



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 04:58 AM UTC

PDB ID : 7PWF / pdb_00007pwf
EMDB ID : EMD-13680
Title : Cryo-EM structure of small subunit of Giardia lamblia ribosome at 2.9 Å resolution
Authors : Hiregange, D.G.; Rivalta, A.; Bose, T.; Breiner-Goldstein, E.; Samiya, S.; Cimicata, G.; Kulakova, L.; Zimmerman, E.; Bashan, A.; Herzberg, O.; Yonath, A.
Deposited on : 2021-10-06
Resolution : 2.85 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:

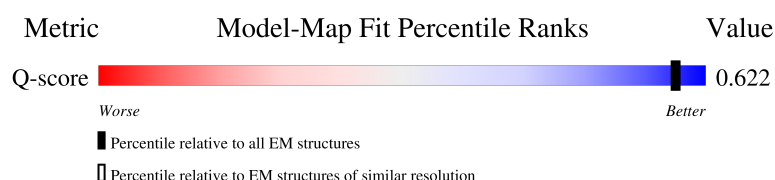
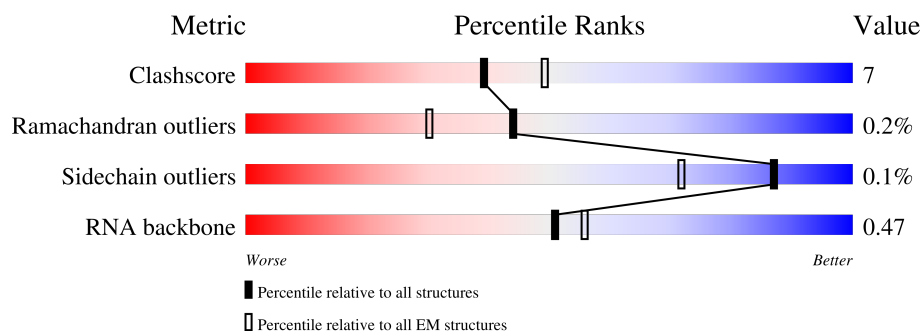
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

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

The reported resolution of this entry is 2.85 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	11965 (2.35 - 3.35)

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

Mol	Chain	Length	Quality of chain
1	d	137	
2	T	139	
3	N	154	

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Mol	Chain	Length	Quality of chain
4	J	189	
5	D	217	
6	X	143	
7	S	154	
8	Q	158	
9	C	242	
10	A	245	
11	B	248	
12	Y	132	
13	b	124	
14	a	109	
15	Z	88	
16	V	89	
17	P	145	
18	R	137	
19	K	134	
20	I	174	
21	e	69	
22	H	190	
23	n	41	
24	c	64	
25	O	145	
26	W	130	
27	E	268	
28	2	1452	

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Mol	Chain	Length	Quality of chain
29	L	199	16% 84% 7% 9%
30	U	126	29% 46% 13% 41%
31	G	248	37% 58% 21% • 21%
32	F	190	35% 64% 21% 15%

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 60466 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal protein S29A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	d	48	Total	C	N	O	S	0	0
			398	253	75	65	5		

- Molecule 2 is a protein called Ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	130	Total	C	N	O	S	0	0
			934	592	176	164	2		

- Molecule 3 is a protein called Ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	152	Total	C	N	O	S	0	0
			1198	762	230	201	5		

- Molecule 4 is a protein called Ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	166	Total	C	N	O	S	0	0
			1322	827	257	232	6		

- Molecule 5 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	182	Total	C	N	O	S	0	0
			1402	890	254	244	14		

- Molecule 6 is a protein called Ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	142	Total	C	N	O	S	0	0
			1104	697	219	184	4		

- Molecule 7 is a protein called Ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	133	Total	C	N	O	S	0	0
			1055	651	210	188	6		

- Molecule 8 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	125	Total	C	N	O	S	0	0
			960	603	190	164	3		

- Molecule 9 is a protein called Ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	212	Total	C	N	O	S	0	0
			1641	1043	298	296	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	194	Total	C	N	O	S	0	0
			1546	998	269	271	8		

- Molecule 11 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	218	Total	C	N	O	S	0	0
			1758	1113	323	309	13		

- Molecule 12 is a protein called Ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	90	Total	C	N	O	S	0	0
			708	451	125	126	6		

- Molecule 13 is a protein called Ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	b	79	Total	C	N	O	S	0	0
			614	389	105	114	6		

- Molecule 14 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	a	97	Total	C	N	O	S	0	0
			785	484	162	131	8		

- Molecule 15 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Z	59	Total	C	N	O	S	0	0
			419	266	73	75	5		

- Molecule 16 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	82	Total	C	N	O	S	0	0
			605	377	112	110	6		

- Molecule 17 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	105	Total	C	N	O	S	0	0
			836	531	166	133	6		

- Molecule 18 is a protein called Ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	101	Total	C	N	O	S	0	0
			780	485	145	147	3		

- Molecule 19 is a protein called Ribosomal protein S10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	83	Total	C	N	O	S	0	0
			689	446	116	123	4		

- Molecule 20 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	I	163	Total	C	N	O	S	0	0
			1282	804	246	229	3		

- Molecule 21 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	e	37	Total	C	N	O	S	0	0
			291	185	59	46	1		

- Molecule 22 is a protein called Ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	162	Total	C	N	O	S	0	0
			1194	772	210	207	5		

- Molecule 23 is a protein called Ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	n	24	Total	C	N	O	S	0	0
			217	134	55	25	3		

- Molecule 24 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	c	55	Total	C	N	O	S	0	0
			439	269	89	80	1		

- Molecule 25 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	126	Total	C	N	O	S	0	0
			935	572	189	170	4		

- Molecule 26 is a protein called Ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	129	Total	C	N	O	S	0	0
			1031	659	192	177	3		

- Molecule 27 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	E	258	Total	C	N	O	S	0	0
			2058	1317	377	352	12		

- Molecule 28 is a RNA chain called rRNA 18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	1355	Total	C	N	O	P	0	0
			29096	12946	5388	9407	1355		

- Molecule 29 is a protein called SSU ribosomal protein S17P.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	L	181	Total	C	N	O	S	0	0
			1481	933	293	248	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	12	SER	GLY	variant	UNP V6TVJ7

- Molecule 30 is a protein called Ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	74	Total	C	N	O	S	0	0
			609	394	111	102	2		

- Molecule 31 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	G	197	Total	C	N	O	S	0	0
			1530	961	296	263	10		

- Molecule 32 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	F	161	Total	C	N	O	S	0	0
			1246	771	240	227	8		

- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
33	d	1	Total	K	0
			1	1	
33	N	7	Total	K	0
			7	7	
33	S	2	Total	K	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
33	A	1	Total 1	K 1	0
33	b	1	Total 1	K 1	0
33	R	1	Total 1	K 1	0
33	O	6	Total 6	K 6	0
33	W	1	Total 1	K 1	0
33	E	3	Total 3	K 3	0
33	2	239	Total 239	K 239	0
33	L	3	Total 3	K 3	0
33	G	1	Total 1	K 1	0

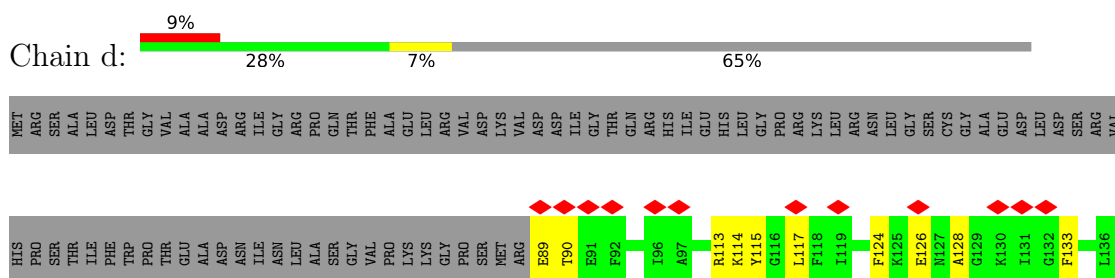
- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
34	N	1	Total 1	Mg 1	0
34	I	1	Total 1	Mg 1	0
34	2	35	Total 35	Mg 35	0

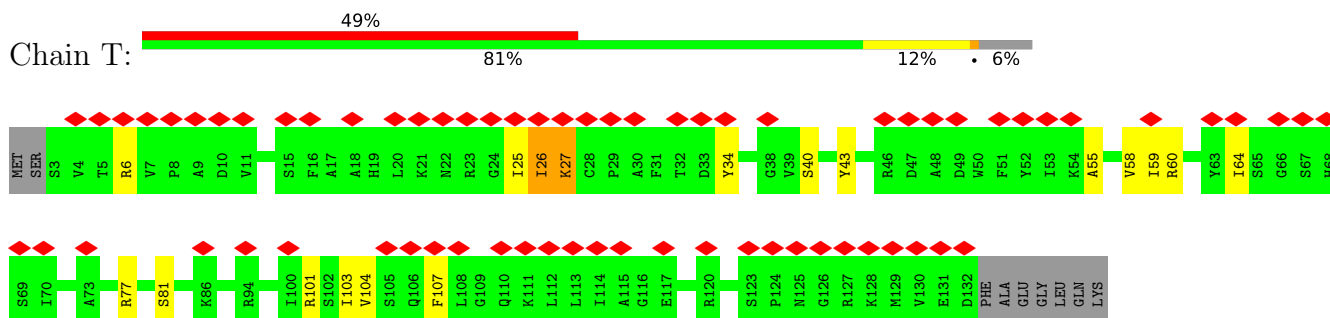
3 Residue-property plots

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.

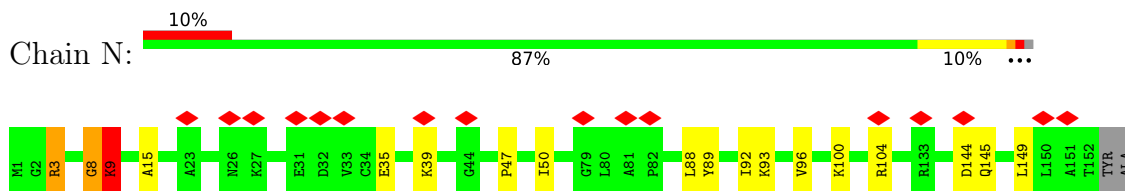
- Molecule 1: Ribosomal protein S29A



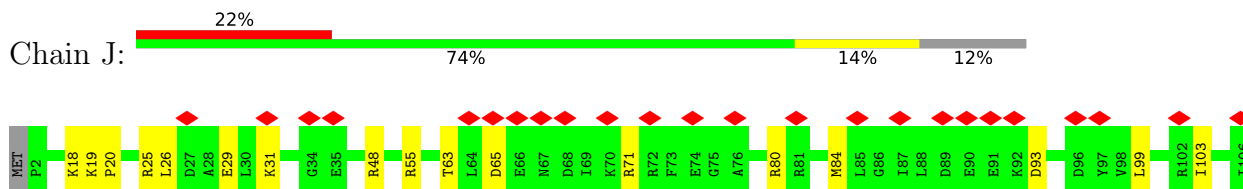
- Molecule 2: Ribosomal protein S19e

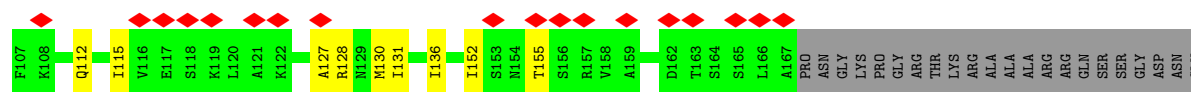


- Molecule 3: Ribosomal protein S13

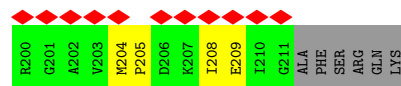
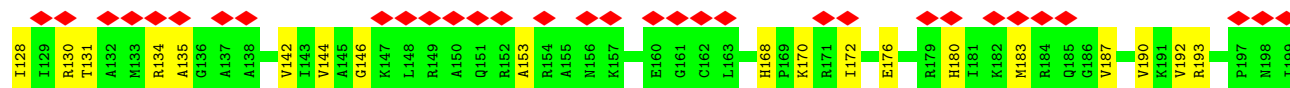
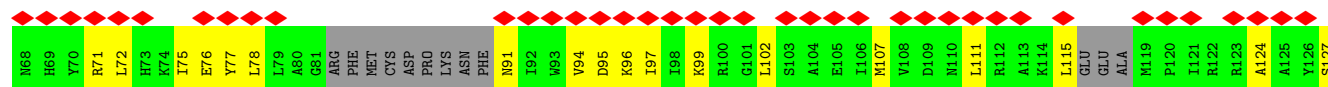
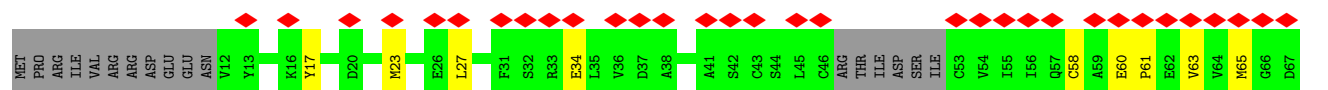


- Molecule 4: Ribosomal protein S9

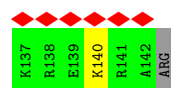
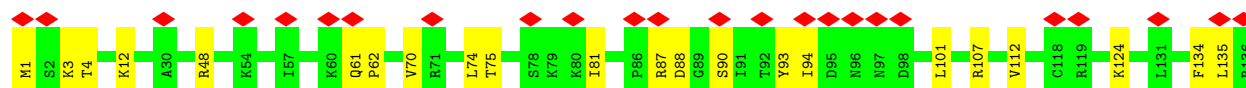
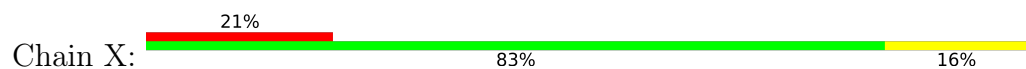




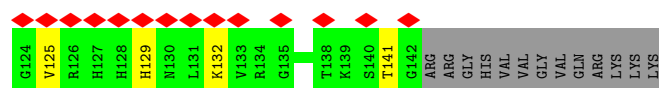
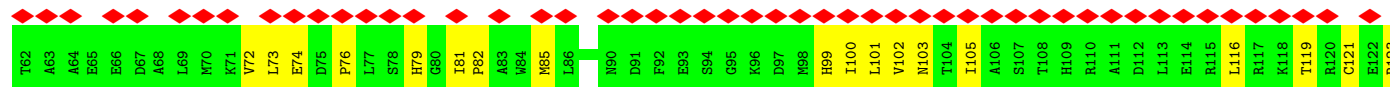
• Molecule 5: Ribosomal protein S3



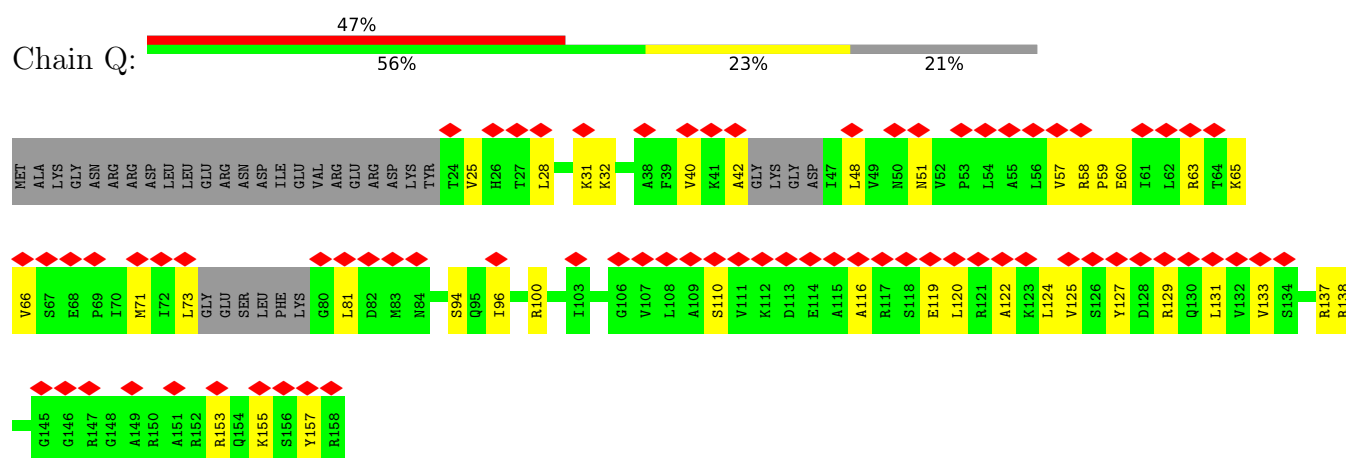
• Molecule 6: Ribosomal protein S23



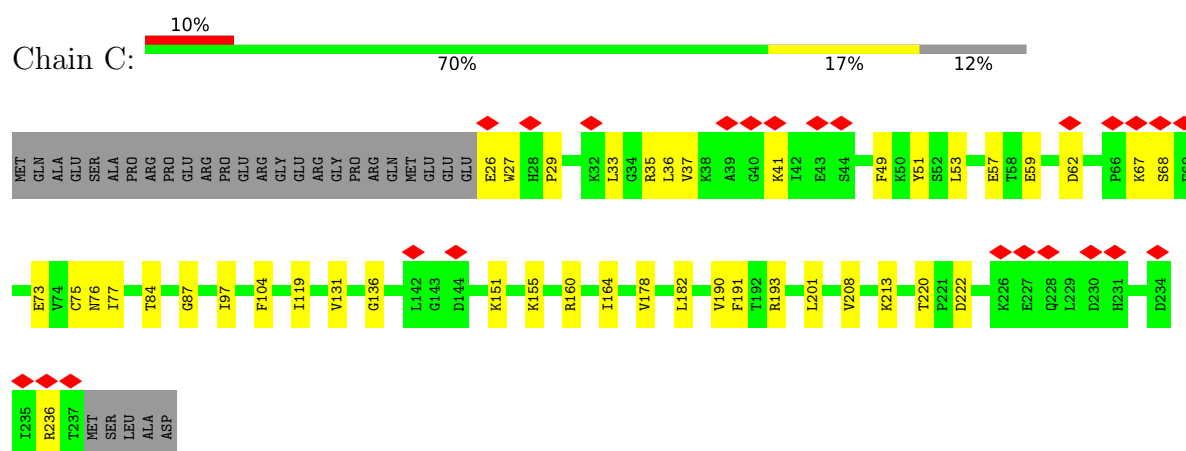
• Molecule 7: Ribosomal protein S18



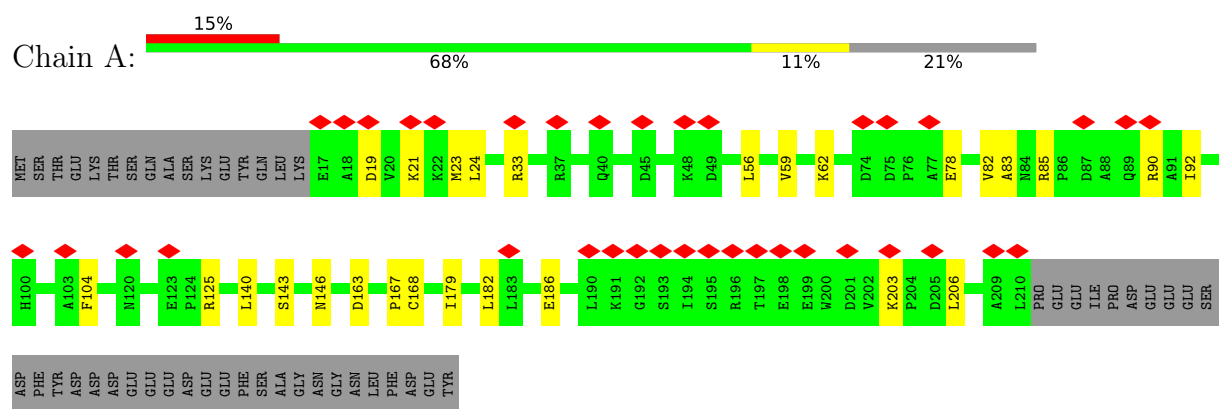
• Molecule 8: Ribosomal protein S16



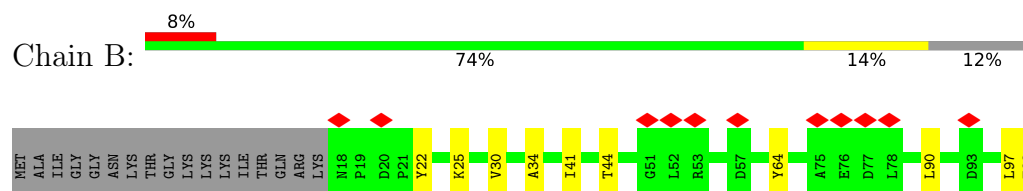
• Molecule 9: Ribosomal protein S2

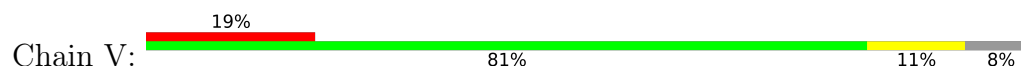


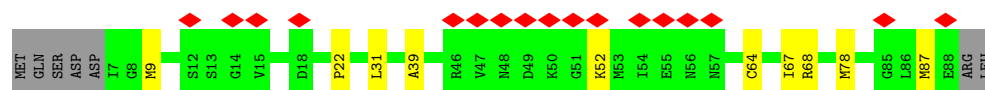
• Molecule 10: 40S ribosomal protein SA



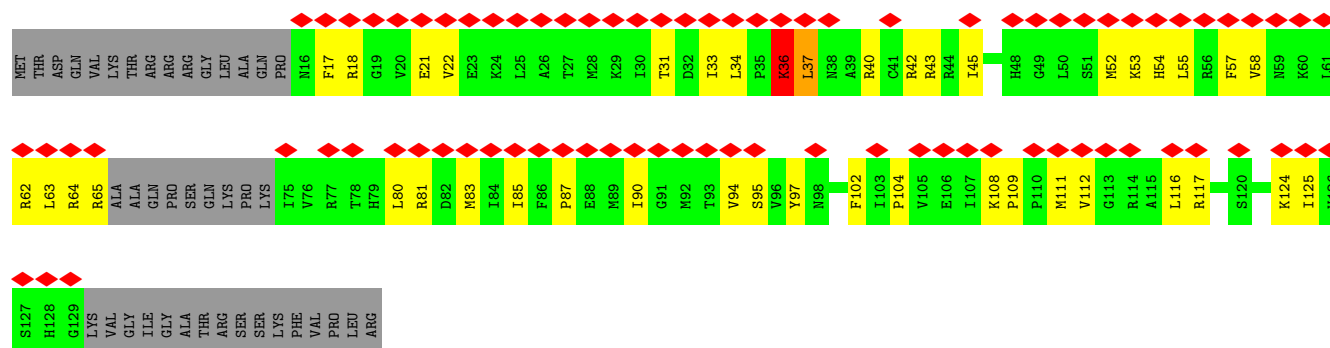
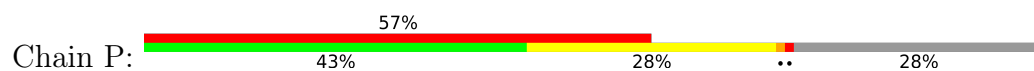
• Molecule 11: 40S ribosomal protein S3a



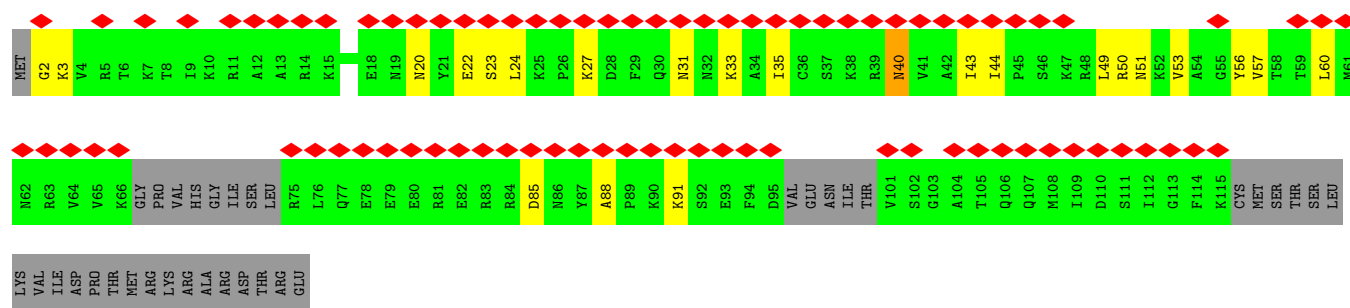




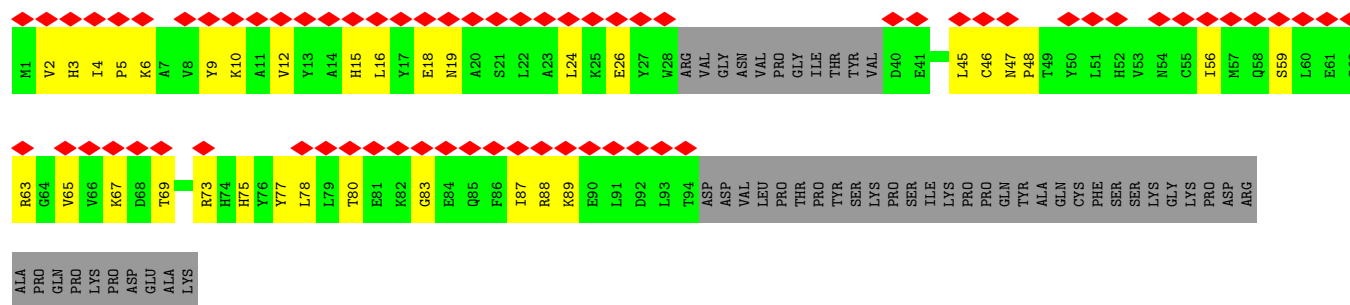
• Molecule 17: Ribosomal protein S15



• Molecule 18: Ribosomal protein S17



• Molecule 19: Ribosomal protein S10B

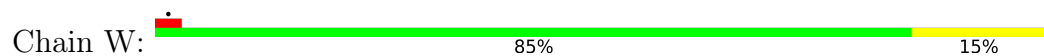


• Molecule 20: 40S ribosomal protein S8

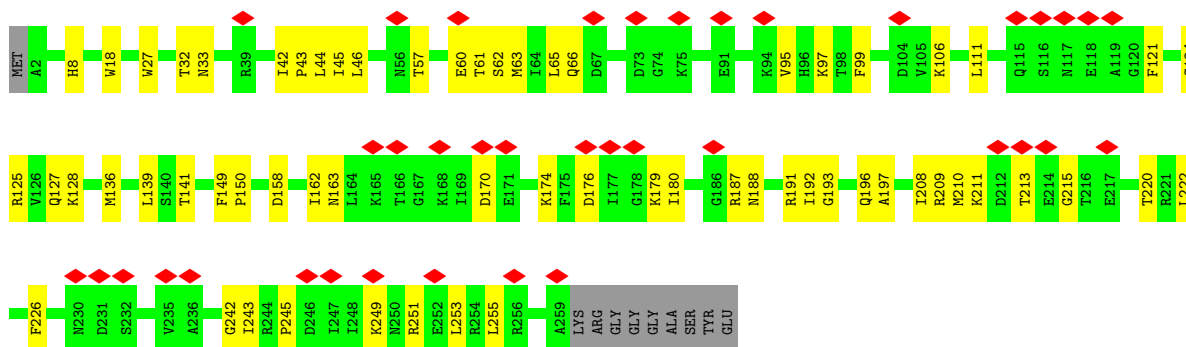




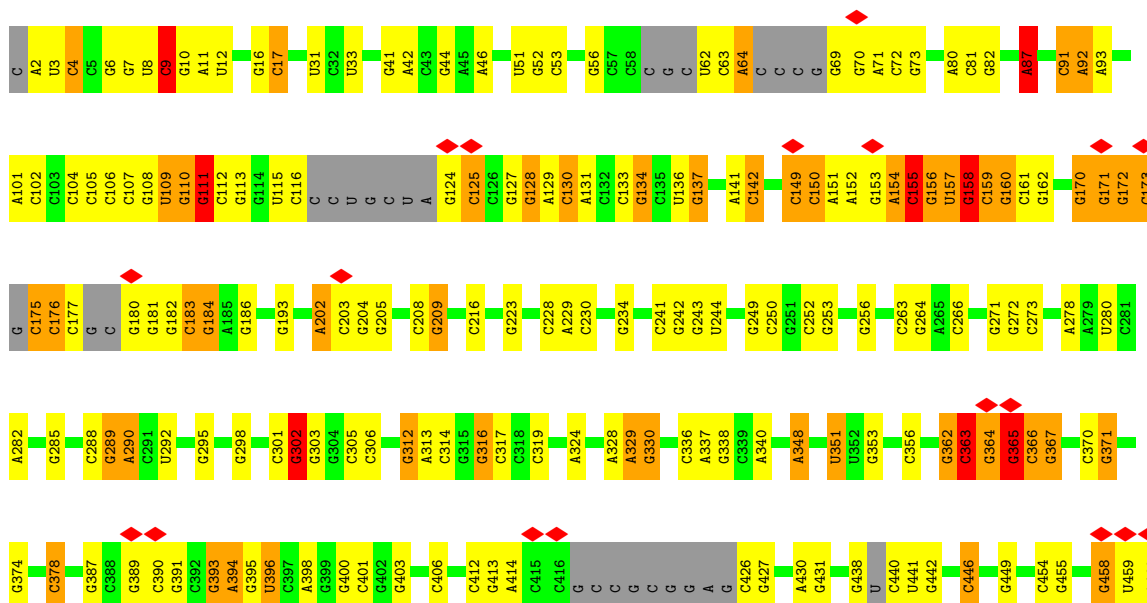
• Molecule 26: Ribosomal protein S15A

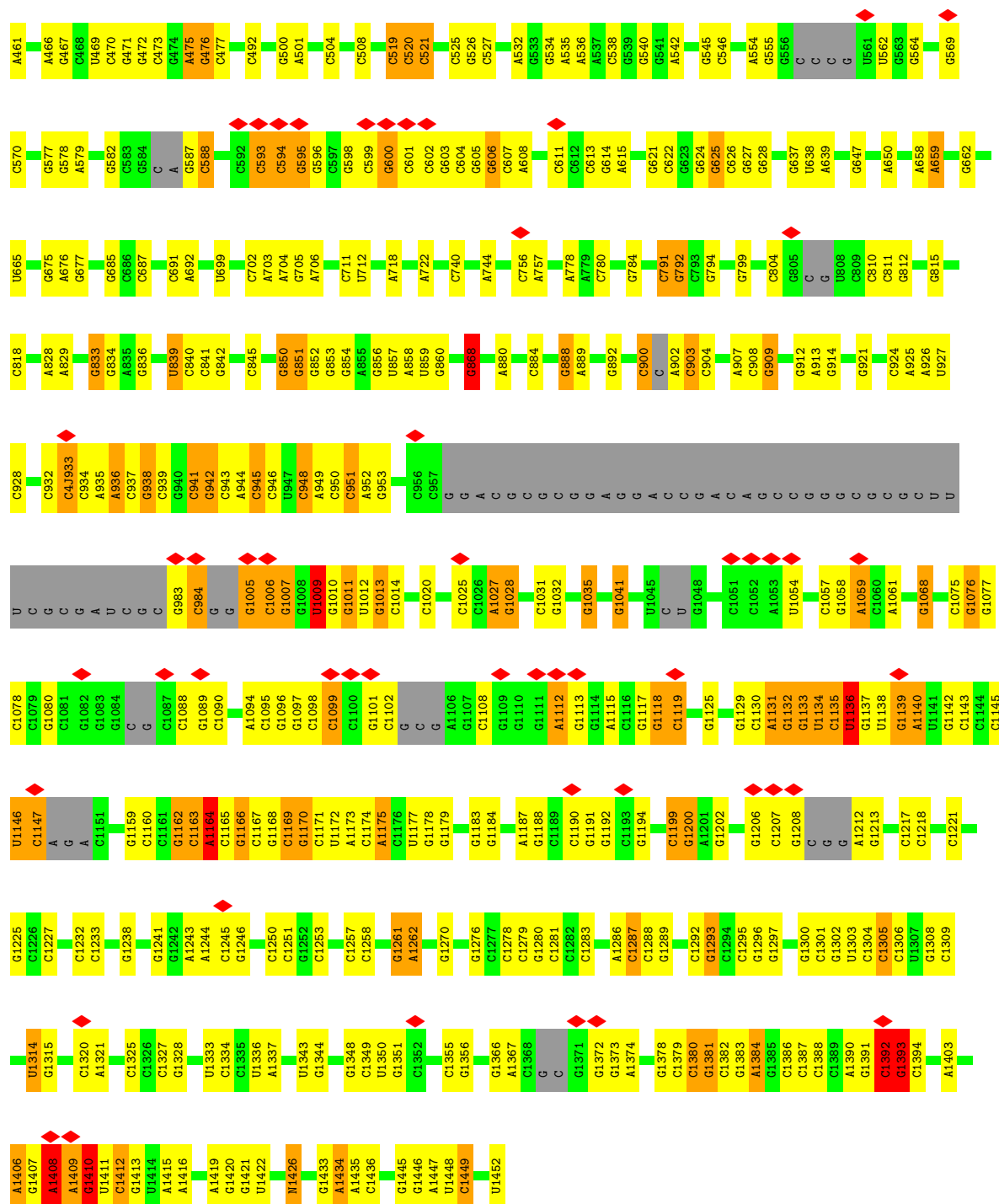


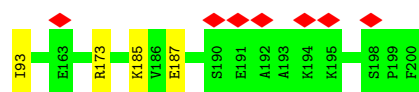
• Molecule 27: 40S ribosomal protein S4



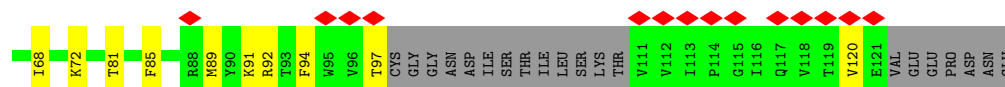
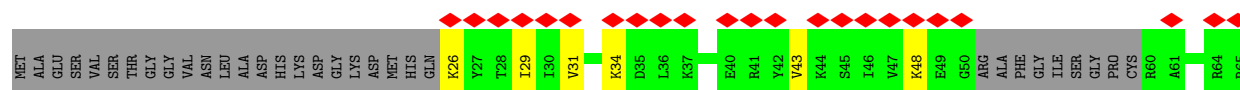
• Molecule 28: rRNA 18S



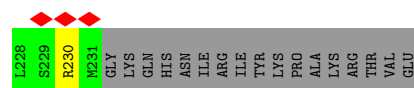
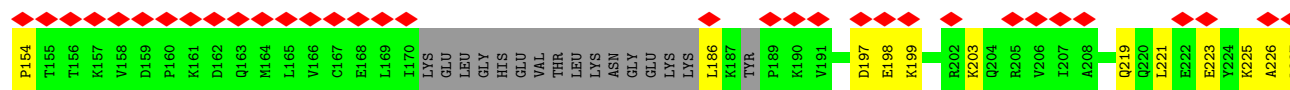
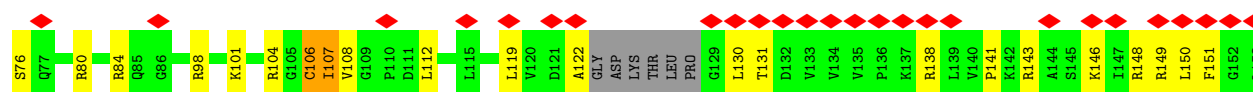




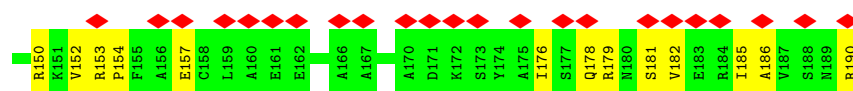
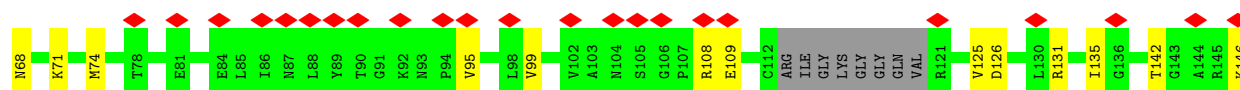
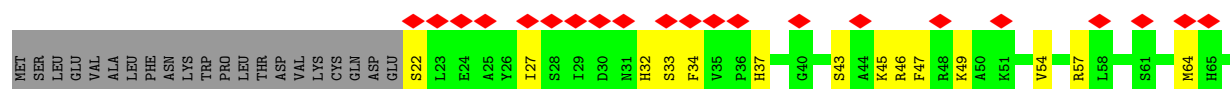
• Molecule 30: Ribosomal protein S20



• Molecule 31: 40S ribosomal protein S6



• Molecule 32: Ribosomal protein S5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91058	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.186	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.027	Depositor
Map size ($\text{\AA}$)	374.0, 374.0, 374.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.85, 0.85, 0.85	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: M7A, C4J, OMG, OMU, K, OMC, A2M, MA6, 4AC, MG, 7MG, 4OC

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	d	0.21	0/406	0.51	0/539
2	T	0.20	0/955	0.58	0/1297
3	N	0.30	0/1221	0.50	0/1641
4	J	0.21	0/1340	0.46	0/1796
5	D	0.21	0/1422	0.51	0/1909
6	X	0.22	0/1119	0.51	0/1498
7	S	0.20	0/1070	0.52	0/1435
8	Q	0.20	0/968	0.51	1/1295 (0.1%)
9	C	0.23	0/1674	0.46	0/2259
10	A	0.24	0/1580	0.47	0/2149
11	B	0.22	0/1793	0.45	0/2419
12	Y	0.19	0/719	0.48	0/964
13	b	0.27	0/628	0.54	0/852
14	a	0.24	0/797	0.45	0/1072
15	Z	0.21	0/422	0.58	0/565
16	V	0.22	0/613	0.47	0/823
17	P	0.22	0/850	0.63	0/1138
18	R	0.22	0/786	0.50	0/1052
19	K	0.23	0/707	0.56	0/957
20	I	0.25	0/1302	0.48	0/1746
21	e	0.20	0/294	0.45	0/392
22	H	0.22	0/1210	0.44	0/1638
23	n	0.26	0/219	0.50	0/280
24	c	0.22	0/439	0.53	0/585
25	O	0.23	0/947	0.49	0/1273
26	W	0.25	0/1048	0.47	0/1412
27	E	0.22	0/2104	0.47	0/2841
28	2	0.35	0/32117	0.57	99/50066 (0.2%)
29	L	0.23	0/1514	0.47	0/2030
30	U	0.21	0/619	0.46	0/833
31	G	0.23	0/1545	0.54	0/2061
32	F	0.21	0/1264	0.43	0/1697

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.29	0/63692	0.54	100/92514 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
17	P	0	1
18	R	0	1
31	G	0	3
All	All	0	5

There are no bond length outliers.

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	175	C	P-O3'-C3'	-12.40	101.60	120.20
28	2	1132	G	P-O3'-C3'	-9.56	105.85	120.20
28	2	363	C	P-O3'-C3'	-8.59	107.32	120.20
28	2	1410	G	P-O3'-C3'	-8.52	107.42	120.20
28	2	366	C	P-O3'-C3'	-8.47	107.49	120.20
28	2	182	G	P-O3'-C3'	-8.32	107.73	120.20
28	2	1392	C	P-O3'-C3'	-7.99	108.22	120.20
28	2	152	A	P-O3'-C3'	-7.96	108.26	120.20
28	2	1168	G	P-O3'-C3'	-7.91	108.34	120.20
28	2	181	G	P-O3'-C3'	-7.88	108.38	120.20
28	2	156	G	P-O3'-C3'	-7.79	108.52	120.20
28	2	1388	C	P-O3'-C3'	-7.50	108.95	120.20
28	2	295	G	P-O3'-C3'	-7.50	108.95	120.20
28	2	1137	G	P-O3'-C3'	-7.49	108.96	120.20
28	2	1035	OMG	P-O3'-C3'	-7.49	108.97	120.20
28	2	1007	G	P-O3'-C3'	-7.49	108.97	120.20
28	2	151	A	P-O3'-C3'	-7.41	109.08	120.20
28	2	1133	G	P-O3'-C3'	-7.40	109.11	120.20
28	2	1391	G	P-O3'-C3'	-7.36	109.16	120.20
28	2	1172	U	P-O3'-C3'	-7.30	109.25	120.20
28	2	1006	C	P-O3'-C3'	-7.29	109.27	120.20
28	2	937	C	P-O3'-C3'	-7.24	109.33	120.20
28	2	7	G	P-O3'-C3'	-7.18	109.43	120.20
28	2	1011	OMG	P-O3'-C3'	-7.16	109.47	120.20
28	2	367	G	P-O3'-C3'	-7.15	109.47	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	290	A	P-O3'-C3'	-7.14	109.49	120.20
28	2	104	OMC	P-O3'-C3'	-7.12	109.52	120.20
28	2	365	G	P-O3'-C3'	-7.08	109.58	120.20
28	2	1166	G	P-O3'-C3'	-7.00	109.70	120.20
28	2	159	C	P-O3'-C3'	-6.96	109.76	120.20
28	2	1408	A	P-O3'-C3'	-6.94	109.79	120.20
28	2	1412	C	P-O3'-C3'	-6.94	109.79	120.20
28	2	1167	C	P-O3'-C3'	-6.93	109.80	120.20
28	2	939	C	P-O3'-C3'	-6.90	109.85	120.20
28	2	109	U	P-O3'-C3'	-6.88	109.89	120.20
28	2	1384	A	P-O3'-C3'	-6.81	109.99	120.20
28	2	1386	C	P-O3'-C3'	-6.65	110.23	120.20
28	2	157	U	P-O3'-C3'	-6.64	110.25	120.20
28	2	110	G	P-O3'-C3'	-6.62	110.26	120.20
28	2	1164	A	P-O3'-C3'	-6.60	110.31	120.20
28	2	155	C	P-O3'-C3'	-6.53	110.41	120.20
28	2	158	G	P-O3'-C3'	-6.48	110.48	120.20
28	2	1131	A	P-O3'-C3'	-6.48	110.48	120.20
28	2	943	C	P-O3'-C3'	-6.46	110.50	120.20
28	2	1169	C	P-O3'-C3'	-6.38	110.62	120.20
28	2	301	C	P-O3'-C3'	-6.38	110.63	120.20
28	2	854	G	P-O3'-C3'	-6.37	110.64	120.20
28	2	815	G	P-O3'-C3'	-6.32	110.72	120.20
28	2	1165	C	P-O3'-C3'	-6.31	110.73	120.20
28	2	853	G	P-O3'-C3'	-6.29	110.76	120.20
28	2	1138	U	P-O3'-C3'	-6.26	110.81	120.20
28	2	180	G	P-O3'-C3'	-6.20	110.89	120.20
28	2	4	C	P-O3'-C3'	-6.19	110.91	120.20
28	2	1136	U	P-O3'-C3'	-6.18	110.93	120.20
28	2	302	G	P-O3'-C3'	-6.15	110.97	120.20
28	2	1393	G	P-O3'-C3'	-6.08	111.08	120.20
28	2	1140	A	P-O3'-C3'	-6.04	111.15	120.20
28	2	1130	C	P-O3'-C3'	-6.02	111.17	120.20
28	2	1387	C	P-O3'-C3'	-6.01	111.18	120.20
28	2	150	C	P-O3'-C3'	-6.01	111.19	120.20
28	2	1411	U	P-O3'-C3'	-6.00	111.20	120.20
28	2	944	A	P-O3'-C3'	-5.98	111.23	120.20
28	2	938	G	P-O3'-C3'	-5.96	111.25	120.20
28	2	1009	U	P-O3'-C3'	-5.96	111.25	120.20
28	2	184	G	P-O3'-C3'	-5.96	111.26	120.20
28	2	1170	G	P-O3'-C3'	-5.95	111.27	120.20
28	2	851	G	P-O3'-C3'	-5.93	111.30	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	9	C	P-O3'-C3'	-5.92	111.33	120.20
28	2	108	G	P-O3'-C3'	-5.92	111.33	120.20
28	2	1134	U	P-O3'-C3'	-5.91	111.33	120.20
28	2	106	C	P-O3'-C3'	-5.91	111.34	120.20
28	2	1005	G	P-O3'-C3'	-5.89	111.37	120.20
28	2	362	G	P-O3'-C3'	-5.82	111.47	120.20
28	2	852	G	P-O3'-C3'	-5.82	111.47	120.20
28	2	946	C	P-O3'-C3'	-5.75	111.58	120.20
28	2	1159	G	P-O3'-C3'	-5.73	111.60	120.20
28	2	364	G	P-O3'-C3'	-5.69	111.67	120.20
28	2	3	U	P-O3'-C3'	-5.65	111.72	120.20
28	2	936	A	P-O3'-C3'	-5.64	111.74	120.20
28	2	945	C	P-O3'-C3'	-5.62	111.77	120.20
28	2	319	C	P-O3'-C3'	-5.56	111.86	120.20
28	2	183	C	P-O3'-C3'	-5.55	111.88	120.20
28	2	12	U	P-O3'-C3'	-5.51	111.94	120.20
28	2	1171	C	P-O3'-C3'	-5.45	112.03	120.20
28	2	1406	A	P-O3'-C3'	-5.42	112.08	120.20
28	2	105	C	P-O3'-C3'	-5.41	112.09	120.20
28	2	107	C	P-O3'-C3'	-5.34	112.19	120.20
28	2	160	G	P-O3'-C3'	-5.33	112.20	120.20
28	2	1139	G	P-O3'-C3'	-5.32	112.22	120.20
28	2	1420	G	P-O3'-C3'	-5.29	112.27	120.20
28	2	6	G	P-O3'-C3'	-5.29	112.27	120.20
8	Q	110	SER	N-CA-C	-5.28	107.49	114.04
28	2	82	G	P-O3'-C3'	-5.28	112.28	120.20
28	2	850	G	P-O3'-C3'	-5.28	112.29	120.20
28	2	111	G	P-O3'-C3'	-5.26	112.31	120.20
28	2	10	G	P-O3'-C3'	-5.25	112.33	120.20
28	2	1135	C	P-O3'-C3'	-5.25	112.33	120.20
28	2	1041	G	P-O3'-C3'	-5.21	112.38	120.20
28	2	1416	A	P-O3'-C3'	-5.14	112.48	120.20
28	2	508	C	P-O3'-C3'	-5.07	112.59	120.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	G	106	CYS	Peptide
31	G	107	ILE	Peptide
31	G	29	LYS	Peptide
17	P	36	LYS	Peptide

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Mol	Chain	Res	Type	Group
18	R	40	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d	398	0	398	10	0
2	T	934	0	882	17	0
3	N	1198	0	1266	11	0
4	J	1322	0	1378	20	0
5	D	1402	0	1424	35	0
6	X	1104	0	1194	13	0
7	S	1055	0	1076	41	0
8	Q	960	0	1037	24	0
9	C	1641	0	1687	26	0
10	A	1546	0	1575	21	0
11	B	1758	0	1797	20	0
12	Y	708	0	724	12	0
13	b	614	0	604	7	0
14	a	785	0	818	6	0
15	Z	419	0	413	13	0
16	V	605	0	606	8	0
17	P	836	0	866	33	0
18	R	780	0	782	19	0
19	K	689	0	671	27	0
20	I	1282	0	1336	24	0
21	e	291	0	306	7	0
22	H	1194	0	1169	24	0
23	n	217	0	259	1	0
24	c	439	0	473	14	0
25	O	935	0	935	11	0
26	W	1031	0	1082	13	0
27	E	2058	0	2135	38	0
28	2	29096	0	14778	266	0
29	L	1481	0	1496	11	0
30	U	609	0	649	12	0
31	G	1530	0	1613	44	0
32	F	1246	0	1268	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	2	239	0	0	0	0
33	A	1	0	0	0	0
33	E	3	0	0	0	0
33	G	1	0	0	0	0
33	L	3	0	0	0	0
33	N	7	0	0	0	0
33	O	6	0	0	0	0
33	R	1	0	0	0	0
33	S	2	0	0	0	0
33	W	1	0	0	0	0
33	b	1	0	0	0	0
33	d	1	0	0	0	0
34	2	35	0	0	0	0
34	I	1	0	0	0	0
34	N	1	0	0	0	0
All	All	60466	0	46697	766	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 7.

All (766) 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)
31:G:27:PHE:HD1	31:G:28:ARG:H	1.23	0.85
2:T:25:ILE:HG22	2:T:26:ILE:H	1.41	0.84
28:2:593:C:H4'	28:2:594:C:H5'	1.58	0.84
5:D:107:MET:HE1	5:D:131:THR:HG23	1.65	0.78
28:2:124:G:H1	31:G:203:LYS:HE2	1.49	0.78
31:G:143:ARG:HB3	31:G:146:LYS:HD3	1.65	0.78
20:I:23:LYS:HE2	28:2:298:G:H5''	1.64	0.78
27:E:210:MET:HE1	27:E:220:THR:HG22	1.66	0.76
4:J:112:GLN:HE22	4:J:128:ARG:HD2	1.50	0.76
8:Q:25:VAL:HB	8:Q:40:VAL:HB	1.68	0.74
11:B:107:ARG:NH1	25:O:127:THR:O	2.20	0.74
12:Y:97:ILE:HG22	12:Y:99:ALA:H	1.52	0.74
28:2:599:C:H2'	28:2:600:G:C8	2.23	0.73
27:E:45:ILE:HG13	27:E:61:THR:HG21	1.71	0.72
5:D:130:ARG:HD3	5:D:134:ARG:HH22	1.54	0.72
32:F:27:ILE:HG23	32:F:54:VAL:HG11	1.71	0.71
19:K:10:LYS:HD2	19:K:56:ILE:HG21	1.73	0.71
28:2:64:A:H2	28:2:71:A:H62	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:E:163:ASN:ND2	27:E:170:ASP:OD2	2.23	0.71
28:2:127:G:H1	28:2:155:C:H5	1.36	0.71
2:T:25:ILE:O	2:T:27:LYS:N	2.21	0.70
1:d:89:GLU:HG2	1:d:90:THR:HG23	1.73	0.70
11:B:190:ASN:HB3	11:B:192:GLU:HG2	1.74	0.70
28:2:705:G:H2'	28:2:706:A:C8	2.27	0.69
11:B:165:ARG:NH1	28:2:699:U:OP1	2.26	0.69
20:I:55:THR:HG23	20:I:63:ILE:HG23	1.75	0.69
15:Z:43:THR:HG23	32:F:152:VAL:HG12	1.75	0.69
31:G:104:ARG:HH21	31:G:107:ILE:HG22	1.58	0.69
7:S:132:LYS:HE3	28:2:1232:C:H5''	1.75	0.68
10:A:206:LEU:HD21	18:R:88:ALA:HB2	1.76	0.68
31:G:221:LEU:HD11	31:G:225:LYS:HZ3	1.57	0.68
28:2:691:C:H2'	28:2:692:A:C8	2.28	0.68
19:K:46:CYS:HB2	19:K:48:PRO:HD3	1.75	0.68
29:L:185:LYS:NZ	29:L:187:GLU:OE1	2.21	0.68
8:Q:65:LYS:NZ	32:F:37:HIS:O	2.25	0.68
25:O:46:THR:HG21	28:2:647:G:H21	1.59	0.68
14:a:28:ARG:NH2	14:a:29:CYS:O	2.27	0.68
7:S:32:LEU:HB3	7:S:38:ILE:HG21	1.76	0.67
28:2:1101:G:H1	28:2:1108:C:H42	1.42	0.67
5:D:34:GLU:HG2	19:K:69:THR:HG21	1.77	0.67
5:D:209:GLU:HB3	18:R:43:ILE:HD13	1.78	0.66
28:2:109:U:H3	28:2:209:G:H1	1.41	0.66
28:2:364:G:O2'	28:2:365:G:OP2	2.13	0.65
5:D:142:VAL:HG22	5:D:192:VAL:HG22	1.79	0.65
27:E:187:ARG:NH1	28:2:532:A:OP2	2.30	0.65
32:F:142:THR:O	32:F:146:LYS:HG3	1.95	0.65
28:2:913:A:H2'	28:2:914:G:C8	2.32	0.65
8:Q:60:GLU:HA	8:Q:63:ARG:HG3	1.78	0.65
15:Z:28:ASN:HA	15:Z:31:LEU:HG	1.78	0.65
10:A:62:LYS:HE3	16:V:87:MET:HE1	1.78	0.65
27:E:208:ILE:HD11	27:E:222:LEU:HD12	1.79	0.64
28:2:302:G:H5''	28:2:302:G:H8	1.62	0.64
28:2:1162:G:H5'	28:2:1163:C:OP2	1.98	0.64
11:B:166:ALA:O	11:B:170:GLU:HG3	1.97	0.64
7:S:38:ILE:HD13	7:S:101:LEU:HD12	1.79	0.64
21:e:31:ARG:HH11	28:2:426:C:H4'	1.62	0.64
15:Z:55:LEU:O	15:Z:59:VAL:HG12	1.98	0.64
19:K:26:GLU:OE2	19:K:73:ARG:NH2	2.31	0.64
28:2:149:C:O2	31:G:138:ARG:NH2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:119:LEU:HD21	31:G:122:ALA:HA	1.78	0.63
30:U:26:LYS:HG2	30:U:97:THR:HA	1.81	0.63
4:J:48:ARG:HA	4:J:103:ILE:HD11	1.80	0.62
28:2:605:G:O2'	28:2:606:G:OP2	2.16	0.62
17:P:85:ILE:HD11	17:P:116:LEU:HG	1.81	0.62
4:J:25:ARG:O	4:J:29:GLU:HB2	1.98	0.62
27:E:106:LYS:NZ	28:2:564:G:OP1	2.33	0.62
22:H:70:LEU:HD13	22:H:97:ALA:HB2	1.80	0.62
5:D:130:ARG:HD3	5:D:134:ARG:NH2	2.12	0.62
28:2:1305:C:H2'	28:2:1306:C:H6	1.65	0.62
14:a:44:ILE:HD11	14:a:65:PRO:HD2	1.82	0.62
28:2:1241:G:N2	28:2:1243:A:H3'	2.15	0.62
8:Q:73:LEU:HD11	8:Q:124:LEU:HD11	1.81	0.62
9:C:182:LEU:HD13	9:C:190:VAL:HG11	1.82	0.62
28:2:175:C:N4	28:2:598:G:H1'	2.15	0.61
22:H:105:ALA:HB3	28:2:520:C:H42	1.65	0.61
28:2:403:G:H22	28:2:406:C:P	2.24	0.61
9:C:136:GLY:HA2	16:V:9:MET:HE1	1.83	0.61
1:d:114:LYS:HD3	1:d:115:TYR:CE2	2.36	0.61
5:D:115:LEU:HB3	5:D:183:MET:HE1	1.83	0.61
2:T:59:ILE:HG13	2:T:107:PHE:CZ	2.36	0.61
28:2:158:G:H22	28:2:202:A:H5'	1.65	0.61
9:C:155:LYS:HD2	9:C:160:ARG:HD3	1.83	0.60
6:X:87:ARG:O	6:X:90:SER:OG	2.16	0.60
8:Q:31:LYS:HG3	8:Q:32:LYS:H	1.65	0.60
22:H:104:ASN:OD1	28:2:521:C:O2'	2.19	0.60
28:2:176:C:H5	28:2:596:G:H1	1.48	0.60
17:P:81:ARG:HG3	17:P:81:ARG:HH11	1.67	0.60
28:2:637:G:H2'	28:2:638:U:C6	2.35	0.60
31:G:141:PRO:HG2	31:G:150:LEU:HD12	1.83	0.60
22:H:147:PRO:HA	26:W:49:ASP:OD1	2.01	0.60
28:2:431:G:H1	28:2:469:U:H3	1.49	0.60
1:d:126:GLU:OE1	1:d:126:GLU:N	2.34	0.60
28:2:1112:A:H2'	28:2:1113:G:C8	2.36	0.60
32:F:109:GLU:HG2	32:F:186:ALA:HB1	1.82	0.60
17:P:124:LYS:NZ	28:2:924:C:H5''	2.16	0.60
20:I:52:LYS:HD2	20:I:69:ARG:HH12	1.66	0.60
27:E:245:PRO:HB3	27:E:249:LYS:HD3	1.84	0.60
18:R:2:GLY:N	28:2:1108:C:OP1	2.35	0.60
27:E:125:ARG:HB2	27:E:226:PHE:CE2	2.36	0.60
28:2:1372:G:H2'	28:2:1373:G:O4'	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:141:PRO:HB3	31:G:146:LYS:HB3	1.84	0.60
2:T:40:SER:OG	2:T:81:SER:OG	2.15	0.59
28:2:1118:G:H4'	28:2:1119:C:O5'	2.02	0.59
11:B:30:VAL:HG12	11:B:41:ILE:HD12	1.85	0.59
28:2:1288:C:H2'	28:2:1289:G:C8	2.37	0.59
28:2:158:G:H5''	28:2:158:G:H8	1.67	0.59
28:2:472:G:H2'	28:2:473:C:C6	2.36	0.59
8:Q:116:ALA:HA	8:Q:119:GLU:HG2	1.84	0.59
17:P:17:PHE:HZ	17:P:37:LEU:HD21	1.66	0.59
28:2:430:A:H61	28:2:470:C:H42	1.51	0.59
28:2:351:U:H3	28:2:374:G:H1	1.50	0.59
6:X:48:ARG:HH12	6:X:75:THR:HG21	1.68	0.59
17:P:55:LEU:HA	17:P:58:VAL:HG22	1.85	0.59
8:Q:57:VAL:HG21	8:Q:66:VAL:HG21	1.83	0.59
22:H:163:TYR:O	22:H:167:SER:OG	2.20	0.59
28:2:926:A:HO2'	28:2:950:C:HO2'	1.49	0.59
29:L:27:PRO:HG2	29:L:30:GLU:HG3	1.85	0.59
7:S:141:THR:HG21	28:2:1166:G:N7	2.17	0.58
28:2:130:C:H2'	28:2:131:A:H8	1.68	0.58
11:B:205:THR:HG22	11:B:206:MET:H	1.69	0.58
18:R:44:ILE:HG21	18:R:50:ARG:HB2	1.85	0.58
25:O:115:ARG:HG2	25:O:115:ARG:HH11	1.68	0.58
26:W:53:VAL:O	26:W:59:ASN:HB3	2.03	0.58
5:D:17:TYR:HD2	30:U:89:MET:HE2	1.68	0.58
12:Y:7:LYS:NZ	12:Y:9:ARG:HD2	2.18	0.58
10:A:182:LEU:O	10:A:186:GLU:HG2	2.03	0.58
28:2:1261:7MG:H2'	28:2:1262:A:C8	2.38	0.58
31:G:104:ARG:NH2	31:G:107:ILE:HG22	2.17	0.58
7:S:36:LYS:HG3	28:2:1253:C:H5''	1.85	0.58
7:S:54:VAL:HG23	7:S:55:HIS:CD2	2.38	0.58
21:e:60:ASN:OD1	21:e:61:LEU:N	2.36	0.58
28:2:141:A:HO2'	28:2:142:C:H6	1.51	0.58
3:N:88:LEU:O	3:N:92:ILE:HG13	2.04	0.58
22:H:106:TYR:HA	22:H:114:ILE:O	2.04	0.58
9:C:49:PHE:HE2	9:C:104:PHE:HE1	1.51	0.58
17:P:31:THR:HB	17:P:34:LEU:HD12	1.86	0.57
28:2:175:C:H5'	28:2:176:C:O2	2.03	0.57
5:D:144:VAL:HG22	5:D:190:VAL:HG12	1.84	0.57
28:2:398:A:H61	28:2:412:C:H42	1.50	0.57
28:2:413:G:H2'	28:2:414:A:C8	2.39	0.57
10:A:33:ARG:HG3	10:A:33:ARG:HH11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:F:45:LYS:HG2	32:F:46:ARG:H	1.69	0.57
1:d:133:PHE:HB3	30:U:85:PHE:HB3	1.85	0.57
28:2:137:G:O5'	31:G:8:LYS:NZ	2.35	0.57
28:2:177:C:H42	28:2:595:G:H1	1.51	0.57
10:A:90:ARG:NH1	18:R:85:ASP:OD1	2.36	0.57
27:E:62:SER:O	27:E:66:GLN:HG3	2.04	0.57
28:2:621:G:H2'	28:2:622:C:C6	2.40	0.57
28:2:1250:C:H2'	28:2:1251:C:C6	2.39	0.57
8:Q:129:ARG:HE	8:Q:133:VAL:HG21	1.69	0.57
28:2:948:C:H42	28:2:1160:C:H5	1.52	0.57
6:X:107:ARG:HD3	6:X:112:VAL:HG12	1.85	0.57
19:K:6:LYS:O	19:K:10:LYS:HG3	2.05	0.57
27:E:249:LYS:HE3	27:E:253:LEU:HD11	1.85	0.57
6:X:70:VAL:HG11	6:X:94:ILE:HG21	1.85	0.57
19:K:16:LEU:HD21	19:K:87:ILE:HG21	1.87	0.57
9:C:151:LYS:NZ	26:W:94:LEU:O	2.38	0.57
17:P:90:ILE:HD11	17:P:109:PRO:HA	1.86	0.57
12:Y:11:VAL:HG23	12:Y:22:CYS:SG	2.44	0.57
17:P:124:LYS:HZ2	28:2:924:C:H5''	1.69	0.57
22:H:105:ALA:HB3	28:2:520:C:N4	2.20	0.56
28:2:587:G:O2'	28:2:588:C:H6	1.88	0.56
27:E:211:LYS:HE2	27:E:215:GLY:HA2	1.87	0.56
28:2:364:G:O2'	28:2:365:G:P	2.63	0.56
28:2:902:A:H2'	28:2:903:C:C6	2.40	0.56
28:2:941:C:O2	28:2:941:C:H2'	2.05	0.56
2:T:58:VAL:HG11	2:T:103:ILE:HG21	1.87	0.56
19:K:88:ARG:HG2	19:K:88:ARG:HH11	1.69	0.56
28:2:1011:OMG:H2'	28:2:1012:U:C6	2.39	0.56
30:U:43:VAL:HG21	30:U:92:ARG:HG3	1.85	0.56
31:G:26:ASP:HA	31:G:31:GLN:HE21	1.70	0.56
28:2:133:C:H2'	28:2:134:G:H8	1.71	0.56
28:2:1175:A:OP1	32:F:150:ARG:NH2	2.35	0.56
19:K:77:TYR:O	19:K:78:LEU:HD23	2.06	0.56
28:2:1187:A:H2'	28:2:1188:G:C8	2.41	0.56
28:2:658:A:H2'	28:2:659:A:C8	2.41	0.55
22:H:45:TYR:CE1	22:H:69:MET:HE1	2.41	0.55
11:B:123:VAL:HG11	11:B:168:ILE:HG21	1.86	0.55
12:Y:82:LEU:O	12:Y:86:GLU:HB2	2.06	0.55
5:D:99:LYS:HE3	5:D:135:ALA:HA	1.89	0.55
28:2:1301:C:P	32:F:46:ARG:HE	2.29	0.55
19:K:80:THR:HG23	19:K:83:GLY:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:91:C:H5''	28:2:92:A:C2	2.40	0.55
32:F:154:PRO:HG2	32:F:157:GLU:HB3	1.88	0.55
9:C:76:ASN:HB2	9:C:201:LEU:HD22	1.88	0.55
28:2:305:C:H2'	28:2:306:C:C6	2.41	0.55
9:C:36:LEU:HD22	9:C:41:LYS:HG3	1.89	0.55
24:c:9:VAL:HA	24:c:27:VAL:HG12	1.88	0.55
3:N:92:ILE:O	3:N:96:VAL:HG23	2.07	0.54
18:R:51:ASN:ND2	28:2:1094:A:H5''	2.22	0.54
31:G:69:MET:HA	31:G:104:ARG:HA	1.88	0.54
28:2:31:U:H3	28:2:378:C:H5	1.54	0.54
28:2:900:C:H5	28:2:904:C:H41	1.55	0.54
18:R:51:ASN:HD22	28:2:1094:A:H5''	1.72	0.54
9:C:160:ARG:NH2	28:2:839:U:O2	2.41	0.54
4:J:80:ARG:O	4:J:84:MET:HG3	2.08	0.54
24:c:22:ILE:HA	24:c:41:VAL:O	2.07	0.54
28:2:130:C:H2'	28:2:131:A:C8	2.42	0.54
25:O:23:ALA:HB2	25:O:84:ILE:HD12	1.90	0.54
28:2:818:C:N4	28:2:833:G:O6	2.31	0.54
28:2:329:A:H4'	28:2:330:G:O5'	2.06	0.54
2:T:25:ILE:CG2	2:T:26:ILE:H	2.17	0.54
8:Q:127:TYR:HH	32:F:33:SER:HG	1.54	0.54
9:C:67:LYS:O	9:C:68:SER:OG	2.23	0.54
17:P:21:GLU:OE1	17:P:22:VAL:HG13	2.08	0.54
25:O:72:THR:O	25:O:76:ILE:HG12	2.08	0.53
20:I:38:LEU:HD12	20:I:39:ILE:H	1.73	0.53
28:2:102:C:OP2	29:L:173:ARG:NH1	2.42	0.53
7:S:100:ILE:HD12	7:S:105:ILE:HG23	1.90	0.53
10:A:168:CYS:HB2	10:A:179:ILE:HD11	1.89	0.53
3:N:35:GLU:O	3:N:39:LYS:HG3	2.09	0.53
5:D:77:TYR:CE2	19:K:19:ASN:HB2	2.43	0.53
7:S:30:CYS:SG	7:S:40:ARG:NH1	2.79	0.53
5:D:111:LEU:HD13	5:D:128:ILE:HG13	1.91	0.53
28:2:907:A:H4'	28:2:1297:G:H22	1.74	0.53
3:N:3:ARG:HD2	3:N:9:LYS:HE3	1.91	0.53
7:S:47:LEU:HD23	7:S:52:ILE:HG22	1.91	0.53
10:A:85:ARG:HG3	10:A:85:ARG:HH11	1.74	0.53
28:2:1278:C:H2'	28:2:1279:C:C6	2.44	0.53
9:C:33:LEU:O	9:C:37:VAL:HG23	2.09	0.52
17:P:81:ARG:HD3	17:P:97:TYR:O	2.09	0.52
22:H:163:TYR:HA	22:H:189:PHE:CE2	2.44	0.52
27:E:43:PRO:HG2	27:E:46:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:E:197:ALA:HB3	27:E:209:ARG:HB3	1.91	0.52
3:N:8:GLY:O	3:N:9:LYS:HB2	2.08	0.52
10:A:19:ASP:N	10:A:19:ASP:OD1	2.43	0.52
10:A:203:LYS:NZ	18:R:91:LYS:O	2.41	0.52
31:G:84:ARG:HE	31:G:98:ARG:HE	1.57	0.52
4:J:112:GLN:NE2	4:J:128:ARG:HD2	2.21	0.52
24:c:15:ARG:NH2	24:c:23:THR:OG1	2.43	0.52
24:c:46:ARG:HG3	32:F:47:PHE:CE2	2.45	0.52
28:2:393:G:O2'	28:2:394:A:H8	1.93	0.52
28:2:624:G:H2'	28:2:625:G:C8	2.45	0.52
10:A:83:ALA:HB3	10:A:92:ILE:HD13	1.91	0.52
22:H:94:ILE:HG21	22:H:133:ILE:HD12	1.91	0.52
27:E:213:THR:HG22	27:E:243:ILE:HD11	1.92	0.52
28:2:1178:G:H2'	28:2:1179:G:C8	2.44	0.52
1:d:114:LYS:HD3	1:d:115:TYR:CZ	2.44	0.52
24:c:57:GLU:HB3	25:O:69:MET:HE2	1.90	0.52
28:2:1300:G:H2'	28:2:1301:C:O4'	2.10	0.52
28:2:127:G:O2'	28:2:128:G:H5'	2.10	0.52
7:S:116:LEU:HD11	7:S:123:ARG:HH21	1.75	0.52
17:P:108:LYS:O	17:P:111:MET:HG2	2.09	0.52
28:2:1206:G:H2'	28:2:1207:C:C6	2.45	0.52
29:L:36:ARG:NH1	29:L:93:ILE:O	2.43	0.52
17:P:81:ARG:HB3	17:P:117:ARG:HB3	1.92	0.51
19:K:15:HIS:HB3	19:K:18:GLU:HB3	1.92	0.51
19:K:16:LEU:HD11	19:K:87:ILE:HB	1.90	0.51
7:S:43:ALA:O	7:S:47:LEU:HD12	2.10	0.51
27:E:176:ASP:HB2	27:E:179:LYS:HE3	1.93	0.51
2:T:40:SER:HG	2:T:81:SER:HG	1.43	0.51
13:b:83:ASP:OD1	13:b:84:ILE:N	2.35	0.51
2:T:25:ILE:HG22	2:T:26:ILE:N	2.18	0.51
15:Z:43:THR:HG21	32:F:153:ARG:HA	1.91	0.51
22:H:158:LEU:O	22:H:190:MET:N	2.38	0.51
10:A:82:VAL:HG22	10:A:104:PHE:HB2	1.93	0.51
24:c:55:GLU:OE2	32:F:190:ARG:HD3	2.11	0.51
28:2:69:G:H8	31:G:186:LEU:HD22	1.75	0.51
12:Y:5:THR:HB	12:Y:27:LEU:HB3	1.92	0.51
28:2:1170:G:O2'	28:2:1288:C:OP1	2.29	0.51
31:G:226:ALA:O	31:G:230:ARG:HG3	2.11	0.51
5:D:204:MET:SD	5:D:205:PRO:HD2	2.50	0.51
24:c:61:ARG:HH11	24:c:62:ARG:HB2	1.75	0.51
28:2:1178:G:H2'	28:2:1179:G:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:K:67:LYS:HE3	19:K:78:LEU:HB2	1.93	0.51
28:2:1336:U:H2'	28:2:1337:A:C8	2.46	0.51
29:L:28:ASP:OD1	29:L:28:ASP:N	2.43	0.51
9:C:27:TRP:CD2	9:C:59:GLU:HG3	2.47	0.50
6:X:4:THR:HG21	6:X:12:LYS:HG2	1.93	0.50
8:Q:137:ARG:O	8:Q:138:ARG:HD3	2.11	0.50
15:Z:29:GLU:O	15:Z:33:PHE:N	2.43	0.50
27:E:18:TRP:CD1	27:E:42:ILE:HD12	2.45	0.50
28:2:828:A:H2'	28:2:829:A:C8	2.46	0.50
28:2:62:U:H2'	28:2:63:C:C6	2.46	0.50
12:Y:34:GLU:O	12:Y:35:SER:OG	2.25	0.50
17:P:53:LYS:HD3	17:P:83:MET:HG2	1.93	0.50
5:D:61:PRO:HD2	5:D:96:LYS:HE2	1.93	0.50
5:D:146:GLY:O	5:D:153:ALA:HA	2.12	0.50
15:Z:41:THR:O	15:Z:45:ILE:HG22	2.11	0.50
17:P:95:SER:HB3	17:P:102:PHE:HB3	1.92	0.50
5:D:99:LYS:HG2	5:D:102:LEU:HD12	1.94	0.50
26:W:103:ILE:HD11	26:W:129:PHE:CE1	2.46	0.50
7:S:56:LYS:HE3	7:S:60:GLU:OE1	2.11	0.50
18:R:3:LYS:NZ	28:2:1119:C:OP1	2.37	0.50
18:R:33:LYS:HD2	18:R:33:LYS:O	2.12	0.50
19:K:47:ASN:N	19:K:48:PRO:HD3	2.27	0.50
22:H:145:LEU:HD13	22:H:153:ARG:HH21	1.77	0.50
28:2:983:G:H5'	28:2:984:C:H5	1.77	0.50
32:F:153:ARG:HG2	32:F:154:PRO:HD2	1.94	0.50
2:T:60:ARG:O	2:T:64:ILE:HG13	2.12	0.49
9:C:73:GLU:OE1	9:C:97:ILE:HD11	2.12	0.49
10:A:59:VAL:HG22	10:A:167:PRO:HG2	1.93	0.49
10:A:140:LEU:O	10:A:143:SER:OG	2.30	0.49
27:E:188:ASN:HB3	27:E:191:ARG:HE	1.76	0.49
28:2:983:G:H3'	28:2:984:C:C6	2.47	0.49
28:2:1408:A:H5'	28:2:1409:A:C6	2.47	0.49
4:J:80:ARG:HH11	27:E:255:LEU:HD21	1.76	0.49
9:C:57:GLU:HB3	9:C:59:GLU:OE1	2.12	0.49
20:I:67:ALA:HB2	20:I:153:GLY:HA2	1.94	0.49
28:2:925:A:N3	28:2:951:C:O2'	2.40	0.49
7:S:42:PHE:HA	7:S:45:VAL:HG12	1.94	0.49
8:Q:48:LEU:HD13	8:Q:51:ASN:HA	1.94	0.49
20:I:166:LEU:HD11	20:I:170:LYS:HZ2	1.78	0.49
28:2:154:A:H2'	28:2:155:C:O4'	2.11	0.49
28:2:348:A2M:O5'	28:2:348:A2M:H8	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:U:43:VAL:HG13	30:U:94:PHE:HZ	1.76	0.49
15:Z:52:SER:OG	15:Z:53:VAL:N	2.45	0.49
28:2:173:C:H1'	29:L:36:ARG:HH21	1.77	0.49
11:B:139:VAL:HG21	11:B:172:LEU:HD11	1.94	0.49
11:B:226:GLU:O	11:B:230:THR:HG23	2.12	0.49
13:b:60:HIS:HD2	13:b:62:LEU:H	1.61	0.49
29:L:63:PHE:HB3	29:L:66:ARG:HG3	1.95	0.49
32:F:95:VAL:O	32:F:99:VAL:HG23	2.13	0.49
31:G:219:GLN:O	31:G:223:GLU:HG2	2.12	0.49
9:C:178:VAL:HG13	9:C:208:VAL:HG21	1.94	0.49
18:R:20:ASN:O	18:R:24:LEU:HG	2.13	0.49
32:F:131:ARG:O	32:F:135:ILE:HG12	2.13	0.49
4:J:55:ARG:HE	4:J:99:LEU:HD22	1.77	0.49
5:D:65:MET:HG3	5:D:72:LEU:HD22	1.95	0.49
20:I:51:GLN:HA	20:I:69:ARG:O	2.12	0.49
24:c:52:VAL:HG11	32:F:108:ARG:HD2	1.94	0.49
5:D:60:GLU:HG2	5:D:63:VAL:HG12	1.94	0.49
17:P:94:VAL:O	17:P:104:PRO:HA	2.13	0.49
21:e:15:ARG:HH21	21:e:15:ARG:HG3	1.76	0.49
26:W:3:ARG:HH12	26:W:28:ARG:NH1	2.10	0.49
28:2:302:G:H5''	28:2:302:G:C8	2.45	0.49
28:2:1058:G:H2'	28:2:1059:A:C8	2.48	0.49
32:F:22:SER:O	32:F:22:SER:OG	2.25	0.49
11:B:44:THR:HG21	11:B:64:TYR:OH	2.12	0.49
28:2:280:U:H5	28:2:285:G:O6	1.96	0.49
31:G:5:SER:HB2	31:G:23:MET:HE1	1.94	0.49
28:2:9:C:H2'	28:2:11:A:OP2	2.13	0.48
28:2:69:G:H2'	28:2:70:G:C8	2.48	0.48
28:2:1027:A:H4'	28:2:1028:G:OP1	2.13	0.48
7:S:49:LYS:HD2	7:S:79:HIS:O	2.13	0.48
27:E:57:THR:O	27:E:61:THR:OG1	2.21	0.48
5:D:94:VAL:HG12	5:D:95:ASP:O	2.14	0.48
17:P:53:LYS:HE3	17:P:80:LEU:HD13	1.96	0.48
22:H:106:TYR:CE1	22:H:115:ARG:HD3	2.48	0.48
28:2:62:U:H5''	28:2:153:G:C5	2.48	0.48
14:a:90:GLU:H	14:a:90:GLU:CD	2.21	0.48
21:e:60:ASN:HB3	21:e:63:ILE:HG12	1.94	0.48
20:I:164:GLU:HG3	29:L:56:TYR:CD2	2.48	0.48
28:2:913:A:H2'	28:2:914:G:H8	1.79	0.48
28:2:1407:G:H2'	28:2:1408:A:H1'	1.94	0.48
7:S:15:LEU:HB2	7:S:22:ILE:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:11:VAL:HG23	12:Y:22:CYS:HG	1.78	0.48
18:R:56:TYR:CZ	18:R:60:LEU:HD21	2.49	0.48
2:T:59:ILE:HG13	2:T:107:PHE:CE1	2.48	0.48
25:O:51:SER:O	25:O:54:MET:HG2	2.13	0.48
5:D:71:ARG:O	5:D:75:ILE:HG12	2.14	0.48
27:E:192:ILE:HG13	27:E:242:GLY:HA3	1.95	0.48
24:c:4:PRO:HB3	24:c:54:MET:SD	2.54	0.48
26:W:113:HIS:O	26:W:117:GLN:HG2	2.12	0.48
28:2:606:G:O2'	28:2:607:C:H5'	2.14	0.48
5:D:124:ALA:O	5:D:128:ILE:HG12	2.14	0.48
5:D:170:LYS:NZ	28:2:1125:G:OP1	2.46	0.47
6:X:74:LEU:HD11	6:X:81:ILE:HG12	1.95	0.47
10:A:33:ARG:HG3	10:A:33:ARG:NH1	2.28	0.47
17:P:17:PHE:CE2	17:P:18:ARG:HG2	2.49	0.47
31:G:197:ASP:OD1	31:G:198:GLU:N	2.46	0.47
6:X:93:TYR:HB3	6:X:140:LYS:HD2	1.97	0.47
7:S:24:GLY:HA2	7:S:58:ALA:HB3	1.97	0.47
8:Q:153:ARG:HD3	28:2:1169:C:O3'	2.14	0.47
28:2:441:U:H2'	28:2:442:G:H8	1.78	0.47
28:2:942:G:H8	28:2:1281:C:H2'	1.78	0.47
31:G:130:LEU:HD23	31:G:131:THR:N	2.29	0.47
28:2:208:C:H2'	28:2:209:G:C8	2.50	0.47
20:I:37:LYS:HA	20:I:37:LYS:HD3	1.76	0.47
22:H:49:VAL:HG22	22:H:63:VAL:HG13	1.95	0.47
27:E:196:GLN:OE1	27:E:211:LYS:HB3	2.15	0.47
28:2:626:C:H2'	28:2:627:G:C8	2.49	0.47
28:2:1163:C:H4'	28:2:1164:A:OP1	2.15	0.47
28:2:1314:OMU:H2'	28:2:1315:G:C8	2.50	0.47
31:G:42:PHE:CE2	31:G:47:LEU:HD21	2.48	0.47
7:S:47:LEU:HD23	7:S:52:ILE:CG2	2.45	0.47
13:b:97:CYS:HB2	13:b:100:CYS:HB2	1.74	0.47
15:Z:30:ALA:HA	15:Z:34:ILE:HD12	1.96	0.47
18:R:53:VAL:O	18:R:57:VAL:HG23	2.14	0.47
28:2:587:G:O2'	28:2:588:C:O5'	2.27	0.47
18:R:22:GLU:OE1	18:R:23:SER:OG	2.27	0.47
18:R:49:LEU:O	18:R:53:VAL:HG23	2.15	0.47
20:I:52:LYS:HD2	20:I:69:ARG:NH1	2.29	0.47
22:H:84:LEU:HB3	22:H:93:PHE:CE2	2.50	0.47
22:H:122:MET:HE3	22:H:126:TYR:CE2	2.50	0.47
28:2:208:C:H2'	28:2:209:G:H8	1.78	0.47
2:T:77:ARG:NH2	28:2:1212:A:H5'	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:57:ARG:HB2	7:S:60:GLU:OE1	2.15	0.47
9:C:131:VAL:HG11	9:C:213:LYS:HG3	1.96	0.47
19:K:45:LEU:HG	19:K:46:CYS:H	1.79	0.47
20:I:131:GLU:O	20:I:135:GLN:HG3	2.14	0.47
28:2:51:U:H2'	28:2:52:G:C8	2.49	0.47
28:2:859:U:H2'	28:2:860:G:C8	2.50	0.47
7:S:47:LEU:HD22	7:S:54:VAL:HA	1.97	0.47
12:Y:7:LYS:HZ1	12:Y:9:ARG:HD2	1.78	0.47
12:Y:36:LYS:HB2	12:Y:36:LYS:HE3	1.72	0.47
20:I:91:VAL:HA	20:I:112:VAL:HG12	1.97	0.47
28:2:1199:C:H2'	28:2:1200:G:O4'	2.14	0.47
5:D:60:GLU:HG2	5:D:60:GLU:O	2.14	0.47
9:C:164:ILE:HB	9:C:191:PHE:HB2	1.97	0.47
28:2:115:U:OP1	28:2:160:G:O2'	2.32	0.47
28:2:1409:A:H4'	28:2:1410:G:OP2	2.14	0.47
32:F:176:ILE:HG23	32:F:179:ARG:HH21	1.80	0.47
7:S:119:THR:HG23	17:P:111:MET:SD	2.55	0.46
8:Q:42:ALA:HA	8:Q:81:LEU:HD22	1.98	0.46
28:2:1212:A:H2'	28:2:1213:G:C8	2.50	0.46
28:2:278:A:OP1	28:2:538:C:O2'	2.28	0.46
28:2:625:G:O2'	28:2:799:G:OP1	2.30	0.46
31:G:38:MET:SD	31:G:104:ARG:NH1	2.88	0.46
7:S:74:GLU:O	7:S:99:HIS:NE2	2.43	0.46
11:B:124:PHE:HA	11:B:137:VAL:O	2.16	0.46
1:d:124:PHE:CZ	30:U:68:ILE:HD12	2.50	0.46
9:C:220:THR:HG22	9:C:222:ASP:H	1.80	0.46
13:b:97:CYS:CB	13:b:100:CYS:H	2.29	0.46
24:c:41:VAL:HG22	32:F:126:ASP:OD1	2.15	0.46
27:E:136:MET:HG2	27:E:149:PHE:HE1	1.80	0.46
28:2:370:C:H3'	28:2:371:OMG:H8	1.80	0.46
31:G:31:GLN:HB3	31:G:34:HIS:ND1	2.31	0.46
31:G:58:ILE:HD12	31:G:58:ILE:H	1.80	0.46
31:G:221:LEU:HD11	31:G:225:LYS:NZ	2.30	0.46
16:V:64:CYS:O	16:V:67:ILE:HG22	2.16	0.46
27:E:95:VAL:HG12	27:E:97:LYS:HG2	1.97	0.46
9:C:26:GLU:HG3	9:C:27:TRP:N	2.30	0.46
17:P:42:ARG:NH1	28:2:1238:G:OP2	2.49	0.46
28:2:1281:C:H42	28:2:1286:A:H2	1.64	0.46
4:J:130:MET:HE3	4:J:136:ILE:HD11	1.97	0.46
27:E:8:HIS:HB3	27:E:27:TRP:CZ3	2.50	0.46
28:2:127:G:OP1	31:G:149:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:F:49:LYS:HE3	32:F:57:ARG:HH12	1.80	0.46
3:N:15:ALA:O	28:2:711:C:H5'	2.16	0.46
19:K:2:VAL:HG12	19:K:3:HIS:CE1	2.51	0.46
25:O:115:ARG:HG2	25:O:115:ARG:NH1	2.30	0.46
28:2:1009:U:H2'	28:2:1136:U:C5	2.51	0.46
28:2:1258:C:H2'	28:2:1258:C:O2	2.16	0.46
31:G:29:LYS:O	31:G:31:GLN:HB2	2.16	0.46
4:J:31:LYS:HG3	21:e:44:PHE:CE2	2.51	0.46
4:J:152:ILE:O	4:J:155:THR:HG22	2.16	0.46
8:Q:155:LYS:HD3	8:Q:157:TYR:CZ	2.51	0.46
9:C:77:ILE:HD11	9:C:119:ILE:HD11	1.98	0.46
17:P:52:MET:HE2	17:P:80:LEU:HD21	1.98	0.46
27:E:128:LYS:HB2	27:E:128:LYS:HE3	1.81	0.46
8:Q:58:ARG:NH2	28:2:1184:G:H1'	2.30	0.45
11:B:175:GLU:HG3	11:B:196:LYS:NZ	2.30	0.45
19:K:9:TYR:O	19:K:12:VAL:HB	2.16	0.45
4:J:19:LYS:O	4:J:25:ARG:NH2	2.49	0.45
20:I:97:SER:HB3	20:I:100:LEU:HD23	1.98	0.45
28:2:80:A:H5'	28:2:81:C:C5	2.51	0.45
32:F:178:GLN:O	32:F:182:VAL:HG23	2.16	0.45
2:T:55:ALA:HB1	2:T:107:PHE:HE2	1.82	0.45
3:N:145:GLN:O	3:N:149:LEU:HD13	2.15	0.45
11:B:131:ASP:OD1	11:B:131:ASP:N	2.49	0.45
13:b:76:ILE:O	13:b:84:ILE:HG13	2.16	0.45
19:K:45:LEU:CG	19:K:46:CYS:H	2.29	0.45
19:K:89:LYS:HA	19:K:89:LYS:HD2	1.75	0.45
20:I:165:LEU:O	20:I:169:GLN:HG3	2.15	0.45
22:H:115:ARG:HH22	28:2:519:C:H5	1.64	0.45
28:2:125:C:H5	31:G:199:LYS:HZ1	1.63	0.45
28:2:952:A:H2'	28:2:953:G:O4'	2.16	0.45
5:D:127:SER:HA	5:D:130:ARG:HG2	1.97	0.45
7:S:50:ALA:HB2	7:S:72:VAL:HG11	1.97	0.45
26:W:103:ILE:HD11	26:W:129:PHE:HE1	1.81	0.45
28:2:72:C:H2'	28:2:73:G:O4'	2.16	0.45
28:2:112:C:H3'	28:2:113:G:N2	2.31	0.45
28:2:363:C:H2'	28:2:363:C:O2	2.16	0.45
28:2:857:U:H2'	28:2:858:A:H8	1.81	0.45
28:2:1378:G:H2'	28:2:1379:C:C6	2.52	0.45
29:L:24:ARG:HH12	29:L:30:GLU:CD	2.23	0.45
10:A:21:LYS:HA	10:A:24:LEU:HD12	1.98	0.45
23:n:23:ARG:O	23:n:24:SER:OG	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:40:ASN:HB2	32:F:125:VAL:HG12	1.98	0.45
28:2:1348:G:H2'	28:2:1349:C:C6	2.52	0.45
28:2:1407:G:H2'	28:2:1408:A:C1'	2.47	0.45
2:T:55:ALA:HA	2:T:58:VAL:HG12	1.98	0.45
8:Q:131:LEU:HD23	8:Q:131:LEU:HA	1.78	0.45
10:A:62:LYS:HE2	10:A:62:LYS:HA	1.99	0.45
17:P:34:LEU:HD11	17:P:45:ILE:HG21	1.99	0.45
28:2:676:A:H2'	28:2:677:G:C8	2.51	0.45
31:G:63:ASP:HA	31:G:112:LEU:HA	1.99	0.45
16:V:22:PRO:HB2	16:V:31:LEU:HD22	1.99	0.45
21:e:15:ARG:HG3	21:e:15:ARG:NH2	2.31	0.45
3:N:89:TYR:CE2	3:N:93:LYS:HD2	2.52	0.45
4:J:63:THR:HB	26:W:87:GLU:OE1	2.17	0.45
18:R:31:ASN:O	18:R:35:ILE:HG12	2.17	0.45
27:E:121:PHE:HA	27:E:162:ILE:O	2.16	0.45
27:E:180:ILE:HD12	27:E:193:GLY:O	2.15	0.45
28:2:158:G:H5''	28:2:158:G:C8	2.48	0.45
28:2:613:C:H2'	28:2:614:G:O4'	2.16	0.45
28:2:1035:OMG:H1'	28:2:1035:OMG:HM23	1.50	0.45
28:2:1333:U:H2'	28:2:1334:C:C6	2.52	0.45
8:Q:71:MET:HE3	32:F:34:PHE:CE1	2.52	0.45
19:K:88:ARG:HG2	19:K:88:ARG:NH1	2.31	0.45
28:2:857:U:H2'	28:2:858:A:C8	2.51	0.45
28:2:1382:C:H2'	28:2:1383:G:O4'	2.17	0.45
7:S:102:VAL:O	7:S:105:ILE:HG13	2.17	0.45
26:W:16:ASN:OD1	26:W:19:ARG:NH2	2.50	0.45
28:2:80:A:H5'	28:2:81:C:H5	1.82	0.45
28:2:675:G:H2'	28:2:676:A:C8	2.52	0.45
31:G:80:ARG:HA	31:G:101:LYS:O	2.16	0.45
4:J:93:ASP:OD1	4:J:93:ASP:N	2.46	0.44
5:D:180:HIS:HB3	5:D:187:VAL:CG1	2.46	0.44
28:2:1117:G:H4'	28:2:1118:G:H5'	1.99	0.44
9:C:29:PRO:HB2	9:C:35:ARG:HG3	1.99	0.44
28:2:466:A:H2'	28:2:467:G:H8	1.82	0.44
28:2:1027:A:N1	28:2:1068:G:O2'	2.45	0.44
2:T:101:ARG:HA	2:T:104:VAL:HG22	1.99	0.44
7:S:40:ARG:O	7:S:44:ASN:ND2	2.50	0.44
10:A:85:ARG:HG3	10:A:85:ARG:NH1	2.32	0.44
24:c:53:LEU:HD23	24:c:53:LEU:HA	1.76	0.44
30:U:72:LYS:HD3	30:U:81:THR:OG1	2.16	0.44
4:J:99:LEU:HD23	4:J:99:LEU:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:1:MET:N	28:2:845:C:H41	2.15	0.44
16:V:52:LYS:HE3	16:V:52:LYS:HB2	1.77	0.44
28:2:364:G:HO2'	28:2:365:G:P	2.36	0.44
28:2:1094:A:H4'	28:2:1095:C:O4'	2.18	0.44
28:2:1217:C:H2'	28:2:1218:C:C6	2.52	0.44
28:2:171:G:O2'	28:2:172:G:C8	2.66	0.44
28:2:1145:C:O2'	28:2:1146:U:H6	1.99	0.44
28:2:1173:A:H2'	28:2:1174:C:C6	2.53	0.44
28:2:1295:C:H2'	28:2:1296:G:O4'	2.17	0.44
5:D:76:GLU:OE2	5:D:91:ASN:HA	2.17	0.44
24:c:26:LYS:HE2	24:c:38:ILE:HD11	1.99	0.44
27:E:139:LEU:HD23	27:E:150:PRO:HB3	2.00	0.44
28:2:92:A:H3'	28:2:93:A:H8	1.82	0.44
28:2:170:G:P	29:L:66:ARG:HH21	2.40	0.44
28:2:1305:C:H2'	28:2:1306:C:C6	2.48	0.44
32:F:43:SER:O	32:F:43:SER:OG	2.32	0.44
15:Z:43:THR:HG21	32:F:154:PRO:HD3	1.99	0.44
27:E:127:GLN:HA	27:E:127:GLN:OE1	2.18	0.44
28:2:364:G:H1'	28:2:365:G:C5	2.52	0.44
28:2:466:A:H2'	28:2:467:G:C8	2.53	0.44
28:2:1177:U:H4'	32:F:74:MET:HE1	1.99	0.44
31:G:107:ILE:O	31:G:108:VAL:C	2.61	0.44
5:D:76:GLU:CD	5:D:91:ASN:HA	2.43	0.44
6:X:61:GLN:HB3	6:X:62:PRO:HD3	2.00	0.44
7:S:28:LEU:HA	7:S:31:ALA:HB3	2.00	0.44
7:S:100:ILE:O	7:S:100:ILE:HG13	2.17	0.44
20:I:31:ARG:NH1	28:2:244:U:OP1	2.45	0.44
10:A:146:ASN:ND2	16:V:39:ALA:O	2.43	0.44
11:B:22:TYR:HA	11:B:25:LYS:CG	2.48	0.44
18:R:27:LYS:HB3	18:R:27:LYS:HE3	1.84	0.44
27:E:180:ILE:HD11	27:E:192:ILE:HG22	1.99	0.44
27:E:187:ARG:HH11	28:2:532:A:P	2.41	0.44
28:2:110:G:H8	28:2:110:G:H5''	1.83	0.44
28:2:1303:U:H2'	28:2:1304:C:C6	2.53	0.44
28:2:1355:C:H2'	28:2:1356:G:O4'	2.18	0.44
7:S:129:HIS:CE1	17:P:125:ILE:HG21	2.53	0.43
28:2:329:A:H5'	28:2:330:G:C4	2.52	0.43
28:2:393:G:O2'	28:2:394:A:O5'	2.36	0.43
28:2:413:G:H2'	28:2:414:A:H8	1.80	0.43
28:2:446:C:H5	28:2:458:G:OP2	2.01	0.43
31:G:20:LYS:HG3	31:G:21:SER:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:81:ILE:HA	7:S:82:PRO:HD3	1.88	0.43
17:P:40:ARG:HH12	28:2:1241:G:H1	1.64	0.43
17:P:81:ARG:HG3	17:P:81:ARG:NH1	2.30	0.43
19:K:26:GLU:HG3	19:K:26:GLU:O	2.18	0.43
31:G:24:ILE:HD11	31:G:31:GLN:HE22	1.83	0.43
32:F:181:SER:O	32:F:185:ILE:HG13	2.18	0.43
3:N:100:LYS:HE2	3:N:104:ARG:HH22	1.83	0.43
26:W:28:ARG:HB3	26:W:60:ARG:HG3	2.00	0.43
27:E:32:THR:HG22	27:E:33:ASN:O	2.18	0.43
28:2:156:G:O2'	28:2:157:U:H5'	2.18	0.43
28:2:1031:C:H2'	28:2:1032:G:H8	1.82	0.43
31:G:76:SER:HA	31:G:106:CYS:HA	2.00	0.43
7:S:26:VAL:HG23	7:S:31:ALA:HB2	2.00	0.43
9:C:84:THR:HB	9:C:87:GLY:O	2.18	0.43
17:P:64:ARG:HG2	17:P:65:ARG:NH2	2.33	0.43
28:2:242:G:H2'	28:2:243:G:C8	2.53	0.43
28:2:1005:G:H2'	28:2:1005:G:N3	2.33	0.43
31:G:108:VAL:HG23	31:G:112:LEU:HD12	2.00	0.43
8:Q:28:LEU:HD23	8:Q:28:LEU:HA	1.87	0.43
17:P:33:ILE:O	17:P:36:LYS:HB2	2.19	0.43
17:P:62:ARG:HG3	17:P:63:LEU:HD12	2.00	0.43
20:I:16:ALA:HB2	28:2:266:C:H5''	2.00	0.43
28:2:16:G:H2'	28:2:17:C:C6	2.53	0.43
28:2:124:G:N1	31:G:203:LYS:HE2	2.27	0.43
28:2:288:C:H2'	28:2:289:G:O4'	2.18	0.43
28:2:868:OMG:H1'	28:2:868:OMG:HM23	1.77	0.43
28:2:1075:C:O2'	28:2:1076:G:H5'	2.18	0.43
7:S:27:VAL:HG12	7:S:29:GLU:HB2	2.01	0.43
20:I:89:LEU:O	20:I:90:GLN:HG2	2.18	0.43
28:2:52:G:H2'	28:2:53:C:C6	2.53	0.43
28:2:621:G:H2'	28:2:622:C:H6	1.83	0.43
28:2:702:C:H2'	28:2:703:A:C8	2.53	0.43
14:a:92:ARG:HB3	28:2:1449:C:O2	2.19	0.43
20:I:117:ALA:HA	20:I:120:LYS:NZ	2.33	0.43
21:e:61:LEU:HD11	28:2:440:C:H5'	2.01	0.43
22:H:103:LYS:O	22:H:116:ARG:NH2	2.52	0.43
28:2:1031:C:H2'	28:2:1032:G:C8	2.54	0.43
28:2:1221:C:H4'	28:2:1227:C:H42	1.83	0.43
32:F:68:ASN:HA	32:F:71:LYS:HD2	2.00	0.43
4:J:65:ASP:O	4:J:71:ARG:HD3	2.19	0.43
9:C:59:GLU:HA	9:C:62:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:98:THR:O	11:B:232:HIS:NE2	2.42	0.43
27:E:251:ARG:HG3	28:2:542:A:O2'	2.18	0.43
28:2:1279:C:H2'	28:2:1280:G:C8	2.54	0.43
32:F:64:MET:O	32:F:64:MET:HG2	2.19	0.43
5:D:17:TYR:HE2	30:U:34:LYS:HB3	1.83	0.43
7:S:41:ARG:NH1	7:S:85:MET:HE1	2.34	0.43
31:G:150:LEU:HD22	31:G:151:PHE:CD1	2.53	0.43
9:C:75:CYS:SG	9:C:97:ILE:HG12	2.59	0.43
9:C:193:ARG:HD3	28:2:2:A:N3	2.33	0.43
22:H:84:LEU:HB3	22:H:93:PHE:CD2	2.54	0.43
28:2:945:C:H6	28:2:945:C:O5'	2.02	0.43
5:D:208:ILE:O	5:D:208:ILE:HG23	2.19	0.42
11:B:90:LEU:HD23	11:B:97:LEU:HD12	2.01	0.42
15:Z:68:ASP:HB3	15:Z:80:ILE:HG22	2.01	0.42
19:K:24:LEU:HB3	19:K:75:HIS:HB2	2.01	0.42
26:W:71:LYS:HE3	28:2:841:C:OP1	2.19	0.42
27:E:44:LEU:HD23	27:E:65:LEU:HD21	2.01	0.42
28:2:366:C:C2	28:2:367:G:C8	3.07	0.42
28:2:1292:C:H2'	28:2:1293:G:C8	2.54	0.42
30:U:29:ILE:HG13	30:U:120:VAL:HG12	2.01	0.42
32:F:32:HIS:HE1	32:F:54:VAL:HG22	1.84	0.42
9:C:236:ARG:HE	9:C:236:ARG:HB2	1.66	0.42
11:B:34:ALA:HB2	11:B:232:HIS:O	2.19	0.42
13:b:44:MET:HE2	13:b:44:MET:HA	2.01	0.42
28:2:155:C:O4'	28:2:155:C:O2	2.36	0.42
28:2:908:C:H2'	28:2:909:G:O4'	2.18	0.42
4:J:26:LEU:HD12	4:J:26:LEU:HA	1.87	0.42
6:X:134:PHE:CD2	6:X:135:LEU:HD23	2.54	0.42
18:R:27:LYS:O	18:R:31:ASN:ND2	2.52	0.42
28:2:935:A:H8	28:2:935:A:OP1	2.02	0.42
4:J:127:ALA:O	4:J:131:ILE:HG12	2.18	0.42
5:D:130:ARG:HG3	5:D:131:THR:N	2.34	0.42
6:X:1:MET:C	6:X:3:LYS:H	2.27	0.42
6:X:74:LEU:CD1	6:X:81:ILE:HG12	2.50	0.42
8:Q:100:ARG:NH1	8:Q:131:LEU:HD21	2.33	0.42
17:P:33:ILE:HD12	17:P:33:ILE:H	1.84	0.42
25:O:39:THR:HG22	25:O:46:THR:HA	2.02	0.42
28:2:365:G:C2	28:2:366:C:N3	2.87	0.42
19:K:59:SER:O	19:K:63:ARG:HG2	2.18	0.42
20:I:169:GLN:HE21	20:I:169:GLN:HB3	1.60	0.42
28:2:141:A:O2'	28:2:142:C:H6	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:1146:U:H2'	28:2:1147:C:O4'	2.20	0.42
28:2:1434:MA6:H8	28:2:1434:MA6:O5'	2.19	0.42
3:N:144:ASP:OD1	3:N:145:GLN:N	2.53	0.42
12:Y:92:ILE:HG23	12:Y:98:GLU:HA	2.01	0.42
28:2:1097:G:C2	28:2:1098:C:C6	3.07	0.42
28:2:1288:C:H2'	28:2:1289:G:H8	1.82	0.42
1:d:124:PHE:O	1:d:128:ALA:HB2	2.20	0.42
5:D:168:HIS:CD2	5:D:172:ILE:HD11	2.55	0.42
7:S:121:CYS:O	7:S:125:VAL:HG23	2.19	0.42
11:B:205:THR:HG22	11:B:206:MET:N	2.32	0.42
13:b:49:LEU:HG	22:H:143:ARG:NH2	2.35	0.42
17:P:54:HIS:HA	17:P:57:PHE:CD2	2.54	0.42
27:E:124:CYS:HB3	27:E:141:THR:HB	2.01	0.42
28:2:252:C:H2'	28:2:253:G:C8	2.55	0.42
28:2:1133:G:H2'	28:2:1134:U:C6	2.55	0.42
28:2:1232:C:H2'	28:2:1233:C:O4'	2.20	0.42
5:D:176:GLU:HG3	5:D:193:ARG:HG2	2.02	0.42
8:Q:66:VAL:HG13	8:Q:96:ILE:HG23	2.01	0.42
11:B:129:THR:OG1	11:B:133:TYR:HB2	2.20	0.42
16:V:78:MET:HE2	16:V:78:MET:HB3	1.80	0.42
20:I:132:ILE:O	20:I:136:ILE:HG13	2.18	0.42
28:2:1407:G:C4	28:2:1408:A:H1'	2.55	0.42
20:I:79:SER:HB2	20:I:161:GLU:OE1	2.19	0.42
31:G:227:LEU:HA	31:G:230:ARG:HE	1.85	0.42
1:d:114:LYS:O	1:d:117:LEU:HD23	2.20	0.41
7:S:73:LEU:HD23	7:S:73:LEU:HA	1.91	0.41
8:Q:59:PRO:HB2	8:Q:96:ILE:HD11	2.02	0.41
22:H:151:ASN:HA	22:H:152:PRO:HD2	1.97	0.41
22:H:163:TYR:HA	22:H:189:PHE:HE2	1.84	0.41
26:W:52:VAL:HG22	26:W:61:ILE:HG12	2.02	0.41
28:2:112:C:H3'	28:2:113:G:H21	1.83	0.41
28:2:1286:A:O2'	28:2:1287:C:OP2	2.30	0.41
31:G:26:ASP:HA	31:G:31:GLN:NE2	2.33	0.41
4:J:18:LYS:HE3	4:J:18:LYS:HB3	1.90	0.41
8:Q:119:GLU:HG3	8:Q:120:LEU:N	2.35	0.41
28:2:70:G:H2'	28:2:71:A:C8	2.56	0.41
28:2:87:A2M:H1'	28:2:87:A2M:HM'3	1.77	0.41
1:d:115:TYR:HB2	1:d:117:LEU:CD2	2.50	0.41
3:N:47:PRO:HA	3:N:50:ILE:HD12	2.03	0.41
8:Q:31:LYS:HG2	8:Q:94:SER:HA	2.01	0.41
10:A:23:MET:SD	10:A:56:LEU:HD22	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Z:59:VAL:O	15:Z:63:LEU:HG	2.19	0.41
28:2:810:C:H2'	28:2:811:C:C6	2.55	0.41
28:2:912:G:C2	28:2:913:A:C8	3.08	0.41
28:2:1327:C:H2'	28:2:1328:G:C8	2.54	0.41
28:2:1380:C:O2'	28:2:1381:G:OP1	2.37	0.41
31:G:84:ARG:HE	31:G:98:ARG:NE	2.19	0.41
7:S:44:ASN:O	7:S:48:LYS:HE3	2.21	0.41
8:Q:122:ALA:HA	8:Q:125:VAL:HG22	2.02	0.41
11:B:136:ARG:HG2	11:B:138:PHE:CE1	2.55	0.41
15:Z:62:GLN:HA	15:Z:65:LYS:NZ	2.36	0.41
19:K:65:VAL:O	19:K:80:THR:HG22	2.20	0.41
28:2:475:A:H4'	28:2:476:G:H5'	2.03	0.41
28:2:587:G:O2'	28:2:588:C:P	2.78	0.41
28:2:859:U:H2'	28:2:860:G:H8	1.84	0.41
31:G:29:LYS:HD3	31:G:29:LYS:HA	1.65	0.41
2:T:6:ARG:HB2	2:T:6:ARG:NH1	2.35	0.41
6:X:101:LEU:HB3	6:X:124:LYS:HB2	2.00	0.41
7:S:76:PRO:HA	7:S:81:ILE:HD12	2.02	0.41
7:S:81:ILE:H	7:S:81:ILE:HG13	1.72	0.41
14:a:2:PRO:HB3	28:2:884:C:H5''	2.02	0.41
19:K:4:ILE:N	19:K:5:PRO:HD2	2.36	0.41
25:O:66:TYR:O	25:O:70:GLN:HG3	2.20	0.41
26:W:104:LEU:HD23	26:W:125:VAL:HA	2.02	0.41
28:2:110:G:H3'	28:2:111:G:H5''	2.01	0.41
28:2:111:G:H2'	28:2:112:C:O4'	2.20	0.41
19:K:46:CYS:C	19:K:48:PRO:HD3	2.46	0.41
22:H:106:TYR:CZ	22:H:115:ARG:HD3	2.55	0.41
28:2:363:C:H6	28:2:363:C:O5'	2.04	0.41
28:2:364:G:H1'	28:2:365:G:C4	2.56	0.41
28:2:1142:G:H2'	28:2:1143:C:O4'	2.21	0.41
28:2:1373:G:OP2	28:2:1373:G:H8	2.03	0.41
29:L:72:ASN:OD1	29:L:72:ASN:O	2.38	0.41
7:S:74:GLU:C	7:S:99:HIS:HE2	2.28	0.41
9:C:51:TYR:O	9:C:53:LEU:HG	2.21	0.41
17:P:45:ILE:HD13	17:P:45:ILE:HA	1.90	0.41
28:2:306:C:H4'	31:G:98:ARG:NH2	2.36	0.41
30:U:26:LYS:HZ1	30:U:97:THR:HB	1.85	0.41
2:T:34:TYR:HB2	7:S:85:MET:SD	2.61	0.41
5:D:23:MET:HE2	5:D:27:LEU:HD11	2.03	0.41
5:D:78:LEU:HD23	5:D:78:LEU:HA	1.96	0.41
28:2:426:C:H5''	28:2:427:G:N7	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:577:G:H2'	28:2:578:G:O4'	2.21	0.41
31:G:75:LYS:O	31:G:107:ILE:HG23	2.20	0.41
4:J:115:ILE:HG21	4:J:136:ILE:HD13	2.03	0.41
10:A:163:ASP:OD1	16:V:68:ARG:NH1	2.53	0.41
12:Y:14:ASN:OD1	12:Y:17:LEU:HB2	2.20	0.41
12:Y:60:PHE:O	28:2:401:C:O2'	2.35	0.41
17:P:43:ARG:NE	28:2:1241:G:O6	2.49	0.41
18:R:40:ASN:O	18:R:40:ASN:CG	2.64	0.41
20:I:52:LYS:HD2	20:I:69:ARG:HH22	1.86	0.41
25:O:127:THR:HA	25:O:128:PRO:HD3	1.94	0.41
27:E:99:PHE:HB3	27:E:111:LEU:HB3	2.03	0.41
28:2:156:G:H2'	28:2:157:U:C6	2.56	0.41
28:2:1098:C:H2'	28:2:1099:C:C6	2.56	0.41
30:U:48:LYS:O	30:U:48:LYS:HG3	2.20	0.41
31:G:148:ARG:HD2	31:G:154:PRO:O	2.21	0.41
17:P:17:PHE:O	17:P:18:ARG:C	2.63	0.41
20:I:130:LYS:HE2	20:I:130:LYS:HB3	1.91	0.41
22:H:58:LYS:HE3	22:H:58:LYS:HB2	1.87	0.41
28:2:395:G:H2'	28:2:396:U:H5'	2.02	0.41
4:J:20:PRO:HA	4:J:25:ARG:HH22	1.85	0.40
7:S:102:VAL:HG22	7:S:103:ASN:N	2.36	0.40
15:Z:69:PHE:CE2	15:Z:83:ASN:HA	2.56	0.40
27:E:158:ASP:CG	27:E:174:LYS:HA	2.46	0.40
28:2:1286:A:N3	28:2:1286:A:H2'	2.36	0.40
30:U:31:VAL:O	30:U:91:LYS:HA	2.21	0.40
2:T:43:TYR:CD1	7:S:40:ARG:HD3	2.56	0.40
19:K:45:LEU:HG	19:K:46:CYS:N	2.37	0.40
27:E:60:GLU:HA	27:E:63:MET:HG2	2.04	0.40
28:2:1013:G:O6	28:2:1134:U:H2'	2.22	0.40
28:2:1308:G:H2'	28:2:1309:C:H6	1.85	0.40
14:a:46:ASP:OD1	14:a:47:ASN:N	2.55	0.40
17:P:87:PRO:HG3	17:P:112:VAL:HG11	2.02	0.40
28:2:888:G:H2'	28:2:889:A:C8	2.56	0.40
28:2:1301:C:H5''	28:2:1302:G:O5'	2.21	0.40
28:2:1392:C:H2'	28:2:1393:G:C8	2.56	0.40
5:D:58:CYS:O	5:D:97:ILE:N	2.46	0.40
10:A:78:GLU:OE1	10:A:125:ARG:HD3	2.21	0.40
28:2:471:G:H2'	28:2:472:G:C8	2.56	0.40
28:2:638:U:C2	28:2:639:A:C8	3.09	0.40
28:2:791:C:H2'	28:2:792:G:O4'	2.20	0.40
28:2:912:G:N3	28:2:912:G:H2'	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:1006:C:H2'	28:2:1007:G:O4'	2.22	0.40
28:2:1078:C:H1'	28:2:1115:A:C4	2.57	0.40
28:2:1380:C:H2'	28:2:1381:G:H8	1.85	0.40
1:d:113:ARG:HG2	28:2:1281:C:OP1	2.22	0.40
7:S:14:LEU:C	7:S:15:LEU:HD12	2.45	0.40
20:I:25:ARG:HA	28:2:312:G:H5''	2.03	0.40
24:c:16:THR:HB	24:c:22:ILE:HG13	2.03	0.40
28:2:316:G:H2'	28:2:317:C:C6	2.56	0.40
28:2:393:G:HO2'	28:2:394:A:H8	1.70	0.40
28:2:1177:U:H4'	32:F:74:MET:CE	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	d	46/137 (34%)	43 (94%)	3 (6%)	0	100	100
2	T	128/139 (92%)	116 (91%)	10 (8%)	2 (2%)	7	17
3	N	150/154 (97%)	145 (97%)	3 (2%)	2 (1%)	9	21
4	J	164/189 (87%)	162 (99%)	2 (1%)	0	100	100
5	D	174/217 (80%)	160 (92%)	14 (8%)	0	100	100
6	X	140/143 (98%)	133 (95%)	6 (4%)	1 (1%)	18	35
7	S	131/154 (85%)	116 (88%)	15 (12%)	0	100	100
8	Q	119/158 (75%)	110 (92%)	9 (8%)	0	100	100
9	C	210/242 (87%)	201 (96%)	9 (4%)	0	100	100
10	A	192/245 (78%)	185 (96%)	7 (4%)	0	100	100
11	B	216/248 (87%)	210 (97%)	6 (3%)	0	100	100
12	Y	86/132 (65%)	82 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	b	77/124 (62%)	74 (96%)	3 (4%)	0	100	100
14	a	95/109 (87%)	91 (96%)	4 (4%)	0	100	100
15	Z	57/88 (65%)	52 (91%)	5 (9%)	0	100	100
16	V	80/89 (90%)	73 (91%)	7 (9%)	0	100	100
17	P	101/145 (70%)	88 (87%)	11 (11%)	2 (2%)	6	13
18	R	95/137 (69%)	91 (96%)	4 (4%)	0	100	100
19	K	79/134 (59%)	69 (87%)	10 (13%)	0	100	100
20	I	159/174 (91%)	155 (98%)	4 (2%)	0	100	100
21	e	31/69 (45%)	31 (100%)	0	0	100	100
22	H	148/190 (78%)	137 (93%)	11 (7%)	0	100	100
23	n	22/41 (54%)	22 (100%)	0	0	100	100
24	c	51/64 (80%)	48 (94%)	3 (6%)	0	100	100
25	O	124/145 (86%)	121 (98%)	3 (2%)	0	100	100
26	W	127/130 (98%)	118 (93%)	9 (7%)	0	100	100
27	E	256/268 (96%)	246 (96%)	10 (4%)	0	100	100
29	L	179/199 (90%)	169 (94%)	10 (6%)	0	100	100
30	U	68/126 (54%)	66 (97%)	2 (3%)	0	100	100
31	G	187/248 (75%)	170 (91%)	17 (9%)	0	100	100
32	F	157/190 (83%)	154 (98%)	3 (2%)	0	100	100
All	All	3849/4828 (80%)	3638 (94%)	204 (5%)	7 (0%)	44	62

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	T	26	ILE
17	P	37	LEU
2	T	27	LYS
3	N	8	GLY
17	P	36	LYS
3	N	9	LYS
6	X	88	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	d	42/116 (36%)	42 (100%)	0	100	100
2	T	86/115 (75%)	86 (100%)	0	100	100
3	N	124/130 (95%)	122 (98%)	2 (2%)	55	76
4	J	141/164 (86%)	141 (100%)	0	100	100
5	D	142/182 (78%)	142 (100%)	0	100	100
6	X	113/114 (99%)	113 (100%)	0	100	100
7	S	112/131 (86%)	112 (100%)	0	100	100
8	Q	101/130 (78%)	101 (100%)	0	100	100
9	C	176/201 (88%)	176 (100%)	0	100	100
10	A	168/217 (77%)	168 (100%)	0	100	100
11	B	196/220 (89%)	196 (100%)	0	100	100
12	Y	77/113 (68%)	77 (100%)	0	100	100
13	b	70/112 (62%)	70 (100%)	0	100	100
14	a	90/103 (87%)	90 (100%)	0	100	100
15	Z	41/79 (52%)	41 (100%)	0	100	100
16	V	62/72 (86%)	62 (100%)	0	100	100
17	P	87/128 (68%)	87 (100%)	0	100	100
18	R	82/123 (67%)	82 (100%)	0	100	100
19	K	73/119 (61%)	73 (100%)	0	100	100
20	I	138/148 (93%)	137 (99%)	1 (1%)	76	87
21	e	30/58 (52%)	30 (100%)	0	100	100
22	H	116/170 (68%)	116 (100%)	0	100	100
23	n	21/38 (55%)	21 (100%)	0	100	100
24	c	49/57 (86%)	49 (100%)	0	100	100
25	O	91/113 (80%)	91 (100%)	0	100	100
26	W	114/115 (99%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	E	224/232 (97%)	224 (100%)	0	100	100
29	L	154/173 (89%)	154 (100%)	0	100	100
30	U	68/110 (62%)	68 (100%)	0	100	100
31	G	162/213 (76%)	162 (100%)	0	100	100
32	F	132/157 (84%)	132 (100%)	0	100	100
All	All	3282/4153 (79%)	3279 (100%)	3 (0%)	87	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	N	3	ARG
3	N	9	LYS
20	I	23	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	d	109	ASN
2	T	42	GLN
3	N	26	ASN
4	J	112	GLN
5	D	28	HIS
7	S	44	ASN
8	Q	84	ASN
8	Q	92	HIS
9	C	125	ASN
10	A	120	ASN
10	A	130	ASN
10	A	169	ASN
11	B	40	HIS
11	B	60	ASN
11	B	155	HIS
11	B	223	ASN
12	Y	52	GLN
14	a	8	ASN
14	a	69	ASN
15	Z	44	GLN
18	R	20	ASN
19	K	3	HIS

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Mol	Chain	Res	Type
19	K	42	ASN
26	W	5	ASN
26	W	44	ASN
26	W	56	HIS
26	W	59	ASN
27	E	50	ASN
27	E	53	HIS
27	E	163	ASN
29	L	64	GLN
29	L	107	ASN
29	L	136	HIS
29	L	182	ASN
31	G	31	GLN
31	G	92	HIS
31	G	192	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	2	1335/1452 (91%)	287 (21%)	15 (1%)

All (287) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
28	2	4	C
28	2	9	C
28	2	17	C
28	2	33	U
28	2	41	G
28	2	42	A
28	2	44	G
28	2	46	A
28	2	56	G
28	2	64	A
28	2	87	A2M
28	2	91	C
28	2	92	A
28	2	101	A
28	2	111	G
28	2	116	C
28	2	125	C

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Mol	Chain	Res	Type
28	2	128	G
28	2	129	A
28	2	130	C
28	2	134	G
28	2	136	U
28	2	137	G
28	2	142	C
28	2	149	C
28	2	150	C
28	2	154	A
28	2	155	C
28	2	158	G
28	2	159	C
28	2	161	C
28	2	162	G
28	2	170	G
28	2	171	G
28	2	172	G
28	2	173	C
28	2	176	C
28	2	183	C
28	2	184	G
28	2	186	G
28	2	193	G
28	2	202	A
28	2	203	C
28	2	204	G
28	2	205	G
28	2	209	G
28	2	216	C
28	2	223	G
28	2	228	C
28	2	229	A
28	2	230	C
28	2	234	G
28	2	241	C
28	2	249	G
28	2	250	C
28	2	256	G
28	2	263	C
28	2	264	G
28	2	271	G

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Mol	Chain	Res	Type
28	2	272	G
28	2	273	C
28	2	282	A
28	2	289	G
28	2	290	A
28	2	292	U
28	2	302	G
28	2	303	G
28	2	312	G
28	2	313	A
28	2	314	C
28	2	316	G
28	2	324	A
28	2	328	A
28	2	329	A
28	2	330	G
28	2	336	C
28	2	337	A
28	2	338	G
28	2	340	A
28	2	351	U
28	2	353	G
28	2	356	C
28	2	362	G
28	2	363	C
28	2	365	G
28	2	378	C
28	2	387	G
28	2	389	G
28	2	390	C
28	2	391	G
28	2	393	G
28	2	394	A
28	2	396	U
28	2	400	G
28	2	438	G
28	2	446	C
28	2	449	G
28	2	454	C
28	2	455	G
28	2	458	G
28	2	459	U

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Mol	Chain	Res	Type
28	2	460	A
28	2	461	A
28	2	475	A
28	2	476	G
28	2	477	C
28	2	492	C
28	2	500	G
28	2	501	A
28	2	504	C
28	2	519	C
28	2	520	C
28	2	521	C
28	2	525	C
28	2	526	G
28	2	527	C
28	2	534	G
28	2	535	A
28	2	536	A
28	2	540	G
28	2	545	G
28	2	546	C
28	2	554	A
28	2	555	G
28	2	562	U
28	2	569	G
28	2	570	C
28	2	579	A
28	2	582	G
28	2	588	C
28	2	593	C
28	2	594	C
28	2	595	G
28	2	601	C
28	2	602	C
28	2	603	G
28	2	604	C
28	2	606	G
28	2	608	A
28	2	611	C
28	2	615	A
28	2	625	G
28	2	628	G

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Mol	Chain	Res	Type
28	2	650	A
28	2	659	A
28	2	662	G
28	2	665	U
28	2	685	G
28	2	687	C
28	2	704	A
28	2	712	U
28	2	718	A
28	2	722	A
28	2	740	C
28	2	744	A
28	2	756	C
28	2	757	A
28	2	778	A
28	2	780	C
28	2	784	G
28	2	791	C
28	2	792	G
28	2	794	G
28	2	804	C
28	2	812	G
28	2	833	G
28	2	834	G
28	2	836	G
28	2	839	U
28	2	840	C
28	2	842	G
28	2	850	G
28	2	851	G
28	2	856	G
28	2	868	OMG
28	2	880	A
28	2	888	G
28	2	892	G
28	2	900	C
28	2	903	C
28	2	909	G
28	2	921	G
28	2	927	U
28	2	928	C
28	2	932	C

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Mol	Chain	Res	Type
28	2	933	C4J
28	2	934	C
28	2	936	A
28	2	938	G
28	2	942	G
28	2	949	A
28	2	951	C
28	2	984	C
28	2	1009	U
28	2	1010	G
28	2	1013	G
28	2	1014	C
28	2	1020	C
28	2	1025	C
28	2	1027	A
28	2	1028	G
28	2	1041	G
28	2	1054	U
28	2	1057	C
28	2	1059	A
28	2	1061	A
28	2	1068	G
28	2	1076	G
28	2	1077	G
28	2	1080	G
28	2	1088	C
28	2	1089	G
28	2	1090	C
28	2	1096	G
28	2	1099	C
28	2	1102	C
28	2	1112	A
28	2	1119	C
28	2	1129	G
28	2	1131	A
28	2	1132	G
28	2	1135	C
28	2	1136	U
28	2	1139	G
28	2	1140	A
28	2	1146	U
28	2	1147	C

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Mol	Chain	Res	Type
28	2	1162	G
28	2	1163	C
28	2	1164	A
28	2	1175	A
28	2	1183	G
28	2	1190	C
28	2	1191	G
28	2	1192	G
28	2	1194	G
28	2	1200	G
28	2	1202	G
28	2	1208	G
28	2	1225	G
28	2	1244	A
28	2	1245	C
28	2	1246	G
28	2	1257	C
28	2	1262	A
28	2	1270	G
28	2	1276	G
28	2	1283	C
28	2	1287	C
28	2	1293	G
28	2	1305	C
28	2	1320	C
28	2	1321	A
28	2	1343	U
28	2	1344	G
28	2	1350	U
28	2	1351	G
28	2	1366	G
28	2	1367	A
28	2	1374	A
28	2	1380	C
28	2	1381	G
28	2	1384	A
28	2	1390	M7A
28	2	1392	C
28	2	1393	G
28	2	1394	C
28	2	1403	A
28	2	1406	A

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Mol	Chain	Res	Type
28	2	1408	A
28	2	1409	A
28	2	1410	G
28	2	1412	C
28	2	1413	G
28	2	1415	A
28	2	1419	A
28	2	1421	G
28	2	1422	U
28	2	1426	4AC
28	2	1433	G
28	2	1436	C
28	2	1445	G
28	2	1446	G
28	2	1447	A
28	2	1448	U
28	2	1449	C
28	2	1452	U

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
28	2	8	U
28	2	158	G
28	2	204	G
28	2	302	G
28	2	329	A
28	2	600	G
28	2	603	G
28	2	850	G
28	2	941	C
28	2	948	C
28	2	1118	G
28	2	1135	C
28	2	1199	C
28	2	1380	C
28	2	1421	G

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

15 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$
28	MA6	2	1434	28	23,26,27	1.43	4 (17%)	33,38,41	3.25	12 (36%)
28	OMC	2	104	28	19,22,23	0.84	0	25,31,34	0.93	2 (8%)
28	OMG	2	1035	28,33	23,26,27	1.21	3 (13%)	32,38,41	2.15	9 (28%)
28	OMU	2	1314	28	19,22,23	2.98	8 (42%)	25,31,34	1.79	4 (16%)
28	A2M	2	87	28,33	22,25,26	3.24	10 (45%)	30,36,39	2.89	12 (40%)
28	OMG	2	371	28,33	23,26,27	2.35	8 (34%)	32,38,41	2.01	8 (25%)
28	7MG	2	1261	28	23,26,27	3.49	11 (47%)	27,39,42	2.21	9 (33%)
28	4AC	2	1426	28,33	21,24,25	4.43	16 (76%)	28,34,37	1.35	3 (10%)
28	MA6	2	1435	28	23,26,27	1.43	4 (17%)	33,38,41	3.36	12 (36%)
28	OMG	2	1011	28	23,26,27	1.21	3 (13%)	32,38,41	2.10	7 (21%)
28	OMG	2	868	28	23,26,27	2.31	8 (34%)	32,38,41	1.66	9 (28%)
28	4OC	2	1325	28	20,23,24	3.14	8 (40%)	25,32,35	1.01	1 (4%)
28	C4J	2	933	28	25,29,30	3.22	9 (36%)	28,42,45	1.49	5 (17%)
28	M7A	2	1390	28	19,25,26	0.39	0	25,37,40	0.61	0
28	A2M	2	348	28,34	22,25,26	3.23	9 (40%)	30,36,39	2.99	11 (36%)

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
28	MA6	2	1434	28	-	0/11/29/30	0/3/3/3
28	OMC	2	104	28	-	0/9/27/28	0/2/2/2
28	OMG	2	1035	28,33	-	1/9/27/28	0/3/3/3
28	OMU	2	1314	28	-	0/9/27/28	0/2/2/2
28	A2M	2	87	28,33	-	3/9/27/28	0/3/3/3
28	OMG	2	371	28,33	-	1/9/27/28	0/3/3/3
28	7MG	2	1261	28	-	0/7/37/38	0/3/3/3
28	4AC	2	1426	28,33	-	2/11/29/30	0/2/2/2
28	MA6	2	1435	28	-	2/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	OMG	2	1011	28	-	3/9/27/28	0/3/3/3
28	OMG	2	868	28	-	5/9/27/28	0/3/3/3
28	4OC	2	1325	28	-	0/9/29/30	0/2/2/2
28	C4J	2	933	28	-	4/16/34/35	0/2/2/2
28	M7A	2	1390	28	-	0/7/37/38	0/3/3/3
28	A2M	2	348	28,34	-	0/9/27/28	0/3/3/3

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	2	933	C4J	C6-C5	11.52	1.51	1.35
28	2	1426	4AC	O4'-C1'	8.98	1.62	1.42
28	2	87	A2M	C3'-C4'	-8.81	1.30	1.53
28	2	348	A2M	C3'-C4'	-8.70	1.30	1.53
28	2	1261	7MG	C8-N9	8.23	1.51	1.45
28	2	87	A2M	O4'-C4'	7.77	1.62	1.45
28	2	348	A2M	O4'-C4'	7.67	1.62	1.45
28	2	1325	4OC	C4-N3	7.09	1.44	1.32
28	2	1314	OMU	C2-N1	7.07	1.49	1.38
28	2	1426	4AC	C4-N3	7.04	1.44	1.32
28	2	1426	4AC	C2'-C1'	-6.98	1.31	1.53
28	2	1426	4AC	C6-C5	6.66	1.50	1.35
28	2	1261	7MG	C5-N7	6.59	1.44	1.35
28	2	1314	OMU	C2-N3	6.45	1.49	1.38
28	2	371	OMG	C4-N3	6.35	1.48	1.34
28	2	1325	4OC	C2-N3	6.27	1.48	1.36
28	2	933	C4J	C2-N3	6.22	1.49	1.38
28	2	1325	4OC	C6-C5	6.00	1.49	1.35
28	2	868	OMG	C4-N3	5.86	1.47	1.34
28	2	1261	7MG	C2-N3	5.84	1.47	1.33
28	2	1261	7MG	C4-N3	5.77	1.47	1.34
28	2	1426	4AC	C2-N1	5.56	1.51	1.40
28	2	1314	OMU	C6-C5	5.45	1.47	1.35
28	2	371	OMG	C2-N3	5.44	1.46	1.33
28	2	1261	7MG	C4-N9	5.35	1.44	1.37
28	2	1426	4AC	O4'-C4'	-5.13	1.33	1.45
28	2	868	OMG	C2-N3	5.11	1.45	1.33
28	2	348	A2M	O4'-C1'	-4.94	1.30	1.42
28	2	1426	4AC	C2-N3	4.92	1.46	1.36
28	2	1261	7MG	C2-N2	4.81	1.45	1.34
28	2	1325	4OC	C4-N4	4.74	1.45	1.36
28	2	87	A2M	O4'-C1'	-4.70	1.31	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	2	1426	4AC	C7-N4	4.37	1.46	1.37
28	2	1325	4OC	C2-N1	4.27	1.49	1.40
28	2	348	A2M	C6-N6	4.22	1.45	1.34
28	2	87	A2M	C6-N6	4.22	1.45	1.34
28	2	868	OMG	C2-N2	4.09	1.43	1.34
28	2	933	C4J	C1'-C5	-4.05	1.41	1.50
28	2	1314	OMU	C4-N3	4.04	1.45	1.38
28	2	371	OMG	C2-N2	3.95	1.43	1.34
28	2	1434	MA6	C6-N6	3.93	1.47	1.36
28	2	1426	4AC	C4-N4	3.87	1.45	1.39
28	2	1435	MA6	C6-N6	3.75	1.47	1.36
28	2	1261	7MG	C2-N1	3.68	1.46	1.37
28	2	1426	4AC	C5-C4	3.63	1.49	1.41
28	2	1426	4AC	CM7-C7	3.60	1.58	1.50
28	2	933	C4J	C6-N1	3.57	1.45	1.36
28	2	933	C4J	C2-N1	3.56	1.49	1.39
28	2	1261	7MG	C5-C6	3.52	1.52	1.43
28	2	1325	4OC	C5-C4	3.46	1.48	1.41
28	2	1426	4AC	O3'-C3'	-3.45	1.34	1.43
28	2	868	OMG	O6-C6	-3.42	1.17	1.23
28	2	933	C4J	C4-N3	3.33	1.46	1.40
28	2	1435	MA6	C5-C4	-3.30	1.33	1.39
28	2	1314	OMU	O4-C4	-3.26	1.18	1.24
28	2	933	C4J	O4-C4	-3.16	1.16	1.23
28	2	348	A2M	C5-C4	-3.15	1.33	1.39
28	2	87	A2M	C5-N7	-3.11	1.33	1.39
28	2	1434	MA6	C5-C4	-3.09	1.33	1.39
28	2	371	OMG	O6-C6	-3.08	1.17	1.23
28	2	87	A2M	C8-N9	-3.05	1.32	1.37
28	2	1325	4OC	O2-C2	-3.03	1.18	1.23
28	2	1325	4OC	C6-N1	2.99	1.45	1.38
28	2	87	A2M	C5-C4	-2.98	1.33	1.39
28	2	371	OMG	C5-N7	-2.98	1.33	1.39
28	2	348	A2M	C8-N9	-2.94	1.32	1.37
28	2	868	OMG	C5-N7	-2.93	1.33	1.39
28	2	1261	7MG	C6-N1	2.92	1.44	1.38
28	2	348	A2M	O3'-C3'	2.85	1.50	1.43
28	2	1011	OMG	C5-C4	2.85	1.46	1.38
28	2	1426	4AC	O7-C7	-2.84	1.16	1.23
28	2	348	A2M	O2'-C2'	-2.79	1.35	1.42
28	2	868	OMG	C2-N1	2.79	1.44	1.37
28	2	1314	OMU	O2-C2	-2.78	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	2	933	C4J	O4'-C1'	-2.73	1.40	1.43
28	2	1035	OMG	C5-C4	2.72	1.46	1.38
28	2	1314	OMU	C6-N1	2.70	1.44	1.38
28	2	87	A2M	O2'-C2'	-2.69	1.36	1.42
28	2	1035	OMG	C6-N1	-2.69	1.33	1.38
28	2	868	OMG	C4-N9	-2.68	1.31	1.38
28	2	1011	OMG	C6-N1	-2.67	1.33	1.38
28	2	1426	4AC	O2'-C2'	2.63	1.49	1.43
28	2	1426	4AC	O5'-C5'	-2.61	1.36	1.44
28	2	87	A2M	O3'-C3'	2.60	1.49	1.43
28	2	1434	MA6	C8-N9	-2.56	1.33	1.37
28	2	1434	MA6	C5-N7	-2.56	1.34	1.39
28	2	1435	MA6	C5-N7	-2.56	1.34	1.39
28	2	1261	7MG	O6-C6	-2.56	1.18	1.23
28	2	348	A2M	C5-N7	-2.54	1.34	1.39
28	2	1426	4AC	C6-N1	2.53	1.44	1.38
28	2	371	OMG	C5-C6	2.44	1.53	1.44
28	2	371	OMG	C2-N1	2.33	1.43	1.37
28	2	1011	OMG	C5-N7	-2.27	1.34	1.39
28	2	1435	MA6	C8-N9	-2.25	1.33	1.37
28	2	933	C4J	O2-C2	-2.19	1.18	1.22
28	2	1314	OMU	C5-C4	2.18	1.48	1.43
28	2	1035	OMG	C5-N7	-2.16	1.34	1.39
28	2	371	OMG	C6-N1	2.15	1.42	1.38
28	2	1261	7MG	C5-C4	2.14	1.44	1.37
28	2	87	A2M	C4-N9	-2.12	1.33	1.37
28	2	868	OMG	C6-N1	2.04	1.42	1.38

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	1435	MA6	N1-C6-N6	-12.27	101.90	116.86
28	2	1434	MA6	N1-C6-N6	-11.72	102.57	116.86
28	2	1435	MA6	C5-C6-N6	8.14	138.21	125.33
28	2	1434	MA6	C5-C6-N6	7.82	137.70	125.33
28	2	348	A2M	N6-C6-N1	-6.64	103.60	118.38
28	2	87	A2M	N6-C6-N1	-6.18	104.62	118.38
28	2	1011	OMG	C5-C4-N3	-6.13	118.63	128.39
28	2	1035	OMG	C5-C4-N3	-6.10	118.69	128.39
28	2	1435	MA6	N1-C2-N3	-5.94	119.59	128.58
28	2	348	A2M	N9-C8-N7	-5.85	105.64	113.94
28	2	348	A2M	N3-C2-N1	-5.67	119.99	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	1434	MA6	N1-C2-N3	-5.60	120.11	128.58
28	2	1314	OMU	C4-N3-C2	-5.56	119.71	126.61
28	2	87	A2M	N9-C8-N7	-5.52	106.11	113.94
28	2	371	OMG	C5-C4-N3	-5.46	119.71	128.39
28	2	87	A2M	N3-C2-N1	-5.41	120.39	128.58
28	2	348	A2M	C4-N9-C8	5.39	111.40	105.74
28	2	348	A2M	C5-C6-N6	5.23	136.24	123.29
28	2	1035	OMG	C2-N3-C4	5.20	121.25	112.30
28	2	87	A2M	C5-C6-N6	5.05	135.79	123.29
28	2	1434	MA6	C5-C4-N3	-5.03	119.80	126.72
28	2	87	A2M	C4-N9-C8	5.01	111.00	105.74
28	2	1011	OMG	C2-N3-C4	4.91	120.76	112.30
28	2	1261	7MG	C5-C6-N1	4.89	119.55	110.94
28	2	371	OMG	C2-N3-C4	4.78	120.53	112.30
28	2	1435	MA6	N9-C8-N7	-4.70	107.27	113.94
28	2	1011	OMG	N9-C4-N3	4.65	135.25	125.95
28	2	87	A2M	C5-C4-N3	-4.64	120.33	126.72
28	2	1261	7MG	C2-N3-C4	4.60	120.22	112.30
28	2	1435	MA6	C5-C4-N3	-4.50	120.52	126.72
28	2	1261	7MG	C5-C4-N3	-4.48	119.73	128.13
28	2	1035	OMG	N9-C4-N3	4.44	134.83	125.95
28	2	348	A2M	C5-C4-N3	-4.42	120.63	126.72
28	2	87	A2M	C1'-N9-C8	-4.30	117.55	127.09
28	2	933	C4J	C4-N3-C2	-4.28	120.36	125.62
28	2	87	A2M	N3-C4-N9	4.11	134.16	127.17
28	2	1434	MA6	N9-C8-N7	-4.10	108.12	113.94
28	2	348	A2M	C1'-N9-C8	-4.04	118.12	127.09
28	2	1434	MA6	C4-C5-C6	4.02	120.07	115.91
28	2	1261	7MG	C4-C5-N7	3.95	110.05	105.38
28	2	1314	OMU	C5-C4-N3	3.93	120.31	114.80
28	2	348	A2M	N3-C4-N9	3.86	133.74	127.17
28	2	868	OMG	C5-C4-N3	-3.77	122.39	128.39
28	2	1035	OMG	C2'-C1'-N9	-3.72	107.18	114.24
28	2	1314	OMU	N3-C2-N1	3.65	119.64	114.89
28	2	868	OMG	C2-N3-C4	3.58	118.47	112.30
28	2	1035	OMG	C6-C5-N7	3.53	136.71	130.29
28	2	1435	MA6	C2-N1-C6	3.52	120.42	111.83
28	2	348	A2M	C5-N7-C8	3.50	108.95	103.45
28	2	1434	MA6	C2-N1-C6	3.43	120.21	111.83
28	2	1435	MA6	C2-N3-C4	3.42	120.19	111.83
28	2	1434	MA6	C2-N3-C4	3.38	120.09	111.83
28	2	1435	MA6	C4-C5-C6	3.38	119.41	115.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	87	A2M	C5-N7-C8	3.35	108.71	103.45
28	2	371	OMG	N9-C4-N3	3.29	132.53	125.95
28	2	1426	4AC	C5'-C4'-C3'	-3.28	103.42	115.21
28	2	348	A2M	C2-N3-C4	3.20	119.64	111.83
28	2	371	OMG	C2-N1-C6	-3.19	119.33	125.11
28	2	1011	OMG	C6-C5-N7	3.15	136.02	130.29
28	2	1434	MA6	N3-C4-N9	3.15	132.52	127.17
28	2	371	OMG	N9-C8-N7	-3.14	107.58	113.40
28	2	1261	7MG	N9-C4-N3	3.10	130.01	125.46
28	2	1011	OMG	C2'-C1'-N9	-3.10	108.35	114.24
28	2	87	A2M	C2-N3-C4	3.09	119.37	111.83
28	2	1435	MA6	C5-N7-C8	3.08	108.29	103.45
28	2	1261	7MG	C5-C4-N9	3.07	110.27	106.33
28	2	1434	MA6	C5-N7-C8	3.02	108.20	103.45
28	2	933	C4J	C3-N3-C4	2.95	121.36	117.18
28	2	1314	OMU	O4-C4-C5	-2.94	120.09	125.16
28	2	1325	4OC	C6-C5-C4	2.83	120.41	117.00
28	2	1435	MA6	C4-N9-C8	2.82	108.70	105.74
28	2	371	OMG	C5-C6-N1	2.78	120.33	113.25
28	2	933	C4J	N3-C2-N1	2.77	120.10	116.72
28	2	1426	4AC	O2-C2-N3	-2.75	117.99	122.33
28	2	1261	7MG	C2-N1-C6	-2.72	120.17	125.11
28	2	1435	MA6	N3-C4-N9	2.72	131.79	127.17
28	2	1035	OMG	C4-C5-N7	-2.70	106.39	110.67
28	2	1261	7MG	O6-C6-C5	-2.68	121.03	127.62
28	2	1261	7MG	N9-C8-N7	2.67	107.16	103.37
28	2	868	OMG	C2-N1-C6	-2.62	120.36	125.11
28	2	1011	OMG	C4-C5-N7	-2.53	106.66	110.67
28	2	348	A2M	C2'-C1'-N9	-2.50	109.64	113.75
28	2	868	OMG	C5-C6-N1	2.47	119.54	113.25
28	2	868	OMG	O6-C6-C5	-2.46	120.03	126.53
28	2	868	OMG	N9-C8-N7	-2.46	108.84	113.40
28	2	371	OMG	O6-C6-C5	-2.43	120.13	126.53
28	2	1434	MA6	C4-C5-N7	-2.39	107.85	110.58
28	2	371	OMG	C8-N7-C5	2.36	108.47	104.26
28	2	1434	MA6	C4-N9-C8	2.30	108.16	105.74
28	2	1011	OMG	O6-C6-C5	-2.28	120.51	126.53
28	2	104	OMC	C2'-C1'-N1	-2.27	109.93	114.24
28	2	1035	OMG	O6-C6-C5	-2.24	120.61	126.53
28	2	868	OMG	N9-C4-N3	2.23	130.41	125.95
28	2	1435	MA6	C4-C5-N7	-2.22	108.04	110.58
28	2	104	OMC	O2-C2-N3	-2.14	118.96	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	868	OMG	C1'-N9-C8	-2.09	120.78	126.73
28	2	868	OMG	C2'-C1'-N9	-2.09	110.27	114.24
28	2	87	A2M	C6-C5-C4	2.08	120.02	117.18
28	2	933	C4J	C1'-C5-C4	2.06	120.73	117.61
28	2	87	A2M	C4-N9-C1'	2.06	131.44	126.63
28	2	933	C4J	C5-C4-N3	2.06	119.89	116.15
28	2	1035	OMG	C5-C6-N1	2.06	118.49	113.25
28	2	1426	4AC	C5-C4-N3	-2.05	119.40	122.60
28	2	1035	OMG	C8-N7-C5	2.01	107.83	104.26

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	2	87	A2M	C1'-C2'-O2'-CM'
28	2	371	OMG	C1'-C2'-O2'-CM2
28	2	868	OMG	C1'-C2'-O2'-CM2
28	2	868	OMG	O4'-C1'-N9-C8
28	2	868	OMG	O4'-C1'-N9-C4
28	2	933	C4J	C3'-C4'-C5'-O5'
28	2	933	C4J	C4'-C5'-O5'-P
28	2	1011	OMG	C1'-C2'-O2'-CM2
28	2	1035	OMG	C1'-C2'-O2'-CM2
28	2	87	A2M	O4'-C4'-C5'-O5'
28	2	1426	4AC	O4'-C4'-C5'-O5'
28	2	1426	4AC	C3'-C4'-C5'-O5'
28	2	1435	MA6	O4'-C4'-C5'-O5'
28	2	933	C4J	O4'-C4'-C5'-O5'
28	2	868	OMG	C3'-C4'-C5'-O5'
28	2	1435	MA6	C3'-C4'-C5'-O5'
28	2	87	A2M	C3'-C4'-C5'-O5'
28	2	868	OMG	O4'-C4'-C5'-O5'
28	2	933	C4J	N3-C3-C31-C32
28	2	1011	OMG	C3'-C2'-O2'-CM2
28	2	1011	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	2	1434	MA6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	2	1035	OMG	1	0
28	2	1314	OMU	1	0
28	2	87	A2M	1	0
28	2	371	OMG	1	0
28	2	1261	7MG	1	0
28	2	1011	OMG	1	0
28	2	868	OMG	1	0
28	2	348	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 303 ligands modelled in this entry, 303 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

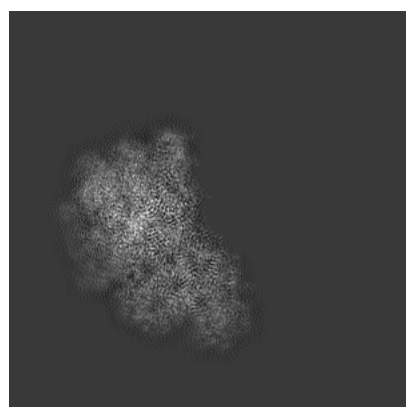
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13680. These allow visual inspection of the internal detail of the map and identification of artifacts.

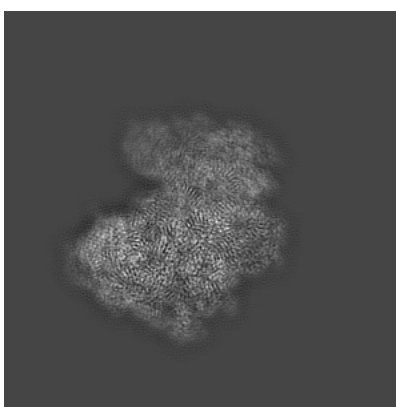
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

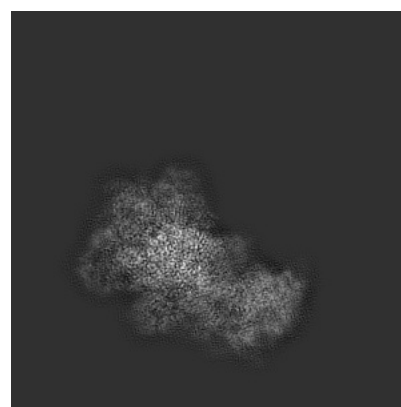
6.1.1 Primary map



X



Y

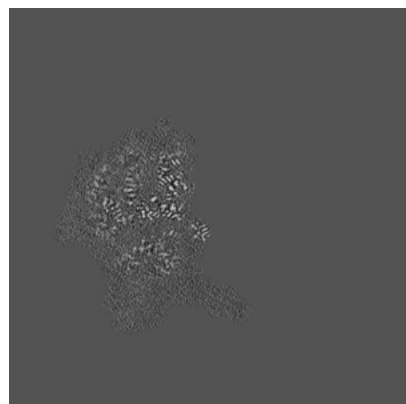


Z

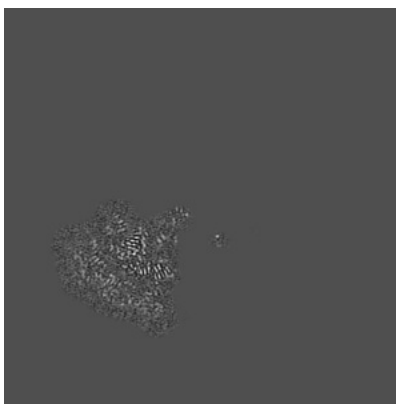
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

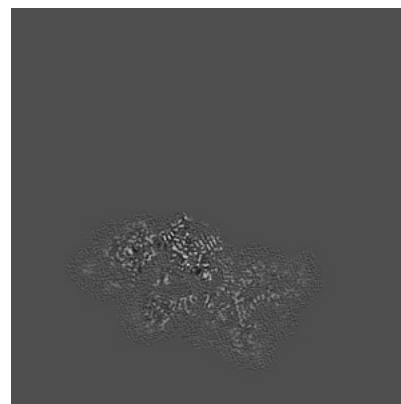
6.2.1 Primary map



X Index: 220



Y Index: 220

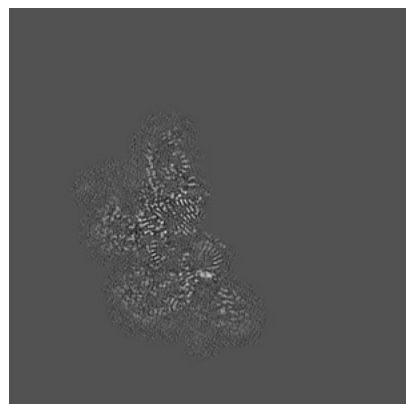


Z Index: 220

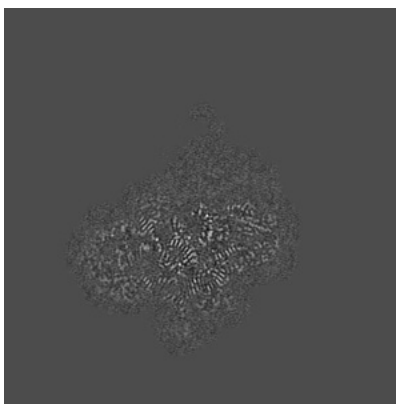
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

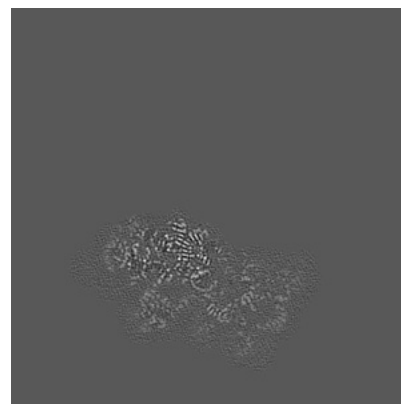
6.3.1 Primary map



X Index: 187



Y Index: 168

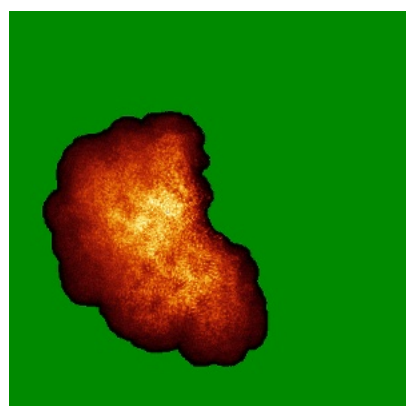


Z Index: 226

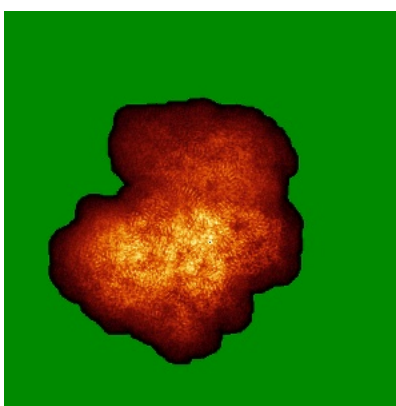
The images above show the largest variance slices of the map in three orthogonal directions.

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

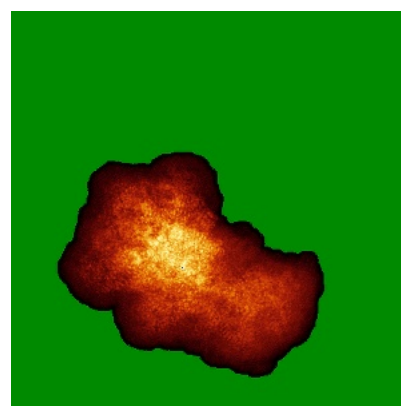
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

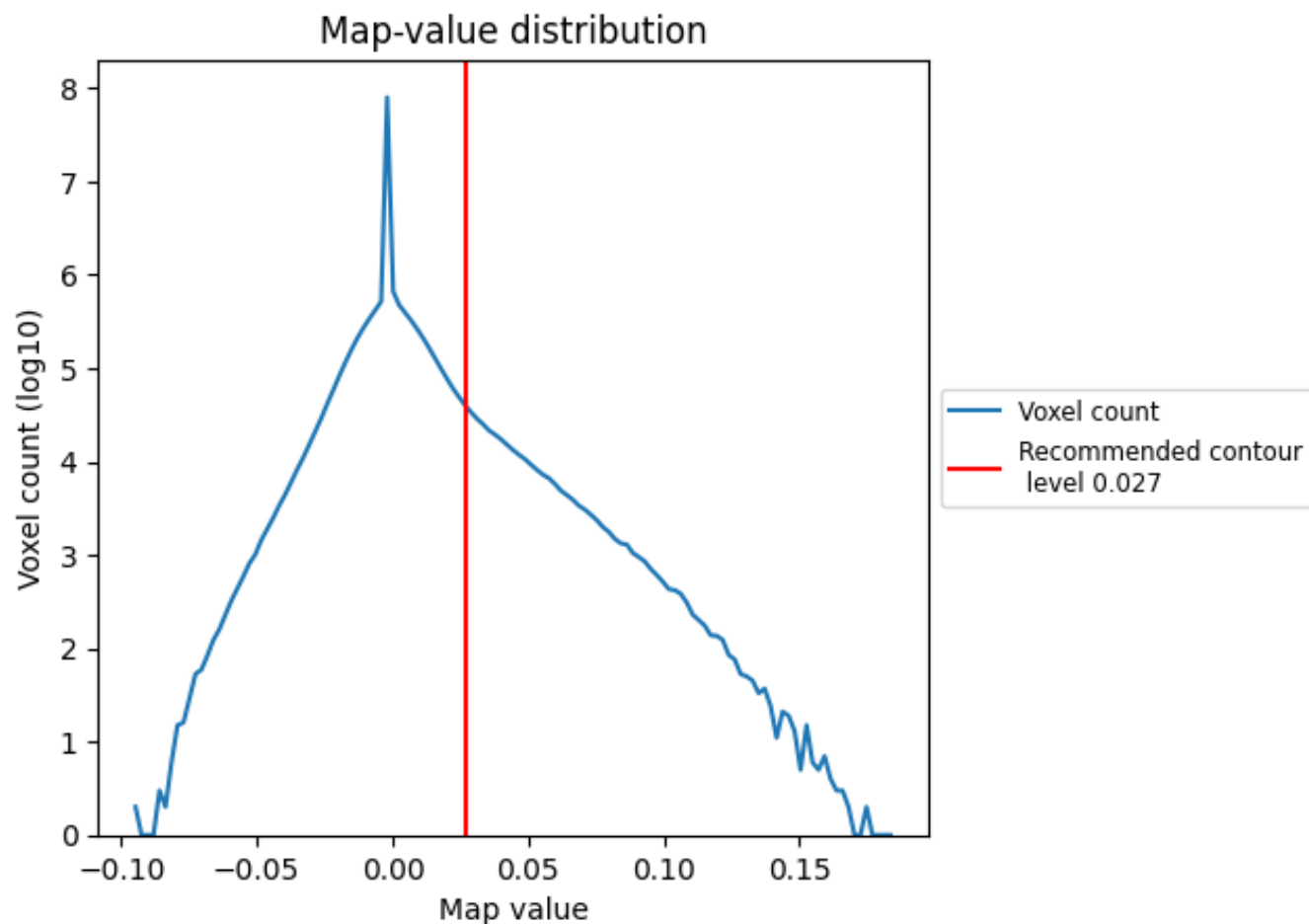
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

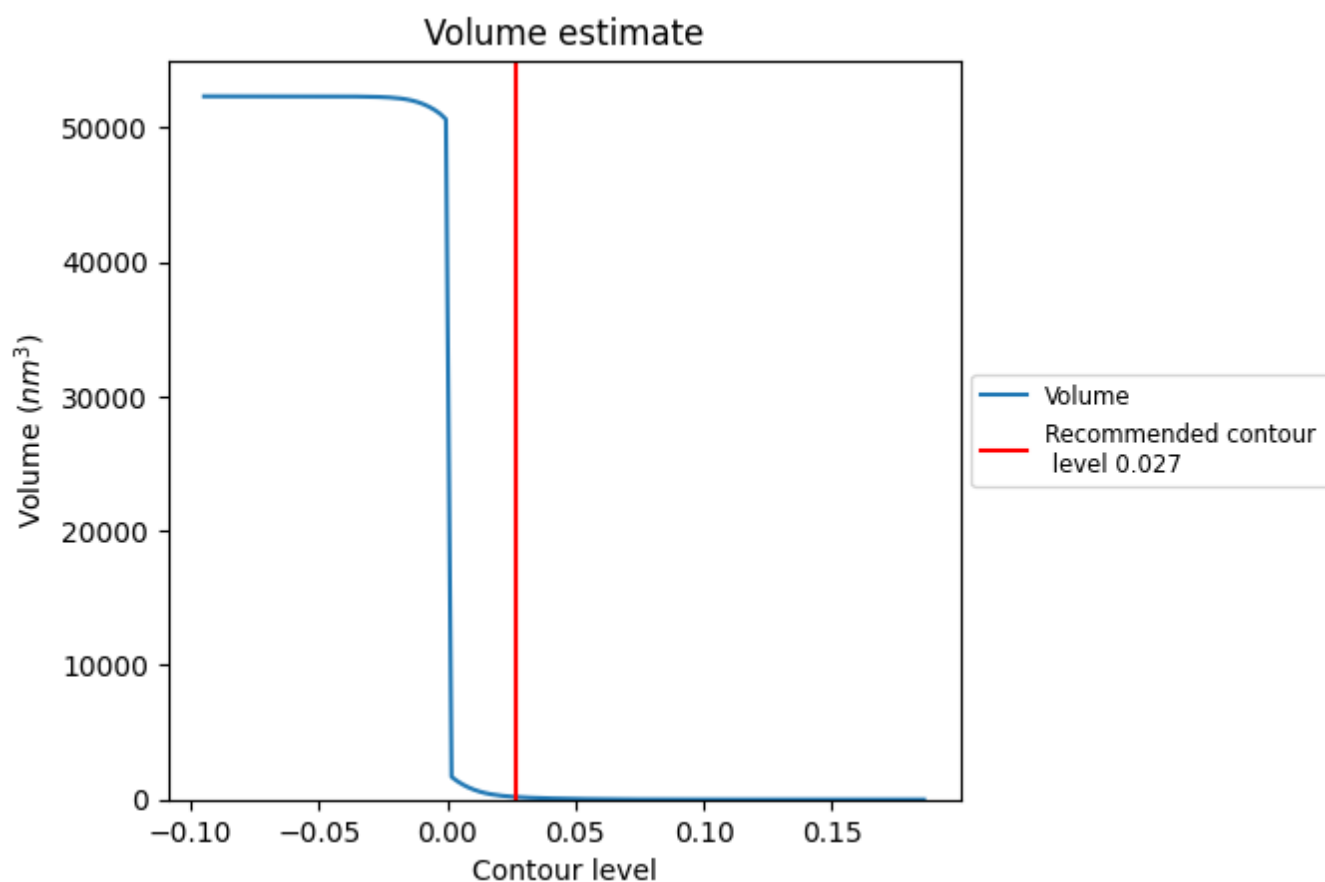
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

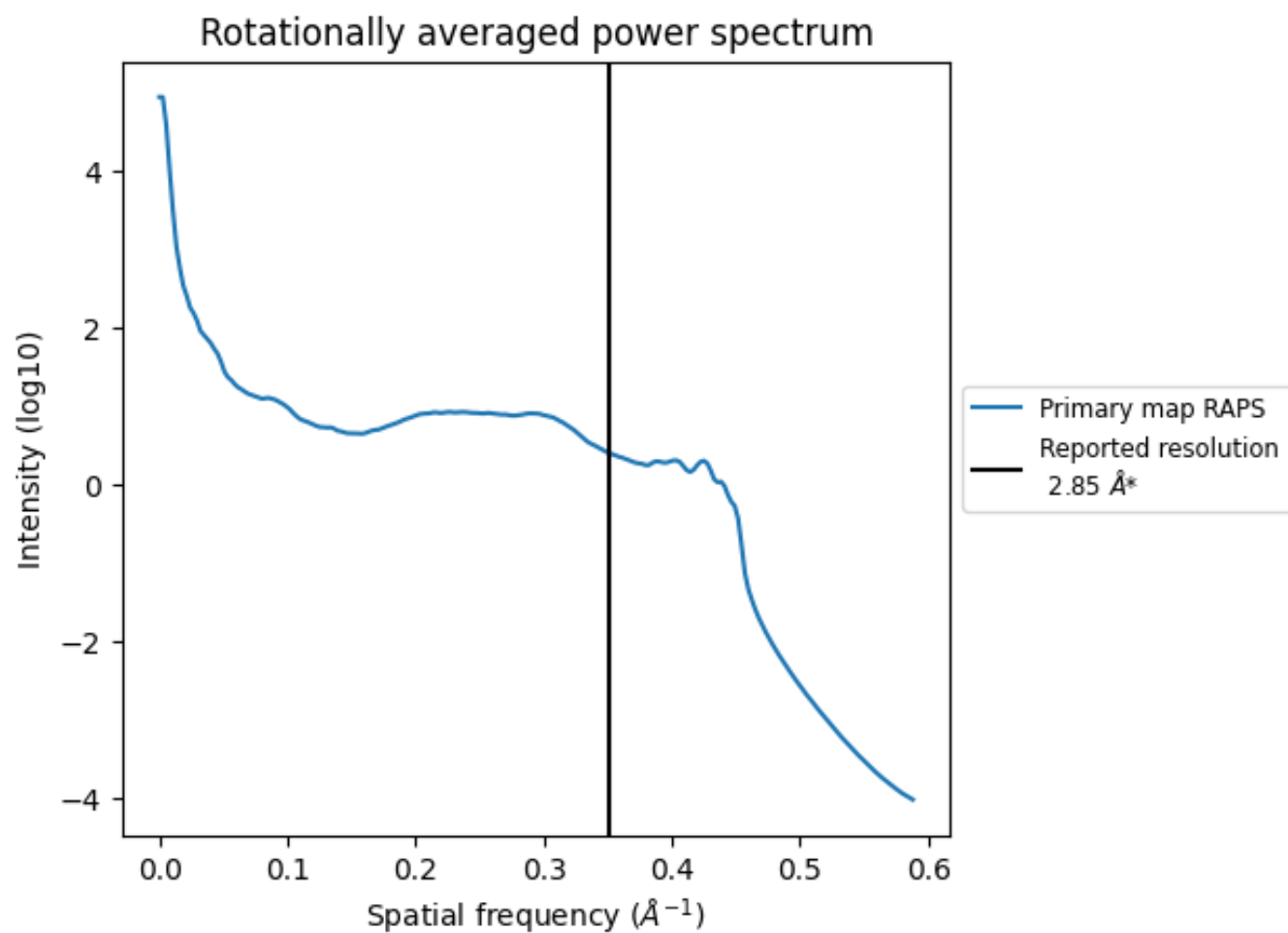
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm³; this corresponds to an approximate mass of 173 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 0.351 Å⁻¹

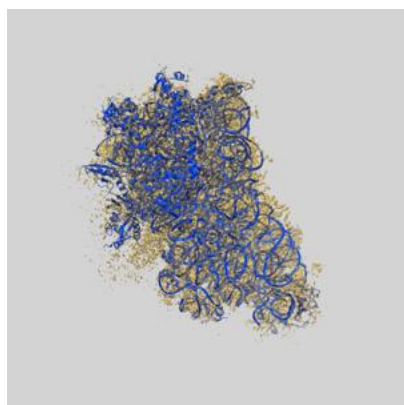
8 Fourier-Shell correlation ⓘ

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

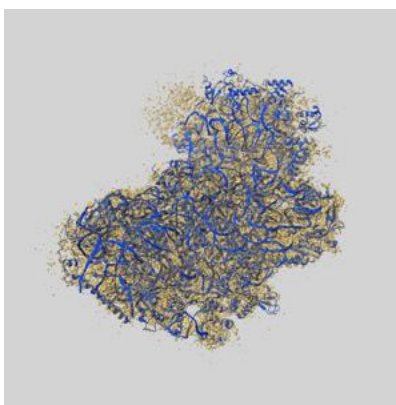
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13680 and PDB model 7PWF. Per-residue inclusion information can be found in section [3](#) on page [11](#).

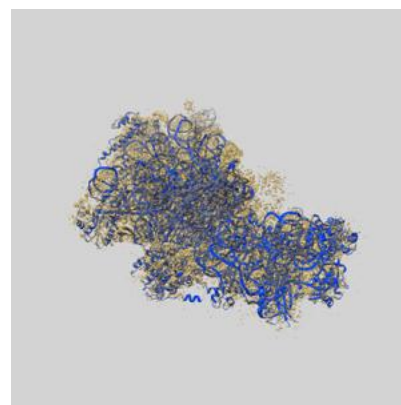
9.1 Map-model overlay [i](#)



X



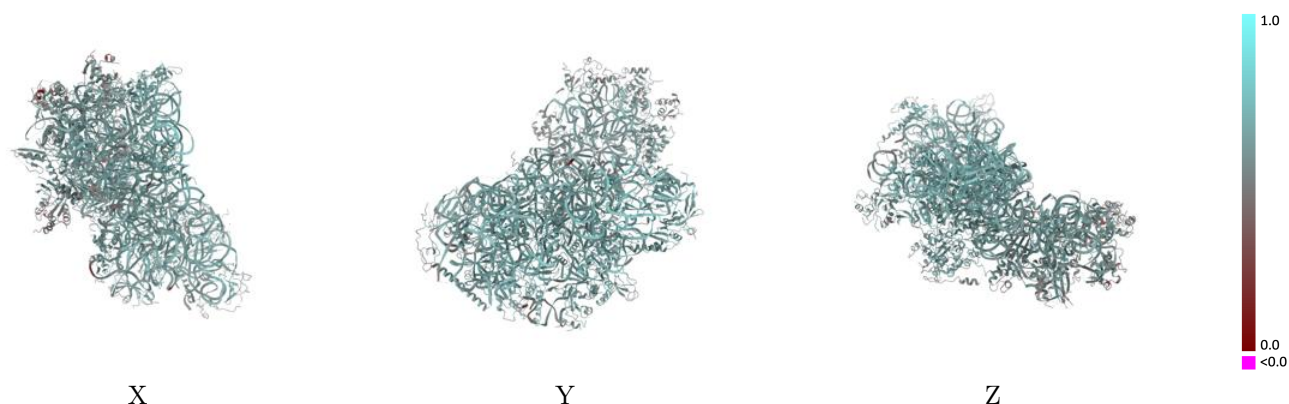
Y



Z

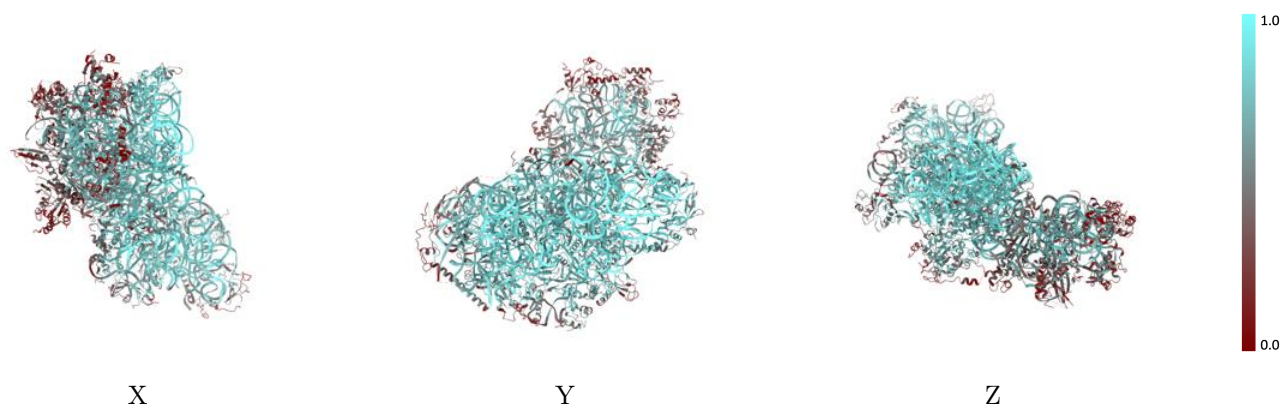
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



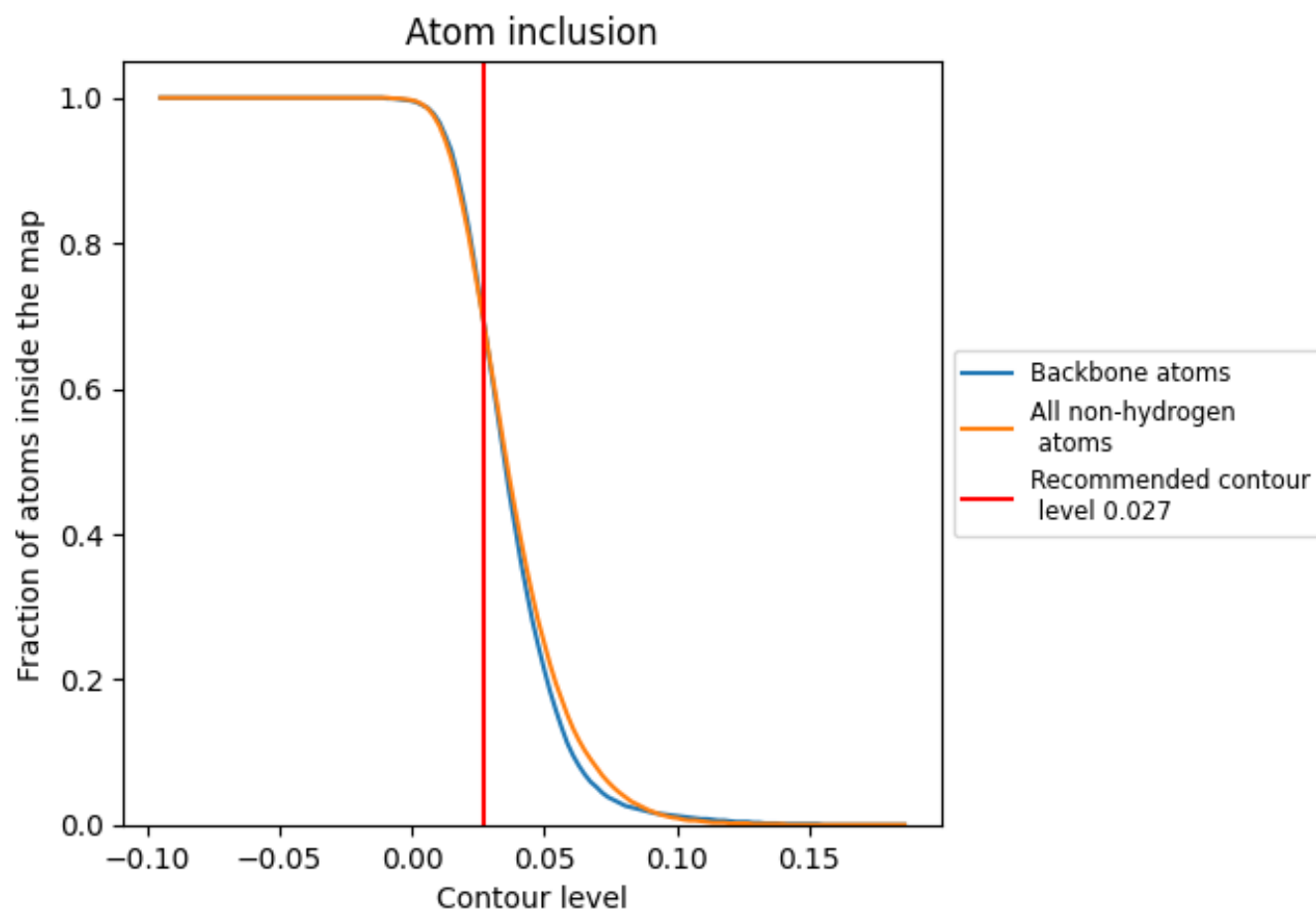
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.027).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 69% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6940	 0.6220
2	 0.8180	 0.6390
A	 0.6070	 0.6120
B	 0.7410	 0.6450
C	 0.7490	 0.6480
D	 0.3610	 0.5670
E	 0.6700	 0.6360
F	 0.5060	 0.6000
G	 0.4570	 0.5680
H	 0.6020	 0.5960
I	 0.7220	 0.6500
J	 0.6000	 0.6200
K	 0.2180	 0.4840
L	 0.7200	 0.6470
N	 0.7540	 0.6600
O	 0.8500	 0.6720
P	 0.2290	 0.5210
Q	 0.3770	 0.5670
R	 0.2430	 0.5160
S	 0.2570	 0.5310
T	 0.4260	 0.5480
U	 0.4520	 0.5900
V	 0.6340	 0.6100
W	 0.8550	 0.6690
X	 0.6420	 0.6310
Y	 0.4990	 0.5940
Z	 0.2230	 0.4780
a	 0.8070	 0.6720
b	 0.5650	 0.5990
c	 0.3470	 0.5650
d	 0.5880	 0.6100
e	 0.4340	 0.5960
n	 0.7770	 0.6750

