0

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.

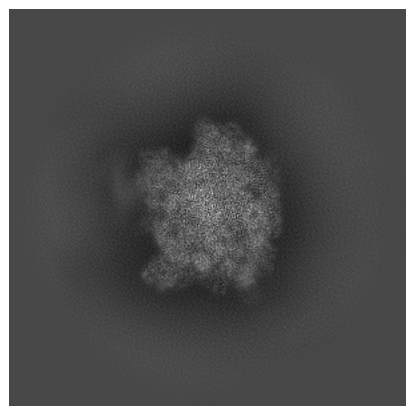
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47578. These allow visual inspection of the internal detail of the map and identification of artifacts.

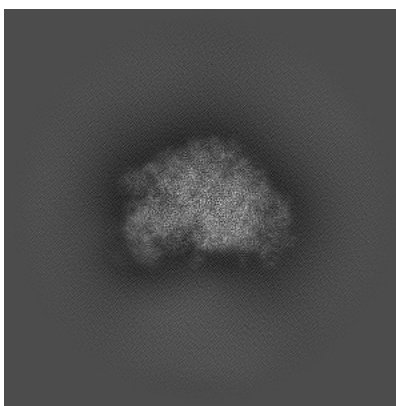
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

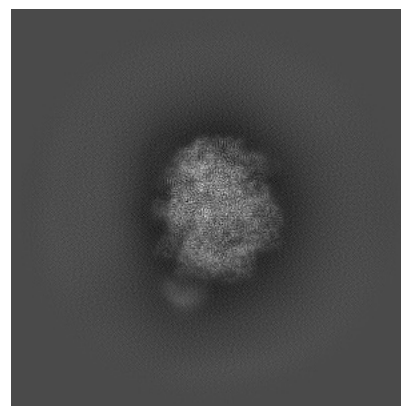
6.1.1 Primary map



X

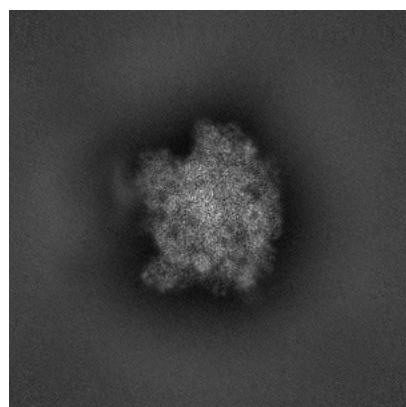


Y

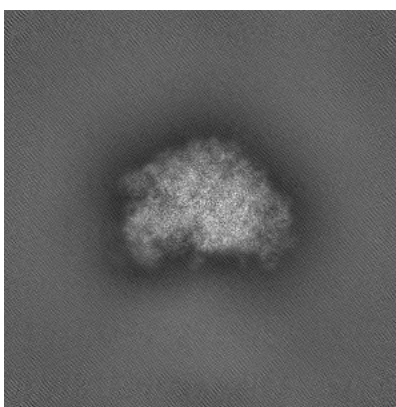


Z

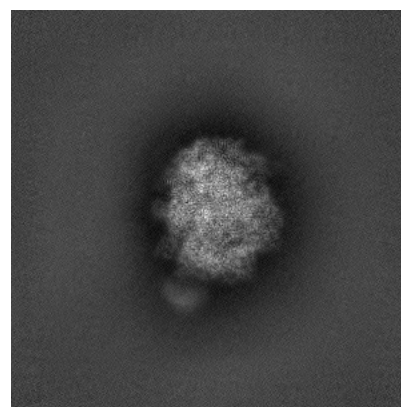
6.1.2 Raw map



X



Y

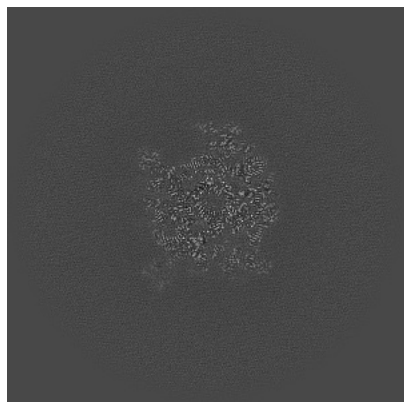


Z

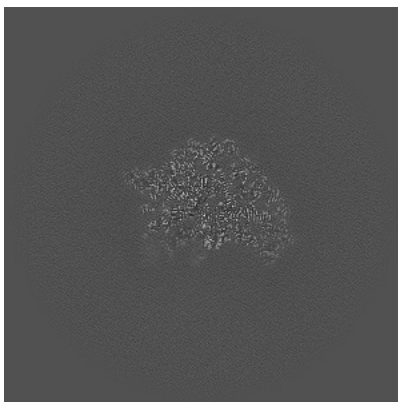
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

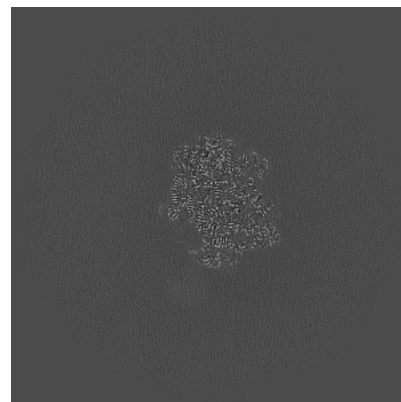
6.2.1 Primary map



X Index: 304

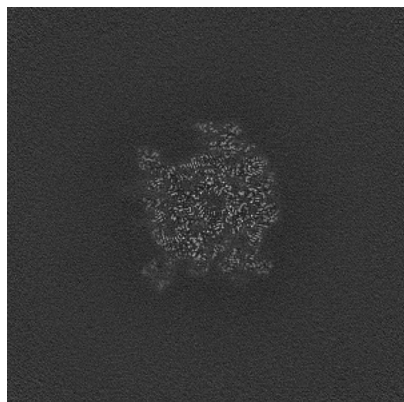


Y Index: 304

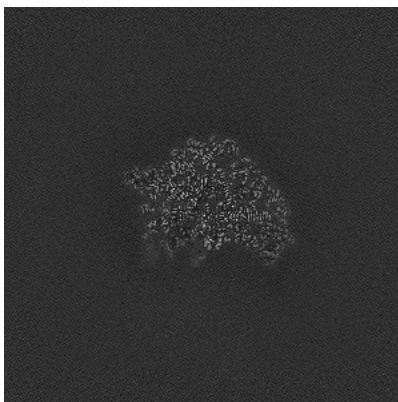


Z Index: 304

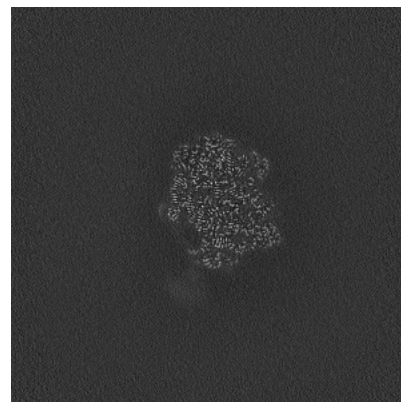
6.2.2 Raw map



X Index: 304



Y Index: 304

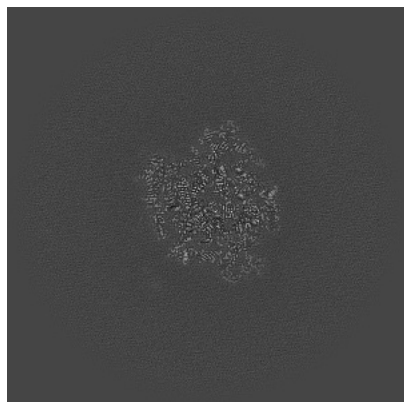


Z Index: 304

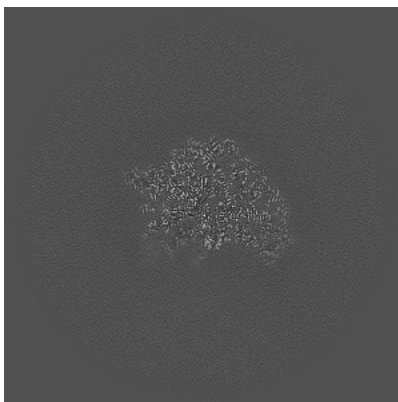
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

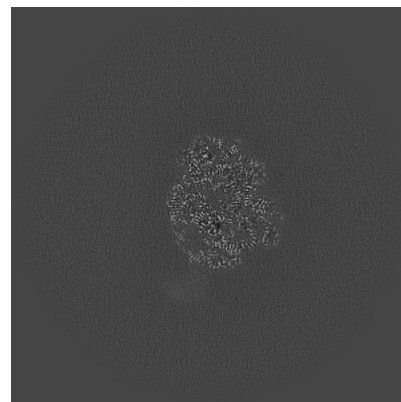
6.3.1 Primary map



X Index: 316

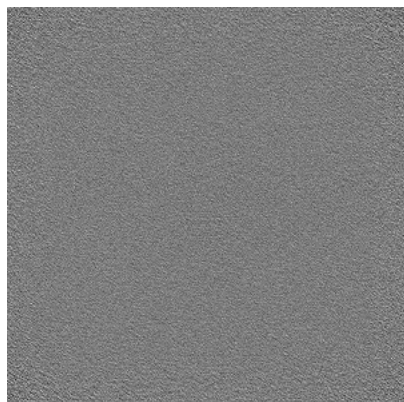


Y Index: 304

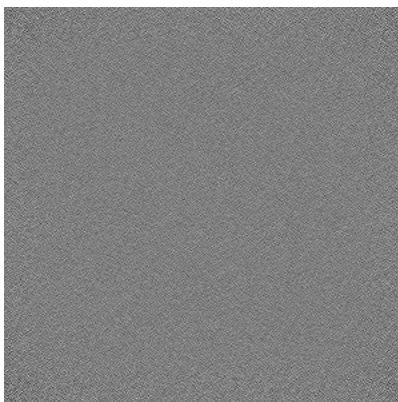


Z Index: 311

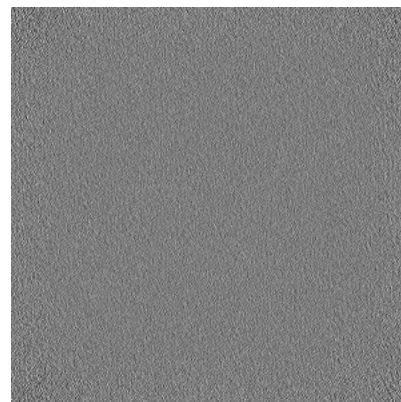
6.3.2 Raw map



X Index: 0



Y Index: 0

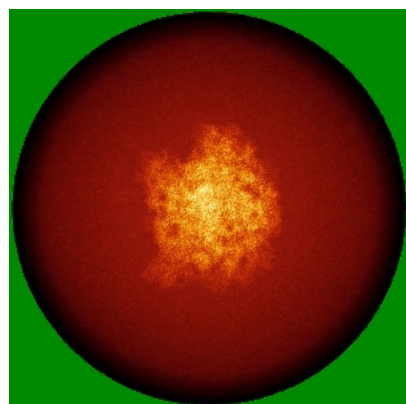


Z Index: 0

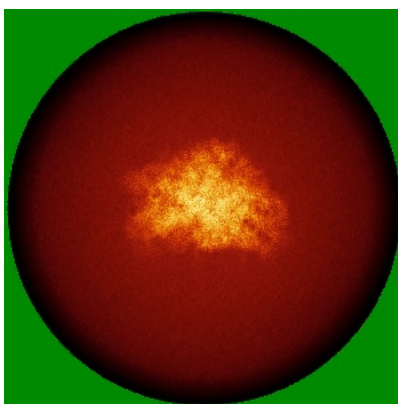
The images above show the largest variance slices of the map in three orthogonal directions.

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

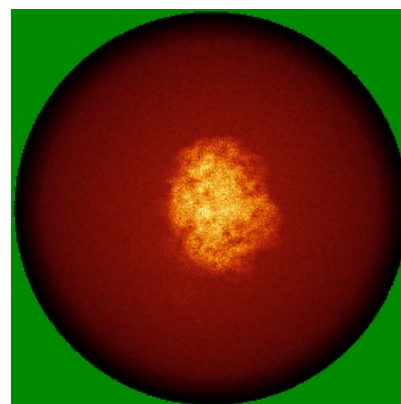
6.4.1 Primary map



X

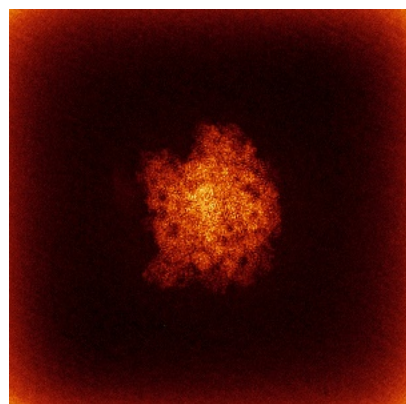


Y

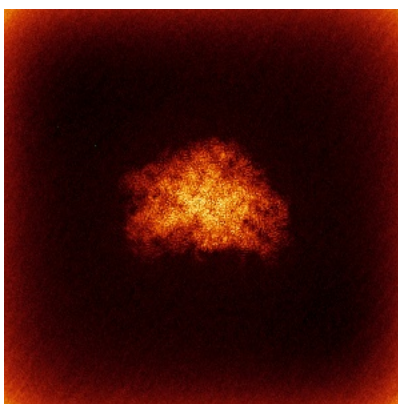


Z

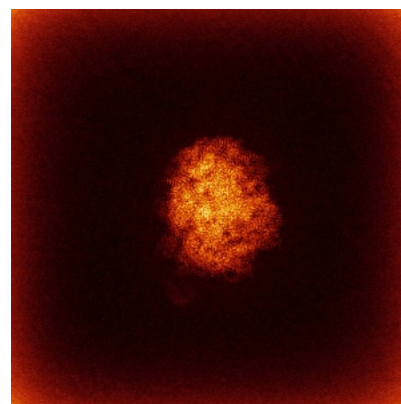
6.4.2 Raw map



X



Y

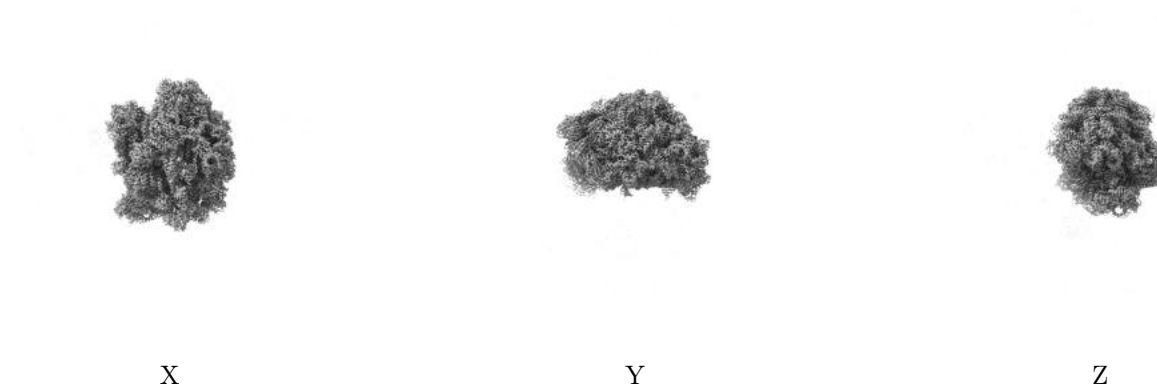


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.152. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

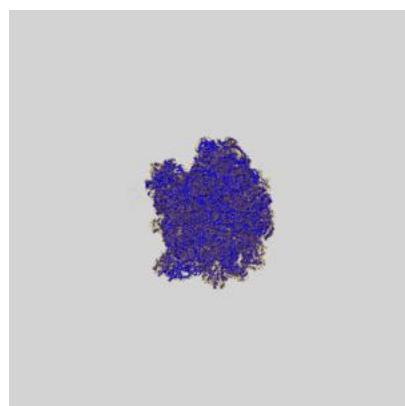
6.6 Mask visualisation [i](#)

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

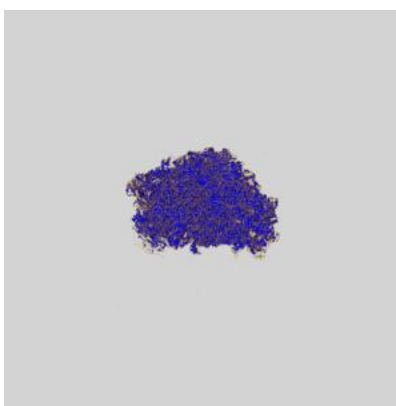
A mask typically either:

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

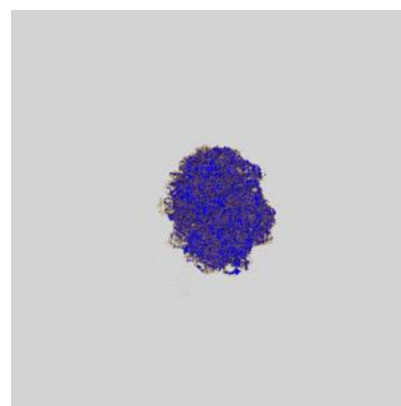
6.6.1 emd_47578_msk_1.map [i](#)



X



Y

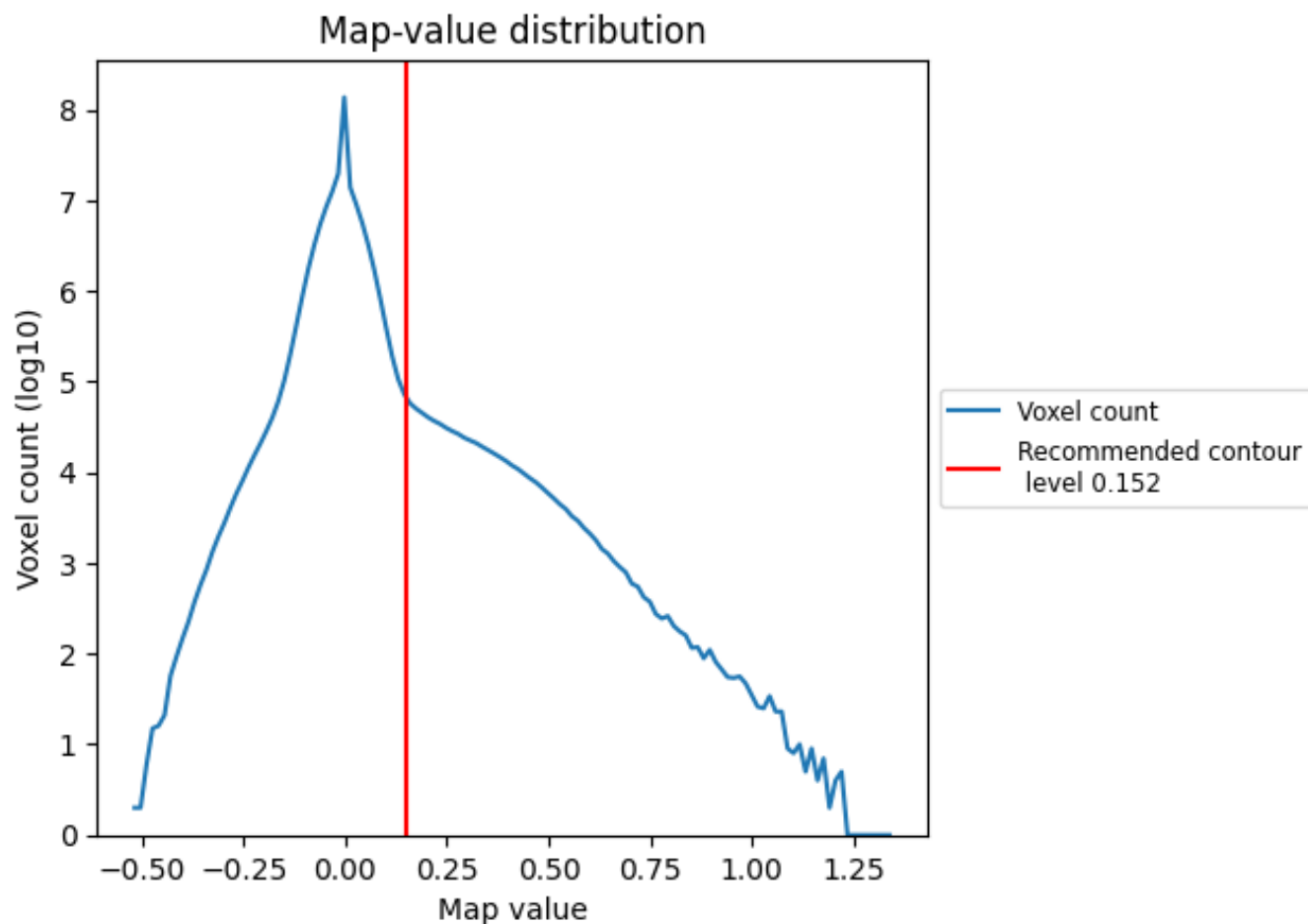


Z

7 Map analysis [i](#)

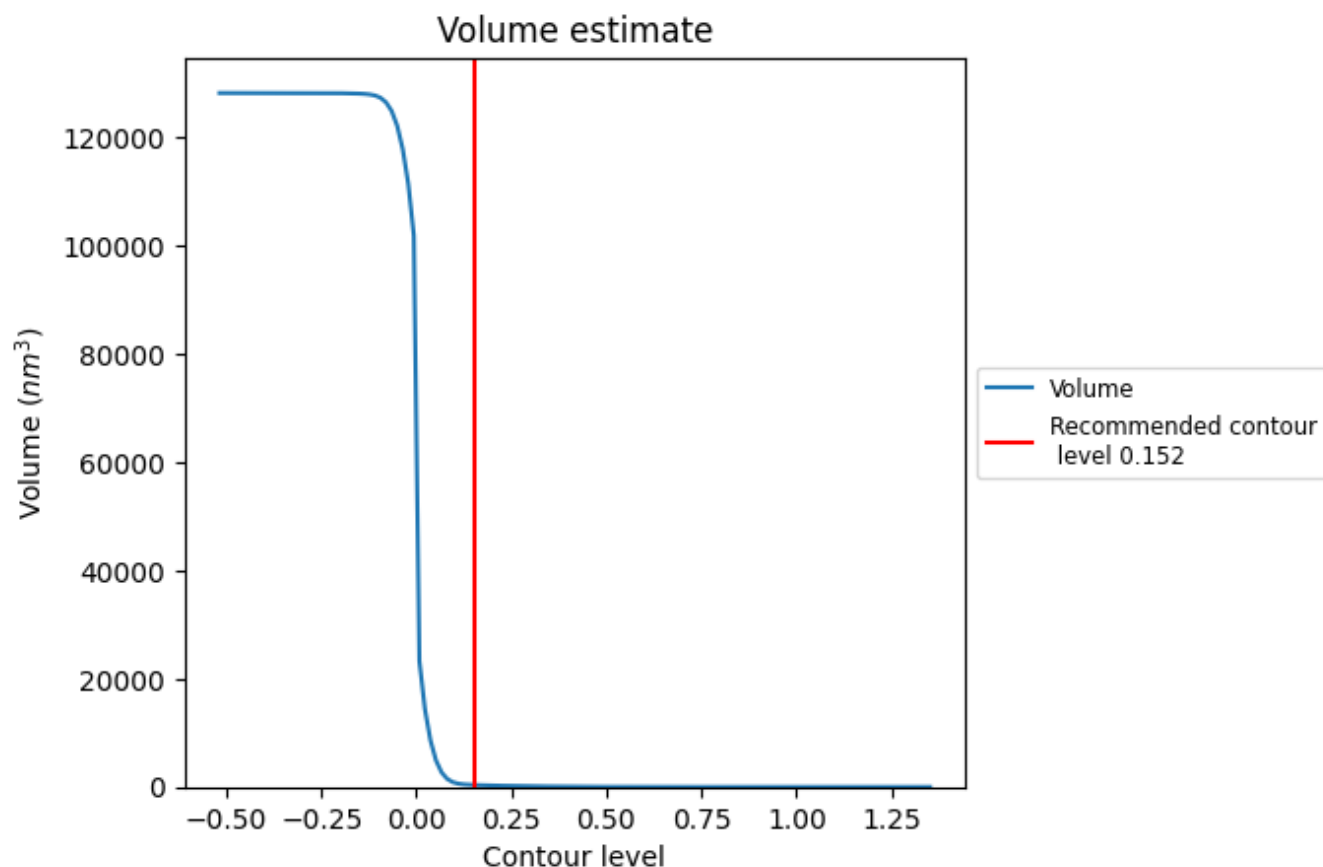
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

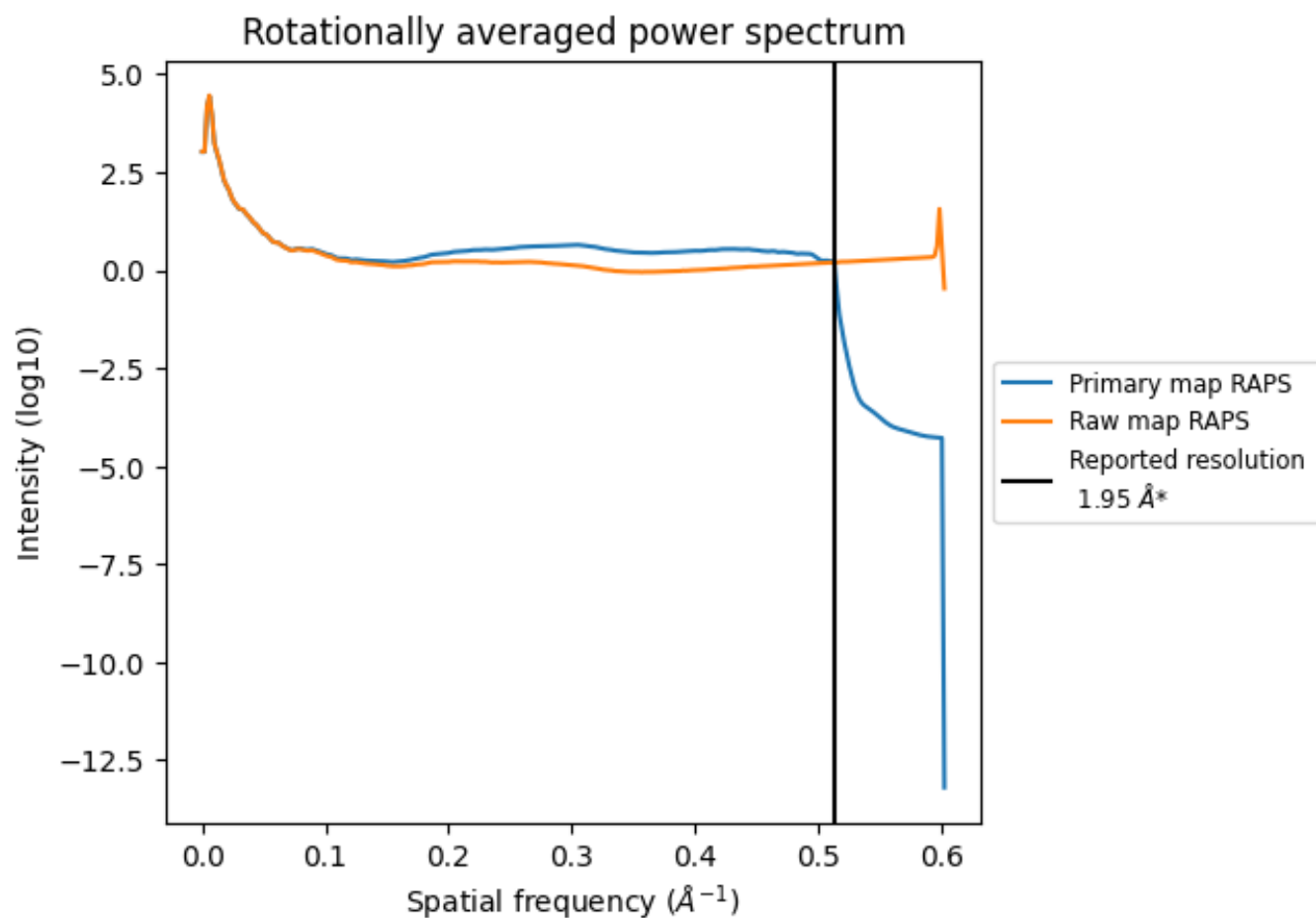
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 360 nm^3 ; this corresponds to an approximate mass of 325 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 ⓘ

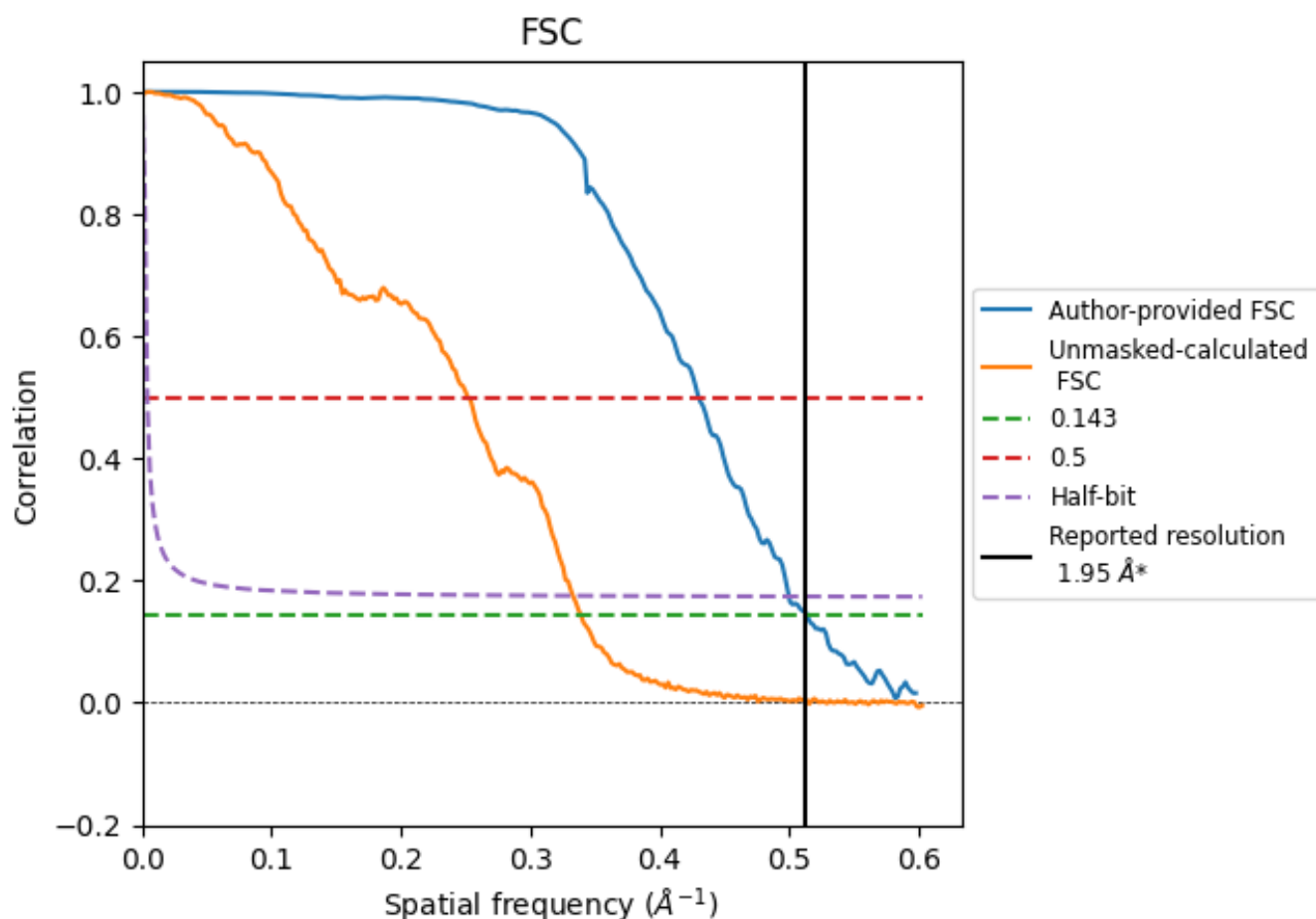


*Reported resolution corresponds to spatial frequency of 0.513 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.513 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

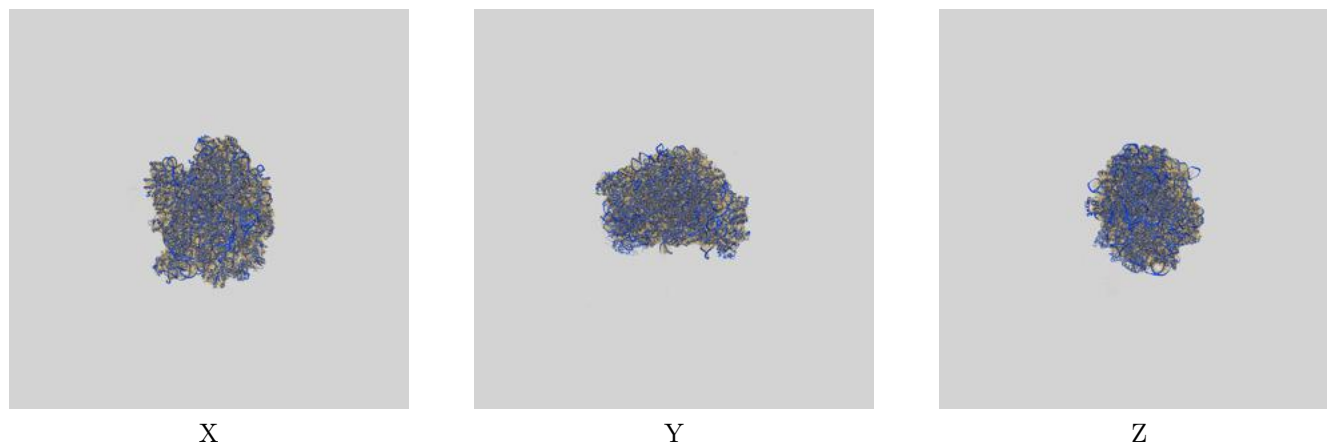
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.95	-	-
Author-provided FSC curve	1.95	2.32	2.00
Unmasked-calculated*	2.95	3.97	3.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.95 differs from the reported value 1.95 by more than 10 %

9 Map-model fit [i](#)

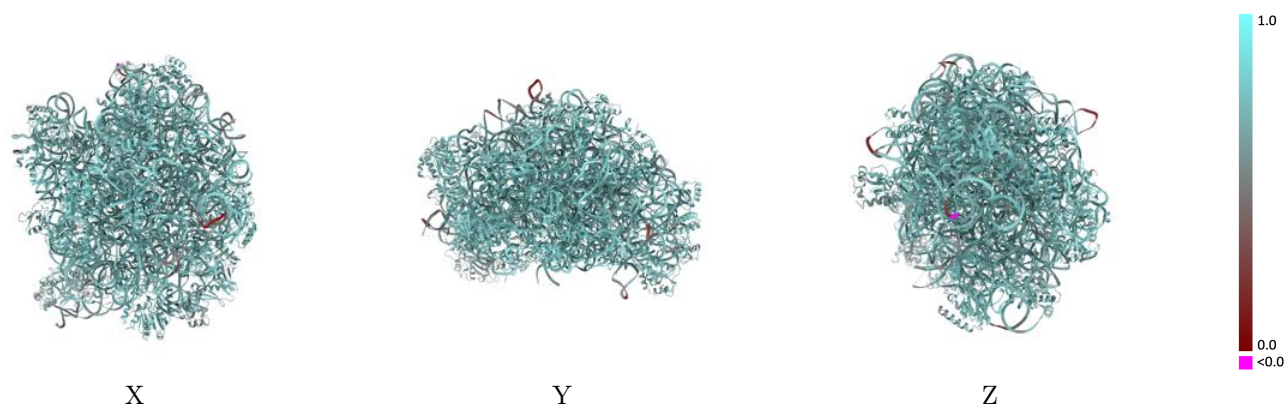
This section contains information regarding the fit between EMDB map EMD-47578 and PDB model 9E6Q. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



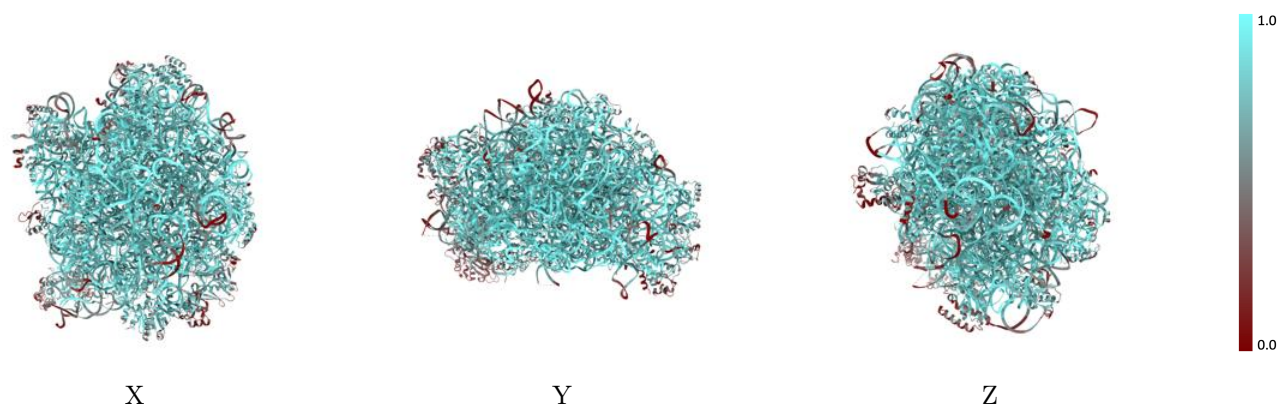
The images above show the 3D surface view of the map at the recommended contour level 0.152 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



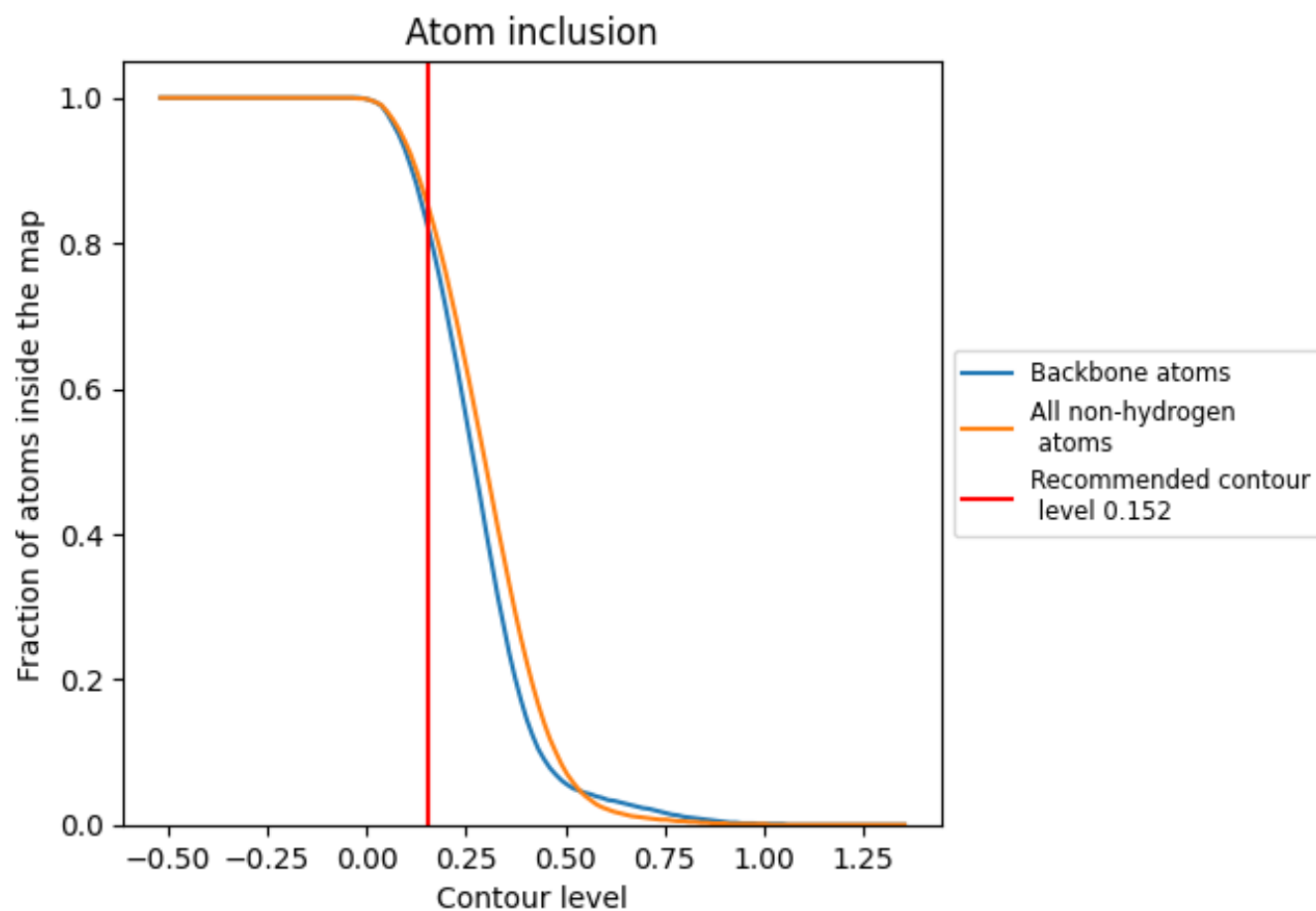
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.152).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 86% 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 (0.152) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8560	 0.7260
1	 0.9130	 0.7290
2	 0.7540	 0.6710
3	 0.7710	 0.7220
AA	 0.9030	 0.7590
AB	 0.8970	 0.7600
AC	 0.8650	 0.7470
AD	 0.2720	 0.5760
AE	 0.6660	 0.6980
AF	 0.6050	 0.6730
AG	 0.8300	 0.7460
AH	 0.8600	 0.7470
AI	 0.8620	 0.7510
AJ	 0.5470	 0.6460
AK	 0.6000	 0.6720
AL	 0.7260	 0.7070
AM	 0.8720	 0.7510
AN	 0.8770	 0.7540
AO	 0.5930	 0.6730
AP	 0.8620	 0.7470
AQ	 0.8160	 0.7380
AR	 0.6980	 0.7080
AS	 0.9020	 0.7540
AT	 0.8960	 0.7620
AU	 0.8540	 0.7510
AV	 0.8030	 0.7280
AW	 0.8430	 0.7430
AX	 0.7160	 0.7100
AY	 0.8510	 0.7400
AZ	 0.5860	 0.6720
Aa	 0.8210	 0.7410
Ab	 0.8490	 0.7490
Ac	 0.9060	 0.7420
Ad	 0.9830	 0.7900
Ae	 0.7940	 0.7310



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Chain	Atom inclusion	Q-score
Af	 0.9240	 0.7650
Ag	 0.6930	 0.6920
Ah	 0.8760	 0.7430
Ai	 0.7120	 0.7150
Aj	 0.7260	 0.7120
Ak	 0.7250	 0.7020