



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 10:08 PM UTC

PDB ID : 7WTU / pdb_00007wtu
EMDB ID : EMD-32801
Title : Cryo-EM structure of a human pre-40S ribosomal subunit - State RRP12-A1 (without CK1)
Authors : Cheng, J.; Lau, B.; Thoms, M.; Ameismeier, M.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on : 2022-02-05
Resolution : 3.00 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:

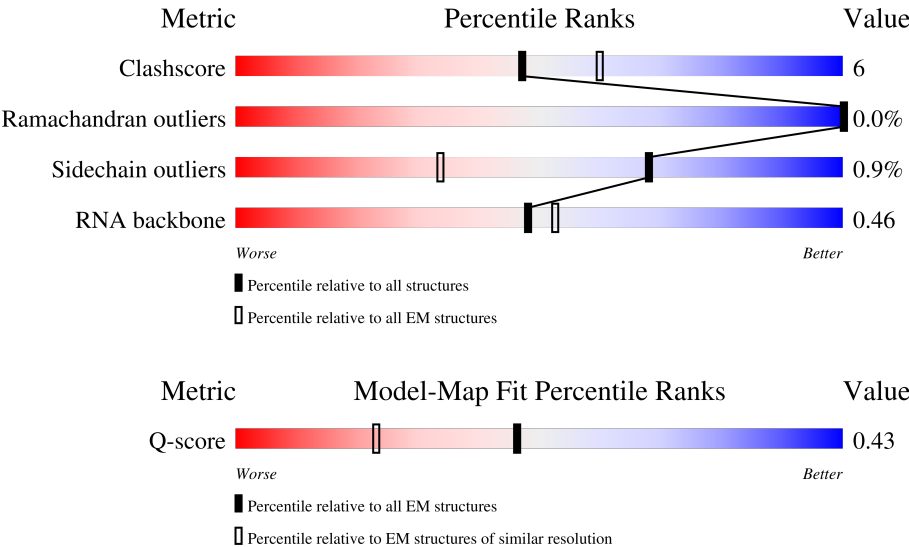
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.00 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.



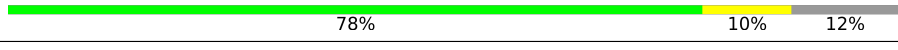
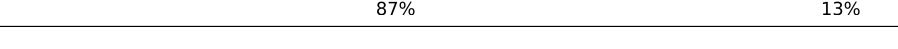
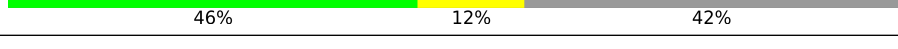
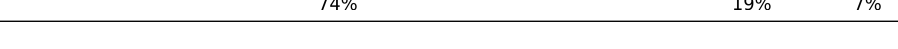
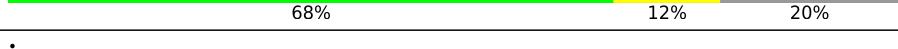
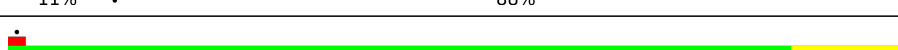
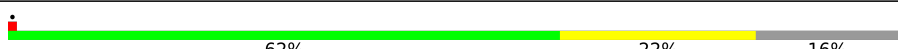
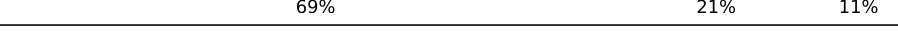
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	1873	
2	R	135	
3	b	84	

Continued on next page...

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Mol	Chain	Length	Quality of chain
4	B	264	
5	c	69	
6	E	263	
7	e	59	
8	F	204	
9	H	194	
10	G	249	
11	Z	125	
12	Y	133	
13	x	252	
14	X	143	
15	w	437	
16	W	130	
17	u	804	
18	t	475	
19	T	145	
20	S	152	
21	Q	146	
22	P	145	
23	O	151	
24	N	151	
25	L	158	
26	J	194	
27	I	208	
28	r	125	

Continued on next page...

Mol	Chain	Length	Quality of chain
29	q	281	
30	K	1297	
31	M	132	
32	f	156	
33	z	230	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 81215 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1575	Total	C	N	O	P	0	0
			33634	15011	6036	11012	1575		

- Molecule 2 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	81	Total	C	N	O	S	0	0
			673	420	137	114	2		

- Molecule 3 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 5 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	c	61	Total	C	N	O	S	0	0
			471	288	95	86	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 7 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	20	Total	C	N	O	S	0	0
			179	110	43	25	1		

- Molecule 8 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	189	Total	C	N	O	S	0	0
			1494	934	284	269	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 10 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 11 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 12 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 13 is a protein called RNA-binding protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	x	175	Total	C	N	O	S	0	0
			1372	881	249	238	4		

- Molecule 14 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 15 is a protein called Bystin.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	w	331	Total	C	N	O	S	0	0
			2610	1671	477	453	9		

- Molecule 16 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	129	Total	C	N	O	S	0	0
			1033	659	193	175	6		

- Molecule 17 is a protein called Pre-rRNA-processing protein TSR1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	u	642	Total	C	N	O	S	0	0
			5168	3315	928	901	24		

- Molecule 18 is a protein called Protein LTV1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	t	59	Total	C	N	O	S	0	0
			520	328	88	101	3		

- Molecule 19 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	144	Total	C	N	O	S	0	0
			1122	703	217	199	3		

- Molecule 20 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	127	Total	C	N	O	S	0	0
			1054	669	205	179	1		

- Molecule 21 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	125	Total	C	N	O	S	0	0
			998	637	185	173	3		

- Molecule 22 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	121	Total	C	N	O	S	0	0
			1006	643	186	170	7		

- Molecule 23 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	135	Total	C	N	O	S	0	0
			1009	618	198	187	6		

- Molecule 24 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 25 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 26 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 27 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 28 is a protein called Multifunctional methyltransferase subunit TRM112-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	r	118	Total	C	N	O	S	0	0
			940	601	166	166	7		

- Molecule 29 is a protein called Probable 18S rRNA (guanine-N(7))-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	q	235	Total	C	N	O	S	0	0
			1869	1182	333	343	11		

- Molecule 30 is a protein called RRP12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	K	1022	Total	C	N	O	S	0	0
			7949	5087	1383	1434	45		

- Molecule 31 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	M	108	Total	C	N	O	S	0	0
			837	530	147	153	7		

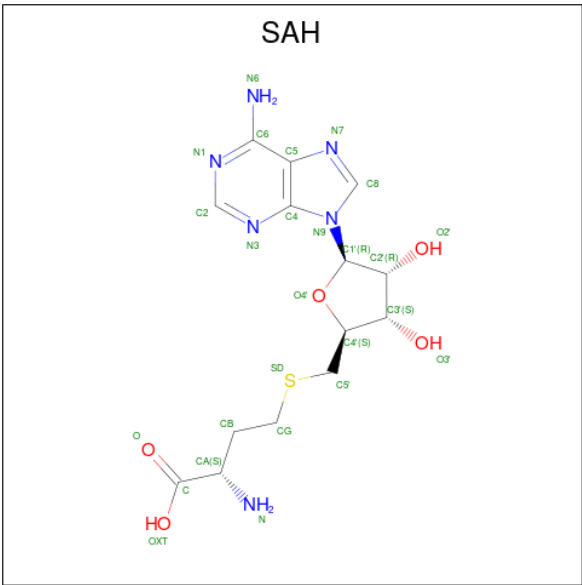
- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	57	Total	C	N	O	S	0	0
			465	295	89	74	7		

- Molecule 33 is a protein called Ribosome biogenesis protein SLX9 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	z	82	Total	C	N	O	S	0	0
			679	424	132	120	3		

- Molecule 34 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					AltConf
34	q	1	Total	C	N	O	S	0
			26	14	6	5	1	

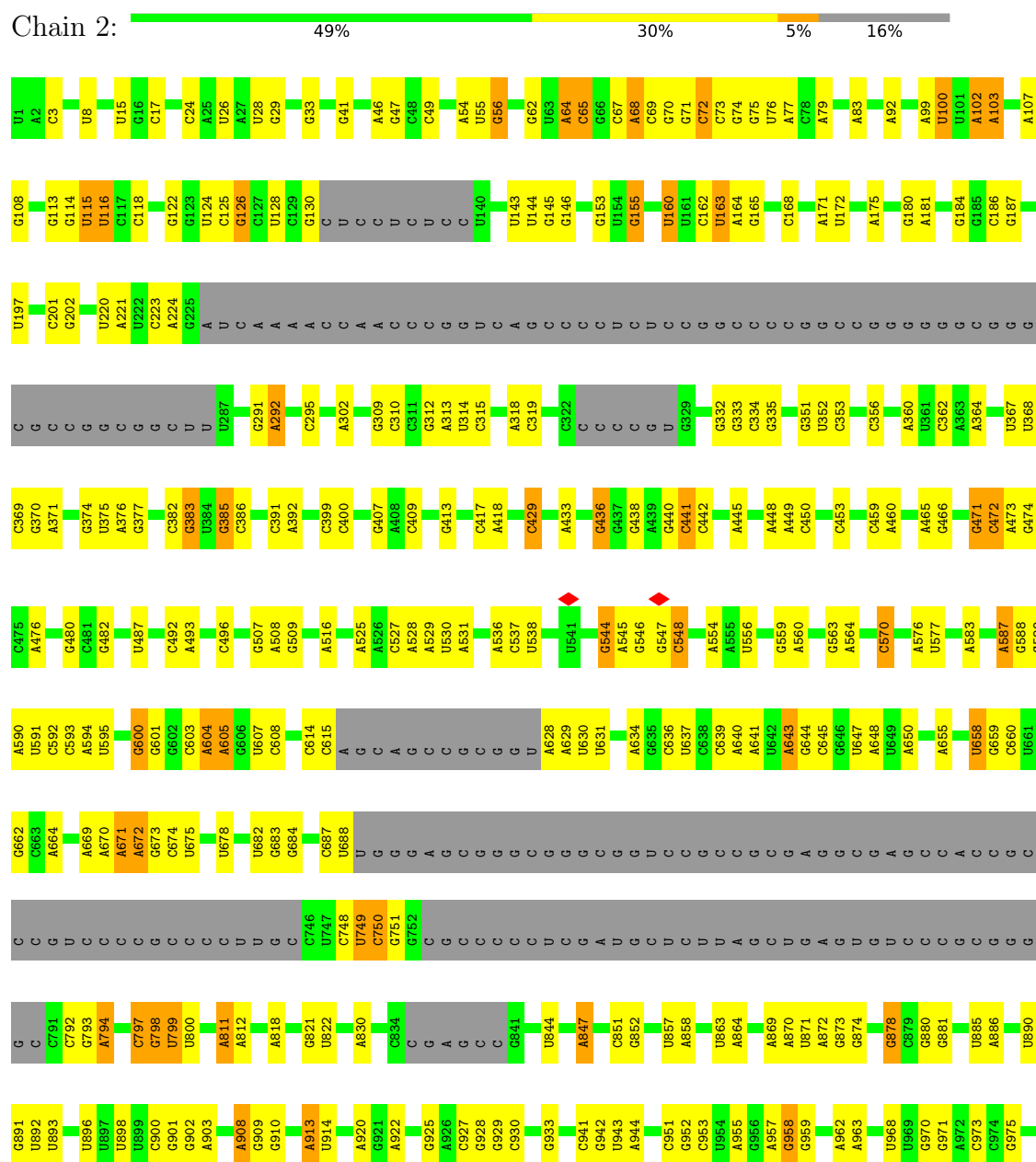
- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
35	f	1	Total	Zn	0
			1	1	

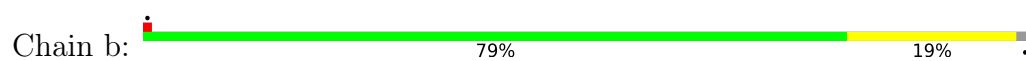
3 Residue-property plots

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.

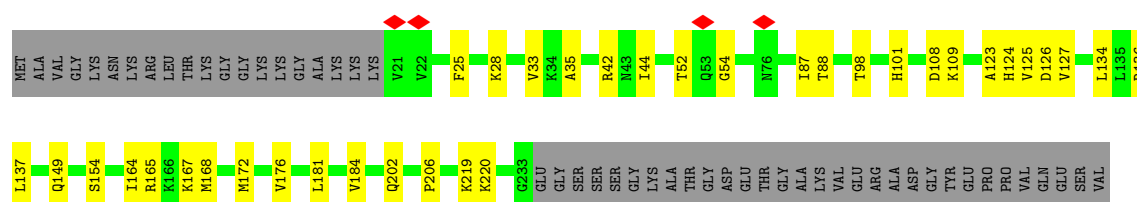
• Molecule 1: 18S rRNA



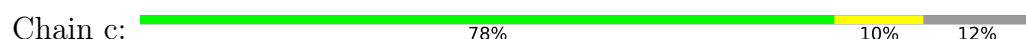




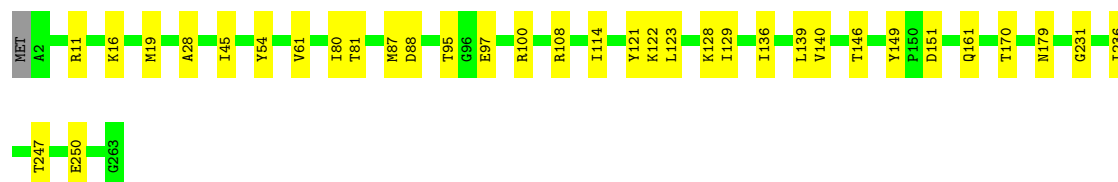
- Molecule 4: 40S ribosomal protein S3a



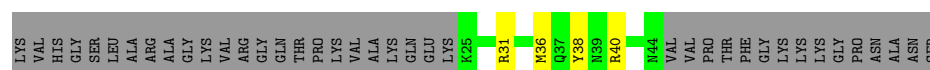
- Molecule 5: 40S ribosomal protein S28



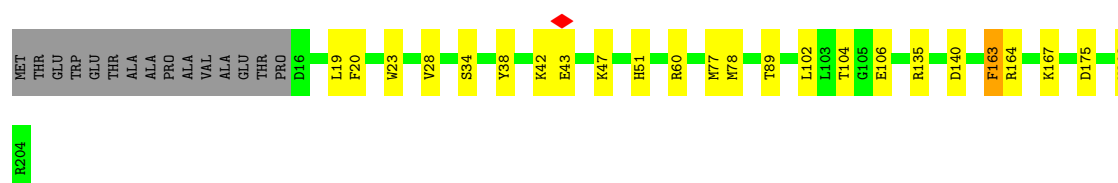
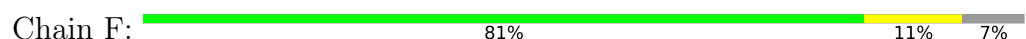
- Molecule 6: 40S ribosomal protein S4, X isoform



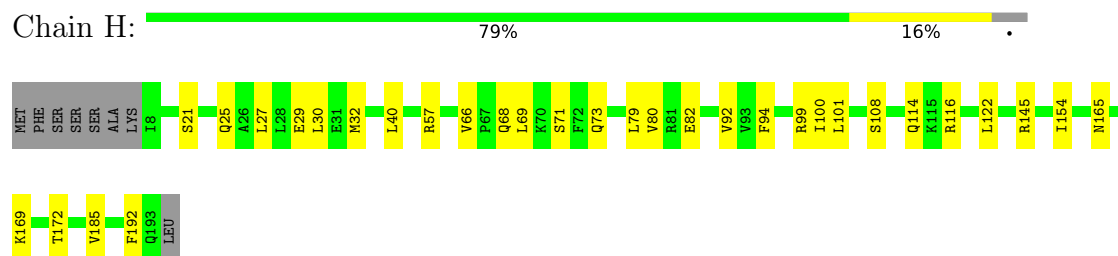
- Molecule 7: 40S ribosomal protein S30



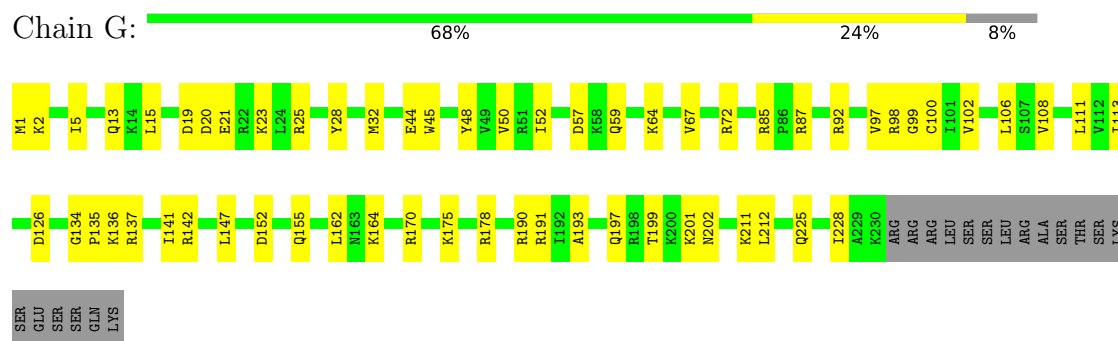
- Molecule 8: 40S ribosomal protein S5



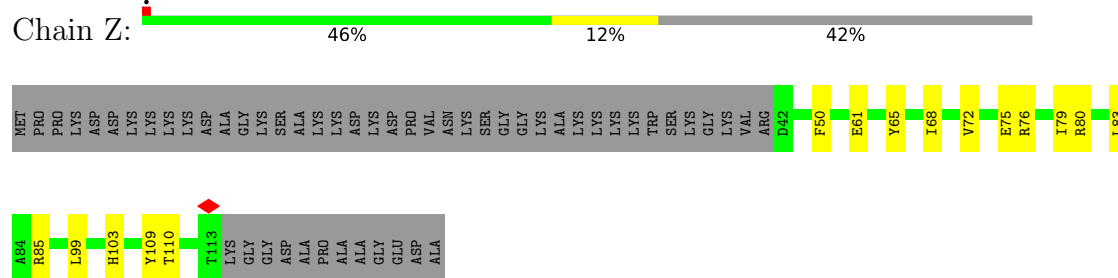
- Molecule 9: 40S ribosomal protein S7



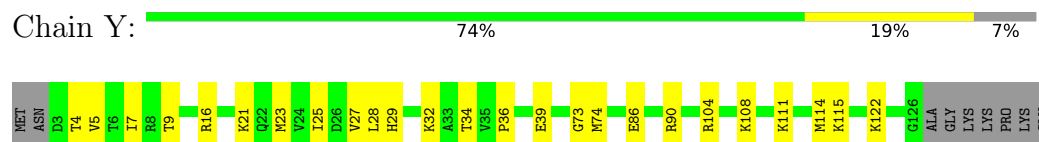
- Molecule 10: 40S ribosomal protein S6



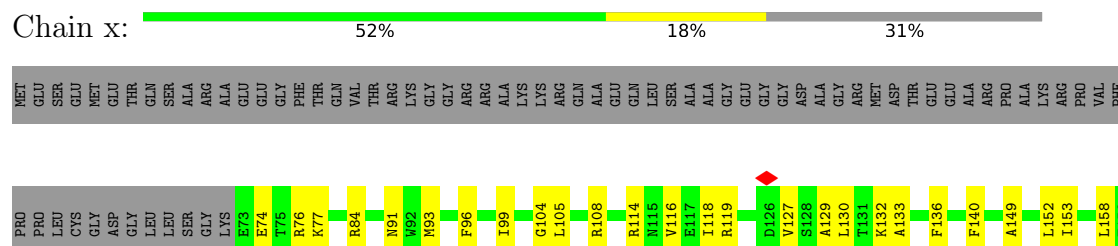
- Molecule 11: 40S ribosomal protein S25



- Molecule 12: 40S ribosomal protein S24



- Molecule 13: RNA-binding protein PNO1

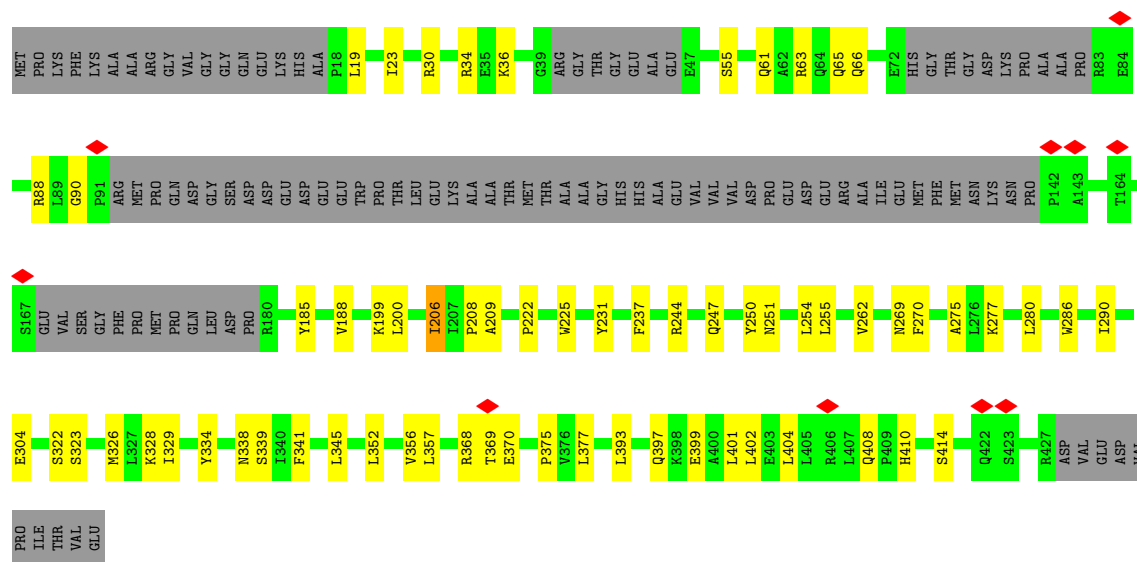




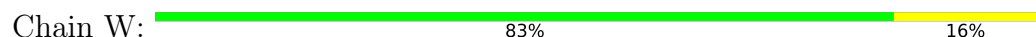
- Molecule 14: 40S ribosomal protein S23



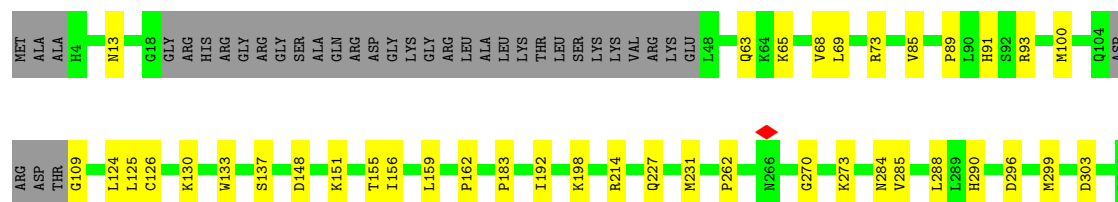
- Molecule 15: Bystin

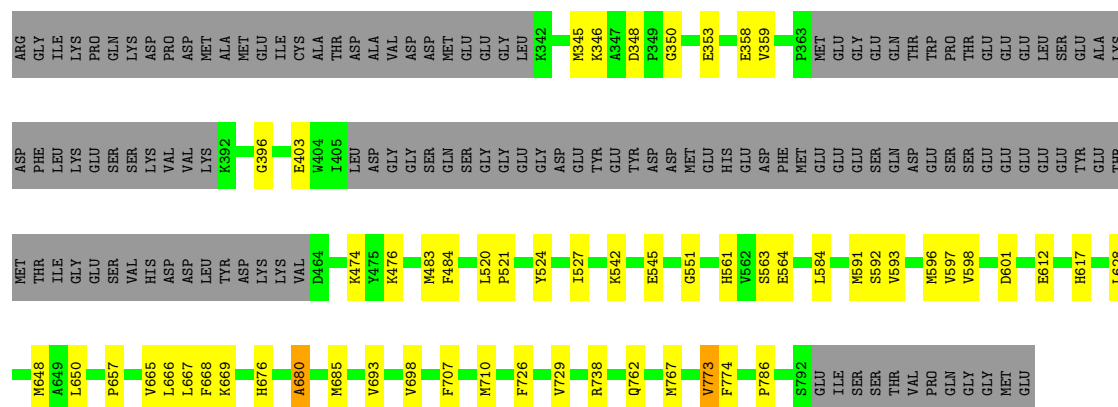


- Molecule 16: 40S ribosomal protein S15a

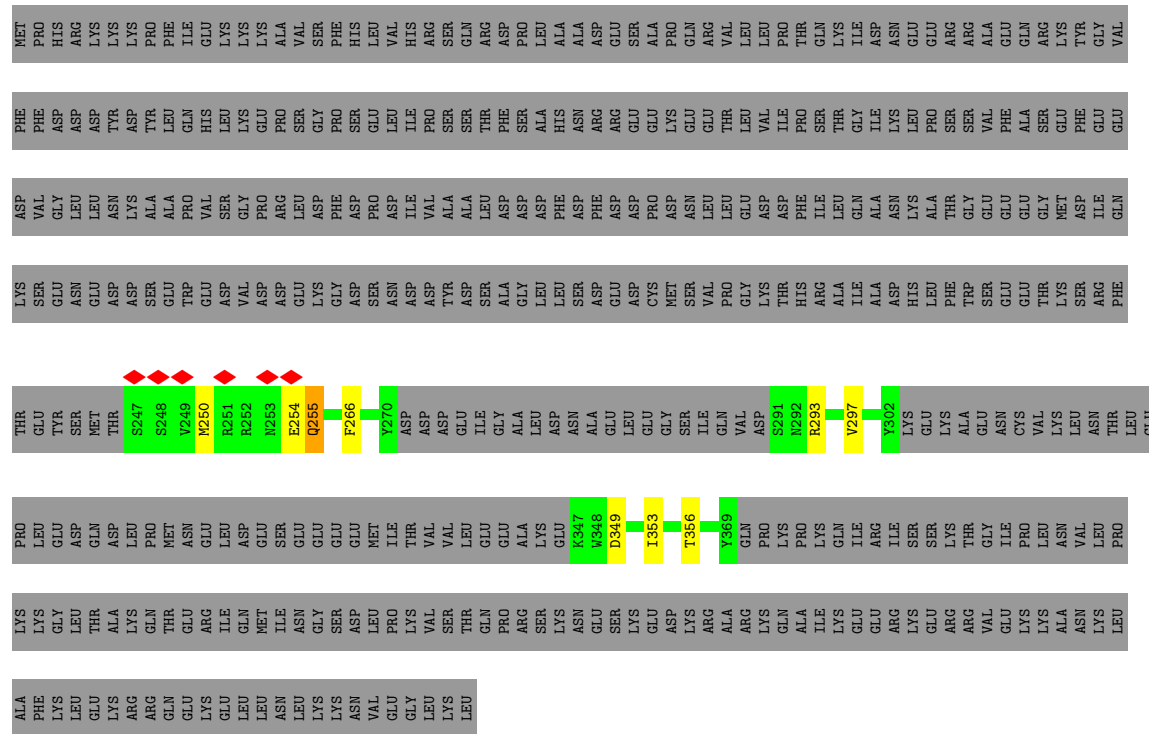


- Molecule 17: Pre-rRNA-processing protein TSR1 homolog

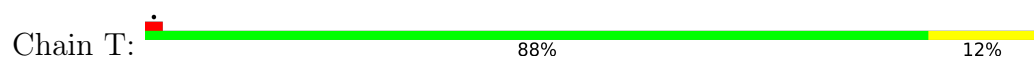




• Molecule 18: Protein LTV1 homolog

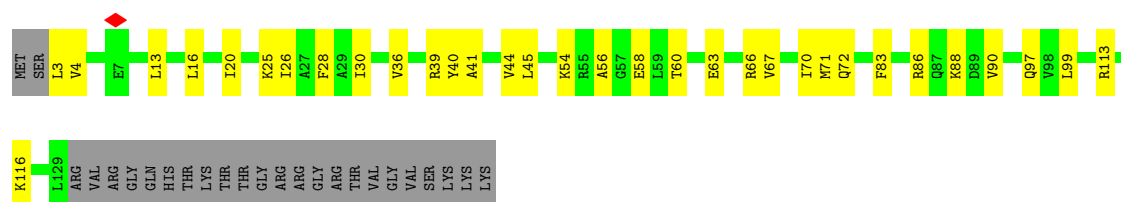


• Molecule 19: 40S ribosomal protein S19



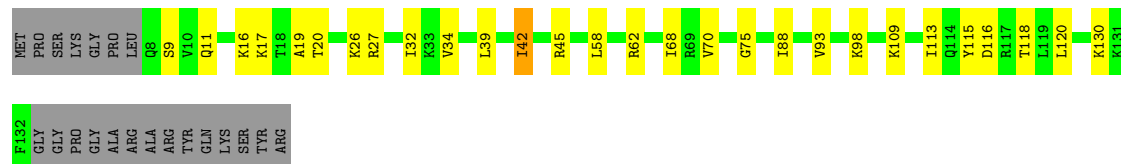
• Molecule 20: 40S ribosomal protein S18





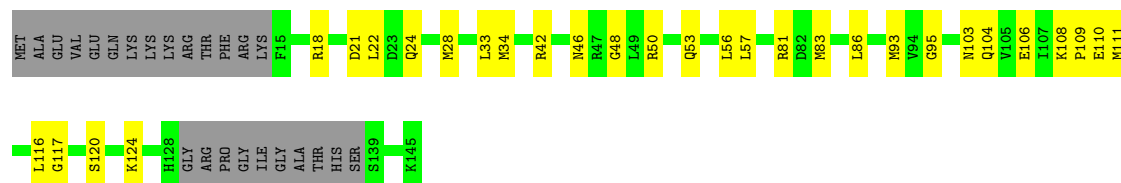
- Molecule 21: 40S ribosomal protein S16

Chain Q: 66% 18% 14%



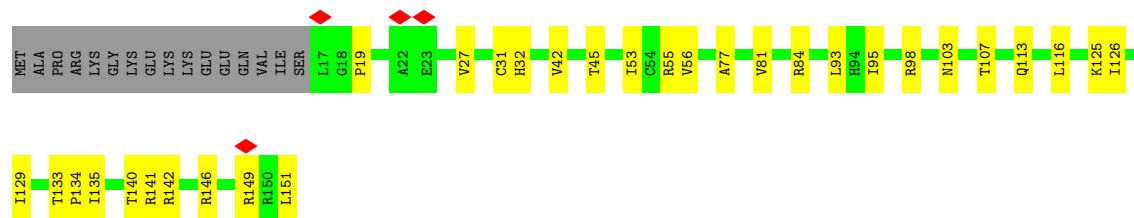
- Molecule 22: 40S ribosomal protein S15

Chain P: 63% 21% 17%



- Molecule 23: 40S ribosomal protein S14

Chain O: 69% 21% 11%



- Molecule 24: 40S ribosomal protein S13

Chain N: 92% 7%



- Molecule 25: 40S ribosomal protein S11

Chain L: 86% 9%



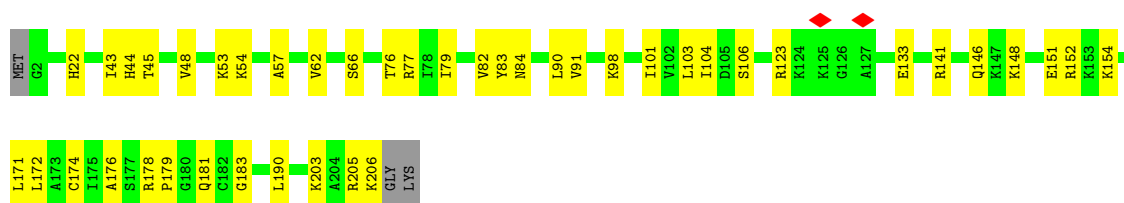
- Molecule 26: 40S ribosomal protein S9

Chain J: 82% 11% 7%



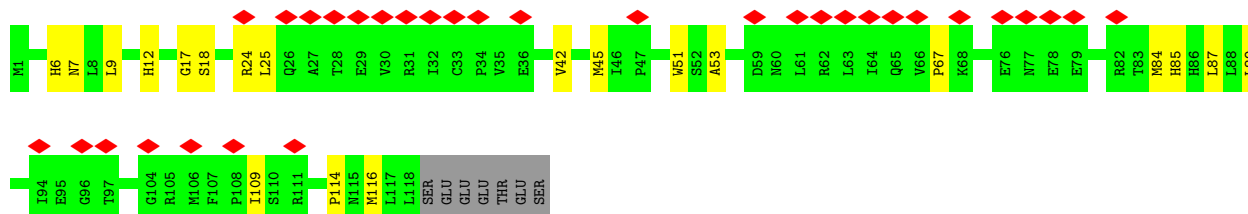
- Molecule 27: 40S ribosomal protein S8

Chain I: 78% 21%



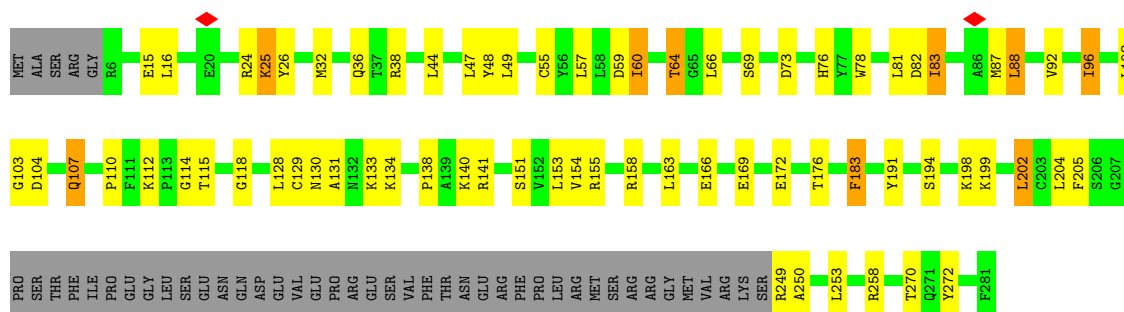
- Molecule 28: Multifunctional methyltransferase subunit TRM112-like protein

Chain r: 26% 78% 16% 6%



- Molecule 29: Probable 18S rRNA (guanine-N(7))-methyltransferase

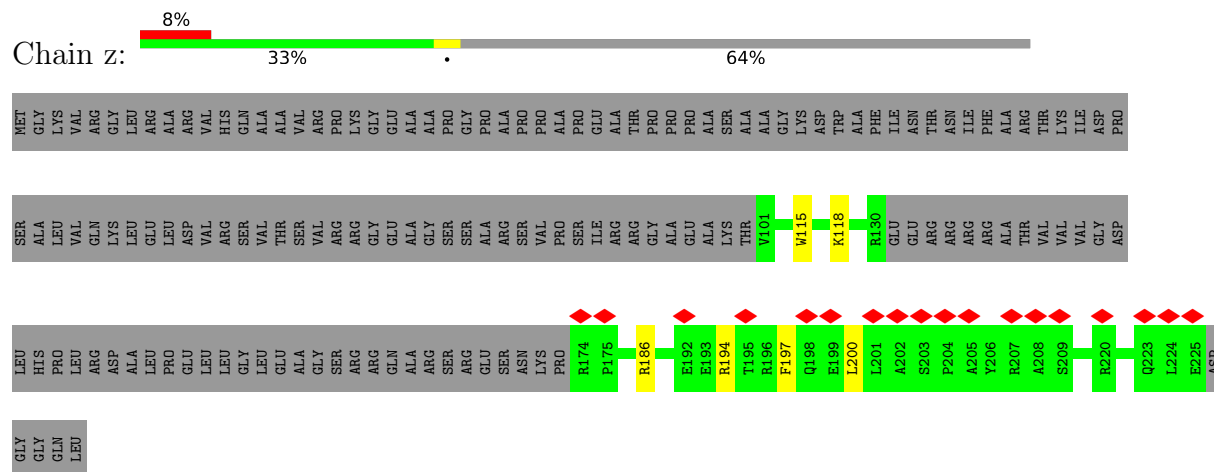
Chain q: 58% 22% 16%



- Molecule 30: RRP12-like protein

Chain K: 5% 68% 11% 21%

- Molecule 33: Ribosome biogenesis protein SLX9 homolog



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104045	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.599	Depositor
Minimum map value	-0.389	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, SAH, ZN

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	0.28	1/37573 (0.0%)	0.39	1/58534 (0.0%)
2	R	0.21	0/680	0.58	0/905
3	b	0.24	0/653	0.46	0/876
4	B	0.22	0/1756	0.55	0/2350
5	c	0.24	0/473	0.57	0/633
6	E	0.33	0/2118	0.56	0/2849
7	e	0.24	0/180	0.50	0/232
8	F	0.20	0/1515	0.50	0/2037
9	H	0.22	0/1524	0.51	0/2042
10	G	0.27	0/1885	0.59	0/2510
11	Z	0.27	0/580	0.66	0/780
12	Y	0.31	0/1031	0.51	0/1370
13	x	0.27	0/1394	0.61	0/1880
14	X	0.29	0/1116	0.58	0/1490
15	w	0.20	0/2656	0.54	2/3586 (0.1%)
16	W	0.30	0/1050	0.58	0/1406
17	u	0.26	0/5296	0.53	2/7154 (0.0%)
18	t	0.19	0/531	0.57	0/713
19	T	0.19	0/1142	0.47	0/1530
20	S	0.22	0/1071	0.54	0/1437
21	Q	0.25	0/1012	0.66	0/1356
22	P	0.21	0/1025	0.55	0/1369
23	O	0.23	0/1022	0.57	0/1372
24	N	0.22	0/1226	0.51	0/1649
25	L	0.31	0/1250	0.53	0/1673
26	J	0.29	0/1524	0.54	0/2035
27	I	0.31	0/1711	0.59	0/2282
28	r	0.21	0/961	0.55	0/1301
29	q	0.89	0/1910	1.09	1/2572 (0.0%)
30	K	0.21	0/8097	0.55	0/10950
31	M	0.14	0/845	0.41	0/1134
32	f	0.14	0/474	0.49	0/626

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	z	0.21	0/686	0.56	0/914
All	All	0.29	1/85967 (0.0%)	0.50	6/123547 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
17	u	0	3
18	t	0	1
21	Q	0	1
27	I	0	1
30	K	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1639	G7M	O3'-P	5.60	1.61	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	w	206	ILE	CA-C-N	6.35	124.24	120.24
15	w	206	ILE	C-N-CA	6.35	124.24	120.24
17	u	773	VAL	CA-C-N	6.28	135.90	122.90
17	u	773	VAL	C-N-CA	6.28	135.90	122.90
29	q	118	GLY	CA-C-O	-6.22	118.18	122.22
1	2	102	A	C4'-C3'-O3'	5.04	116.96	109.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	I	66	SER	Peptide
30	K	378	VAL	Peptide
21	Q	42	ILE	Peptide
18	t	255	GLN	Peptide
17	u	345	MET	Peptide
17	u	348	ASP	Peptide

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Mol	Chain	Res	Type	Group
17	u	680	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	33634	0	16988	325	0
2	R	673	0	722	19	0
3	b	640	0	665	10	0
4	B	1729	0	1803	20	0
5	c	471	0	499	5	0
6	E	2076	0	2177	23	0
7	e	179	0	200	3	0
8	F	1494	0	1549	19	0
9	H	1501	0	1593	20	0
10	G	1862	0	2018	42	0
11	Z	574	0	627	14	0
12	Y	1014	0	1082	16	0
13	x	1372	0	1453	35	0
14	X	1098	0	1167	10	0
15	w	2610	0	2644	48	0
16	W	1033	0	1080	15	0
17	u	5168	0	5230	62	0
18	t	520	0	479	7	0
19	T	1122	0	1153	10	0
20	S	1054	0	1105	21	0
21	Q	998	0	1065	20	0
22	P	1006	0	1056	19	0
23	O	1009	0	1034	29	0
24	N	1202	0	1289	6	0
25	L	1229	0	1302	12	0
26	J	1499	0	1618	14	0
27	I	1682	0	1769	25	0
28	r	940	0	958	13	0
29	q	1869	0	1854	33	0
30	K	7949	0	8223	95	0
31	M	837	0	870	12	0
32	f	465	0	482	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	z	679	0	719	5	0
34	q	26	0	19	1	0
35	f	1	0	0	0	0
All	All	81215	0	66492	866	0

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

All (866) 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)
16:W:101:PHE:O	16:W:128:PHE:HA	1.27	1.29
1:2:8:U:O4	1:2:15:U:O4	1.59	1.20
1:2:748:C:N4	1:2:794:A:H61	1.43	1.15
1:2:536:A:N6	1:2:548:C:H42	1.48	1.12
1:2:536:A:H61	1:2:548:C:N4	1.48	1.11
1:2:748:C:H42	1:2:794:A:N6	1.47	1.10
1:2:1710:C:H42	1:2:1823:A:N6	1.49	1.10
1:2:1710:C:N4	1:2:1823:A:H61	1.49	1.09
1:2:1609:C:N4	1:2:1630:A:H61	1.51	1.09
23:O:42:VAL:O	23:O:55:ARG:HA	1.58	1.04
1:2:1609:C:H42	1:2:1630:A:N6	1.54	1.04
1:2:24:C:N4	1:2:650:A:H61	1.59	1.01
1:2:614:C:H42	1:2:629:A:N6	1.59	0.99
1:2:24:C:H42	1:2:650:A:N6	1.61	0.98
29:q:26:TYR:CD2	29:q:64:THR:HG21	2.06	0.91
1:2:1534:C:C2	1:2:1598:G:N2	2.39	0.90
1:2:614:C:N4	1:2:629:A:H61	1.72	0.88
29:q:26:TYR:HD2	29:q:64:THR:HG21	1.40	0.87
1:2:615:C:H42	1:2:628:A:N6	1.71	0.86
13:x:133:ALA:O	13:x:136:PHE:HB3	1.75	0.86
1:2:1398:G:H1	1:2:1448:A:H2	1.21	0.84
16:W:101:PHE:O	16:W:128:PHE:CA	2.22	0.82
30:K:538:ALA:O	30:K:542:MET:HB3	1.80	0.81
1:2:615:C:N4	1:2:628:A:N6	2.28	0.81
1:2:615:C:N4	1:2:628:A:H61	1.79	0.81
1:2:1335:G:H1	1:2:1492:U:H3	1.28	0.81
1:2:1037:G:C2	1:2:1079:C:O2	2.37	0.76
13:x:76:ARG:HH22	23:O:126:ILE:HD13	1.51	0.76
13:x:168:VAL:HG23	23:O:149:ARG:HH11	1.52	0.75
1:2:748:C:H42	1:2:794:A:H61	0.76	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1743:G:H21	1:2:1791:A:H62	1.36	0.74
29:q:26:TYR:CD2	29:q:64:THR:CG2	2.71	0.73
1:2:748:C:N4	1:2:794:A:N6	2.20	0.73
1:2:925:G:H1	1:2:1017:U:H3	1.36	0.73
1:2:1710:C:N3	1:2:1823:A:N1	2.35	0.73
1:2:749:U:O4	1:2:793:G:O6	2.07	0.72
1:2:957:A:H3'	1:2:958:G:H21	1.54	0.72
1:2:1177:U:H3	1:2:1184:G:H1	1.38	0.71
17:u:617:HIS:HB2	17:u:666:LEU:HB2	1.71	0.71
14:X:112:VAL:HG12	14:X:114:ASP:H	1.54	0.70
30:K:908:PRO:HB3	33:z:200:LEU:HD23	1.71	0.70
1:2:536:A:N1	1:2:548:C:N3	2.39	0.70
17:u:726:PHE:HB3	17:u:767:MET:HE1	1.73	0.69
1:2:614:C:N4	1:2:629:A:N6	2.30	0.69
10:G:2:LYS:HB2	10:G:108:VAL:HG12	1.74	0.69
17:u:667:LEU:HB2	17:u:680:ALA:HB3	1.73	0.69
28:r:116:MET:HE3	29:q:103:GLY:HA3	1.73	0.69
1:2:1652:G:H1	1:2:1672:U:H3	1.40	0.69
1:2:64:A:H2	1:2:83:A:H62	1.38	0.69
1:2:1609:C:N3	1:2:1630:A:N1	2.40	0.68
1:2:1275:G:O6	1:2:1324:G:C2	2.47	0.68
1:2:991:G:H22	1:2:1099:G:H22	1.41	0.68
17:u:109:GLY:HA2	17:u:125:LEU:O	1.95	0.67
10:G:67:VAL:HG13	10:G:99:GLY:HA2	1.77	0.67
15:w:397:GLN:HG3	18:t:250:MET:HE1	1.76	0.67
21:Q:32:ILE:HD12	21:Q:39:LEU:HD12	1.75	0.67
4:B:125:VAL:HG22	4:B:172:MET:HE3	1.77	0.67
1:2:1610:G:O2'	20:S:86:ARG:NH1	2.29	0.66
22:P:28:MET:HE2	22:P:33:LEU:HA	1.76	0.66
25:L:4:ILE:HG23	25:L:5:GLN:HG2	1.77	0.66
1:2:1037:G:N2	1:2:1079:C:O2	2.29	0.66
29:q:158:ARG:HA	29:q:205:PHE:HA	1.78	0.66
12:Y:5:VAL:HA	12:Y:28:LEU:O	1.96	0.66
6:E:247:THR:OG1	6:E:250:GLU:OE1	2.13	0.65
1:2:24:C:H42	1:2:650:A:H61	0.78	0.65
14:X:139:GLU:OE2	17:u:214:ARG:NH1	2.29	0.65
10:G:57:ASP:HB3	10:G:98:ARG:HD2	1.77	0.65
1:2:1302:G:C6	1:2:1306:U:O4	2.49	0.65
1:2:1471:C:N3	30:K:711:ARG:NH2	2.44	0.65
17:u:284:ASN:OD1	17:u:346:LYS:NZ	2.29	0.65
21:Q:34:VAL:HG22	21:Q:70:VAL:HB	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:I:45:THR:HB	27:I:53:LYS:HD2	1.79	0.64
1:2:1227:G:N2	1:2:1635:C:O2'	2.31	0.64
2:R:34:VAL:HA	2:R:37:GLU:HG2	1.79	0.64
30:K:1021:LYS:O	30:K:1029:HIS:NE2	2.29	0.64
26:J:59:GLU:OE2	26:J:69:ARG:NH2	2.31	0.64
1:2:1761:U:H3	1:2:1771:G:H1	1.46	0.64
1:2:1227:G:O6	1:2:1531:A:N1	2.31	0.63
13:x:127:VAL:O	13:x:130:LEU:HB3	1.98	0.63
6:E:140:VAL:HG22	6:E:146:THR:HG22	1.80	0.63
1:2:1550:G:H3'	1:2:1579:A:H61	1.64	0.63
9:H:21:SER:O	9:H:25:GLN:NE2	2.31	0.63
1:2:507:G:OP2	12:Y:104:ARG:NH2	2.32	0.62
13:x:76:ARG:HB2	13:x:118:ILE:HB	1.80	0.62
10:G:32:MET:HG3	10:G:100:CYS:HB2	1.82	0.62
1:2:885:U:O2	1:2:901:G:O6	2.17	0.62
5:c:17:VAL:HA	5:c:30:VAL:HG23	1.81	0.62
1:2:1277:C:O2	1:2:1322:G:N2	2.33	0.62
17:u:346:LYS:HD2	17:u:551:GLY:HA2	1.79	0.62
1:2:1682:C:OP2	15:w:34:ARG:NH2	2.33	0.62
21:Q:42:ILE:O	21:Q:45:ARG:NH2	2.33	0.62
1:2:643:A:OP1	26:J:39:ASN:ND2	2.33	0.61
13:x:229:ILE:O	23:O:149:ARG:NH2	2.31	0.61
5:c:46:VAL:HG12	8:F:140:ASP:HB3	1.81	0.61
6:E:87:MET:HE1	6:E:236:ILE:HG21	1.83	0.61
1:2:103:A:OP2	1:2:356:C:N4	2.27	0.61
1:2:614:C:N3	1:2:629:A:N1	2.48	0.61
1:2:1593:C:OP1	11:Z:103:HIS:NE2	2.32	0.61
30:K:334:MET:HE3	30:K:346:MET:HE3	1.81	0.61
10:G:64:LYS:HG3	10:G:97:VAL:HG21	1.82	0.61
30:K:863:ILE:HG22	30:K:919:CYS:HB3	1.82	0.61
1:2:1285:G:H5'	31:M:35:ILE:HD12	1.83	0.60
1:2:24:C:N3	1:2:650:A:N1	2.49	0.60
1:2:1453:C:OP2	2:R:45:LYS:NZ	2.32	0.60
1:2:1871:C:OP2	13:x:114:ARG:NH2	2.34	0.60
22:P:34:MET:SD	22:P:46:ASN:ND2	2.74	0.60
29:q:104:ASP:HB3	29:q:107:GLN:HB2	1.81	0.60
1:2:1236:G:H21	1:2:1522:A:H62	1.49	0.60
3:b:40:CYS:SG	3:b:42:LYS:NZ	2.72	0.60
1:2:24:C:OP1	26:J:11:LYS:NZ	2.32	0.60
1:2:615:C:N3	1:2:628:A:N1	2.49	0.60
1:2:847:A:OP2	6:E:16:LYS:NZ	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1091:C:HO2'	16:W:2:VAL:N	2.00	0.60
5:c:55:VAL:HG23	8:F:34:SER:HA	1.83	0.60
20:S:116:LYS:NZ	22:P:110:GLU:OE2	2.35	0.60
15:w:206:ILE:HG21	18:t:297:VAL:HG21	1.82	0.59
15:w:338:ASN:HA	15:w:341:PHE:HD2	1.66	0.59
1:2:1332:A:C6	1:2:1497:G:N1	2.70	0.59
1:2:1502:C:O2'	17:u:762:GLN:NE2	2.35	0.59
13:x:197:VAL:HG11	13:x:241:ILE:HG13	1.83	0.59
27:I:57:ALA:HB2	27:I:183:GLY:HA2	1.83	0.59
22:P:81:ARG:NH2	22:P:117:GLY:O	2.36	0.59
1:2:312:G:O2'	10:G:191:ARG:NH1	2.36	0.59
1:2:507:G:OP1	12:Y:108:LYS:NZ	2.35	0.59
13:x:197:VAL:HG13	13:x:245:ALA:HB2	1.85	0.59
15:w:368:ARG:HH21	15:w:404:LEU:HG	1.65	0.59
22:P:22:LEU:HD11	22:P:109:PRO:HB3	1.84	0.59
15:w:250:TYR:HB3	15:w:290:ILE:HG12	1.85	0.59
1:2:1753:C:H2'	1:2:1754:G:H8	1.67	0.59
1:2:630:U:OP1	29:q:249:ARG:NH1	2.36	0.59
6:E:128:LYS:HG2	6:E:140:VAL:HB	1.85	0.59
17:u:126:CYS:O	17:u:130:LYS:N	2.35	0.59
1:2:634:A:OP1	14:X:134:TYR:OH	2.19	0.58
8:F:135:ARG:HG2	29:q:131:ALA:HB3	1.84	0.58
6:E:100:ARG:HG3	6:E:114:ILE:HD13	1.85	0.58
10:G:193:ALA:O	10:G:197:GLN:NE2	2.36	0.58
13:x:149:ALA:HA	13:x:152:LEU:HD13	1.83	0.58
1:2:1216:C:H2'	30:K:1188:ARG:HG2	1.85	0.58
1:2:1336:C:OP1	30:K:1036:ARG:NH2	2.37	0.58
1:2:594:A:H61	1:2:643:A:H5''	1.69	0.58
26:J:107:GLU:O	26:J:113:GLN:NE2	2.36	0.58
1:2:429:C:O2'	1:2:811:A:N1	2.35	0.58
1:2:1598:G:OP1	11:Z:80:ARG:NH2	2.37	0.58
1:2:1563:G:OP1	19:T:121:ARG:NH1	2.36	0.58
3:b:11:SER:OG	3:b:14:GLU:OE1	2.20	0.58
30:K:112:ARG:HH21	30:K:126:ALA:HB2	1.69	0.58
31:M:86:GLY:HA3	31:M:105:GLY:HA2	1.85	0.57
32:f:133:ALA:O	32:f:139:HIS:HA	2.04	0.57
1:2:1277:C:C2	1:2:1322:G:N2	2.73	0.57
28:r:84:MET:HA	28:r:87:LEU:HD12	1.86	0.57
26:J:93:LYS:NZ	26:J:95:ASP:OD2	2.37	0.57
1:2:1534:C:O2	1:2:1598:G:N2	2.36	0.57
1:2:1761:U:O2	1:2:1771:G:N2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:577:U:H5''	17:u:198:LYS:HE3	1.86	0.57
10:G:1:MET:HE2	10:G:106:LEU:HB3	1.87	0.57
1:2:1811:C:O2'	17:u:63:GLN:OE1	2.23	0.57
2:R:27:ASP:O	2:R:31:ASN:ND2	2.38	0.57
9:H:154:ILE:HB	9:H:185:VAL:HG12	1.86	0.57
12:Y:4:THR:OG1	12:Y:32:LYS:NZ	2.37	0.57
14:X:101:LEU:HB3	14:X:124:LYS:HB2	1.87	0.57
1:2:1222:G:H5''	8:F:78:MET:HE1	1.86	0.56
9:H:69:LEU:O	9:H:73:GLN:N	2.37	0.56
26:J:170:PRO:O	26:J:175:ARG:NH1	2.38	0.56
1:2:334:C:OP2	10:G:190:ARG:NH2	2.38	0.56
11:Z:68:ILE:HB	11:Z:109:TYR:HB2	1.87	0.56
19:T:77:LYS:HD3	19:T:94:ARG:HH21	1.69	0.56
1:2:1453:C:OP1	2:R:48:ASN:ND2	2.38	0.56
3:b:36:LYS:HD2	3:b:43:ILE:HG12	1.86	0.56
6:E:54:TYR:OH	6:E:97:GLU:OE2	2.22	0.56
15:w:209:ALA:HB1	18:t:293:ARG:HH12	1.68	0.56
16:W:28:ARG:HB3	16:W:60:LYS:HG2	1.86	0.56
17:u:273:LYS:HG2	17:u:561:HIS:HD2	1.70	0.56
1:2:1398:G:N1	1:2:1448:A:C2	2.62	0.56
18:t:254:GLU:HG2	18:t:255:GLN:HG2	1.86	0.56
1:2:153:G:N3	10:G:13:GLN:NE2	2.54	0.56
1:2:1332:A:N6	1:2:1497:G:C6	2.73	0.56
1:2:1653:U:H3	1:2:1671:G:H1	1.52	0.56
1:2:615:C:H41	17:u:738:ARG:HH12	1.54	0.56
1:2:530:U:H2'	1:2:531:A:H8	1.70	0.56
1:2:1367:U:N3	1:2:1373:C:N4	2.54	0.56
1:2:1757:G:C6	1:2:1776:G:C2	2.94	0.56
20:S:60:THR:OG1	20:S:63:GLU:OE1	2.23	0.56
23:O:103:ASN:HB3	23:O:142:ARG:HG3	1.85	0.56
20:S:30:ILE:HG13	20:S:45:LEU:HD21	1.88	0.56
20:S:88:LYS:O	22:P:18:ARG:NH1	2.38	0.56
1:2:1272:C:OP1	1:2:1303:C:O2'	2.24	0.56
22:P:48:GLY:O	22:P:50:ARG:NH1	2.39	0.56
1:2:536:A:H61	1:2:548:C:H42	0.71	0.55
1:2:1398:G:O6	1:2:1448:A:N1	2.39	0.55
15:w:375:PRO:HB2	15:w:377:LEU:HG	1.89	0.55
1:2:1301:A:H5''	15:w:199:LYS:HB2	1.88	0.55
1:2:1329:U:O2	1:2:1500:G:O6	2.24	0.55
23:O:140:THR:HG22	23:O:141:ARG:H	1.70	0.55
30:K:621:GLN:O	30:K:624:THR:OG1	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:164:A:H3'	1:2:165:G:H21	1.72	0.55
1:2:171:A:OP2	10:G:137:ARG:NH1	2.39	0.55
1:2:436:G:OP2	1:2:471:G:O2'	2.24	0.55
1:2:973:C:N3	23:O:55:ARG:NH1	2.55	0.55
1:2:1743:G:N2	1:2:1791:A:H62	2.02	0.55
23:O:53:ILE:O	23:O:84:ARG:NH1	2.35	0.55
1:2:1217:A:H2'	1:2:1218:C:H6	1.72	0.55
30:K:538:ALA:O	30:K:542:MET:CB	2.53	0.55
4:B:126:ASP:OD1	4:B:136:ARG:NE	2.34	0.55
26:J:136:ARG:NH2	26:J:158:ASP:OD2	2.35	0.55
1:2:480:G:H4'	17:u:68:VAL:HG11	1.89	0.55
6:E:87:MET:HE2	6:E:123:LEU:HB2	1.89	0.55
1:2:1367:U:O2	1:2:1373:C:N3	2.40	0.55
2:R:63:ARG:O	30:K:574:ARG:NH2	2.39	0.55
24:N:66:VAL:HG13	24:N:67:THR:HG23	1.88	0.55
30:K:860:PRO:HG2	33:z:194:ARG:HG2	1.87	0.55
1:2:56:G:OP1	12:Y:111:LYS:NZ	2.35	0.55
17:u:227:GLN:NE2	17:u:231:MET:SD	2.80	0.55
1:2:587:A:H5'	1:2:592:C:H41	1.72	0.54
1:2:1398:G:N1	1:2:1448:A:H2	1.98	0.54
27:I:178:ARG:HE	27:I:181:GLN:HG3	1.72	0.54
3:b:45:THR:OG1	3:b:82:LYS:NZ	2.40	0.54
4:B:124:HIS:HA	4:B:137:LEU:O	2.08	0.54
17:u:358:GLU:HG2	17:u:359:VAL:HG23	1.88	0.54
1:2:944:A:H61	1:2:982:G:H1	1.55	0.54
30:K:830:SER:OG	33:z:186:ARG:NH1	2.40	0.54
1:2:928:G:N2	3:b:68:GLY:O	2.37	0.54
1:2:922:A:OP1	16:W:28:ARG:NH2	2.41	0.54
1:2:1740:C:OP1	27:I:44:HIS:ND1	2.30	0.54
27:I:82:VAL:O	27:I:205:ARG:NH1	2.39	0.54
11:Z:61:GLU:HG2	11:Z:65:TYR:HE1	1.73	0.54
15:w:368:ARG:HG3	15:w:369:THR:HG23	1.90	0.54
30:K:1110:LYS:NZ	30:K:1115:ASP:OD2	2.41	0.54
31:M:61:TYR:HB3	32:f:103:LEU:HD21	1.89	0.54
1:2:145:G:O6	10:G:178:ARG:NH2	2.41	0.54
1:2:1536:G:H2'	1:2:1537:A:C8	2.43	0.54
17:u:612:GLU:OE2	17:u:669:LYS:NZ	2.41	0.54
25:L:119:ASP:O	25:L:147:LYS:NZ	2.40	0.54
8:F:102:LEU:HD11	11:Z:110:THR:HB	1.89	0.54
1:2:1050:A:OP1	1:2:1846:G:N2	2.36	0.54
1:2:1062:A:H4'	1:2:1853:C:H4'	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1302:G:O6	1:2:1307:U:O4	2.26	0.54
15:w:55:SER:HB2	30:K:1109:LEU:HG	1.88	0.54
17:u:597:VAL:HG23	17:u:685:MET:HB2	1.89	0.54
1:2:851:C:H5''	1:2:852:G:H5'	1.88	0.54
1:2:1606:G:H22	1:2:1632:G:H1'	1.72	0.54
3:b:12:PRO:HB3	9:H:192:PHE:HD2	1.73	0.53
27:I:98:LYS:NZ	27:I:176:ALA:O	2.33	0.53
28:r:24:ARG:NH1	28:r:25:LEU:O	2.41	0.53
30:K:837:LEU:HA	30:K:840:LEU:HD12	1.88	0.53
1:2:943:U:H2'	1:2:944:A:H8	1.74	0.53
1:2:1285:G:O6	31:M:82:ASN:ND2	2.41	0.53
4:B:35:ALA:HB3	4:B:42:ARG:HA	1.91	0.53
15:w:61:GLN:NE2	21:Q:20:THR:OG1	2.41	0.53
21:Q:16:LYS:HG3	21:Q:17:LYS:H	1.72	0.53
1:2:1275:G:O6	1:2:1324:G:N3	2.41	0.53
1:2:1348:G:O6	1:2:1381:G:O6	2.27	0.53
1:2:1536:G:H2'	1:2:1537:A:H8	1.72	0.53
30:K:574:ARG:NH1	30:K:575:ASP:OD1	2.41	0.53
10:G:135:PRO:HG2	10:G:141:ILE:HD13	1.91	0.53
14:X:11:ARG:NH2	25:L:104:LYS:O	2.41	0.53
1:2:1332:A:N6	1:2:1497:G:O6	2.42	0.53
15:w:231:TYR:HA	15:w:275:ALA:HB2	1.91	0.53
17:u:474:LYS:NZ	17:u:612:GLU:OE1	2.42	0.53
21:Q:116:ASP:OD2	21:Q:118:THR:OG1	2.26	0.53
30:K:112:ARG:NH2	30:K:120:ALA:O	2.41	0.53
1:2:1177:U:O2	1:2:1184:G:N2	2.33	0.53
20:S:13:LEU:HB2	20:S:20:ILE:HB	1.90	0.53
21:Q:11:GLN:HB3	30:K:1120:PHE:HB2	1.91	0.53
1:2:1562:C:H2'	1:2:1563:G:H8	1.72	0.53
1:2:1736:G:H2'	1:2:1737:G:C8	2.44	0.53
6:E:151:ASP:HA	10:G:212:LEU:HD21	1.90	0.53
1:2:197:U:H3	1:2:202:G:H1	1.58	0.52
22:P:56:LEU:HD23	22:P:83:MET:HE3	1.91	0.52
1:2:1289:U:OP2	32:f:95:ARG:NH1	2.42	0.52
6:E:161:GLN:O	6:E:170:THR:OG1	2.27	0.52
24:N:5:HIS:CD2	24:N:121:ARG:HE	2.27	0.52
29:q:114:GLY:HA2	29:q:154:VAL:HA	1.90	0.52
6:E:11:ARG:HA	6:E:28:ALA:HB2	1.90	0.52
7:e:31:ARG:HD3	26:J:127:ARG:HD3	1.92	0.52
15:w:334:TYR:HE1	15:w:339:SER:HB3	1.74	0.52
1:2:1681:U:O4	15:w:36:LYS:NZ	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:M:35:ILE:HG22	32:f:102:VAL:HG11	1.91	0.52
1:2:1212:G:OP1	15:w:30:ARG:NH2	2.35	0.52
1:2:160:U:O2'	1:2:162:C:OP2	2.26	0.52
20:S:71:MET:HE2	20:S:99:LEU:HD13	1.91	0.52
27:I:43:ILE:HG22	27:I:57:ALA:HA	1.91	0.52
1:2:943:U:H2'	1:2:944:A:C8	2.45	0.52
1:2:1367:U:O2	1:2:1373:C:C4	2.62	0.52
6:E:95:THR:HG22	12:Y:16:ARG:HB2	1.92	0.52
11:Z:79:ILE:HG23	11:Z:83:LEU:HD23	1.91	0.52
30:K:983:GLN:HG3	30:K:1023:LEU:HD13	1.91	0.52
1:2:115:U:OP1	1:2:382:C:O2'	2.26	0.52
1:2:1309:C:OP1	32:f:118:ARG:NE	2.42	0.52
1:2:1854:U:H2'	1:2:1855:G:H8	1.74	0.52
2:R:67:ARG:NH2	30:K:563:ASP:OD2	2.43	0.52
15:w:410:HIS:O	15:w:414:SER:OG	2.25	0.52
27:I:91:VAL:HG11	27:I:205:ARG:HH12	1.75	0.52
1:2:433:A:H5''	27:I:22:HIS:HB3	1.92	0.51
1:2:878:G:H1	1:2:908:A:H61	1.58	0.51
1:2:991:G:H1	1:2:1099:G:N2	2.08	0.51
3:b:3:LEU:HD22	16:W:22:LYS:HD3	1.91	0.51
22:P:81:ARG:NH2	22:P:120:SER:O	2.43	0.51
30:K:1024:LEU:HD12	30:K:1032:LEU:HD11	1.91	0.51
1:2:885:U:O2	1:2:902:G:C6	2.64	0.51
1:2:1228:A:H2'	1:2:1229:G:C8	2.45	0.51
1:2:1637:A:H5''	29:q:25:LYS:HE3	1.92	0.51
9:H:100:ILE:HD12	9:H:122:LEU:HD12	1.91	0.51
16:W:18:GLU:HB2	16:W:65:LEU:HD13	1.91	0.51
31:M:56:CYS:HG	31:M:61:TYR:HH	1.58	0.51
1:2:991:G:H1	1:2:1099:G:H21	1.59	0.51
15:w:254:LEU:HB3	15:w:290:ILE:HD11	1.92	0.51
21:Q:93:VAL:HG21	21:Q:120:LEU:HD21	1.91	0.51
30:K:108:SER:O	30:K:111:GLN:NE2	2.40	0.51
1:2:8:U:OP1	29:q:258:ARG:NH1	2.43	0.51
9:H:69:LEU:O	9:H:73:GLN:HG2	2.11	0.51
30:K:975:VAL:HA	30:K:978:LEU:HB2	1.92	0.51
31:M:32:ALA:HB1	31:M:37:GLU:HB3	1.91	0.51
1:2:1858:G:OP2	23:O:146:ARG:NH2	2.41	0.51
13:x:162:SER:HB3	23:O:107:THR:HG21	1.92	0.51
15:w:326:MET:HE1	15:w:345:LEU:HB3	1.91	0.51
27:I:106:SER:HB3	27:I:171:LEU:HG	1.91	0.51
1:2:49:C:H2'	1:2:472:C:H41	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:101:LEU:O	9:H:116:ARG:NH1	2.42	0.51
1:2:391:C:H2'	1:2:392:A:H8	1.76	0.51
1:2:812:A:H5'	6:E:16:LYS:HD2	1.92	0.51
9:H:145:ARG:HD2	16:W:51:GLU:HB2	1.91	0.51
30:K:421:VAL:HA	30:K:424:LEU:HD12	1.93	0.51
1:2:980:A:H2'	1:2:981:A:C8	2.46	0.51
6:E:80:ILE:HG13	6:E:81:THR:HG23	1.93	0.51
17:u:648:MET:HE3	17:u:650:LEU:HD21	1.91	0.51
26:J:19:PRO:O	26:J:24:ARG:NH2	2.44	0.51
29:q:250:ALA:HA	29:q:253:LEU:HD12	1.92	0.51
1:2:1478:U:OP1	30:K:874:ARG:NH1	2.43	0.51
11:Z:50:PHE:HB2	20:S:4:VAL:HA	1.92	0.50
17:u:262:PRO:HA	17:u:270:GLY:HA3	1.93	0.50
30:K:535:VAL:HG12	30:K:572:VAL:HG11	1.93	0.50
1:2:1332:A:C6	1:2:1497:G:C6	2.99	0.50
6:E:100:ARG:NH2	6:E:121:TYR:O	2.39	0.50
29:q:191:TYR:HB3	29:q:194:SER:HB2	1.92	0.50
1:2:1598:G:H5''	11:Z:80:ARG:HH21	1.75	0.50
2:R:72:LYS:HD2	30:K:1073:ILE:HG21	1.94	0.50
19:T:22:LEU:HD23	19:T:28:LEU:HD11	1.94	0.50
21:Q:9:SER:HB3	21:Q:26:LYS:HD3	1.93	0.50
1:2:367:U:H4'	1:2:371:A:C8	2.47	0.50
1:2:1454:A:H8	1:2:1455:A:H62	1.59	0.50
22:P:95:GLY:HA2	22:P:103:ASN:O	2.11	0.50
28:r:116:MET:HG3	29:q:110:PRO:HG3	1.92	0.50
30:K:633:PRO:HB2	30:K:636:VAL:HB	1.92	0.50
30:K:869:VAL:O	30:K:874:ARG:NH2	2.42	0.50
15:w:399:GLU:HA	15:w:402:LEU:HD12	1.92	0.50
17:u:124:LEU:HB3	17:u:133:TRP:HB2	1.92	0.50
1:2:1367:U:C2	1:2:1373:C:N3	2.80	0.50
1:2:1707:U:H3	1:2:1827:U:H3	1.57	0.50
7:e:36:MET:SD	7:e:40:ARG:NH1	2.85	0.50
30:K:334:MET:HE2	30:K:345:ALA:HB3	1.93	0.50
1:2:1161:U:O4	14:X:2:GLY:N	2.45	0.50
13:x:105:LEU:HD11	13:x:130:LEU:HA	1.94	0.50
1:2:1033:G:H1	1:2:1080:A:HO2'	1.60	0.50
16:W:69:LEU:HD11	16:W:129:PHE:HB2	1.94	0.50
21:Q:19:ALA:HB2	21:Q:75:GLY:HA3	1.94	0.50
8:F:104:THR:HG23	8:F:106:GLU:H	1.77	0.49
15:w:247:GLN:O	15:w:251:ASN:ND2	2.45	0.49
17:u:592:SER:OG	17:u:593:VAL:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:42:VAL:O	23:O:55:ARG:CA	2.47	0.49
29:q:249:ARG:NH2	29:q:270:THR:O	2.45	0.49
23:O:133:THR:HG23	23:O:135:ILE:HG13	1.94	0.49
30:K:510:ARG:HA	30:K:513:LEU:HD12	1.94	0.49
1:2:1597:C:OP2	11:Z:85:ARG:NH2	2.46	0.49
2:R:30:THR:HG22	2:R:33:ARG:HH21	1.78	0.49
17:u:698:VAL:HA	17:u:767:MET:O	2.13	0.49
1:2:1776:G:H2'	1:2:1777:G:H8	1.77	0.49
20:S:30:ILE:HG22	20:S:36:VAL:HG11	1.94	0.49
2:R:5:ARG:HB3	2:R:10:LYS:HE3	1.93	0.49
3:b:38:PRO:HD3	3:b:77:CYS:HA	1.95	0.49
9:H:27:LEU:HD23	9:H:40:LEU:HD11	1.93	0.49
9:H:66:VAL:HA	9:H:69:LEU:HD23	1.94	0.49
10:G:142:ARG:HG2	10:G:147:LEU:HB2	1.94	0.49
15:w:65:GLN:OE1	21:Q:11:GLN:NE2	2.37	0.49
15:w:66:GLN:NE2	21:Q:11:GLN:OE1	2.41	0.49
15:w:334:TYR:HA	15:w:338:ASN:HD21	1.76	0.49
30:K:498:PHE:HD1	30:K:509:MET:HE2	1.76	0.49
30:K:993:SER:HB2	30:K:996:MET:HB3	1.95	0.49
32:f:123:SER:HB3	32:f:146:LEU:HD11	1.94	0.49
1:2:953:C:O2	23:O:55:ARG:NH2	2.46	0.49
1:2:1213:C:OP2	15:w:34:ARG:NH1	2.45	0.49
1:2:1473:G:N2	1:2:1476:A:OP2	2.37	0.49
1:2:1685:U:H2'	1:2:1686:G:C8	2.48	0.49
17:u:290:HIS:HA	17:u:296:ASP:HA	1.95	0.49
29:q:26:TYR:CE2	29:q:64:THR:HG23	2.48	0.49
1:2:201:C:H3'	1:2:202:G:H8	1.77	0.49
1:2:674:C:H2'	1:2:675:U:C6	2.48	0.49
17:u:598:VAL:HB	17:u:680:ALA:HB1	1.95	0.49
26:J:136:ARG:HG2	26:J:160:SER:H	1.77	0.49
30:K:472:PHE:HA	30:K:475:VAL:HG12	1.95	0.49
1:2:671:A:O2'	1:2:1089:G:OP2	2.29	0.49
1:2:1144:A:H2'	1:2:1145:A:C8	2.48	0.49
1:2:1275:G:O6	1:2:1324:G:N2	2.45	0.49
9:H:68:GLN:O	9:H:71:SER:OG	2.25	0.49
13:x:227:ASN:HA	13:x:230:LEU:HG	1.94	0.49
30:K:863:ILE:O	30:K:866:THR:OG1	2.26	0.49
6:E:88:ASP:OD1	6:E:122:LYS:NZ	2.45	0.49
17:u:89:PRO:HA	17:u:159:LEU:HB2	1.95	0.49
1:2:981:A:H2'	1:2:982:G:C8	2.48	0.49
8:F:167:LYS:NZ	8:F:175:ASP:OD2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:q:26:TYR:CE2	29:q:64:THR:CG2	2.96	0.48
30:K:928:LEU:HD23	30:K:968:VAL:HG12	1.95	0.48
10:G:45:TRP:HA	10:G:48:TYR:HD2	1.78	0.48
1:2:1685:U:H2'	1:2:1686:G:H8	1.79	0.48
11:Z:99:LEU:HD12	11:Z:109:TYR:HE1	1.78	0.48
28:r:6:HIS:HA	28:r:9:LEU:HD12	1.95	0.48
1:2:1736:G:H2'	1:2:1737:G:H8	1.76	0.48
1:2:1036:A:N3	1:2:1844:U:O2'	2.47	0.48
1:2:1648:G:N2	1:2:1675:A:OP2	2.32	0.48
13:x:169:LYS:HA	23:O:142:ARG:HH22	1.79	0.48
1:2:570:C:O2'	12:Y:34:THR:O	2.26	0.48
12:Y:86:GLU:OE2	12:Y:90:ARG:NE	2.36	0.48
17:u:69:LEU:HG	17:u:73:ARG:HE	1.78	0.48
30:K:652:SER:O	30:K:658:ARG:NH2	2.39	0.48
30:K:780:LEU:O	30:K:788:GLN:NE2	2.41	0.48
1:2:1286:G:H2'	1:2:1312:G:H22	1.78	0.48
4:B:181:LEU:HA	4:B:184:VAL:HB	1.94	0.48
17:u:483:MET:HE3	17:u:484:PHE:CE2	2.48	0.48
19:T:140:ALA:HA	19:T:144:LYS:HD3	1.94	0.48
23:O:42:VAL:HG11	23:O:81:VAL:HG11	1.96	0.48
30:K:909:GLY:HA2	30:K:916:MET:HE1	1.95	0.48
8:F:19:LEU:HB3	8:F:23:TRP:HB2	1.95	0.48
16:W:45:GLY:O	16:W:68:ARG:NH1	2.46	0.48
29:q:183:PHE:HB3	29:q:204:LEU:HD22	1.96	0.48
1:2:385:G:H3'	25:L:136:LYS:HB2	1.96	0.48
1:2:1722:G:O6	1:2:1812:U:O2	2.31	0.48
20:S:90:VAL:HG21	20:S:113:ARG:HH12	1.78	0.48
29:q:202:LEU:HD23	29:q:204:LEU:HD11	1.95	0.48
1:2:145:G:H2'	1:2:146:G:C8	2.48	0.48
1:2:1472:C:OP2	30:K:834:ARG:NH2	2.47	0.48
4:B:127:VAL:HG11	4:B:176:VAL:HG11	1.95	0.48
5:c:54:ASP:OD1	8:F:38:TYR:OH	2.31	0.48
19:T:11:GLN:OE1	19:T:62:ARG:NH1	2.38	0.48
25:L:136:LYS:O	25:L:139:ARG:NH1	2.46	0.48
28:r:42:VAL:HA	28:r:45:MET:HE2	1.95	0.48
30:K:113:PHE:HD1	30:K:127:VAL:HG21	1.79	0.48
1:2:8:U:H3	1:2:1196:A:H62	1.62	0.47
1:2:383:G:O2'	25:L:133:PRO:O	2.29	0.47
2:R:36:GLU:OE2	2:R:47:ARG:NH1	2.47	0.47
9:H:79:LEU:HD22	9:H:94:PHE:HZ	1.78	0.47
13:x:99:ILE:O	13:x:104:GLY:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:u:162:PRO:HB3	17:u:192:ILE:HD13	1.95	0.47
27:I:76:THR:HG21	27:I:104:ILE:HD12	1.96	0.47
1:2:913:A:H1'	9:H:66:VAL:HB	1.96	0.47
1:2:1030:A:H2'	1:2:1031:A:H8	1.80	0.47
1:2:1588:A:H2'	1:2:1589:A:C8	2.49	0.47
10:G:211:LYS:HB3	10:G:211:LYS:HE2	1.75	0.47
10:G:225:GLN:HA	10:G:228:ILE:HG22	1.96	0.47
15:w:185:TYR:HA	15:w:188:VAL:HG22	1.95	0.47
15:w:262:VAL:HG11	15:w:304:GLU:HG2	1.96	0.47
17:u:350:GLY:HA2	17:u:353:GLU:HB3	1.96	0.47
30:K:245:THR:HG21	30:K:310:LEU:HD11	1.94	0.47
30:K:353:PHE:O	30:K:356:ARG:NH1	2.46	0.47
1:2:1685:U:O3'	30:K:1195:LEU:HD11	2.15	0.47
12:Y:36:PRO:HG2	12:Y:39:GLU:HG3	1.96	0.47
17:u:100:MET:HE2	17:u:137:SER:HB3	1.96	0.47
30:K:264:LEU:HD11	30:K:284:THR:HG21	1.96	0.47
27:I:79:ILE:HB	27:I:103:LEU:HD12	1.96	0.47
1:2:1037:G:N2	1:2:1079:C:C2	2.83	0.47
1:2:1227:G:C6	1:2:1531:A:N1	2.82	0.47
13:x:194:ILE:O	13:x:198:THR:OG1	2.29	0.47
17:u:396:GLY:HA3	22:P:104:GLN:HB3	1.96	0.47
1:2:153:G:H21	10:G:13:GLN:HE22	1.61	0.47
1:2:955:A:N1	1:2:968:U:O2'	2.45	0.47
9:H:29:GLU:HA	9:H:32:MET:HE2	1.95	0.47
4:B:108:ASP:OD2	13:x:77:LYS:NZ	2.45	0.47
4:B:123:ALA:HB2	4:B:165:ARG:HG3	1.96	0.47
4:B:164:ILE:O	4:B:168:MET:HG2	2.14	0.47
8:F:28:VAL:O	8:F:42:LYS:NZ	2.47	0.47
17:u:285:VAL:HG12	17:u:346:LYS:HE2	1.96	0.47
28:r:12:HIS:HB3	29:q:110:PRO:HB3	1.97	0.47
1:2:28:U:H2'	1:2:29:G:H8	1.79	0.47
1:2:885:U:O2	1:2:901:G:C6	2.68	0.47
17:u:521:PRO:HD3	17:u:774:PHE:CE2	2.49	0.47
29:q:60:ILE:HD13	29:q:60:ILE:HA	1.69	0.47
1:2:1486:A:OP1	30:K:1030:ARG:NH2	2.47	0.47
17:u:285:VAL:HG23	17:u:299:MET:HE2	1.97	0.47
32:f:141:CYS:HB3	32:f:146:LEU:HB2	1.96	0.47
1:2:223:C:H2'	1:2:224:A:C8	2.50	0.47
27:I:203:LYS:HA	27:I:206:LYS:HE3	1.96	0.47
1:2:107:A:H2'	1:2:108:G:C8	2.50	0.46
19:T:14:PHE:HE1	19:T:134:ILE:HG23	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:I:83:TYR:HB3	27:I:101:ILE:HB	1.97	0.46
1:2:1172:U:H2'	1:2:1173:A:C8	2.51	0.46
1:2:1331:C:H2'	1:2:1332:A:C8	2.51	0.46
10:G:19:ASP:OD1	10:G:19:ASP:N	2.48	0.46
28:r:109:ILE:HG12	28:r:114:PRO:HG3	1.97	0.46
30:K:171:LEU:O	30:K:175:LEU:HB2	2.16	0.46
30:K:535:VAL:HG11	30:K:568:TRP:HZ3	1.80	0.46
1:2:1076:G:O6	1:2:1077:A:N6	2.49	0.46
1:2:1334:G:H2'	1:2:1335:G:H8	1.80	0.46
21:Q:26:LYS:HZ3	21:Q:27:ARG:HH21	1.64	0.46
16:W:87:GLU:OE2	16:W:117:ARG:NH1	2.48	0.46
28:r:116:MET:HE2	29:q:110:PRO:HD3	1.97	0.46
9:H:57:ARG:HH22	9:H:172:THR:HB	1.81	0.46
20:S:97:GLN:HG3	20:S:99:LEU:HD21	1.97	0.46
1:2:857:U:H2'	1:2:858:A:C8	2.51	0.46
1:2:1759:G:H2'	1:2:1760:G:C8	2.51	0.46
2:R:24:LEU:HD13	2:R:34:VAL:HG21	1.96	0.46
1:2:983:A:OP1	1:2:1073:U:O2'	2.25	0.46
20:S:39:ARG:HG3	20:S:83:PHE:HZ	1.80	0.46
1:2:659:G:O2'	1:2:662:G:O2'	2.25	0.46
1:2:1232:U:H2'	1:2:1233:G:H8	1.81	0.46
1:2:1674:G:OP1	8:F:51:HIS:NE2	2.34	0.46
12:Y:114:MET:O	12:Y:122:LYS:NZ	2.46	0.46
15:w:255:LEU:HD13	15:w:290:ILE:HG23	1.97	0.46
27:I:151:GLU:HA	27:I:154:LYS:HG3	1.98	0.46
1:2:658:U:N3	14:X:20:GLN:O	2.42	0.46
1:2:1776:G:H2'	1:2:1777:G:C8	2.50	0.46
4:B:25:PHE:HA	4:B:28:LYS:HG2	1.98	0.46
8:F:47:LYS:NZ	21:Q:115:TYR:O	2.49	0.46
10:G:162:LEU:HB2	10:G:170:ARG:O	2.15	0.46
27:I:84:ASN:HD22	27:I:90:LEU:HB2	1.81	0.46
20:S:3:LEU:HB3	20:S:4:VAL:H	1.58	0.45
27:I:148:LYS:HD3	27:I:152:ARG:HH21	1.81	0.45
1:2:975:G:OP1	23:O:98:ARG:NH1	2.43	0.45
4:B:33:VAL:HG13	4:B:44:ILE:HG13	1.98	0.45
11:Z:99:LEU:HA	11:Z:109:TYR:HD1	1.80	0.45
30:K:638:ILE:O	30:K:641:LYS:NZ	2.49	0.45
1:2:1010:G:H2'	1:2:1011:A:C8	2.51	0.45
8:F:42:LYS:HG3	8:F:43:GLU:OE1	2.16	0.45
17:u:563:SER:OG	17:u:564:GLU:N	2.49	0.45
32:f:119:ARG:HH12	32:f:122:PRO:HD3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:85:ARG:O	10:G:87:ARG:NH1	2.50	0.45
27:I:172:LEU:HB3	27:I:190:LEU:HD12	1.98	0.45
30:K:127:VAL:HG12	30:K:131:VAL:HG21	1.99	0.45
24:N:92:ILE:O	24:N:96:VAL:HG23	2.15	0.45
31:M:71:GLU:HG3	32:f:114:ILE:HG23	1.99	0.45
1:2:749:U:C4	1:2:750:C:N4	2.84	0.45
1:2:1367:U:H3	1:2:1373:C:N4	2.14	0.45
1:2:1839:U:O2	17:u:13:ASN:ND2	2.48	0.45
10:G:25:ARG:HH11	10:G:28:TYR:HD2	1.62	0.45
13:x:76:ARG:HH12	23:O:129:ILE:HD11	1.82	0.45
14:X:67:ARG:HD2	14:X:67:ARG:HA	1.78	0.45
21:Q:98:LYS:HE2	30:K:1119:ASN:HD22	1.81	0.45
1:2:8:U:H3	1:2:1196:A:N6	2.15	0.45
1:2:1004:U:H2'	1:2:1005:G:H8	1.81	0.45
15:w:222:PRO:HA	15:w:225:TRP:CZ3	2.50	0.45
30:K:187:PHE:HD1	30:K:220:LEU:HD11	1.82	0.45
30:K:210:LEU:HA	30:K:213:VAL:HG12	1.99	0.45
30:K:730:ASN:ND2	30:K:765:ASP:OD1	2.45	0.45
1:2:1560:U:H2'	1:2:1561:A:H8	1.82	0.45
10:G:50:VAL:HG21	10:G:111:LEU:HD12	1.99	0.45
15:w:352:LEU:HD23	15:w:357:LEU:HD12	1.97	0.45
28:r:17:GLY:HA2	28:r:18:SER:HA	1.61	0.45
30:K:865:CYS:HA	30:K:868:GLU:HB2	1.98	0.45
33:z:115:TRP:HE3	33:z:118:LYS:HE3	1.80	0.45
1:2:47:G:O2'	17:u:65:LYS:NZ	2.43	0.45
1:2:1331:C:N4	1:2:1499:U:H3	2.14	0.45
19:T:104:LEU:HD13	19:T:121:ARG:HD3	1.99	0.45
22:P:42:ARG:O	22:P:46:ASN:ND2	2.39	0.45
1:2:615:C:N4	17:u:738:ARG:HH12	2.15	0.44
1:2:962:A:N1	1:2:1055:A:O2'	2.48	0.44
1:2:1064:C:H2'	1:2:1065:G:H8	1.82	0.44
8:F:20:PHE:HB2	8:F:23:TRP:HD1	1.82	0.44
17:u:707:PHE:HB2	17:u:710:MET:HB3	1.99	0.44
21:Q:68:ILE:HD12	21:Q:88:ILE:HG12	1.99	0.44
1:2:1174:U:H2'	1:2:1175:G:H8	1.82	0.44
2:R:27:ASP:OD1	2:R:27:ASP:N	2.48	0.44
17:u:591:MET:HA	17:u:657:PRO:HA	1.98	0.44
30:K:619:GLN:HA	30:K:622:MET:HG3	1.99	0.44
30:K:928:LEU:HD12	30:K:935:MET:HE3	1.98	0.44
30:K:947:VAL:HA	30:K:950:LEU:HD12	1.98	0.44
1:2:1679:A:H2'	8:F:60:ARG:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:77:MET:HG3	8:F:89:THR:HG21	1.99	0.44
13:x:84:ARG:HA	13:x:84:ARG:HD2	1.71	0.44
17:u:542:LYS:HA	17:u:545:GLU:HG2	1.99	0.44
26:J:60:LEU:HD22	26:J:70:ARG:HA	1.98	0.44
27:I:178:ARG:HA	27:I:179:PRO:HD3	1.82	0.44
29:q:199:LYS:HA	29:q:199:LYS:HD3	1.83	0.44
1:2:1669:G:H5'	21:Q:130:LYS:HB2	2.00	0.44
1:2:1780:G:H2'	1:2:1781:A:C8	2.52	0.44
27:I:62:VAL:HG22	27:I:77:ARG:HG2	1.99	0.44
30:K:108:SER:HB3	30:K:111:GLN:HE21	1.83	0.44
30:K:332:ARG:O	30:K:335:THR:OG1	2.24	0.44
30:K:725:ASP:OD1	30:K:725:ASP:N	2.51	0.44
32:f:107:LYS:O	32:f:114:ILE:N	2.50	0.44
32:f:121:CYS:HB2	32:f:146:LEU:HD12	1.99	0.44
1:2:124:U:OP1	10:G:201:LYS:NZ	2.38	0.44
1:2:125:C:OP1	10:G:202:ASN:ND2	2.47	0.44
1:2:913:A:H2	9:H:99:ARG:H	1.63	0.44
1:2:1264:C:O2'	1:2:1265:A:O5'	2.35	0.44
13:x:169:LYS:HB3	23:O:149:ARG:CZ	2.47	0.44
29:q:44:LEU:HD21	29:q:76:HIS:HD2	1.81	0.44
30:K:585:PHE:O	30:K:589:PHE:HB2	2.18	0.44
31:M:43:ASP:OD2	32:f:106:TYR:OH	2.35	0.44
1:2:1101:U:H2'	1:2:1102:G:C8	2.53	0.44
1:2:1172:U:H2'	1:2:1173:A:H8	1.82	0.44
1:2:1609:C:H42	1:2:1630:A:H61	0.70	0.44
15:w:328:LYS:HB2	18:t:266:PHE:HE2	1.82	0.44
16:W:111:MET:HE2	16:W:111:MET:HB3	1.94	0.44
17:u:601:ASP:OD1	17:u:601:ASP:N	2.51	0.44
1:2:1758:G:H2'	1:2:1759:G:C8	2.52	0.44
23:O:95:ILE:HG21	23:O:116:LEU:HD13	2.00	0.44
25:L:111:VAL:HG11	25:L:128:VAL:HG11	1.99	0.44
30:K:585:PHE:HA	30:K:589:PHE:HD2	1.82	0.44
1:2:682:U:O2'	16:W:4:MET:SD	2.76	0.44
15:w:280:LEU:HD13	15:w:286:TRP:CE3	2.53	0.44
27:I:178:ARG:NE	27:I:181:GLN:HG3	2.31	0.44
30:K:142:GLU:HA	30:K:143:THR:HA	1.58	0.44
10:G:136:LYS:NZ	10:G:175:LYS:O	2.40	0.44
15:w:63:ARG:NH2	30:K:381:GLU:OE1	2.50	0.44
15:w:208:PRO:HD3	15:w:237:PHE:HE1	1.83	0.44
15:w:269:ASN:OD1	15:w:270:PHE:N	2.50	0.44
15:w:401:LEU:HA	15:w:404:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1279:C:H2'	1:2:1280:G:C8	2.53	0.43
1:2:1465:A:OP1	2:R:60:ARG:NH1	2.51	0.43
4:B:219:LYS:NZ	4:B:220:LYS:O	2.51	0.43
8:F:42:LYS:HD3	8:F:42:LYS:HA	1.88	0.43
10:G:50:VAL:HG12	10:G:113:ILE:HA	2.00	0.43
10:G:52:ILE:HD13	10:G:102:VAL:HG21	2.00	0.43
13:x:136:PHE:HB2	13:x:153:ILE:HD11	1.99	0.43
29:q:16:LEU:HD23	29:q:16:LEU:HA	1.82	0.43
29:q:78:TRP:HH2	29:q:96:ILE:HD12	1.83	0.43
29:q:83:ILE:HD12	29:q:83:ILE:HA	1.78	0.43
1:2:115:U:H2'	1:2:116:U:C6	2.53	0.43
1:2:118:C:H1'	1:2:445:A:C5	2.53	0.43
1:2:818:A:OP1	26:J:80:ARG:NH2	2.52	0.43
1:2:1545:A:H2'	1:2:1546:G:C8	2.54	0.43
20:S:25:LYS:HB2	20:S:28:PHE:HD2	1.83	0.43
25:L:111:VAL:HG12	25:L:140:PHE:HB2	2.00	0.43
1:2:56:G:OP2	12:Y:115:LYS:NZ	2.45	0.43
1:2:292:A:O2'	25:L:39:ASN:O	2.36	0.43
1:2:600:G:C5	29:q:272:TYR:HB3	2.54	0.43
1:2:640:A:H2'	1:2:641:A:C8	2.54	0.43
1:2:1286:G:N2	1:2:1312:G:O2'	2.50	0.43
1:2:1643:U:H2'	1:2:1644:C:C6	2.53	0.43
13:x:129:ALA:HA	13:x:132:LYS:HB2	1.99	0.43
14:X:67:ARG:HE	14:X:84:PHE:HE1	1.66	0.43
27:I:141:ARG:HG3	27:I:146:GLN:HB3	1.99	0.43
1:2:122:G:H21	6:E:146:THR:HG21	1.82	0.43
1:2:1283:C:O2'	1:2:1313:A:N1	2.47	0.43
3:b:67:THR:OG1	3:b:70:LYS:O	2.36	0.43
6:E:19:MET:SD	6:E:108:ARG:HD2	2.59	0.43
14:X:52:LEU:HD11	14:X:73:GLN:HB2	2.00	0.43
15:w:277:LYS:HB3	15:w:277:LYS:HE2	1.84	0.43
15:w:370:GLU:O	15:w:408:GLN:NE2	2.51	0.43
22:P:57:LEU:HD21	22:P:86:LEU:HD12	2.00	0.43
23:O:19:PRO:HG2	23:O:27:VAL:HG21	2.00	0.43
1:2:374:G:OP1	25:L:59:LYS:NZ	2.46	0.43
1:2:928:G:H2'	1:2:929:G:C8	2.54	0.43
1:2:1333:U:H2'	1:2:1495:G:H1	1.83	0.43
1:2:1348:G:N7	1:2:1381:G:N1	2.59	0.43
1:2:1606:G:H5'	19:T:86:GLY:HA2	2.01	0.43
1:2:1854:U:H2'	1:2:1855:G:C8	2.53	0.43
4:B:108:ASP:OD1	4:B:109:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:59:GLN:OE1	10:G:72:ARG:NH1	2.49	0.43
13:x:169:LYS:HB3	23:O:149:ARG:NH1	2.33	0.43
12:Y:7:ILE:HD13	12:Y:27:VAL:HG22	2.00	0.43
1:2:155:G:H4'	10:G:15:LEU:HD13	2.00	0.43
1:2:951:C:H2'	1:2:952:G:H8	1.82	0.43
4:B:167:LYS:HB2	4:B:167:LYS:HE2	1.71	0.43
10:G:152:ASP:OD2	10:G:155:GLN:N	2.51	0.43
13:x:108:ARG:NH1	13:x:119:ARG:HH12	2.17	0.43
13:x:199:ARG:HD3	15:w:23:ILE:HG12	2.01	0.43
23:O:56:VAL:HG23	23:O:77:ALA:HB1	1.99	0.43
1:2:1276:A:N1	1:2:1322:G:N2	2.67	0.43
10:G:126:ASP:OD1	10:G:126:ASP:N	2.50	0.43
15:w:323:SER:HB2	15:w:356:VAL:HG21	2.00	0.43
17:u:85:VAL:HG13	17:u:155:THR:HG23	2.01	0.43
29:q:128:LEU:HD23	29:q:128:LEU:HA	1.86	0.43
1:2:671:A:H4'	1:2:672:A:H5''	2.00	0.43
1:2:1189:A:H2'	1:2:1190:A:C8	2.54	0.43
1:2:1367:U:C2	1:2:1373:C:C4	3.07	0.43
6:E:179:ASN:OD1	6:E:231:GLY:N	2.49	0.43
13:x:158:LEU:HD21	15:w:19:LEU:HD23	2.01	0.43
18:t:349:ASP:OD1	18:t:349:ASP:N	2.52	0.43
19:T:51:ASN:HB3	19:T:54:TYR:HD2	1.83	0.43
29:q:131:ALA:HB2	29:q:138:PRO:HD3	2.01	0.43
1:2:798:G:O2'	9:H:108:SER:OG	2.21	0.43
1:2:944:A:H5''	23:O:134:PRO:HB3	2.00	0.43
2:R:62:GLN:HB3	30:K:620:TRP:HZ3	1.82	0.43
10:G:5:ILE:HG13	10:G:111:LEU:HD21	2.01	0.43
16:W:30:CYS:SG	16:W:31:SER:N	2.92	0.43
22:P:83:MET:HB3	22:P:116:LEU:HD12	1.99	0.43
30:K:467:SER:O	30:K:471:MET:HG2	2.18	0.43
1:2:544:G:H2'	1:2:545:A:C8	2.54	0.42
1:2:909:G:H2'	1:2:910:G:C8	2.55	0.42
1:2:1471:C:O3'	30:K:793:ARG:NH1	2.52	0.42
13:x:246:SER:OG	13:x:247:ARG:NH1	2.52	0.42
15:w:88:ARG:HH11	15:w:90:GLY:H	1.67	0.42
16:W:103:VAL:N	16:W:127:GLY:O	2.33	0.42
17:u:527:ILE:HB	17:u:592:SER:HA	2.00	0.42
17:u:668:PHE:HB3	17:u:676:HIS:HB3	2.01	0.42
30:K:710:ARG:NH1	30:K:752:SER:OG	2.47	0.42
1:2:604:A:H2'	1:2:605:A:C8	2.54	0.42
1:2:1606:G:N2	1:2:1632:G:H1'	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:20:ASP:HB3	10:G:23:LYS:HD3	2.01	0.42
13:x:223:THR:HG23	23:O:151:LEU:HG	2.01	0.42
20:S:26:ILE:HA	20:S:56:ALA:HB2	2.01	0.42
30:K:338:HIS:CE1	30:K:340:LEU:HB2	2.54	0.42
1:2:220:U:H2'	1:2:221:A:C8	2.55	0.42
1:2:797:C:O2'	1:2:798:G:O4'	2.36	0.42
1:2:1725:U:H2'	1:2:1726:G:H8	1.84	0.42
4:B:134:LEU:HB3	4:B:219:LYS:HB3	2.01	0.42
12:Y:25:ILE:HD11	12:Y:73:GLY:HA3	2.02	0.42
17:u:91:HIS:CE1	17:u:93:ARG:HE	2.37	0.42
34:q:301:SAH:HG2	34:q:301:SAH:H4'	1.51	0.42
30:K:998:ARG:HG3	30:K:1001:ARG:HH21	1.84	0.42
1:2:68:A:OP2	10:G:164:LYS:NZ	2.40	0.42
8:F:203:ASN:HA	29:q:134:LYS:HG2	2.01	0.42
13:x:93:MET:HA	13:x:96:PHE:CE1	2.55	0.42
15:w:88:ARG:HH12	30:K:324:LYS:HE2	1.83	0.42
21:Q:109:LYS:O	21:Q:113:ILE:HG12	2.19	0.42
27:I:123:ARG:NH2	27:I:133:GLU:OE2	2.52	0.42
28:r:7:ASN:HD21	28:r:53:ALA:C	2.27	0.42
1:2:530:U:H2'	1:2:531:A:C8	2.53	0.42
30:K:901:CYS:HA	30:K:904:VAL:HG22	2.02	0.42
1:2:941:C:H2'	1:2:942:G:C8	2.54	0.42
1:2:1113:A:H5''	1:2:1114:U:H4'	2.02	0.42
4:B:88:THR:HA	4:B:98:THR:HA	2.02	0.42
9:H:80:VAL:HG13	9:H:92:VAL:HB	2.01	0.42
13:x:91:ASN:HD22	13:x:140:PHE:HZ	1.65	0.42
17:u:628:LEU:HD11	17:u:774:PHE:C	2.45	0.42
17:u:693:VAL:HB	17:u:773:VAL:HG23	2.02	0.42
4:B:87:ILE:HG22	4:B:101:HIS:HB2	2.01	0.42
4:B:149:GLN:NE2	4:B:154:SER:OG	2.52	0.42
11:Z:72:VAL:O	11:Z:76:ARG:HG2	2.20	0.42
15:w:244:ARG:NH2	15:w:247:GLN:OE1	2.48	0.42
17:u:520:LEU:HD22	17:u:524:TYR:CD2	2.55	0.42
22:P:93:MET:HE1	22:P:106:GLU:OE1	2.20	0.42
1:2:163:U:H2'	1:2:164:A:H8	1.85	0.42
1:2:375:U:H2'	1:2:376:A:C8	2.54	0.42
1:2:1293:A:O4'	32:f:138:ARG:NH1	2.53	0.42
1:2:1502:C:HO2'	17:u:762:GLN:NE2	2.17	0.42
2:R:78:ARG:HD3	2:R:81:ARG:HH21	1.85	0.42
8:F:163:PHE:HE2	8:F:164:ARG:HH21	1.67	0.42
11:Z:61:GLU:HG2	11:Z:65:TYR:CE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:x:183:ILE:HA	13:x:228:LEU:HD13	2.01	0.42
1:2:798:G:H8	1:2:799:U:H5'	1.84	0.42
1:2:1013:U:OP1	1:2:1129:G:O2'	2.36	0.42
1:2:1289:U:H2'	1:2:1290:G:C8	2.55	0.42
1:2:1325:G:O2'	1:2:1327:G:OP2	2.35	0.42
1:2:1523:C:H2'	1:2:1524:G:H8	1.85	0.42
4:B:52:THR:HG22	4:B:54:GLY:H	1.84	0.42
7:e:38:TYR:CG	26:J:33:GLY:HA3	2.55	0.42
12:Y:5:VAL:HG12	12:Y:29:HIS:HB3	2.02	0.42
13:x:74:GLU:OE2	23:O:125:LYS:NZ	2.43	0.42
17:u:288:LEU:HB2	17:u:584:LEU:HD12	2.01	0.42
17:u:476:LYS:HB3	17:u:476:LYS:HE3	1.80	0.42
23:O:32:HIS:NE2	23:O:45:THR:OG1	2.46	0.42
28:r:85:HIS:CD2	28:r:89:LEU:HD12	2.55	0.42
1:2:1004:U:H2'	1:2:1005:G:C8	2.55	0.42
13:x:228:LEU:HG	13:x:237:VAL:HG11	2.02	0.42
20:S:67:VAL:O	20:S:71:MET:HG3	2.20	0.42
1:2:71:G:H2'	1:2:72:C:O4'	2.20	0.41
1:2:508:A:H3'	1:2:509:G:H8	1.85	0.41
1:2:604:A:H5''	26:J:22:LYS:HG2	2.02	0.41
1:2:1394:G:OP2	1:2:1394:G:N2	2.33	0.41
1:2:1717:C:H2'	1:2:1718:G:O4'	2.20	0.41
2:R:15:VAL:HG21	30:K:1146:PHE:HE2	1.85	0.41
2:R:17:ILE:HD11	2:R:54:VAL:HG23	2.02	0.41
30:K:903:LEU:HD11	30:K:935:MET:HG3	2.01	0.41
31:M:21:VAL:HA	31:M:24:THR:HG22	2.01	0.41
32:f:100:LEU:HD13	32:f:103:LEU:HD22	2.03	0.41
1:2:17:C:O2'	1:2:1194:A:N1	2.47	0.41
1:2:28:U:H2'	1:2:29:G:C8	2.55	0.41
1:2:126:G:H8	10:G:199:THR:HG21	1.84	0.41
1:2:900:C:H2'	1:2:901:G:H8	1.85	0.41
1:2:1279:C:H2'	1:2:1280:G:H8	1.86	0.41
6:E:136:ILE:HG23	6:E:149:TYR:CE1	2.55	0.41
1:2:352:U:H2'	1:2:353:C:C6	2.56	0.41
1:2:1023:A:H5''	24:N:4:MET:HE2	2.03	0.41
2:R:66:VAL:HG21	30:K:618:LEU:HD23	2.02	0.41
6:E:45:ILE:HG13	6:E:61:VAL:HG21	2.02	0.41
17:u:666:LEU:HD23	17:u:666:LEU:HA	1.87	0.41
30:K:304:THR:HA	30:K:307:MET:HE2	2.02	0.41
1:2:453:C:O2'	10:G:92:ARG:O	2.33	0.41
1:2:544:G:H2'	1:2:545:A:H8	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1228:A:H2'	1:2:1229:G:H8	1.84	0.41
17:u:156:ILE:HG13	17:u:183:PRO:HG2	2.02	0.41
22:P:108:LYS:HB2	22:P:111:MET:HG3	2.01	0.41
23:O:116:LEU:HD11	23:O:126:ILE:HD11	2.03	0.41
29:q:88:LEU:HD23	29:q:88:LEU:HA	1.75	0.41
30:K:182:VAL:O	30:K:186:LYS:HG3	2.20	0.41
30:K:720:TYR:HA	30:K:723:ILE:HG12	2.02	0.41
30:K:1195:LEU:HA	30:K:1198:GLN:HB3	2.01	0.41
1:2:1302:G:O6	1:2:1306:U:O4	2.39	0.41
1:2:1318:G:H2'	1:2:1319:U:C6	2.56	0.41
6:E:129:ILE:HD13	6:E:139:LEU:HB3	2.03	0.41
9:H:165:ASN:O	9:H:169:LYS:NZ	2.54	0.41
19:T:42:HIS:NE2	19:T:43:LYS:HE2	2.36	0.41
20:S:54:LYS:HE2	20:S:58:GLU:OE2	2.21	0.41
21:Q:42:ILE:N	21:Q:45:ARG:HH22	2.18	0.41
24:N:87:ASP:N	24:N:87:ASP:OD1	2.53	0.41
27:I:174:CYS:HB2	27:I:190:LEU:HD21	2.03	0.41
1:2:996:A:H2'	1:2:997:A:C8	2.55	0.41
1:2:1179:G:N2	1:2:1182:A:OP2	2.44	0.41
1:2:1277:C:H2'	1:2:1278:A:H8	1.85	0.41
13:x:77:LYS:HA	13:x:116:VAL:O	2.21	0.41
13:x:160:LEU:O	23:O:113:GLN:NE2	2.52	0.41
17:u:403:GLU:HG3	22:P:124:LYS:HE2	2.03	0.41
25:L:134:LEU:HB2	25:L:138:VAL:HG23	2.02	0.41
1:2:537:C:H2'	1:2:538:U:C6	2.56	0.41
1:2:944:A:N6	1:2:982:G:H1	2.17	0.41
2:R:7:LYS:HD3	2:R:7:LYS:HA	1.84	0.41
15:w:200:LEU:HD23	15:w:200:LEU:HA	1.88	0.41
15:w:329:ILE:HD12	15:w:329:ILE:HA	1.92	0.41
17:u:148:ASP:HA	17:u:151:LYS:HG2	2.02	0.41
17:u:676:HIS:CD2	17:u:786:PRO:HG3	2.55	0.41
20:S:66:ARG:O	20:S:70:ILE:HG13	2.20	0.41
23:O:31:CYS:HB2	23:O:93:LEU:HD23	2.02	0.41
27:I:48:VAL:HG11	27:I:54:LYS:HD2	2.03	0.41
30:K:860:PRO:HG3	33:z:197:PHE:CD2	2.55	0.41
30:K:941:GLU:CD	30:K:981:HIS:CE1	2.98	0.41
31:M:77:ILE:HD11	31:M:128:PHE:HZ	1.86	0.41
1:2:1562:C:H2'	1:2:1563:G:C8	2.54	0.41
10:G:44:GLU:HG2	10:G:45:TRP:CD1	2.56	0.41
12:Y:21:LYS:O	12:Y:74:MET:HA	2.20	0.41
15:w:322:SER:O	15:w:326:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:K:1029:HIS:HA	30:K:1032:LEU:HD12	2.02	0.41
1:2:99:A:H2'	1:2:100:U:O4'	2.21	0.41
1:2:639:C:H2'	1:2:640:A:C8	2.55	0.41
1:2:1743:G:H21	1:2:1791:A:N6	2.13	0.41
1:2:1753:C:H2'	1:2:1754:G:C8	2.51	0.41
1:2:1817:G:H2'	1:2:1818:A:C8	2.56	0.41
3:b:8:LEU:HA	3:b:8:LEU:HD23	1.90	0.41
9:H:30:LEU:HD11	9:H:82:GLU:HB3	2.02	0.41
18:t:353:ILE:O	18:t:356:THR:HG22	2.20	0.41
21:Q:58:LEU:HB3	21:Q:62:ARG:HD2	2.02	0.41
30:K:384:LEU:HD11	30:K:430:GLN:HB2	2.02	0.41
30:K:407:ASP:OD1	30:K:407:ASP:N	2.53	0.41
30:K:531:LEU:O	30:K:535:VAL:HG23	2.21	0.41
32:f:94:LYS:HE3	32:f:94:LYS:HB3	1.88	0.41
32:f:96:LYS:HD2	32:f:96:LYS:HA	1.86	0.41
1:2:527:C:H2'	1:2:528:A:H8	1.86	0.41
1:2:641:A:O2'	1:2:645:C:OP1	2.39	0.41
1:2:1217:A:H2'	1:2:1218:C:C6	2.53	0.41
17:u:596:MET:HB2	17:u:665:VAL:HG21	2.03	0.41
25:L:104:LYS:HE2	25:L:104:LYS:HB3	1.85	0.41
30:K:338:HIS:HB3	30:K:341:VAL:HG12	2.03	0.41
1:2:459:C:H2'	1:2:460:A:O4'	2.21	0.40
1:2:863:U:O4	1:2:864:A:N6	2.54	0.40
10:G:32:MET:HE2	10:G:32:MET:HB3	1.81	0.40
22:P:53:GLN:HA	22:P:83:MET:HE1	2.02	0.40
30:K:733:LEU:HD23	30:K:768:ALA:HB1	2.03	0.40
1:2:65:C:N4	10:G:134:GLY:O	2.45	0.40
10:G:21:GLU:O	10:G:25:ARG:HG2	2.21	0.40
20:S:41:ALA:HA	20:S:44:VAL:HG12	2.03	0.40
22:P:21:ASP:H	22:P:24:GLN:NE2	2.19	0.40
29:q:169:GLU:H	29:q:169:GLU:HG2	1.74	0.40
30:K:379:PRO:HD2	30:K:387:LEU:HD13	2.03	0.40
1:2:186:C:H2'	1:2:187:G:H8	1.87	0.40
1:2:441:C:H2'	1:2:442:C:C6	2.56	0.40
15:w:357:LEU:HD21	15:w:393:LEU:HD23	2.02	0.40
20:S:36:VAL:HG13	20:S:40:TYR:HD2	1.86	0.40
24:N:99:ARG:NH2	24:N:119:GLU:OE2	2.54	0.40
30:K:568:TRP:CD1	30:K:568:TRP:H	2.38	0.40
1:2:1546:G:H2'	1:2:1547:C:C6	2.57	0.40
1:2:1726:G:H2'	1:2:1727:G:H8	1.86	0.40
5:c:29:GLN:HE21	5:c:43:ILE:HG21	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:u:303:ASP:OD1	17:u:303:ASP:N	2.55	0.40
30:K:223:LYS:HA	30:K:223:LYS:HD3	1.90	0.40
30:K:624:THR:HG22	30:K:660:THR:HG21	2.03	0.40
30:K:889:LEU:HD22	30:K:895:GLN:HG2	2.02	0.40
1:2:528:A:H2'	1:2:529:A:H8	1.85	0.40
1:2:647:U:H2'	1:2:648:A:C8	2.57	0.40
1:2:951:C:H2'	1:2:952:G:C8	2.56	0.40
1:2:1051:G:H2'	1:2:1052:A:H8	1.86	0.40
4:B:202:GLN:HE21	4:B:206:PRO:HB3	1.86	0.40
6:E:45:ILE:HD12	6:E:80:ILE:HD12	2.03	0.40
11:Z:72:VAL:HA	11:Z:75:GLU:HG2	2.04	0.40
12:Y:9:THR:HB	12:Y:23:MET:HG3	2.03	0.40
17:u:729:VAL:HB	17:u:767:MET:HE3	2.03	0.40
20:S:16:LEU:HD11	20:S:72:GLN:HE22	1.87	0.40
28:r:51:TRP:NE1	28:r:67:PRO:O	2.43	0.40
31:M:43:ASP:HA	31:M:72:HIS:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	R	79/135 (58%)	77 (98%)	2 (2%)	0	100	100
3	b	80/84 (95%)	76 (95%)	4 (5%)	0	100	100
4	B	211/264 (80%)	202 (96%)	9 (4%)	0	100	100
5	c	59/69 (86%)	56 (95%)	3 (5%)	0	100	100
6	E	260/263 (99%)	254 (98%)	6 (2%)	0	100	100
7	e	18/59 (30%)	18 (100%)	0	0	100	100
8	F	187/204 (92%)	178 (95%)	8 (4%)	1 (0%)	24	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	H	184/194 (95%)	174 (95%)	10 (5%)	0	100	100
10	G	228/249 (92%)	222 (97%)	6 (3%)	0	100	100
11	Z	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
12	Y	122/133 (92%)	120 (98%)	2 (2%)	0	100	100
13	x	173/252 (69%)	165 (95%)	8 (5%)	0	100	100
14	X	139/143 (97%)	138 (99%)	1 (1%)	0	100	100
15	w	321/437 (74%)	310 (97%)	11 (3%)	0	100	100
16	W	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
17	u	630/804 (78%)	601 (95%)	29 (5%)	0	100	100
18	t	53/475 (11%)	43 (81%)	10 (19%)	0	100	100
19	T	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
20	S	125/152 (82%)	117 (94%)	8 (6%)	0	100	100
21	Q	123/146 (84%)	118 (96%)	5 (4%)	0	100	100
22	P	117/145 (81%)	113 (97%)	4 (3%)	0	100	100
23	O	133/151 (88%)	124 (93%)	9 (7%)	0	100	100
24	N	147/151 (97%)	147 (100%)	0	0	100	100
25	L	149/158 (94%)	142 (95%)	7 (5%)	0	100	100
26	J	178/194 (92%)	170 (96%)	8 (4%)	0	100	100
27	I	203/208 (98%)	196 (97%)	7 (3%)	0	100	100
28	r	116/125 (93%)	106 (91%)	10 (9%)	0	100	100
29	q	231/281 (82%)	214 (93%)	17 (7%)	0	100	100
30	K	1000/1297 (77%)	955 (96%)	45 (4%)	0	100	100
31	M	102/132 (77%)	101 (99%)	1 (1%)	0	100	100
32	f	53/156 (34%)	47 (89%)	6 (11%)	0	100	100
33	z	78/230 (34%)	75 (96%)	3 (4%)	0	100	100
All	All	5838/7691 (76%)	5584 (96%)	253 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	F	163	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	72/122 (59%)	72 (100%)	0	100	100
3	b	74/76 (97%)	74 (100%)	0	100	100
4	B	194/231 (84%)	194 (100%)	0	100	100
5	c	52/62 (84%)	52 (100%)	0	100	100
6	E	224/225 (100%)	224 (100%)	0	100	100
7	e	18/48 (38%)	18 (100%)	0	100	100
8	F	159/170 (94%)	159 (100%)	0	100	100
9	H	167/174 (96%)	166 (99%)	1 (1%)	78	88
10	G	200/218 (92%)	200 (100%)	0	100	100
11	Z	64/103 (62%)	64 (100%)	0	100	100
12	Y	108/115 (94%)	108 (100%)	0	100	100
13	x	148/208 (71%)	148 (100%)	0	100	100
14	X	113/115 (98%)	113 (100%)	0	100	100
15	w	262/370 (71%)	262 (100%)	0	100	100
16	W	112/113 (99%)	112 (100%)	0	100	100
17	u	561/705 (80%)	561 (100%)	0	100	100
18	t	59/434 (14%)	59 (100%)	0	100	100
19	T	114/115 (99%)	114 (100%)	0	100	100
20	S	111/132 (84%)	111 (100%)	0	100	100
21	Q	106/121 (88%)	106 (100%)	0	100	100
22	P	111/130 (85%)	111 (100%)	0	100	100
23	O	105/119 (88%)	105 (100%)	0	100	100
24	N	130/131 (99%)	130 (100%)	0	100	100
25	L	135/142 (95%)	135 (100%)	0	100	100
26	J	160/168 (95%)	160 (100%)	0	100	100
27	I	178/180 (99%)	178 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	r	105/112 (94%)	105 (100%)	0	100	100
29	q	198/240 (82%)	155 (78%)	43 (22%)	1	6
30	K	871/1094 (80%)	871 (100%)	0	100	100
31	M	91/108 (84%)	91 (100%)	0	100	100
32	f	51/140 (36%)	51 (100%)	0	100	100
33	z	72/185 (39%)	72 (100%)	0	100	100
All	All	5125/6606 (78%)	5081 (99%)	44 (1%)	68	85

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	H	114	GLN
29	q	15	GLU
29	q	24	ARG
29	q	25	LYS
29	q	32	MET
29	q	36	GLN
29	q	38	ARG
29	q	47	LEU
29	q	48	TYR
29	q	49	LEU
29	q	55	CYS
29	q	57	LEU
29	q	59	ASP
29	q	60	ILE
29	q	64	THR
29	q	66	LEU
29	q	69	SER
29	q	73	ASP
29	q	81	LEU
29	q	82	ASP
29	q	83	ILE
29	q	87	MET
29	q	88	LEU
29	q	92	VAL
29	q	96	ILE
29	q	102	LEU
29	q	107	GLN
29	q	112	LYS
29	q	115	THR

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Mol	Chain	Res	Type
29	q	129	CYS
29	q	130	ASN
29	q	133	LYS
29	q	140	LYS
29	q	141	ARG
29	q	151	SER
29	q	153	LEU
29	q	155	ARG
29	q	163	LEU
29	q	166	GLU
29	q	172	GLU
29	q	176	THR
29	q	183	PHE
29	q	198	LYS
29	q	202	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	202	GLN
5	c	29	GLN
6	E	197	ASN
6	E	209	HIS
9	H	25	GLN
9	H	33	ASN
9	H	114	GLN
10	G	13	GLN
10	G	81	HIS
13	x	102	HIS
13	x	106	GLN
13	x	227	ASN
14	X	61	GLN
15	w	61	GLN
15	w	251	ASN
15	w	422	GLN
16	W	70	ASN
17	u	226	GLN
17	u	242	GLN
17	u	301	GLN
17	u	312	ASN
17	u	604	ASN
17	u	683	HIS

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Mol	Chain	Res	Type
17	u	762	GLN
18	t	292	ASN
18	t	299	ASN
22	P	104	GLN
23	O	20	GLN
24	N	62	GLN
25	L	19	ASN
25	L	94	HIS
25	L	141	ASN
27	I	52	ASN
27	I	84	ASN
27	I	167	GLN
28	r	6	HIS
29	q	36	GLN
29	q	76	HIS
29	q	107	GLN
29	q	130	ASN
29	q	193	ASN
30	K	338	HIS
30	K	466	GLN
30	K	484	HIS
30	K	492	GLN
30	K	886	HIS
30	K	900	GLN
30	K	981	HIS
30	K	1189	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1557/1873 (83%)	351 (22%)	26 (1%)

All (351) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	26	U
1	2	33	G
1	2	41	G
1	2	46	A
1	2	54	A

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Mol	Chain	Res	Type
1	2	55	U
1	2	56	G
1	2	62	G
1	2	64	A
1	2	65	C
1	2	67	C
1	2	68	A
1	2	69	C
1	2	70	G
1	2	72	C
1	2	73	C
1	2	74	G
1	2	75	G
1	2	76	U
1	2	77	A
1	2	79	A
1	2	92	A
1	2	100	U
1	2	103	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	116	U
1	2	126	G
1	2	128	U
1	2	130	G
1	2	143	U
1	2	144	U
1	2	155	G
1	2	160	U
1	2	163	U
1	2	168	C
1	2	172	U
1	2	175	A
1	2	181	A
1	2	184	G
1	2	291	G
1	2	292	A
1	2	295	C
1	2	302	A
1	2	309	G
1	2	310	C

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Mol	Chain	Res	Type
1	2	313	A
1	2	315	C
1	2	318	A
1	2	319	C
1	2	333	G
1	2	335	G
1	2	351	G
1	2	360	A
1	2	362	C
1	2	364	A
1	2	368	U
1	2	369	C
1	2	370	G
1	2	377	G
1	2	383	G
1	2	385	G
1	2	386	C
1	2	399	C
1	2	400	C
1	2	407	G
1	2	409	C
1	2	413	G
1	2	418	A
1	2	429	C
1	2	436	G
1	2	438	G
1	2	441	C
1	2	448	A
1	2	449	A
1	2	450	C
1	2	465	A
1	2	466	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	476	A
1	2	482	G
1	2	487	U
1	2	492	C
1	2	493	A
1	2	496	C

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Mol	Chain	Res	Type
1	2	516	A
1	2	525	A
1	2	544	G
1	2	546	G
1	2	547	G
1	2	548	C
1	2	554	A
1	2	556	U
1	2	559	G
1	2	560	A
1	2	563	G
1	2	564	A
1	2	570	C
1	2	576	A
1	2	583	A
1	2	587	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	593	C
1	2	595	U
1	2	600	G
1	2	601	G
1	2	603	C
1	2	604	A
1	2	605	A
1	2	607	U
1	2	608	C
1	2	631	U
1	2	637	U
1	2	643	A
1	2	644	G
1	2	655	A
1	2	658	U
1	2	660	C
1	2	664	A
1	2	669	A
1	2	670	A
1	2	671	A
1	2	672	A
1	2	673	G

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Mol	Chain	Res	Type
1	2	678	U
1	2	683	G
1	2	684	G
1	2	687	C
1	2	688	U
1	2	749	U
1	2	750	C
1	2	751	G
1	2	792	C
1	2	794	A
1	2	797	C
1	2	798	G
1	2	799	U
1	2	800	U
1	2	811	A
1	2	821	G
1	2	822	U
1	2	830	A
1	2	844	U
1	2	847	A
1	2	869	A
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	874	G
1	2	878	G
1	2	880	G
1	2	881	G
1	2	886	A
1	2	890	U
1	2	891	G
1	2	892	U
1	2	893	U
1	2	896	U
1	2	898	U
1	2	903	A
1	2	908	A
1	2	913	A
1	2	914	U
1	2	920	A
1	2	927	C

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Mol	Chain	Res	Type
1	2	930	C
1	2	933	G
1	2	959	G
1	2	963	A
1	2	970	G
1	2	971	G
1	2	981	A
1	2	990	A
1	2	992	A
1	2	1002	U
1	2	1017	U
1	2	1023	A
1	2	1039	C
1	2	1041	G
1	2	1044	G
1	2	1045	U
1	2	1049	A
1	2	1083	A
1	2	1085	C
1	2	1089	G
1	2	1096	G
1	2	1099	G
1	2	1114	U
1	2	1116	C
1	2	1117	C
1	2	1118	C
1	2	1120	U
1	2	1121	G
1	2	1123	C
1	2	1130	G
1	2	1138	C
1	2	1140	G
1	2	1149	A
1	2	1153	C
1	2	1154	U
1	2	1157	G
1	2	1165	G
1	2	1170	A
1	2	1171	G
1	2	1172	U
1	2	1195	A
1	2	1200	A

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Mol	Chain	Res	Type
1	2	1202	U
1	2	1206	G
1	2	1211	G
1	2	1215	C
1	2	1217	A
1	2	1221	G
1	2	1224	G
1	2	1227	G
1	2	1232	U
1	2	1238	U
1	2	1242	U
1	2	1243	U
1	2	1265	A
1	2	1272	C
1	2	1273	C
1	2	1274	G
1	2	1275	G
1	2	1284	A
1	2	1285	G
1	2	1286	G
1	2	1296	U
1	2	1299	A
1	2	1300	U
1	2	1301	A
1	2	1302	G
1	2	1303	C
1	2	1305	C
1	2	1307	U
1	2	1308	U
1	2	1309	C
1	2	1312	G
1	2	1313	A
1	2	1315	U
1	2	1317	C
1	2	1322	G
1	2	1323	U
1	2	1325	G
1	2	1327	G
1	2	1335	G
1	2	1364	U
1	2	1371	U
1	2	1372	U

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Mol	Chain	Res	Type
1	2	1376	A
1	2	1383	A
1	2	1387	G
1	2	1388	A
1	2	1389	C
1	2	1396	A
1	2	1397	U
1	2	1398	G
1	2	1445	U
1	2	1446	A
1	2	1447	G
1	2	1454	A
1	2	1462	U
1	2	1463	U
1	2	1465	A
1	2	1476	A
1	2	1477	U
1	2	1487	A
1	2	1489	A
1	2	1490	G
1	2	1491	G
1	2	1494	U
1	2	1495	G
1	2	1498	A
1	2	1503	C
1	2	1512	C
1	2	1519	U
1	2	1533	A
1	2	1534	C
1	2	1535	U
1	2	1551	U
1	2	1559	C
1	2	1560	U
1	2	1566	G
1	2	1570	G
1	2	1571	G
1	2	1580	A
1	2	1584	G
1	2	1585	U
1	2	1586	U
1	2	1588	A
1	2	1601	A

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Mol	Chain	Res	Type
1	2	1606	G
1	2	1617	G
1	2	1618	C
1	2	1621	U
1	2	1623	A
1	2	1637	A
1	2	1638	G
1	2	1639	G7M
1	2	1640	A
1	2	1641	A
1	2	1647	A
1	2	1648	G
1	2	1654	G
1	2	1660	C
1	2	1661	A
1	2	1662	U
1	2	1663	A
1	2	1664	A
1	2	1665	G
1	2	1671	G
1	2	1675	A
1	2	1686	G
1	2	1689	C
1	2	1694	U
1	2	1704	C
1	2	1705	C
1	2	1721	U
1	2	1722	G
1	2	1723	G
1	2	1727	G
1	2	1728	U
1	2	1729	U
1	2	1744	G
1	2	1756	C
1	2	1761	U
1	2	1783	C
1	2	1784	G
1	2	1786	U
1	2	1800	A
1	2	1801	A
1	2	1805	G
1	2	1806	A

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Mol	Chain	Res	Type
1	2	1826	G
1	2	1829	G
1	2	1836	G
1	2	1839	U
1	2	1841	C
1	2	1861	G
1	2	1863	A
1	2	1864	U
1	2	1872	G

All (26) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	102	A
1	2	114	G
1	2	143	U
1	2	180	G
1	2	291	G
1	2	314	U
1	2	332	G
1	2	417	C
1	2	440	G
1	2	465	A
1	2	604	A
1	2	636	C
1	2	750	C
1	2	958	G
1	2	980	A
1	2	1231	C
1	2	1264	C
1	2	1295	A
1	2	1304	U
1	2	1386	A
1	2	1497	G
1	2	1511	U
1	2	1534	C
1	2	1565	C
1	2	1693	G
1	2	1726	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	G7M	2	1639	1	23,26,27	4.37	14 (60%)	34,39,42	1.96	9 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G7M	2	1639	1	-	2/7/25/26	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1639	G7M	C3'-C4'	-10.05	1.27	1.53
1	2	1639	G7M	C2'-C1'	-8.12	1.27	1.53
1	2	1639	G7M	C4-N3	6.68	1.49	1.34
1	2	1639	G7M	C2-N2	6.57	1.49	1.34
1	2	1639	G7M	C2-N3	5.69	1.47	1.33
1	2	1639	G7M	C2'-C3'	5.35	1.67	1.53
1	2	1639	G7M	O4'-C4'	5.17	1.56	1.45
1	2	1639	G7M	O4'-C1'	5.10	1.53	1.42
1	2	1639	G7M	C5-C6	4.09	1.54	1.43
1	2	1639	G7M	C5-N7	-4.04	1.34	1.39
1	2	1639	G7M	C2-N1	3.00	1.44	1.37
1	2	1639	G7M	C6-N1	2.88	1.44	1.38
1	2	1639	G7M	O6-C6	-2.51	1.18	1.23
1	2	1639	G7M	O3'-C3'	2.22	1.48	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1639	G7M	C2-N3-C4	4.63	120.27	112.30
1	2	1639	G7M	C5-C4-N3	-4.01	120.57	128.15
1	2	1639	G7M	C5-C6-N1	3.92	119.94	111.84
1	2	1639	G7M	CN7-N7-C5	3.51	131.17	126.80
1	2	1639	G7M	CN7-N7-C8	-3.17	119.98	124.79
1	2	1639	G7M	C2-N1-C6	-2.93	119.80	125.11
1	2	1639	G7M	N9-C4-N3	2.88	131.72	125.95
1	2	1639	G7M	O6-C6-C5	-2.87	121.61	128.01
1	2	1639	G7M	N9-C8-N7	-2.12	107.33	112.48

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	1639	G7M	C2'-C1'-N9-C8
1	2	1639	G7M	C2'-C1'-N9-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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	$\# Z > 2$
34	SAH	q	301	-	27,28,28	0.46	0	36,40,40	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	SAH	q	301	-	-	6/15/31/31	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

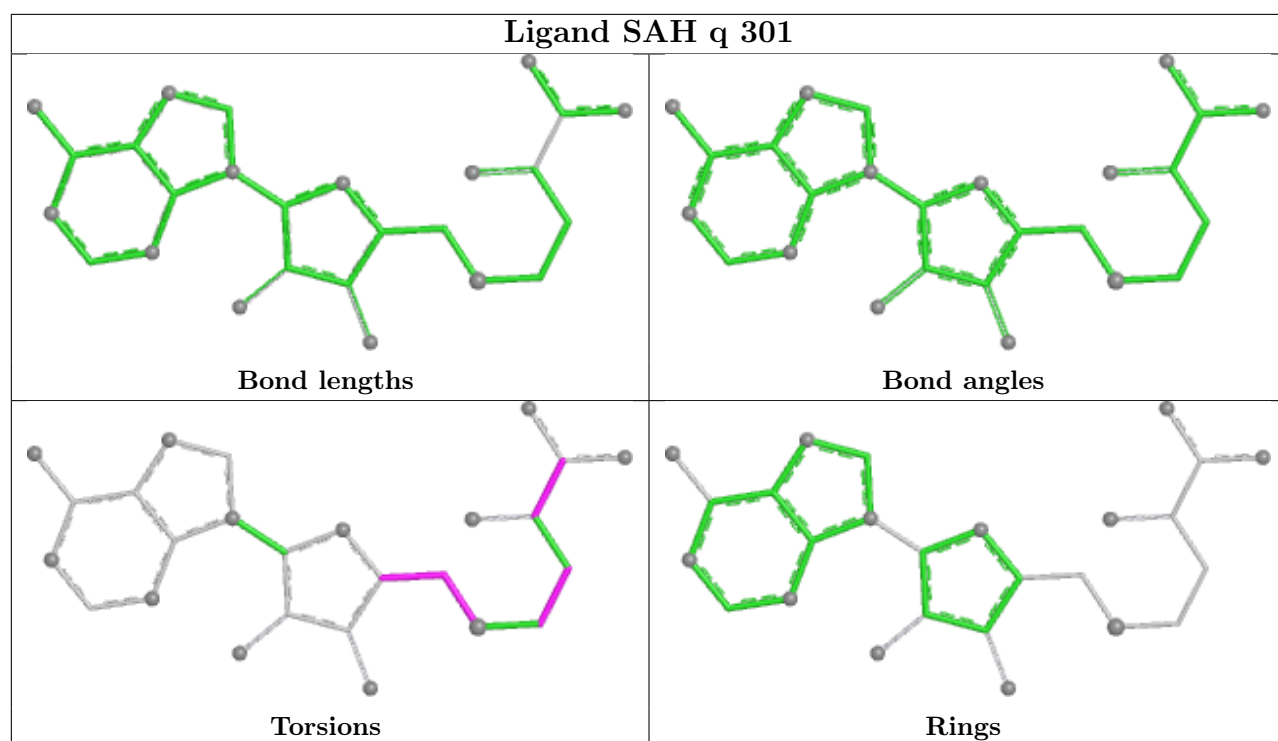
Mol	Chain	Res	Type	Atoms
34	q	301	SAH	O4'-C4'-C5'-SD
34	q	301	SAH	C3'-C4'-C5'-SD
34	q	301	SAH	CA-CB-CG-SD
34	q	301	SAH	OXT-C-CA-N
34	q	301	SAH	O-C-CA-N
34	q	301	SAH	C4'-C5'-SD-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	q	301	SAH	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

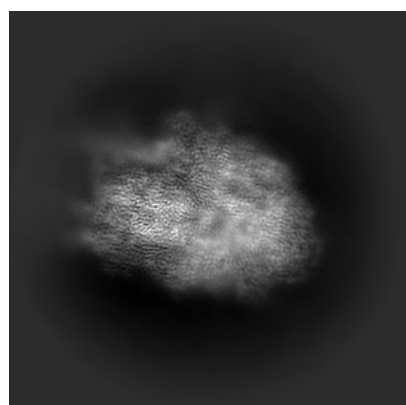
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32801. These allow visual inspection of the internal detail of the map and identification of artifacts.

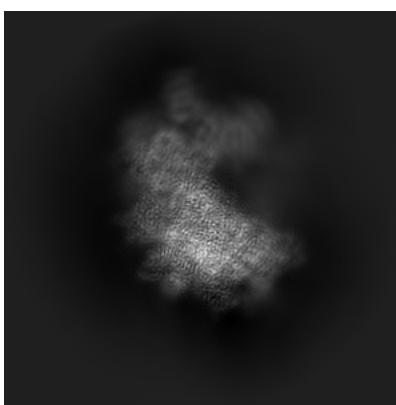
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

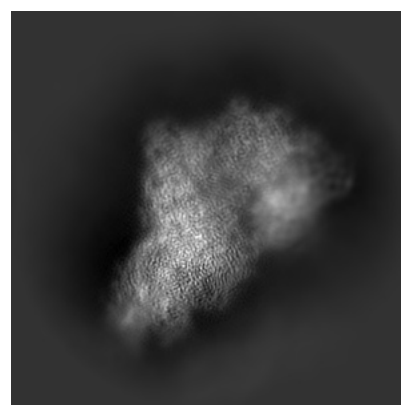
6.1.1 Primary map



X



Y

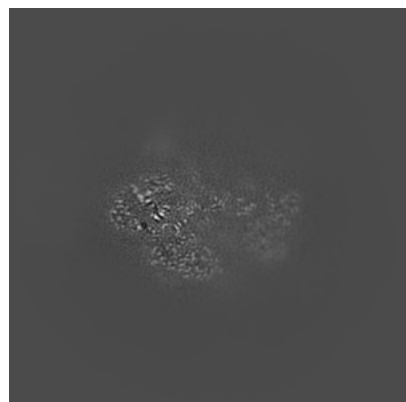


Z

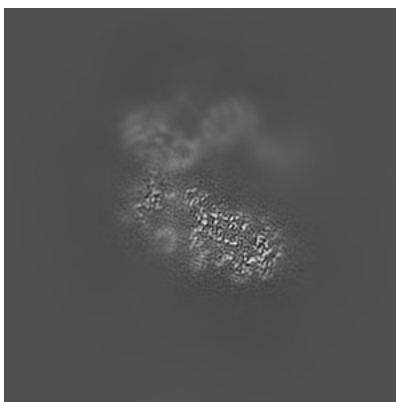
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

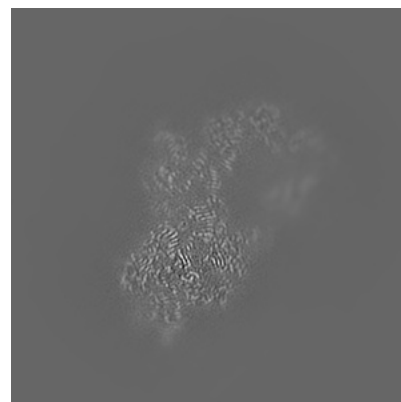
6.2.1 Primary map



X Index: 180



Y Index: 180

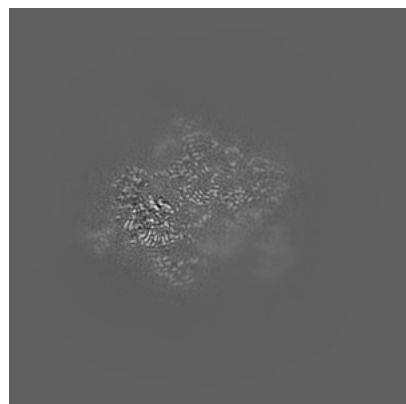


Z Index: 180

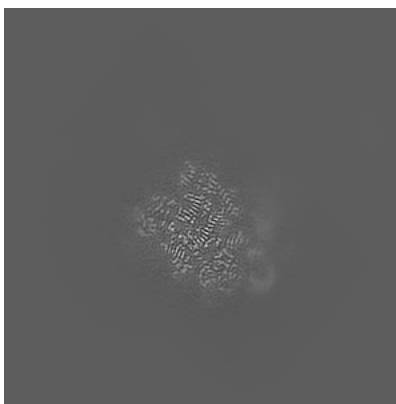
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

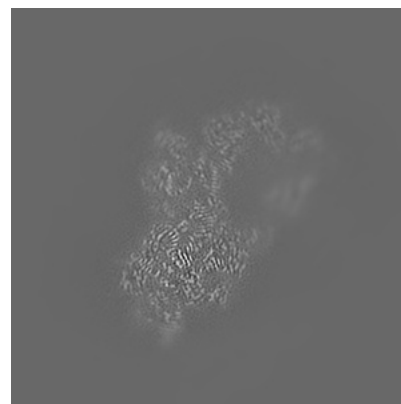
6.3.1 Primary map



X Index: 159



Y Index: 134

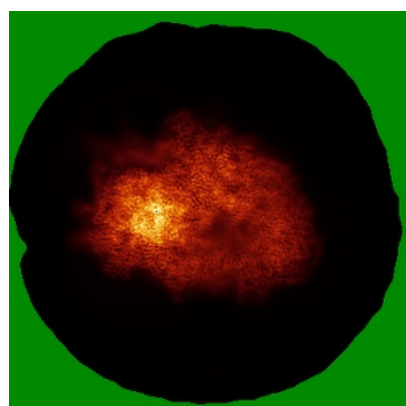


Z Index: 181

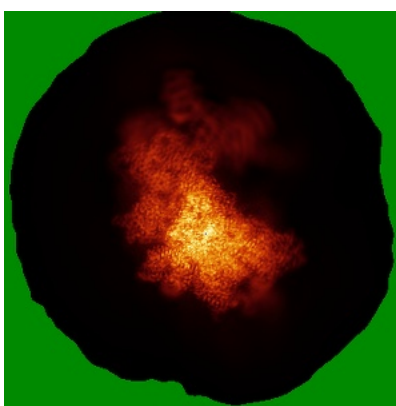
The images above show the largest variance slices of the map in three orthogonal directions.

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

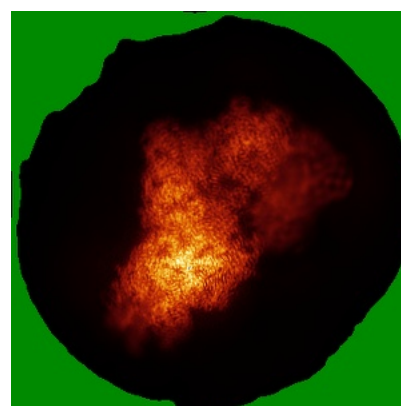
6.4.1 Primary map



X



Y

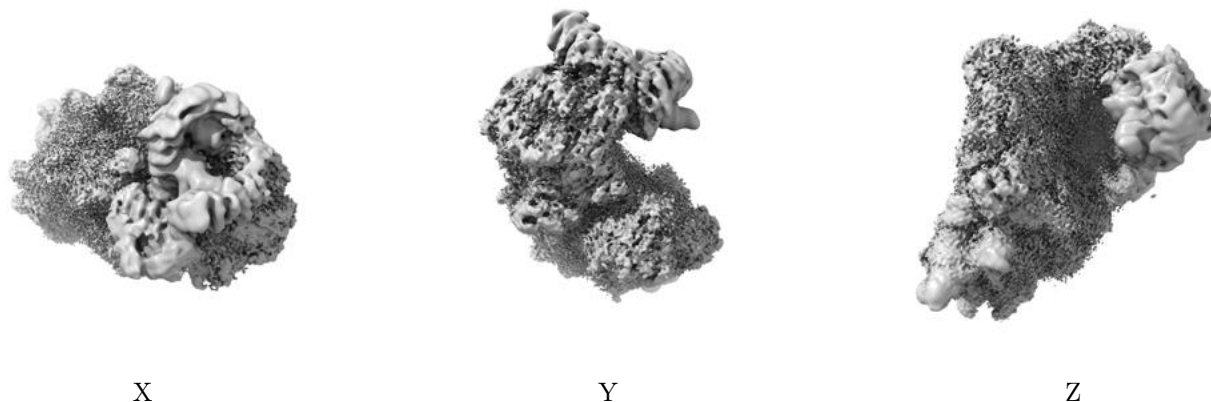


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

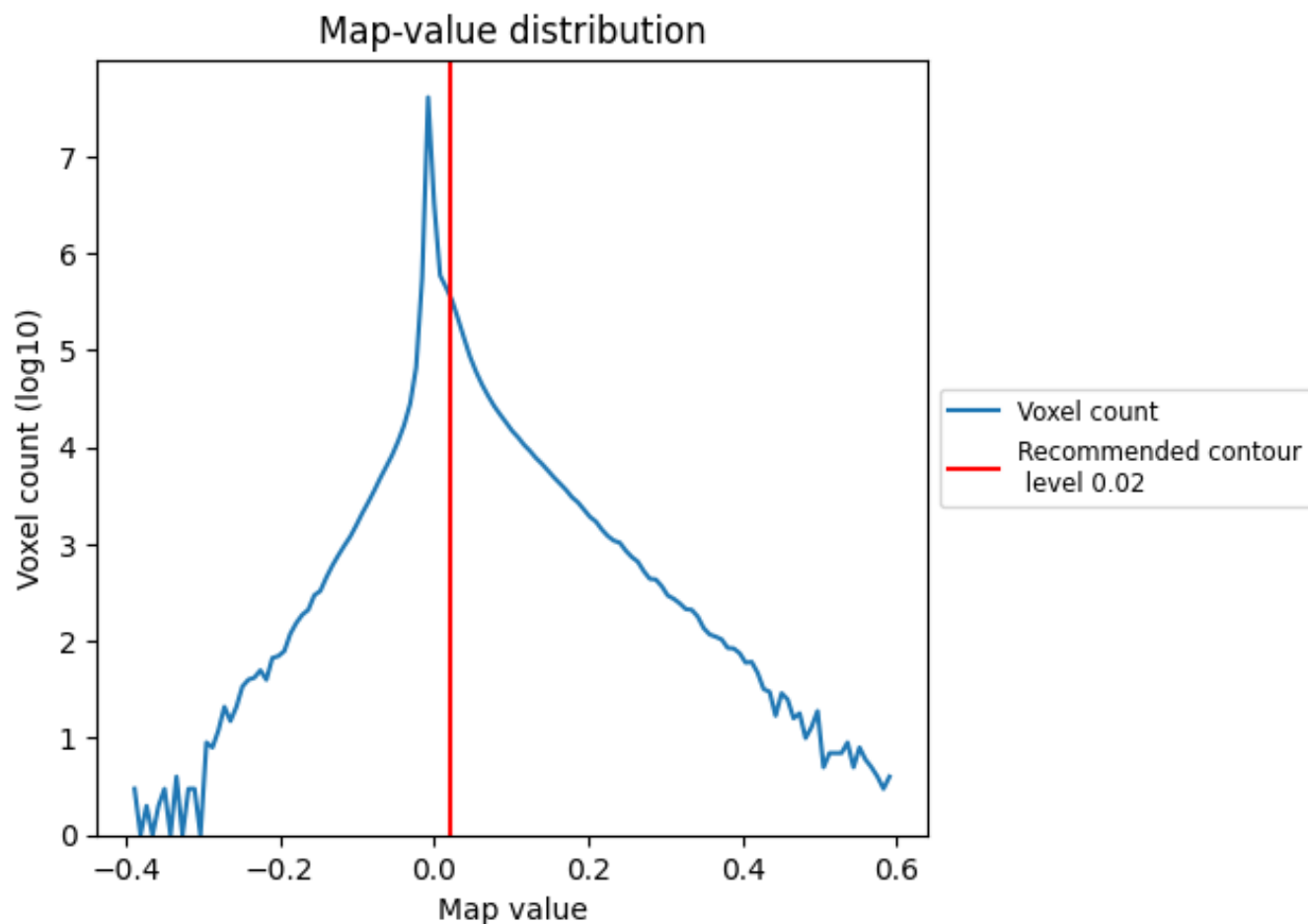
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

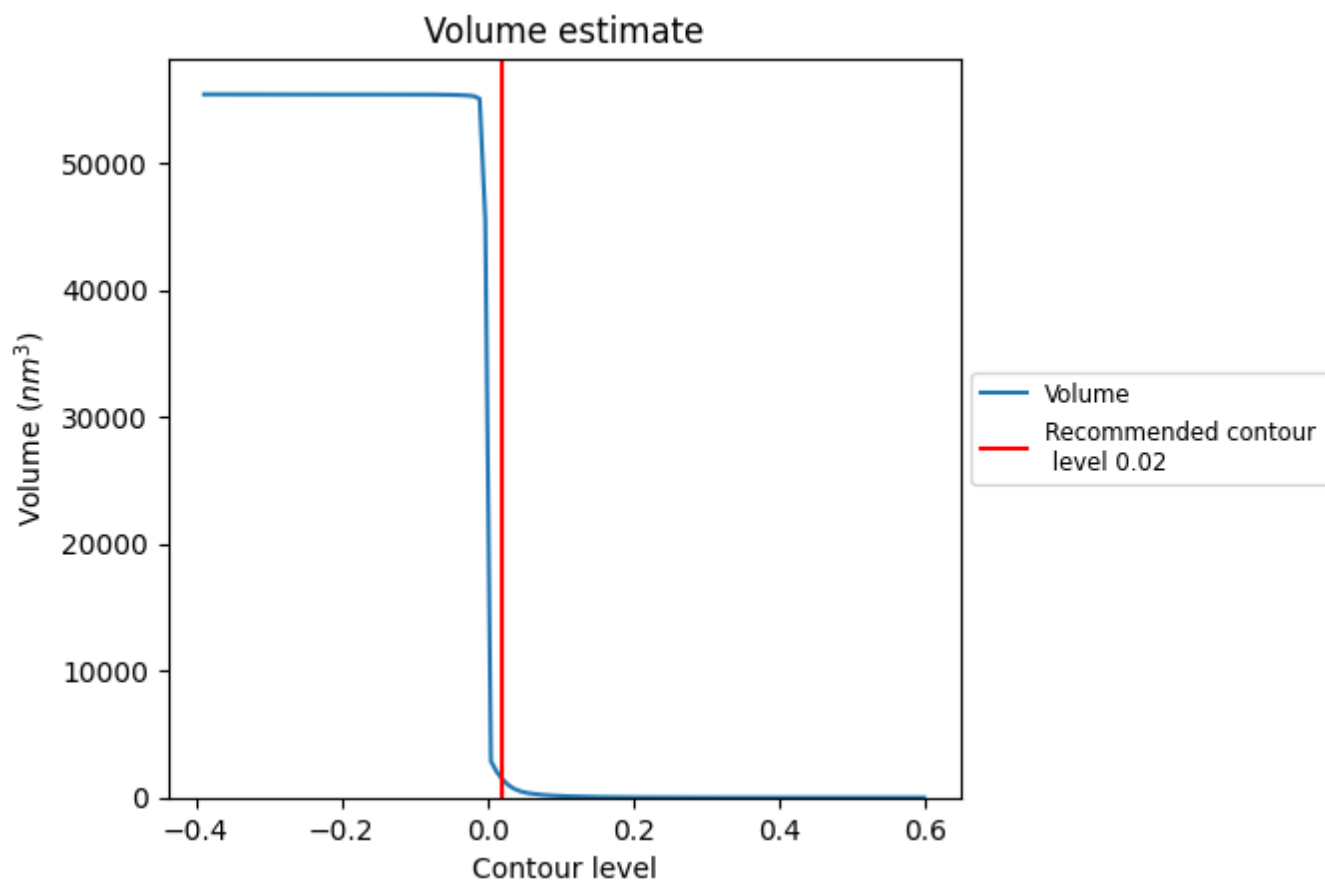
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

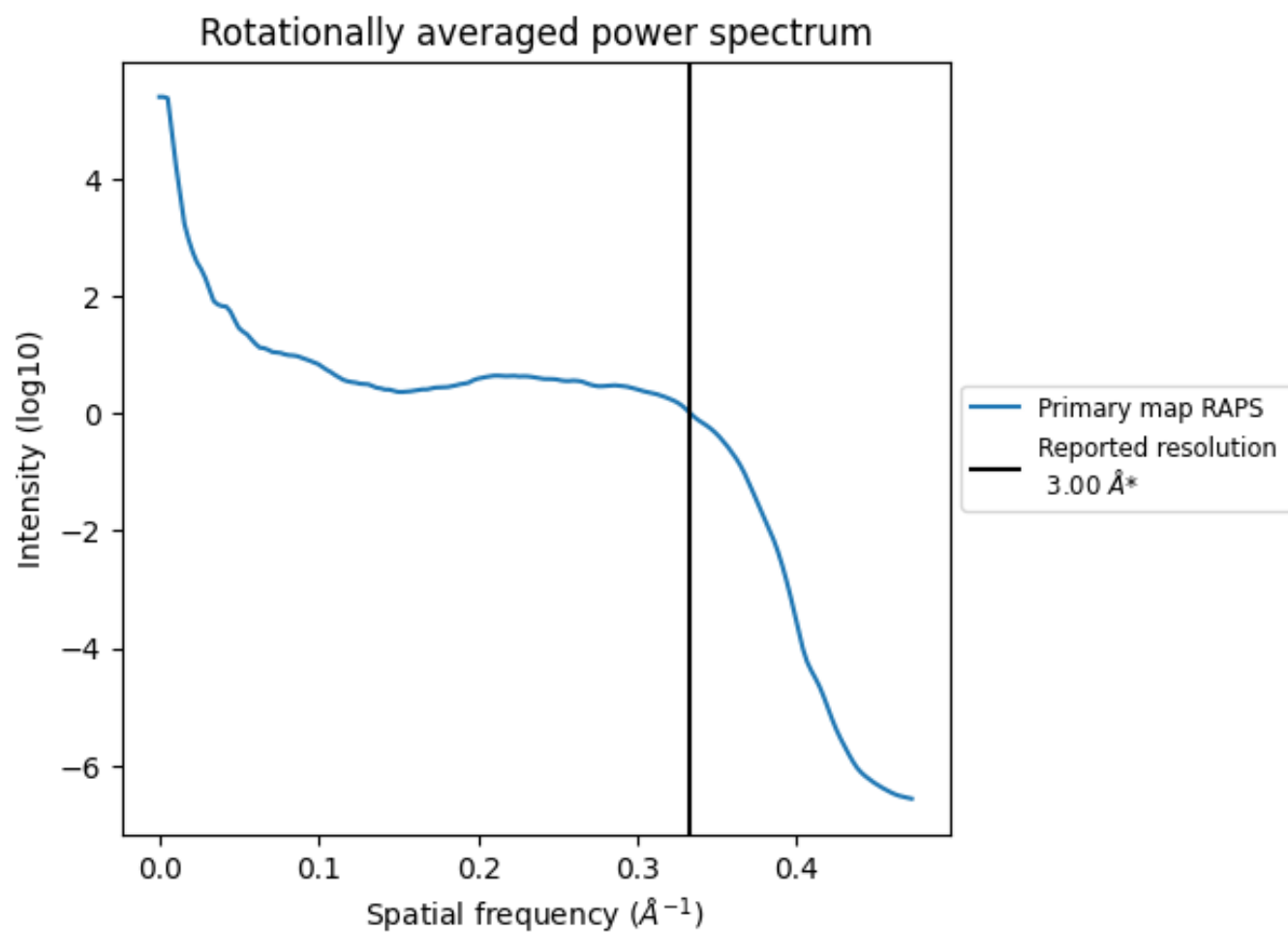
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1484 nm^3 ; this corresponds to an approximate mass of 1340 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 ⓘ

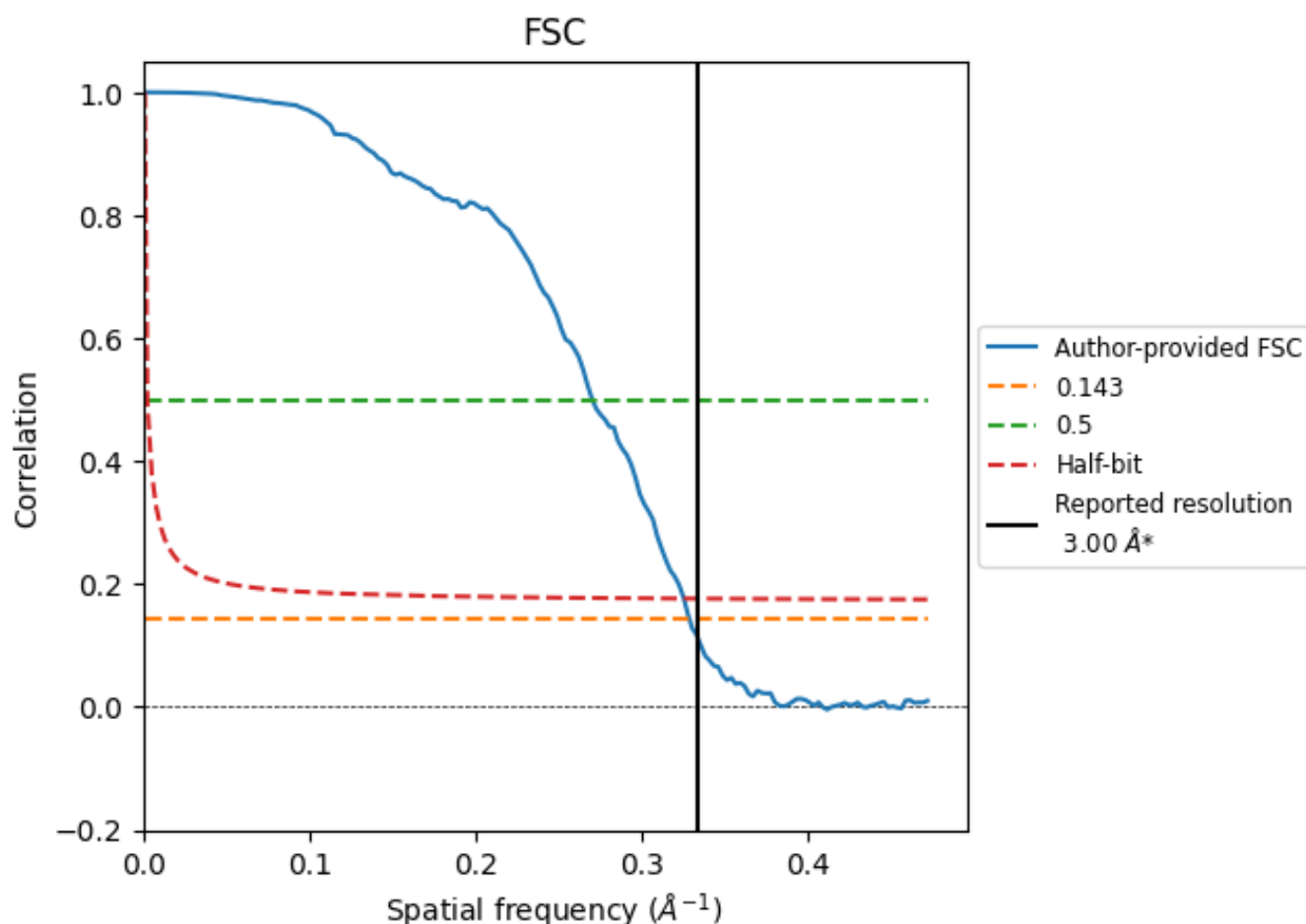


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

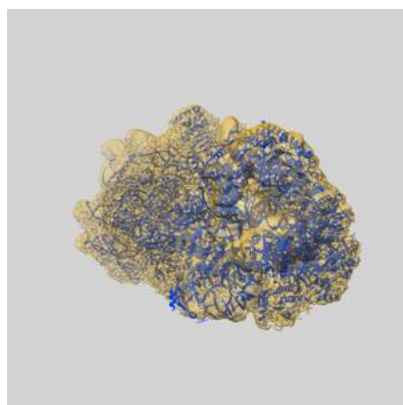
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.04	3.70	3.07
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

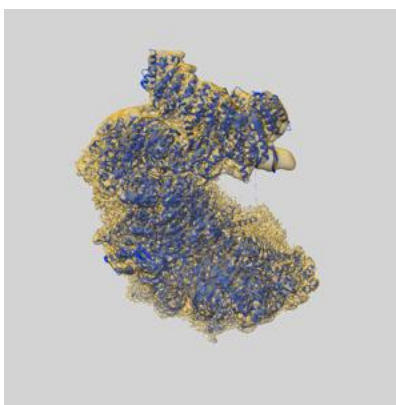
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32801 and PDB model 7WTU. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

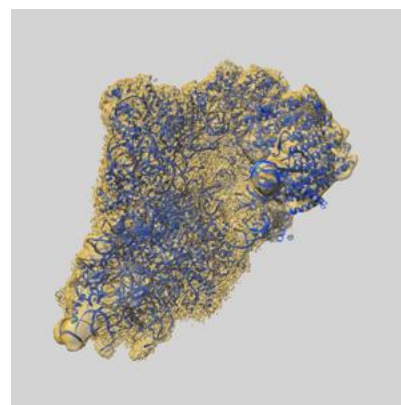
9.1 Map-model overlay [i](#)



X



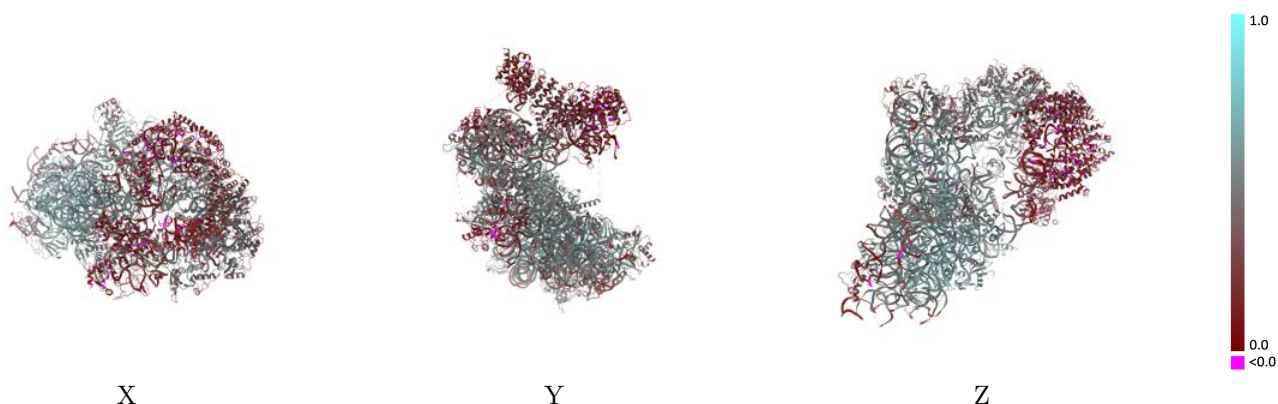
Y



Z

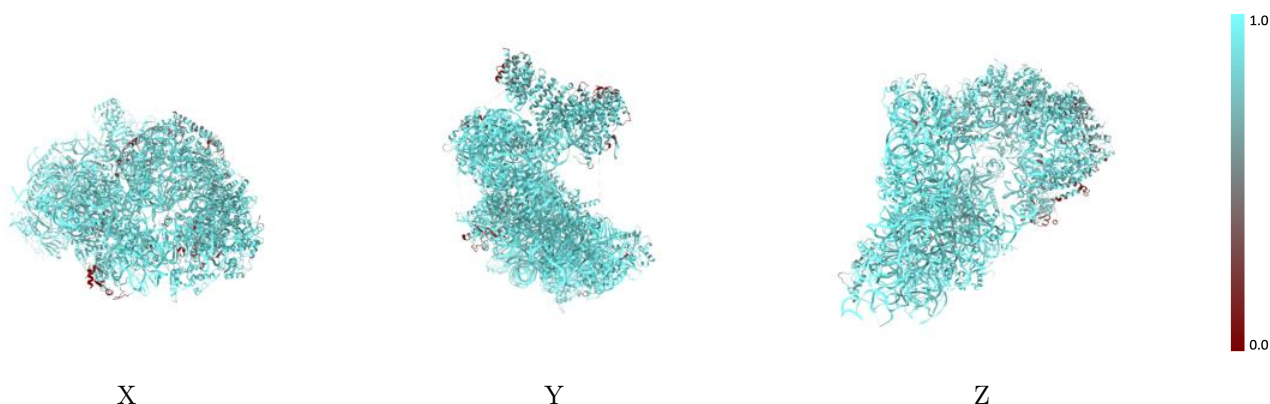
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



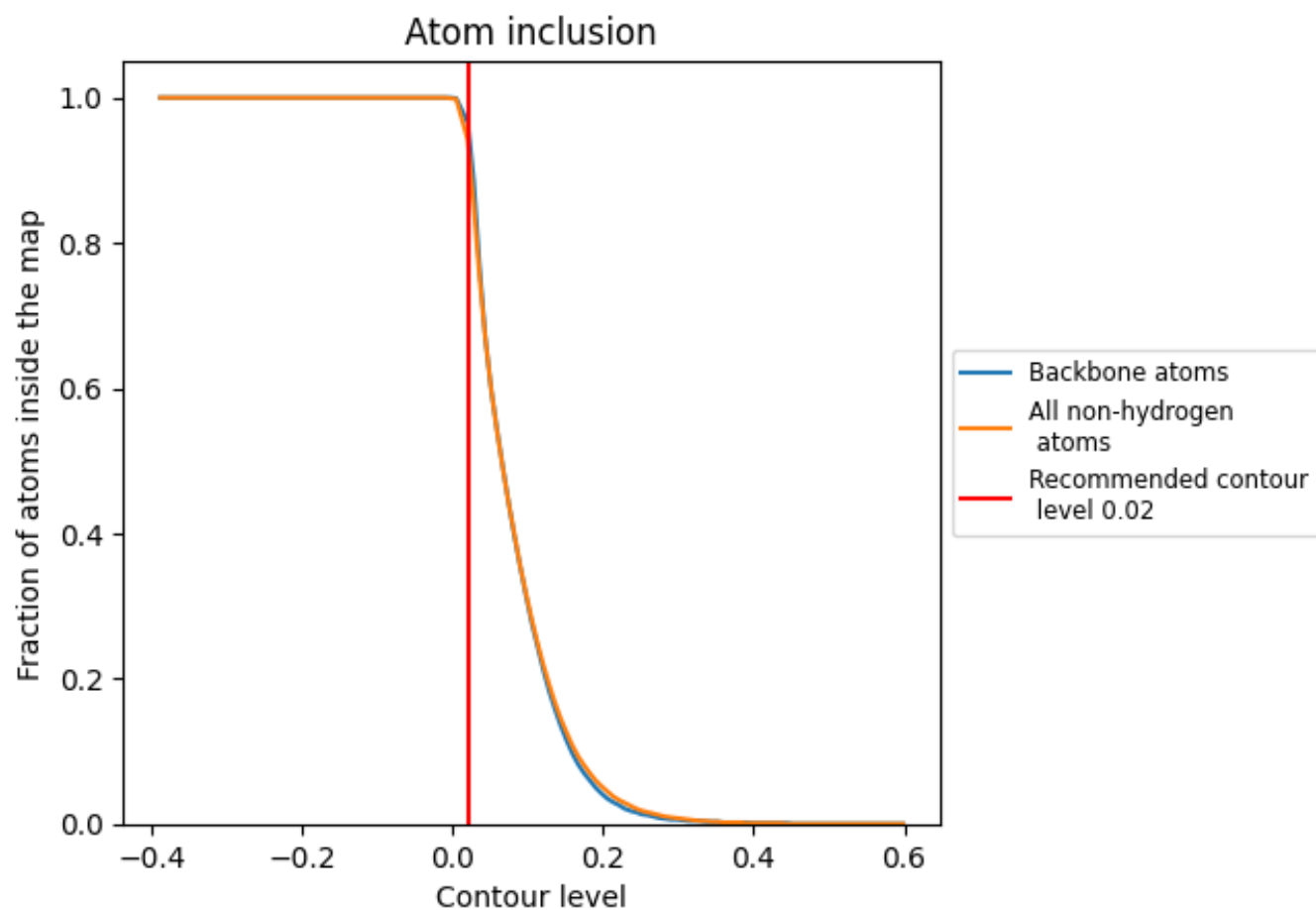
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9420	 0.4300
2	 0.9860	 0.4770
B	 0.9200	 0.4390
E	 0.9880	 0.6060
F	 0.9460	 0.4630
G	 0.9660	 0.4940
H	 0.9400	 0.4160
I	 0.9420	 0.4920
J	 0.9850	 0.5730
K	 0.8280	 0.1910
L	 0.9580	 0.5510
M	 0.4630	 0.1300
N	 0.9800	 0.5140
O	 0.9280	 0.4410
P	 0.9570	 0.4360
Q	 0.9280	 0.4310
R	 0.9160	 0.1710
S	 0.9220	 0.4180
T	 0.9200	 0.4490
W	 0.9940	 0.5630
X	 0.9810	 0.5220
Y	 0.9930	 0.5910
Z	 0.8720	 0.3640
b	 0.9650	 0.5120
c	 0.9250	 0.4370
e	 0.9880	 0.5320
f	 0.7520	 0.1230
q	 0.9040	 0.3080
r	 0.6380	 0.1420
t	 0.8610	 0.2990
u	 0.9820	 0.5260
w	 0.9110	 0.2270
x	 0.9750	 0.4880
z	 0.6830	 0.2150

