



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:08 AM UTC

PDB ID : 8G4I / pdb_00008g4i
EMDB ID : EMD-29721
Title : 40S ribosomal subunit of the 80S Giardia intestinalis assemblage A ribosome
with Emetine bound in V1 conformation
Authors : Eiler, D.R.; Wimberly, B.T.; Bilodeau, D.Y.; Rissland, O.S.; Kieft, J.S.
Deposited on : 2023-02-09
Resolution : 3.24 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

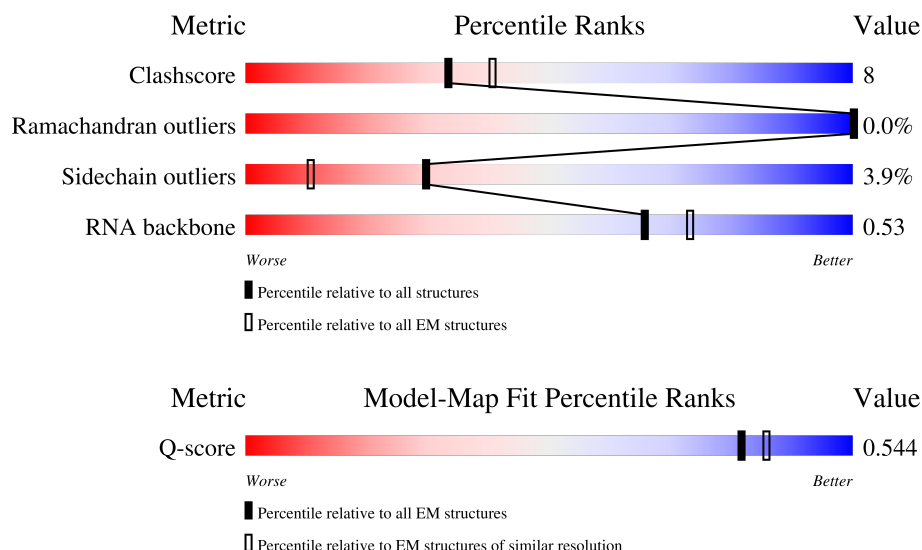
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.24 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	14594 (2.74 - 3.74)

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	2	1451	
2	A	245	
3	B	248	

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Mol	Chain	Length	Quality of chain
4	C	242	
5	D	217	
6	E	268	
7	F	190	
8	G	248	
9	H	201	
10	I	174	
11	J	189	
12	K	134	
13	L	199	
14	N	154	
15	O	145	
16	P	145	
17	Q	158	
18	R	137	
19	S	154	
20	T	158	
21	U	126	
22	V	89	
23	W	130	
24	X	143	
25	Y	132	
26	Z	88	
27	a	109	
28	b	124	

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Mol	Chain	Length	Quality of chain
29	c	64	23%53%38%6%
30	d	137	22%47%12%39%
31	f	137	16%7%77%
32	g	74	35%95%53%12%
33	M	125	15%28%36%33%
34	e	69	67%46%23%30%

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 118402 atoms, of which 51286 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 18S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	2	1441	Total	C	H	N	O	P	0	0
			46630	13746	15711	5742	9991	1440		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	932	C	U	conflict	GB 2333213660

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	199	Total	C	H	N	O	S	0	0
			3194	1025	1608	275	278	8		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	B	212	Total	C	H	N	O	S	0	0
			3470	1092	1754	317	295	12		

- Molecule 4 is a protein called Ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	C	209	Total	C	H	N	O	S	0	0
			3250	1025	1638	292	291	4		

- Molecule 5 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	D	204	Total	C	H	N	O	S	0	0
			3222	1013	1620	289	284	16		

- Molecule 6 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	E	258	Total	C	H	N	O	S	0	0
			4204	1321	2140	378	352	13		

- Molecule 7 is a protein called SSU ribosomal protein S7P (Fragment).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	F	186	Total	C	H	N	O	S	0	0
			2905	899	1460	273	263	10		

- Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	G	201	Total	C	H	N	O	S	0	0
			3277	1004	1680	310	275	8		

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	H	165	Total	C	H	N	O	S	0	0
			2681	846	1363	227	239	6		

- Molecule 10 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	I	167	Total	C	H	N	O	S	0	0
			2644	817	1338	250	236	3		

- Molecule 11 is a protein called Ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	J	164	Total	C	H	N	O	S	0	0
			2706	828	1383	260	229	6		

- Molecule 12 is a protein called Ribosomal protein S10B.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	K	104	Total	C	H	N	O	S	0	0
			1678	551	827	143	154	3		

- Molecule 13 is a protein called SSU ribosomal protein S17P.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	L	170	Total	C	H	N	O	S	0	0
			2841	888	1436	278	232	7		

- Molecule 14 is a protein called Ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	153	Total	C	H	N	O	S	0	0
			2532	780	1304	237	206	5		

- Molecule 15 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	139	Total	C	H	N	O	S	0	0
			2113	645	1058	210	196	4		

- Molecule 16 is a protein called Ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	108	Total	C	H	N	O	S	0	0
			1803	560	925	171	139	8		

- Molecule 17 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	158	Total	C	H	N	O	S	0	0
			2523	766	1293	243	217	4		

- Molecule 18 is a protein called Ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	81	Total	C	H	N	O	S	0	0
			1349	405	699	130	113	2		

- Molecule 19 is a protein called Ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	143	Total	C	H	N	O	S	0	0
			2294	701	1156	228	202	7		

- Molecule 20 is a protein called SSU ribosomal protein S19E (Fragment).

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	137	Total	C	H	N	O	S	0	0
			2163	683	1089	203	185	3		

- Molecule 21 is a protein called Ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	103	Total	C	H	N	O	S	0	0
			1634	516	824	146	144	4		

- Molecule 22 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	81	Total	C	H	N	O	S	0	0
			1212	377	607	112	110	6		

- Molecule 23 is a protein called SSU ribosomal protein S8P (Fragment).

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	129	Total	C	H	N	O	S	0	0
			2104	659	1074	192	176	3		

- Molecule 24 is a protein called SSU ribosomal protein S12P.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	X	138	Total	C	H	N	O	S	0	0
			2231	680	1153	216	178	4		

- Molecule 25 is a protein called Ribosomal protein S24.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	122	Total	C	H	N	O	S	0	0
			1979	611	1014	181	166	7		

- Molecule 26 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	73	Total	C	H	N	O	S	0	0
			1182	366	605	104	101	6		

- Molecule 27 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	a	96	Total	C	H	N	O	S	0	0
			1575	480	795	161	132	7		

- Molecule 28 is a protein called Ribosomal protein S27.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	b	65	Total	C	H	N	O	S	0	0
			1009	327	503	86	89	4		

- Molecule 29 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	c	60	Total	C	H	N	O	S	0	0
			957	293	483	91	88	2		

- Molecule 30 is a protein called Ribosomal protein S29A.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	d	84	Total	C	H	N	O	S	0	0
			1309	418	639	127	118	7		

- Molecule 31 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	f	32	Total	C	H	N	O	S	0	0
			503	156	251	49	44	3		

- Molecule 32 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	g	74	Total	C	H	N	O	P	0	0
			2314	701	745	274	521	73		

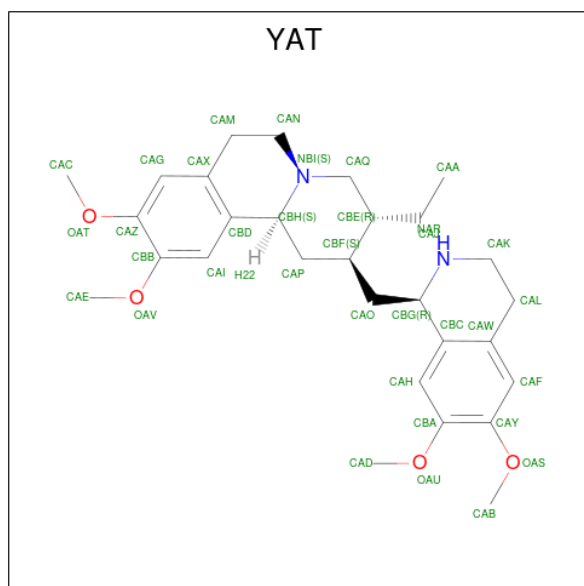
- Molecule 33 is a protein called Ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	M	84	Total	C	H	N	O	S	0	0
			1339	428	665	125	114	7		

- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	48	Total	C	H	N	O	0	0
			798	246	406	80	66		

- Molecule 35 is emetine (CCD ID: YAT) (formula: $C_{29}H_{40}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
35	2	1	Total	C	H	N	O	0
			75	29	40	2	4	

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	2	22	Total	Mg	0
			22	22	
36	a	1	Total	Mg	0
			1	1	

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	a	1	Total	Zn	0
			1	1	
37	d	1	Total	Zn	0
			1	1	

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	AltConf
38	2	579	Total O 579 579	0
38	B	2	Total O 2 2	0
38	C	9	Total O 9 9	0
38	D	1	Total O 1 1	0
38	E	11	Total O 11 11	0
38	F	5	Total O 5 5	0
38	G	1	Total O 1 1	0
38	I	8	Total O 8 8	0
38	K	1	Total O 1 1	0
38	L	4	Total O 4 4	0
38	N	11	Total O 11 11	0
38	O	3	Total O 3 3	0
38	P	2	Total O 2 2	0
38	Q	7	Total O 7 7	0
38	R	1	Total O 1 1	0
38	S	3	Total O 3 3	0
38	T	3	Total O 3 3	0
38	U	3	Total O 3 3	0
38	W	4	Total O 4 4	0
38	X	3	Total O 3 3	0
38	Z	2	Total O 2 2	0
38	a	8	Total O 8 8	0

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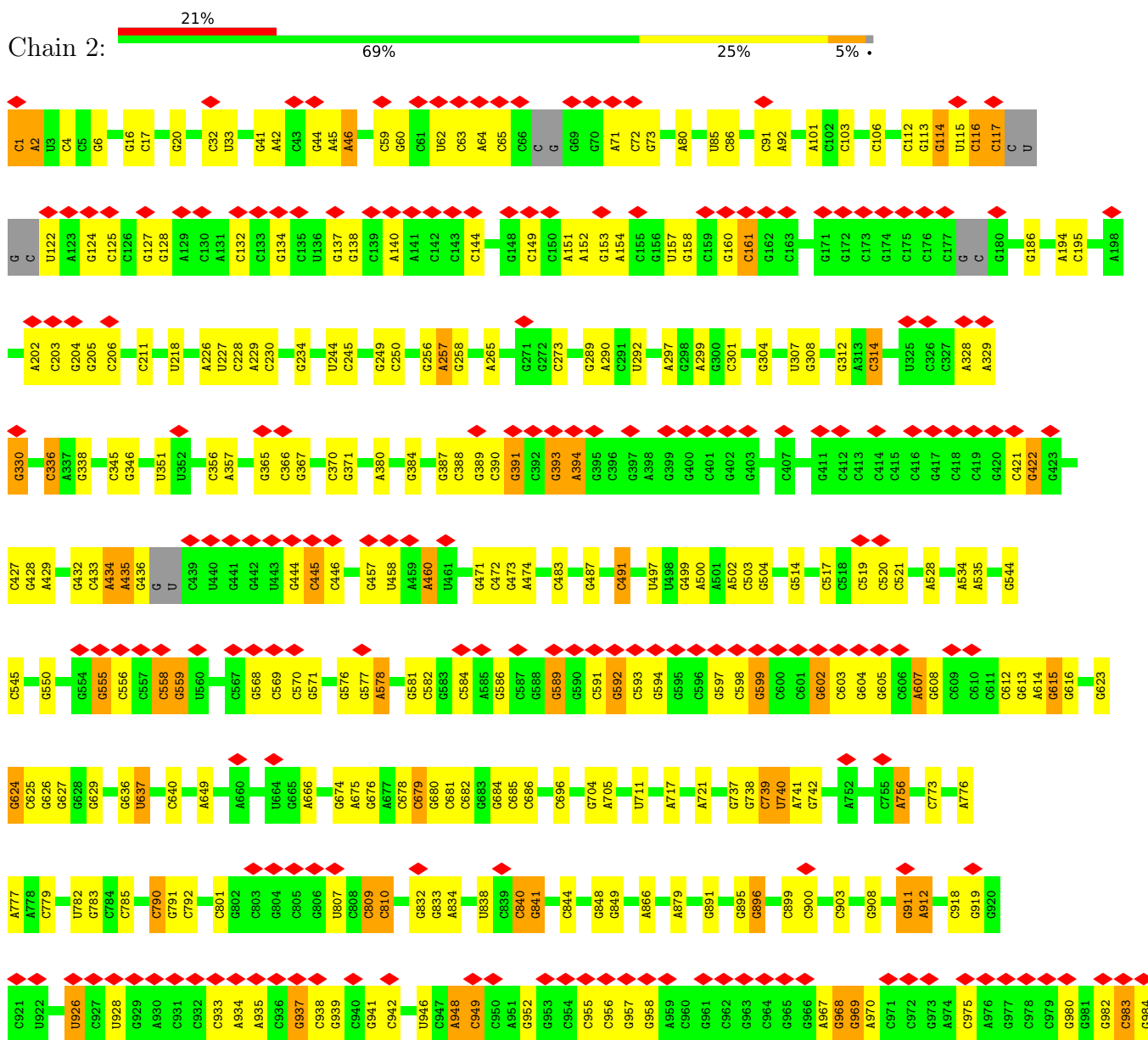
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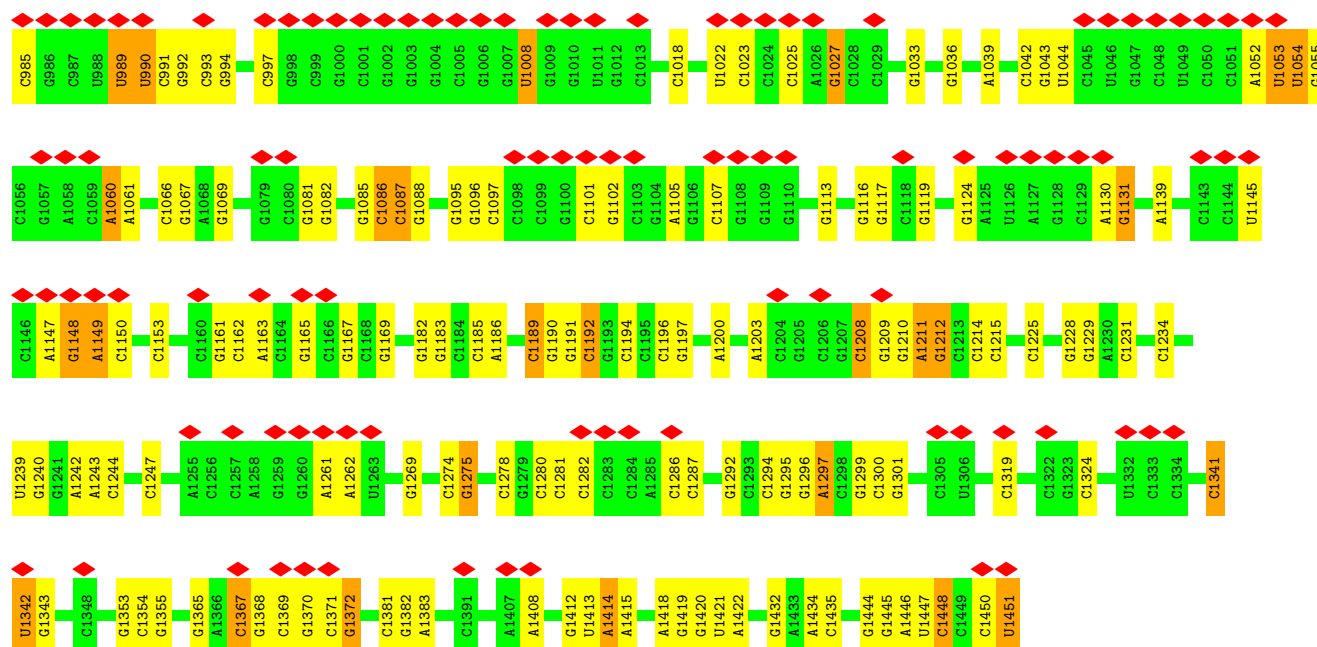
Mol	Chain	Residues	Atoms		AltConf
38	b	2	Total 2	O 2	0
38	d	2	Total 2	O 2	0
38	g	2	Total 2	O 2	0

3 Residue-property plots

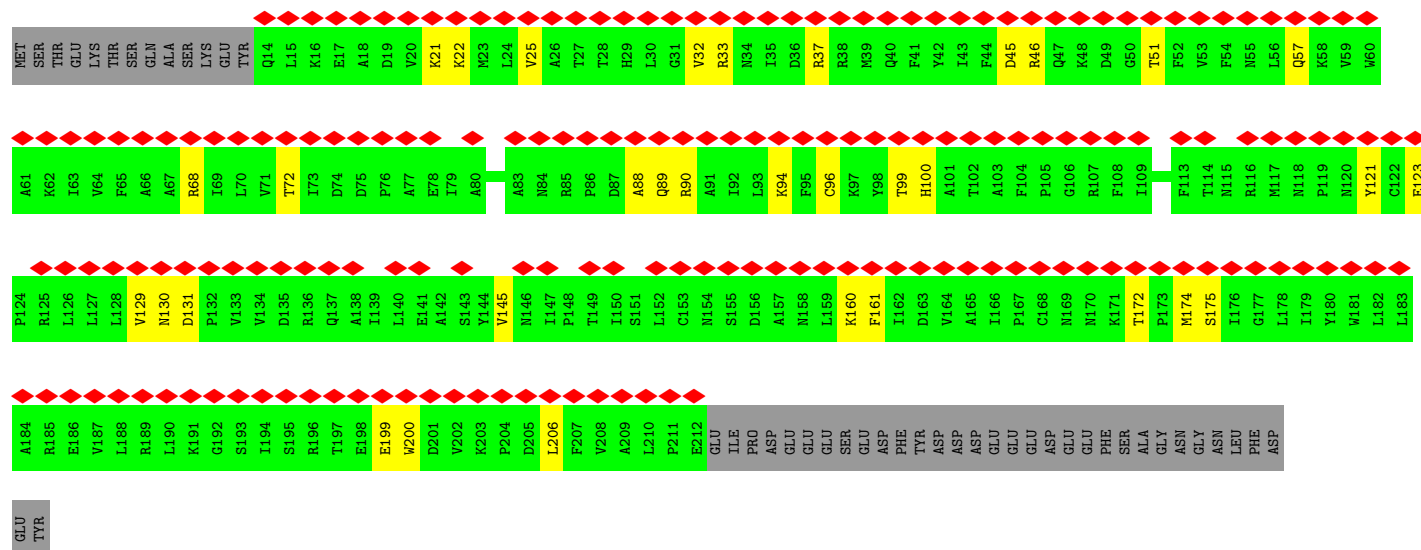
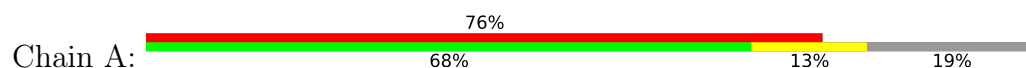
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 18S rRNA

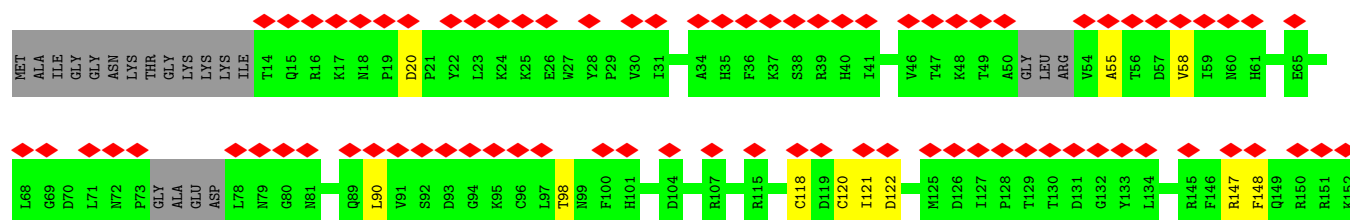
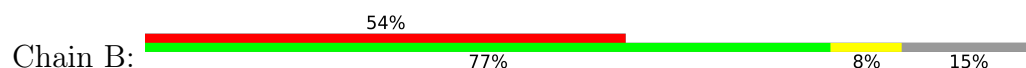




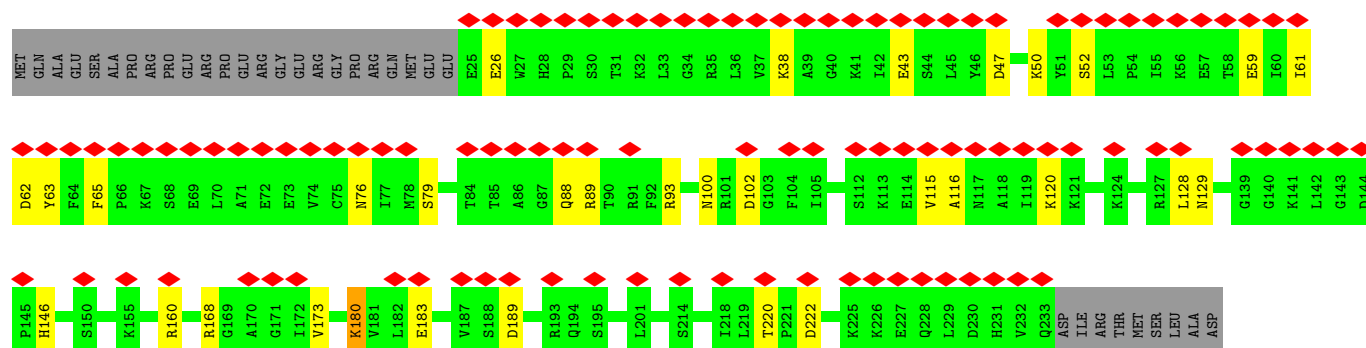
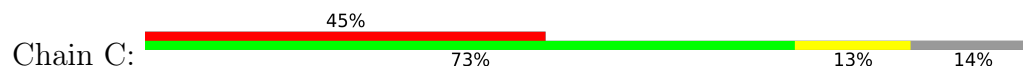
• Molecule 2: 40S ribosomal protein SA



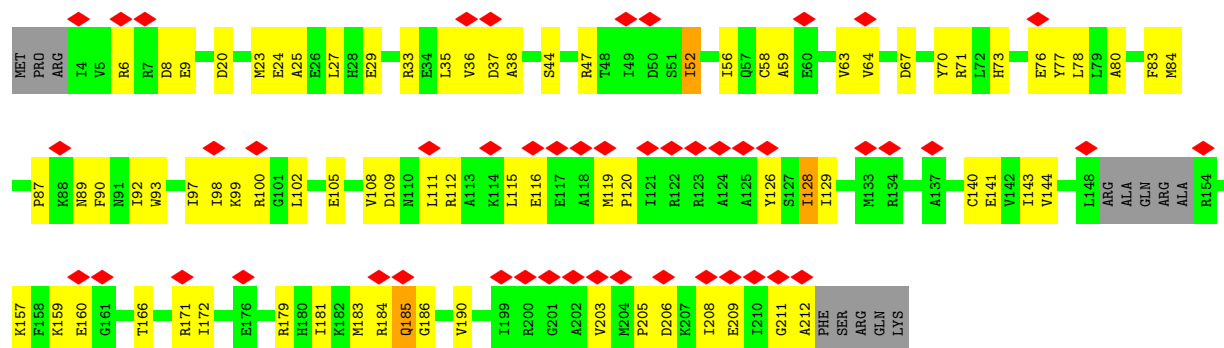
• Molecule 3: 40S ribosomal protein S3a



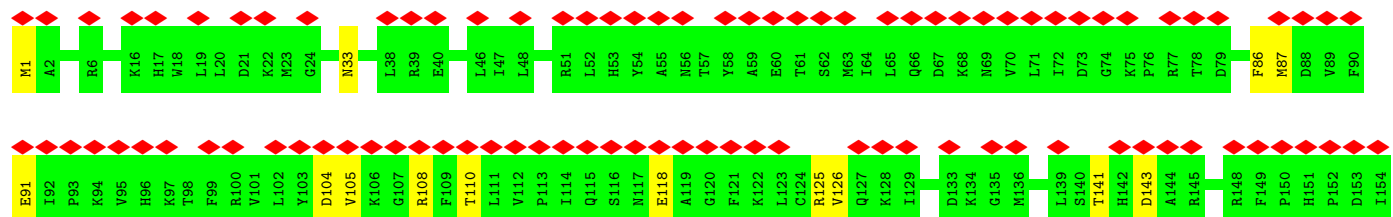
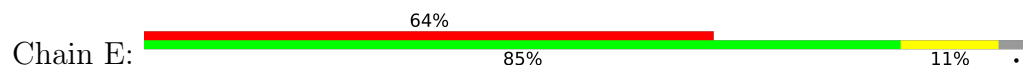
- Molecule 4: Ribosomal protein S2

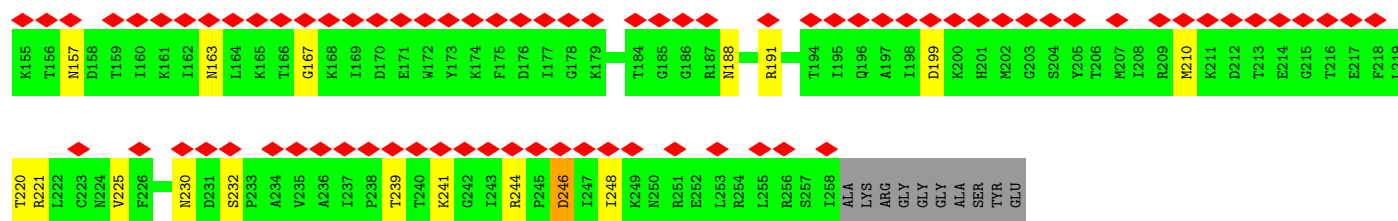


- Molecule 5: Ribosomal protein S3

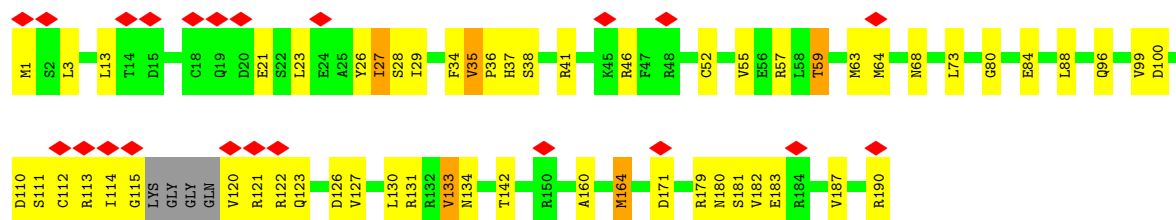


- Molecule 6: 40S ribosomal protein S4

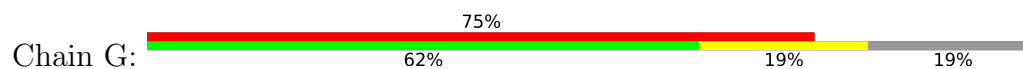




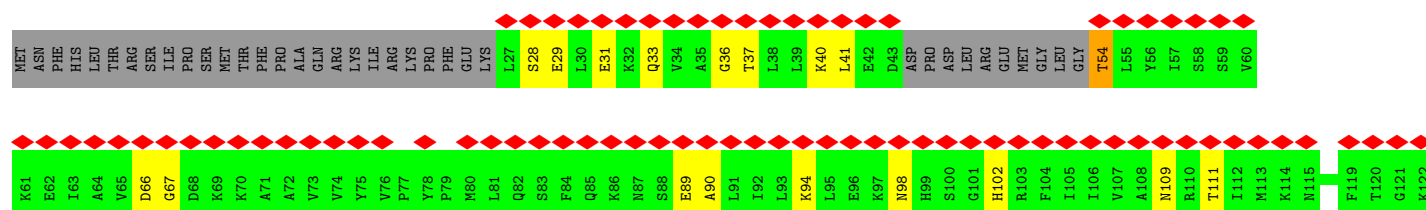
• Molecule 7: SSU ribosomal protein S7P (Fragment)

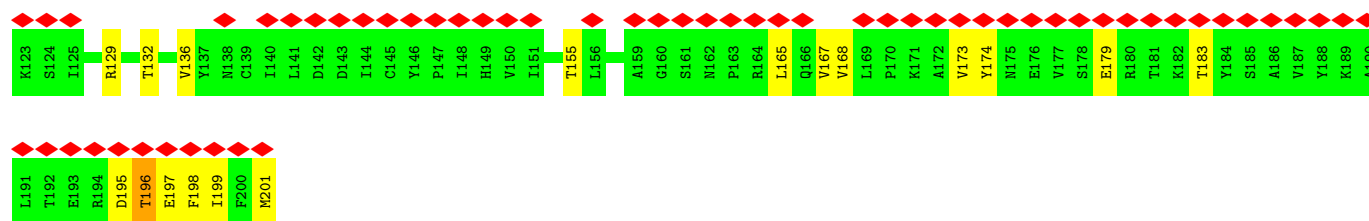


• Molecule 8: 40S ribosomal protein S6

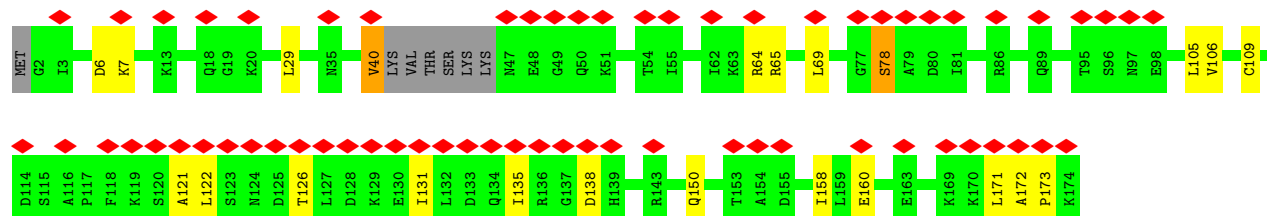
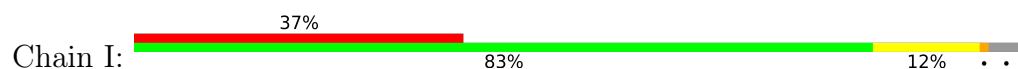


• Molecule 9: 40S ribosomal protein S7

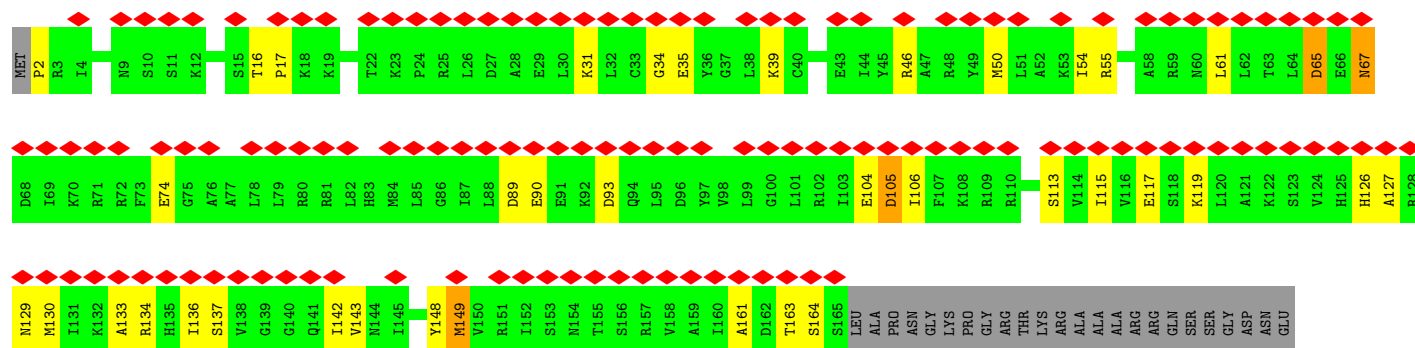




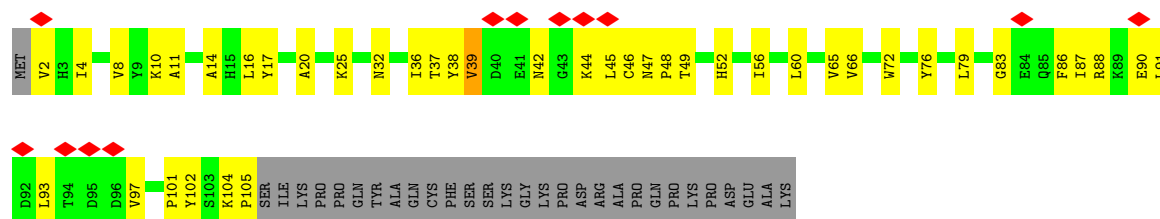
• Molecule 10: 40S ribosomal protein S8



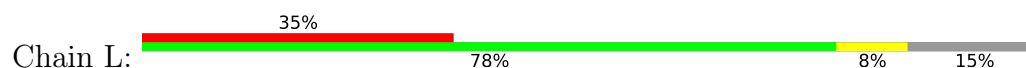
• Molecule 11: Ribosomal protein S9

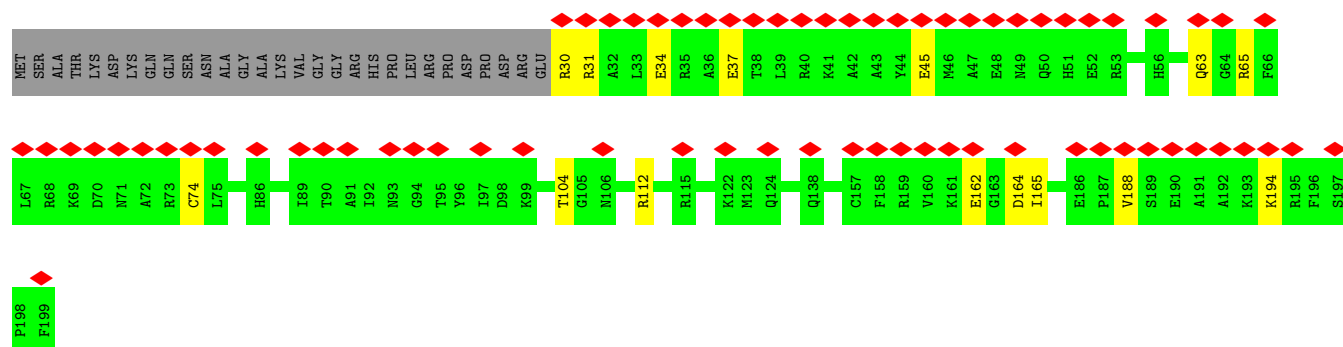


• Molecule 12: Ribosomal protein S10B

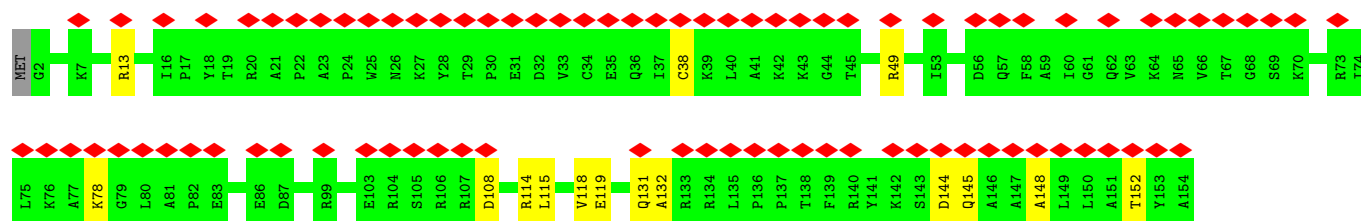
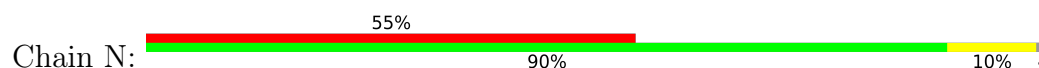


• Molecule 13: SSU ribosomal protein S17P

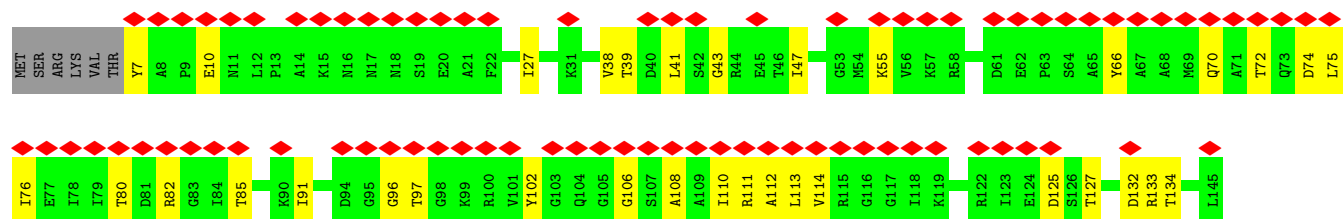
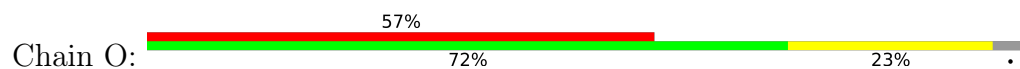




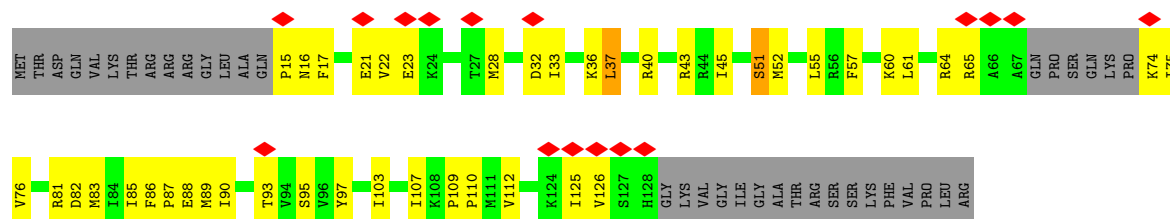
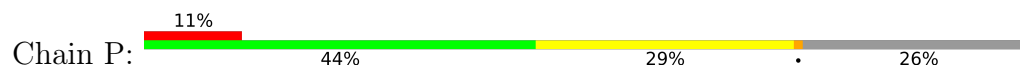
• Molecule 14: Ribosomal protein S13



• Molecule 15: Ribosomal protein S14

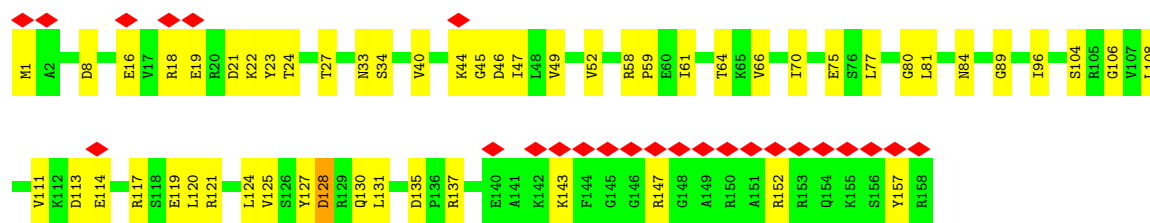


• Molecule 16: Ribosomal protein S15

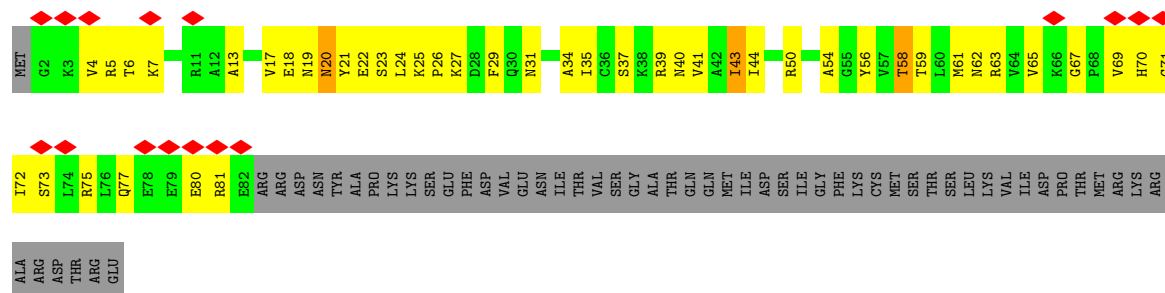
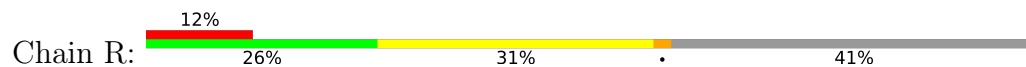


• Molecule 17: Ribosomal protein S16

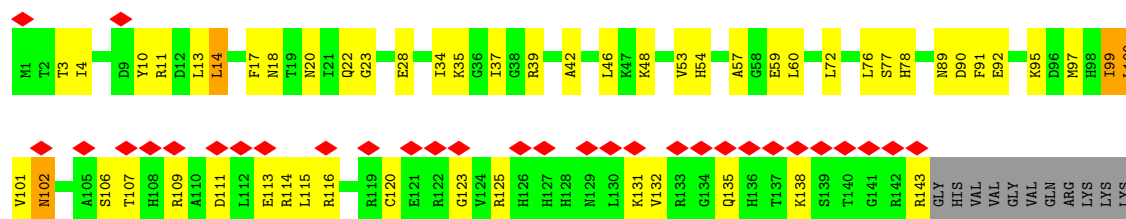




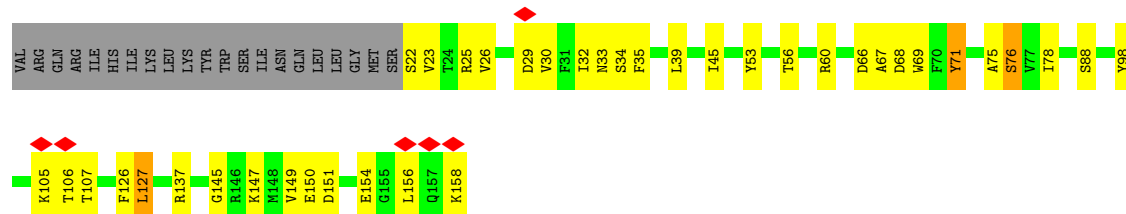
• Molecule 18: Ribosomal protein S17



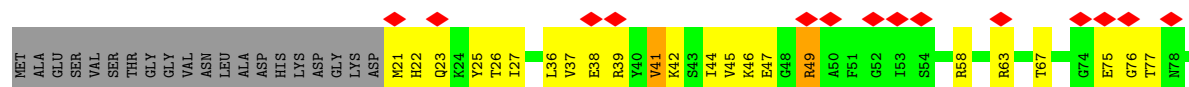
• Molecule 19: Ribosomal protein S18

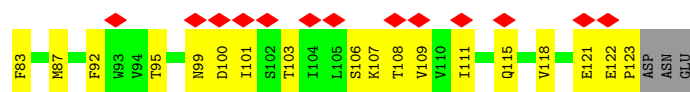


• Molecule 20: SSU ribosomal protein S19E (Fragment)

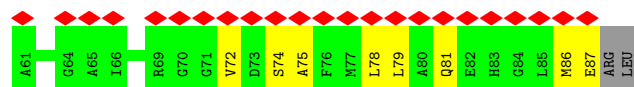
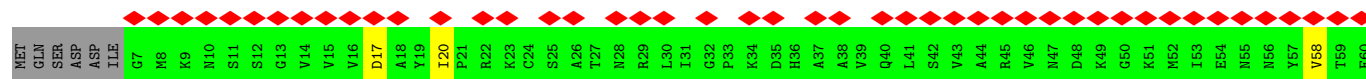
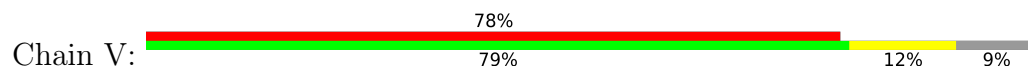


• Molecule 21: Ribosomal protein S20

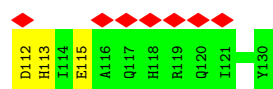
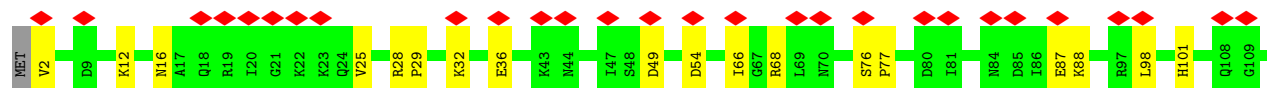
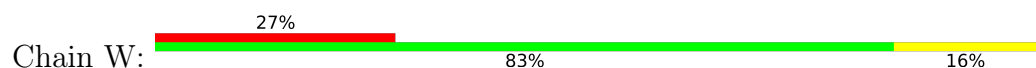




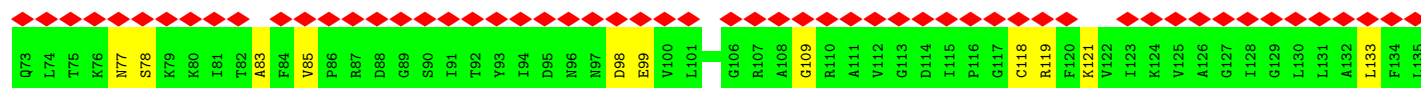
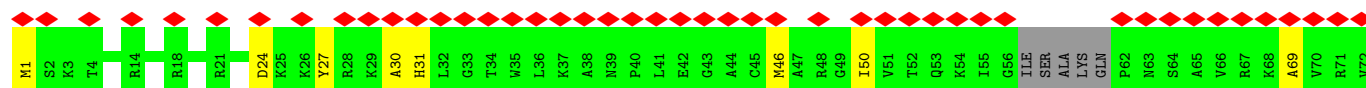
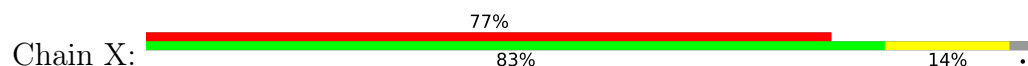
- Molecule 22: 40S ribosomal protein S21



- Molecule 23: SSU ribosomal protein S8P (Fragment)



- Molecule 24: SSU ribosomal protein S12P

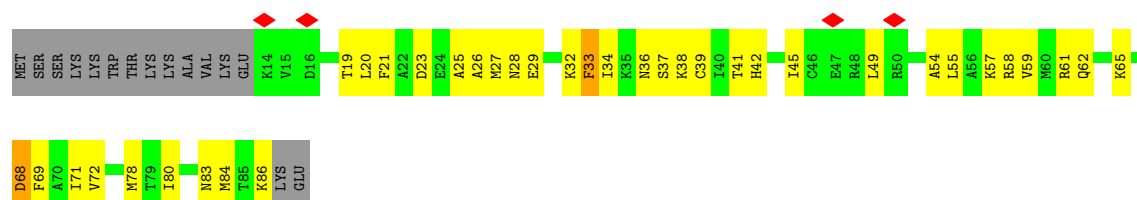


- Molecule 25: Ribosomal protein S24

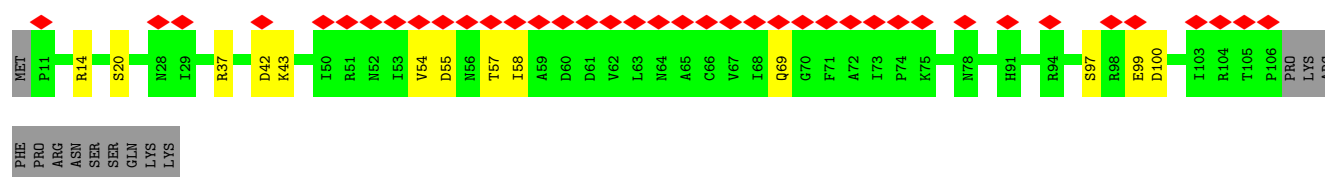
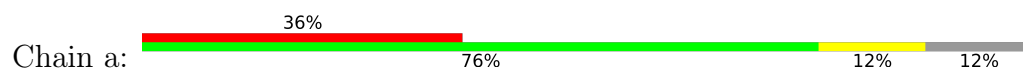




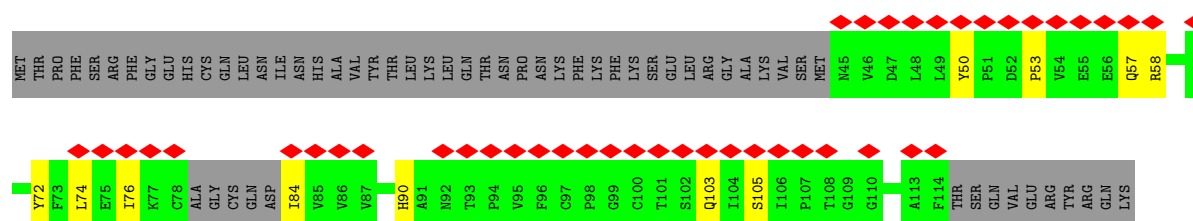
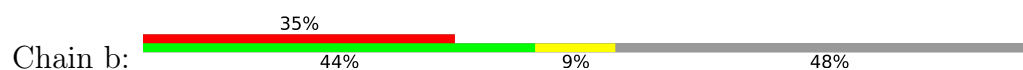
- Molecule 26: 40S ribosomal protein S25



- Molecule 27: 40S ribosomal protein S26



- Molecule 28: Ribosomal protein S27

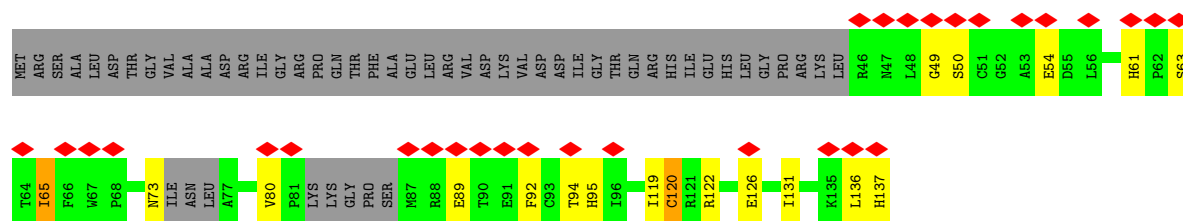


- Molecule 29: Ribosomal protein S28

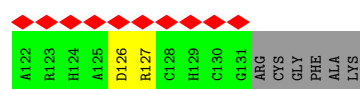
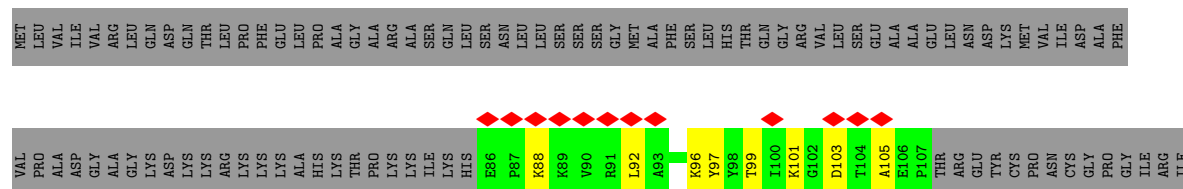


- Molecule 30: Ribosomal protein S29A

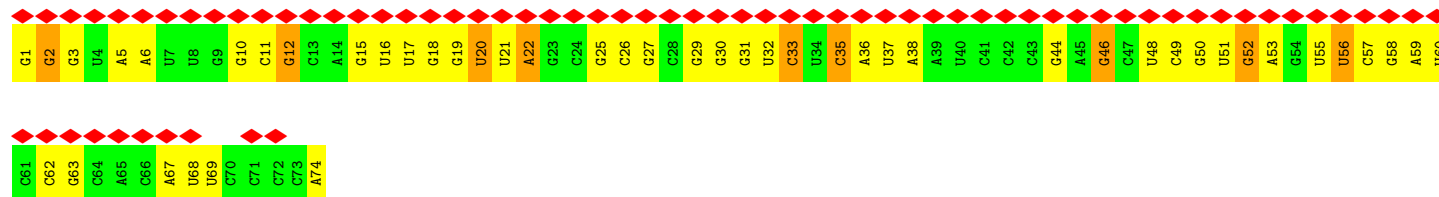




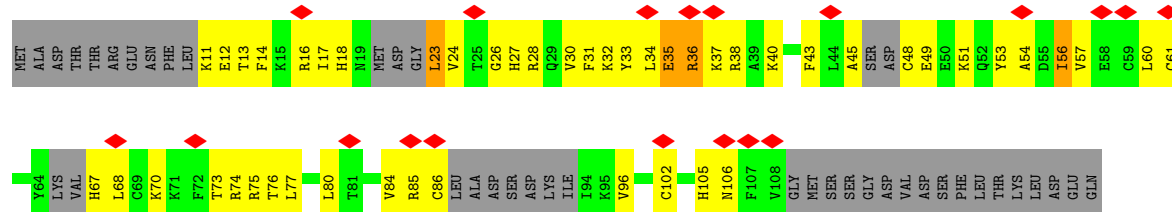
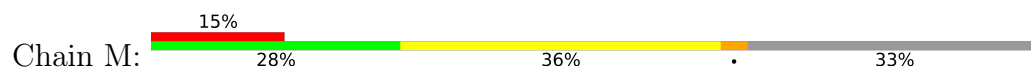
• Molecule 31: Ribosomal protein S27a



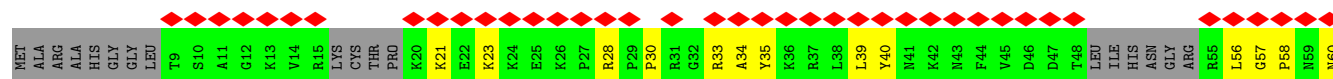
• Molecule 32: tRNA



• Molecule 33: Ribosomal protein S12



• Molecule 34: 40S ribosomal protein S30



I61	I62	I63	R64	Q65	K66	LEU	GLY	PHE
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143395	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 ($e^-/\text{\AA}^2$)	72.26	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	23.022	Depositor
Minimum map value	-10.703	Depositor
Average map value	0.003	Depositor
Map value standard deviation	1.048	Depositor
Recommended contour level	4.54	Depositor
Map size ($\text{\AA}$)	369.495, 369.495, 369.495	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8211, 0.8211, 0.8211	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, YAT, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	2	0.13	0/34573	0.26	0/53952
2	A	0.13	0/1620	0.28	0/2203
3	B	0.18	0/1749	0.31	0/2354
4	C	0.14	0/1645	0.28	0/2218
5	D	0.24	0/1627	0.38	0/2186
6	E	0.12	0/2110	0.26	0/2847
7	F	0.25	0/1467	0.40	0/1974
8	G	0.13	0/1618	0.28	0/2156
9	H	0.13	0/1341	0.29	0/1810
10	I	0.15	0/1326	0.28	0/1780
11	J	0.14	0/1341	0.31	0/1794
12	K	0.26	0/876	0.40	0/1193
13	L	0.16	0/1435	0.26	0/1919
14	N	0.16	0/1252	0.29	0/1681
15	O	0.16	0/1070	0.29	0/1436
16	P	0.25	0/893	0.40	0/1192
17	Q	0.23	0/1242	0.40	0/1660
18	R	0.24	0/656	0.43	0/875
19	S	0.24	0/1154	0.35	0/1549
20	T	0.25	0/1098	0.32	0/1476
21	U	0.22	0/826	0.36	0/1119
22	V	0.15	0/613	0.28	0/822
23	W	0.16	0/1047	0.30	0/1412
24	X	0.14	0/1092	0.30	0/1459
25	Y	0.14	0/979	0.32	0/1309
26	Z	0.26	0/583	0.37	0/777
27	a	0.16	0/792	0.28	0/1065
28	b	0.17	0/518	0.33	0/702
29	c	0.25	0/477	0.41	0/638
30	d	0.21	0/684	0.34	0/915
31	f	0.25	0/256	0.50	0/341
32	g	0.09	0/1751	0.23	0/2727

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	M	0.20	0/682	0.39	0/909
34	e	0.20	0/396	0.37	0/523
All	All	0.16	0/70789	0.29	0/102973

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	Q	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	Q	58	ARG	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	2	30919	15711	15718	225	0
2	A	1586	1608	1613	25	0
3	B	1716	1754	1760	15	0
4	C	1612	1638	1645	18	0
5	D	1602	1620	1623	65	0
6	E	2064	2140	2151	17	0
7	F	1445	1460	1472	52	0
8	G	1597	1680	1686	27	0
9	H	1318	1363	1370	26	0
10	I	1306	1338	1349	16	0
11	J	1323	1383	1395	26	0
12	K	851	827	833	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	L	1405	1436	1443	12	0
14	N	1228	1304	1308	8	0
15	O	1055	1058	1068	23	0
16	P	878	925	938	46	0
17	Q	1230	1293	1306	40	0
18	R	650	699	704	40	0
19	S	1138	1156	1169	44	0
20	T	1074	1089	1101	28	0
21	U	810	824	830	28	0
22	V	605	607	612	5	0
23	W	1030	1074	1082	12	0
24	X	1078	1153	1166	9	0
25	Y	965	1014	1020	22	0
26	Z	577	605	617	26	0
27	a	780	795	808	9	0
28	b	506	503	510	9	0
29	c	474	483	503	18	0
30	d	670	639	642	11	0
31	f	252	251	252	8	0
32	g	1569	745	798	40	0
33	M	674	665	669	45	0
34	e	392	406	416	12	0
35	2	35	40	0	0	0
36	2	22	0	0	0	0
36	a	1	0	0	0	0
37	a	1	0	0	0	0
37	d	1	0	0	0	0
38	2	579	0	0	56	0
38	B	2	0	0	0	0
38	C	9	0	0	2	0
38	D	1	0	0	0	0
38	E	11	0	0	0	0
38	F	5	0	0	5	0
38	G	1	0	0	0	0
38	I	8	0	0	3	0
38	K	1	0	0	0	0
38	L	4	0	0	1	0
38	N	11	0	0	0	0
38	O	3	0	0	0	0
38	P	2	0	0	1	0
38	Q	7	0	0	2	0
38	R	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	S	3	0	0	0	0
38	T	3	0	0	3	0
38	U	3	0	0	1	0
38	W	4	0	0	1	0
38	X	3	0	0	0	0
38	Z	2	0	0	2	0
38	a	8	0	0	2	0
38	b	2	0	0	1	0
38	d	2	0	0	1	0
38	g	2	0	0	0	0
All	All	67116	51286	51577	969	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 8.

All (969) 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)
15:O:102:TYR:OH	15:O:125:ASP:OD1	1.84	0.94
32:g:12:G:O6	32:g:22:A:N1	2.03	0.90
1:2:1102:G:N2	1:2:1105:A:OP2	2.04	0.89
1:2:257:A:O2'	1:2:258:G:O4'	1.90	0.89
1:2:297:A:OP2	6:E:1:MET:N	2.05	0.89
17:Q:23:TYR:OH	17:Q:84:ASN:OD1	1.90	0.89
12:K:10:LYS:NZ	12:K:90:GLU:OE1	2.05	0.89
32:g:2:G:H1	32:g:69:U:H3	1.21	0.87
1:2:1191:G:O2'	1:2:1192:C:OP2	1.90	0.87
1:2:678:C:O2'	15:O:132:ASP:OD2	1.92	0.86
5:D:211:GLY:O	18:R:19:ASN:ND2	2.07	0.86
20:T:29:ASP:O	20:T:33:ASN:ND2	2.07	0.86
7:F:113:ARG:NH2	7:F:114:ILE:O	2.08	0.86
6:E:141:THR:OG1	6:E:143:ASP:OD1	1.93	0.85
19:S:10:TYR:OH	19:S:23:GLY:O	1.91	0.85
5:D:109:ASP:OD1	5:D:179:ARG:NH1	2.10	0.85
17:Q:44:LYS:NZ	17:Q:45:GLY:O	2.10	0.85
25:Y:28:HIS:ND1	25:Y:31:CYS:O	2.10	0.85
26:Z:32:LYS:NZ	26:Z:36:ASN:OD1	2.10	0.84
32:g:29:G:H1	32:g:38:A:H2	1.22	0.84
7:F:110:ASP:OD1	7:F:111:SER:N	2.10	0.84
1:2:555:G:N2	1:2:558:C:O2	2.11	0.82
9:H:31:GLU:OE1	9:H:31:GLU:N	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:928:U:O4	38:2:1601:HOH:O	1.96	0.82
1:2:218:U:O2	13:L:112:ARG:NH1	2.13	0.82
20:T:30:VAL:O	38:T:201:HOH:O	1.98	0.82
1:2:591:C:N4	38:2:1630:HOH:O	2.12	0.81
1:2:384:G:OP2	38:2:1603:HOH:O	1.98	0.81
1:2:918:C:OP1	38:2:1601:HOH:O	1.99	0.81
28:b:76:ILE:O	28:b:84:ILE:N	2.15	0.80
1:2:1211:A:O2'	1:2:1212:G:OP2	2.00	0.80
18:R:22:GLU:OE2	18:R:22:GLU:N	2.14	0.80
7:F:180:ASN:OD1	38:F:201:HOH:O	1.98	0.80
32:g:12:G:H1	32:g:22:A:H2	1.29	0.80
1:2:1420:G:OP2	38:2:1604:HOH:O	1.99	0.79
19:S:143:ARG:H	19:S:143:ARG:HD2	1.46	0.79
1:2:63:C:OP1	8:G:142:LYS:NZ	2.15	0.79
32:g:21:U:O4	32:g:44:G:N1	2.15	0.79
7:F:126:ASP:OD1	38:F:202:HOH:O	2.00	0.79
1:2:741:A:OP2	38:2:1606:HOH:O	2.01	0.79
7:F:183:GLU:O	7:F:187:VAL:HG23	1.83	0.79
23:W:112:ASP:OD1	23:W:113:HIS:N	2.15	0.79
4:C:220:THR:OG1	4:C:222:ASP:OD1	2.01	0.78
26:Z:84:MET:O	38:Z:101:HOH:O	2.01	0.78
1:2:629:G:O6	38:2:1608:HOH:O	2.02	0.78
1:2:933:C:OP2	1:2:934:A:O2'	2.02	0.78
17:Q:40:VAL:O	38:Q:201:HOH:O	2.00	0.78
1:2:550:G:N7	38:2:1638:HOH:O	2.16	0.78
1:2:739:C:O2'	1:2:740:U:OP2	2.01	0.78
6:E:125:ARG:NH2	6:E:157:ASN:OD1	2.17	0.77
7:F:187:VAL:O	7:F:190:ARG:HG2	1.83	0.77
1:2:393:G:O2'	1:2:394:A:O4'	2.02	0.77
10:I:158:ILE:O	38:I:201:HOH:O	2.03	0.77
1:2:487:G:OP2	38:2:1607:HOH:O	2.02	0.77
5:D:63:VAL:O	5:D:71:ARG:NH2	2.18	0.76
15:O:55:LYS:NZ	15:O:74:ASP:OD2	2.18	0.76
33:M:48:CYS:SG	33:M:49:GLU:N	2.57	0.76
12:K:83:GLY:O	12:K:87:ILE:HD12	1.85	0.76
1:2:72:C:O2	1:2:132:C:O2'	2.04	0.76
1:2:640:C:O2'	1:2:740:U:OP1	2.01	0.76
1:2:1042:C:O2'	1:2:1061:A:OP2	2.03	0.76
21:U:25:TYR:HA	21:U:123:PRO:HA	1.69	0.75
1:2:1209:G:OP2	1:2:1209:G:N2	2.20	0.75
5:D:160:GLU:N	5:D:160:GLU:OE2	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:429:A:OP1	38:2:1609:HOH:O	2.04	0.74
1:2:299:A:N7	38:2:1644:HOH:O	2.19	0.74
18:R:73:SER:OG	18:R:75:ARG:NH1	2.20	0.74
1:2:390:C:OP2	38:2:1613:HOH:O	2.05	0.74
4:C:168:ARG:O	11:J:55:ARG:NH2	2.19	0.74
1:2:1169:G:O2'	1:2:1287:C:OP1	2.05	0.74
1:2:1415:A:OP2	38:2:1604:HOH:O	2.06	0.74
19:S:97:MET:SD	19:S:97:MET:N	2.61	0.74
1:2:427:C:O2'	38:2:1610:HOH:O	2.04	0.74
1:2:446:C:OP1	38:2:1612:HOH:O	2.05	0.74
33:M:57:VAL:O	33:M:61:CYS:N	2.20	0.74
2:A:33:ARG:NH1	2:A:51:THR:OG1	2.20	0.74
8:G:196:THR:OG1	8:G:198:GLU:OE1	2.05	0.74
24:X:109:GLY:O	24:X:119:ARG:NH1	2.21	0.74
32:g:48:U:H3	32:g:62:C:H42	1.35	0.74
1:2:103:C:O2'	1:2:245:C:O2	2.05	0.74
1:2:336:C:O2'	1:2:338:G:OP1	2.01	0.73
1:2:514:G:OP2	38:2:1611:HOH:O	2.05	0.73
5:D:140:CYS:SG	5:D:141:GLU:N	2.61	0.73
10:I:40:VAL:O	38:I:202:HOH:O	2.06	0.73
7:F:127:VAL:O	38:F:202:HOH:O	2.05	0.73
26:Z:38:LYS:NZ	26:Z:83:ASN:O	2.21	0.73
31:f:88:LYS:HA	31:f:88:LYS:HE2	1.69	0.73
32:g:35:C:H42	32:g:36:A:H62	1.36	0.73
1:2:1131:G:OP2	38:2:1615:HOH:O	2.07	0.73
30:d:95:HIS:O	38:d:301:HOH:O	2.07	0.72
1:2:491:C:OP1	38:2:1614:HOH:O	2.06	0.72
11:J:161:ALA:O	11:J:164:SER:OG	2.06	0.72
16:P:28:MET:HE1	16:P:33:ILE:HB	1.70	0.72
1:2:154:A:OP2	38:2:1617:HOH:O	2.07	0.72
9:H:33:GLN:O	9:H:37:THR:HG23	1.89	0.72
1:2:1299:G:OP1	38:2:1616:HOH:O	2.07	0.72
18:R:34:ALA:O	18:R:37:SER:OG	2.04	0.72
1:2:393:G:O2'	1:2:394:A:O5'	2.08	0.71
5:D:35:LEU:HD13	5:D:64:VAL:HG22	1.71	0.71
7:F:21:GLU:N	7:F:21:GLU:OE1	2.23	0.71
1:2:1018:C:OP2	38:2:1618:HOH:O	2.07	0.71
27:a:43:LYS:NZ	38:a:1101:HOH:O	2.21	0.71
3:B:20:ASP:OD2	15:O:7:TYR:OH	2.05	0.71
4:C:180:LYS:NZ	4:C:183:GLU:OE1	2.23	0.71
7:F:179:ARG:NE	38:F:201:HOH:O	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:M:11:LYS:N	33:M:80:LEU:HD21	2.06	0.71
1:2:205:G:O6	8:G:210:LYS:NZ	2.23	0.71
29:c:31:THR:OG1	29:c:33:GLU:OE1	2.08	0.71
1:2:1242:A:O2'	16:P:82:ASP:OD2	2.09	0.70
12:K:16:LEU:O	12:K:20:ALA:N	2.24	0.70
1:2:968:G:O2'	1:2:969:G:OP1	2.09	0.70
10:I:150:GLN:OE1	38:I:203:HOH:O	2.09	0.70
20:T:34:SER:OG	38:T:201:HOH:O	1.97	0.70
1:2:834:A:O2'	38:2:1619:HOH:O	2.09	0.70
1:2:1042:C:OP2	38:2:1622:HOH:O	2.09	0.70
30:d:61:HIS:ND1	30:d:63:SER:OG	2.25	0.70
20:T:145:GLY:O	20:T:149:VAL:HG23	1.91	0.70
7:F:190:ARG:NH1	29:c:55:GLU:OE2	2.24	0.69
12:K:42:ASN:ND2	12:K:46:CYS:SG	2.64	0.69
25:Y:78:ASN:OD1	25:Y:80:ASP:N	2.25	0.69
1:2:1192:C:O3'	38:2:1623:HOH:O	2.10	0.69
1:2:134:G:N3	38:2:1654:HOH:O	2.24	0.69
8:G:63:ASP:OD1	8:G:67:PHE:N	2.24	0.69
1:2:20:G:N3	38:2:1660:HOH:O	2.26	0.69
16:P:15:PRO:HB2	19:S:92:GLU:OE2	1.93	0.69
27:a:57:THR:HG23	27:a:58:ILE:HG23	1.74	0.69
1:2:1008:U:OP2	38:2:1620:HOH:O	2.09	0.69
20:T:66:ASP:OD1	20:T:67:ALA:N	2.26	0.69
5:D:73:HIS:HB3	12:K:105:PRO:HG2	1.74	0.69
1:2:937:G:O2'	1:2:1287:C:O2'	2.11	0.69
1:2:756:A:OP2	38:2:1628:HOH:O	2.12	0.68
8:G:26:ASP:OD1	8:G:28:ARG:N	2.25	0.68
1:2:387:G:O2'	1:2:422:G:N2	2.26	0.68
1:2:1422:A:OP2	38:2:1624:HOH:O	2.10	0.68
7:F:121:ARG:NH1	7:F:122:ARG:O	2.26	0.68
5:D:119:MET:SD	5:D:120:PRO:HD2	2.34	0.68
1:2:113:G:O2'	1:2:114:G:OP1	2.10	0.68
1:2:194:A:N7	38:2:1661:HOH:O	2.26	0.68
1:2:528:A:OP2	38:2:1625:HOH:O	2.10	0.68
1:2:1355:G:O2'	1:2:1383:A:N6	2.27	0.68
24:X:77:ASN:O	24:X:78:SER:OG	2.12	0.68
1:2:46:A:OP2	38:2:1626:HOH:O	2.11	0.68
17:Q:24:THR:OG1	38:Q:201:HOH:O	2.12	0.68
22:V:86:MET:SD	22:V:86:MET:N	2.66	0.68
16:P:23:GLU:N	16:P:23:GLU:OE1	2.26	0.68
16:P:57:PHE:O	16:P:61:LEU:HD12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:122:U:O4	1:2:202:A:N6	2.28	0.67
16:P:125:ILE:HD12	16:P:125:ILE:O	1.94	0.67
1:2:32:C:OP2	38:2:1627:HOH:O	2.11	0.67
1:2:989:U:O2'	1:2:990:U:OP1	2.13	0.67
5:D:64:VAL:O	5:D:71:ARG:NE	2.27	0.67
30:d:49:GLY:O	30:d:50:SER:OG	2.11	0.67
1:2:85:U:O4	38:2:1621:HOH:O	2.09	0.67
1:2:903:C:OP2	38:2:1632:HOH:O	2.13	0.67
13:L:104:THR:OG1	38:L:201:HOH:O	2.13	0.67
30:d:54:GLU:N	30:d:54:GLU:OE1	2.28	0.67
5:D:76:GLU:OE1	12:K:105:PRO:HB2	1.95	0.67
7:F:171:ASP:OD2	7:F:180:ASN:ND2	2.27	0.67
19:S:3:THR:C	19:S:4:ILE:HD13	2.20	0.66
19:S:89:ASN:OD1	19:S:90:ASP:N	2.28	0.66
33:M:45:ALA:O	33:M:70:LYS:NZ	2.28	0.66
32:g:3:G:H1	32:g:68:U:H3	1.42	0.66
1:2:289:G:OP2	38:2:1635:HOH:O	2.14	0.66
4:C:146:HIS:ND1	4:C:189:ASP:OD2	2.22	0.66
4:C:89:ARG:NH1	38:C:301:HOH:O	2.27	0.66
10:I:6:ASP:OD1	10:I:7:LYS:N	2.27	0.66
10:I:78:SER:OG	10:I:160:GLU:OE1	2.12	0.66
7:F:115:GLY:O	29:c:18:SER:N	2.29	0.66
12:K:49:THR:OG1	12:K:52:HIS:ND1	2.28	0.66
1:2:86:C:OP2	1:2:290:A:O2'	2.14	0.66
1:2:483:C:OP2	38:2:1631:HOH:O	2.12	0.66
6:E:91:GLU:N	6:E:91:GLU:OE1	2.24	0.66
19:S:111:ASP:OD1	19:S:114:ARG:NH2	2.28	0.66
20:T:34:SER:N	38:T:201:HOH:O	2.28	0.65
1:2:106:C:N3	38:2:1667:HOH:O	2.29	0.65
1:2:211:C:O2	6:E:33:ASN:ND2	2.30	0.65
16:P:65:ARG:NH1	38:P:201:HOH:O	2.29	0.65
1:2:993:C:OP1	33:M:32:LYS:NZ	2.20	0.65
5:D:67:ASP:OD2	12:K:102:TYR:OH	2.13	0.65
19:S:37:ILE:HD11	19:S:100:LEU:HD21	1.77	0.65
17:Q:66:VAL:HG13	17:Q:96:ILE:HG23	1.77	0.65
1:2:497:U:OP1	38:2:1633:HOH:O	2.13	0.65
20:T:147:LYS:NZ	20:T:151:ASP:OD1	2.26	0.64
2:A:45:ASP:OD1	2:A:46:ARG:N	2.29	0.64
19:S:28:GLU:OE2	19:S:39:ARG:NE	2.30	0.64
5:D:52:ILE:HD12	5:D:52:ILE:O	1.97	0.64
32:g:20:U:N3	32:g:46:G:N7	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:132:ASP:OD1	15:O:133:ARG:N	2.31	0.64
1:2:218:U:O4	38:2:1634:HOH:O	2.14	0.64
21:U:26:THR:N	21:U:122:GLU:O	2.30	0.64
17:Q:46:ASP:OD1	17:Q:47:ILE:N	2.31	0.64
5:D:119:MET:HA	5:D:119:MET:HE2	1.79	0.64
7:F:55:VAL:O	7:F:59:THR:HG23	1.97	0.64
33:M:36:ARG:O	33:M:38:ARG:NH1	2.30	0.64
1:2:445:C:O2'	1:2:457:G:N2	2.30	0.64
1:2:776:A:OP2	38:2:1636:HOH:O	2.14	0.64
1:2:1036:G:N2	1:2:1039:A:OP2	2.30	0.63
1:2:370:C:O2'	38:2:1637:HOH:O	2.15	0.63
1:2:1086:C:O2'	1:2:1087:C:OP2	2.12	0.63
1:2:1231:C:OP1	19:S:135:GLN:NE2	2.31	0.63
4:C:160:ARG:NH1	38:C:302:HOH:O	2.29	0.63
5:D:44:SER:OG	21:U:115:GLN:NE2	2.31	0.63
1:2:1367:C:OP2	8:G:71:GLN:NE2	2.31	0.63
5:D:9:GLU:OE1	5:D:9:GLU:N	2.32	0.62
1:2:1365:G:OP2	38:2:1639:HOH:O	2.16	0.62
8:G:26:ASP:OD1	8:G:27:PHE:N	2.32	0.62
1:2:314:C:O2	38:2:1629:HOH:O	2.12	0.62
17:Q:77:LEU:HD23	17:Q:77:LEU:H	1.64	0.62
18:R:77:GLN:O	18:R:81:ARG:N	2.31	0.62
32:g:1:G:O2'	32:g:2:G:OP1	2.15	0.62
12:K:66:VAL:HG12	12:K:79:LEU:HA	1.81	0.62
17:Q:80:GLY:C	17:Q:81:LEU:HD12	2.25	0.62
1:2:592:G:N1	1:2:597:G:O6	2.33	0.62
9:H:168:VAL:CG1	9:H:201:MET:HB3	2.30	0.62
4:C:26:GLU:OE2	4:C:38:LYS:NZ	2.28	0.61
33:M:56:ILE:HG23	33:M:57:VAL:H	1.65	0.61
20:T:56:THR:HG22	20:T:56:THR:O	2.00	0.61
1:2:937:G:HO2'	1:2:1287:C:HO2'	1.49	0.61
13:L:65:ARG:NH1	13:L:74:CYS:O	2.34	0.61
2:A:68:ARG:O	2:A:72:THR:HG23	2.01	0.60
8:G:127:LEU:HD23	8:G:128:PRO:HD2	1.83	0.60
8:G:85:GLN:NE2	8:G:95:ASN:O	2.34	0.60
20:T:66:ASP:OD1	20:T:68:ASP:N	2.26	0.60
11:J:115:ILE:HD11	11:J:127:ALA:HB1	1.84	0.60
14:N:114:ARG:O	14:N:118:VAL:HG23	2.02	0.60
2:A:174:MET:HE2	2:A:174:MET:H	1.67	0.60
1:2:992:G:OP2	33:M:28:ARG:NH2	2.34	0.60
29:c:11:GLU:OE1	29:c:12:VAL:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:24:GLU:O	5:D:27:LEU:N	2.34	0.59
5:D:111:LEU:O	5:D:115:LEU:HD23	2.03	0.59
26:Z:19:THR:OG1	26:Z:20:LEU:HD12	2.02	0.59
28:b:90:HIS:NE2	38:b:201:HOH:O	2.31	0.59
29:c:40:ASN:N	29:c:40:ASN:OD1	2.35	0.59
32:g:30:G:H1	32:g:37:U:H3	1.48	0.59
5:D:52:ILE:HD11	5:D:90:PHE:CZ	2.37	0.59
7:F:23:LEU:HD13	7:F:27:ILE:HD12	1.84	0.59
4:C:88:GLN:OE1	4:C:88:GLN:N	2.35	0.59
15:O:47:ILE:O	15:O:82:ARG:NH1	2.34	0.59
34:e:57:GLY:N	34:e:58:PRO:HD3	2.18	0.59
1:2:791:G:OP1	2:A:37:ARG:NH1	2.34	0.59
12:K:93:LEU:HD12	12:K:97:VAL:HG21	1.84	0.59
14:N:38:CYS:SG	14:N:78:LYS:NZ	2.69	0.59
11:J:104:GLU:N	11:J:104:GLU:OE1	2.36	0.59
17:Q:46:ASP:O	17:Q:47:ILE:HD13	2.02	0.59
29:c:33:GLU:O	29:c:35:ARG:NE	2.35	0.59
20:T:76:SER:OG	20:T:98:TYR:OH	2.20	0.59
33:M:75:ARG:NH2	33:M:96:VAL:HG13	2.18	0.59
1:2:900:C:O2'	17:Q:157:TYR:OH	2.21	0.59
7:F:113:ARG:HE	7:F:113:ARG:C	2.11	0.59
16:P:76:VAL:O	16:P:76:VAL:HG13	2.02	0.59
26:Z:86:LYS:HB2	38:Z:101:HOH:O	2.03	0.59
1:2:517:C:O2	9:H:129:ARG:NH2	2.32	0.58
1:2:785:C:HO2'	23:W:2:VAL:N	2.01	0.58
32:g:50:G:N2	32:g:60:U:O2	2.36	0.58
4:C:62:ASP:OD1	4:C:63:TYR:N	2.36	0.58
9:H:196:THR:OG1	9:H:197:GLU:N	2.34	0.58
7:F:13:LEU:HD23	7:F:13:LEU:O	2.04	0.58
21:U:87:MET:HE2	21:U:87:MET:HA	1.86	0.58
1:2:989:U:HO2'	1:2:990:U:P	2.27	0.58
5:D:29:GLU:OE2	5:D:33:ARG:NE	2.36	0.58
1:2:292:U:H4'	11:J:2:PRO:HG3	1.85	0.58
1:2:1192:C:O2	20:T:137:ARG:NH2	2.37	0.58
5:D:185:GLN:OE1	5:D:185:GLN:N	2.36	0.58
1:2:704:G:H2'	1:2:705:A:C8	2.38	0.58
4:C:59:GLU:OE1	4:C:59:GLU:N	2.36	0.58
7:F:112:CYS:SG	7:F:113:ARG:N	2.76	0.58
1:2:391:G:N2	1:2:393:G:O6	2.38	0.57
6:E:104:ASP:OD1	6:E:108:ARG:N	2.34	0.57
33:M:73:THR:HG22	33:M:75:ARG:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:55:ALA:HA	3:B:58:VAL:HG12	1.85	0.57
5:D:78:LEU:HD11	12:K:76:TYR:HD1	1.68	0.57
25:Y:94:CYS:HB3	25:Y:96:LEU:HD23	1.86	0.57
1:2:810:C:O2'	28:b:58:ARG:NH2	2.37	0.57
7:F:34:PHE:HB2	17:Q:64:THR:HG21	1.87	0.57
22:V:74:SER:O	22:V:78:LEU:HD23	2.03	0.57
9:H:201:MET:HE1	28:b:50:TYR:CE1	2.39	0.57
12:K:38:TYR:O	12:K:46:CYS:N	2.37	0.57
12:K:65:VAL:HG13	12:K:66:VAL:HG13	1.85	0.57
26:Z:23:ASP:O	26:Z:25:ALA:N	2.36	0.57
5:D:77:TYR:HE1	12:K:105:PRO:HB3	1.69	0.57
19:S:113:GLU:OE1	19:S:113:GLU:HA	2.05	0.57
6:E:125:ARG:NH1	6:E:225:VAL:O	2.38	0.57
16:P:125:ILE:HD12	16:P:125:ILE:C	2.30	0.57
7:F:190:ARG:HD3	15:O:66:TYR:OH	2.05	0.57
11:J:67:ASN:O	11:J:67:ASN:ND2	2.36	0.57
1:2:629:G:O2'	14:N:108:ASP:OD1	2.23	0.57
1:2:1239:U:HO2'	1:2:1282:C:HO2'	1.48	0.57
32:g:35:C:H42	32:g:36:A:N6	2.03	0.57
33:M:12:GLU:O	33:M:16:ARG:NH2	2.37	0.56
12:K:104:LYS:O	12:K:104:LYS:NZ	2.28	0.56
23:W:12:LYS:NZ	38:W:201:HOH:O	2.37	0.56
1:2:1225:C:O2'	38:2:1643:HOH:O	2.18	0.56
9:H:201:MET:HE1	28:b:50:TYR:CD1	2.41	0.56
16:P:88:GLU:OE1	16:P:88:GLU:N	2.37	0.56
27:a:37:ARG:NH2	38:a:1102:HOH:O	2.36	0.56
1:2:1281:C:O2	38:2:1640:HOH:O	2.16	0.56
19:S:60:LEU:C	19:S:60:LEU:HD12	2.30	0.56
9:H:66:ASP:OD1	9:H:67:GLY:N	2.39	0.56
12:K:11:ALA:C	12:K:36:ILE:HD11	2.31	0.56
17:Q:16:GLU:OE1	17:Q:18:ARG:N	2.39	0.56
1:2:432:G:OP2	1:2:433:C:O2'	2.24	0.55
1:2:460:A:OP2	38:2:1642:HOH:O	2.18	0.55
1:2:1186:A:OP2	17:Q:1:MET:N	2.39	0.55
32:g:29:G:O6	32:g:38:A:N1	2.39	0.55
9:H:37:THR:HG22	9:H:98:ASN:ND2	2.21	0.55
4:C:129:ASN:OD1	4:C:129:ASN:O	2.25	0.55
9:H:129:ARG:O	9:H:132:THR:OG1	2.20	0.55
19:S:99:ILE:HD12	19:S:107:THR:HG21	1.87	0.55
3:B:90:LEU:HD13	3:B:225:MET:CE	2.36	0.55
14:N:148:ALA:O	14:N:152:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:20:ASN:OD1	18:R:20:ASN:N	2.39	0.55
16:P:60:LYS:O	16:P:64:ARG:HG3	2.07	0.55
21:U:67:THR:N	38:U:201:HOH:O	2.33	0.55
1:2:1027:G:N7	1:2:1053:U:O2'	2.31	0.54
18:R:25:LYS:HE3	18:R:25:LYS:HA	1.87	0.54
1:2:975:C:N4	38:2:1653:HOH:O	2.37	0.54
21:U:23:GLN:NE2	21:U:101:ILE:HG23	2.22	0.54
33:M:35:GLU:O	33:M:36:ARG:NE	2.40	0.54
1:2:969:G:O2'	1:2:970:A:OP2	2.21	0.54
18:R:63:ARG:NH2	18:R:67:GLY:O	2.37	0.54
21:U:49:ARG:HD3	21:U:49:ARG:N	2.22	0.54
28:b:103:GLN:NE2	28:b:105:SER:O	2.40	0.54
30:d:126:GLU:OE1	30:d:126:GLU:N	2.40	0.54
18:R:31:ASN:O	18:R:35:ILE:HG12	2.08	0.54
1:2:1189:C:OP2	21:U:63:ARG:NE	2.39	0.54
4:C:100:ASN:OD1	4:C:102:ASP:N	2.40	0.54
17:Q:127:TYR:O	17:Q:128:ASP:C	2.51	0.54
7:F:64:MET:HE2	7:F:64:MET:HA	1.89	0.54
13:L:37:GLU:N	13:L:37:GLU:OE2	2.40	0.54
21:U:99:ASN:OD1	21:U:100:ASP:N	2.40	0.54
25:Y:55:ILE:HD12	25:Y:55:ILE:O	2.08	0.54
19:S:143:ARG:HD2	19:S:143:ARG:N	2.20	0.54
1:2:948:A:O2'	1:2:949:C:O5'	2.24	0.54
11:J:65:ASP:OD1	11:J:65:ASP:N	2.37	0.54
8:G:239:ILE:O	8:G:240:TYR:HB2	2.06	0.54
1:2:792:C:OP2	2:A:37:ARG:NH2	2.37	0.54
7:F:96:GLN:O	7:F:99:VAL:HG22	2.08	0.54
12:K:60:LEU:O	12:K:65:VAL:HG12	2.08	0.54
18:R:73:SER:O	18:R:75:ARG:NH2	2.35	0.54
15:O:38:VAL:HG23	15:O:75:LEU:HD21	1.89	0.53
26:Z:27:MET:SD	26:Z:28:ASN:N	2.81	0.53
26:Z:68:ASP:OD1	26:Z:68:ASP:N	2.41	0.53
5:D:38:ALA:CB	5:D:64:VAL:HG23	2.39	0.53
26:Z:86:LYS:HD2	26:Z:86:LYS:O	2.09	0.53
5:D:97:ILE:HD12	5:D:97:ILE:N	2.24	0.53
19:S:46:LEU:HD13	19:S:53:VAL:HG12	1.88	0.53
1:2:1153:C:O2'	30:d:92:PHE:O	2.23	0.53
1:2:1208:C:H42	5:D:6:ARG:HG3	1.72	0.53
2:A:172:THR:OG1	2:A:175:SER:OG	2.00	0.53
1:2:434:A:O2'	1:2:435:A:O5'	2.22	0.53
19:S:35:LYS:HB3	19:S:101:VAL:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:34:PHE:CB	17:Q:64:THR:HG21	2.39	0.53
7:F:160:ALA:O	7:F:164:MET:SD	2.67	0.53
17:Q:66:VAL:CG1	17:Q:96:ILE:HG23	2.39	0.53
32:g:12:G:C6	32:g:22:A:N1	2.76	0.53
7:F:37:HIS:O	7:F:38:SER:OG	2.25	0.53
18:R:69:VAL:HG22	18:R:70:HIS:N	2.24	0.53
1:2:840:C:O2'	1:2:841:G:OP1	2.24	0.52
2:A:99:THR:HG22	2:A:99:THR:O	2.08	0.52
5:D:73:HIS:CB	12:K:105:PRO:HG2	2.39	0.52
6:E:230:ASN:O	6:E:232:SER:N	2.41	0.52
9:H:197:GLU:OE1	9:H:198:PHE:N	2.42	0.52
1:2:615:G:OP1	14:N:13:ARG:NH1	2.41	0.52
1:2:636:G:H2'	1:2:637:U:C6	2.43	0.52
1:2:637:U:OP2	38:2:1646:HOH:O	2.19	0.52
18:R:20:ASN:ND2	18:R:41:VAL:HG13	2.25	0.52
19:S:106:SER:O	19:S:106:SER:OG	2.25	0.52
34:e:35:TYR:O	34:e:39:LEU:HD12	2.09	0.52
13:L:31:ARG:HD3	13:L:31:ARG:H	1.74	0.52
17:Q:18:ARG:O	17:Q:22:LYS:NZ	2.41	0.52
25:Y:34:GLU:O	25:Y:35:SER:OG	2.25	0.52
33:M:75:ARG:HH22	33:M:96:VAL:HG13	1.75	0.52
1:2:1197:G:N2	1:2:1200:A:OP2	2.43	0.52
8:G:104:ARG:NE	8:G:111:ASP:OD2	2.34	0.52
17:Q:27:THR:HG21	17:Q:106:GLY:N	2.25	0.52
25:Y:23:VAL:HG13	25:Y:23:VAL:O	2.09	0.52
1:2:1055:G:O2'	1:2:1105:A:O2'	2.22	0.52
11:J:89:ASP:OD1	11:J:90:GLU:N	2.43	0.52
11:J:106:ILE:HG23	11:J:149:MET:HE1	1.92	0.52
17:Q:108:LEU:HD21	17:Q:121:ARG:HG2	1.92	0.52
27:a:97:SER:OG	27:a:99:GLU:OE2	2.25	0.52
1:2:612:C:H2'	1:2:613:G:O4'	2.09	0.51
18:R:23:SER:C	18:R:24:LEU:HD22	2.35	0.51
1:2:1194:C:H42	1:2:1203:A:H61	1.58	0.51
18:R:23:SER:O	18:R:24:LEU:HD22	2.10	0.51
19:S:95:LYS:C	19:S:97:MET:HE1	2.36	0.51
21:U:99:ASN:ND2	21:U:103:THR:OG1	2.42	0.51
8:G:13:ASN:OD1	8:G:16:THR:OG1	2.27	0.51
34:e:60:ASN:OD1	34:e:61:LEU:N	2.44	0.51
1:2:844:C:N4	24:X:1:MET:O	2.44	0.51
1:2:1280:C:OP2	1:2:1281:C:N4	2.43	0.51
2:A:32:VAL:HG12	2:A:33:ARG:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:15:VAL:HG13	8:G:16:THR:HG23	1.93	0.51
9:H:28:SER:OG	9:H:29:GLU:N	2.42	0.51
17:Q:21:ASP:OD1	17:Q:21:ASP:N	2.39	0.51
1:2:740:U:O2'	38:2:1647:HOH:O	2.19	0.51
7:F:41:ARG:H	7:F:41:ARG:HD2	1.75	0.51
19:S:42:ALA:O	19:S:46:LEU:HD12	2.11	0.51
24:X:98:ASP:OD1	24:X:99:GLU:N	2.44	0.51
1:2:801:C:H42	1:2:809:C:H42	1.58	0.51
8:G:38:MET:SD	8:G:38:MET:N	2.84	0.51
21:U:108:THR:HA	21:U:111:ILE:HD11	1.91	0.51
1:2:140:A:N6	1:2:330:G:O6	2.43	0.51
5:D:8:ASP:OD1	5:D:8:ASP:N	2.36	0.51
24:X:139:GLU:OE1	24:X:139:GLU:HA	2.10	0.51
1:2:1239:U:O4	16:P:40:ARG:NH2	2.44	0.51
18:R:18:GLU:OE1	18:R:19:ASN:N	2.44	0.51
15:O:39:THR:HG21	15:O:43:GLY:HA2	1.92	0.51
15:O:72:THR:HG21	15:O:112:ALA:HB3	1.92	0.51
26:Z:57:LYS:O	26:Z:61:ARG:HG2	2.11	0.51
29:c:24:GLN:O	29:c:25:VAL:HG23	2.11	0.50
31:f:126:ASP:OD1	31:f:127:ARG:N	2.44	0.50
1:2:675:A:H2'	1:2:676:G:C8	2.47	0.50
2:A:96:CYS:O	2:A:100:HIS:N	2.44	0.50
21:U:103:THR:O	21:U:107:LYS:N	2.38	0.50
32:g:5:A:H2'	32:g:6:A:C8	2.46	0.50
10:I:138:ASP:OD1	10:I:138:ASP:N	2.45	0.50
33:M:51:LYS:O	33:M:54:ALA:N	2.40	0.50
3:B:98:THR:O	3:B:232:HIS:NE2	2.43	0.50
5:D:205:PRO:O	5:D:206:ASP:OD1	2.30	0.50
8:G:73:VAL:HG21	8:G:105:GLY:HA2	1.94	0.50
14:N:144:ASP:OD1	14:N:145:GLN:N	2.45	0.50
1:2:919:G:C6	1:2:1165:G:O6	2.64	0.50
7:F:26:TYR:CD1	7:F:130:LEU:HD13	2.46	0.50
15:O:110:ILE:O	15:O:114:VAL:HG23	2.12	0.50
32:g:51:U:H2'	32:g:52:G:C5	2.46	0.50
1:2:114:G:O2'	1:2:161:C:O2'	2.29	0.50
1:2:1113:G:N1	1:2:1116:G:OP2	2.40	0.50
33:M:33:TYR:HA	33:M:36:ARG:HH21	1.77	0.50
1:2:1240:G:N1	1:2:1243:A:OP2	2.37	0.50
8:G:51:TYR:CE1	8:G:127:LEU:HD11	2.45	0.50
11:J:34:GLY:HA3	34:e:40:TYR:CE2	2.46	0.50
16:P:65:ARG:NH2	16:P:90:ILE:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:75:GLU:N	17:Q:75:GLU:OE1	2.44	0.50
25:Y:39:ILE:HG22	25:Y:39:ILE:O	2.11	0.50
29:c:61:ARG:HA	29:c:61:ARG:HH11	1.77	0.50
1:2:678:C:C2'	15:O:132:ASP:OD2	2.59	0.50
1:2:1300:C:OP1	7:F:46:ARG:NH2	2.39	0.50
1:2:1371:C:O2'	1:2:1372:G:OP2	2.26	0.50
11:J:67:ASN:HD22	11:J:67:ASN:C	2.20	0.50
13:L:194:LYS:HD2	13:L:194:LYS:C	2.36	0.50
18:R:43:ILE:O	18:R:44:ILE:HD13	2.12	0.50
34:e:56:LEU:C	34:e:58:PRO:HD3	2.37	0.50
1:2:918:C:H41	19:S:138:LYS:HE2	1.77	0.49
5:D:183:MET:HB2	5:D:185:GLN:OE1	2.12	0.49
7:F:1:MET:HE2	7:F:3:LEU:HD23	1.93	0.49
7:F:41:ARG:HG2	7:F:41:ARG:O	2.12	0.49
7:F:57:ARG:NH2	7:F:134:ASN:OD1	2.38	0.49
18:R:62:ASN:HA	18:R:65:VAL:HG12	1.94	0.49
21:U:27:ILE:HB	21:U:92:PHE:HB2	1.94	0.49
25:Y:38:ALA:O	25:Y:42:LYS:NZ	2.45	0.49
33:M:56:ILE:HG23	33:M:57:VAL:HG23	1.94	0.49
5:D:116:GLU:HA	5:D:116:GLU:OE2	2.12	0.49
16:P:95:SER:HA	16:P:103:ILE:O	2.12	0.49
17:Q:77:LEU:O	17:Q:81:LEU:HD13	2.12	0.49
17:Q:119:GLU:OE1	17:Q:120:LEU:HD23	2.12	0.49
18:R:18:GLU:OE1	18:R:18:GLU:C	2.55	0.49
26:Z:55:LEU:O	26:Z:59:VAL:HG23	2.12	0.49
33:M:34:LEU:HD23	33:M:60:LEU:HD23	1.94	0.49
1:2:371:G:OP1	25:Y:109:LYS:NZ	2.40	0.49
5:D:203:VAL:O	5:D:203:VAL:HG13	2.12	0.49
12:K:38:TYR:C	12:K:45:LEU:HD13	2.37	0.49
33:M:14:PHE:CD2	33:M:80:LEU:HD13	2.48	0.49
7:F:73:LEU:N	38:F:204:HOH:O	2.46	0.49
15:O:106:GLY:O	15:O:110:ILE:HG12	2.13	0.49
16:P:52:MET:SD	16:P:52:MET:C	2.96	0.49
16:P:107:ILE:N	16:P:107:ILE:HD12	2.27	0.49
20:T:22:SER:OG	20:T:25:ARG:NH2	2.33	0.49
33:M:61:CYS:HB3	33:M:68:LEU:HB3	1.95	0.49
1:2:444:G:N1	1:2:460:A:OP1	2.42	0.49
17:Q:59:PRO:O	17:Q:61:ILE:N	2.42	0.49
18:R:6:THR:HG22	18:R:7:LYS:N	2.28	0.49
19:S:90:ASP:OD1	19:S:91:PHE:N	2.45	0.49
19:S:125:ARG:NE	19:S:131:LYS:O	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:35:PHE:O	20:T:39:LEU:HD13	2.13	0.49
33:M:17:ILE:HG22	33:M:23:LEU:HD21	1.95	0.49
1:2:679:C:O2'	1:2:696:C:OP2	2.17	0.49
11:J:126:HIS:O	11:J:130:MET:HG3	2.13	0.49
20:T:75:ALA:O	20:T:78:ILE:HG22	2.13	0.49
23:W:101:HIS:ND1	23:W:112:ASP:OD2	2.38	0.49
33:M:26:GLY:O	33:M:30:VAL:HG12	2.13	0.49
1:2:1039:A:OP1	4:C:93:ARG:NH1	2.45	0.49
12:K:8:VAL:HG22	12:K:38:TYR:CD2	2.48	0.49
19:S:22:GLN:OE1	19:S:22:GLN:HA	2.12	0.49
20:T:151:ASP:O	20:T:154:GLU:HG3	2.13	0.49
26:Z:34:ILE:C	26:Z:34:ILE:HD12	2.37	0.49
5:D:73:HIS:CD2	12:K:105:PRO:HD2	2.48	0.49
11:J:105:ASP:OD1	11:J:105:ASP:N	2.46	0.49
26:Z:29:GLU:O	26:Z:33:PHE:N	2.34	0.49
31:f:96:LYS:HD2	31:f:96:LYS:H	1.77	0.49
18:R:17:VAL:HG23	18:R:61:MET:SD	2.53	0.48
19:S:53:VAL:HG23	19:S:54:HIS:ND1	2.28	0.48
1:2:589:G:N1	1:2:602:G:O6	2.46	0.48
1:2:1033:G:O2'	1:2:1060:A:N1	2.43	0.48
9:H:36:GLY:O	9:H:40:LYS:HG2	2.12	0.48
10:I:106:VAL:HG22	10:I:109:CYS:SG	2.53	0.48
32:g:1:G:HO2'	32:g:2:G:P	2.34	0.48
2:A:199:GLU:OE1	2:A:200:TRP:N	2.42	0.48
5:D:212:ALA:HA	18:R:19:ASN:HD21	1.78	0.48
7:F:1:MET:HE2	7:F:3:LEU:CD2	2.43	0.48
18:R:20:ASN:ND2	18:R:41:VAL:HG22	2.28	0.48
32:g:1:G:O2'	32:g:2:G:P	2.70	0.48
1:2:576:G:H2'	1:2:577:G:O4'	2.14	0.48
1:2:1240:G:O6	16:P:43:ARG:NH1	2.46	0.48
1:2:982:G:C2'	1:2:983:C:H5'	2.43	0.48
5:D:208:ILE:HG22	5:D:209:GLU:N	2.29	0.48
12:K:32:ASN:ND2	12:K:47:ASN:O	2.47	0.48
18:R:56:TYR:O	18:R:59:THR:HG22	2.14	0.48
19:S:143:ARG:O	19:S:143:ARG:HG2	2.12	0.48
23:W:115:GLU:HA	23:W:115:GLU:OE1	2.13	0.48
1:2:336:C:O4'	1:2:336:C:O2	2.32	0.48
5:D:159:LYS:C	5:D:160:GLU:OE2	2.56	0.48
7:F:29:ILE:HD12	7:F:29:ILE:C	2.38	0.48
15:O:96:GLY:O	15:O:97:THR:OG1	2.20	0.48
5:D:80:ALA:O	5:D:84:MET:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:76:ILE:O	15:O:80:THR:HG23	2.14	0.48
17:Q:135:ASP:OD2	17:Q:137:ARG:NH1	2.46	0.48
32:g:50:G:N1	32:g:60:U:N3	2.48	0.48
1:2:387:G:H2'	1:2:388:C:O2	2.14	0.48
1:2:840:C:C2'	1:2:841:G:OP1	2.62	0.48
16:P:75:ILE:HD12	16:P:93:THR:CG2	2.44	0.48
3:B:120:CYS:C	3:B:121:ILE:HD12	2.39	0.47
9:H:173:VAL:HG23	9:H:174:TYR:N	2.28	0.47
20:T:71:TYR:CD1	20:T:71:TYR:N	2.82	0.47
33:M:14:PHE:CG	33:M:80:LEU:HD22	2.49	0.47
12:K:14:ALA:HA	12:K:91:LEU:HD11	1.97	0.47
18:R:6:THR:HG22	18:R:7:LYS:H	1.77	0.47
24:X:30:ALA:HB3	24:X:31:HIS:CE1	2.49	0.47
25:Y:51:ASP:OD1	25:Y:51:ASP:C	2.57	0.47
33:M:77:LEU:H	33:M:77:LEU:HD12	1.77	0.47
5:D:59:ALA:HB1	5:D:100:ARG:HD2	1.96	0.47
17:Q:34:SER:HA	17:Q:89:GLY:HA3	1.97	0.47
18:R:37:SER:O	18:R:39:ARG:NH2	2.47	0.47
27:a:99:GLU:H	27:a:99:GLU:CD	2.21	0.47
1:2:113:G:H3'	1:2:114:G:H5''	1.95	0.47
1:2:301:C:OP1	38:2:1649:HOH:O	2.20	0.47
6:E:105:VAL:O	6:E:244:ARG:NH1	2.47	0.47
1:2:1:C:O2'	1:2:2:A:OP1	2.30	0.47
13:L:162:GLU:N	13:L:162:GLU:OE2	2.48	0.47
20:T:26:VAL:HG21	20:T:156:LEU:HD11	1.96	0.47
9:H:37:THR:HG22	9:H:98:ASN:HD22	1.79	0.47
23:W:76:SER:HB3	23:W:77:PRO:HD3	1.96	0.47
7:F:27:ILE:CG2	7:F:29:ILE:HG23	2.44	0.47
7:F:114:ILE:HG22	7:F:123:GLN:HG3	1.96	0.47
7:F:122:ARG:NH2	32:g:31:G:O3'	2.46	0.47
11:J:31:LYS:HG3	11:J:35:GLU:OE2	2.15	0.47
17:Q:147:ARG:NH1	17:Q:152:ARG:O	2.48	0.47
19:S:116:ARG:HB3	19:S:116:ARG:CZ	2.45	0.47
23:W:87:GLU:OE2	23:W:88:LYS:HG3	2.14	0.47
29:c:7:ALA:N	29:c:51:LEU:O	2.36	0.47
2:A:121:TYR:OH	2:A:123:GLU:OE2	2.30	0.47
8:G:227:LEU:O	8:G:228:LEU:HB2	2.14	0.47
9:H:199:ILE:HD12	9:H:201:MET:HE3	1.97	0.47
33:M:53:TYR:CD1	33:M:53:TYR:O	2.68	0.47
1:2:678:C:HO2'	15:O:132:ASP:CG	2.16	0.47
5:D:105:GLU:O	5:D:108:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:30:ARG:HD3	13:L:31:ARG:H	1.80	0.47
19:S:3:THR:O	19:S:4:ILE:HD13	2.14	0.47
19:S:115:LEU:N	19:S:115:LEU:HD23	2.30	0.47
26:Z:34:ILE:O	26:Z:37:SER:N	2.48	0.47
7:F:113:ARG:CZ	7:F:114:ILE:O	2.62	0.47
8:G:38:MET:HE3	8:G:69:MET:HE3	1.97	0.47
18:R:59:THR:O	18:R:62:ASN:OD1	2.32	0.47
19:S:77:SER:O	19:S:77:SER:OG	2.23	0.47
1:2:682:C:O2'	3:B:118:CYS:O	2.34	0.46
5:D:185:GLN:OE1	5:D:186:GLY:N	2.48	0.46
16:P:76:VAL:O	16:P:76:VAL:CG1	2.62	0.46
21:U:37:VAL:O	21:U:41:VAL:HG13	2.15	0.46
2:A:160:LYS:O	2:A:161:PHE:HB2	2.13	0.46
7:F:35:VAL:HG13	7:F:37:HIS:H	1.80	0.46
10:I:29:LEU:HD12	10:I:29:LEU:C	2.40	0.46
27:a:42:ASP:OD1	27:a:42:ASP:C	2.57	0.46
1:2:1234:C:O2'	19:S:89:ASN:O	2.31	0.46
5:D:144:VAL:HG22	5:D:190:VAL:HG23	1.97	0.46
12:K:44:LYS:HD3	12:K:44:LYS:C	2.40	0.46
12:K:65:VAL:HG23	12:K:83:GLY:HA2	1.97	0.46
32:g:48:U:H3	32:g:62:C:N4	2.09	0.46
5:D:56:ILE:HD13	5:D:58:CYS:SG	2.56	0.46
5:D:92:ILE:HG22	5:D:93:TRP:N	2.31	0.46
10:I:69:LEU:HD11	10:I:105:LEU:HD13	1.98	0.46
12:K:36:ILE:HG23	12:K:48:PRO:HG3	1.96	0.46
16:P:109:PRO:O	16:P:112:VAL:HG23	2.15	0.46
17:Q:81:LEU:HD12	17:Q:81:LEU:N	2.31	0.46
20:T:127:LEU:C	20:T:127:LEU:HD23	2.40	0.46
1:2:345:C:H2'	1:2:346:G:O4'	2.15	0.46
1:2:1414:A:OP2	38:2:1650:HOH:O	2.21	0.46
5:D:111:LEU:C	5:D:111:LEU:HD23	2.41	0.46
7:F:113:ARG:NE	7:F:114:ILE:O	2.48	0.46
10:I:171:LEU:HD12	10:I:171:LEU:O	2.15	0.46
16:P:21:GLU:HA	16:P:21:GLU:OE1	2.15	0.46
34:e:57:GLY:N	34:e:58:PRO:CD	2.78	0.46
1:2:577:G:O2'	1:2:578:A:N7	2.42	0.46
5:D:143:ILE:HG23	5:D:157:LYS:HG2	1.97	0.46
12:K:39:VAL:HB	12:K:45:LEU:HD22	1.98	0.46
20:T:66:ASP:OD1	20:T:66:ASP:C	2.59	0.46
23:W:66:ILE:HD12	23:W:68:ARG:HD2	1.96	0.46
25:Y:9:ARG:HB2	25:Y:23:VAL:HG13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:100:ASP:N	27:a:100:ASP:OD1	2.47	0.46
1:2:1081:G:H21	21:U:58:ARG:HH12	1.62	0.46
32:g:52:G:H1	32:g:56:U:H5	1.63	0.46
33:M:13:THR:O	33:M:16:ARG:HB2	2.16	0.46
1:2:674:G:H2'	1:2:675:A:C8	2.51	0.46
1:2:1161:G:N3	1:2:1161:G:H2'	2.31	0.46
6:E:86:PHE:CE2	6:E:87:MET:HE2	2.51	0.46
1:2:307:U:H2'	1:2:308:G:O4'	2.16	0.46
1:2:739:C:O2'	1:2:740:U:H6	1.98	0.46
4:C:43:GLU:N	4:C:43:GLU:OE1	2.49	0.46
5:D:67:ASP:O	5:D:70:TYR:N	2.49	0.46
6:E:239:THR:O	6:E:241:LYS:NZ	2.37	0.46
15:O:27:ILE:HB	15:O:91:ILE:HD12	1.98	0.46
16:P:83:MET:HE1	16:P:86:PHE:CE1	2.50	0.46
33:M:56:ILE:HG23	33:M:57:VAL:N	2.29	0.46
1:2:116:C:H2'	1:2:117:C:O4'	2.16	0.46
1:2:625:C:H2'	1:2:626:G:C8	2.51	0.46
11:J:39:LYS:HA	34:e:33:ARG:HG2	1.98	0.46
15:O:41:LEU:HD22	15:O:41:LEU:H	1.81	0.46
20:T:154:GLU:O	20:T:158:LYS:HE3	2.16	0.46
32:g:52:G:H2'	32:g:53:A:C8	2.51	0.46
33:M:35:GLU:HG3	33:M:36:ARG:HD3	1.96	0.46
1:2:739:C:O2'	1:2:740:U:P	2.73	0.45
1:2:1066:C:C2	1:2:1067:G:C8	3.04	0.45
1:2:1162:C:H5'	16:P:126:VAL:HG21	1.98	0.45
3:B:90:LEU:HD13	3:B:225:MET:HE1	1.97	0.45
7:F:80:GLY:O	7:F:84:GLU:OE2	2.34	0.45
9:H:132:THR:O	9:H:136:VAL:HG23	2.16	0.45
12:K:44:LYS:HD3	12:K:45:LEU:N	2.31	0.45
16:P:32:ASP:OD1	16:P:32:ASP:C	2.58	0.45
33:M:76:THR:O	33:M:80:LEU:N	2.32	0.45
1:2:1043:G:OP2	1:2:1044:U:O2'	2.27	0.45
2:A:21:LYS:HZ1	2:A:22:LYS:HG3	1.80	0.45
2:A:145:VAL:HG12	2:A:145:VAL:O	2.15	0.45
5:D:105:GLU:N	5:D:105:GLU:OE1	2.49	0.45
19:S:14:LEU:HD11	19:S:57:ALA:HB1	1.98	0.45
25:Y:115:ARG:HG3	25:Y:122:GLU:HG3	1.98	0.45
29:c:8:ARG:NH2	29:c:50:ILE:HD11	2.31	0.45
1:2:256:G:H2'	1:2:257:A:O4'	2.16	0.45
1:2:649:A:C2	1:2:666:A:C5	3.05	0.45
19:S:17:PHE:HD2	19:S:34:ILE:HD13	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:69:TRP:H	20:T:69:TRP:CD1	2.34	0.45
28:b:53:PRO:O	28:b:57:GLN:NE2	2.47	0.45
34:e:30:PRO:HB2	34:e:34:ALA:HB3	1.97	0.45
1:2:1212:G:H21	1:2:1274:C:H1'	1.81	0.45
1:2:1341:C:H5''	1:2:1342:U:H5'	1.98	0.45
9:H:37:THR:O	9:H:41:LEU:HG	2.17	0.45
20:T:150:GLU:O	20:T:154:GLU:HG2	2.17	0.45
30:d:61:HIS:ND1	30:d:61:HIS:O	2.50	0.45
31:f:92:LEU:HD13	33:M:27:HIS:HE1	1.82	0.45
1:2:1116:G:O2'	1:2:1117:G:N7	2.47	0.45
16:P:86:PHE:HB3	16:P:88:GLU:OE1	2.17	0.45
17:Q:128:ASP:OD1	17:Q:130:GLN:N	2.50	0.45
18:R:21:TYR:CE1	18:R:61:MET:HE1	2.51	0.45
19:S:3:THR:HG21	19:S:59:GLU:OE2	2.16	0.45
26:Z:78:MET:SD	26:Z:80:ILE:HD11	2.56	0.45
29:c:8:ARG:N	29:c:30:MET:SD	2.90	0.45
32:g:12:G:N1	32:g:22:A:C2	2.75	0.45
1:2:472:C:H2'	1:2:473:G:O4'	2.17	0.45
1:2:1354:C:H2'	1:2:1355:G:O4'	2.16	0.45
8:G:127:LEU:HD23	8:G:128:PRO:CD	2.47	0.45
16:P:74:LYS:C	16:P:75:ILE:HD13	2.41	0.45
24:X:69:ALA:HB1	24:X:83:ALA:O	2.17	0.45
1:2:1194:C:H42	1:2:1203:A:N6	2.14	0.45
11:J:133:ALA:C	11:J:134:ARG:HG2	2.42	0.45
18:R:27:LYS:O	18:R:27:LYS:HG2	2.16	0.45
21:U:42:LYS:NZ	21:U:46:LYS:HB2	2.32	0.45
26:Z:45:ILE:O	26:Z:49:LEU:N	2.43	0.45
3:B:192:GLU:HB3	3:B:196:LYS:NZ	2.32	0.45
8:G:212:GLU:O	8:G:216:LYS:HG3	2.16	0.45
11:J:50:MET:O	11:J:54:ILE:HG12	2.17	0.45
28:b:72:TYR:HE1	28:b:74:LEU:HD23	1.81	0.45
1:2:428:G:O2'	1:2:435:A:N1	2.47	0.45
1:2:1274:C:H2'	1:2:1275:G:O4'	2.17	0.45
3:B:192:GLU:HB3	3:B:196:LYS:HZ1	1.82	0.45
5:D:87:PRO:O	5:D:89:ASN:N	2.41	0.45
5:D:111:LEU:HD21	5:D:190:VAL:HG21	1.99	0.45
10:I:121:ALA:HB1	10:I:122:LEU:HD22	1.98	0.45
11:J:143:VAL:HG11	11:J:148:TYR:CD2	2.52	0.45
11:J:163:THR:O	11:J:163:THR:HG22	2.17	0.45
12:K:11:ALA:HB1	12:K:36:ILE:HD11	1.97	0.45
12:K:38:TYR:C	12:K:38:TYR:CD1	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:22:SER:N	20:T:25:ARG:HE	2.15	0.45
5:D:77:TYR:CE1	12:K:105:PRO:HB3	2.51	0.45
6:E:246:ASP:OD2	6:E:248:ILE:N	2.46	0.45
9:H:90:ALA:O	9:H:94:LYS:HG3	2.16	0.45
11:J:93:ASP:OD1	11:J:93:ASP:N	2.50	0.45
22:V:81:GLN:HB3	22:V:87:GLU:HB2	1.99	0.45
1:2:790:C:H2'	1:2:791:G:O4'	2.17	0.44
1:2:1191:G:HO2'	1:2:1192:C:P	2.31	0.44
1:2:1239:U:OP2	16:P:43:ARG:NH2	2.50	0.44
26:Z:54:ALA:O	26:Z:58:ARG:HG2	2.17	0.44
26:Z:61:ARG:O	26:Z:65:LYS:HD3	2.17	0.44
9:H:201:MET:HE3	9:H:201:MET:HB2	1.80	0.44
13:L:164:ASP:N	13:L:164:ASP:OD1	2.49	0.44
17:Q:124:LEU:HD11	17:Q:131:LEU:HD13	1.98	0.44
29:c:16:THR:HG21	29:c:24:GLN:CG	2.47	0.44
29:c:60:ALA:O	29:c:61:ARG:HB2	2.16	0.44
1:2:388:C:O2	1:2:388:C:O4'	2.32	0.44
1:2:1124:G:O2'	5:D:166:THR:OG1	2.27	0.44
5:D:126:TYR:O	5:D:129:ILE:HG13	2.17	0.44
11:J:137:SER:HA	11:J:142:ILE:HA	1.99	0.44
18:R:75:ARG:HG3	18:R:75:ARG:HH11	1.82	0.44
26:Z:33:PHE:O	26:Z:36:ASN:ND2	2.51	0.44
33:M:37:LYS:HE2	33:M:37:LYS:HA	1.98	0.44
15:O:72:THR:HG23	15:O:113:LEU:HD23	1.99	0.44
20:T:156:LEU:HD12	20:T:156:LEU:O	2.17	0.44
21:U:42:LYS:O	21:U:45:VAL:HG12	2.18	0.44
21:U:47:GLU:O	21:U:49:ARG:NH1	2.44	0.44
1:2:607:A:OP1	9:H:111:THR:HG21	2.18	0.44
2:A:94:LYS:HE2	2:A:94:LYS:HA	2.00	0.44
7:F:187:VAL:HG12	7:F:190:ARG:HD2	2.00	0.44
16:P:16:ASN:N	19:S:92:GLU:OE2	2.40	0.44
20:T:71:TYR:N	20:T:71:TYR:HD1	2.15	0.44
21:U:115:GLN:HA	21:U:115:GLN:OE1	2.17	0.44
31:f:97:TYR:OH	31:f:101:LYS:N	2.50	0.44
2:A:57:GLN:OE1	2:A:57:GLN:N	2.37	0.44
5:D:37:ASP:OD1	5:D:37:ASP:N	2.49	0.44
7:F:131:ARG:HG3	7:F:131:ARG:HH11	1.82	0.44
9:H:29:GLU:CD	9:H:29:GLU:H	2.26	0.44
16:P:57:PHE:CE1	16:P:61:LEU:HD11	2.52	0.44
18:R:26:PRO:HB2	18:R:62:ASN:HB3	2.00	0.44
25:Y:22:CYS:HB3	25:Y:73:CYS:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:57:C:H2'	32:g:57:C:O2	2.17	0.44
33:M:30:VAL:HG13	33:M:31:PHE:N	2.33	0.44
33:M:37:LYS:HD2	33:M:37:LYS:N	2.32	0.44
3:B:224:THR:O	3:B:224:THR:OG1	2.27	0.44
16:P:83:MET:HE1	16:P:86:PHE:HE1	1.81	0.44
32:g:62:C:H2'	32:g:63:G:O4'	2.18	0.44
1:2:16:G:OP1	38:2:1651:HOH:O	2.21	0.44
1:2:948:A:N3	1:2:948:A:H2'	2.33	0.44
1:2:968:G:HO2'	1:2:969:G:P	2.40	0.44
3:B:121:ILE:HD12	3:B:121:ILE:N	2.33	0.44
4:C:116:ALA:O	4:C:120:LYS:HG2	2.17	0.44
5:D:98:ILE:HG13	5:D:99:LYS:N	2.33	0.44
5:D:184:ARG:H	5:D:184:ARG:HD2	1.83	0.44
7:F:96:GLN:O	7:F:100:ASP:OD2	2.36	0.44
10:I:126:THR:O	10:I:126:THR:OG1	2.35	0.44
17:Q:49:VAL:O	17:Q:52:VAL:N	2.51	0.44
18:R:44:ILE:HG21	18:R:50:ARG:N	2.33	0.44
19:S:13:LEU:HD21	19:S:20:ASN:HB2	2.00	0.44
33:M:105:HIS:CG	33:M:106:ASN:N	2.85	0.44
1:2:1448:C:OP2	27:a:14:ARG:NH1	2.51	0.44
5:D:20:ASP:N	5:D:20:ASP:OD1	2.49	0.44
5:D:171:ARG:HG3	5:D:172:ILE:HG23	2.00	0.44
1:2:471:G:H2'	1:2:472:C:C6	2.53	0.43
1:2:1096:G:C2	1:2:1097:C:C6	3.06	0.43
1:2:1182:G:O2'	1:2:1183:G:H5'	2.18	0.43
15:O:10:GLU:H	15:O:10:GLU:CD	2.26	0.43
16:P:75:ILE:HD12	16:P:93:THR:HG23	2.00	0.43
20:T:105:LYS:O	20:T:106:THR:HG22	2.18	0.43
21:U:106:SER:HA	21:U:109:VAL:HG22	2.00	0.43
33:M:40:LYS:C	33:M:67:HIS:CE1	2.96	0.43
1:2:556:C:OP2	25:Y:9:ARG:HD2	2.18	0.43
1:2:602:G:H2'	1:2:603:C:O4'	2.16	0.43
1:2:969:G:N2	1:2:994:G:O2'	2.50	0.43
8:G:150:LEU:O	8:G:151:PHE:HB3	2.17	0.43
8:G:202:ARG:O	8:G:206:VAL:HG23	2.18	0.43
11:J:16:THR:HG23	11:J:17:PRO:HD2	2.00	0.43
14:N:131:GLN:O	14:N:132:ALA:HB3	2.18	0.43
21:U:21:MET:SD	21:U:22:HIS:N	2.90	0.43
25:Y:92:ILE:HD12	25:Y:99:ALA:HB2	2.00	0.43
31:f:99:THR:HG22	31:f:105:ALA:HB2	2.00	0.43
2:A:129:VAL:HG12	2:A:130:ASN:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:122:ASP:N	3:B:122:ASP:OD1	2.51	0.43
3:B:175:GLU:HA	3:B:175:GLU:OE1	2.18	0.43
7:F:23:LEU:HD22	7:F:133:VAL:HG12	2.00	0.43
1:2:773:C:O2'	1:2:866:A:N1	2.52	0.43
11:J:61:LEU:HD11	11:J:74:GLU:HB3	2.00	0.43
16:P:33:ILE:HD12	16:P:36:LYS:HB2	2.00	0.43
5:D:73:HIS:CG	12:K:105:PRO:HG2	2.54	0.43
16:P:15:PRO:HB2	16:P:16:ASN:H	1.63	0.43
16:P:85:ILE:HG23	16:P:89:MET:HE2	2.00	0.43
18:R:75:ARG:NH1	18:R:75:ARG:HG3	2.34	0.43
25:Y:82:LEU:HD23	25:Y:82:LEU:O	2.17	0.43
26:Z:58:ARG:O	26:Z:62:GLN:HG2	2.18	0.43
1:2:742:G:O6	38:2:1645:HOH:O	2.19	0.43
8:G:230:ARG:H	8:G:230:ARG:HD3	1.83	0.43
10:I:131:ILE:O	10:I:135:ILE:HG12	2.18	0.43
16:P:45:ILE:HD13	16:P:45:ILE:N	2.32	0.43
16:P:125:ILE:C	16:P:125:ILE:CD1	2.91	0.43
17:Q:130:GLN:N	17:Q:130:GLN:OE1	2.43	0.43
23:W:49:ASP:OD1	23:W:49:ASP:N	2.52	0.43
1:2:989:U:O2'	1:2:990:U:P	2.75	0.43
1:2:1294:C:H2'	1:2:1295:G:O4'	2.18	0.43
5:D:24:GLU:OE1	5:D:25:ALA:N	2.52	0.43
19:S:101:VAL:HG23	19:S:102:ASN:N	2.33	0.43
28:b:103:GLN:HG2	28:b:105:SER:H	1.82	0.43
32:g:20:U:O2'	32:g:44:G:O6	2.31	0.43
1:2:1381:C:H2'	1:2:1382:G:O4'	2.18	0.43
17:Q:108:LEU:O	17:Q:117:ARG:NH1	2.51	0.43
33:M:57:VAL:O	33:M:61:CYS:SG	2.77	0.43
1:2:1054:U:O2	18:R:4:VAL:HG11	2.19	0.43
1:2:1148:G:H3'	1:2:1149:A:C5'	2.48	0.43
1:2:1262:A:OP1	32:g:33:C:O2'	2.25	0.43
12:K:17:TYR:CE2	12:K:88:ARG:HG3	2.53	0.43
21:U:75:GLU:HG2	21:U:76:GLY:N	2.33	0.43
33:M:34:LEU:HD23	33:M:60:LEU:CD2	2.48	0.43
2:A:22:LYS:O	2:A:25:VAL:HG22	2.19	0.43
18:R:54:ALA:O	18:R:58:THR:HG22	2.18	0.43
29:c:38:ILE:HG22	29:c:39:ARG:N	2.34	0.43
32:g:11:C:H2'	32:g:12:G:C8	2.54	0.43
32:g:31:G:H22	32:g:35:C:H5	1.67	0.43
1:2:737:G:O2'	1:2:738:G:H5'	2.19	0.42
5:D:35:LEU:CD1	5:D:64:VAL:HG13	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:28:SER:OG	7:F:52:CYS:O	2.33	0.42
19:S:48:LYS:NZ	19:S:78:HIS:O	2.51	0.42
26:Z:41:THR:HG22	26:Z:42:HIS:N	2.32	0.42
29:c:6:ASN:C	29:c:30:MET:HE1	2.44	0.42
31:f:99:THR:CG2	31:f:105:ALA:H	2.32	0.42
33:M:84:VAL:HG22	33:M:96:VAL:HA	2.01	0.42
7:F:122:ARG:HH11	7:F:122:ARG:HG2	1.83	0.42
12:K:91:LEU:HB3	12:K:93:LEU:HD23	2.00	0.42
16:P:17:PHE:CE1	19:S:91:PHE:HE1	2.37	0.42
17:Q:113:ASP:OD1	17:Q:114:GLU:N	2.52	0.42
18:R:59:THR:HA	18:R:62:ASN:OD1	2.19	0.42
34:e:21:LYS:O	34:e:23:LYS:NZ	2.52	0.42
1:2:623:G:H2'	1:2:624:G:C8	2.54	0.42
7:F:113:ARG:C	7:F:113:ARG:NE	2.77	0.42
29:c:16:THR:HG21	29:c:24:GLN:HG3	2.01	0.42
33:M:18:HIS:ND1	33:M:18:HIS:O	2.52	0.42
33:M:84:VAL:HG12	33:M:85:ARG:H	1.85	0.42
1:2:244:U:P	10:I:65:ARG:HH22	2.42	0.42
8:G:104:ARG:NH1	8:G:105:GLY:O	2.53	0.42
16:P:109:PRO:N	16:P:110:PRO:HD2	2.35	0.42
18:R:71:GLY:O	18:R:72:ILE:HD13	2.19	0.42
19:S:76:LEU:HD12	19:S:76:LEU:HA	1.87	0.42
24:X:24:ASP:OD1	24:X:27:TYR:N	2.36	0.42
26:Z:21:PHE:CD2	26:Z:26:ALA:HB2	2.54	0.42
17:Q:19:GLU:HA	17:Q:22:LYS:HE2	2.02	0.42
33:M:43:PHE:H	33:M:102:CYS:HB2	1.84	0.42
33:M:85:ARG:O	33:M:86:CYS:C	2.63	0.42
1:2:926:U:O2	1:2:926:U:H2'	2.20	0.42
5:D:47:ARG:HA	5:D:52:ILE:HG22	2.02	0.42
5:D:73:HIS:CG	12:K:105:PRO:HD2	2.55	0.42
9:H:41:LEU:HD22	9:H:94:LYS:HE3	2.02	0.42
21:U:39:ARG:HG2	21:U:39:ARG:HH11	1.85	0.42
1:2:127:G:H2'	1:2:128:G:C8	2.54	0.42
1:2:558:C:H2'	1:2:559:G:OP1	2.19	0.42
5:D:128:ILE:HD13	5:D:128:ILE:N	2.35	0.42
6:E:220:THR:HG22	6:E:221:ARG:N	2.35	0.42
7:F:187:VAL:CG1	7:F:190:ARG:HD2	2.49	0.42
12:K:65:VAL:HG13	12:K:66:VAL:N	2.34	0.42
14:N:115:LEU:O	14:N:119:GLU:HG2	2.20	0.42
30:d:65:ILE:O	30:d:65:ILE:HD12	2.19	0.42
1:2:1353:G:H2'	1:2:1354:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:46:ARG:HB3	11:J:50:MET:HE3	2.02	0.42
16:P:81:ARG:NH1	16:P:97:TYR:O	2.46	0.42
18:R:40:ASN:OD1	18:R:40:ASN:N	2.52	0.42
32:g:19:G:H2'	32:g:20:U:H4'	2.01	0.42
1:2:598:C:H2'	1:2:599:G:O4'	2.20	0.42
1:2:848:G:O2'	1:2:849:G:H5'	2.20	0.42
1:2:1451:U:O2	1:2:1451:U:O4'	2.38	0.42
4:C:50:LYS:NZ	22:V:20:ILE:O	2.46	0.42
5:D:93:TRP:HA	5:D:93:TRP:CE3	2.55	0.42
7:F:35:VAL:HG22	7:F:36:PRO:HD2	2.02	0.42
7:F:88:LEU:HG	26:Z:39:CYS:HB3	2.02	0.42
8:G:220:GLN:O	8:G:223:GLU:HG3	2.20	0.42
19:S:11:ARG:HH22	19:S:60:LEU:HD11	1.85	0.42
23:W:28:ARG:CB	23:W:29:PRO:HD3	2.49	0.42
1:2:911:G:C2	1:2:912:A:C8	3.08	0.41
2:A:90:ARG:NH1	2:A:206:LEU:O	2.53	0.41
4:C:128:LEU:HD23	4:C:128:LEU:HA	1.93	0.41
5:D:112:ARG:HG3	5:D:181:ILE:HG12	2.01	0.41
6:E:210:MET:HE2	6:E:210:MET:HB3	1.95	0.41
16:P:51:SER:O	16:P:55:LEU:HG	2.20	0.41
31:f:97:TYR:CE1	31:f:99:THR:OG1	2.70	0.41
33:M:73:THR:HG22	33:M:75:ARG:N	2.34	0.41
2:A:21:LYS:O	2:A:25:VAL:HG13	2.20	0.41
9:H:54:THR:O	9:H:54:THR:HG23	2.20	0.41
13:L:34:GLU:OE1	13:L:34:GLU:CA	2.69	0.41
19:S:4:ILE:HD13	19:S:4:ILE:N	2.34	0.41
19:S:109:ARG:HH11	19:S:109:ARG:HG2	1.84	0.41
21:U:121:GLU:C	21:U:122:GLU:OE2	2.63	0.41
25:Y:82:LEU:O	25:Y:86:GLU:HB2	2.19	0.41
25:Y:90:ARG:HH11	25:Y:90:ARG:HG3	1.85	0.41
25:Y:122:GLU:OE2	25:Y:122:GLU:N	2.50	0.41
32:g:50:G:O6	32:g:60:U:O4	2.37	0.41
1:2:1081:G:H2'	1:2:1082:G:O4'	2.20	0.41
3:B:199:GLU:OE1	3:B:200:ALA:N	2.53	0.41
19:S:18:ASN:OD1	19:S:18:ASN:N	2.53	0.41
21:U:39:ARG:HB3	21:U:39:ARG:CZ	2.50	0.41
23:W:76:SER:HB3	23:W:77:PRO:CD	2.50	0.41
27:a:55:ASP:OD1	27:a:55:ASP:N	2.52	0.41
33:M:30:VAL:O	33:M:34:LEU:N	2.43	0.41
1:2:304:G:N7	38:2:1685:HOH:O	2.37	0.41
2:A:88:ALA:O	2:A:89:GLN:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:104:ASP:HB3	6:E:110:THR:HG21	2.03	0.41
16:P:64:ARG:NH2	16:P:74:LYS:HG2	2.35	0.41
17:Q:143:LYS:HB2	17:Q:152:ARG:HH12	1.86	0.41
34:e:28:ARG:HB2	34:e:28:ARG:NH1	2.35	0.41
2:A:90:ARG:O	2:A:94:LYS:HG2	2.20	0.41
24:X:119:ARG:NH1	24:X:119:ARG:HB3	2.36	0.41
7:F:63:MET:HB2	7:F:68:ASN:O	2.20	0.41
10:I:172:ALA:N	10:I:173:PRO:CD	2.84	0.41
21:U:99:ASN:OD1	21:U:103:THR:OG1	2.35	0.41
26:Z:34:ILE:HG22	26:Z:45:ILE:HD12	2.02	0.41
30:d:120:CYS:SG	30:d:122:ARG:N	2.93	0.41
1:2:1214:C:C2	1:2:1215:C:C5	3.07	0.41
1:2:1296:G:O2'	1:2:1297:A:P	2.78	0.41
17:Q:121:ARG:O	17:Q:125:VAL:HG12	2.20	0.41
18:R:13:ALA:O	18:R:17:VAL:HG12	2.21	0.41
19:S:120:CYS:SG	19:S:123:GLY:N	2.83	0.41
20:T:158:LYS:HB3	20:T:158:LYS:HE2	1.84	0.41
29:c:47:LYS:NZ	29:c:47:LYS:HB3	2.36	0.41
34:e:28:ARG:HB2	34:e:28:ARG:CZ	2.50	0.41
1:2:112:C:H2'	1:2:113:G:O4'	2.21	0.41
1:2:1190:G:N2	1:2:1209:G:O2'	2.54	0.41
16:P:33:ILE:HG13	16:P:37:LEU:CD2	2.51	0.41
18:R:77:GLN:HA	18:R:80:GLU:HG2	2.03	0.41
30:d:89:GLU:CD	30:d:89:GLU:C	2.88	0.41
32:g:10:G:C2	32:g:11:C:C5	3.09	0.41
38:2:1647:HOH:O	15:O:134:THR:OG1	2.22	0.41
8:G:135:VAL:HG13	8:G:135:VAL:O	2.21	0.41
8:G:209:GLU:O	8:G:212:GLU:HG3	2.21	0.41
9:H:168:VAL:HG11	9:H:201:MET:HB3	2.01	0.41
11:J:113:SER:O	11:J:117:GLU:HG2	2.21	0.41
12:K:101:PRO:O	12:K:105:PRO:HD3	2.20	0.41
17:Q:111:VAL:HG11	17:Q:117:ARG:HB2	2.02	0.41
18:R:29:PHE:O	18:R:29:PHE:CG	2.74	0.41
21:U:38:GLU:O	21:U:41:VAL:HG22	2.21	0.41
22:V:75:ALA:O	22:V:79:LEU:HD23	2.21	0.41
23:W:32:LYS:O	23:W:36:GLU:HG2	2.21	0.41
32:g:26:C:H2'	32:g:27:G:C8	2.55	0.41
32:g:49:C:N3	32:g:62:C:N4	2.69	0.41
33:M:74:ARG:HA	33:M:77:LEU:HD13	2.02	0.41
1:2:982:G:H2'	1:2:983:C:H5'	2.02	0.41
1:2:1022:U:OP2	1:2:1023:C:O2'	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1186:A:H5''	17:Q:1:MET:H2	1.85	0.41
6:E:163:ASN:O	6:E:167:GLY:N	2.51	0.41
9:H:179:GLU:H	9:H:179:GLU:CD	2.28	0.41
16:P:28:MET:SD	16:P:28:MET:C	3.03	0.41
16:P:87:PRO:O	16:P:90:ILE:HG12	2.21	0.41
26:Z:71:ILE:CG2	26:Z:72:VAL:N	2.84	0.41
26:Z:80:ILE:HD12	26:Z:80:ILE:N	2.36	0.41
11:J:136:ILE:HG22	11:J:137:SER:N	2.36	0.40
12:K:17:TYR:HE2	12:K:88:ARG:HG3	1.86	0.40
20:T:56:THR:O	20:T:60:ARG:HD3	2.21	0.40
30:d:136:LEU:HD12	30:d:136:LEU:O	2.20	0.40
32:g:15:G:C6	32:g:46:G:N2	2.90	0.40
1:2:895:G:H3'	1:2:896:G:H5''	2.02	0.40
2:A:129:VAL:HG12	2:A:131:ASP:H	1.85	0.40
4:C:61:ILE:O	4:C:65:PHE:N	2.54	0.40
6:E:188:ASN:HB3	6:E:191:ARG:HD3	2.03	0.40
10:I:64:ARG:HB3	10:I:64:ARG:NH1	2.36	0.40
25:Y:34:GLU:OE1	25:Y:38:ALA:HB2	2.21	0.40
25:Y:70:VAL:HG22	25:Y:71:GLY:N	2.36	0.40
32:g:25:G:N1	32:g:26:C:C4	2.89	0.40
1:2:955:C:H2'	1:2:956:C:C6	2.56	0.40
12:K:11:ALA:O	12:K:36:ILE:HD11	2.22	0.40
17:Q:70:ILE:HG22	17:Q:75:GLU:OE2	2.21	0.40
34:e:62:LEU:O	34:e:66:LYS:HE3	2.20	0.40
1:2:229:A:C2	1:2:265:A:C5	3.09	0.40
2:A:21:LYS:HE3	2:A:21:LYS:HB3	1.98	0.40
12:K:86:PHE:CD1	12:K:86:PHE:C	2.99	0.40
15:O:66:TYR:O	15:O:70:GLN:HG3	2.21	0.40
16:P:28:MET:HE1	16:P:33:ILE:CB	2.45	0.40
16:P:28:MET:HE2	16:P:32:ASP:HB3	2.03	0.40
25:Y:22:CYS:HB3	25:Y:73:CYS:O	2.22	0.40
33:M:77:LEU:HD12	33:M:77:LEU:N	2.36	0.40
1:2:157:U:H2'	1:2:158:G:O4'	2.22	0.40
1:2:990:U:HO2'	1:2:991:C:H6	1.68	0.40
1:2:1161:G:H5''	1:2:1162:C:OP2	2.21	0.40
3:B:147:ARG:HD3	3:B:148:PHE:CE1	2.57	0.40
5:D:23:MET:HE3	5:D:83:PHE:CG	2.56	0.40
13:L:31:ARG:H	13:L:31:ARG:CD	2.33	0.40
13:L:165:ILE:HD12	13:L:188:VAL:CG2	2.50	0.40
15:O:108:ALA:HA	15:O:111:ARG:HG2	2.03	0.40
21:U:23:GLN:HE21	21:U:101:ILE:HG23	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:61:ARG:HA	29:c:61:ARG:HD2	1.81	0.40
32:g:56:U:O2'	32:g:58:G:OP2	2.35	0.40
32:g:67:A:C2	32:g:68:U:C5	3.09	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	
2	A	197/245 (80%)	189 (96%)	8 (4%)	0	100	100
3	B	206/248 (83%)	198 (96%)	8 (4%)	0	100	100
4	C	207/242 (86%)	197 (95%)	10 (5%)	0	100	100
5	D	200/217 (92%)	180 (90%)	20 (10%)	0	100	100
6	E	256/268 (96%)	251 (98%)	5 (2%)	0	100	100
7	F	182/190 (96%)	170 (93%)	12 (7%)	0	100	100
8	G	195/248 (79%)	189 (97%)	6 (3%)	0	100	100
9	H	161/201 (80%)	154 (96%)	7 (4%)	0	100	100
10	I	163/174 (94%)	157 (96%)	6 (4%)	0	100	100
11	J	162/189 (86%)	159 (98%)	3 (2%)	0	100	100
12	K	102/134 (76%)	91 (89%)	11 (11%)	0	100	100
13	L	168/199 (84%)	161 (96%)	7 (4%)	0	100	100
14	N	151/154 (98%)	146 (97%)	5 (3%)	0	100	100
15	O	137/145 (94%)	132 (96%)	5 (4%)	0	100	100
16	P	104/145 (72%)	95 (91%)	9 (9%)	0	100	100
17	Q	156/158 (99%)	144 (92%)	11 (7%)	1 (1%)	21	53
18	R	79/137 (58%)	76 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	141/154 (92%)	126 (89%)	15 (11%)	0	100	100
20	T	135/158 (85%)	126 (93%)	9 (7%)	0	100	100
21	U	101/126 (80%)	94 (93%)	7 (7%)	0	100	100
22	V	79/89 (89%)	77 (98%)	2 (2%)	0	100	100
23	W	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
24	X	134/143 (94%)	126 (94%)	8 (6%)	0	100	100
25	Y	118/132 (89%)	112 (95%)	6 (5%)	0	100	100
26	Z	71/88 (81%)	59 (83%)	12 (17%)	0	100	100
27	a	94/109 (86%)	94 (100%)	0	0	100	100
28	b	61/124 (49%)	58 (95%)	3 (5%)	0	100	100
29	c	58/64 (91%)	51 (88%)	7 (12%)	0	100	100
30	d	78/137 (57%)	67 (86%)	11 (14%)	0	100	100
31	f	28/137 (20%)	21 (75%)	7 (25%)	0	100	100
33	M	74/125 (59%)	61 (82%)	13 (18%)	0	100	100
34	e	42/69 (61%)	40 (95%)	2 (5%)	0	100	100
All	All	4167/5079 (82%)	3918 (94%)	248 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	Q	128	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	
2	A	170/217 (78%)	170 (100%)	0	100	100
3	B	190/220 (86%)	188 (99%)	2 (1%)	65	77
4	C	171/201 (85%)	164 (96%)	7 (4%)	27	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	D	167/182 (92%)	162 (97%)	5 (3%)	36	63
6	E	226/232 (97%)	222 (98%)	4 (2%)	51	71
7	F	154/157 (98%)	145 (94%)	9 (6%)	18	48
8	G	169/213 (79%)	159 (94%)	10 (6%)	18	48
9	H	147/181 (81%)	137 (93%)	10 (7%)	14	43
10	I	140/148 (95%)	138 (99%)	2 (1%)	59	74
11	J	143/164 (87%)	137 (96%)	6 (4%)	26	56
12	K	91/119 (76%)	84 (92%)	7 (8%)	12	39
13	L	147/171 (86%)	145 (99%)	2 (1%)	59	74
14	N	129/130 (99%)	128 (99%)	1 (1%)	73	80
15	O	107/113 (95%)	105 (98%)	2 (2%)	50	70
16	P	93/128 (73%)	90 (97%)	3 (3%)	34	62
17	Q	128/130 (98%)	125 (98%)	3 (2%)	44	68
18	R	71/123 (58%)	67 (94%)	4 (6%)	19	49
19	S	122/131 (93%)	116 (95%)	6 (5%)	22	53
20	T	113/133 (85%)	103 (91%)	10 (9%)	9	33
21	U	89/110 (81%)	81 (91%)	8 (9%)	9	32
22	V	63/72 (88%)	60 (95%)	3 (5%)	23	53
23	W	114/115 (99%)	110 (96%)	4 (4%)	32	60
24	X	110/114 (96%)	104 (94%)	6 (6%)	19	50
25	Y	104/113 (92%)	104 (100%)	0	100	100
26	Z	65/79 (82%)	62 (95%)	3 (5%)	24	55
27	a	90/103 (87%)	87 (97%)	3 (3%)	33	62
28	b	58/112 (52%)	58 (100%)	0	100	100
29	c	53/57 (93%)	47 (89%)	6 (11%)	5	23
30	d	71/116 (61%)	63 (89%)	8 (11%)	5	23
31	f	26/112 (23%)	25 (96%)	1 (4%)	29	59
33	M	71/112 (63%)	66 (93%)	5 (7%)	14	42
34	e	41/58 (71%)	41 (100%)	0	100	100
All	All	3633/4366 (83%)	3493 (96%)	140 (4%)	30	58

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	223	ASN
3	B	224	THR
4	C	47	ASP
4	C	52	SER
4	C	76	ASN
4	C	79	SER
4	C	115	VAL
4	C	173	VAL
4	C	180	LYS
5	D	36	VAL
5	D	52	ILE
5	D	102	LEU
5	D	128	ILE
5	D	185	GLN
6	E	118	GLU
6	E	126	VAL
6	E	199	ASP
6	E	246	ASP
7	F	27	ILE
7	F	35	VAL
7	F	59	THR
7	F	120	VAL
7	F	133	VAL
7	F	142	THR
7	F	164	MET
7	F	181	SER
7	F	182	VAL
8	G	15	VAL
8	G	32	THR
8	G	54	CYS
8	G	81	LEU
8	G	89	CYS
8	G	102	SER
8	G	115	LEU
8	G	118	VAL
8	G	120	VAL
8	G	195	VAL
9	H	54	THR
9	H	89	GLU
9	H	102	HIS
9	H	109	ASN
9	H	155	THR
9	H	165	LEU

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Mol	Chain	Res	Type
9	H	167	VAL
9	H	183	THR
9	H	195	ASP
9	H	196	THR
10	I	40	VAL
10	I	78	SER
11	J	65	ASP
11	J	67	ASN
11	J	105	ASP
11	J	119	LYS
11	J	129	ASN
11	J	149	MET
12	K	2	VAL
12	K	4	ILE
12	K	25	LYS
12	K	37	THR
12	K	39	VAL
12	K	56	ILE
12	K	72	TRP
13	L	45	GLU
13	L	63	GLN
14	N	49	ARG
15	O	85	THR
15	O	127	THR
16	P	22	VAL
16	P	37	LEU
16	P	51	SER
17	Q	8	ASP
17	Q	33	ASN
17	Q	104	SER
18	R	5	ARG
18	R	20	ASN
18	R	43	ILE
18	R	58	THR
19	S	14	LEU
19	S	72	LEU
19	S	99	ILE
19	S	100	LEU
19	S	102	ASN
19	S	132	VAL
20	T	23	VAL
20	T	32	ILE

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Mol	Chain	Res	Type
20	T	45	ILE
20	T	53	TYR
20	T	71	TYR
20	T	76	SER
20	T	88	SER
20	T	107	THR
20	T	126	PHE
20	T	127	LEU
21	U	36	LEU
21	U	41	VAL
21	U	44	ILE
21	U	49	ARG
21	U	77	THR
21	U	83	PHE
21	U	95	THR
21	U	118	VAL
22	V	17	ASP
22	V	58	VAL
22	V	72	VAL
23	W	16	ASN
23	W	25	VAL
23	W	54	ASP
23	W	98	LEU
24	X	46	MET
24	X	50	ILE
24	X	85	VAL
24	X	118	CYS
24	X	121	LYS
24	X	133	LEU
26	Z	33	PHE
26	Z	68	ASP
26	Z	69	PHE
27	a	20	SER
27	a	54	VAL
27	a	69	GLN
29	c	17	SER
29	c	24	GLN
29	c	27	VAL
29	c	37	ILE
29	c	40	ASN
29	c	48	ASP
30	d	65	ILE

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Mol	Chain	Res	Type
30	d	73	ASN
30	d	80	VAL
30	d	94	THR
30	d	119	ILE
30	d	120	CYS
30	d	131	ILE
30	d	137	HIS
31	f	103	ASP
33	M	23	LEU
33	M	24	VAL
33	M	35	GLU
33	M	36	ARG
33	M	56	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	112	ASN
2	A	118	ASN
3	B	18	ASN
3	B	87	GLN
3	B	190	ASN
6	E	127	GLN
6	E	201	HIS
7	F	68	ASN
9	H	87	ASN
10	I	71	HIS
11	J	129	ASN
11	J	154	ASN
12	K	54	ASN
13	L	181	ASN
14	N	5	HIS
15	O	136	HIS
18	R	19	ASN
19	S	128	HIS
19	S	136	HIS
20	T	33	ASN
20	T	80	HIS
21	U	78	ASN
21	U	115	GLN
22	V	28	ASN
22	V	83	HIS

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Mol	Chain	Res	Type
23	W	5	ASN
24	X	96	ASN
25	Y	54	ASN
27	a	28	ASN
30	d	137	HIS
33	M	27	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1437/1451 (99%)	240 (16%)	9 (0%)
32	g	73/74 (98%)	16 (21%)	0
All	All	1510/1525 (99%)	256 (16%)	9 (0%)

All (256) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	6	G
1	2	17	C
1	2	33	U
1	2	41	G
1	2	42	A
1	2	44	G
1	2	45	A
1	2	46	A
1	2	59	C
1	2	60	G
1	2	62	U
1	2	64	A
1	2	65	C
1	2	71	A
1	2	73	G
1	2	80	A
1	2	91	C
1	2	92	A
1	2	101	A
1	2	114	G
1	2	116	C
1	2	117	C

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Mol	Chain	Res	Type
1	2	124	G
1	2	125	C
1	2	137	G
1	2	138	G
1	2	144	C
1	2	149	C
1	2	151	A
1	2	152	A
1	2	153	G
1	2	160	G
1	2	161	C
1	2	186	G
1	2	195	C
1	2	204	G
1	2	206	C
1	2	226	A
1	2	227	U
1	2	228	C
1	2	230	C
1	2	234	G
1	2	249	G
1	2	250	C
1	2	257	A
1	2	273	C
1	2	312	G
1	2	314	C
1	2	328	A
1	2	329	A
1	2	330	G
1	2	336	C
1	2	351	U
1	2	356	C
1	2	357	A
1	2	365	G
1	2	366	C
1	2	367	G
1	2	380	A
1	2	389	G
1	2	391	G
1	2	393	G
1	2	394	A
1	2	422	G

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Mol	Chain	Res	Type
1	2	434	A
1	2	435	A
1	2	436	G
1	2	445	C
1	2	458	U
1	2	460	A
1	2	474	A
1	2	491	C
1	2	499	G
1	2	500	A
1	2	502	A
1	2	503	C
1	2	504	G
1	2	519	C
1	2	520	C
1	2	521	C
1	2	534	A
1	2	535	A
1	2	544	G
1	2	545	C
1	2	555	G
1	2	558	C
1	2	559	G
1	2	568	G
1	2	569	C
1	2	570	C
1	2	571	G
1	2	578	A
1	2	581	G
1	2	582	C
1	2	584	C
1	2	586	G
1	2	589	G
1	2	592	G
1	2	593	C
1	2	594	G
1	2	599	G
1	2	602	G
1	2	604	G
1	2	605	G
1	2	607	A
1	2	608	G

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Mol	Chain	Res	Type
1	2	614	A
1	2	615	G
1	2	616	G
1	2	624	G
1	2	627	G
1	2	637	U
1	2	679	C
1	2	680	G
1	2	681	C
1	2	684	G
1	2	685	C
1	2	686	C
1	2	711	U
1	2	717	A
1	2	721	A
1	2	739	C
1	2	740	U
1	2	756	A
1	2	777	A
1	2	779	C
1	2	782	U
1	2	783	G
1	2	790	C
1	2	807	U
1	2	809	C
1	2	810	C
1	2	832	G
1	2	833	G
1	2	838	U
1	2	841	G
1	2	879	A
1	2	891	G
1	2	896	G
1	2	899	C
1	2	908	G
1	2	911	G
1	2	912	A
1	2	926	U
1	2	935	A
1	2	937	G
1	2	938	C
1	2	939	G

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Mol	Chain	Res	Type
1	2	941	G
1	2	942	C
1	2	946	U
1	2	948	A
1	2	949	C
1	2	952	G
1	2	957	G
1	2	958	G
1	2	967	A
1	2	968	G
1	2	969	G
1	2	980	G
1	2	983	C
1	2	984	G
1	2	985	C
1	2	990	U
1	2	997	C
1	2	1008	U
1	2	1025	C
1	2	1027	G
1	2	1052	A
1	2	1053	U
1	2	1054	U
1	2	1060	A
1	2	1069	G
1	2	1085	G
1	2	1086	C
1	2	1087	C
1	2	1088	G
1	2	1095	G
1	2	1101	C
1	2	1107	C
1	2	1119	G
1	2	1130	A
1	2	1131	G
1	2	1139	A
1	2	1145	U
1	2	1147	A
1	2	1148	G
1	2	1149	A
1	2	1150	C
1	2	1163	A

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Mol	Chain	Res	Type
1	2	1167	G
1	2	1185	C
1	2	1189	C
1	2	1192	C
1	2	1196	C
1	2	1208	C
1	2	1210	G
1	2	1211	A
1	2	1212	G
1	2	1228	G
1	2	1229	G
1	2	1244	C
1	2	1247	C
1	2	1261	A
1	2	1269	G
1	2	1275	G
1	2	1278	C
1	2	1286	C
1	2	1292	G
1	2	1297	A
1	2	1301	G
1	2	1319	C
1	2	1324	C
1	2	1341	C
1	2	1342	U
1	2	1343	G
1	2	1367	C
1	2	1368	G
1	2	1369	C
1	2	1370	G
1	2	1372	G
1	2	1408	A
1	2	1412	G
1	2	1413	U
1	2	1414	A
1	2	1418	A
1	2	1419	G
1	2	1421	U
1	2	1432	G
1	2	1434	A
1	2	1435	C
1	2	1444	G

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Mol	Chain	Res	Type
1	2	1445	G
1	2	1446	A
1	2	1447	U
1	2	1448	C
1	2	1450	C
1	2	1451	U
32	g	2	G
32	g	12	G
32	g	16	U
32	g	17	U
32	g	18	G
32	g	20	U
32	g	22	A
32	g	32	U
32	g	33	C
32	g	35	C
32	g	46	G
32	g	52	G
32	g	55	U
32	g	56	U
32	g	59	A
32	g	74	A

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1	C
1	2	115	U
1	2	203	C
1	2	393	G
1	2	421	C
1	2	604	G
1	2	679	C
1	2	840	C
1	2	989	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 25 are monoatomic - leaving 1 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	$\# Z > 2$
35	YAT	2	1501	-	39,39,39	3.23	18 (46%)	51,56,56	2.55	18 (35%)

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
35	YAT	2	1501	-	-	8/14/49/49	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	2	1501	YAT	CAN-CAM	-10.67	1.31	1.51
35	2	1501	YAT	CAN-NBI	10.28	1.66	1.47
35	2	1501	YAT	CAQ-NBI	4.21	1.54	1.47
35	2	1501	YAT	CBC-CBG	4.14	1.55	1.52
35	2	1501	YAT	OAT-CAZ	4.05	1.43	1.37
35	2	1501	YAT	CAI-CBB	3.75	1.45	1.38
35	2	1501	YAT	CAF-CAW	3.72	1.45	1.39
35	2	1501	YAT	CAX-CBD	3.44	1.45	1.40
35	2	1501	YAT	CAW-CBC	-3.23	1.34	1.40
35	2	1501	YAT	CBG-NAR	2.96	1.50	1.47
35	2	1501	YAT	CAG-CAX	2.94	1.44	1.39
35	2	1501	YAT	CAH-CBC	2.94	1.44	1.39
35	2	1501	YAT	CAG-CAZ	2.83	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	2	1501	YAT	OAS-CAY	2.76	1.41	1.37
35	2	1501	YAT	OAV-CBB	2.74	1.41	1.37
35	2	1501	YAT	OAU-CBA	2.55	1.41	1.37
35	2	1501	YAT	CAO-CBF	2.39	1.58	1.53
35	2	1501	YAT	CAI-CBD	2.35	1.43	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	2	1501	YAT	CAN-NBI-CAQ	11.51	132.44	110.32
35	2	1501	YAT	CAP-CBH-CBD	-4.99	105.97	113.07
35	2	1501	YAT	CAQ-CBE-CBF	4.42	116.74	108.12
35	2	1501	YAT	OAU-CBA-CAY	3.77	120.52	115.40
35	2	1501	YAT	CAL-CAK-NAR	3.69	114.02	109.02
35	2	1501	YAT	OAT-CAZ-CBB	3.43	120.06	115.40
35	2	1501	YAT	OAS-CAY-CBA	3.39	120.00	115.40
35	2	1501	YAT	CAJ-CBE-CAQ	-3.05	104.65	111.77
35	2	1501	YAT	CAP-CBF-CBE	2.91	115.34	110.57
35	2	1501	YAT	CAK-CAL-CAW	2.85	115.72	110.66
35	2	1501	YAT	CBE-CAQ-NBI	2.82	115.89	112.17
35	2	1501	YAT	OAV-CBB-CAZ	2.74	119.11	115.40
35	2	1501	YAT	CAC-OAT-CAZ	-2.68	113.58	117.51
35	2	1501	YAT	CAB-OAS-CAY	-2.57	113.75	117.51
35	2	1501	YAT	OAU-CBA-CAH	-2.54	119.70	124.08
35	2	1501	YAT	OAT-CAZ-CAG	-2.50	119.76	124.08
35	2	1501	YAT	CAJ-CBE-CBF	-2.32	108.62	114.56
35	2	1501	YAT	OAS-CAY-CAF	-2.29	120.13	124.08

There are no chirality outliers.

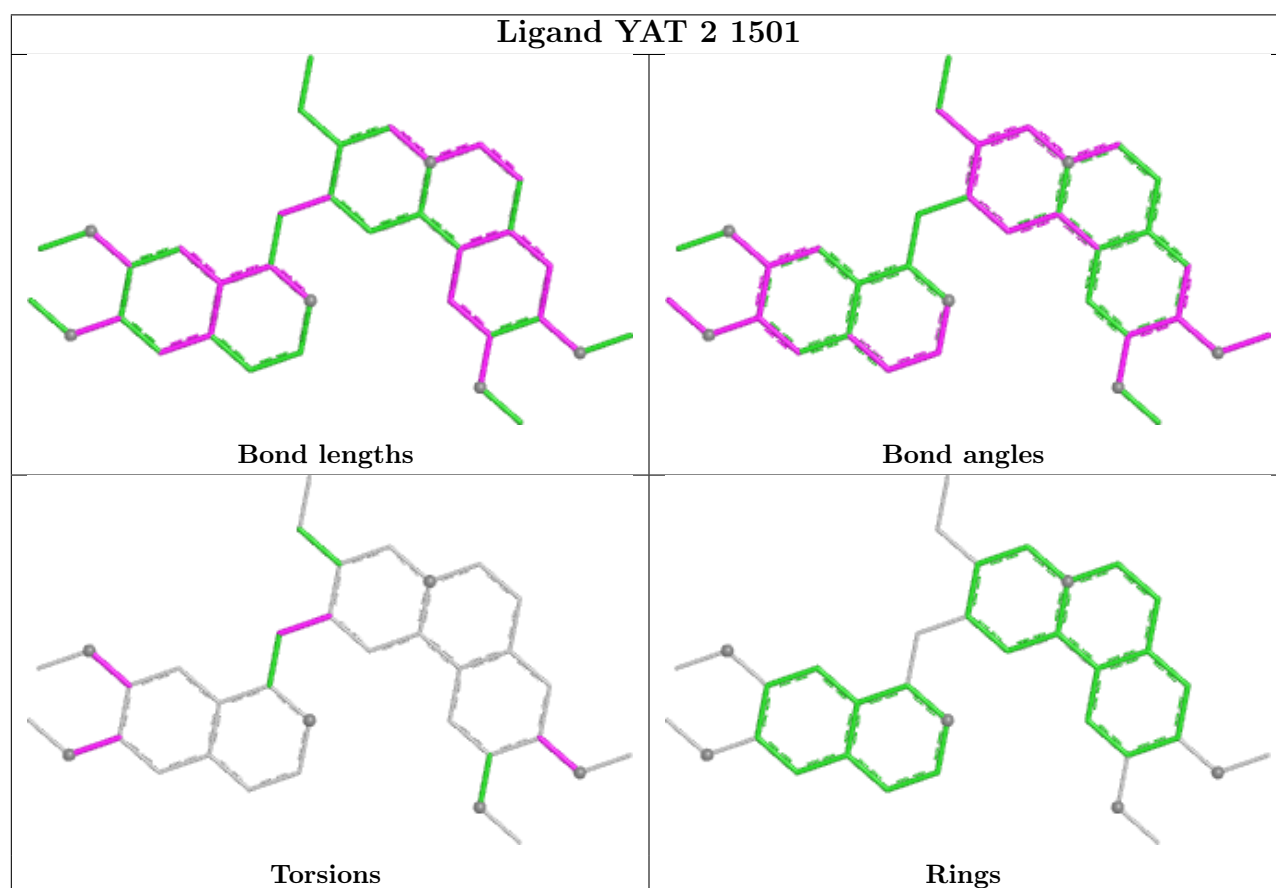
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	2	1501	YAT	CAF-CAY-OAS-CAB
35	2	1501	YAT	CAG-CAZ-OAT-CAC
35	2	1501	YAT	CBA-CAY-OAS-CAB
35	2	1501	YAT	CAY-CBA-OAU-CAD
35	2	1501	YAT	CBB-CAZ-OAT-CAC
35	2	1501	YAT	CAH-CBA-OAU-CAD
35	2	1501	YAT	CBG-CAO-CBF-CBE
35	2	1501	YAT	CBG-CAO-CBF-CAP

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

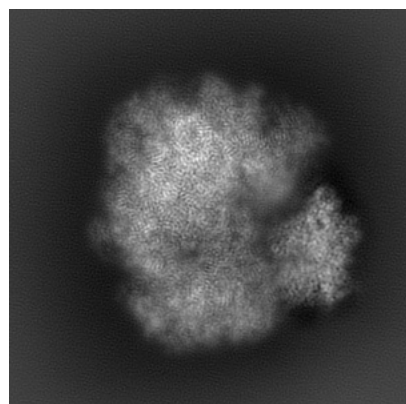
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29721. These allow visual inspection of the internal detail of the map and identification of artifacts.

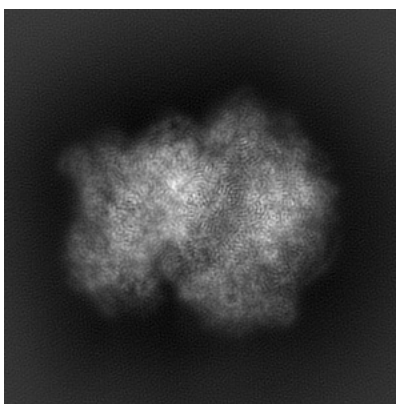
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

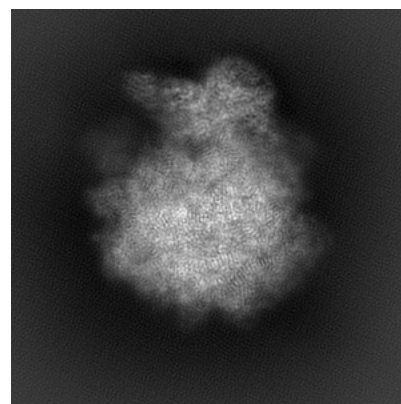
6.1.1 Primary map



X

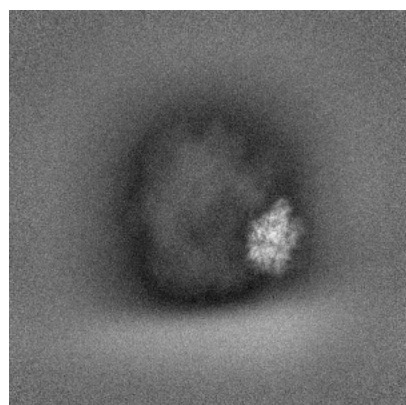


Y

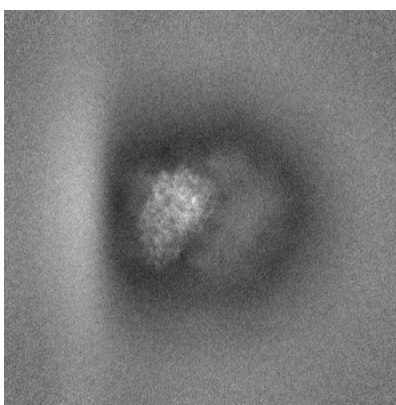


Z

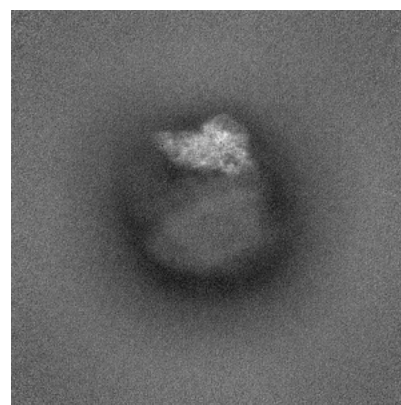
6.1.2 Raw map



X



Y

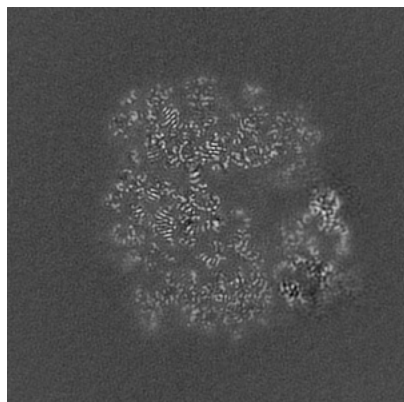


Z

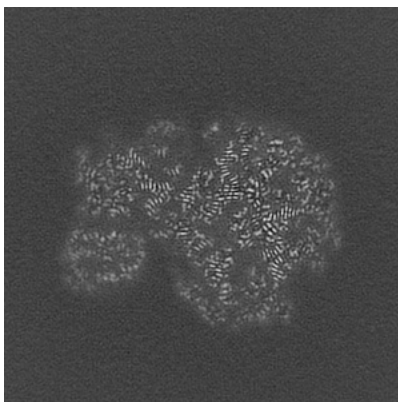
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

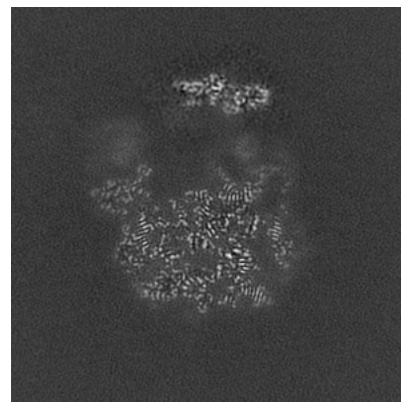
6.2.1 Primary map



X Index: 225

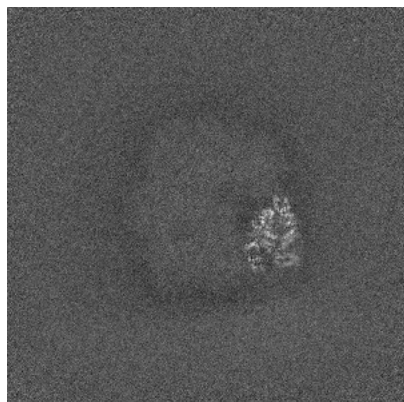


Y Index: 225

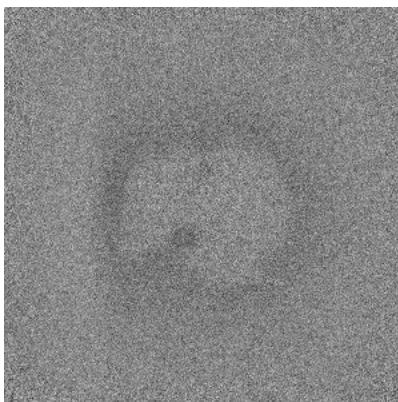


Z Index: 225

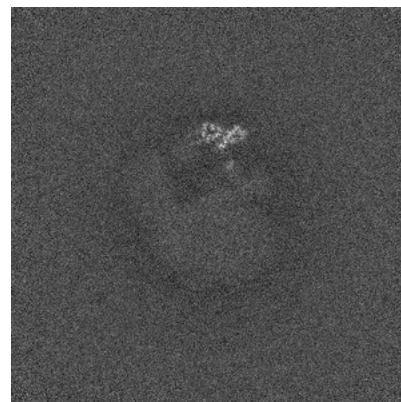
6.2.2 Raw map



X Index: 351



Y Index: 351

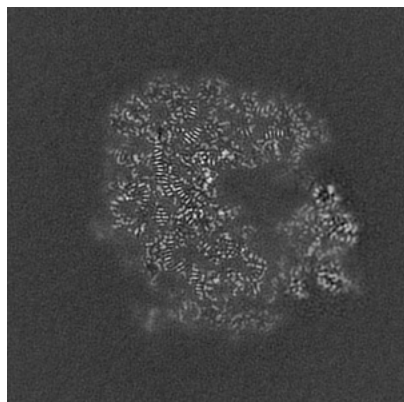


Z Index: 351

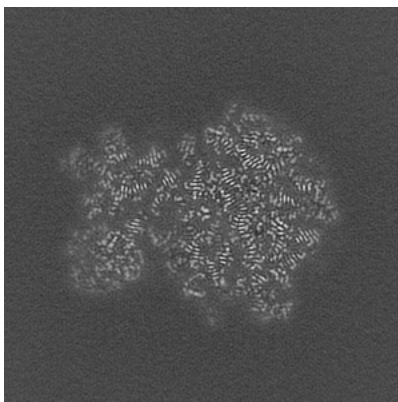
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

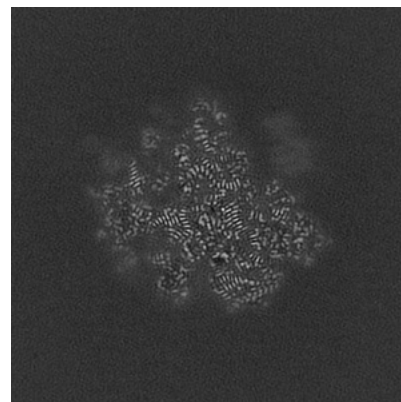
6.3.1 Primary map



X Index: 239

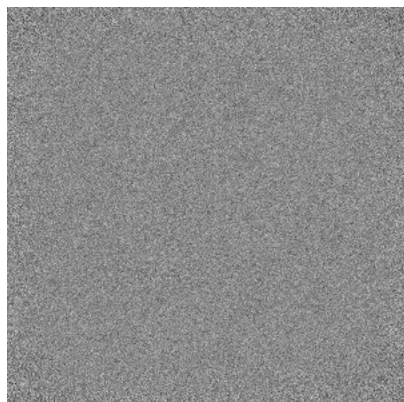


Y Index: 217

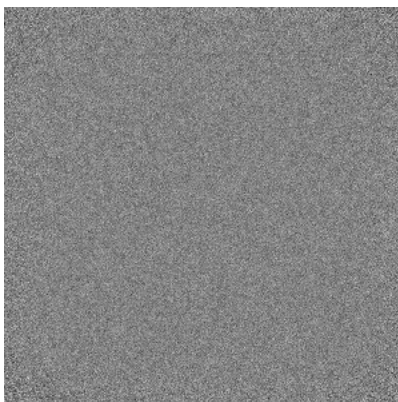


Z Index: 280

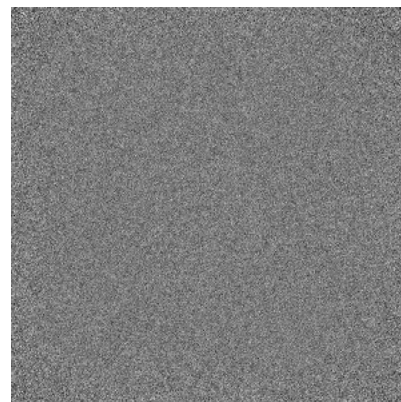
6.3.2 Raw map



X Index: 0



Y Index: 0

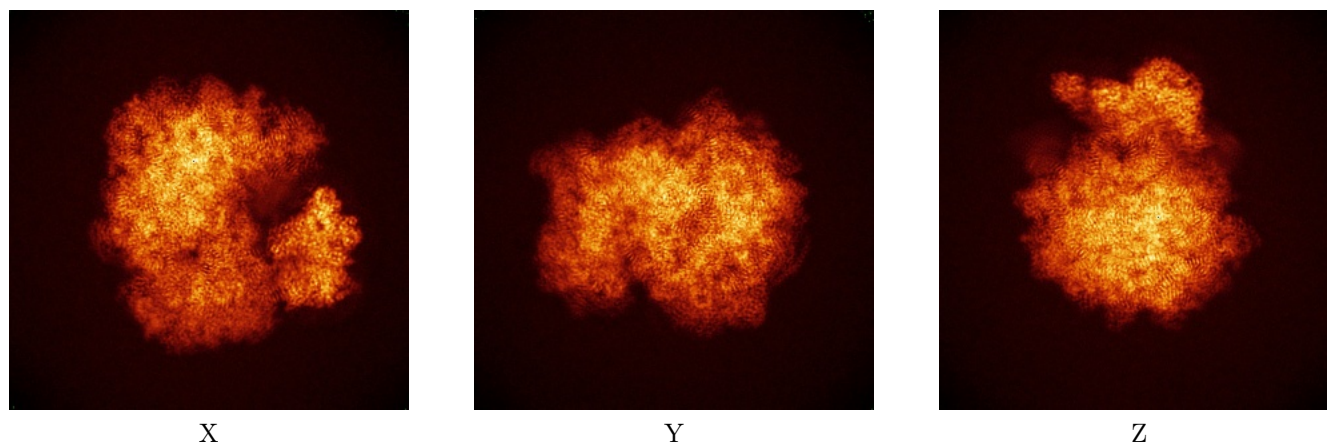


Z Index: 0

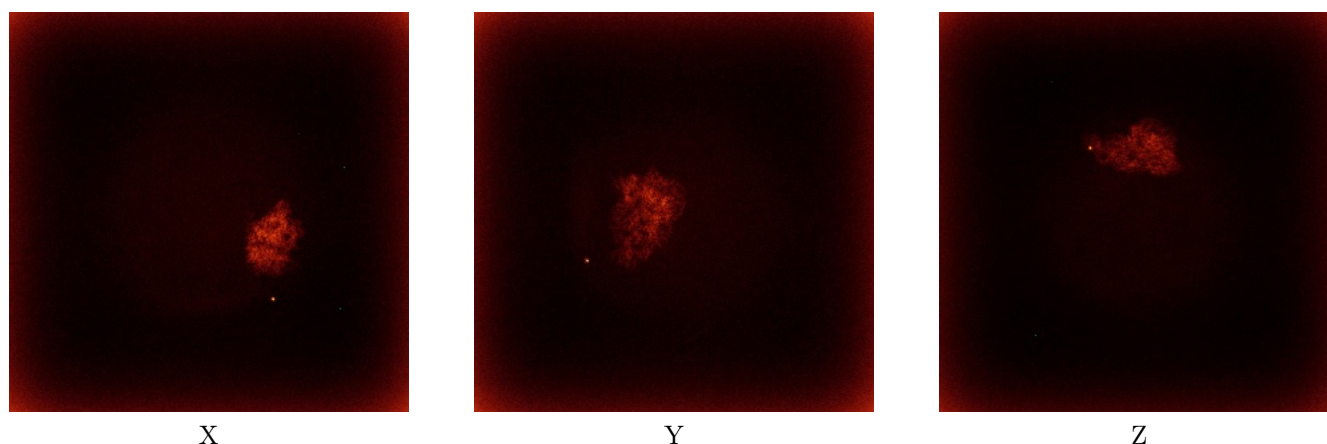
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

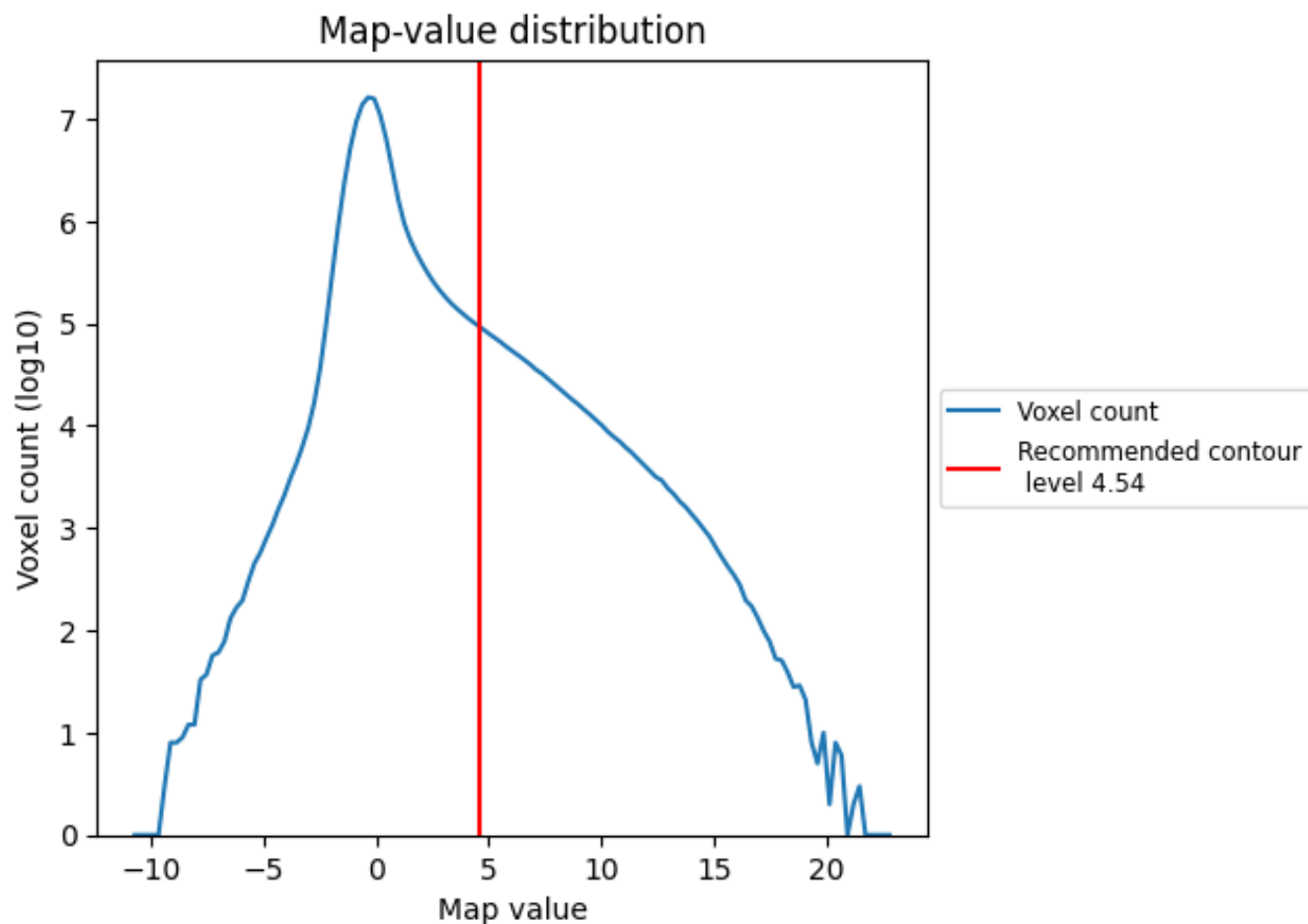
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

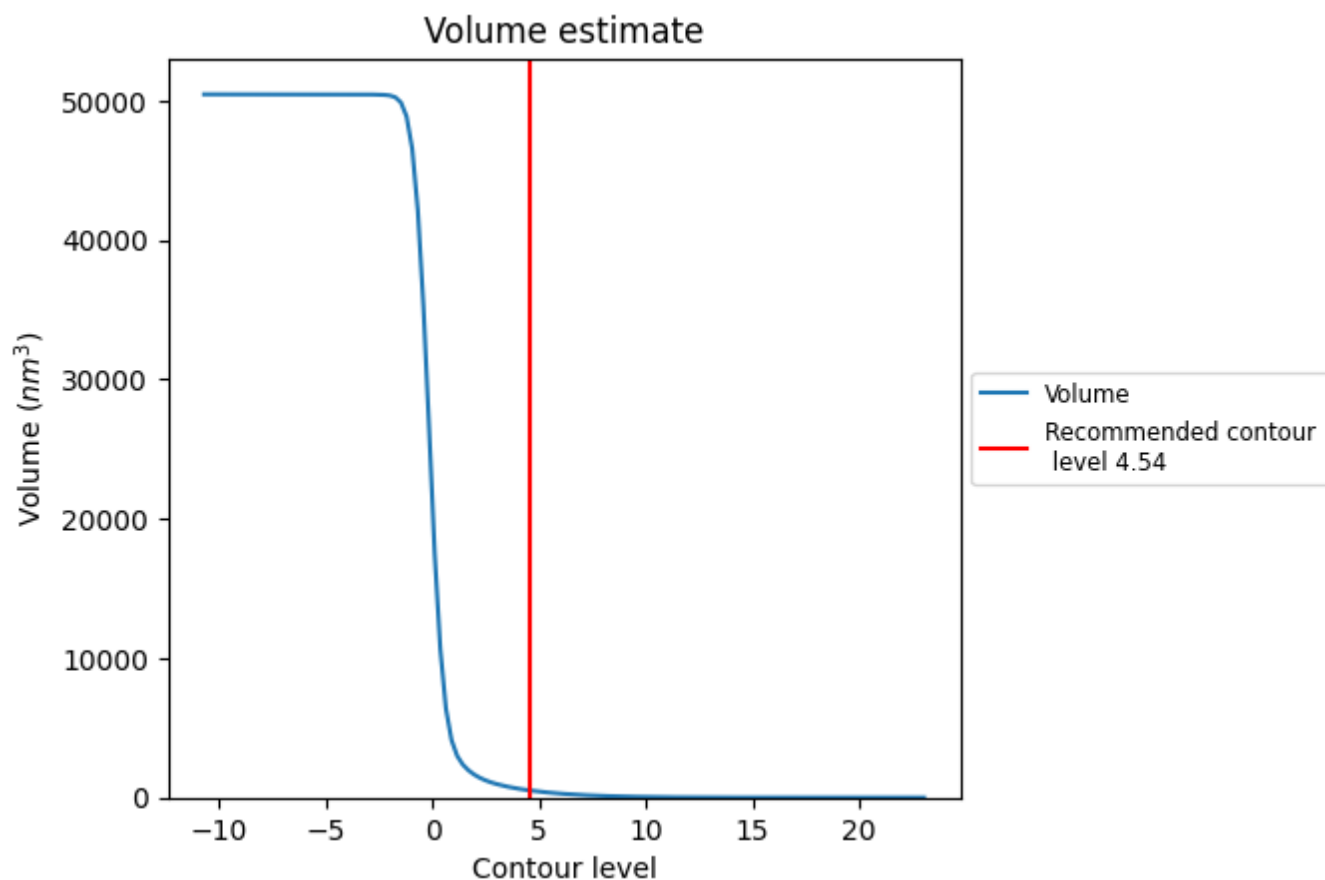
This section contains the results of statistical analysis of the map.

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.

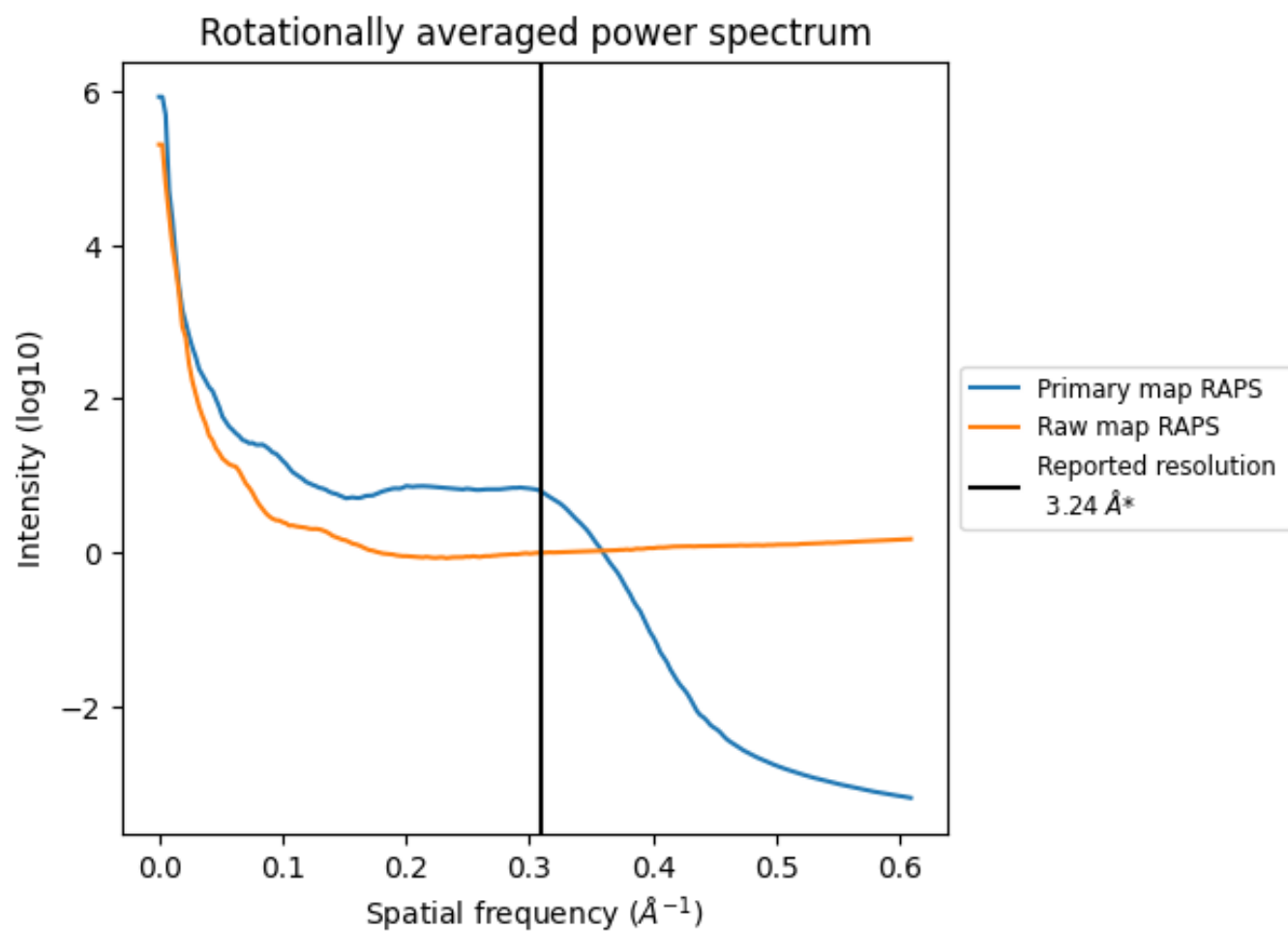
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 516 nm³; this corresponds to an approximate mass of 466 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 ⓘ

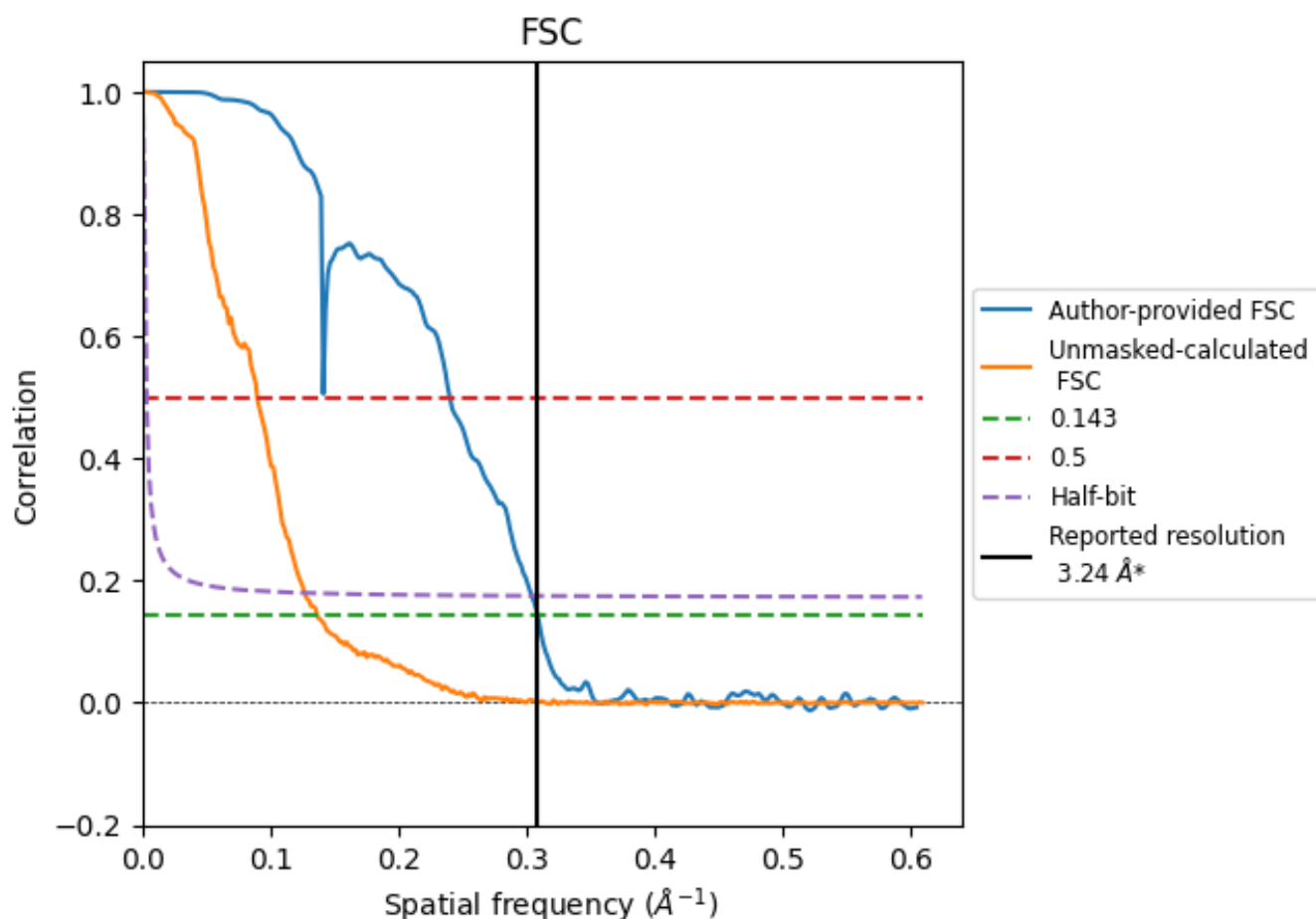


*Reported resolution corresponds to spatial frequency of 0.309 $\text{\AA}^{-1}$

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 0.309 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.24	-	-
Author-provided FSC curve	3.24	4.16	3.29
Unmasked-calculated*	7.32	11.14	7.89

*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 7.32 differs from the reported value 3.24 by more than 10 %

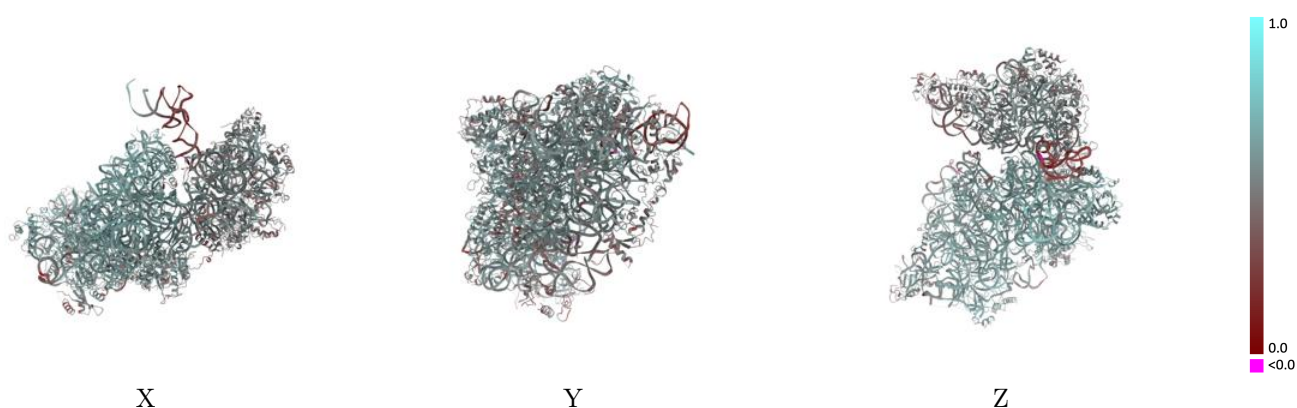
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29721 and PDB model 8G4I. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)

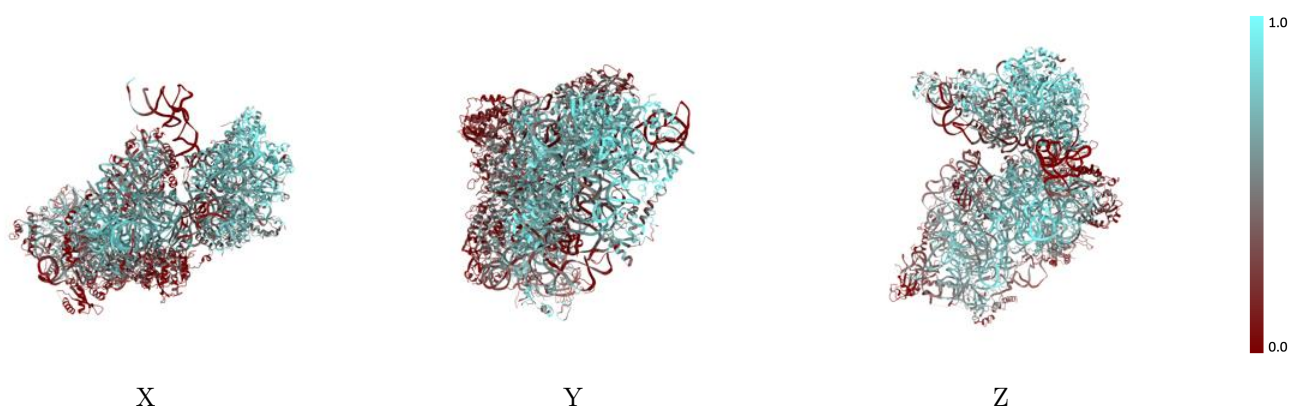
This section was not generated.

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



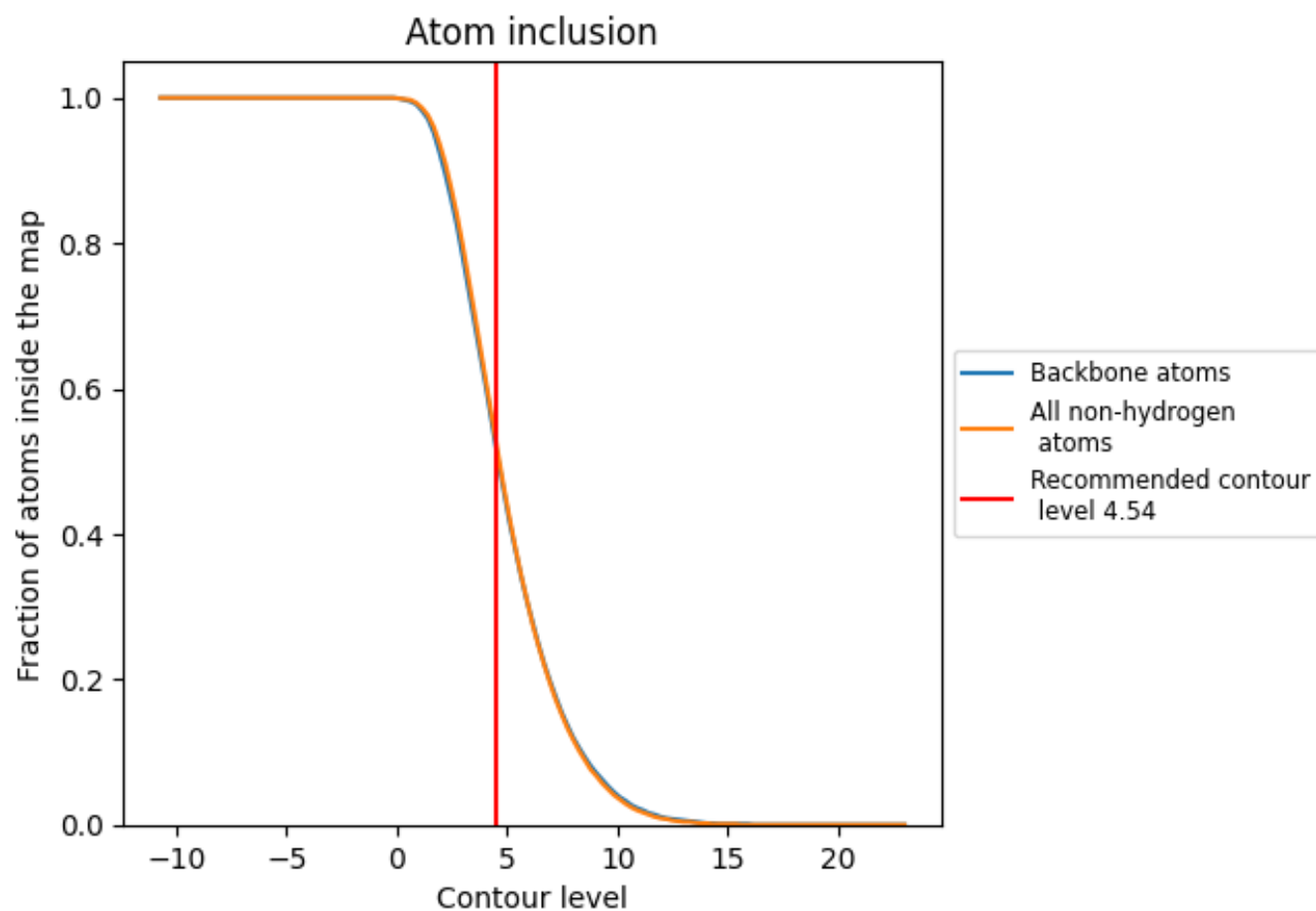
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.54).

9.4 Atom inclusion [i](#)



At the recommended contour level, 51% of all backbone atoms, 52% 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 (4.54) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5210	 0.5440
2	 0.6420	 0.5730
A	 0.1440	 0.5250
B	 0.3310	 0.5910
C	 0.3820	 0.5750
D	 0.6000	 0.4760
E	 0.3360	 0.5820
F	 0.7060	 0.4950
G	 0.1190	 0.5030
H	 0.1620	 0.5150
I	 0.4850	 0.6030
J	 0.2640	 0.5470
K	 0.6880	 0.4730
L	 0.4760	 0.6120
M	 0.6130	 0.4170
N	 0.3500	 0.5770
O	 0.3500	 0.5890
P	 0.6600	 0.4760
Q	 0.6710	 0.4900
R	 0.5870	 0.4360
S	 0.6560	 0.4900
T	 0.7920	 0.5130
U	 0.5740	 0.4690
V	 0.1870	 0.5270
W	 0.5280	 0.6010
X	 0.2320	 0.5840
Y	 0.0710	 0.4880
Z	 0.7880	 0.4820
a	 0.4640	 0.6060
b	 0.2910	 0.5700
c	 0.6050	 0.4720
d	 0.5380	 0.4950
e	 0.0710	 0.3340
f	 0.3160	 0.3310
g	 0.0650	 0.2900

