



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:29 AM UTC

PDB ID : 7WTT / pdb_00007wtt
EMDB ID : EMD-32800
Title : Cryo-EM structure of a human pre-40S ribosomal subunit - State RRP12-A1 (with CK1)
Authors : Cheng, J.; Lau, B.; Thoms, M.; Ameismeier, M.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on : 2022-02-05
Resolution : 3.10 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 : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

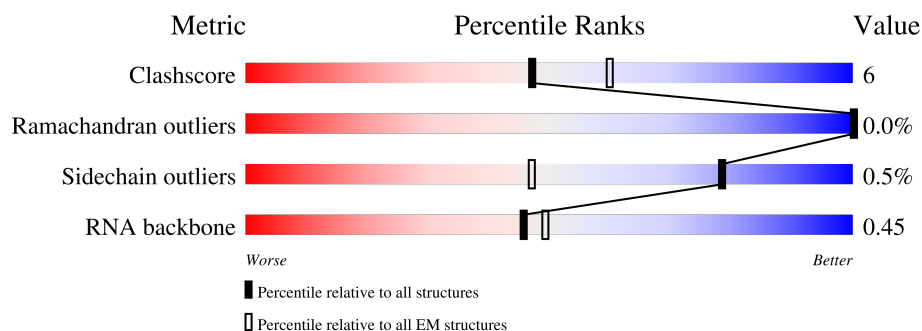
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	2	1873	51% 29% 5% 16%
2	R	135	47% 13% 40%
3	b	84	83% 14% .
4	B	264	66% 15% 19%
5	c	69	72% 16% 12%
6	E	263	89% 11%
7	e	59	34% 66%

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

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Mol	Chain	Length	Quality of chain
33	a	337	 72%17%12%
34	z	230	 31%5%64%

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 83677 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 Casein kinase I isoform alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	297	Total	C	N	O	S	1	0
			2462	1581	432	434	15		

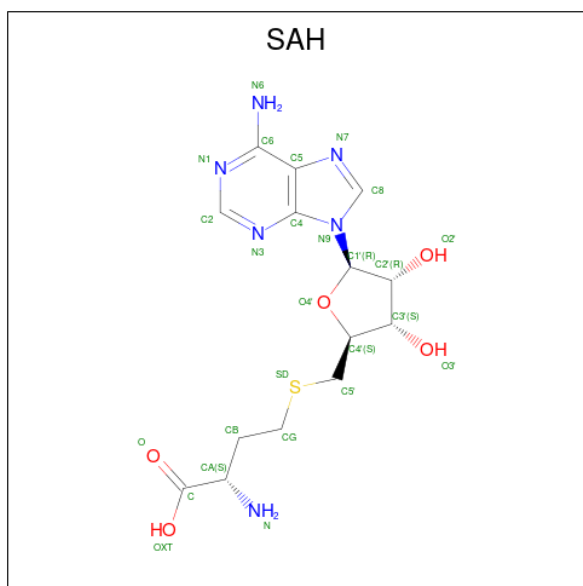
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	20	GLY	VAL	conflict	UNP P48729
a	35	THR	ILE	conflict	UNP P48729
a	58	HIS	LEU	conflict	UNP P48729

- Molecule 34 is a protein called Ribosome biogenesis protein SLX9 homolog.

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

- Molecule 35 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

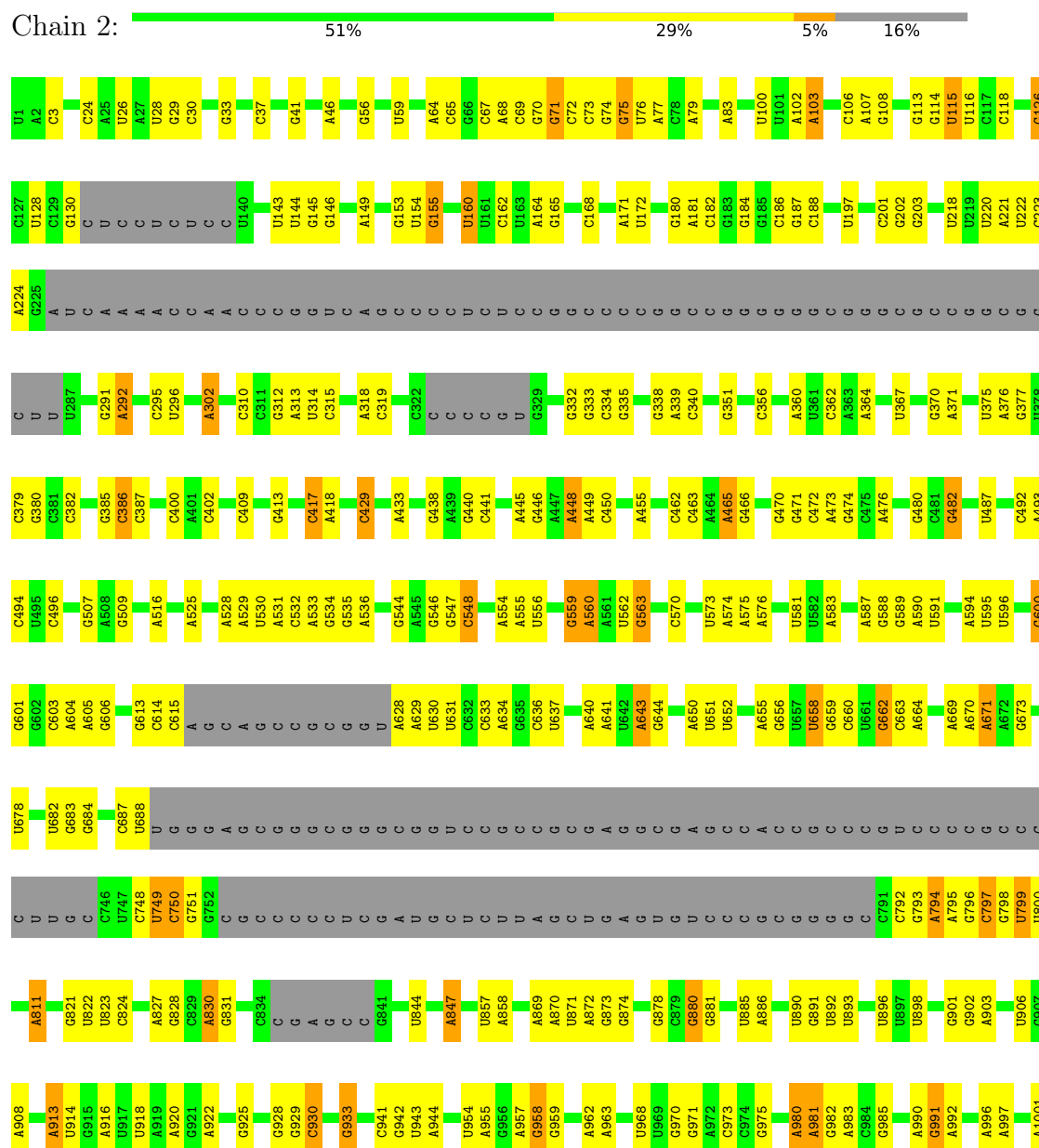
- Molecule 36 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

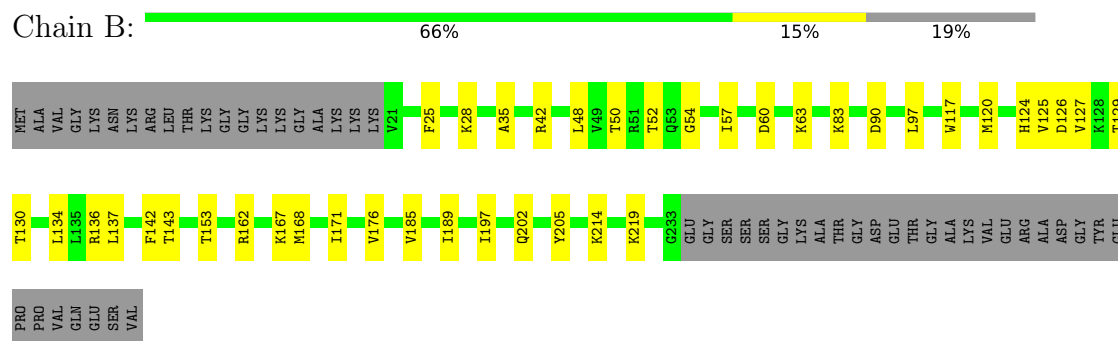
3 Residue-property plots

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. 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. 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.

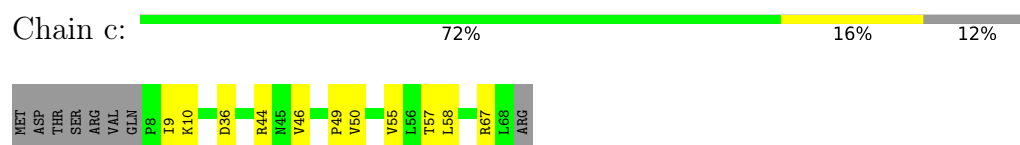
• Molecule 1: 18S rRNA



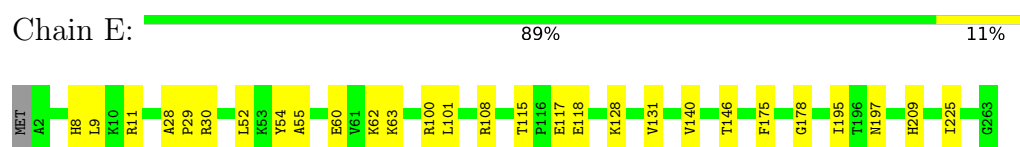
- Molecule 4: 40S ribosomal protein S3a



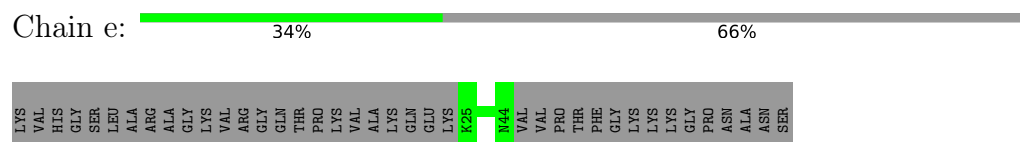
- Molecule 5: 40S ribosomal protein S28



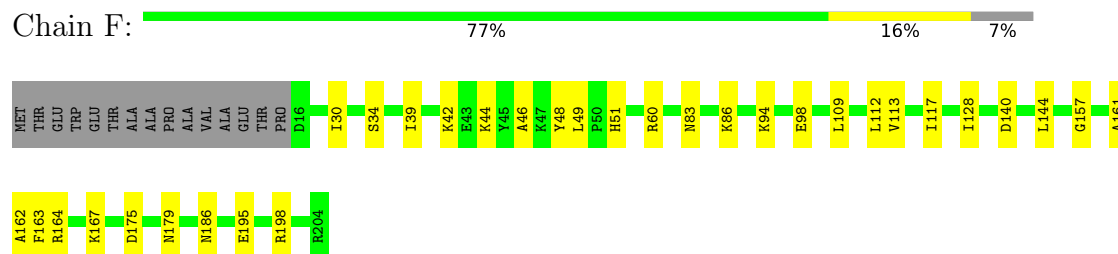
- Molecule 6: 40S ribosomal protein S4, X isoform



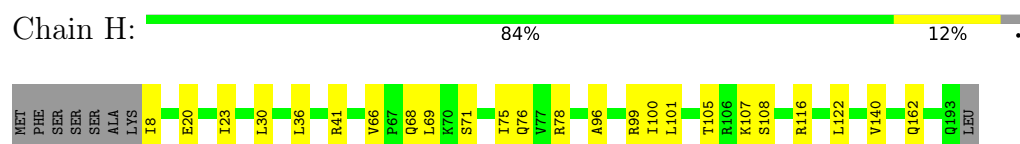
- Molecule 7: 40S ribosomal protein S30



- Molecule 8: 40S ribosomal protein S5

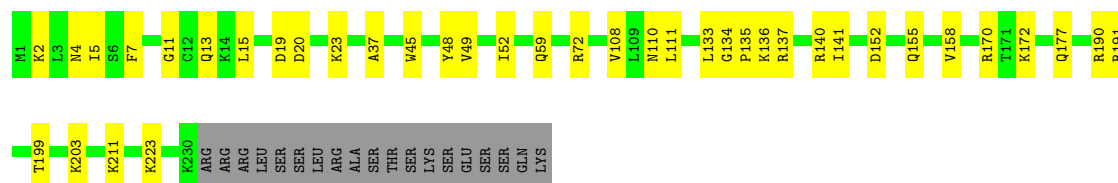


- Molecule 9: 40S ribosomal protein S7

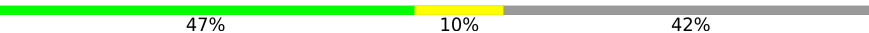


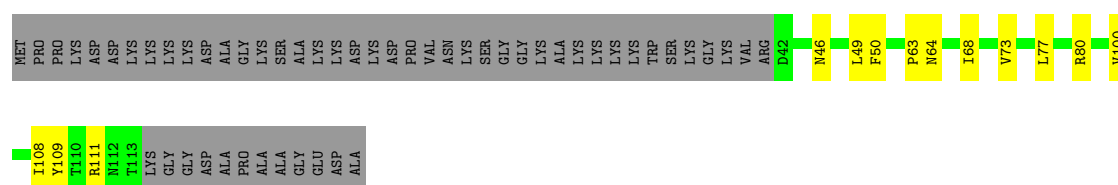
- Molecule 10: 40S ribosomal protein S6

Chain G: 



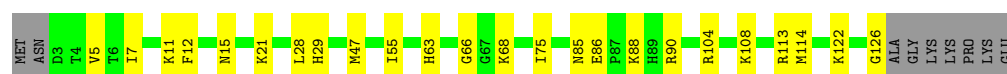
- Molecule 11: 40S ribosomal protein S25

Chain Z: 



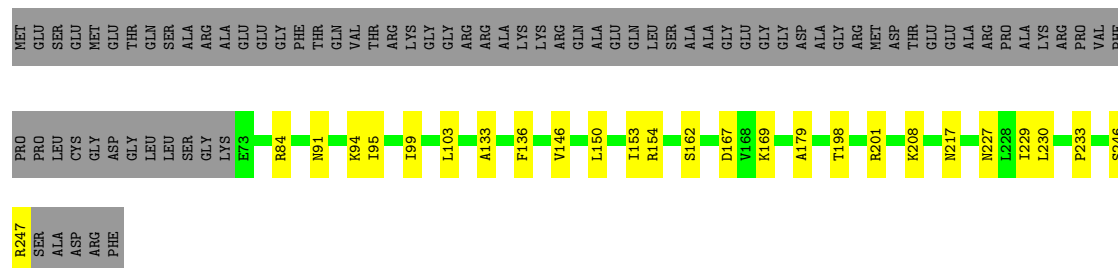
- Molecule 12: 40S ribosomal protein S24

Chain Y: 



- Molecule 13: RNA-binding protein PNO1

Chain x: 



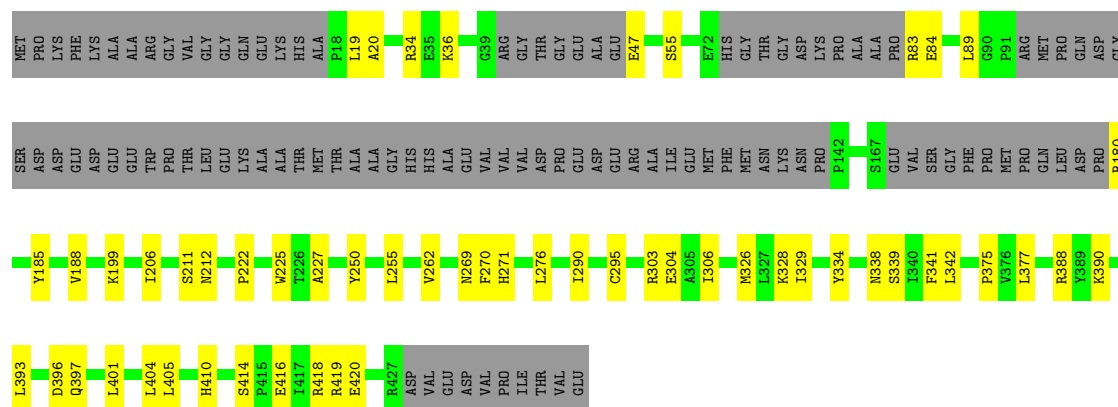
- Molecule 14: 40S ribosomal protein S23

Chain X: 



- Molecule 15: Bystin

Chain w: 



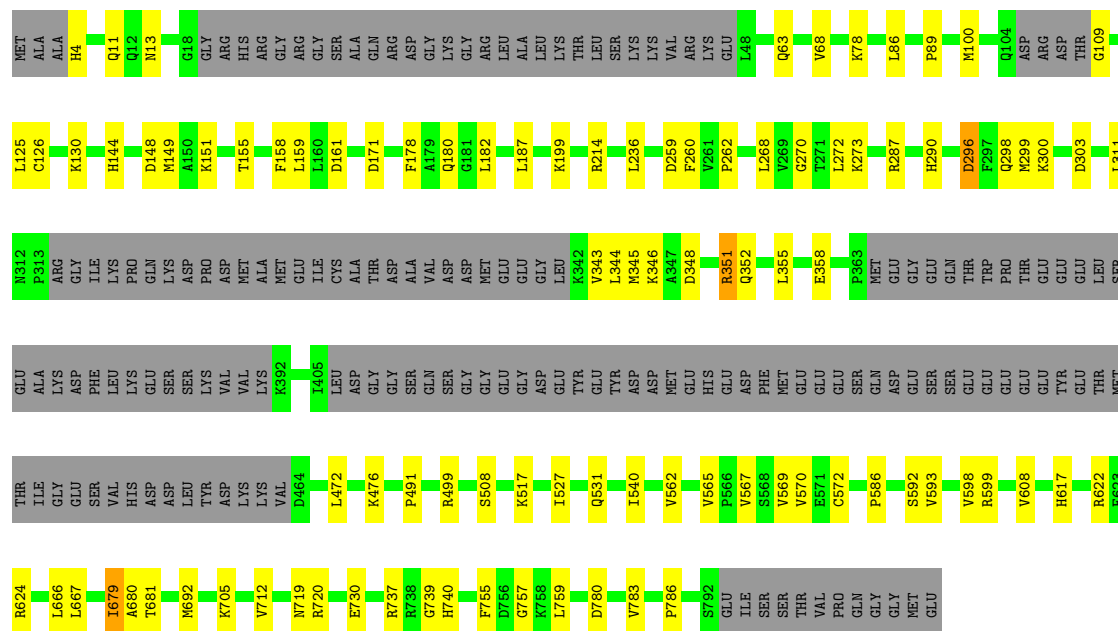
• Molecule 16: 40S ribosomal protein S15a

Chain W: 88% 12% .



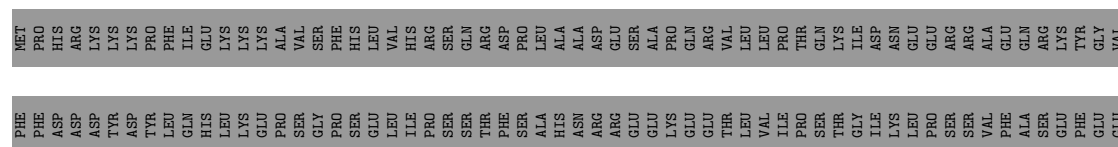
• Molecule 17: Pre-rRNA-processing protein TSR1 homolog

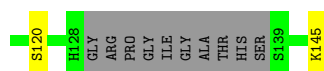
Chain u: 68% 12% 20%



• Molecule 18: Protein LTV1 homolog

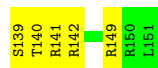
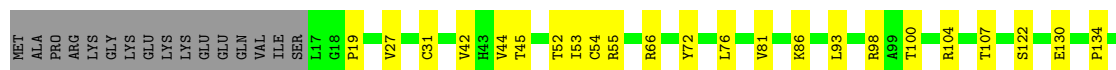
Chain t: 10% 88%





- Molecule 23: 40S ribosomal protein S14

Chain O: 71% 19% 11%



- Molecule 24: 40S ribosomal protein S13

Chain N: 88% 11%



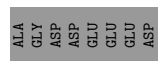
- Molecule 25: 40S ribosomal protein S11

Chain L: 84% 12%



- Molecule 26: 40S ribosomal protein S9

Chain J: 78% 15% 7%



- Molecule 27: 40S ribosomal protein S8

Chain I: 81% 17%

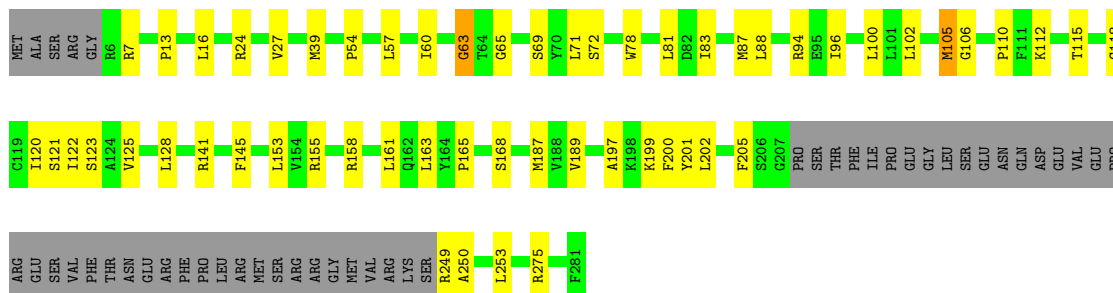


- Molecule 28: Multifunctional methyltransferase subunit TRM112-like protein

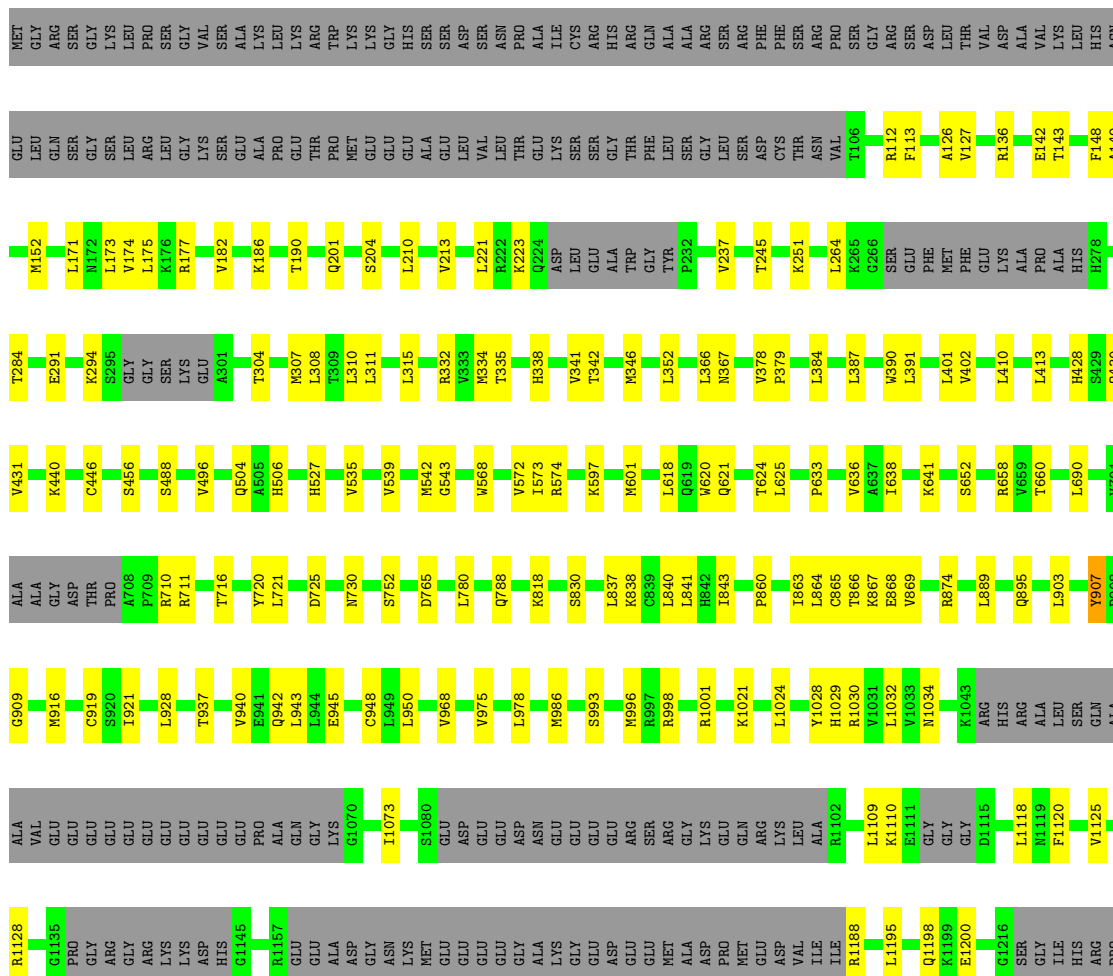
Chain r: 71% 23% 6%



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



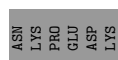
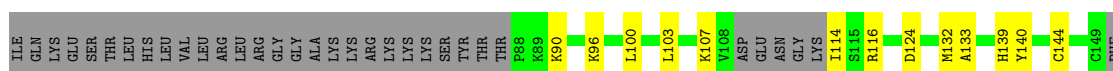
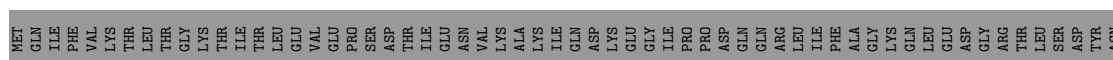
• Molecule 30: RRP12-like protein



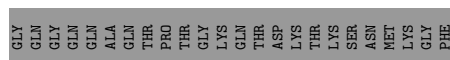
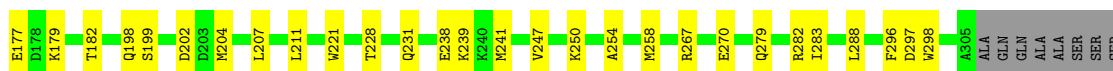
- Molecule 31: 40S ribosomal protein S12



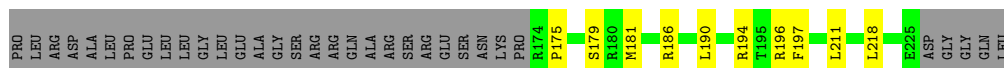
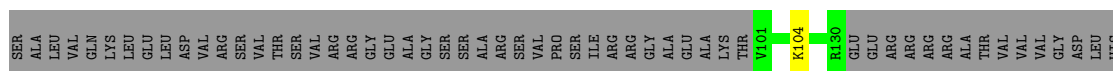
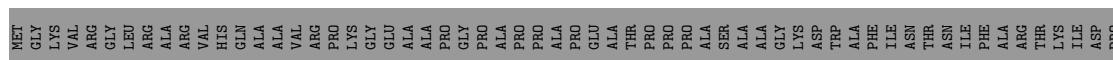
- Molecule 32: Ubiquitin-40S ribosomal protein S27a



- Molecule 33: Casein kinase I isoform alpha



- Molecule 34: 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	103616	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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.32	0/37573	0.43	2/58534 (0.0%)
2	R	0.24	0/680	0.64	0/905
3	b	0.26	0/653	0.47	0/876
4	B	0.24	0/1756	0.54	0/2350
5	c	0.26	0/473	0.59	0/633
6	E	0.38	0/2118	0.57	0/2849
7	e	0.29	0/180	0.43	0/232
8	F	0.24	0/1515	0.53	0/2037
9	H	0.21	0/1524	0.54	1/2042 (0.0%)
10	G	0.28	0/1885	0.50	0/2510
11	Z	0.28	0/580	0.65	2/780 (0.3%)
12	Y	0.34	0/1031	0.53	0/1370
13	x	0.28	0/1394	0.59	0/1880
14	X	0.32	0/1116	0.59	0/1490
15	w	0.21	0/2656	0.54	2/3586 (0.1%)
16	W	0.32	0/1050	0.59	0/1406
17	u	0.37	0/5296	0.59	2/7154 (0.0%)
18	t	0.21	0/531	0.63	0/713
19	T	0.23	0/1142	0.48	0/1530
20	S	0.24	0/1071	0.56	0/1437
21	Q	0.24	0/1012	0.57	0/1356
22	P	0.26	0/1025	0.59	0/1369
23	O	0.26	0/1022	0.61	0/1372
24	N	0.25	0/1226	0.50	0/1649
25	L	0.35	0/1250	0.53	0/1673
26	J	0.42	0/1524	0.59	0/2035
27	I	0.38	0/1711	0.61	0/2282
28	r	0.20	0/961	0.57	0/1301
29	q	0.41	0/1910	0.64	1/2572 (0.0%)
30	K	0.21	1/8097 (0.0%)	0.53	0/10950
31	M	0.14	0/845	0.43	0/1134
32	f	0.18	0/474	0.54	0/626

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	a	0.18	0/2520	0.53	0/3385
34	z	0.15	0/686	0.40	0/914
All	All	0.30	1/88487 (0.0%)	0.50	10/126932 (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
18	t	0	1
30	K	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	907	TYR	C-N	5.04	1.39	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	q	13	PRO	O-C-N	-7.39	117.68	121.15
9	H	162	GLN	CA-CB-CG	6.30	126.70	114.10
11	Z	63	PRO	CA-N-CD	-6.24	103.27	112.00
1	2	1494	U	C2'-C3'-O3'	5.83	118.24	109.50
11	Z	63	PRO	N-CD-CG	-5.75	94.57	103.20
1	2	1494	U	P-O3'-C3'	5.71	128.76	120.20
15	w	295	CYS	CA-C-N	-5.29	113.46	122.56
15	w	295	CYS	C-N-CA	-5.29	113.46	122.56
17	u	692	MET	CA-C-N	-5.15	115.55	122.91
17	u	692	MET	C-N-CA	-5.15	115.55	122.91

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	K	378	VAL	Peptide
18	t	255	GLN	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	333	0
2	R	673	0	722	14	0
3	b	640	0	665	8	0
4	B	1729	0	1803	25	0
5	c	471	0	499	9	0
6	E	2076	0	2177	19	0
7	e	179	0	200	0	0
8	F	1494	0	1549	23	0
9	H	1501	0	1593	17	0
10	G	1862	0	2018	35	0
11	Z	574	0	627	8	0
12	Y	1014	0	1082	17	0
13	x	1372	0	1453	22	0
14	X	1098	0	1167	12	0
15	w	2610	0	2644	40	0
16	W	1033	0	1080	11	0
17	u	5168	0	5230	53	0
18	t	520	0	479	10	0
19	T	1122	0	1153	17	0
20	S	1054	0	1105	14	0
21	Q	998	0	1065	15	0
22	P	1006	0	1056	20	0
23	O	1009	0	1034	25	0
24	N	1202	0	1289	11	0
25	L	1229	0	1302	13	0
26	J	1499	0	1618	18	0
27	I	1682	0	1769	27	0
28	r	940	0	958	23	0
29	q	1869	0	1854	42	0
30	K	7949	0	8223	112	0
31	M	837	0	870	13	0
32	f	465	0	481	10	0
33	a	2462	0	2466	34	0
34	z	679	0	719	10	0
35	q	26	0	19	1	0
36	f	1	0	0	0	0
All	All	83677	0	68957	890	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 (890) 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	1.37	1.25
1:2:748:C:N4	1:2:794:A:H61	1.42	1.15
1:2:748:C:H42	1:2:794:A:N6	1.46	1.12
1:2:536:A:N6	1:2:548:C:H42	1.49	1.11
1:2:615:C:N4	1:2:628:A:H61	1.49	1.11
1:2:615:C:H42	1:2:628:A:N6	1.48	1.10
1:2:536:A:H61	1:2:548:C:N4	1.47	1.10
1:2:24:C:H42	1:2:650:A:N6	1.50	1.09
1:2:24:C:N4	1:2:650:A:H61	1.50	1.09
1:2:1710:C:N4	1:2:1823:A:H61	1.51	1.09
1:2:1710:C:H42	1:2:1823:A:N6	1.50	1.09
1:2:1609:C:N4	1:2:1630:A:H61	1.54	1.04
23:O:42:VAL:O	23:O:55:ARG:HA	1.58	1.04
1:2:1609:C:H42	1:2:1630:A:N6	1.56	1.02
1:2:614:C:H42	1:2:629:A:N6	1.61	0.97
1:2:1177:U:H3	1:2:1184:G:H1	0.94	0.94
1:2:1335:G:H1	1:2:1492:U:H3	1.10	0.94
17:u:109:GLY:HA3	17:u:125:LEU:O	1.70	0.92
1:2:614:C:N4	1:2:629:A:H61	1.69	0.90
1:2:925:G:H1	1:2:1017:U:H3	1.19	0.89
1:2:1398:G:H1	1:2:1448:A:H2	1.17	0.86
1:2:1287:A:C8	1:2:1312:G:N2	2.49	0.80
1:2:614:C:H42	1:2:629:A:H61	1.21	0.79
1:2:1534:C:C2	1:2:1598:G:N2	2.50	0.78
1:2:944:A:H61	1:2:982:G:H1	1.30	0.78
1:2:1301:A:H5''	15:w:199:LYS:HB2	1.66	0.78
17:u:287:ARG:HH12	17:u:586:PRO:HD3	1.50	0.76
1:2:1033:G:H1	1:2:1080:A:HO2'	1.32	0.75
1:2:1236:G:H21	1:2:1522:A:H62	1.32	0.75
1:2:615:C:N3	1:2:628:A:N1	2.34	0.75
1:2:1287:A:N7	1:2:1312:G:C2	2.55	0.75
1:2:1710:C:N3	1:2:1823:A:N1	2.35	0.74
1:2:1288:U:H3	1:2:1311:C:N4	1.85	0.74
30:K:149:ALA:HA	30:K:152:MET:HE2	1.71	0.73
14:X:112:VAL:HG12	14:X:114:ASP:H	1.54	0.73
28:r:113:ILE:HD12	29:q:100:LEU:HB2	1.71	0.72
30:K:291:GLU:HB3	30:K:307:MET:HE2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:749:U:O4	1:2:793:G:O6	2.07	0.71
29:q:161:LEU:HD23	29:q:202:LEU:HD23	1.72	0.71
1:2:1302:G:C6	1:2:1306:U:O4	2.44	0.71
1:2:614:C:N3	1:2:629:A:N1	2.39	0.70
30:K:716:THR:O	30:K:720:TYR:HB3	1.92	0.69
30:K:863:ILE:HG22	30:K:919:CYS:HB3	1.74	0.69
1:2:24:C:N3	1:2:650:A:N1	2.41	0.69
1:2:928:G:H1	1:2:1013:U:H3	1.38	0.69
28:r:98:LEU:HB2	28:r:107:PHE:HB2	1.75	0.69
1:2:75:G:H1	10:G:155:GLN:HA	1.58	0.69
30:K:1118:LEU:HD13	30:K:1128:ARG:HD2	1.75	0.69
1:2:1275:G:O6	1:2:1324:G:C2	2.46	0.68
12:Y:5:VAL:HA	12:Y:28:LEU:O	1.93	0.68
1:2:1609:C:N3	1:2:1630:A:N1	2.41	0.68
1:2:64:A:H2	1:2:83:A:H62	1.41	0.68
1:2:536:A:N1	1:2:548:C:N3	2.42	0.68
1:2:1277:C:O2	1:2:1322:G:N2	2.27	0.68
1:2:1652:G:H1	1:2:1672:U:H3	1.41	0.67
1:2:594:A:H61	1:2:643:A:H5'	1.60	0.67
10:G:134:GLY:HA3	10:G:158:VAL:HG11	1.77	0.66
30:K:1021:LYS:O	30:K:1029:HIS:NE2	2.27	0.66
1:2:1037:G:N2	1:2:1079:C:O2	2.29	0.66
20:S:13:LEU:HB2	20:S:20:ILE:HB	1.78	0.66
15:w:334:TYR:HA	15:w:338:ASN:HD21	1.61	0.65
1:2:1227:G:N2	1:2:1635:C:O2'	2.29	0.65
29:q:60:ILE:HG22	29:q:81:LEU:HB3	1.78	0.65
1:2:991:G:H22	1:2:1099:G:H22	1.45	0.65
1:2:1010:G:H2'	1:2:1011:A:H8	1.61	0.65
1:2:1288:U:H3	1:2:1311:C:H42	1.43	0.65
1:2:1285:G:H5'	31:M:35:ILE:HD12	1.79	0.64
1:2:1037:G:C2	1:2:1079:C:O2	2.51	0.64
24:N:130:LYS:HE2	24:N:139:TRP:HB3	1.80	0.64
17:u:290:HIS:HA	17:u:296:ASP:HA	1.80	0.64
1:2:1496:U:H5'	15:w:375:PRO:HB3	1.80	0.64
1:2:1682:C:OP2	15:w:34:ARG:NH2	2.30	0.64
1:2:1398:G:N1	1:2:1448:A:H2	1.94	0.64
32:f:133:ALA:HB3	32:f:140:TYR:HB3	1.79	0.64
1:2:944:A:N6	1:2:982:G:H1	1.96	0.63
1:2:197:U:H3	1:2:202:G:H1	1.47	0.63
1:2:1216:C:H2'	30:K:1188:ARG:HG2	1.81	0.63
4:B:124:HIS:HA	4:B:137:LEU:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:q:158:ARG:HG2	29:q:205:PHE:HB3	1.81	0.62
30:K:334:MET:HE1	30:K:342:THR:HA	1.81	0.62
1:2:1550:G:H3'	1:2:1579:A:H61	1.64	0.62
1:2:748:C:N4	1:2:794:A:N6	2.21	0.62
6:E:55:ALA:HB1	6:E:60:GLU:HG3	1.81	0.62
23:O:42:VAL:HG11	23:O:81:VAL:HG11	1.82	0.62
1:2:630:U:OP1	29:q:249:ARG:NH1	2.33	0.62
13:x:133:ALA:O	13:x:136:PHE:HB3	2.00	0.62
30:K:986:MET:HE1	30:K:1024:LEU:HG	1.82	0.62
17:u:755:PHE:HD2	17:u:759:LEU:HD11	1.65	0.62
24:N:101:HIS:HA	24:N:104:ARG:HE	1.65	0.62
1:2:1471:C:N3	30:K:711:ARG:NH2	2.43	0.62
27:I:57:ALA:HB2	27:I:183:GLY:HA2	1.82	0.61
1:2:71:G:O6	10:G:170:ARG:NH2	2.32	0.61
19:T:18:LEU:HD13	19:T:134:ILE:HG21	1.83	0.61
26:J:107:GLU:O	26:J:113:GLN:NE2	2.32	0.61
1:2:748:C:H42	1:2:794:A:H61	0.69	0.61
17:u:171:ASP:OD1	17:u:214:ARG:NH2	2.34	0.61
1:2:560:A:H5'	26:J:174:LYS:HE3	1.83	0.61
33:a:136:ASP:OD2	33:a:141:ASN:ND2	2.34	0.61
1:2:885:U:O2	1:2:901:G:O6	2.19	0.60
12:Y:12:PHE:HZ	12:Y:21:LYS:HD2	1.66	0.60
27:I:82:VAL:O	27:I:205:ARG:NH2	2.35	0.60
1:2:975:G:OP1	23:O:98:ARG:NH1	2.35	0.60
1:2:1679:A:H2'	8:F:60:ARG:HD2	1.83	0.60
31:M:86:GLY:HA3	31:M:105:GLY:HA2	1.84	0.60
1:2:798:G:O2'	9:H:108:SER:OG	2.20	0.60
2:R:63:ARG:O	30:K:574:ARG:NH2	2.35	0.60
22:P:49:LEU:HD12	22:P:53:GLN:HG3	1.84	0.60
29:q:106:GLY:HA2	29:q:145:PHE:HB2	1.84	0.60
1:2:1534:C:O2	1:2:1598:G:N2	2.34	0.60
1:2:1599:U:OP2	11:Z:46:ASN:ND2	2.34	0.60
1:2:1761:U:H3	1:2:1771:G:H1	1.48	0.60
10:G:5:ILE:HG22	10:G:111:LEU:HB2	1.84	0.60
18:t:254:GLU:HG2	18:t:255:GLN:HG2	1.84	0.60
30:K:690:LEU:HD21	30:K:721:LEU:HD21	1.83	0.60
1:2:1275:G:O6	1:2:1324:G:N2	2.35	0.60
13:x:230:LEU:HD12	23:O:149:ARG:HD2	1.84	0.60
6:E:100:ARG:NH1	6:E:118:GLU:OE2	2.34	0.59
30:K:440:LYS:HG3	30:K:496:VAL:HG21	1.83	0.59
29:q:163:LEU:HG	29:q:165:PRO:HD3	1.83	0.59

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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	0.59
17:u:617:HIS:HB2	17:u:666:LEU:HB2	1.85	0.59
33:a:198:GLN:NE2	33:a:199:SER:O	2.35	0.59
21:Q:53:GLU:OE1	21:Q:85:ARG:NH2	2.35	0.59
1:2:1761:U:O2	1:2:1771:G:N2	2.35	0.59
3:b:40:CYS:SG	3:b:42:LYS:NZ	2.75	0.59
1:2:1213:C:OP2	15:w:34:ARG:NH1	2.36	0.59
1:2:1398:G:N1	1:2:1448:A:C2	2.59	0.59
21:Q:16:LYS:HG3	21:Q:17:LYS:H	1.66	0.59
9:H:100:ILE:HD12	9:H:122:LEU:HD12	1.83	0.59
27:I:11:ARG:NH1	27:I:15:GLY:O	2.36	0.58
1:2:1398:G:O6	1:2:1448:A:N1	2.36	0.58
1:2:1588:A:H2'	1:2:1589:A:C8	2.39	0.58
1:2:1606:G:H5'	19:T:86:GLY:HA2	1.85	0.58
19:T:140:ALA:HA	19:T:144:LYS:HD3	1.84	0.58
21:Q:40:GLU:O	21:Q:45:ARG:NH1	2.33	0.58
27:I:119:LEU:HD11	27:I:153:LYS:HG3	1.84	0.58
1:2:1856:C:H2'	1:2:1857:G:H8	1.69	0.58
13:x:150:LEU:HD23	13:x:153:ILE:HD12	1.85	0.58
1:2:1757:G:C6	1:2:1776:G:C2	2.92	0.58
1:2:828:G:N2	1:2:830:A:O2'	2.37	0.58
17:u:540:ILE:HD13	17:u:586:PRO:HG2	1.86	0.58
1:2:160:U:O2'	1:2:162:C:OP2	2.20	0.58
1:2:1486:A:OP1	30:K:1030:ARG:NH2	2.36	0.58
20:S:20:ILE:HD11	20:S:33:ILE:HG23	1.86	0.58
5:c:49:PRO:HG2	8:F:144:LEU:HD23	1.86	0.58
30:K:379:PRO:HD2	30:K:387:LEU:HD13	1.84	0.58
1:2:913:A:H1'	9:H:66:VAL:HB	1.86	0.57
1:2:1227:G:O6	1:2:1531:A:N1	2.37	0.57
1:2:462:C:OP1	17:u:130:LYS:NZ	2.37	0.57
1:2:1177:U:O2	1:2:1184:G:N2	2.32	0.57
9:H:20:GLU:HA	9:H:23:ILE:HG12	1.86	0.57
26:J:149:VAL:HG11	26:J:157:ILE:HD11	1.85	0.57
14:X:94:ILE:HG12	14:X:125:VAL:HG21	1.85	0.57
22:P:81:ARG:NH2	22:P:120:SER:O	2.37	0.57
1:2:103:A:OP2	1:2:356:C:N4	2.31	0.57
6:E:140:VAL:HG22	6:E:146:THR:HG22	1.86	0.57
10:G:137:ARG:HE	10:G:140:ARG:HH21	1.50	0.57
13:x:246:SER:OG	13:x:247:ARG:NH1	2.37	0.57
17:u:608:VAL:HG21	17:u:679:ILE:HD12	1.86	0.57
1:2:75:G:N2	10:G:155:GLN:O	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:11:ARG:HA	6:E:28:ALA:HB2	1.86	0.57
22:P:22:LEU:HD21	22:P:109:PRO:HB3	1.87	0.57
1:2:1722:G:O6	1:2:1812:U:O2	2.23	0.57
16:W:28:ARG:HB3	16:W:60:LYS:HG2	1.87	0.57
1:2:65:C:H4'	10:G:172:LYS:HE2	1.86	0.56
1:2:334:C:OP2	10:G:190:ARG:NH2	2.36	0.56
17:u:259:ASP:HB3	17:u:273:LYS:HZ3	1.70	0.56
1:2:1332:A:C6	1:2:1497:G:N1	2.73	0.56
1:2:1867:U:O2'	13:x:84:ARG:NH1	2.39	0.56
13:x:169:LYS:HD2	23:O:149:ARG:HE	1.69	0.56
25:L:119:ASP:O	25:L:147:LYS:NZ	2.38	0.56
17:u:531:GLN:HB2	18:t:366:LEU:HD21	1.86	0.56
25:L:4:ILE:HG23	25:L:5:GLN:HG2	1.86	0.56
30:K:410:LEU:HD13	30:K:413:LEU:HD12	1.87	0.56
1:2:1333:U:H2'	1:2:1495:G:H1	1.69	0.56
17:u:667:LEU:HB2	17:u:680:ALA:HB3	1.88	0.56
19:T:42:HIS:ND1	19:T:93:SER:OG	2.37	0.56
23:O:44:VAL:HG13	23:O:53:ILE:HB	1.87	0.56
30:K:171:LEU:O	30:K:175:LEU:HB2	2.06	0.56
1:2:954:U:O2	23:O:55:ARG:NH2	2.38	0.56
30:K:730:ASN:ND2	30:K:765:ASP:OD1	2.38	0.56
1:2:1536:G:H2'	1:2:1537:A:H8	1.71	0.56
8:F:179:ASN:HD21	8:F:186:ASN:HB2	1.70	0.56
27:I:76:THR:HG21	27:I:104:ILE:HD12	1.88	0.56
10:G:152:ASP:HB3	10:G:155:GLN:HG2	1.88	0.56
25:L:60:CYS:HG	25:L:114:SER:HG	1.54	0.56
1:2:164:A:H3'	1:2:165:G:H21	1.71	0.56
11:Z:100:VAL:HB	11:Z:108:ILE:HG13	1.88	0.56
29:q:168:SER:HB2	30:K:1200:GLU:HG2	1.86	0.56
1:2:1285:G:O6	31:M:82:ASN:ND2	2.39	0.55
9:H:101:LEU:O	9:H:116:ARG:NH1	2.38	0.55
1:2:973:C:N3	23:O:55:ARG:NH1	2.54	0.55
5:c:44:ARG:HH21	5:c:58:LEU:HD23	1.72	0.55
20:S:73:ASN:ND2	20:S:76:GLN:OE1	2.39	0.55
30:K:113:PHE:HD1	30:K:127:VAL:HG21	1.71	0.55
1:2:1030:A:H2'	1:2:1031:A:H8	1.72	0.55
12:Y:7:ILE:HB	12:Y:47:MET:HE1	1.87	0.55
15:w:83:ARG:NH1	15:w:84:GLU:O	2.40	0.55
30:K:597:LYS:HG3	30:K:601:MET:HE2	1.87	0.55
30:K:652:SER:O	30:K:658:ARG:NH2	2.39	0.55
1:2:573:U:O2'	1:2:575:A:N7	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:981:A:H2'	1:2:982:G:C8	2.41	0.55
11:Z:50:PHE:HB2	20:S:4:VAL:HA	1.88	0.55
26:J:128:VAL:O	26:J:132:GLN:HG3	2.07	0.55
1:2:507:G:OP2	12:Y:104:ARG:NH2	2.37	0.55
5:c:55:VAL:HG23	8:F:34:SER:HA	1.89	0.55
1:2:1753:C:H2'	1:2:1754:G:H8	1.72	0.55
28:r:116:MET:HG2	29:q:110:PRO:HG3	1.89	0.55
4:B:25:PHE:HA	4:B:28:LYS:HG2	1.89	0.55
13:x:167:ASP:O	23:O:142:ARG:NH2	2.33	0.55
29:q:189:VAL:HB	30:K:1252:ALA:HB3	1.89	0.55
12:Y:55:ILE:HG12	12:Y:75:ILE:HG12	1.88	0.54
1:2:312:G:O2'	10:G:191:ARG:NH1	2.41	0.54
25:L:22:ARG:HE	25:L:27:GLU:HA	1.72	0.54
1:2:536:A:H61	1:2:548:C:H42	0.71	0.54
1:2:1005:G:OP2	4:B:162:ARG:NH2	2.40	0.54
1:2:1367:U:O2	1:2:1373:C:N3	2.40	0.54
15:w:55:SER:HB2	30:K:1109:LEU:HG	1.88	0.54
1:2:1348:G:O6	1:2:1381:G:O6	2.25	0.54
6:E:9:LEU:HB2	6:E:30:ARG:HD3	1.89	0.54
11:Z:73:VAL:O	11:Z:77:LEU:HB2	2.08	0.54
1:2:614:C:N4	1:2:629:A:N6	2.34	0.54
1:2:1217:A:H2'	1:2:1218:C:H6	1.72	0.54
6:E:54:TYR:O	12:Y:15:ASN:ND2	2.41	0.54
1:2:1272:C:OP1	1:2:1303:C:O2'	2.26	0.54
30:K:245:THR:HG21	30:K:310:LEU:HD11	1.90	0.54
1:2:145:G:H2'	1:2:146:G:C8	2.43	0.54
1:2:1329:U:O2	1:2:1500:G:O6	2.26	0.54
6:E:115:THR:HG22	6:E:117:GLU:H	1.73	0.54
10:G:20:ASP:HB3	10:G:23:LYS:HD2	1.91	0.53
30:K:869:VAL:O	30:K:874:ARG:NH2	2.39	0.53
8:F:44:LYS:NZ	21:Q:114:GLN:OE1	2.37	0.53
17:u:262:PRO:HA	17:u:270:GLY:HA3	1.89	0.53
17:u:624:ARG:NH2	17:u:780:ASP:OD2	2.39	0.53
21:Q:34:VAL:HG12	21:Q:70:VAL:HB	1.90	0.53
1:2:1302:G:O6	1:2:1307:U:O4	2.27	0.53
9:H:105:THR:HG23	9:H:107:LYS:H	1.73	0.53
22:P:81:ARG:NH2	22:P:117:GLY:O	2.41	0.53
1:2:1228:A:H2'	1:2:1229:G:C8	2.43	0.53
28:r:8:LEU:HD22	29:q:115:THR:HG23	1.91	0.53
1:2:1536:G:H2'	1:2:1537:A:C8	2.44	0.53
3:b:67:THR:OG1	3:b:70:LYS:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:r:6:HIS:CE1	28:r:25:LEU:HD11	2.43	0.53
1:2:1465:A:OP1	2:R:60:ARG:NH1	2.41	0.53
26:J:128:VAL:HG13	26:J:132:GLN:HE21	1.73	0.53
30:K:837:LEU:HA	30:K:840:LEU:HD12	1.89	0.53
11:Z:64:ASN:HA	11:Z:111:ARG:HD3	1.91	0.53
33:a:71:VAL:O	33:a:123:ARG:NH1	2.42	0.53
6:E:197:ASN:HB3	6:E:209:HIS:HB2	1.91	0.53
12:Y:114:MET:O	12:Y:122:LYS:NZ	2.38	0.53
6:E:8:HIS:O	6:E:30:ARG:NH1	2.42	0.53
8:F:195:GLU:HG2	29:q:16:LEU:HD13	1.91	0.53
30:K:334:MET:HE3	30:K:346:MET:HE3	1.90	0.53
30:K:710:ARG:NH1	30:K:752:SER:OG	2.40	0.53
1:2:446:G:OP2	27:I:47:ARG:NH2	2.39	0.53
23:O:86:LYS:NZ	23:O:122:SER:O	2.41	0.53
33:a:110:MET:HE2	33:a:288:LEU:HD22	1.91	0.53
1:2:64:A:OP1	10:G:177:GLN:NE2	2.42	0.52
1:2:1562:C:H2'	1:2:1563:G:H8	1.74	0.52
13:x:162:SER:HB3	23:O:107:THR:HG21	1.91	0.52
28:r:113:ILE:HG21	29:q:88:LEU:HD13	1.89	0.52
30:K:113:PHE:HB2	30:K:127:VAL:HG11	1.89	0.52
1:2:1016:U:H5''	24:N:14:SER:HB2	1.90	0.52
22:P:24:GLN:O	22:P:28:MET:N	2.42	0.52
30:K:633:PRO:HB2	30:K:636:VAL:HB	1.90	0.52
8:F:167:LYS:NZ	8:F:175:ASP:OD2	2.43	0.52
29:q:153:LEU:O	29:q:155:ARG:NH1	2.42	0.52
1:2:155:G:H4'	10:G:15:LEU:HD13	1.92	0.52
25:L:86:ILE:HD13	25:L:113:LEU:HD22	1.92	0.52
1:2:957:A:H3'	1:2:958:G:H21	1.74	0.52
1:2:1856:C:H2'	1:2:1857:G:C8	2.45	0.52
4:B:168:MET:HG2	4:B:197:ILE:HG21	1.91	0.52
17:u:158:PHE:HB2	17:u:187:LEU:HD13	1.92	0.52
30:K:865:CYS:HA	30:K:868:GLU:HB2	1.92	0.52
8:F:49:LEU:HD12	21:Q:50:LYS:HG2	1.92	0.52
27:I:34:ALA:HB2	27:I:56:ARG:HD2	1.91	0.52
17:u:155:THR:HG21	17:u:236:LEU:HD22	1.92	0.52
1:2:847:A:OP1	6:E:108:ARG:NH1	2.43	0.52
14:X:101:LEU:HB3	14:X:124:LYS:HB2	1.91	0.52
1:2:1143:A:H5'	34:z:104:LYS:HD2	1.91	0.51
15:w:419:ARG:NH1	15:w:420:GLU:OE2	2.41	0.51
18:t:293:ARG:NH2	32:f:144:CYS:O	2.40	0.51
30:K:864:LEU:HD12	34:z:190:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:943:U:H2'	1:2:944:A:H8	1.75	0.51
32:f:114:ILE:O	32:f:116:ARG:NH1	2.43	0.51
1:2:171:A:OP1	10:G:137:ARG:NH1	2.42	0.51
1:2:1366:G:OP2	30:K:251:LYS:NZ	2.42	0.51
2:R:26:ASN:HD22	30:K:620:TRP:HH2	1.58	0.51
1:2:367:U:H4'	1:2:371:A:C8	2.45	0.51
21:Q:44:PRO:HG2	21:Q:81:ILE:HD11	1.91	0.51
32:f:107:LYS:O	32:f:114:ILE:N	2.44	0.51
1:2:943:U:OP1	4:B:214:LYS:NZ	2.41	0.51
4:B:117:TRP:HB3	4:B:153:THR:HG22	1.92	0.51
1:2:433:A:H5''	27:I:22:HIS:HB3	1.91	0.51
1:2:1811:C:O2'	17:u:63:GLN:OE1	2.20	0.51
4:B:90:ASP:HB2	4:B:97:LEU:HB2	1.91	0.51
22:P:57:LEU:HD21	22:P:89:MET:HE2	1.93	0.51
30:K:201:GLN:HB3	30:K:210:LEU:HD13	1.92	0.51
30:K:506:HIS:HB3	30:K:542:MET:HE2	1.93	0.51
1:2:153:G:N3	10:G:13:GLN:NE2	2.59	0.51
25:L:85:THR:HG22	25:L:112:HIS:HA	1.93	0.51
31:M:56:CYS:HG	31:M:61:TYR:HH	1.59	0.51
1:2:918:U:O2'	16:W:56:HIS:O	2.29	0.51
14:X:50:ILE:HG12	14:X:75:ILE:HD11	1.91	0.51
25:L:60:CYS:SG	25:L:114:SER:OG	2.65	0.51
27:I:190:LEU:HD21	27:I:198:TYR:HD2	1.75	0.51
30:K:535:VAL:HG12	30:K:572:VAL:HG11	1.93	0.51
1:2:831:G:N7	12:Y:11:LYS:NZ	2.56	0.51
1:2:1669:G:H5'	21:Q:130:LYS:HB2	1.93	0.51
1:2:1685:U:O3'	30:K:1195:LEU:HD11	2.10	0.51
4:B:52:THR:HG22	4:B:54:GLY:H	1.75	0.51
1:2:928:G:H2'	1:2:929:G:C8	2.46	0.51
1:2:943:U:H2'	1:2:944:A:C8	2.45	0.51
1:2:1214:A:OP2	15:w:36:LYS:NZ	2.42	0.51
1:2:1653:U:H3	1:2:1671:G:H1	1.59	0.51
3:b:38:PRO:HD3	3:b:77:CYS:HA	1.93	0.51
10:G:45:TRP:HA	10:G:48:TYR:HD2	1.76	0.51
13:x:99:ILE:HA	13:x:103:LEU:HD12	1.93	0.51
30:K:830:SER:OG	34:z:186:ARG:NH1	2.44	0.51
1:2:857:U:H2'	1:2:858:A:C8	2.46	0.50
1:2:1227:G:C6	1:2:1531:A:N1	2.79	0.50
8:F:30:ILE:HG13	8:F:117:ILE:HD11	1.93	0.50
30:K:838:LYS:O	30:K:841:LEU:HB3	2.10	0.50
9:H:140:VAL:HG12	24:N:19:ARG:HE	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:u:719:ASN:OD1	17:u:720:ARG:N	2.43	0.50
23:O:45:THR:HG22	23:O:52:THR:HA	1.93	0.50
1:2:659:G:HO2'	1:2:662:G:HO2'	1.59	0.50
25:L:23:VAL:HG23	25:L:26:GLY:H	1.75	0.50
30:K:367:ASN:HB3	30:K:401:LEU:HD13	1.92	0.50
11:Z:68:ILE:HB	11:Z:109:TYR:HB2	1.94	0.50
15:w:339:SER:HA	15:w:342:LEU:HD12	1.94	0.50
27:I:83:TYR:HB3	27:I:101:ILE:HB	1.94	0.50
1:2:223:C:H2'	1:2:224:A:C8	2.46	0.50
6:E:128:LYS:HG2	6:E:140:VAL:HB	1.91	0.50
30:K:136:ARG:NH2	30:K:173:LEU:O	2.44	0.50
33:a:123:ARG:HE	33:a:155:LEU:HB2	1.77	0.50
1:2:1348:G:N7	1:2:1381:G:N1	2.52	0.50
3:b:34:ASP:O	3:b:79:PHE:HA	2.12	0.50
8:F:39:ILE:HG21	8:F:113:VAL:HG23	1.94	0.50
28:r:115:ASN:HA	29:q:102:LEU:HB3	1.94	0.50
30:K:998:ARG:HG3	30:K:1001:ARG:HH21	1.76	0.50
1:2:1161:U:O4	14:X:2:GLY:N	2.45	0.50
1:2:1748:G:H2'	1:2:1749:G:H8	1.77	0.50
8:F:198:ARG:HH12	29:q:16:LEU:HD21	1.77	0.50
10:G:7:PHE:O	10:G:11:GLY:N	2.42	0.50
23:O:31:CYS:HB2	23:O:93:LEU:HD13	1.93	0.50
28:r:3:LEU:HB2	28:r:88:LEU:HA	1.92	0.50
1:2:643:A:OP1	26:J:39:ASN:ND2	2.45	0.50
8:F:157:GLY:O	8:F:161:ALA:HB2	2.12	0.50
30:K:264:LEU:HD11	30:K:284:THR:HG21	1.93	0.50
30:K:1247:ARG:NH2	30:K:1251:TYR:OH	2.45	0.50
23:O:139:SER:OG	23:O:140:THR:N	2.44	0.49
29:q:63:GLY:HA2	29:q:87:MET:HB3	1.94	0.49
1:2:885:U:O2	1:2:902:G:C6	2.65	0.49
17:u:78:LYS:HG2	17:u:311:LEU:HB3	1.94	0.49
27:I:61:ASP:OD1	27:I:61:ASP:N	2.43	0.49
1:2:614:C:OP1	17:u:508:SER:OG	2.24	0.49
2:R:13:ALA:O	2:R:17:ILE:HG12	2.12	0.49
10:G:135:PRO:HG2	10:G:141:ILE:HG12	1.94	0.49
15:w:328:LYS:HE3	18:t:267:TYR:HB2	1.94	0.49
1:2:1277:C:C2	1:2:1322:G:N2	2.79	0.49
1:2:1332:A:C6	1:2:1497:G:C6	3.00	0.49
1:2:658:U:N3	14:X:20:GLN:O	2.37	0.49
1:2:913:A:H2	9:H:99:ARG:H	1.59	0.49
1:2:955:A:N1	1:2:968:U:O2'	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:66:VAL:HG21	30:K:618:LEU:HD21	1.95	0.49
27:I:98:LYS:NZ	27:I:176:ALA:O	2.42	0.49
14:X:93:PHE:O	14:X:140:ARG:NH1	2.39	0.49
20:S:68:ILE:O	20:S:72:GLN:HG2	2.13	0.49
30:K:638:ILE:O	30:K:641:LYS:NZ	2.45	0.49
33:a:123:ARG:HH22	33:a:126:TYR:HD2	1.60	0.49
1:2:991:G:H5''	1:2:991:G:H8	1.78	0.49
5:c:46:VAL:HG12	8:F:140:ASP:HB2	1.95	0.49
15:w:375:PRO:HB2	15:w:377:LEU:HG	1.93	0.49
17:u:739:GLY:HA3	17:u:755:PHE:HD1	1.78	0.49
28:r:38:ASN:HB3	28:r:41:PHE:HD2	1.77	0.49
29:q:88:LEU:HD22	29:q:100:LEU:HD13	1.94	0.49
1:2:494:C:N4	1:2:509:G:H21	2.10	0.49
3:b:3:LEU:HD22	16:W:22:LYS:HD3	1.93	0.49
4:B:143:THR:HB	4:B:205:TYR:CE2	2.48	0.49
2:R:78:ARG:HD3	2:R:81:ARG:HH21	1.78	0.49
8:F:42:LYS:O	8:F:46:ALA:N	2.45	0.49
12:Y:113:ARG:NH2	12:Y:126:GLY:O	2.46	0.49
30:K:1024:LEU:HD12	30:K:1032:LEU:HD11	1.94	0.49
1:2:1331:C:H2'	1:2:1332:A:C8	2.48	0.49
17:u:730:GLU:HG3	17:u:740:HIS:CE1	2.47	0.49
1:2:682:U:OP2	14:X:8:ARG:NH1	2.46	0.48
1:2:1839:U:O2	17:u:13:ASN:ND2	2.45	0.48
4:B:126:ASP:OD1	4:B:136:ARG:NE	2.38	0.48
12:Y:5:VAL:HG22	12:Y:29:HIS:HB3	1.95	0.48
28:r:44:ARG:HD2	29:q:54:PRO:HG2	1.95	0.48
33:a:31:ILE:HA	33:a:45:VAL:O	2.13	0.48
28:r:8:LEU:HD23	29:q:112:LYS:HE3	1.95	0.48
1:2:1047:C:H1'	23:O:141:ARG:HD3	1.94	0.48
1:2:1681:U:O4	15:w:36:LYS:NZ	2.43	0.48
2:R:21:TYR:HA	2:R:24:LEU:HD12	1.95	0.48
5:c:36:ASP:N	5:c:36:ASP:OD1	2.46	0.48
1:2:201:C:H3'	1:2:202:G:H8	1.77	0.48
1:2:1332:A:N6	1:2:1497:G:O6	2.47	0.48
1:2:1606:G:H22	1:2:1632:G:H1'	1.79	0.48
4:B:127:VAL:HG11	4:B:176:VAL:HG11	1.96	0.48
22:P:95:GLY:HA2	22:P:103:ASN:O	2.13	0.48
1:2:153:G:H21	10:G:13:GLN:HE22	1.60	0.48
1:2:1302:G:O6	1:2:1306:U:O4	2.32	0.48
28:r:18:SER:OG	28:r:19:ARG:NH2	2.33	0.48
28:r:51:TRP:NE1	28:r:67:PRO:O	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:q:69:SER:OG	29:q:94:ARG:NH2	2.46	0.48
1:2:402:C:OP1	27:I:14:THR:OG1	2.31	0.48
1:2:1331:C:N4	1:2:1499:U:H3	2.11	0.48
8:F:48:TYR:HD2	21:Q:53:GLU:HG2	1.78	0.48
10:G:52:ILE:HA	10:G:111:LEU:HD23	1.96	0.48
10:G:59:GLN:OE1	10:G:72:ARG:NH2	2.46	0.48
28:r:3:LEU:HA	28:r:6:HIS:CD2	2.48	0.48
33:a:128:HIS:HE1	33:a:133:ILE:HG22	1.78	0.48
1:2:682:U:O2'	16:W:4:MET:SD	2.72	0.48
2:R:34:VAL:HA	2:R:37:GLU:HG3	1.96	0.48
13:x:198:THR:O	13:x:217:ASN:ND2	2.33	0.48
24:N:46:THR:OG1	24:N:49:GLN:OE1	2.25	0.48
33:a:204:MET:HA	33:a:207:LEU:HB2	1.96	0.48
33:a:67:LEU:HB3	33:a:73:ILE:HG13	1.95	0.48
15:w:180:ARG:HG3	18:t:298:LEU:HD11	1.96	0.48
22:P:75:VAL:HG22	22:P:104:GLN:HE21	1.79	0.48
30:K:780:LEU:O	30:K:788:GLN:NE2	2.43	0.48
1:2:496:C:H5'	6:E:29:PRO:HA	1.96	0.47
1:2:1685:U:H2'	1:2:1686:G:H8	1.78	0.47
30:K:993:SER:HB2	30:K:996:MET:HB2	1.96	0.47
1:2:115:U:OP1	1:2:382:C:O2'	2.30	0.47
13:x:230:LEU:HD12	23:O:149:ARG:HH11	1.79	0.47
17:u:86:LEU:HD13	17:u:149:MET:HB3	1.96	0.47
28:r:6:HIS:HA	28:r:9:LEU:HD12	1.97	0.47
1:2:640:A:H2'	1:2:641:A:C8	2.49	0.47
1:2:980:A:H2'	1:2:981:A:C8	2.49	0.47
1:2:1264:C:H1'	1:2:1265:A:C5	2.49	0.47
4:B:57:ILE:HG23	4:B:60:ASP:H	1.80	0.47
13:x:84:ARG:HA	13:x:84:ARG:HD2	1.72	0.47
30:K:942:GLN:HB3	34:z:211:LEU:HD13	1.95	0.47
1:2:380:G:OP1	27:I:56:ARG:NH2	2.41	0.47
1:2:996:A:H2'	1:2:997:A:C8	2.49	0.47
15:w:262:VAL:HG21	15:w:304:GLU:HG2	1.96	0.47
29:q:128:LEU:HD23	29:q:141:ARG:HG2	1.96	0.47
33:a:124:ILE:HG13	33:a:128:HIS:CD2	2.49	0.47
1:2:386:C:H5''	27:I:10:LYS:HD2	1.96	0.47
1:2:1228:A:H2'	1:2:1229:G:H8	1.79	0.47
1:2:1494:U:O2'	1:2:1495:G:OP2	2.31	0.47
2:R:64:GLY:O	30:K:621:GLN:NE2	2.43	0.47
2:R:69:ILE:HG22	30:K:1073:ILE:HD11	1.96	0.47
12:Y:86:GLU:OE2	12:Y:90:ARG:NE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:q:125:VAL:HB	29:q:161:LEU:HD11	1.96	0.47
30:K:201:GLN:OE1	30:K:204:SER:OG	2.33	0.47
2:R:24:LEU:HD23	2:R:34:VAL:HG21	1.97	0.47
6:E:178:GLY:N	6:E:195:ILE:O	2.45	0.47
15:w:227:ALA:HB1	15:w:271:HIS:HB2	1.95	0.47
31:M:61:TYR:HB3	32:f:103:LEU:HD21	1.97	0.47
1:2:795:A:H2'	1:2:796:G:C8	2.49	0.47
1:2:1275:G:O6	1:2:1324:G:N3	2.48	0.47
1:2:1759:G:H2'	1:2:1760:G:C8	2.50	0.47
15:w:185:TYR:HA	15:w:188:VAL:HG22	1.95	0.47
17:u:299:MET:HA	17:u:562:VAL:HA	1.95	0.47
17:u:476:LYS:HD3	17:u:476:LYS:HA	1.73	0.47
24:N:92:ILE:O	24:N:96:VAL:HG23	2.15	0.47
32:f:124:ASP:OD1	32:f:124:ASP:N	2.47	0.47
1:2:531:A:H2'	1:2:532:C:C6	2.50	0.47
1:2:1663:A:O2'	1:2:1664:A:O4'	2.30	0.47
15:w:47:GLU:OE2	21:Q:15:ARG:NH2	2.47	0.47
17:u:89:PRO:HA	17:u:159:LEU:HB2	1.96	0.47
30:K:428:HIS:HB2	30:K:431:VAL:HG12	1.96	0.47
4:B:28:LYS:HD2	4:B:50:THR:HA	1.97	0.47
23:O:19:PRO:HG2	23:O:27:VAL:HG21	1.97	0.47
30:K:863:ILE:O	30:K:866:THR:OG1	2.23	0.47
30:K:921:ILE:HD11	30:K:950:LEU:HD13	1.96	0.47
1:2:1648:G:N2	1:2:1675:A:OP2	2.29	0.47
8:F:109:LEU:HD12	8:F:112:LEU:HD23	1.97	0.47
10:G:223:LYS:HA	10:G:223:LYS:HD3	1.69	0.47
13:x:94:LYS:HG3	13:x:146:VAL:HG11	1.97	0.47
13:x:179:ALA:HB1	13:x:229:ILE:HG22	1.96	0.47
30:K:975:VAL:HA	30:K:978:LEU:HB2	1.96	0.47
31:M:55:ASN:ND2	31:M:82:ASN:OD1	2.47	0.47
33:a:124:ILE:HA	33:a:127:VAL:HG12	1.97	0.47
1:2:1513:C:H2'	1:2:1514:G:H8	1.79	0.46
10:G:37:ALA:HA	10:G:49:VAL:HG12	1.97	0.46
9:H:68:GLN:O	9:H:71:SER:OG	2.24	0.46
17:u:144:HIS:CE1	17:u:786:PRO:HD3	2.49	0.46
1:2:1325:G:O2'	1:2:1327:G:OP2	2.29	0.46
30:K:148:PHE:HE2	30:K:190:THR:HG22	1.80	0.46
30:K:928:LEU:HD23	30:K:968:VAL:HG12	1.97	0.46
1:2:1189:A:H2'	1:2:1190:A:H8	1.80	0.46
5:c:46:VAL:HG21	5:c:50:VAL:HG21	1.98	0.46
9:H:8:ILE:HD11	9:H:41:ARG:HH12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:983:A:OP1	1:2:1073:U:O2'	2.25	0.46
1:2:991:G:H1	1:2:1099:G:H21	1.63	0.46
1:2:1236:G:N2	1:2:1522:A:H62	2.07	0.46
1:2:1320:G:O2'	1:2:1322:G:N7	2.47	0.46
1:2:1736:G:H2'	1:2:1737:G:C8	2.51	0.46
16:W:30:CYS:SG	16:W:31:SER:N	2.89	0.46
30:K:1030:ARG:O	30:K:1034:ASN:ND2	2.46	0.46
33:a:238:GLU:HA	33:a:241:MET:HE2	1.96	0.46
1:2:218:U:O2	27:I:184:ARG:NH2	2.49	0.46
4:B:120:MET:HG3	4:B:142:PHE:CE1	2.50	0.46
6:E:63:LYS:HE3	12:Y:85:ASN:HA	1.98	0.46
17:u:268:LEU:HD22	17:u:567:VAL:HG11	1.97	0.46
17:u:592:SER:OG	17:u:593:VAL:N	2.47	0.46
1:2:1367:U:O2	1:2:1373:C:C4	2.68	0.46
10:G:136:LYS:HB3	10:G:136:LYS:HE3	1.72	0.46
26:J:103:GLU:O	26:J:107:GLU:HG2	2.16	0.46
29:q:250:ALA:HA	29:q:253:LEU:HD12	1.97	0.46
1:2:1334:G:H2'	1:2:1335:G:H8	1.81	0.46
1:2:1736:G:H2'	1:2:1737:G:H8	1.80	0.46
15:w:326:MET:HA	15:w:329:ILE:HG22	1.97	0.46
24:N:115:LEU:O	24:N:119:GLU:HG3	2.16	0.46
1:2:1473:G:N2	1:2:1476:A:OP2	2.39	0.46
15:w:401:LEU:HA	15:w:404:LEU:HD12	1.98	0.46
22:P:108:LYS:HB2	22:P:111:MET:HG3	1.97	0.46
29:q:39:MET:SD	29:q:201:TYR:OH	2.70	0.46
1:2:480:G:H4'	17:u:68:VAL:HG11	1.98	0.46
1:2:1143:A:H2'	1:2:1144:A:C8	2.51	0.46
27:I:87:ASN:HB3	27:I:90:LEU:HG	1.98	0.46
29:q:72:SER:OG	29:q:78:TRP:NE1	2.42	0.46
30:K:1110:LYS:HB3	30:K:1128:ARG:HG2	1.97	0.46
1:2:387:C:OP2	27:I:10:LYS:NZ	2.46	0.45
1:2:455:A:O2'	1:2:1735:A:N3	2.45	0.45
1:2:1299:A:H4'	22:P:59:ARG:HH12	1.81	0.45
30:K:112:ARG:HH21	30:K:126:ALA:HB2	1.81	0.45
1:2:220:U:H2'	1:2:221:A:C8	2.52	0.45
1:2:615:C:H42	1:2:628:A:H61	0.67	0.45
1:2:798:G:H8	1:2:799:U:H5'	1.79	0.45
1:2:1183:A:H2'	1:2:1184:G:H8	1.80	0.45
1:2:1685:U:H2'	1:2:1686:G:C8	2.51	0.45
15:w:397:GLN:HG3	18:t:250:MET:HE1	1.98	0.45
16:W:71:LYS:O	16:W:129:PHE:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:138:LYS:HG2	33:a:141:ASN:HB2	1.98	0.45
1:2:530:U:H2'	1:2:531:A:H8	1.81	0.45
15:w:416:GLU:HG3	15:w:419:ARG:HH21	1.81	0.45
22:P:21:ASP:H	22:P:24:GLN:NE2	2.14	0.45
30:K:221:LEU:HD11	30:K:237:VAL:HG12	1.99	0.45
1:2:417:C:OP1	26:J:17:ARG:NH2	2.50	0.45
1:2:1144:A:H2'	1:2:1145:A:C8	2.51	0.45
1:2:1367:U:N3	1:2:1373:C:N4	2.64	0.45
1:2:1630:A:H5''	20:S:37:GLY:H	1.82	0.45
19:T:60:THR:HG23	19:T:75:MET:HE2	1.97	0.45
29:q:187:MET:HE1	29:q:200:PHE:HB3	1.99	0.45
10:G:2:LYS:HB2	10:G:108:VAL:HG23	1.98	0.45
19:T:60:THR:O	19:T:64:LEU:HG	2.17	0.45
29:q:202:LEU:HD11	30:K:1256:LEU:HD11	1.98	0.45
1:2:30:C:O2'	1:2:596:U:OP1	2.33	0.45
1:2:944:A:H5''	23:O:134:PRO:HB3	1.97	0.45
9:H:69:LEU:HD22	9:H:96:ALA:HB2	1.98	0.45
19:T:45:LEU:HD22	20:S:42:HIS:CE1	2.50	0.45
30:K:142:GLU:HA	30:K:143:THR:HA	1.58	0.45
30:K:539:VAL:O	30:K:543:GLY:N	2.50	0.45
1:2:186:C:H2'	1:2:187:G:H8	1.82	0.45
1:2:1367:U:C2	1:2:1373:C:N3	2.85	0.45
1:2:292:A:O2'	25:L:39:ASN:O	2.33	0.45
1:2:562:U:H2'	1:2:563:G:C8	2.51	0.45
1:2:962:A:H5'	23:O:66:ARG:HD3	1.99	0.45
1:2:1272:C:OP1	32:f:90:LYS:NZ	2.43	0.45
1:2:1595:U:H2'	1:2:1596:U:C6	2.52	0.45
30:K:136:ARG:HG2	30:K:177:ARG:HG3	1.99	0.45
30:K:308:LEU:HD23	30:K:311:LEU:HD12	1.98	0.45
24:N:87:ASP:N	24:N:87:ASP:OD1	2.50	0.45
30:K:384:LEU:HD11	30:K:430:GLN:HB2	1.98	0.45
1:2:507:G:P	12:Y:104:ARG:HH22	2.41	0.45
1:2:1018:U:O2'	24:N:86:GLU:OE2	2.34	0.45
1:2:1275:G:C6	1:2:1324:G:N2	2.85	0.45
1:2:1758:G:H2'	1:2:1759:G:C8	2.51	0.45
6:E:175:PHE:HE2	6:E:225:ILE:HG21	1.81	0.45
20:S:67:VAL:O	20:S:71:MET:HG2	2.17	0.45
34:z:175:PRO:HG2	34:z:181:MET:HB3	1.98	0.45
1:2:429:C:O2'	1:2:811:A:N1	2.45	0.44
1:2:1776:G:H2'	1:2:1777:G:C8	2.52	0.44
1:2:1798:C:H2'	1:2:1799:G:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Q:112:LEU:HD12	21:Q:120:LEU:HD11	1.98	0.44
29:q:105:MET:HB2	29:q:145:PHE:CE1	2.52	0.44
30:K:488:SER:HB3	30:K:527:HIS:CE1	2.53	0.44
30:K:568:TRP:CD1	30:K:568:TRP:H	2.35	0.44
30:K:624:THR:HG22	30:K:660:THR:HG21	1.99	0.44
33:a:221:TRP:HB3	33:a:239:LYS:HD3	2.00	0.44
33:a:267:ARG:H	33:a:270:GLU:HG2	1.82	0.44
14:X:67:ARG:HE	14:X:84:PHE:HE1	1.65	0.44
15:w:255:LEU:HD13	15:w:290:ILE:HG23	1.98	0.44
30:K:112:ARG:HE	30:K:126:ALA:HA	1.82	0.44
13:x:91:ASN:O	13:x:95:ILE:HG12	2.16	0.44
30:K:315:LEU:HB3	30:K:352:LEU:HD13	1.99	0.44
31:M:32:ALA:HB1	31:M:37:GLU:HB3	1.98	0.44
1:2:535:G:H2'	1:2:536:A:H8	1.81	0.44
17:u:737:ARG:HH21	17:u:757:GLY:HA3	1.80	0.44
19:T:14:PHE:HA	19:T:138:VAL:HG21	1.98	0.44
22:P:24:GLN:O	22:P:28:MET:HG3	2.17	0.44
25:L:39:ASN:OD1	25:L:39:ASN:N	2.47	0.44
30:K:210:LEU:HA	30:K:213:VAL:HG12	1.99	0.44
1:2:1010:G:H2'	1:2:1011:A:C8	2.46	0.44
22:P:145:LYS:HA	22:P:145:LYS:HD2	1.88	0.44
31:M:122:ASP:HA	31:M:125:GLU:HG2	1.98	0.44
1:2:296:U:O2'	6:E:131:VAL:O	2.32	0.44
1:2:991:G:H1	1:2:1099:G:N2	2.16	0.44
1:2:1189:A:H2'	1:2:1190:A:C8	2.53	0.44
2:R:16:ILE:HD12	2:R:16:ILE:HA	1.91	0.44
19:T:31:PRO:HG3	19:T:102:ARG:HG2	1.99	0.44
26:J:24:ARG:NH1	26:J:28:GLU:OE2	2.44	0.44
30:K:136:ARG:HG3	30:K:174:VAL:HG13	2.00	0.44
30:K:1029:HIS:HA	30:K:1032:LEU:HD12	2.00	0.44
33:a:135:ARG:HH21	33:a:182:THR:HG21	1.83	0.44
1:2:885:U:O2	1:2:901:G:C6	2.71	0.44
1:2:1753:C:H2'	1:2:1754:G:C8	2.52	0.44
1:2:1776:G:H2'	1:2:1777:G:H8	1.82	0.44
4:B:60:ASP:HA	4:B:63:LYS:HE2	2.00	0.44
13:x:201:ARG:HG2	15:w:19:LEU:HD12	1.99	0.44
15:w:276:LEU:HD12	15:w:276:LEU:HA	1.84	0.44
17:u:260:PHE:HB2	17:u:570:VAL:HG21	2.00	0.44
26:J:120:ALA:HB2	26:J:129:LEU:HD12	2.00	0.44
31:M:80:ASP:OD1	31:M:80:ASP:N	2.51	0.44
1:2:1579:A:O2'	1:2:1581:C:OP2	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:4:ASN:O	10:G:110:ASN:HA	2.18	0.44
15:w:269:ASN:OD1	15:w:270:PHE:N	2.49	0.44
19:T:104:LEU:HD13	19:T:121:ARG:HD3	2.00	0.44
28:r:2:LYS:O	28:r:5:THR:OG1	2.28	0.44
28:r:116:MET:N	29:q:102:LEU:O	2.48	0.44
30:K:456:SER:HA	30:K:504:GLN:HB3	2.00	0.44
9:H:76:GLN:HE21	9:H:76:GLN:HA	1.82	0.44
10:G:19:ASP:OD1	10:G:19:ASP:N	2.49	0.44
15:w:211:SER:HB2	33:a:168:ARG:HH12	1.82	0.44
1:2:581:U:H4'	12:Y:66:GLY:HA2	2.00	0.43
17:u:126:CYS:O	17:u:130:LYS:N	2.50	0.43
22:P:51:ARG:O	22:P:55:SER:OG	2.26	0.43
27:I:3:ILE:O	27:I:30:GLY:N	2.35	0.43
1:2:126:G:H8	10:G:199:THR:HG21	1.83	0.43
1:2:1279:C:H2'	1:2:1280:G:C8	2.53	0.43
1:2:1289:U:H2'	1:2:1290:G:C8	2.53	0.43
28:r:1:MET:HG3	28:r:109:ILE:HD13	1.98	0.43
30:K:338:HIS:HB3	30:K:341:VAL:HG12	2.00	0.43
33:a:279:GLN:OE1	33:a:282:ARG:NH2	2.51	0.43
1:2:1222:G:H2'	1:2:1223:A:C8	2.53	0.43
1:2:1276:A:N1	1:2:1322:G:N2	2.66	0.43
1:2:1331:C:H42	1:2:1499:U:H3	1.65	0.43
1:2:1332:A:N6	1:2:1497:G:C6	2.87	0.43
1:2:1513:C:H2'	1:2:1514:G:C8	2.52	0.43
4:B:28:LYS:HG3	4:B:48:LEU:HD21	1.99	0.43
10:G:203:LYS:HE2	10:G:203:LYS:HB2	1.86	0.43
15:w:206:ILE:HD13	18:t:297:VAL:HG21	2.00	0.43
32:f:132:MET:SD	32:f:139:HIS:HB3	2.57	0.43
1:2:448:A:H3'	27:I:23:LYS:HE2	2.00	0.43
1:2:528:A:H2'	1:2:529:A:C8	2.53	0.43
2:R:30:THR:HG22	2:R:33:ARG:HH21	1.83	0.43
5:c:67:ARG:NH2	8:F:128:ILE:HD13	2.33	0.43
6:E:52:LEU:HD13	6:E:54:TYR:HE2	1.83	0.43
13:x:227:ASN:HA	13:x:230:LEU:HB2	1.99	0.43
15:w:338:ASN:HA	15:w:341:PHE:CD2	2.54	0.43
1:2:1030:A:H2'	1:2:1031:A:C8	2.53	0.43
1:2:1286:G:H2'	1:2:1312:G:H22	1.83	0.43
1:2:1563:G:OP1	19:T:121:ARG:NH1	2.40	0.43
18:t:260:ASP:H	18:t:262:ARG:HH12	1.65	0.43
22:P:145:LYS:O	30:K:1253:TYR:OH	2.37	0.43
25:L:99:TYR:O	25:L:101:ARG:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:r:66:VAL:HG12	28:r:87:LEU:HD13	2.00	0.43
29:q:197:ALA:HA	29:q:199:LYS:HE2	2.00	0.43
30:K:945:GLU:O	30:K:948:CYS:HB2	2.19	0.43
1:2:1657:G:H1	1:2:1667:U:H3	1.67	0.43
9:H:101:LEU:HD23	9:H:101:LEU:HA	1.83	0.43
26:J:111:GLN:NE2	26:J:127:ARG:HB2	2.33	0.43
1:2:533:A:H2'	1:2:534:G:H8	1.83	0.43
1:2:1036:A:H4'	1:2:1855:G:N2	2.34	0.43
1:2:1333:U:O2	1:2:1495:G:C6	2.72	0.43
1:2:1610:G:O2'	20:S:86:ARG:NH1	2.52	0.43
1:2:1780:G:H2'	1:2:1781:A:C8	2.54	0.43
2:R:7:LYS:HA	2:R:7:LYS:HD3	1.84	0.43
15:w:396:ASP:OD1	15:w:396:ASP:N	2.49	0.43
15:w:405:LEU:HD13	15:w:418:ARG:HD3	2.00	0.43
26:J:131:ARG:HA	26:J:131:ARG:HD2	1.89	0.43
28:r:17:GLY:HA2	28:r:18:SER:HA	1.66	0.43
29:q:121:SER:HB3	29:q:161:LEU:HD12	2.01	0.43
30:K:294:LYS:HB3	30:K:294:LYS:HE2	1.86	0.43
32:f:96:LYS:HD2	32:f:96:LYS:HA	1.86	0.43
1:2:171:A:OP2	10:G:137:ARG:NH2	2.52	0.43
1:2:633:C:H2'	1:2:634:A:H8	1.84	0.43
1:2:1398:G:C6	1:2:1448:A:N1	2.87	0.43
4:B:125:VAL:O	4:B:136:ARG:HA	2.19	0.43
17:u:151:LYS:HB3	17:u:180:GLN:NE2	2.34	0.43
20:S:40:TYR:CZ	20:S:97:GLN:HG2	2.54	0.43
21:Q:108:ILE:O	21:Q:112:LEU:HG	2.19	0.43
27:I:22:HIS:ND1	27:I:23:LYS:O	2.39	0.43
30:K:390:TRP:HE3	30:K:391:LEU:HD22	1.84	0.43
33:a:297:ASP:OD1	33:a:298:TRP:N	2.52	0.43
1:2:962:A:N1	1:2:1055:A:O2'	2.51	0.43
6:E:62:LYS:HE2	6:E:62:LYS:HB3	1.80	0.43
8:F:162:ALA:O	8:F:164:ARG:N	2.46	0.43
17:u:705:LYS:HB3	17:u:712:VAL:HB	2.01	0.43
1:2:203:G:OP1	27:I:147:LYS:NZ	2.38	0.43
1:2:482:G:H5'	14:X:76:LYS:HB3	2.01	0.43
30:K:840:LEU:HA	30:K:843:ILE:HG12	2.01	0.43
30:K:975:VAL:HA	30:K:978:LEU:HD12	2.00	0.43
1:2:107:A:H2'	1:2:108:G:C8	2.54	0.42
1:2:379:C:H5'	27:I:33:ALA:HA	2.00	0.42
1:2:1454:A:H8	1:2:1455:A:H62	1.66	0.42
5:c:9:ILE:HG23	5:c:57:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:w:89:LEU:HD23	30:K:366:LEU:HD11	2.01	0.42
15:w:250:TYR:HB3	15:w:290:ILE:HG12	2.01	0.42
17:u:178:PHE:CE1	17:u:182:LEU:HD11	2.54	0.42
21:Q:49:TYR:O	21:Q:53:GLU:HG3	2.18	0.42
23:O:72:TYR:CZ	23:O:76:LEU:HD11	2.54	0.42
30:K:1120:PHE:HA	30:K:1125:VAL:HG21	2.01	0.42
1:2:463:C:H2'	1:2:465:A:N7	2.33	0.42
1:2:651:U:H2'	1:2:652:U:C6	2.55	0.42
33:a:120:MET:HE1	33:a:211:LEU:HB2	2.01	0.42
1:2:1665:G:P	19:T:88:MET:HE1	2.59	0.42
1:2:1674:G:OP1	8:F:51:HIS:NE2	2.41	0.42
4:B:185:VAL:O	4:B:189:ILE:HG12	2.19	0.42
15:w:390:LYS:HA	15:w:393:LEU:HD12	2.01	0.42
16:W:101:PHE:O	16:W:128:PHE:CA	2.32	0.42
17:u:148:ASP:HA	17:u:151:LYS:HG2	2.00	0.42
18:t:261:GLU:HB2	18:t:263:PHE:CE2	2.55	0.42
1:2:1546:G:H2'	1:2:1547:C:C6	2.55	0.42
23:O:54:CYS:HB3	23:O:81:VAL:HG23	2.00	0.42
28:r:66:VAL:O	28:r:68:LYS:NZ	2.40	0.42
31:M:23:LYS:O	31:M:27:ILE:HG12	2.20	0.42
33:a:115:MET:HG3	33:a:296:PHE:HE1	1.84	0.42
11:Z:49:LEU:HD23	20:S:5:ILE:HA	2.02	0.42
13:x:154:ARG:HH11	15:w:20:ALA:HB1	1.84	0.42
16:W:81:VAL:HG11	16:W:86:LEU:HD13	2.02	0.42
21:Q:96:TYR:HA	21:Q:100:VAL:HB	2.02	0.42
22:P:96:VAL:HG23	22:P:120:SER:HB3	2.02	0.42
33:a:179:LYS:HA	33:a:179:LYS:HD3	1.85	0.42
1:2:65:C:C2	10:G:133:LEU:HD22	2.55	0.42
1:2:75:G:O6	10:G:155:GLN:NE2	2.53	0.42
1:2:671:A:O2'	1:2:1089:G:OP1	2.24	0.42
30:K:937:THR:O	30:K:940:VAL:HB	2.19	0.42
30:K:1195:LEU:HA	30:K:1198:GLN:HB3	2.01	0.42
1:2:560:A:H5'	26:J:174:LYS:HB2	2.01	0.42
1:2:929:G:H2'	1:2:930:C:O4'	2.20	0.42
1:2:1182:A:C5	1:2:1183:A:H1'	2.54	0.42
1:2:1330:G:H2'	1:2:1331:C:C6	2.54	0.42
4:B:83:LYS:NZ	23:O:130:GLU:OE2	2.51	0.42
8:F:94:LYS:O	8:F:98:GLU:HG2	2.20	0.42
12:Y:63:HIS:CE1	12:Y:68:LYS:HD2	2.54	0.42
17:u:472:LEU:HD23	17:u:472:LEU:HA	1.89	0.42
17:u:491:PRO:HG3	17:u:499:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:K:725:ASP:OD1	30:K:725:ASP:N	2.53	0.42
1:2:1121:G:N2	4:B:202:GLN:O	2.53	0.42
1:2:1620:A:OP1	22:P:115:TYR:OH	2.27	0.42
15:w:303:ARG:HD3	15:w:306:ILE:HD11	2.02	0.42
17:u:287:ARG:NH1	17:u:586:PRO:HD3	2.26	0.42
25:L:113:LEU:HD11	25:L:117:PHE:HB2	2.02	0.42
29:q:63:GLY:HA3	35:q:301:SAH:HB1	2.01	0.42
30:K:716:THR:O	30:K:720:TYR:CB	2.65	0.42
33:a:198:GLN:HG2	33:a:202:ASP:HB2	2.01	0.42
1:2:302:A:H1'	27:I:73:THR:CG2	2.50	0.42
1:2:1675:A:OP1	8:F:86:LYS:NZ	2.41	0.42
30:K:889:LEU:HD22	30:K:895:GLN:HG2	2.00	0.42
33:a:124:ILE:HG13	33:a:128:HIS:HD2	1.85	0.42
1:2:1277:C:H2'	1:2:1278:A:H8	1.85	0.42
1:2:1605:G:OP1	19:T:84:ARG:NH2	2.42	0.42
1:2:1609:C:H42	1:2:1630:A:H61	0.71	0.42
29:q:153:LEU:HD23	29:q:153:LEU:HA	1.93	0.42
30:K:182:VAL:O	30:K:186:LYS:HG3	2.19	0.42
30:K:223:LYS:HA	30:K:223:LYS:HD3	1.89	0.42
1:2:28:U:H2'	1:2:29:G:C8	2.55	0.41
17:u:272:LEU:HD22	17:u:565:VAL:HG11	2.01	0.41
17:u:569:VAL:O	17:u:572:CYS:HB2	2.20	0.41
22:P:83:MET:HB3	22:P:116:LEU:HD12	2.02	0.41
26:J:28:GLU:HG2	26:J:43:VAL:HG11	2.02	0.41
27:I:44:HIS:O	27:I:56:ARG:N	2.45	0.41
30:K:264:LEU:HD23	30:K:264:LEU:HA	1.90	0.41
30:K:943:LEU:HD23	30:K:943:LEU:HA	1.94	0.41
34:z:218:LEU:HD23	34:z:218:LEU:HA	1.94	0.41
1:2:1564:C:OP1	19:T:121:ARG:NH2	2.47	0.41
1:2:1781:A:H2'	1:2:1782:G:C8	2.55	0.41
3:b:5:LYS:HD3	3:b:5:LYS:HA	1.85	0.41
4:B:167:LYS:O	4:B:171:ILE:HG12	2.20	0.41
9:H:75:ILE:HG22	9:H:78:ARG:HH21	1.84	0.41
13:x:233:PRO:HB3	17:u:11:GLN:HB2	2.02	0.41
14:X:125:VAL:HG23	14:X:130:LEU:HD21	2.03	0.41
17:u:161:ASP:OD1	17:u:161:ASP:N	2.51	0.41
17:u:303:ASP:OD1	17:u:303:ASP:N	2.49	0.41
19:T:128:GLN:HG2	19:T:129:ARG:HH22	1.85	0.41
30:K:860:PRO:HG3	34:z:197:PHE:HD2	1.84	0.41
33:a:228:THR:HG23	33:a:231:GLN:H	1.85	0.41
33:a:254:ALA:O	33:a:258:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:106:C:H2'	1:2:107:A:C8	2.55	0.41
1:2:375:U:H2'	1:2:376:A:C8	2.55	0.41
1:2:1018:U:H5''	24:N:71:ILE:HD12	2.02	0.41
1:2:1651:A:O2'	8:F:83:ASN:OD1	2.32	0.41
4:B:35:ALA:HB3	4:B:42:ARG:HA	2.01	0.41
9:H:30:LEU:HD21	9:H:36:LEU:HD12	2.01	0.41
17:u:100:MET:HE3	17:u:100:MET:HB3	1.93	0.41
21:Q:85:ARG:HA	21:Q:88:ILE:HG22	2.02	0.41
28:r:42:VAL:HA	28:r:45:MET:HG2	2.00	0.41
29:q:71:LEU:HD21	29:q:120:ILE:HD12	2.03	0.41
4:B:134:LEU:HB3	4:B:219:LYS:HB3	2.02	0.41
10:G:137:ARG:HE	10:G:140:ARG:NH2	2.16	0.41
29:q:57:LEU:HA	29:q:118:GLY:O	2.20	0.41
30:K:903:LEU:O	30:K:907:TYR:N	2.53	0.41
32:f:100:LEU:HB3	32:f:103:LEU:HD13	2.03	0.41
33:a:143:LEU:HD11	33:a:156:ILE:HD13	2.00	0.41
1:2:507:G:OP1	12:Y:108:LYS:NZ	2.53	0.41
1:2:1064:C:H2'	1:2:1065:G:H8	1.85	0.41
1:2:1797:U:H2'	1:2:1798:C:C6	2.55	0.41
13:x:208:LYS:HE2	13:x:208:LYS:HB3	1.87	0.41
29:q:78:TRP:HH2	29:q:96:ILE:HD12	1.85	0.41
30:K:308:LEU:HD23	30:K:308:LEU:HA	1.88	0.41
30:K:402:VAL:HG11	30:K:446:CYS:HB3	2.03	0.41
33:a:131:ASN:OD1	33:a:165:ARG:NE	2.42	0.41
33:a:279:GLN:HE21	33:a:283:ILE:HG13	1.85	0.41
1:2:1393:G:N2	34:z:179:SER:OG	2.48	0.41
12:Y:88:LYS:HD3	12:Y:88:LYS:HA	1.82	0.41
17:u:527:ILE:HB	17:u:592:SER:HA	2.02	0.41
1:2:600:G:N1	29:q:275:ARG:HB3	2.35	0.41
1:2:749:U:C4	1:2:750:C:N4	2.89	0.41
1:2:1279:C:H2'	1:2:1280:G:H8	1.86	0.41
28:r:40:ASN:HB3	29:q:54:PRO:HG3	2.03	0.41
31:M:18:LEU:HD22	31:M:77:ILE:HG21	2.03	0.41
1:2:1004:U:H2'	1:2:1005:G:C8	2.56	0.41
1:2:1217:A:H2'	1:2:1218:C:C6	2.54	0.41
23:O:100:THR:HG23	23:O:104:ARG:HB2	2.03	0.41
33:a:13:VAL:HG23	33:a:82:GLU:HG2	2.03	0.41
33:a:93:LEU:HD23	33:a:93:LEU:HA	1.92	0.41
1:2:933:G:H1'	1:2:1001:A:O4'	2.21	0.41
1:2:941:C:H2'	1:2:942:G:C8	2.56	0.41
1:2:1598:G:H2'	11:Z:80:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1845:A:H2'	1:2:1846:G:C8	2.56	0.41
3:b:25:VAL:HG13	16:W:55:ASP:HB3	2.03	0.41
8:F:42:LYS:HA	8:F:42:LYS:HD2	1.71	0.41
15:w:410:HIS:O	15:w:414:SER:OG	2.27	0.41
17:u:199:LYS:HE2	17:u:199:LYS:HB2	1.89	0.41
17:u:517:LYS:HD2	18:t:363:HIS:CE1	2.56	0.41
17:u:622:ARG:HG2	17:u:783:VAL:HG21	2.02	0.41
22:P:44:ARG:HG2	22:P:84:ILE:HD11	2.02	0.41
26:J:60:LEU:HD22	26:J:70:ARG:HA	2.03	0.41
30:K:304:THR:HA	30:K:307:MET:SD	2.61	0.41
30:K:818:LYS:HB3	30:K:818:LYS:HE2	1.88	0.41
30:K:860:PRO:HG2	34:z:194:ARG:HG2	2.03	0.41
1:2:559:G:O2'	1:2:560:A:H8	2.03	0.41
1:2:1177:U:O4	1:2:1184:G:O6	2.39	0.41
1:2:1296:U:H3	1:2:1301:A:H62	1.69	0.41
1:2:1726:G:H2'	1:2:1727:G:H8	1.86	0.41
15:w:222:PRO:HA	15:w:225:TRP:CD1	2.55	0.41
26:J:18:ARG:HA	26:J:19:PRO:HD3	1.97	0.41
29:q:65:GLY:O	29:q:69:SER:N	2.50	0.41
29:q:187:MET:HE3	29:q:187:MET:HB3	1.88	0.41
30:K:916:MET:HE1	34:z:196:ARG:HH21	1.86	0.41
1:2:28:U:H2'	1:2:29:G:H8	1.85	0.40
1:2:222:U:H5''	25:L:17:PHE:CG	2.56	0.40
1:2:535:G:H2'	1:2:536:A:C8	2.56	0.40
9:H:36:LEU:HD21	9:H:78:ARG:HE	1.85	0.40
13:x:169:LYS:HD2	23:O:149:ARG:NE	2.35	0.40
14:X:75:ILE:HD13	14:X:75:ILE:HA	1.90	0.40
19:T:13:GLU:OE2	19:T:16:ARG:NH2	2.34	0.40
20:S:26:ILE:HA	20:S:56:ALA:HB2	2.02	0.40
20:S:79:ILE:HA	20:S:80:PRO:HD3	1.95	0.40
20:S:102:GLY:HA2	20:S:105:ASN:HD22	1.86	0.40
30:K:332:ARG:O	30:K:335:THR:OG1	2.25	0.40
31:M:43:ASP:HA	31:M:72:HIS:CE1	2.57	0.40
1:2:115:U:H2'	1:2:116:U:C6	2.56	0.40
1:2:1306:U:C4	1:2:1307:U:O4	2.74	0.40
1:2:1817:G:H2'	1:2:1818:A:C8	2.56	0.40
4:B:167:LYS:HE2	4:B:167:LYS:HB2	1.74	0.40
6:E:101:LEU:HD23	6:E:101:LEU:HA	1.89	0.40
9:H:76:GLN:HA	9:H:76:GLN:NE2	2.35	0.40
15:w:211:SER:OG	15:w:212:ASN:N	2.55	0.40
17:u:272:LEU:HB3	17:u:562:VAL:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:88:MET:HE3	19:T:88:MET:HB3	1.66	0.40
22:P:15:PHE:HD2	22:P:22:LEU:HD11	1.86	0.40
30:K:867:LYS:HB2	30:K:919:CYS:SG	2.61	0.40
30:K:909:GLY:HA2	30:K:916:MET:HE1	2.02	0.40
33:a:176:ARG:HD3	33:a:177:GLU:O	2.22	0.40
1:2:24:C:H42	1:2:650:A:H61	0.69	0.40
1:2:118:C:H1'	1:2:445:A:C5	2.56	0.40
1:2:656:G:N2	1:2:663:C:H5''	2.35	0.40
1:2:796:G:H2'	1:2:797:C:H4'	2.02	0.40
1:2:1036:A:N3	1:2:1844:U:O2'	2.54	0.40
1:2:1205:C:O2	17:u:4:HIS:ND1	2.50	0.40
1:2:1606:G:N2	1:2:1632:G:H1'	2.36	0.40
4:B:129:THR:OG1	4:B:130:THR:N	2.54	0.40
13:x:230:LEU:HD12	23:O:149:ARG:NH1	2.36	0.40
15:w:388:ARG:HA	15:w:388:ARG:HD2	1.93	0.40
30:K:1024:LEU:HD13	30:K:1028:TYR:HB3	2.04	0.40
1:2:880:G:O6	1:2:906:U:O2	2.39	0.40
1:2:916:A:N1	24:N:76:LYS:NZ	2.60	0.40
1:2:1276:A:N6	1:2:1322:G:H1	2.20	0.40
3:b:24:LEU:HD12	3:b:24:LEU:HA	1.95	0.40
5:c:10:LYS:HE2	5:c:10:LYS:HB3	1.84	0.40
27:I:21:TYR:CZ	27:I:22:HIS:HD2	2.40	0.40
27:I:165:GLN:HE22	27:I:172:LEU:HG	1.86	0.40
29:q:24:ARG:HA	29:q:27:VAL:HG22	2.03	0.40
31:M:21:VAL:HA	31:M:24:THR:HG22	2.02	0.40
1:2:154:U:O2	10:G:4:ASN:ND2	2.45	0.40
1:2:1286:G:N2	1:2:1312:G:O2'	2.54	0.40
10:G:211:LYS:HB3	10:G:211:LYS:HE2	1.89	0.40
26:J:53:ILE:HD13	26:J:81:LEU:HD21	2.03	0.40
26:J:88:ASP:HB3	26:J:91:LYS:HG3	2.02	0.40
30:K:573:ILE:HG22	30:K:625:LEU:HD22	2.04	0.40
30:K:916:MET:HA	30:K:919:CYS:HB2	2.02	0.40
33:a:247:VAL:HA	33:a:250:LYS:HG2	2.04	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%)	78 (99%)	1 (1%)	0	100	100
3	b	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
4	B	211/264 (80%)	201 (95%)	10 (5%)	0	100	100
5	c	59/69 (86%)	57 (97%)	2 (3%)	0	100	100
6	E	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
7	e	18/59 (30%)	18 (100%)	0	0	100	100
8	F	187/204 (92%)	174 (93%)	12 (6%)	1 (0%)	24	57
9	H	184/194 (95%)	178 (97%)	6 (3%)	0	100	100
10	G	228/249 (92%)	221 (97%)	7 (3%)	0	100	100
11	Z	70/125 (56%)	66 (94%)	4 (6%)	0	100	100
12	Y	122/133 (92%)	120 (98%)	2 (2%)	0	100	100
13	x	173/252 (69%)	166 (96%)	7 (4%)	0	100	100
14	X	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
15	w	321/437 (74%)	309 (96%)	12 (4%)	0	100	100
16	W	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
17	u	630/804 (78%)	602 (96%)	27 (4%)	1 (0%)	43	73
18	t	53/475 (11%)	44 (83%)	9 (17%)	0	100	100
19	T	142/145 (98%)	139 (98%)	3 (2%)	0	100	100
20	S	125/152 (82%)	120 (96%)	5 (4%)	0	100	100
21	Q	123/146 (84%)	120 (98%)	3 (2%)	0	100	100
22	P	117/145 (81%)	117 (100%)	0	0	100	100
23	O	133/151 (88%)	124 (93%)	9 (7%)	0	100	100
24	N	147/151 (97%)	144 (98%)	3 (2%)	0	100	100
25	L	149/158 (94%)	140 (94%)	9 (6%)	0	100	100
26	J	178/194 (92%)	173 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	I	203/208 (98%)	195 (96%)	8 (4%)	0	100	100
28	r	116/125 (93%)	109 (94%)	7 (6%)	0	100	100
29	q	231/281 (82%)	222 (96%)	8 (4%)	1 (0%)	30	61
30	K	1000/1297 (77%)	954 (95%)	46 (5%)	0	100	100
31	M	102/132 (77%)	100 (98%)	2 (2%)	0	100	100
32	f	53/156 (34%)	48 (91%)	5 (9%)	0	100	100
33	a	296/337 (88%)	285 (96%)	11 (4%)	0	100	100
34	z	78/230 (34%)	75 (96%)	3 (4%)	0	100	100
All	All	6134/8028 (76%)	5886 (96%)	245 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	F	163	PHE
17	u	351	ARG
29	q	63	GLY

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%)	167 (100%)	0	100	100
10	G	200/218 (92%)	200 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	545 (97%)	16 (3%)	37	66
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%)	157 (98%)	3 (2%)	50	73
27	I	178/180 (99%)	177 (99%)	1 (1%)	78	83
28	r	105/112 (94%)	105 (100%)	0	100	100
29	q	198/240 (82%)	193 (98%)	5 (2%)	42	69
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	a	262/291 (90%)	262 (100%)	0	100	100
34	z	72/185 (39%)	72 (100%)	0	100	100
All	All	5387/6897 (78%)	5362 (100%)	25 (0%)	78	85

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	u	296	ASP
17	u	298	GLN
17	u	300	LYS
17	u	343	VAL
17	u	344	LEU

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Mol	Chain	Res	Type
17	u	345	MET
17	u	346	LYS
17	u	348	ASP
17	u	351	ARG
17	u	352	GLN
17	u	355	LEU
17	u	358	GLU
17	u	598	VAL
17	u	599	ARG
17	u	679	ILE
17	u	681	THR
26	J	138	ARG
26	J	139	LYS
26	J	158	ASP
27	I	73	THR
29	q	7	ARG
29	q	83	ILE
29	q	105	MET
29	q	122	ILE
29	q	123	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	118	GLN
4	B	159	GLN
6	E	17	HIS
6	E	142	HIS
6	E	201	HIS
8	F	31	ASN
8	F	83	ASN
9	H	114	GLN
9	H	157	HIS
10	G	13	GLN
12	Y	15	ASN
13	x	110	ASN
14	X	61	GLN
15	w	61	GLN
15	w	380	GLN
15	w	410	HIS
16	W	90	GLN
16	W	120	HIS

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Mol	Chain	Res	Type
17	u	243	HIS
17	u	638	HIS
18	t	292	ASN
19	T	126	GLN
20	S	10	GLN
20	S	73	ASN
20	S	125	HIS
21	Q	86	GLN
23	O	20	GLN
25	L	11	GLN
25	L	19	ASN
25	L	94	HIS
27	I	138	ASN
27	I	165	GLN
30	K	527	HIS
30	K	688	ASN
30	K	886	HIS
30	K	1006	ASN
30	K	1189	ASN
31	M	28	HIS
33	a	54	HIS
33	a	68	GLN
33	a	81	GLN
33	a	128	HIS
33	a	134	HIS
33	a	231	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1557/1873 (83%)	341 (21%)	28 (1%)

All (341) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	26	U
1	2	33	G
1	2	37	C
1	2	41	G
1	2	46	A

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Mol	Chain	Res	Type
1	2	56	G
1	2	59	U
1	2	67	C
1	2	68	A
1	2	69	C
1	2	70	G
1	2	71	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	100	U
1	2	103	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	126	G
1	2	128	U
1	2	130	G
1	2	143	U
1	2	144	U
1	2	149	A
1	2	155	G
1	2	160	U
1	2	168	C
1	2	172	U
1	2	181	A
1	2	182	C
1	2	184	G
1	2	188	C
1	2	291	G
1	2	292	A
1	2	295	C
1	2	302	A
1	2	310	C
1	2	313	A
1	2	315	C
1	2	318	A
1	2	319	C

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Mol	Chain	Res	Type
1	2	332	G
1	2	333	G
1	2	335	G
1	2	338	G
1	2	339	A
1	2	340	C
1	2	351	G
1	2	360	A
1	2	362	C
1	2	364	A
1	2	370	G
1	2	377	G
1	2	385	G
1	2	386	C
1	2	400	C
1	2	409	C
1	2	413	G
1	2	418	A
1	2	429	C
1	2	438	G
1	2	441	C
1	2	448	A
1	2	449	A
1	2	450	C
1	2	466	G
1	2	470	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	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

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Mol	Chain	Res	Type
1	2	555	A
1	2	556	U
1	2	559	G
1	2	560	A
1	2	563	G
1	2	570	C
1	2	574	A
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	595	U
1	2	600	G
1	2	601	G
1	2	603	C
1	2	604	A
1	2	605	A
1	2	606	G
1	2	613	G
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	662	G
1	2	664	A
1	2	669	A
1	2	670	A
1	2	671	A
1	2	673	G
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

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Mol	Chain	Res	Type
1	2	751	G
1	2	792	C
1	2	794	A
1	2	797	C
1	2	799	U
1	2	800	U
1	2	811	A
1	2	821	G
1	2	822	U
1	2	823	U
1	2	824	C
1	2	827	A
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	922	A
1	2	930	C
1	2	933	G
1	2	959	G
1	2	963	A
1	2	970	G

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Mol	Chain	Res	Type
1	2	971	G
1	2	981	A
1	2	985	G
1	2	990	A
1	2	991	G
1	2	992	A
1	2	1002	U
1	2	1017	U
1	2	1023	A
1	2	1034	A
1	2	1041	G
1	2	1044	G
1	2	1045	U
1	2	1049	A
1	2	1050	A
1	2	1083	A
1	2	1085	C
1	2	1086	G
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	1121	G
1	2	1130	G
1	2	1138	C
1	2	1139	C
1	2	1149	A
1	2	1153	C
1	2	1154	U
1	2	1157	G
1	2	1171	G
1	2	1183	A
1	2	1200	A
1	2	1203	G
1	2	1204	A
1	2	1206	G
1	2	1211	G
1	2	1215	C
1	2	1217	A

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Mol	Chain	Res	Type
1	2	1221	G
1	2	1224	G
1	2	1227	G
1	2	1232	U
1	2	1235	G
1	2	1238	U
1	2	1242	U
1	2	1243	U
1	2	1265	A
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	1298	G
1	2	1299	A
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
1	2	1376	A
1	2	1383	A
1	2	1387	G
1	2	1388	A
1	2	1389	C

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Mol	Chain	Res	Type
1	2	1396	A
1	2	1397	U
1	2	1398	G
1	2	1444	U
1	2	1445	U
1	2	1446	A
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	1497	G
1	2	1498	A
1	2	1512	C
1	2	1519	U
1	2	1528	G
1	2	1533	A
1	2	1534	C
1	2	1535	U
1	2	1548	G
1	2	1551	U
1	2	1559	C
1	2	1560	U
1	2	1566	G
1	2	1569	A
1	2	1570	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
1	2	1606	G
1	2	1618	C
1	2	1621	U

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Mol	Chain	Res	Type
1	2	1623	A
1	2	1639	G7M
1	2	1640	A
1	2	1641	A
1	2	1648	G
1	2	1654	G
1	2	1660	C
1	2	1661	A
1	2	1663	A
1	2	1664	A
1	2	1665	G
1	2	1669	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	1729	U
1	2	1744	G
1	2	1756	C
1	2	1761	U
1	2	1772	C
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
1	2	1826	G
1	2	1829	G
1	2	1839	U
1	2	1841	C
1	2	1861	G
1	2	1864	U
1	2	1872	G

All (28) 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	1494	U
1	2	1497	G
1	2	1511	U
1	2	1534	C
1	2	1565	C
1	2	1640	A
1	2	1693	G
1	2	1726	G

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

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	4.41	13 (56%)	34,39,42	1.98	10 (29%)

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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1639	G7M	C3'-C4'	-10.53	1.26	1.53
1	2	1639	G7M	C2'-C1'	-7.91	1.28	1.53
1	2	1639	G7M	C4-N3	6.72	1.49	1.34
1	2	1639	G7M	C2-N2	6.60	1.49	1.34
1	2	1639	G7M	C2-N3	5.69	1.47	1.33
1	2	1639	G7M	O4'-C1'	5.52	1.54	1.42
1	2	1639	G7M	O4'-C4'	5.37	1.56	1.45
1	2	1639	G7M	C2'-C3'	4.98	1.66	1.53
1	2	1639	G7M	C5-C6	4.15	1.54	1.43
1	2	1639	G7M	C5-N7	-4.08	1.34	1.39
1	2	1639	G7M	C2-N1	2.91	1.44	1.37
1	2	1639	G7M	C6-N1	2.82	1.44	1.38
1	2	1639	G7M	O6-C6	-2.42	1.19	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1639	G7M	C2-N3-C4	4.93	120.78	112.30
1	2	1639	G7M	C5-C4-N3	-4.29	120.05	128.15
1	2	1639	G7M	C5-C6-N1	3.93	119.96	111.84
1	2	1639	G7M	CN7-N7-C5	3.44	131.09	126.80
1	2	1639	G7M	CN7-N7-C8	-3.27	119.84	124.79
1	2	1639	G7M	N9-C4-N3	3.11	132.18	125.95
1	2	1639	G7M	C2-N1-C6	-2.87	119.90	125.11
1	2	1639	G7M	O6-C6-C5	-2.75	121.87	128.01
1	2	1639	G7M	N9-C8-N7	-2.09	107.41	112.48
1	2	1639	G7M	N1-C2-N3	-2.03	119.60	123.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	1639	G7M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	2	1639	G7M	O4'-C4'-C5'-O5'

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	$\# Z > 2$
35	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
35	SAH	q	301	-	-	3/15/31/31	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

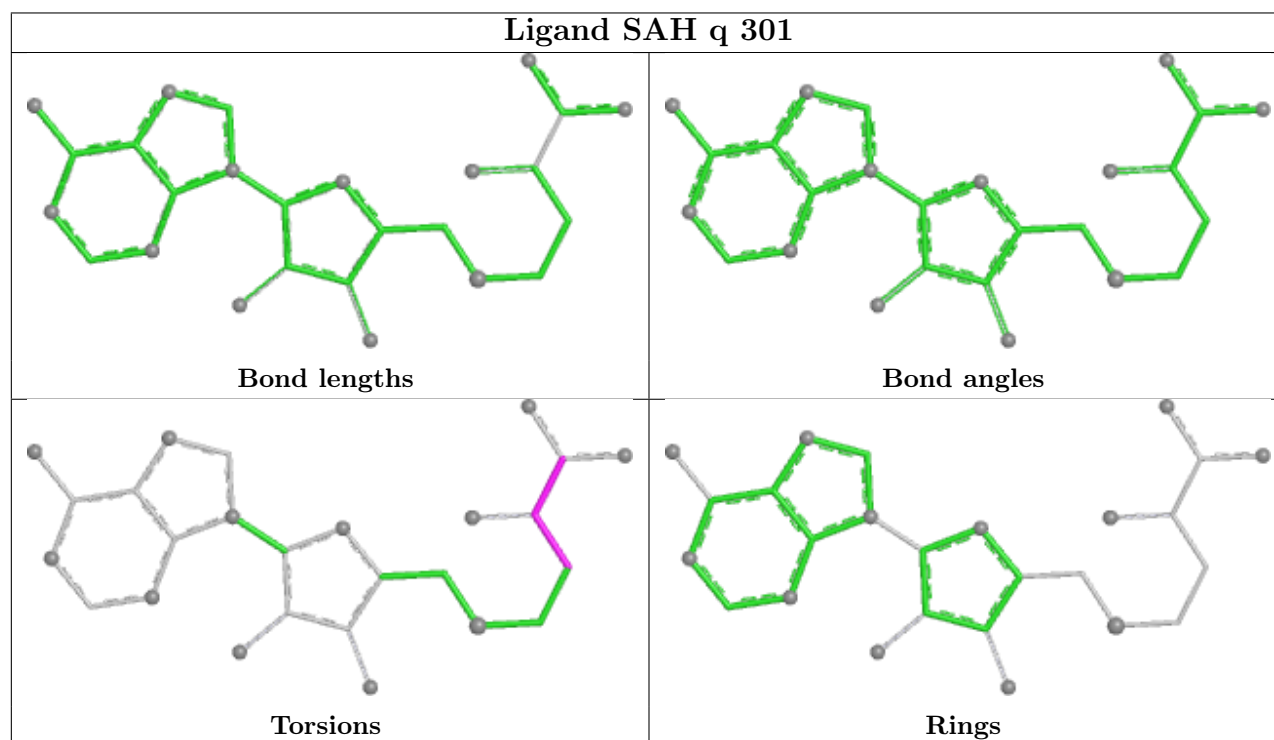
Mol	Chain	Res	Type	Atoms
35	q	301	SAH	OXT-C-CA-N
35	q	301	SAH	O-C-CA-N
35	q	301	SAH	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	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

This section contains visualisations of the EMDB entry EMD-32800. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit ⓘ

This section was not generated.