



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:05 PM UTC

PDB ID : 5XYI / pdb_00005xyi
EMDB ID : EMD-6788
Title : Small subunit of Trichomonas vaginalis ribosome
Authors : Li, Z.; Guo, Q.; Zheng, L.; Ji, Y.; Xie, Y.; Lai, D.; Lun, Z.; Suo, X.; Gao, N.
Deposited on : 2017-07-08
Resolution : 3.35 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:

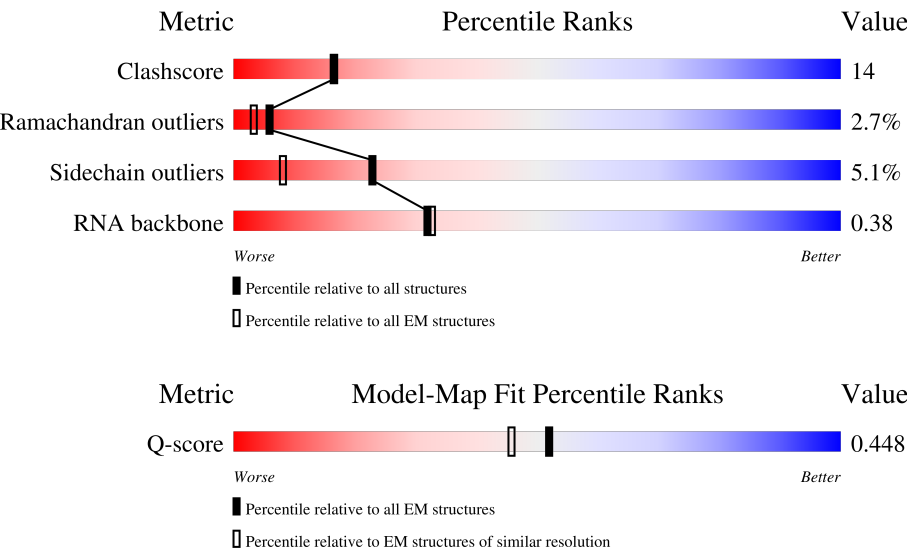
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.35 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.



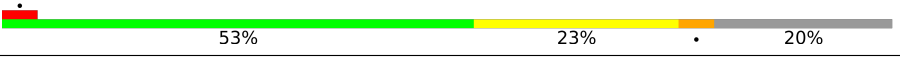
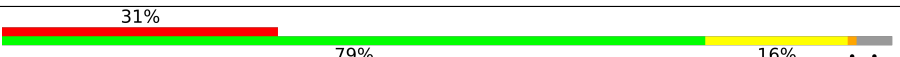
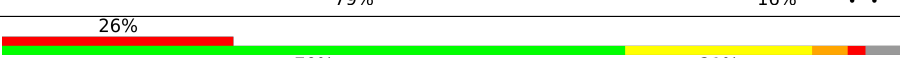
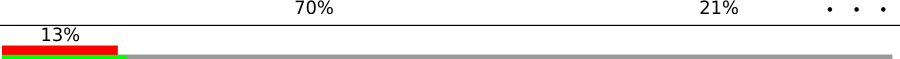
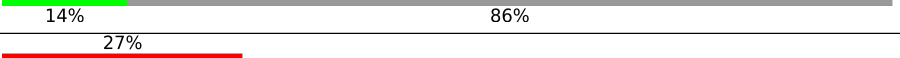
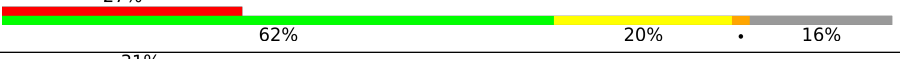
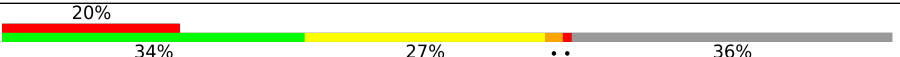
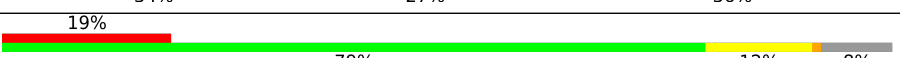
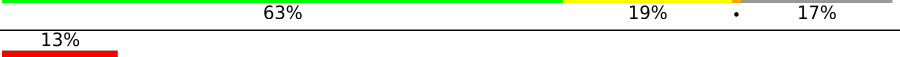
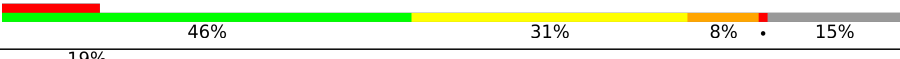
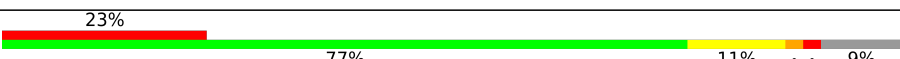
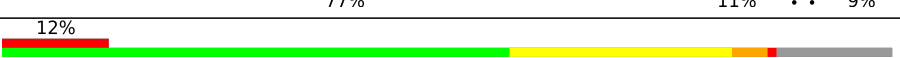
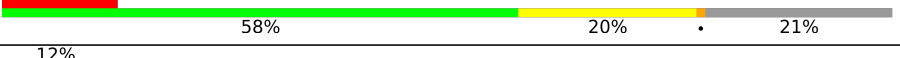
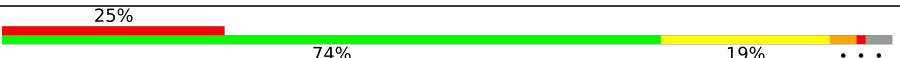
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14390 (2.85 - 3.85)

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	1577	8% 64% 27% • 6%
2	A	256	9% 54% 22% • 20%
3	B	247	21% 55% 30% • 11%

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Mol	Chain	Length	Quality of chain
4	C	272	
5	D	216	
6	E	255	
7	F	193	
8	G	216	
9	H	168	
10	I	197	
11	J	185	
12	K	141	
13	L	155	
14	M	124	
15	N	151	
16	O	159	
17	P	144	
18	Q	140	
19	R	129	
20	S	155	
21	T	148	
22	U	123	
23	V	89	
24	W	130	
25	X	144	
26	Y	140	
27	Z	115	
28	a	118	

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Mol	Chain	Length	Quality of chain
29	b	86	21%72%20%5%
30	c	68	35%41%37%12%10%
31	d	57	7%68%16%7%9%
32	e	62	31%53%13%32%
33	g	335	37%69%20%9%
34	n	25	24%20%56%20%

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 65924 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1490	Total	C	N	O	P	0	0
			31820	14210	5694	10426	1490		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	204	Total	C	N	O	S	0	0
			1603	1028	266	294	15		

- Molecule 3 is a protein called Ribosomal protein S3Ae, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	219	Total	C	N	O	S	0	0
			1747	1103	314	318	12		

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	217	Total	C	N	O	S	0	0
			1685	1082	299	298	6		

- Molecule 5 is a protein called Ribosomal protein S3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	208	Total	C	N	O	S	0	0
			1655	1039	311	296	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	246	Total	C	N	O	S	0	0
			1935	1236	362	329	8		

- Molecule 7 is a protein called 40s ribosomal protein S5-B, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	186	Total	C	N	O	S	0	0
			1476	915	279	273	9		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	G	31	Total	C	N	O	0	0
			155	93	31	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	163	Total	C	N	O	S	0	0
			1276	811	230	234	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	166	Total	C	N	O	S	0	0
			1300	811	253	232	4		

- Molecule 11 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	162	Total	C	N	O	S	0	0
			1321	833	252	233	3		

- Molecule 12 is a protein called Plectin/S10 domain containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	90	Total	C	N	O	S	0	0
			731	472	125	128	6		

- Molecule 13 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	142	Total	C	N	O	S	0	0
			1160	742	222	193	3		

- Molecule 14 is a protein called Ribosomal protein L7Ae, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	M	103	Total	C	N	O	0	0
			509	303	103	103		

- Molecule 15 is a protein called 40S ribosomal protein S13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	150	Total	C	N	O	S	0	0
			1190	749	234	202	5		

- Molecule 16 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	135	Total	C	N	O	S	0	0
			1005	615	205	182	3		

- Molecule 17 is a protein called Ribosomal protein S19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	118	Total	C	N	O	S	0	0
			962	624	176	159	3		

- Molecule 18 is a protein called 40S ribosomal protein S16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	133	Total	C	N	O	S	0	0
			1043	660	196	182	5		

- Molecule 19 is a protein called 40S ribosomal protein S17-B, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	118	Total	C	N	O	S	0	0
			961	603	181	171	6		

- Molecule 20 is a protein called Ribosomal protein S13p/S18e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	135	Total	C	N	O	S	0	0
			1077	668	219	183	7		

- Molecule 21 is a protein called Ribosomal protein S19e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	146	Total	C	N	O	S	0	0
			1148	725	219	200	4		

- Molecule 22 is a protein called Ribosomal protein S10p/S20e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	97	Total	C	N	O	S	0	0
			777	487	150	137	3		

- Molecule 23 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	87	Total	C	N	O	S	0	0
			671	418	118	131	4		

- Molecule 24 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	128	Total	C	N	O	S	0	0
			1001	637	182	175	7		

- Molecule 25 is a protein called 40S ribosomal protein S23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	140	Total	C	N	O	S	0	0
			1062	670	206	182	4		

- Molecule 26 is a protein called Ribosomal protein S24e, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	105	Total	C	N	O	S	0	0
			792	506	144	141	1		

- Molecule 27 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	73	Total	C	N	O	S	0	0
			560	356	99	102	3		

- Molecule 28 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	100	Total	C	N	O	S	0	0
			815	503	168	136	8		

- Molecule 29 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	82	Total	C	N	O	S	0	0
			632	395	114	119	4		

- Molecule 30 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	c	61	Total	C	N	O	0	0
			475	290	96	89		

- Molecule 31 is a protein called 40S ribosomal protein S29, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	52	Total	C	N	O	S	0	0
			438	272	95	67	4		

- Molecule 32 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	42	Total	C	N	O	S	0	0
			337	211	71	54	1		

- Molecule 33 is a protein called Guanine nucleotide-binding protein beta subunit, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	305	Total	C	N	O	S	0	0
			2380	1509	417	443	11		

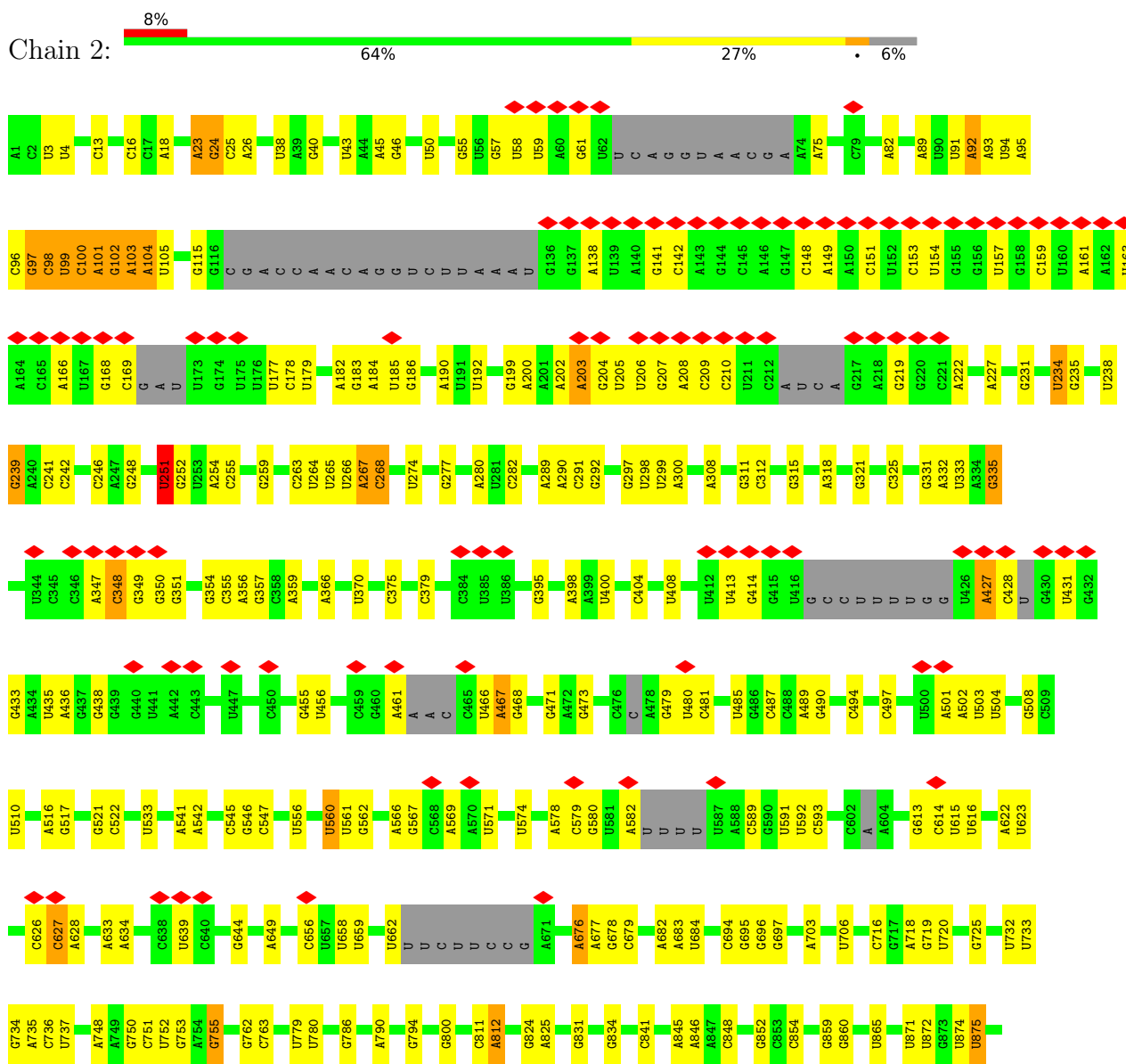
- Molecule 34 is a protein called eL41.

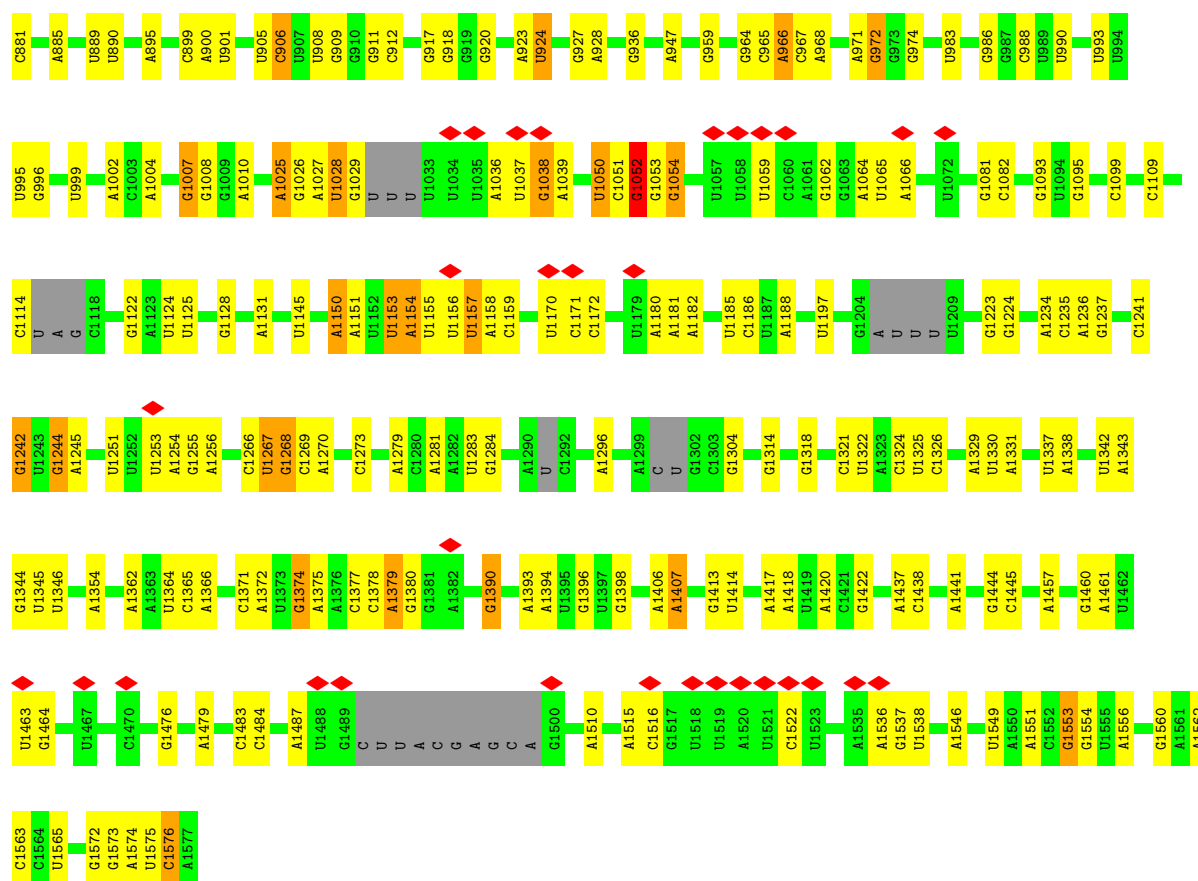
Mol	Chain	Residues	Atoms				AltConf	Trace
34	n	24	Total	C	N	O	0	0
			225	137	62	26		

3 Residue-property plots [i](#)

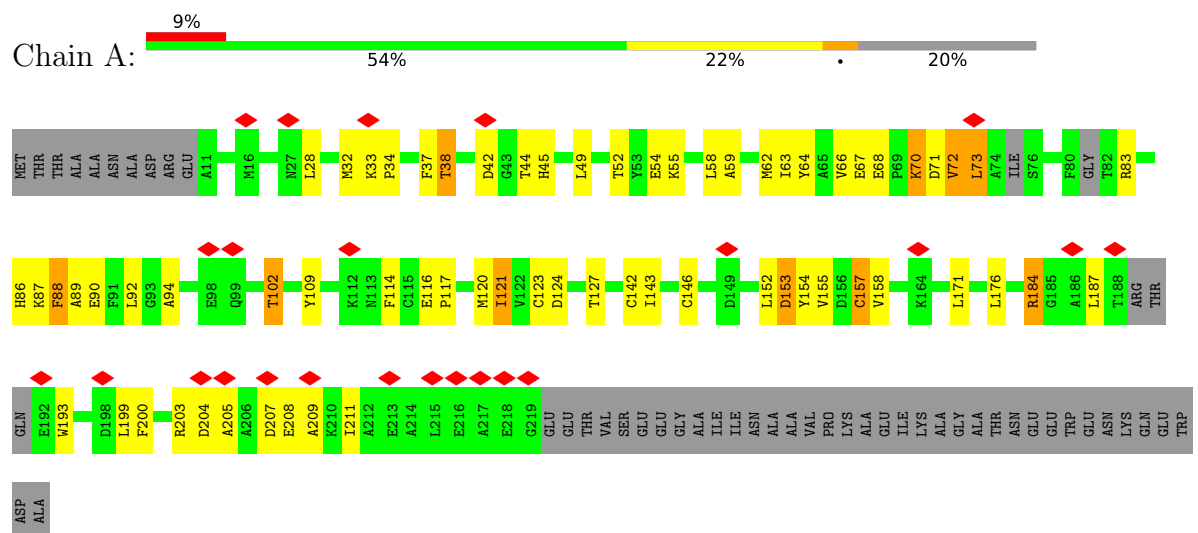
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

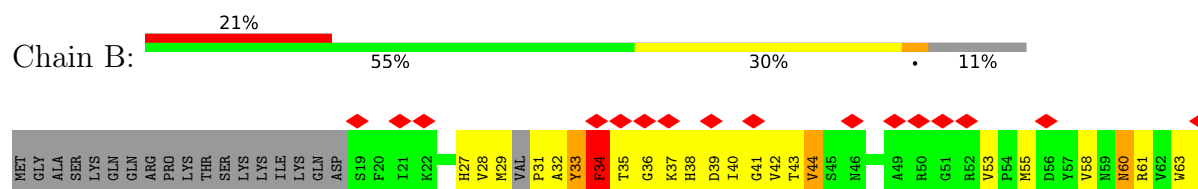


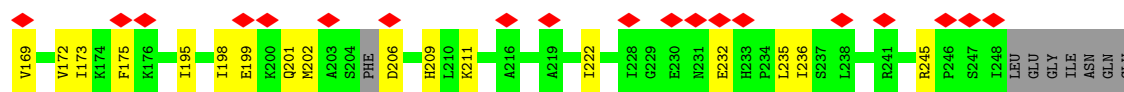


• Molecule 2: 40S ribosomal protein SA

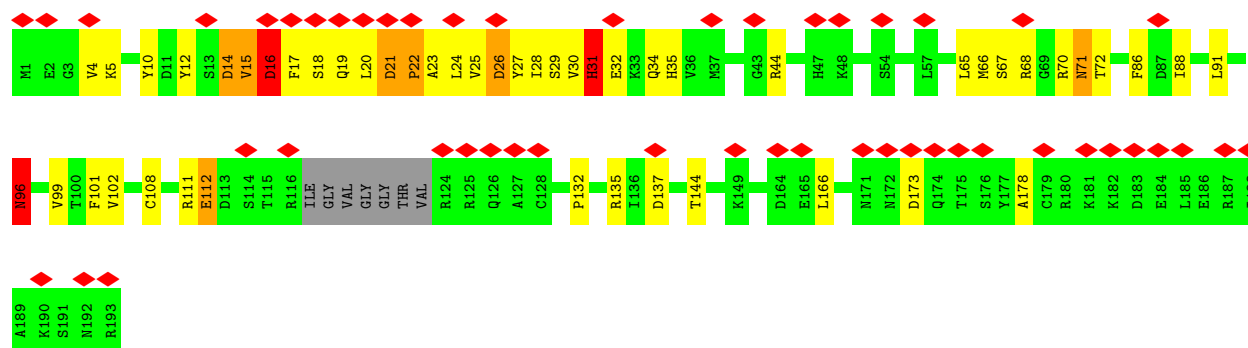


• Molecule 3: Ribosomal protein S3Ae, putative

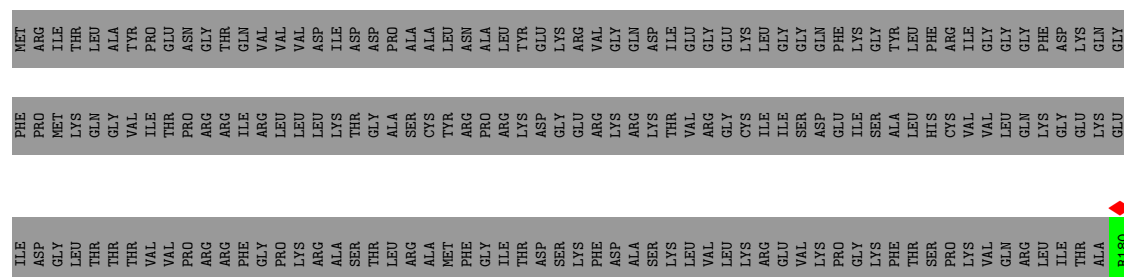




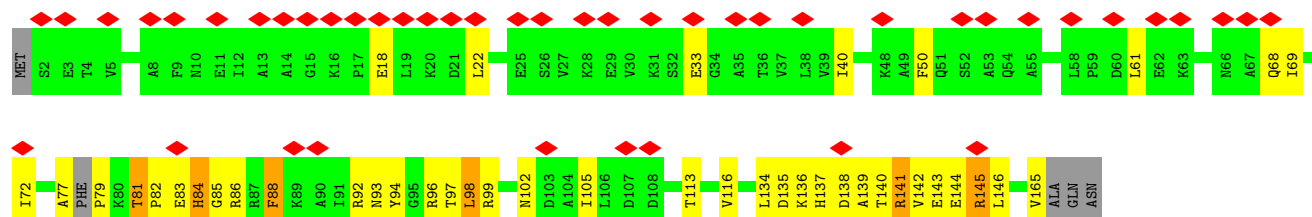
- Molecule 7: 40s ribosomal protein S5-B, putative



- Molecule 8: 40S ribosomal protein S6

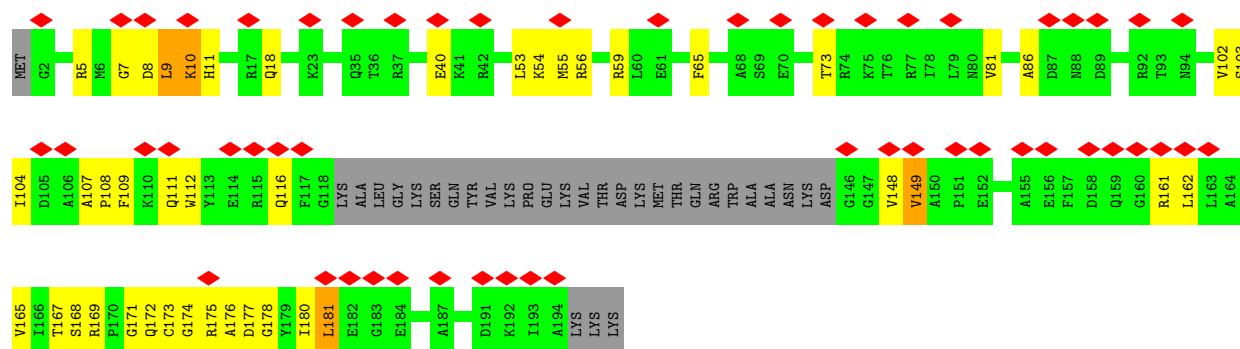


- Molecule 9: 40S ribosomal protein S7, putative

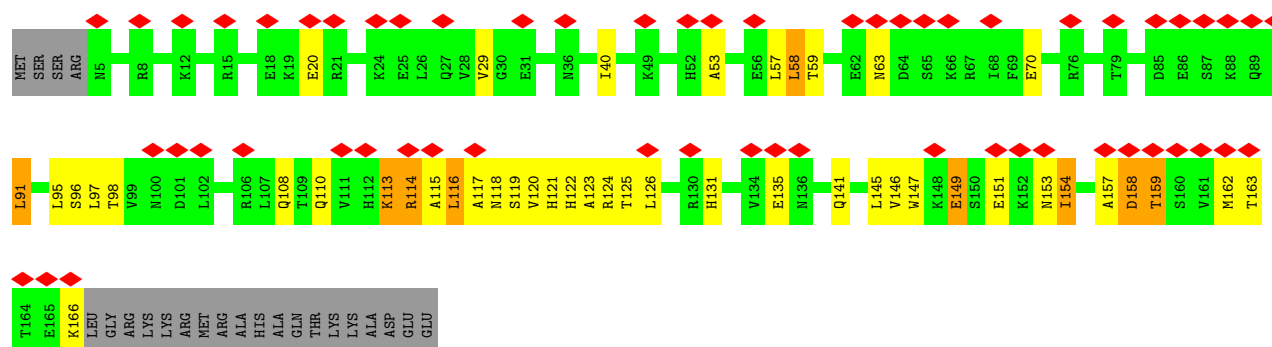


- Molecule 10: 40S ribosomal protein S8

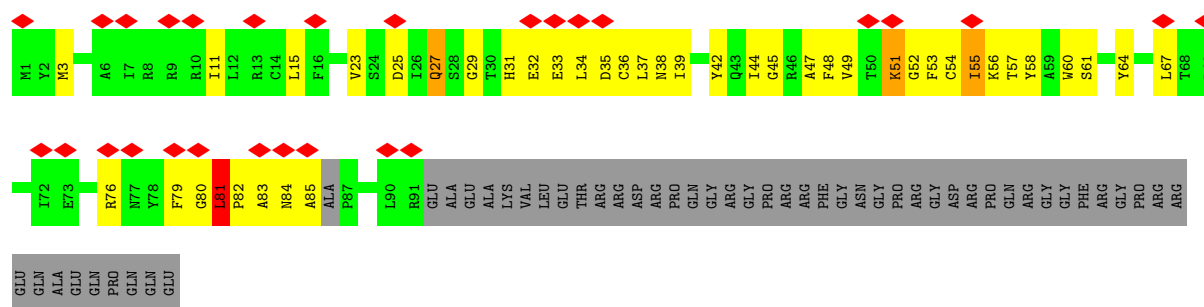




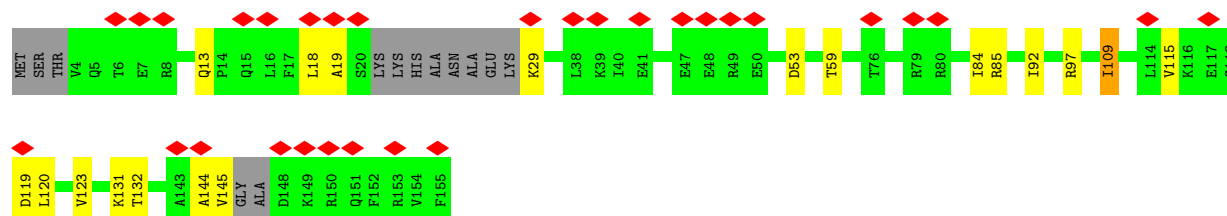
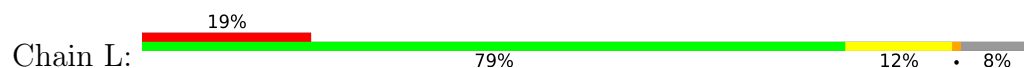
• Molecule 11: Uncharacterized protein



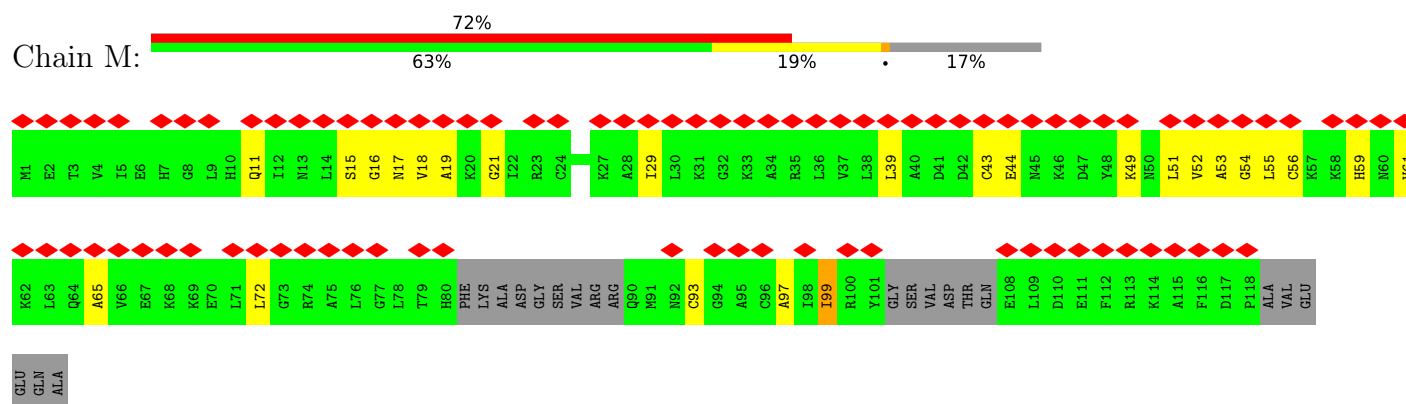
• Molecule 12: Plectin/S10 domain containing protein



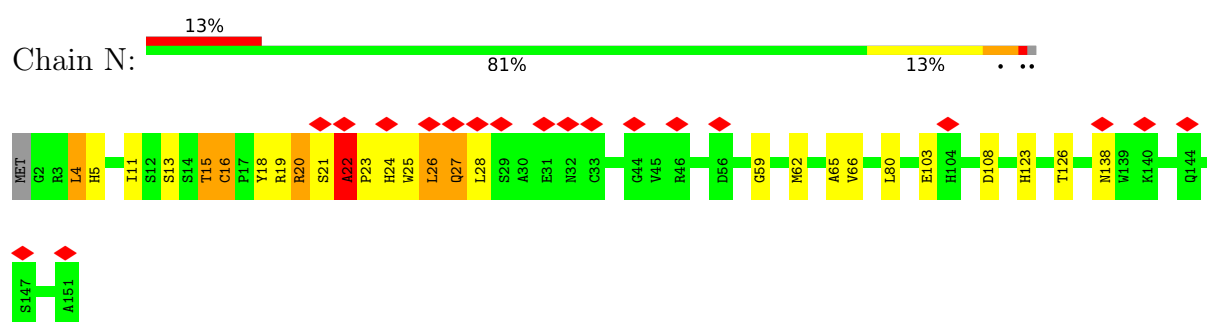
• Molecule 13: Uncharacterized protein



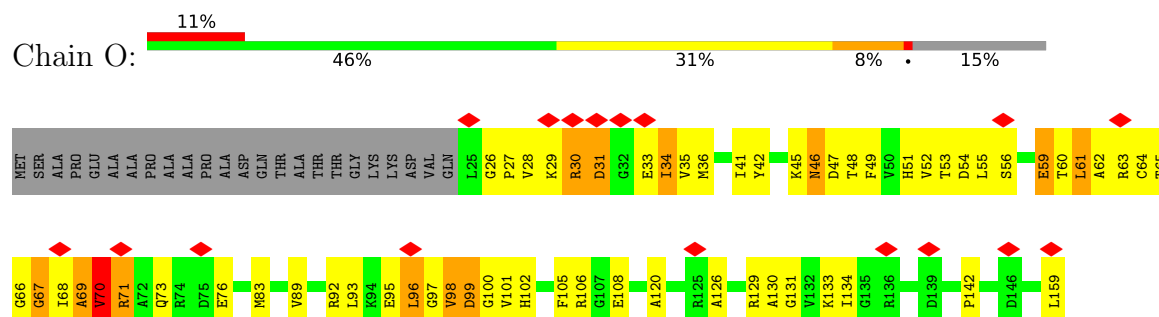
- Molecule 14: Ribosomal protein L7Ae, putative



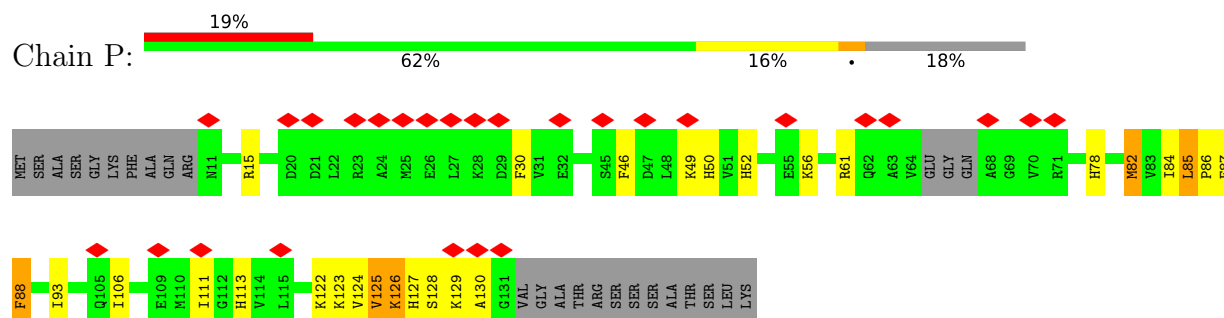
- Molecule 15: 40S ribosomal protein S13, putative



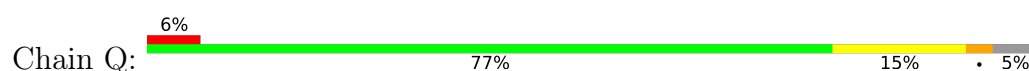
- Molecule 16: Ribosomal protein S14

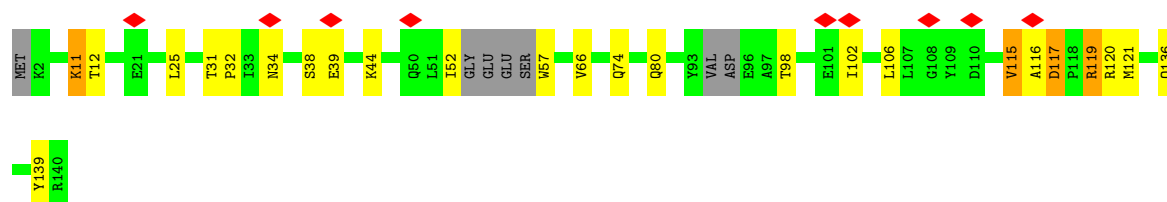


- Molecule 17: Ribosomal protein S19, putative

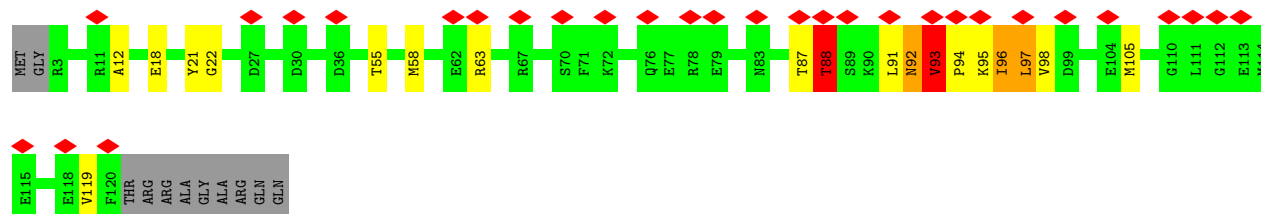
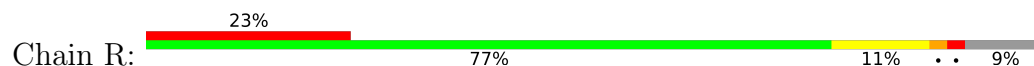


- Molecule 18: 40S ribosomal protein S16, putative

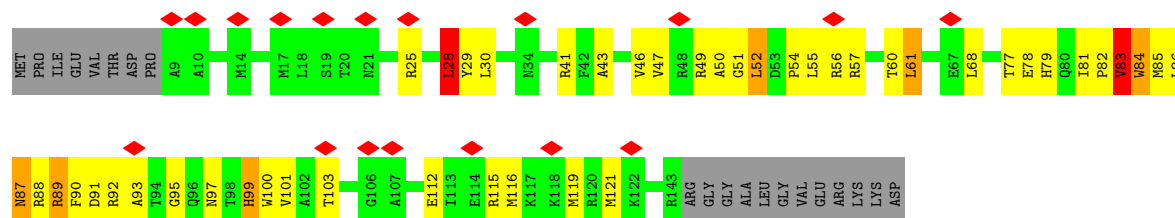




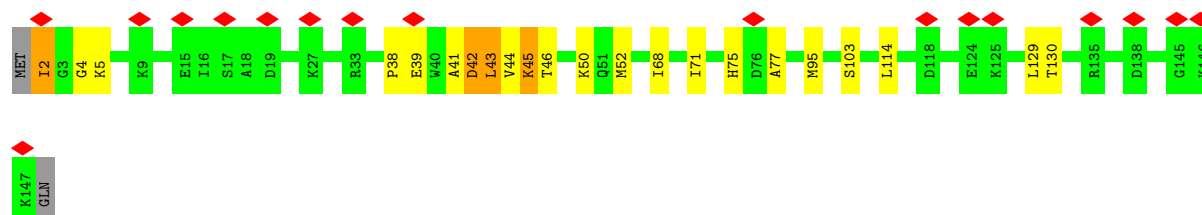
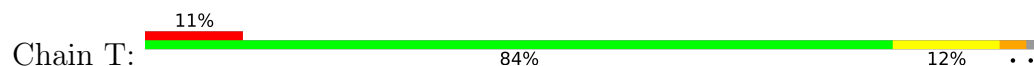
- Molecule 19: 40S ribosomal protein S17-B, putative



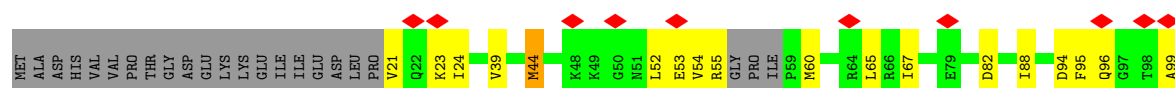
- Molecule 20: Ribosomal protein S13p/S18e, putative

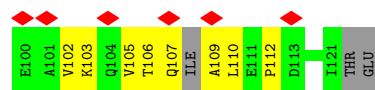


- Molecule 21: Ribosomal protein S19e, putative

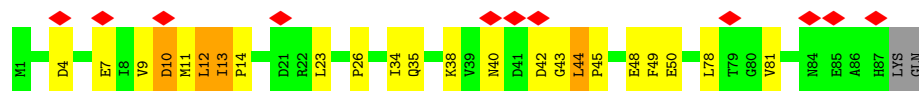
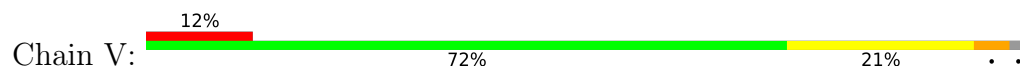


- Molecule 22: Ribosomal protein S10p/S20e, putative

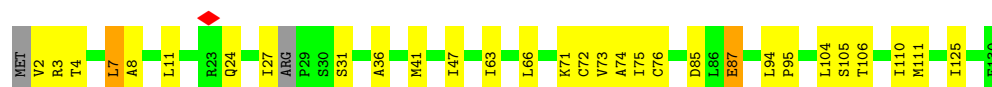




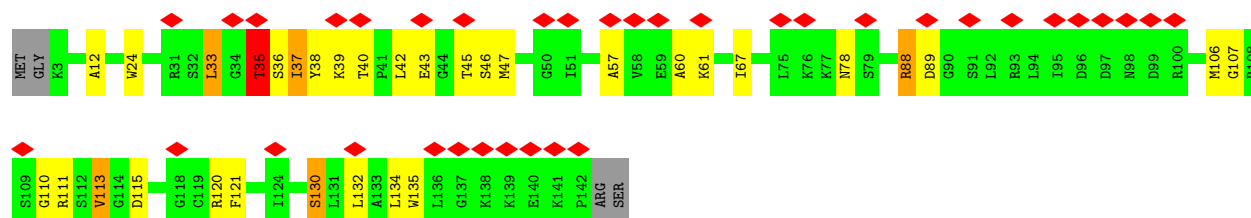
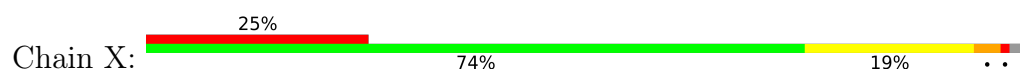
- Molecule 23: 40S ribosomal protein S21



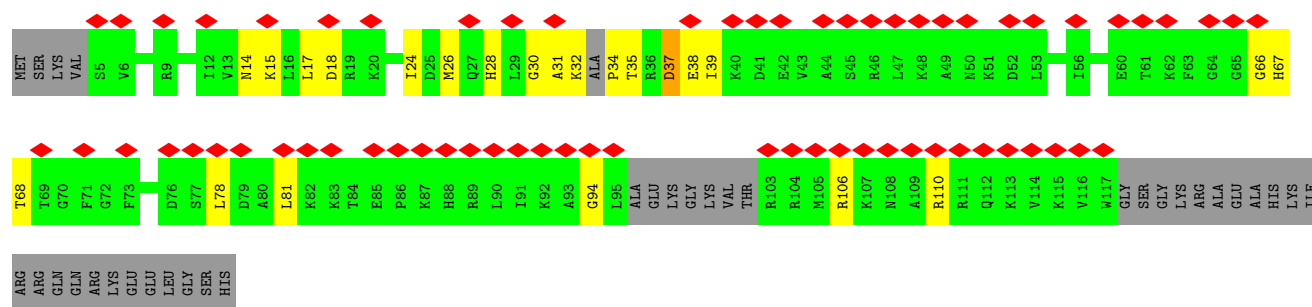
- Molecule 24: Ribosomal protein S15a



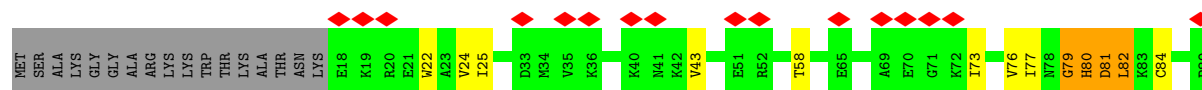
- Molecule 25: 40S ribosomal protein S23, putative

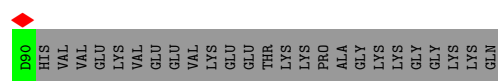


- Molecule 26: Ribosomal protein S24e, putative

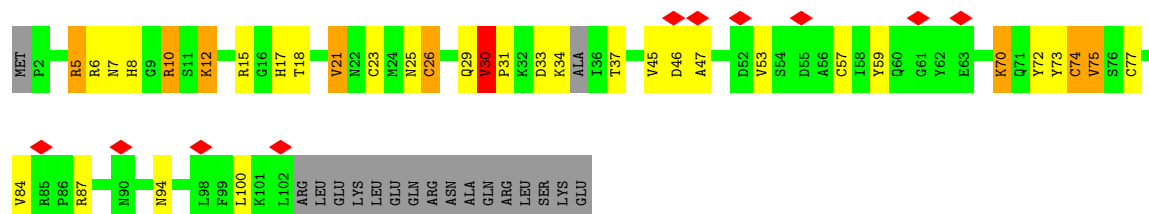


- Molecule 27: Uncharacterized protein





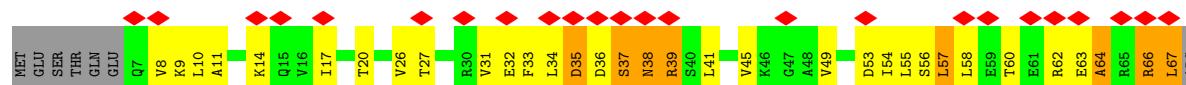
- Molecule 28: 40S ribosomal protein S26



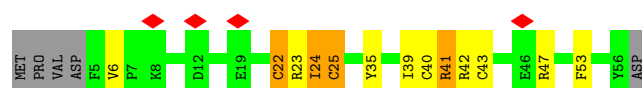
- Molecule 29: 40S ribosomal protein S27



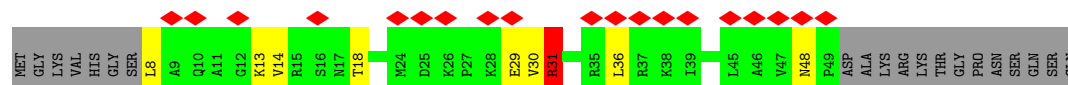
- Molecule 30: Uncharacterized protein



- Molecule 31: 40S ribosomal protein S29, putative

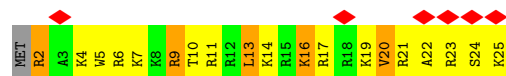


- Molecule 32: 40S ribosomal protein S30



- Molecule 33: Guanine nucleotide-binding protein beta subunit, putative





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.268	Depositor
Minimum map value	-0.139	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.036	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.37	0/35582	0.69	12/55428 (0.0%)
2	A	0.54	0/1634	0.85	4/2210 (0.2%)
3	B	0.50	0/1777	0.86	5/2389 (0.2%)
4	C	0.54	0/1722	0.88	3/2318 (0.1%)
5	D	0.53	0/1675	0.80	1/2242 (0.0%)
6	E	0.52	0/1974	0.73	1/2657 (0.0%)
7	F	0.53	0/1497	0.94	2/2010 (0.1%)
8	G	0.63	0/154	0.94	0/214
9	H	0.54	0/1295	0.91	6/1746 (0.3%)
10	I	0.56	0/1322	0.83	0/1778
11	J	0.50	0/1344	0.85	2/1808 (0.1%)
12	K	0.56	0/749	0.93	3/1013 (0.3%)
13	L	0.48	0/1181	0.65	0/1585
14	M	0.60	0/507	1.16	3/701 (0.4%)
15	N	0.56	0/1213	0.89	3/1634 (0.2%)
16	O	0.53	0/1017	0.98	5/1366 (0.4%)
17	P	0.58	0/983	0.84	2/1320 (0.2%)
18	Q	0.58	1/1057 (0.1%)	0.88	3/1418 (0.2%)
19	R	0.59	1/975 (0.1%)	0.88	1/1305 (0.1%)
20	S	0.59	0/1093	0.98	3/1467 (0.2%)
21	T	0.54	0/1172	0.82	1/1576 (0.1%)
22	U	0.52	0/785	0.83	2/1053 (0.2%)
23	V	0.59	0/682	0.93	5/924 (0.5%)
24	W	0.49	0/1015	0.74	0/1358
25	X	0.52	0/1076	0.88	5/1441 (0.3%)
26	Y	0.52	0/802	0.76	0/1073
27	Z	0.55	0/570	0.85	2/770 (0.3%)
28	a	0.58	0/829	1.02	6/1110 (0.5%)
29	b	0.59	0/645	0.87	2/880 (0.2%)
30	c	0.51	0/475	0.90	2/635 (0.3%)
31	d	0.54	0/445	1.01	3/588 (0.5%)
32	e	0.53	0/341	0.86	1/454 (0.2%)
33	g	0.53	0/2440	0.78	8/3324 (0.2%)
34	n	0.83	0/226	1.12	1/290 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.46	2/70254 (0.0%)	0.77	97/102085 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Q	117	ASP	C-N	6.05	1.39	1.33
19	R	93	VAL	CA-CB	5.24	1.57	1.53

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Q	115	VAL	N-CA-C	11.40	122.23	110.72
1	2	92	A	C4'-C3'-O3'	8.83	122.64	109.40
14	M	18	VAL	N-CA-C	8.49	119.56	108.35
1	2	1374	G	C4'-C3'-O3'	8.35	121.92	109.40
7	F	31	HIS	N-CA-C	8.06	121.71	109.62
15	N	22	ALA	C-N-CD	7.67	137.48	120.60
1	2	348	C	C4'-C3'-O3'	7.47	120.60	109.40
19	R	93	VAL	C-N-CD	7.40	136.87	120.60
31	d	22	CYS	N-CA-C	-7.39	98.87	109.96
1	2	251	U	C2'-C3'-O3'	7.37	120.55	109.50
9	H	145	ARG	N-CA-C	6.90	120.59	112.72
1	2	1150	A	C2'-C3'-O3'	6.88	119.82	109.50
1	2	1052	G	C2'-C3'-O3'	6.66	119.50	109.50
9	H	144	GLU	N-CA-C	6.64	118.52	111.28
3	B	86	ILE	N-CA-C	6.63	117.38	110.62
2	A	155	VAL	N-CA-C	6.63	117.67	108.12
3	B	34	PHE	N-CA-C	6.41	118.27	111.28
14	M	54	GLY	N-CA-C	-6.35	104.64	112.77
34	n	6	ARG	N-CA-C	-6.27	104.44	111.28
17	P	127	HIS	N-CA-C	6.26	118.93	108.73
20	S	84	TRP	N-CA-C	-6.22	104.58	111.36
1	2	1379	A	C2'-C3'-O3'	6.21	118.81	109.50
33	g	110	SER	N-CA-C	6.19	118.11	111.36
9	H	146	LEU	N-CA-C	6.12	117.94	111.28
23	V	13	ILE	CA-C-N	-6.10	113.66	119.76
23	V	13	ILE	C-N-CA	-6.10	113.66	119.76
1	2	627	C	C2'-C3'-O3'	6.09	118.64	109.50
1	2	966	A	C2'-C3'-O3'	6.09	118.64	109.50
22	U	106	THR	N-CA-C	6.09	117.92	111.28
31	d	41	ARG	N-CA-C	5.96	117.78	111.28
2	A	205	ALA	N-CA-C	-5.86	104.89	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	81	LEU	CA-C-N	-5.78	114.31	120.03
12	K	81	LEU	C-N-CA	-5.78	114.31	120.03
27	Z	25	ILE	N-CA-C	5.78	116.20	108.11
20	S	79	HIS	N-CA-C	5.74	118.66	110.68
16	O	30	ARG	N-CA-C	5.74	117.53	111.28
28	a	30	VAL	CA-C-N	-5.72	114.08	119.85
28	a	30	VAL	C-N-CA	-5.72	114.08	119.85
29	b	62	THR	CA-C-N	-5.70	114.06	119.76
29	b	62	THR	C-N-CA	-5.70	114.06	119.76
9	H	141	ARG	N-CA-C	5.69	117.48	111.28
25	X	33	LEU	N-CA-C	5.67	117.46	111.28
30	c	37	SER	N-CA-C	-5.64	105.14	111.28
1	2	24	G	C2'-C3'-O3'	5.63	117.94	109.50
4	C	50	GLN	CA-C-N	-5.62	114.14	119.76
4	C	50	GLN	C-N-CA	-5.62	114.14	119.76
33	g	171	ALA	CA-C-N	-5.61	114.48	120.03
33	g	171	ALA	C-N-CA	-5.61	114.48	120.03
33	g	178	SER	CA-C-N	-5.60	113.99	119.76
33	g	178	SER	C-N-CA	-5.60	113.99	119.76
33	g	226	ILE	N-CA-C	5.60	115.95	108.11
5	D	49	ILE	N-CA-C	5.59	116.05	107.77
28	a	70	LYS	N-CA-C	-5.59	100.12	109.24
3	B	44	VAL	N-CA-C	5.58	115.98	108.17
20	S	87	ASN	N-CA-C	5.58	117.36	111.28
22	U	105	VAL	N-CA-C	5.56	116.29	110.62
16	O	59	GLU	N-CA-C	5.55	118.58	109.76
1	2	427	A	C2'-C3'-O3'	5.53	117.80	109.50
11	J	154	ILE	N-CA-C	-5.49	100.42	108.11
1	2	23	A	C4'-C3'-O3'	5.49	117.63	109.40
18	Q	117	ASP	CA-C-N	-5.48	114.26	120.89
18	Q	117	ASP	C-N-CA	-5.48	114.26	120.89
28	a	17	HIS	N-CA-C	5.48	118.16	109.50
9	H	81	THR	CA-C-N	-5.47	113.92	119.83
9	H	81	THR	C-N-CA	-5.47	113.92	119.83
7	F	70	ARG	N-CA-C	-5.46	107.26	114.04
33	g	51	ALA	N-CA-C	-5.46	102.20	110.28
3	B	148	ASN	N-CA-C	5.46	117.23	111.28
4	C	180	ILE	N-CA-C	5.46	117.49	109.63
15	N	16	CYS	CA-C-N	-5.43	114.19	119.78
15	N	16	CYS	C-N-CA	-5.43	114.19	119.78
25	X	37	ILE	N-CA-C	-5.42	108.56	113.71
31	d	25	CYS	N-CA-C	5.42	117.27	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	V	44	LEU	CA-C-N	-5.34	114.42	119.76
23	V	44	LEU	C-N-CA	-5.34	114.42	119.76
25	X	35	THR	CA-C-N	5.32	131.28	121.70
25	X	35	THR	C-N-CA	5.32	131.28	121.70
16	O	70	VAL	N-CA-C	5.31	120.38	109.34
11	J	113	LYS	N-CA-C	-5.30	105.50	111.28
33	g	112	ARG	CB-CA-C	-5.28	110.50	116.63
32	e	31	ARG	N-CA-C	5.27	117.33	110.53
27	Z	79	GLY	N-CA-C	5.26	117.52	111.36
6	E	95	SER	N-CA-C	-5.23	104.68	111.74
16	O	69	ALA	N-CA-C	5.20	116.63	111.07
25	X	35	THR	N-CA-C	5.19	118.41	111.24
12	K	51	LYS	N-CA-C	-5.17	105.72	111.36
21	T	44	VAL	N-CA-C	5.17	116.25	109.58
23	V	43	GLY	N-CA-C	5.15	123.03	113.76
28	a	12	LYS	N-CA-C	5.13	117.60	109.24
2	A	72	VAL	N-CA-C	5.10	115.25	108.11
3	B	196	LYS	N-CA-C	5.09	116.91	111.36
28	a	75	VAL	N-CA-C	5.09	115.81	110.62
17	P	130	ALA	CB-CA-C	-5.07	110.71	116.54
14	M	99	ILE	N-CA-C	5.06	117.01	108.81
2	A	88	PHE	N-CA-C	-5.05	105.77	111.28
16	O	96	LEU	N-CA-C	5.05	116.47	111.07
30	c	35	ASP	N-CA-C	-5.03	105.93	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	31820	0	16032	220	0
2	A	1603	0	1602	81	0
3	B	1747	0	1773	124	0
4	C	1685	0	1733	109	0
5	D	1655	0	1739	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1935	0	2023	56	0
7	F	1476	0	1494	76	0
8	G	155	0	73	0	0
9	H	1276	0	1326	63	0
10	I	1300	0	1315	56	0
11	J	1321	0	1344	60	0
12	K	731	0	726	81	0
13	L	1160	0	1216	8	0
14	M	509	0	249	23	0
15	N	1190	0	1245	41	0
16	O	1005	0	1036	141	0
17	P	962	0	1009	55	0
18	Q	1043	0	1093	36	0
19	R	961	0	998	31	0
20	S	1077	0	1125	82	0
21	T	1148	0	1175	36	0
22	U	777	0	825	21	0
23	V	671	0	661	31	0
24	W	1001	0	1043	31	0
25	X	1062	0	1150	53	0
26	Y	792	0	784	42	0
27	Z	560	0	587	15	0
28	a	815	0	840	46	0
29	b	632	0	645	20	0
30	c	475	0	503	71	0
31	d	438	0	460	44	0
32	e	337	0	370	10	0
33	g	2380	0	2322	94	0
34	n	225	0	272	23	0
All	All	65924	0	50788	1649	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 14.

All (1649) 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)
33:g:209:HIS:CE1	33:g:228:GLY:HA2	1.24	1.62
16:O:61:LEU:CD2	16:O:89:VAL:HG23	1.36	1.52
33:g:191:VAL:CG2	33:g:208:ALA:HB3	1.46	1.43
16:O:61:LEU:HD21	16:O:89:VAL:CG2	1.44	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:95:SER:HB2	26:Y:15:LYS:CB	1.50	1.41
6:E:95:SER:CB	26:Y:15:LYS:HB2	1.49	1.39
25:X:24:TRP:CH2	25:X:33:LEU:HD23	1.58	1.39
16:O:65:THR:HA	16:O:69:ALA:CB	1.51	1.37
16:O:65:THR:O	16:O:69:ALA:HB3	1.22	1.36
2:A:73:LEU:HD13	2:A:88:PHE:CE2	1.60	1.35
3:B:43:THR:HB	3:B:63:TRP:CH2	1.63	1.34
2:A:73:LEU:HD13	2:A:88:PHE:CD2	1.62	1.33
17:P:84:ILE:HA	17:P:88:PHE:CZ	1.63	1.33
6:E:199:GLU:OE2	6:E:209:HIS:NE2	1.62	1.32
12:K:11:ILE:HD13	12:K:34:LEU:CD2	1.58	1.32
16:O:65:THR:C	16:O:69:ALA:HB3	1.53	1.32
28:a:23:CYS:HB3	28:a:73:TYR:O	1.26	1.31
3:B:61:ARG:CD	16:O:56:SER:OG	1.78	1.29
2:A:59:ALA:O	2:A:63:ILE:HG12	1.29	1.28
31:d:25:CYS:HB2	31:d:43:CYS:SG	1.75	1.26
3:B:79:ARG:NH1	3:B:99:MET:CE	1.99	1.26
33:g:209:HIS:CE1	33:g:228:GLY:CA	2.19	1.25
1:2:1554:G:N7	34:n:4:LYS:NZ	1.83	1.24
28:a:23:CYS:SG	28:a:26:CYS:SG	2.36	1.24
14:M:52:VAL:O	14:M:56:CYS:N	1.69	1.23
26:Y:106:ARG:O	26:Y:110:ARG:CB	1.85	1.23
6:E:95:SER:CB	26:Y:15:LYS:CB	2.09	1.22
1:2:750:G:N2	3:B:110:MET:HE2	1.55	1.22
1:2:1522:C:OP1	25:X:39:LYS:NZ	1.75	1.20
16:O:63:ARG:NH2	16:O:68:ILE:HB	1.56	1.19
9:H:68:GLN:HG2	9:H:145:ARG:CD	1.73	1.18
16:O:63:ARG:HH21	16:O:68:ILE:CB	1.55	1.18
14:M:51:LEU:O	14:M:55:LEU:CB	1.90	1.17
17:P:84:ILE:HG23	17:P:88:PHE:CE1	1.79	1.17
33:g:191:VAL:CG2	33:g:208:ALA:CB	2.21	1.17
16:O:65:THR:CA	16:O:69:ALA:CB	2.21	1.16
18:Q:52:ILE:CG2	18:Q:102:ILE:HD11	1.76	1.16
7:F:16:ASP:HB3	7:F:19:GLN:HB3	1.25	1.16
3:B:35:THR:HG21	3:B:71:VAL:CG1	1.74	1.15
14:M:19:ALA:HB3	14:M:97:ALA:CB	1.75	1.15
3:B:43:THR:CB	3:B:63:TRP:HH2	1.59	1.15
33:g:93:SER:O	33:g:109:LEU:HB2	1.47	1.13
1:2:678:G:O3'	9:H:93:ASN:ND2	1.81	1.12
6:E:95:SER:HB2	26:Y:15:LYS:HB3	1.27	1.12
1:2:695:G:OP2	3:B:154:SER:OG	1.68	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:73:LEU:HD22	2:A:88:PHE:HD2	1.10	1.12
20:S:25:ARG:HB2	27:Z:24:VAL:HG21	1.27	1.12
1:2:750:G:H21	3:B:110:MET:CE	1.61	1.12
1:2:203:A:N6	10:I:175:ARG:NH1	1.98	1.11
33:g:191:VAL:HG21	33:g:208:ALA:CB	1.80	1.11
3:B:28:VAL:HG23	3:B:41:GLY:O	1.48	1.11
9:H:68:GLN:HG2	9:H:145:ARG:HD3	1.27	1.11
9:H:134:LEU:CD1	9:H:142:VAL:HG21	1.80	1.11
26:Y:35:THR:HB	26:Y:38:GLU:HG3	1.12	1.11
12:K:79:PHE:HB3	12:K:81:LEU:HD11	1.19	1.10
10:I:162:LEU:HD23	10:I:180:ILE:HD13	1.26	1.10
33:g:209:HIS:NE2	33:g:228:GLY:HA2	1.66	1.10
1:2:578:A:C4	9:H:86:ARG:NH2	2.20	1.10
31:d:23:ARG:HG3	31:d:24:ILE:HD12	1.34	1.10
28:a:10:ARG:HB2	28:a:10:ARG:HH21	1.08	1.09
1:2:102:G:N2	1:2:234:U:C2	2.20	1.09
16:O:63:ARG:HH21	16:O:68:ILE:HB	0.94	1.09
19:R:97:LEU:HD13	19:R:98:VAL:N	1.67	1.09
33:g:92:ALA:O	33:g:109:LEU:CD1	2.00	1.08
14:M:19:ALA:CB	14:M:97:ALA:HB3	1.84	1.08
18:Q:52:ILE:HG23	18:Q:102:ILE:HD11	1.15	1.08
28:a:23:CYS:CB	28:a:73:TYR:O	1.99	1.08
2:A:70:LYS:HE3	2:A:70:LYS:HA	1.33	1.07
23:V:38:LYS:HZ3	23:V:50:GLU:HG2	1.14	1.07
6:E:95:SER:HB3	26:Y:15:LYS:HB2	1.33	1.07
7:F:12:TYR:CG	7:F:35:HIS:ND1	2.22	1.07
1:2:102:G:N2	1:2:234:U:O2	1.86	1.07
12:K:79:PHE:CB	12:K:81:LEU:HD11	1.84	1.07
20:S:47:VAL:HG13	20:S:52:LEU:CD1	1.84	1.07
5:D:17:LEU:HD21	31:d:23:ARG:NH2	1.68	1.06
16:O:63:ARG:HE	16:O:68:ILE:HG21	1.11	1.06
25:X:24:TRP:CH2	25:X:33:LEU:CD2	2.36	1.06
15:N:22:ALA:HB1	15:N:23:PRO:HA	1.31	1.06
1:2:96:C:C2'	1:2:97:G:H5'	1.86	1.05
14:M:49:LYS:O	14:M:53:ALA:N	1.89	1.05
1:2:26:A:N3	25:X:47:MET:HE1	1.72	1.05
2:A:204:ASP:N	2:A:207:ASP:OD2	1.88	1.05
3:B:79:ARG:NH1	3:B:99:MET:HE1	1.70	1.05
7:F:12:TYR:HB3	7:F:35:HIS:CE1	1.90	1.05
17:P:84:ILE:CG2	17:P:88:PHE:HE1	1.68	1.05
23:V:38:LYS:NZ	23:V:50:GLU:HG2	1.70	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:41:ARG:CD	22:U:110:LEU:HG	1.87	1.05
12:K:11:ILE:CD1	12:K:34:LEU:CD2	2.35	1.05
9:H:134:LEU:HD13	9:H:142:VAL:HG21	1.39	1.04
7:F:12:TYR:CD1	7:F:35:HIS:ND1	2.25	1.04
3:B:35:THR:HG21	3:B:71:VAL:HG12	1.34	1.04
16:O:36:MET:HE2	16:O:102:HIS:NE2	1.73	1.04
33:g:191:VAL:HG23	33:g:208:ALA:HB3	1.07	1.03
1:2:456:U:H5''	26:Y:31:ALA:CB	1.89	1.03
1:2:456:U:H5''	26:Y:31:ALA:HB1	1.40	1.03
23:V:38:LYS:HZ2	23:V:50:GLU:CD	1.65	1.03
25:X:24:TRP:CZ2	25:X:33:LEU:CD2	2.42	1.03
2:A:73:LEU:CD1	2:A:88:PHE:CD2	2.41	1.03
2:A:68:GLU:OE1	2:A:184:ARG:NH2	1.91	1.02
3:B:29:MET:HE1	3:B:39:ASP:HB2	1.38	1.02
3:B:79:ARG:NH1	3:B:99:MET:SD	2.29	1.02
9:H:113:THR:HG22	9:H:138:ASP:HB3	1.37	1.02
31:d:22:CYS:HB3	31:d:25:CYS:HB3	1.40	1.02
3:B:61:ARG:HD3	16:O:56:SER:OG	0.86	1.02
9:H:113:THR:HA	9:H:138:ASP:OD2	1.59	1.02
4:C:67:ILE:HD12	4:C:67:ILE:H	1.18	1.01
5:D:41:ARG:HD3	22:U:110:LEU:CG	1.90	1.00
16:O:61:LEU:CB	16:O:92:ARG:HD3	1.91	1.00
3:B:32:ALA:HA	3:B:33:TYR:HB2	1.44	1.00
16:O:61:LEU:HB3	16:O:92:ARG:HD3	1.43	1.00
17:P:84:ILE:CA	17:P:88:PHE:HZ	1.73	1.00
1:2:13:C:OP1	4:C:179:SER:HB3	1.62	1.00
11:J:131:HIS:O	11:J:157:ALA:N	1.94	0.99
33:g:92:ALA:O	33:g:109:LEU:HD13	1.58	0.99
4:C:126:ILE:HD11	4:C:202:LEU:HD22	1.41	0.99
12:K:32:GLU:N	12:K:32:GLU:OE1	1.96	0.99
1:2:100:C:H2'	1:2:101:A:H5'	1.44	0.99
5:D:41:ARG:HH21	22:U:112:PRO:HD3	1.23	0.99
1:2:936:G:OP1	34:n:11:ARG:NH2	1.95	0.99
19:R:93:VAL:HG22	19:R:95:LYS:N	1.77	0.99
2:A:72:VAL:HG12	2:A:117:PRO:HB3	1.43	0.99
20:S:81:ILE:HG23	20:S:82:PRO:HD2	1.45	0.99
11:J:114:ARG:HB3	11:J:116:LEU:HD13	1.45	0.98
16:O:65:THR:HA	16:O:69:ALA:HB1	1.41	0.98
7:F:32:GLU:HA	7:F:35:HIS:HD2	1.28	0.98
5:D:17:LEU:CD2	31:d:23:ARG:NH2	2.26	0.98
16:O:45:LYS:HG2	16:O:46:ASN:ND2	1.77	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1461:A:OP1	34:n:24:SER:OG	1.79	0.98
12:K:11:ILE:HD13	12:K:34:LEU:HD22	1.01	0.98
1:2:578:A:C5	9:H:86:ARG:NH2	2.32	0.98
33:g:173:MET:SD	33:g:175:ASP:N	2.35	0.98
1:2:1244:G:H22	12:K:56:LYS:NZ	1.62	0.98
12:K:11:ILE:CD1	12:K:34:LEU:HD22	1.92	0.98
2:A:72:VAL:HG12	2:A:117:PRO:CB	1.93	0.98
1:2:1242:G:O2'	31:d:25:CYS:SG	2.21	0.97
4:C:61:SER:HB3	4:C:261:TRP:CH2	1.98	0.97
19:R:93:VAL:HG11	19:R:96:ILE:HA	1.46	0.97
9:H:68:GLN:CG	9:H:145:ARG:HD3	1.93	0.97
16:O:105:PHE:HE1	16:O:120:ALA:HB1	1.29	0.97
16:O:65:THR:C	16:O:69:ALA:CB	2.38	0.97
25:X:35:THR:HB	25:X:38:TYR:CE1	2.00	0.97
25:X:106:MET:HG2	25:X:120:ARG:C	1.89	0.96
15:N:23:PRO:HB2	15:N:25:TRP:CD1	1.99	0.96
16:O:65:THR:HA	16:O:69:ALA:HB2	1.43	0.95
29:b:49:SER:O	29:b:72:ILE:HG23	1.66	0.95
20:S:92:ARG:HD2	20:S:115:ARG:HH22	1.28	0.95
11:J:135:GLU:HG2	11:J:153:ASN:HD22	1.29	0.95
2:A:59:ALA:O	2:A:63:ILE:CG1	2.13	0.95
9:H:134:LEU:CD1	9:H:142:VAL:CG2	2.44	0.95
1:2:456:U:C5'	26:Y:31:ALA:HB1	1.96	0.95
2:A:73:LEU:HD22	2:A:88:PHE:CD2	2.02	0.94
3:B:33:TYR:OH	3:B:177:VAL:HG13	1.67	0.94
31:d:25:CYS:CB	31:d:43:CYS:SG	2.54	0.94
12:K:27:GLN:HE21	12:K:27:GLN:HA	1.32	0.94
34:n:9:ARG:HG3	34:n:9:ARG:HH11	1.31	0.94
1:2:467:A:C2'	32:e:31:ARG:HH11	1.79	0.94
7:F:12:TYR:CB	7:F:35:HIS:CE1	2.50	0.94
25:X:37:ILE:O	25:X:40:THR:HG23	1.67	0.94
11:J:117:ALA:HA	11:J:126:LEU:HD11	1.50	0.94
12:K:84:ASN:N	12:K:85:ALA:HB3	1.82	0.94
14:M:19:ALA:HB3	14:M:97:ALA:HB3	0.94	0.94
6:E:94:LYS:HE3	6:E:94:LYS:HA	1.49	0.93
26:Y:35:THR:OG1	26:Y:38:GLU:OE2	1.85	0.93
33:g:206:PHE:CE1	33:g:208:ALA:HB2	2.04	0.93
9:H:82:PRO:HG3	9:H:88:PHE:CE2	2.04	0.93
1:2:467:A:H2'	32:e:31:ARG:HH11	1.31	0.93
16:O:42:TYR:CE1	16:O:106:ARG:NE	2.36	0.93
20:S:47:VAL:HG13	20:S:52:LEU:HD11	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:87:LYS:HD2	2:A:199:LEU:HD21	1.52	0.92
3:B:79:ARG:HH11	3:B:99:MET:CE	1.72	0.92
25:X:24:TRP:CZ2	25:X:33:LEU:HD23	2.03	0.92
1:2:467:A:C2'	32:e:31:ARG:NH1	2.33	0.92
16:O:52:VAL:HG22	16:O:61:LEU:O	1.68	0.92
4:C:68:GLU:HG3	23:V:12:LEU:HB3	1.50	0.92
20:S:88:ARG:NH2	20:S:100:TRP:CH2	2.38	0.92
33:g:225:VAL:C	33:g:226:ILE:HD13	1.94	0.92
9:H:68:GLN:HE21	9:H:145:ARG:HG2	1.35	0.91
25:X:35:THR:N	25:X:36:SER:HB3	1.86	0.91
16:O:65:THR:O	16:O:69:ALA:CB	2.15	0.91
33:g:49:VAL:HG13	33:g:58:LEU:O	1.70	0.91
33:g:191:VAL:HG21	33:g:208:ALA:HB3	1.33	0.91
21:T:45:LYS:NZ	21:T:50:LYS:O	2.04	0.91
16:O:63:ARG:NE	16:O:68:ILE:HG21	1.86	0.91
31:d:22:CYS:HB2	31:d:40:CYS:HB2	1.54	0.91
1:2:1038:G:N1	14:M:21:GLY:HA3	1.86	0.90
2:A:73:LEU:CD1	2:A:88:PHE:CE2	2.52	0.90
4:C:211:LEU:HD12	4:C:212:PHE:H	1.36	0.90
11:J:114:ARG:HG3	11:J:116:LEU:HD11	1.53	0.90
33:g:209:HIS:HE1	33:g:228:GLY:HA2	1.16	0.90
26:Y:35:THR:HB	26:Y:38:GLU:CG	1.99	0.90
2:A:70:LYS:HD3	4:C:54:LYS:HE3	1.53	0.90
4:C:68:GLU:HG3	23:V:12:LEU:CB	2.02	0.90
16:O:51:HIS:NE2	16:O:59:GLU:HG3	1.85	0.89
1:2:96:C:H2'	1:2:97:G:H5'	1.51	0.89
11:J:117:ALA:O	11:J:122:HIS:ND1	2.05	0.89
31:d:22:CYS:HG	31:d:25:CYS:HB2	1.36	0.89
1:2:97:G:H2'	1:2:98:C:C6	2.07	0.89
1:2:97:G:H2'	1:2:98:C:H6	1.33	0.89
7:F:5:LYS:HB2	7:F:10:TYR:O	1.73	0.89
1:2:456:U:OP1	26:Y:31:ALA:CB	2.21	0.89
2:A:73:LEU:CD2	2:A:88:PHE:HD2	1.86	0.88
6:E:199:GLU:OE2	6:E:209:HIS:CD2	2.25	0.88
9:H:82:PRO:HG3	9:H:88:PHE:CZ	2.08	0.88
16:O:42:TYR:HE1	16:O:106:ARG:NE	1.68	0.88
33:g:191:VAL:HG23	33:g:208:ALA:CB	1.92	0.88
4:C:52:ARG:O	4:C:53:THR:OG1	1.90	0.88
18:Q:52:ILE:HD11	18:Q:106:LEU:HD11	1.56	0.88
30:c:17:ILE:CD1	30:c:67:LEU:HD21	2.04	0.88
33:g:93:SER:O	33:g:109:LEU:CB	2.22	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:103:A:P	1:2:103:A:H3'	2.14	0.87
10:I:109:PHE:CE2	10:I:180:ILE:HD11	2.09	0.87
1:2:102:G:O3'	1:2:103:A:H3'	1.74	0.87
17:P:84:ILE:CA	17:P:88:PHE:CZ	2.52	0.87
1:2:203:A:N6	10:I:175:ARG:HH12	1.64	0.87
9:H:139:ALA:HB2	9:H:142:VAL:H	1.38	0.87
28:a:10:ARG:HB2	28:a:10:ARG:NH2	1.89	0.87
1:2:467:A:O2'	32:e:31:ARG:NH1	2.08	0.87
4:C:68:GLU:OE2	23:V:12:LEU:HA	1.74	0.87
3:B:61:ARG:HD3	16:O:56:SER:HG	1.05	0.87
12:K:34:LEU:CD1	12:K:36:CYS:SG	2.63	0.87
16:O:65:THR:CA	16:O:69:ALA:HB3	1.92	0.87
9:H:134:LEU:HD12	9:H:142:VAL:HG21	1.56	0.87
4:C:172:THR:HG22	4:C:186:PRO:HD2	1.56	0.86
7:F:28:ILE:HD11	7:F:102:VAL:HG13	1.58	0.86
19:R:93:VAL:N	19:R:94:PRO:HA	1.87	0.86
23:V:38:LYS:NZ	23:V:50:GLU:CG	2.36	0.86
4:C:61:SER:HB3	4:C:261:TRP:CZ2	2.10	0.86
7:F:65:LEU:CD1	7:F:144:THR:HG23	2.06	0.86
33:g:53:ARG:O	33:g:82:PHE:HD1	1.56	0.86
1:2:1038:G:H1	14:M:21:GLY:HA3	1.40	0.86
2:A:72:VAL:CG1	2:A:117:PRO:HB3	2.05	0.86
12:K:11:ILE:CD1	12:K:34:LEU:HD21	2.03	0.86
30:c:17:ILE:HD13	30:c:67:LEU:CD2	2.06	0.86
4:C:52:ARG:HG2	4:C:79:GLU:OE2	1.75	0.86
4:C:126:ILE:HD11	4:C:202:LEU:CD2	2.06	0.86
5:D:17:LEU:CD2	31:d:23:ARG:HH22	1.86	0.86
9:H:139:ALA:HA	9:H:140:THR:HB	1.57	0.86
30:c:45:VAL:HG11	30:c:55:LEU:HD21	1.58	0.85
16:O:105:PHE:CE1	16:O:120:ALA:HB1	2.10	0.85
17:P:84:ILE:HG23	17:P:88:PHE:HE1	1.16	0.85
33:g:212:ARG:O	33:g:230:SER:HB2	1.76	0.85
26:Y:26:MET:HE3	26:Y:68:THR:HG23	1.58	0.85
19:R:93:VAL:CG2	19:R:96:ILE:H	1.89	0.85
1:2:96:C:O2'	1:2:97:G:H5'	1.76	0.85
2:A:70:LYS:HA	2:A:70:LYS:CE	2.07	0.85
1:2:1283:U:C6	7:F:71:ASN:ND2	2.44	0.85
1:2:1553:G:OP2	34:n:2:ARG:HD2	1.76	0.85
2:A:68:GLU:CD	2:A:184:ARG:NH2	2.35	0.85
1:2:467:A:H2'	32:e:31:ARG:NH1	1.92	0.85
6:E:95:SER:HB2	26:Y:15:LYS:CG	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:104:LEU:CD1	24:W:106:THR:HG23	2.07	0.84
4:C:52:ARG:CG	4:C:79:GLU:OE2	2.25	0.84
28:a:23:CYS:SG	28:a:77:CYS:SG	2.66	0.84
17:P:84:ILE:HA	17:P:88:PHE:HZ	0.77	0.84
3:B:28:VAL:CG2	3:B:41:GLY:O	2.25	0.84
12:K:79:PHE:CB	12:K:81:LEU:CD1	2.56	0.84
1:2:720:U:P	16:O:66:GLY:HA3	2.17	0.84
6:E:202:MET:HA	6:E:202:MET:HE2	1.59	0.84
25:X:24:TRP:CZ2	25:X:33:LEU:HD21	2.11	0.84
25:X:37:ILE:O	25:X:40:THR:CG2	2.26	0.84
1:2:750:G:H21	3:B:110:MET:HE2	0.72	0.83
2:A:184:ARG:HG3	2:A:184:ARG:HH11	1.43	0.83
5:D:41:ARG:HD3	22:U:110:LEU:HG	0.94	0.83
20:S:88:ARG:NH2	20:S:100:TRP:CZ3	2.46	0.83
9:H:98:LEU:HD12	9:H:98:LEU:O	1.79	0.83
3:B:36:GLY:HA2	3:B:37:LYS:HB3	1.59	0.83
2:A:86:HIS:NE2	2:A:90:GLU:OE2	2.11	0.83
12:K:29:GLY:O	12:K:38:ASN:CG	2.21	0.83
30:c:66:ARG:HG3	30:c:66:ARG:HH11	1.42	0.83
9:H:139:ALA:CB	9:H:142:VAL:H	1.91	0.83
31:d:22:CYS:SG	31:d:25:CYS:HB2	2.19	0.82
2:A:72:VAL:O	2:A:120:MET:HA	1.76	0.82
9:H:134:LEU:HD12	9:H:142:VAL:CG2	2.06	0.82
3:B:32:ALA:HA	3:B:33:TYR:CB	2.08	0.82
17:P:86:PRO:N	17:P:111:ILE:HD11	1.94	0.82
7:F:32:GLU:HA	7:F:35:HIS:CD2	2.13	0.82
26:Y:35:THR:O	26:Y:39:ILE:HG13	1.80	0.82
3:B:197:CYS:HB3	3:B:201:CYS:O	1.78	0.82
5:D:41:ARG:NH2	22:U:112:PRO:HD3	1.94	0.82
7:F:16:ASP:HB3	7:F:19:GLN:CB	2.09	0.81
31:d:23:ARG:HG3	31:d:24:ILE:CD1	2.09	0.81
1:2:924:U:OP1	34:n:14:LYS:NZ	2.14	0.81
17:P:15:ARG:CZ	20:S:90:PHE:CE2	2.64	0.81
9:H:94:TYR:O	9:H:97:THR:HG22	1.80	0.81
20:S:41:ARG:NH1	21:T:43:LEU:O	2.11	0.81
6:E:94:LYS:HE3	6:E:94:LYS:CA	2.11	0.81
18:Q:80:GLN:NE2	18:Q:116:ALA:HB2	1.96	0.81
19:R:93:VAL:HG22	19:R:95:LYS:H	1.45	0.81
3:B:84:ARG:HB2	3:B:84:ARG:NH2	1.96	0.81
16:O:106:ARG:HH22	16:O:142:PRO:CG	1.94	0.81
33:g:173:MET:SD	33:g:174:ALA:N	2.54	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:106:LEU:HD23	3:B:106:LEU:O	1.81	0.80
7:F:12:TYR:HB3	7:F:35:HIS:HE1	1.42	0.80
30:c:33:PHE:HD2	30:c:39:ARG:HG3	1.46	0.80
9:H:134:LEU:HD13	9:H:142:VAL:CG2	2.08	0.80
2:A:88:PHE:CE1	2:A:92:LEU:HD12	2.17	0.80
7:F:24:LEU:HD11	7:F:135:ARG:NH2	1.97	0.80
3:B:153:ASN:OD1	3:B:154:SER:N	2.15	0.80
12:K:58:TYR:OH	12:K:61:SER:HA	1.81	0.80
19:R:97:LEU:HD13	19:R:98:VAL:H	1.44	0.80
1:2:100:C:H2'	1:2:101:A:C5'	2.12	0.80
1:2:865:U:OP1	3:B:149:HIS:HE1	1.65	0.80
7:F:65:LEU:HD12	7:F:144:THR:HG23	1.64	0.79
24:W:36:ALA:C	24:W:110:ILE:HD11	2.06	0.79
30:c:14:LYS:HD2	30:c:32:GLU:CD	2.07	0.79
10:I:54:LYS:HE3	10:I:172:GLN:HG3	1.63	0.79
16:O:106:ARG:HH22	16:O:142:PRO:HG3	1.46	0.79
1:2:1038:G:C6	14:M:21:GLY:HA3	2.18	0.79
3:B:43:THR:HB	3:B:63:TRP:HH2	0.70	0.79
24:W:104:LEU:HD12	24:W:104:LEU:O	1.82	0.79
32:e:8:LEU:HD12	32:e:8:LEU:O	1.83	0.79
6:E:90:ILE:HG22	6:E:92:LEU:HD11	1.62	0.79
3:B:32:ALA:CA	3:B:33:TYR:HB2	2.13	0.79
10:I:65:PHE:CD2	10:I:104:ILE:HD13	2.18	0.79
16:O:53:THR:HG22	16:O:59:GLU:HA	1.65	0.79
20:S:47:VAL:CG1	20:S:52:LEU:CD1	2.60	0.79
1:2:268:C:H5'	10:I:10:LYS:HD3	1.64	0.79
1:2:521:G:H5'	25:X:107:GLY:HA2	1.65	0.79
7:F:29:SER:C	7:F:34:GLN:HG3	2.08	0.79
1:2:177:U:H4'	10:I:173:CYS:SG	2.22	0.78
3:B:88:ALA:HB3	3:B:92:VAL:HA	1.64	0.78
12:K:11:ILE:HD13	12:K:34:LEU:HD21	1.58	0.78
15:N:18:TYR:HD1	29:b:26:VAL:HG13	1.49	0.78
10:I:9:LEU:HD13	10:I:9:LEU:O	1.83	0.78
12:K:31:HIS:HB2	12:K:38:ASN:OD1	1.82	0.78
2:A:64:TYR:OH	2:A:184:ARG:HA	1.83	0.78
16:O:36:MET:CE	16:O:102:HIS:NE2	2.46	0.78
22:U:53:GLU:O	22:U:95:PHE:HB2	1.83	0.78
26:Y:35:THR:CB	26:Y:38:GLU:HG3	2.06	0.78
30:c:9:LYS:HE3	30:c:35:ASP:OD1	1.82	0.78
15:N:16:CYS:SG	15:N:62:MET:HE3	2.24	0.78
16:O:47:ASP:OD1	16:O:48:THR:N	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:125:VAL:HG13	17:P:126:LYS:H	1.48	0.78
9:H:77:ALA:HB1	9:H:96:ARG:O	1.84	0.78
11:J:117:ALA:HA	11:J:126:LEU:CD1	2.13	0.78
1:2:97:G:C6	1:2:239:G:N1	2.52	0.78
3:B:40:ILE:HG21	3:B:65:LEU:CD1	2.14	0.78
17:P:84:ILE:CG2	17:P:88:PHE:CE1	2.51	0.78
5:D:43:THR:HG22	5:D:44:PRO:HD2	1.66	0.78
6:E:90:ILE:HG22	6:E:92:LEU:CD1	2.14	0.77
16:O:61:LEU:HG	16:O:92:ARG:HD3	1.66	0.77
18:Q:25:LEU:HD22	21:T:5:LYS:O	1.84	0.77
1:2:97:G:C6	1:2:239:G:C6	2.73	0.77
18:Q:25:LEU:HD23	21:T:5:LYS:HG3	1.66	0.77
22:U:52:LEU:HD22	22:U:96:GLN:O	1.83	0.77
16:O:129:ARG:CZ	30:c:39:ARG:HH22	1.97	0.77
1:2:97:G:O6	1:2:239:G:C6	2.37	0.77
16:O:61:LEU:HB3	16:O:92:ARG:CD	2.14	0.77
16:O:129:ARG:NH2	30:c:39:ARG:HH22	1.81	0.77
2:A:66:VAL:HG12	2:A:67:GLU:OE2	1.83	0.77
33:g:53:ARG:O	33:g:82:PHE:CD1	2.38	0.77
6:E:48:LEU:HD13	6:E:64:ILE:HD11	1.67	0.77
25:X:106:MET:HB3	25:X:113:VAL:HG21	1.64	0.77
15:N:28:LEU:HD23	15:N:66:VAL:HG21	1.67	0.77
16:O:63:ARG:HE	16:O:68:ILE:CG2	1.96	0.77
9:H:93:ASN:OD1	9:H:94:TYR:N	2.18	0.76
15:N:16:CYS:SG	15:N:62:MET:SD	2.83	0.76
16:O:63:ARG:HH21	16:O:68:ILE:CG2	1.98	0.76
9:H:68:GLN:HG2	9:H:145:ARG:CG	2.14	0.76
20:S:25:ARG:HB2	27:Z:24:VAL:CG2	2.11	0.76
4:C:206:ALA:HB1	4:C:208:PHE:HE2	1.48	0.76
19:R:93:VAL:HG11	19:R:96:ILE:CA	2.15	0.76
3:B:40:ILE:HG21	3:B:65:LEU:HD11	1.66	0.76
11:J:117:ALA:O	11:J:118:ASN:HB3	1.85	0.76
16:O:61:LEU:CG	16:O:92:ARG:HD3	2.15	0.76
20:S:57:ARG:NH2	27:Z:58:THR:HG21	2.01	0.76
10:I:168:SER:OG	10:I:176:ALA:HA	1.86	0.76
15:N:22:ALA:HB1	15:N:23:PRO:CA	2.14	0.76
28:a:10:ARG:HH21	28:a:10:ARG:CB	1.95	0.76
1:2:456:U:OP1	26:Y:31:ALA:HB2	1.85	0.76
15:N:26:LEU:HG	15:N:27:GLN:N	1.99	0.76
3:B:84:ARG:HB2	3:B:84:ARG:HH21	1.49	0.75
4:C:176:LYS:HB3	4:C:181:ARG:HD3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:129:ARG:CZ	30:c:39:ARG:NH2	2.49	0.75
28:a:18:THR:HG21	28:a:33:ASP:CG	2.11	0.75
12:K:27:GLN:HE21	12:K:27:GLN:CA	2.00	0.75
31:d:22:CYS:HB2	31:d:40:CYS:CB	2.16	0.75
16:O:61:LEU:HD11	16:O:93:LEU:HD11	1.69	0.75
1:2:101:A:N1	1:2:235:G:C6	2.55	0.75
1:2:265:U:O4	10:I:5:ARG:NH1	2.19	0.75
15:N:20:ARG:CD	15:N:20:ARG:H	2.00	0.75
17:P:125:VAL:HG13	17:P:126:LYS:N	2.02	0.75
3:B:29:MET:CE	3:B:39:ASP:HB2	2.17	0.75
18:Q:80:GLN:HE22	18:Q:116:ALA:HB2	1.51	0.75
30:c:17:ILE:CD1	30:c:67:LEU:CD2	2.64	0.74
21:T:43:LEU:N	21:T:43:LEU:HD12	2.02	0.74
9:H:79:PRO:HD2	9:H:88:PHE:HB2	1.66	0.74
22:U:24:ILE:HD12	22:U:102:VAL:HG21	1.69	0.74
3:B:31:PRO:O	3:B:33:TYR:HB2	1.88	0.74
4:C:211:LEU:HD12	4:C:212:PHE:N	2.01	0.74
7:F:12:TYR:CG	7:F:35:HIS:CE1	2.75	0.74
15:N:18:TYR:CD1	29:b:26:VAL:HG13	2.23	0.74
3:B:29:MET:HE1	3:B:39:ASP:CB	2.16	0.74
9:H:77:ALA:CB	9:H:96:ARG:O	2.36	0.74
1:2:875:U:O4	3:B:200:ILE:O	2.04	0.74
5:D:17:LEU:HD23	31:d:23:ARG:HH22	1.52	0.74
10:I:169:ARG:NH2	10:I:172:GLN:OE1	2.20	0.74
16:O:52:VAL:CG2	16:O:61:LEU:HD13	2.18	0.74
2:A:73:LEU:CD2	2:A:88:PHE:CD2	2.67	0.74
2:A:171:LEU:HD21	19:R:91:LEU:HD11	1.69	0.74
3:B:29:MET:SD	3:B:39:ASP:HA	2.28	0.74
10:I:162:LEU:CD2	10:I:180:ILE:HD13	2.11	0.74
16:O:61:LEU:HD22	16:O:89:VAL:HG23	1.65	0.74
26:Y:35:THR:HG1	26:Y:38:GLU:CD	1.95	0.74
1:2:906:C:O2'	4:C:174:THR:HG21	1.86	0.74
20:S:47:VAL:HG13	20:S:52:LEU:HD12	1.69	0.74
11:J:58:LEU:CD1	11:J:91:LEU:HD12	2.18	0.73
21:T:46:THR:HG22	21:T:50:LYS:HG3	1.70	0.73
12:K:81:LEU:HD12	12:K:81:LEU:N	2.03	0.73
33:g:225:VAL:O	33:g:226:ILE:HD13	1.89	0.73
12:K:45:GLY:O	12:K:49:VAL:HG23	1.87	0.73
5:D:43:THR:HG22	5:D:44:PRO:CD	2.19	0.73
1:2:1414:U:C5	18:Q:121:MET:HE1	2.24	0.73
10:I:81:VAL:HA	10:I:102:VAL:HG12	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:58:LEU:CD1	11:J:91:LEU:CD1	2.66	0.73
20:S:82:PRO:HB2	20:S:84:TRP:CD1	2.22	0.73
2:A:70:LYS:HD3	4:C:54:LYS:CE	2.18	0.73
4:C:154:VAL:HG11	4:C:208:PHE:CZ	2.24	0.72
11:J:57:LEU:HD11	11:J:70:GLU:HG3	1.71	0.72
4:C:61:SER:CB	4:C:261:TRP:CH2	2.72	0.72
16:O:45:LYS:HG2	16:O:46:ASN:HD21	1.49	0.72
4:C:67:ILE:HG22	4:C:71:PHE:CE2	2.23	0.72
23:V:38:LYS:NZ	23:V:50:GLU:CD	2.47	0.72
1:2:1266:C:OP1	17:P:122:LYS:NZ	2.18	0.72
16:O:61:LEU:HD22	16:O:61:LEU:C	2.15	0.72
11:J:135:GLU:CG	11:J:153:ASN:HD22	2.00	0.72
31:d:24:ILE:HD12	31:d:24:ILE:N	2.04	0.72
16:O:93:LEU:O	16:O:97:GLY:HA2	1.90	0.72
20:S:47:VAL:CG1	20:S:52:LEU:HD12	2.19	0.72
21:T:2:ILE:HD13	21:T:2:ILE:N	2.05	0.72
23:V:38:LYS:HZ3	23:V:50:GLU:CG	1.98	0.72
18:Q:11:LYS:O	18:Q:120:ARG:NH1	2.22	0.72
28:a:10:ARG:CG	28:a:12:LYS:HG2	2.20	0.72
29:b:55:VAL:O	29:b:64:LEU:N	2.23	0.72
1:2:97:G:C4	1:2:239:G:N2	2.58	0.72
7:F:16:ASP:O	7:F:20:LEU:HD13	1.90	0.72
11:J:114:ARG:HG3	11:J:116:LEU:CD1	2.19	0.72
26:Y:28:HIS:O	26:Y:66:GLY:HA3	1.90	0.72
1:2:720:U:OP2	16:O:66:GLY:HA3	1.90	0.71
20:S:92:ARG:HD2	20:S:115:ARG:NH2	2.04	0.71
28:a:30:VAL:HG23	28:a:31:PRO:HD2	1.71	0.71
1:2:97:G:C5	1:2:239:G:C2	2.78	0.71
1:2:854:C:HO2'	24:W:2:VAL:N	1.88	0.71
15:N:22:ALA:CB	15:N:23:PRO:HA	2.06	0.71
17:P:46:PHE:HA	17:P:50:HIS:HD2	1.56	0.71
3:B:34:PHE:H	3:B:34:PHE:HD2	1.36	0.71
15:N:26:LEU:HG	15:N:27:GLN:H	1.52	0.71
19:R:93:VAL:CG1	19:R:96:ILE:HG12	2.20	0.71
30:c:67:LEU:C	30:c:67:LEU:HD13	2.15	0.71
1:2:98:C:C2	1:2:99:U:C5	2.78	0.71
4:C:172:THR:HG22	4:C:186:PRO:CD	2.21	0.71
1:2:1575:U:O4	28:a:34:LYS:HE3	1.91	0.71
17:P:15:ARG:CZ	20:S:90:PHE:HE2	2.02	0.71
9:H:140:THR:HG22	9:H:141:ARG:N	2.04	0.71
18:Q:52:ILE:HD11	18:Q:106:LEU:CD1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:911:G:H5'	24:W:4:THR:HG21	1.71	0.71
18:Q:52:ILE:HG21	18:Q:102:ILE:HD11	1.73	0.71
31:d:24:ILE:HD12	31:d:24:ILE:H	1.55	0.71
1:2:456:U:H5''	26:Y:31:ALA:HB3	1.73	0.71
7:F:132:PRO:HG2	30:c:53:ASP:OD1	1.91	0.71
16:O:106:ARG:NH2	16:O:142:PRO:HG3	2.06	0.71
23:V:12:LEU:C	23:V:12:LEU:HD12	2.15	0.71
16:O:100:GLY:HA2	16:O:133:LYS:O	1.90	0.71
1:2:103:A:C2	1:2:190:A:C4	2.79	0.70
16:O:42:TYR:HE1	16:O:106:ARG:CZ	2.04	0.70
2:A:83:ARG:NH1	2:A:87:LYS:HZ3	1.89	0.70
3:B:79:ARG:NH1	3:B:99:MET:HE3	2.03	0.70
4:C:94:GLU:HB3	4:C:205:MET:HE1	1.73	0.70
4:C:167:HIS:HD2	4:C:210:ASP:OD2	1.74	0.70
4:C:211:LEU:CD1	4:C:212:PHE:H	2.04	0.70
23:V:38:LYS:HZ1	23:V:49:PHE:C	1.99	0.70
1:2:97:G:C4	1:2:98:C:C5	2.79	0.70
16:O:54:ASP:OD1	16:O:55:LEU:N	2.24	0.70
23:V:9:VAL:O	23:V:10:ASP:HB2	1.91	0.70
29:b:48:PHE:HD2	29:b:51:SER:H	1.39	0.70
31:d:42:ARG:HG3	31:d:42:ARG:HH11	1.56	0.70
1:2:644:G:H4'	6:E:201:GLN:HE22	1.55	0.70
7:F:111:ARG:HD2	30:c:58:LEU:HD21	1.74	0.70
33:g:209:HIS:NE2	33:g:228:GLY:CA	2.42	0.70
4:C:174:THR:CG2	4:C:183:ARG:HG3	2.21	0.70
6:E:95:SER:OG	26:Y:15:LYS:HG3	1.91	0.70
1:2:98:C:HO2'	1:2:99:U:H6	1.35	0.70
16:O:61:LEU:O	16:O:61:LEU:HD13	1.92	0.70
1:2:203:A:N6	10:I:175:ARG:HH11	1.90	0.70
7:F:132:PRO:HD2	30:c:53:ASP:OD2	1.92	0.70
12:K:54:CYS:C	12:K:55:ILE:HD12	2.17	0.70
1:2:100:C:C2'	1:2:101:A:H5'	2.19	0.70
4:C:51:PRO:HD3	4:C:60:LYS:HE2	1.72	0.70
7:F:65:LEU:HD12	7:F:144:THR:CG2	2.21	0.70
16:O:134:ILE:HD11	28:a:53:VAL:HG13	1.73	0.70
34:n:9:ARG:HG3	34:n:9:ARG:NH1	1.99	0.70
2:A:62:MET:HE3	23:V:34:ILE:HG23	1.73	0.69
23:V:38:LYS:HZ2	23:V:50:GLU:CG	2.00	0.69
25:X:106:MET:HG3	25:X:120:ARG:HA	1.73	0.69
4:C:172:THR:CG2	4:C:186:PRO:HD2	2.22	0.69
1:2:1244:G:H22	12:K:56:LYS:HZ3	1.37	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:97:G:C5	1:2:239:G:N1	2.60	0.69
4:C:210:ASP:OD2	4:C:210:ASP:N	2.25	0.69
20:S:50:ALA:N	20:S:51:GLY:HA2	2.08	0.69
12:K:76:ARG:NH2	12:K:83:ALA:HB1	2.07	0.69
19:R:22:GLY:O	33:g:212:ARG:HD2	1.92	0.69
19:R:93:VAL:HG21	19:R:96:ILE:H	1.56	0.69
1:2:456:U:OP1	26:Y:31:ALA:HB1	1.93	0.69
11:J:58:LEU:CD2	11:J:95:LEU:HD11	2.22	0.69
1:2:26:A:N3	25:X:47:MET:CE	2.54	0.69
20:S:92:ARG:HH11	20:S:115:ARG:NH2	1.90	0.69
28:a:23:CYS:HB3	28:a:74:CYS:SG	2.32	0.69
1:2:203:A:H61	10:I:175:ARG:NH1	1.86	0.69
7:F:91:LEU:HD13	27:Z:76:VAL:HG11	1.75	0.69
30:c:10:LEU:O	30:c:34:LEU:HB3	1.93	0.69
4:C:94:GLU:CB	4:C:205:MET:HE1	2.23	0.68
9:H:139:ALA:CB	9:H:142:VAL:N	2.55	0.68
1:2:679:C:P	9:H:93:ASN:HD21	2.15	0.68
7:F:65:LEU:HD13	7:F:144:THR:HG23	1.75	0.68
6:E:95:SER:CB	26:Y:15:LYS:CG	2.67	0.68
7:F:14:ASP:OD1	7:F:14:ASP:N	2.27	0.68
33:g:92:ALA:O	33:g:109:LEU:HD12	1.90	0.68
1:2:97:G:C6	1:2:239:G:C2	2.81	0.68
24:W:11:LEU:HD12	24:W:74:ALA:HB2	1.76	0.68
2:A:83:ARG:CZ	2:A:87:LYS:HZ1	2.06	0.68
7:F:12:TYR:CD1	7:F:35:HIS:CE1	2.81	0.68
9:H:94:TYR:OH	9:H:99:ARG:NH2	2.26	0.68
11:J:114:ARG:CB	11:J:116:LEU:HD13	2.22	0.68
31:d:22:CYS:HB3	31:d:25:CYS:CB	2.20	0.68
6:E:95:SER:OG	26:Y:15:LYS:HB2	1.94	0.68
23:V:44:LEU:HD12	23:V:45:PRO:HD2	1.76	0.68
34:n:16:LYS:O	34:n:20:VAL:HG23	1.94	0.68
1:2:97:G:C2'	1:2:98:C:H6	2.05	0.68
3:B:43:THR:CB	3:B:63:TRP:CH2	2.47	0.68
17:P:15:ARG:NH1	20:S:90:PHE:CD2	2.61	0.68
10:I:65:PHE:HD2	10:I:104:ILE:HD13	1.58	0.67
12:K:34:LEU:HD11	12:K:36:CYS:SG	2.33	0.67
30:c:56:SER:C	30:c:57:LEU:HD12	2.19	0.67
1:2:560:U:O2'	9:H:92:ARG:NH1	2.27	0.67
16:O:51:HIS:NE2	16:O:59:GLU:CG	2.58	0.67
20:S:89:ARG:HA	20:S:97:ASN:HA	1.75	0.67
22:U:99:ALA:O	22:U:103:LYS:HG3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:15:SER:N	14:M:16:GLY:HA2	2.08	0.67
2:A:171:LEU:HD21	19:R:91:LEU:CD1	2.24	0.67
4:C:168:THR:HG22	4:C:169:VAL:N	2.08	0.67
33:g:53:ARG:HG3	33:g:82:PHE:CD1	2.30	0.67
16:O:34:ILE:C	16:O:34:ILE:HD12	2.19	0.67
16:O:65:THR:CA	16:O:69:ALA:HB2	2.08	0.67
28:a:18:THR:HG21	28:a:33:ASP:OD1	1.94	0.67
2:A:83:ARG:NH1	2:A:87:LYS:NZ	2.42	0.67
10:I:7:GLY:O	10:I:10:LYS:HG2	1.94	0.67
18:Q:25:LEU:CD2	21:T:5:LYS:O	2.42	0.67
12:K:34:LEU:HD12	12:K:34:LEU:O	1.95	0.67
16:O:129:ARG:NH2	30:c:39:ARG:NH2	2.43	0.67
15:N:18:TYR:HD1	29:b:26:VAL:CG1	2.08	0.67
16:O:64:CYS:O	16:O:69:ALA:HB2	1.95	0.67
16:O:65:THR:OG1	16:O:76:GLU:O	2.13	0.67
12:K:79:PHE:HB2	12:K:81:LEU:CD1	2.26	0.66
30:c:33:PHE:CE2	30:c:39:ARG:HD2	2.30	0.66
31:d:22:CYS:SG	31:d:43:CYS:SG	2.86	0.66
33:g:112:ARG:O	33:g:113:THR:HG22	1.95	0.66
15:N:16:CYS:SG	15:N:62:MET:CE	2.83	0.66
20:S:87:ASN:C	20:S:87:ASN:HD22	2.03	0.66
25:X:35:THR:HB	25:X:38:TYR:HE1	1.54	0.66
9:H:83:GLU:O	9:H:84:HIS:HB3	1.94	0.66
9:H:140:THR:HG22	9:H:141:ARG:H	1.60	0.66
30:c:17:ILE:HD13	30:c:67:LEU:HD23	1.75	0.66
12:K:55:ILE:HD12	12:K:55:ILE:N	2.10	0.66
18:Q:52:ILE:HG23	18:Q:102:ILE:CD1	2.10	0.66
20:S:46:VAL:O	20:S:50:ALA:N	2.29	0.66
7:F:32:GLU:CA	7:F:35:HIS:HD2	2.04	0.66
31:d:22:CYS:SG	31:d:40:CYS:HB3	2.35	0.66
2:A:109:TYR:CD1	4:C:52:ARG:HD3	2.30	0.66
5:D:29:GLU:OE1	12:K:57:THR:HG21	1.95	0.66
12:K:82:PRO:O	12:K:85:ALA:HB2	1.96	0.66
15:N:18:TYR:CD1	29:b:26:VAL:CG1	2.78	0.66
17:P:15:ARG:HA	20:S:92:ARG:O	1.95	0.66
25:X:106:MET:CG	25:X:120:ARG:C	2.67	0.66
11:J:131:HIS:HD2	11:J:159:THR:OG1	1.78	0.66
4:C:57:ARG:NH2	4:C:262:LEU:O	2.29	0.66
12:K:80:GLY:C	12:K:81:LEU:HD12	2.20	0.66
23:V:9:VAL:HG12	23:V:10:ASP:N	2.10	0.66
26:Y:24:ILE:HG22	26:Y:26:MET:HG3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:35:THR:HG21	3:B:71:VAL:HG13	1.70	0.65
9:H:113:THR:HG22	9:H:138:ASP:CB	2.19	0.65
16:O:36:MET:CE	16:O:102:HIS:CE1	2.79	0.65
30:c:33:PHE:CD2	30:c:39:ARG:HG3	2.30	0.65
20:S:87:ASN:H	20:S:99:HIS:HB2	1.61	0.65
3:B:66:SER:OG	3:B:77:ALA:O	2.12	0.65
4:C:147:ALA:O	4:C:150:SER:O	2.14	0.65
4:C:153:PRO:HG2	4:C:237:PHE:CE2	2.32	0.65
7:F:20:LEU:O	7:F:21:ASP:HB3	1.95	0.65
20:S:85:MET:O	20:S:86:LEU:HD12	1.95	0.65
11:J:117:ALA:HB2	11:J:126:LEU:HD12	1.78	0.65
16:O:61:LEU:O	16:O:61:LEU:HD22	1.97	0.65
33:g:55:LYS:HG2	33:g:81:HIS:C	2.21	0.65
33:g:109:LEU:C	33:g:109:LEU:HD23	2.21	0.65
16:O:98:VAL:HG12	16:O:99:ASP:N	2.11	0.65
3:B:87:ALA:HB2	3:B:219:LEU:HD11	1.77	0.65
16:O:52:VAL:HG21	16:O:61:LEU:CD1	2.27	0.65
19:R:87:THR:O	19:R:88:THR:HG22	1.97	0.65
4:C:176:LYS:HB3	4:C:181:ARG:CD	2.26	0.65
16:O:42:TYR:CD1	16:O:106:ARG:NE	2.65	0.65
30:c:9:LYS:HE3	30:c:35:ASP:CG	2.22	0.65
33:g:182:ILE:HD11	33:g:196:ILE:HD11	1.79	0.65
19:R:93:VAL:HG13	19:R:96:ILE:CG1	2.27	0.65
20:S:54:PRO:HG2	20:S:55:LEU:CD2	2.27	0.65
20:S:82:PRO:O	20:S:83:VAL:HG13	1.97	0.65
20:S:82:PRO:O	20:S:83:VAL:HG22	1.96	0.65
30:c:31:VAL:HG22	30:c:41:LEU:O	1.97	0.65
33:g:226:ILE:HG21	33:g:266:ILE:HD11	1.79	0.65
1:2:26:A:C2	25:X:47:MET:HE1	2.32	0.65
12:K:32:GLU:O	12:K:33:GLU:HB2	1.96	0.65
17:P:93:ILE:HD12	17:P:106:ILE:HD11	1.79	0.65
28:a:12:LYS:HG3	28:a:12:LYS:O	1.97	0.65
31:d:25:CYS:SG	31:d:43:CYS:SG	2.95	0.65
16:O:34:ILE:HD12	16:O:34:ILE:O	1.97	0.65
33:g:173:MET:O	33:g:174:ALA:HB3	1.96	0.65
11:J:58:LEU:HD11	11:J:91:LEU:HD12	1.79	0.64
17:P:15:ARG:HD3	20:S:92:ARG:HA	1.79	0.64
20:S:88:ARG:O	20:S:89:ARG:HG2	1.97	0.64
23:V:12:LEU:HD12	23:V:13:ILE:N	2.12	0.64
14:M:17:ASN:CB	14:M:99:ILE:O	2.46	0.64
16:O:106:ARG:NH2	16:O:142:PRO:CG	2.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:89:ALA:HB1	2:A:94:ALA:O	1.98	0.64
18:Q:80:GLN:HE22	18:Q:116:ALA:CB	2.09	0.64
33:g:212:ARG:O	33:g:230:SER:CB	2.45	0.64
6:E:198:ILE:HG13	6:E:198:ILE:O	1.95	0.64
18:Q:57:TRP:CH2	21:T:2:ILE:HG21	2.33	0.64
6:E:202:MET:HA	6:E:202:MET:CE	2.21	0.64
16:O:61:LEU:HD11	16:O:93:LEU:CD1	2.28	0.64
25:X:43:GLU:OE1	25:X:78:ASN:OD1	2.15	0.64
1:2:268:C:C5'	10:I:10:LYS:HD3	2.28	0.64
12:K:31:HIS:ND1	12:K:32:GLU:O	2.31	0.64
28:a:21:VAL:HG11	28:a:72:TYR:CE2	2.33	0.64
30:c:9:LYS:HE2	30:c:35:ASP:OD2	1.97	0.64
30:c:14:LYS:HD2	30:c:32:GLU:OE2	1.97	0.64
17:P:85:LEU:HD12	17:P:85:LEU:H	1.62	0.64
1:2:97:G:C5	1:2:98:C:C5	2.86	0.64
3:B:74:LEU:O	3:B:75:SER:HB3	1.96	0.64
4:C:180:ILE:CD1	4:C:219:THR:HA	2.28	0.64
30:c:66:ARG:HH11	30:c:66:ARG:CG	2.10	0.64
3:B:159:GLN:HG2	3:B:200:ILE:HD13	1.78	0.64
9:H:79:PRO:HD2	9:H:88:PHE:CB	2.27	0.64
11:J:58:LEU:HD23	11:J:95:LEU:HD11	1.78	0.64
1:2:720:U:OP1	16:O:66:GLY:HA3	1.98	0.64
1:2:1414:U:H5	18:Q:121:MET:HE1	1.62	0.64
16:O:29:LYS:HA	16:O:33:GLU:OE1	1.97	0.64
1:2:676:A:OP2	9:H:96:ARG:NH1	2.30	0.63
16:O:42:TYR:CD1	16:O:106:ARG:HG2	2.33	0.63
16:O:42:TYR:HD1	16:O:106:ARG:CD	2.10	0.63
21:T:42:ASP:C	21:T:43:LEU:HD12	2.23	0.63
7:F:17:PHE:HB2	7:F:25:VAL:HG21	1.81	0.63
16:O:52:VAL:HG23	16:O:60:THR:OG1	1.98	0.63
25:X:42:LEU:HG	25:X:121:PHE:CE1	2.34	0.63
1:2:102:G:N2	1:2:234:U:N3	2.46	0.63
1:2:719:G:C5'	16:O:67:GLY:HA2	2.29	0.63
4:C:189:ARG:HA	4:C:210:ASP:OD1	1.99	0.63
1:2:694:C:H5''	3:B:153:ASN:HD21	1.63	0.63
2:A:152:LEU:HD11	2:A:158:VAL:CG2	2.29	0.63
20:S:82:PRO:HB2	20:S:84:TRP:NE1	2.14	0.63
7:F:29:SER:O	7:F:34:GLN:HG3	1.99	0.63
3:B:87:ALA:HB2	3:B:219:LEU:CD1	2.28	0.63
10:I:54:LYS:CE	10:I:172:GLN:HG3	2.28	0.63
16:O:52:VAL:CG2	16:O:61:LEU:O	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:50:HIS:HB3	17:P:82:MET:HE2	1.79	0.63
1:2:1371:C:H4'	20:S:85:MET:HG3	1.78	0.63
12:K:51:LYS:HB2	12:K:53:PHE:CE2	2.33	0.63
3:B:60:ASN:HB2	3:B:84:ARG:HE	1.64	0.63
16:O:98:VAL:O	16:O:99:ASP:HB2	1.98	0.63
28:a:18:THR:CB	28:a:33:ASP:OD2	2.47	0.63
30:c:10:LEU:O	30:c:34:LEU:CB	2.46	0.63
31:d:22:CYS:CB	31:d:25:CYS:HB3	2.24	0.63
1:2:13:C:P	4:C:179:SER:HB3	2.38	0.62
3:B:106:LEU:HD23	3:B:106:LEU:C	2.24	0.62
9:H:139:ALA:HB1	9:H:142:VAL:N	2.14	0.62
4:C:54:LYS:O	4:C:58:LEU:HD13	1.98	0.62
12:K:29:GLY:O	12:K:38:ASN:OD1	2.17	0.62
17:P:86:PRO:CA	17:P:111:ILE:HD11	2.28	0.62
20:S:49:ARG:NH2	21:T:43:LEU:HD11	2.14	0.62
34:n:22:ALA:HA	34:n:25:LYS:HG3	1.81	0.62
20:S:86:LEU:O	20:S:89:ARG:NH1	2.33	0.62
30:c:45:VAL:CG1	30:c:55:LEU:HD21	2.28	0.62
33:g:194:TRP:HA	33:g:202:LEU:HA	1.80	0.62
1:2:644:G:C4'	6:E:201:GLN:HE22	2.12	0.62
6:E:94:LYS:HA	6:E:94:LYS:CE	2.27	0.62
12:K:47:ALA:O	12:K:51:LYS:HG3	1.99	0.62
30:c:53:ASP:OD1	30:c:54:ILE:N	2.33	0.62
1:2:695:G:P	3:B:154:SER:OG	2.57	0.62
11:J:29:VAL:HG23	11:J:40:ILE:HD11	1.81	0.62
13:L:109:ILE:HD11	13:L:115:VAL:HG21	1.81	0.62
16:O:70:VAL:HG12	16:O:71:ARG:N	2.15	0.62
24:W:110:ILE:HG13	24:W:110:ILE:O	2.00	0.62
1:2:1082:C:H2'	1:2:1082:C:O2	1.97	0.62
4:C:180:ILE:HD11	4:C:219:THR:HA	1.82	0.62
12:K:83:ALA:C	12:K:85:ALA:HB3	2.24	0.62
19:R:92:ASN:N	19:R:92:ASN:OD1	2.32	0.62
6:E:173:ILE:HD11	6:E:235:LEU:HD12	1.81	0.62
30:c:33:PHE:HE1	30:c:60:THR:HG22	1.64	0.62
18:Q:52:ILE:HG22	18:Q:52:ILE:O	2.00	0.62
33:g:214:THR:OG1	33:g:228:GLY:O	2.15	0.62
1:2:1153:U:O4	1:2:1188:A:N1	2.33	0.61
2:A:87:LYS:CD	2:A:199:LEU:HD21	2.29	0.61
2:A:184:ARG:HH11	2:A:184:ARG:CG	2.10	0.61
7:F:15:VAL:HA	7:F:99:VAL:HG22	1.82	0.61
9:H:68:GLN:NE2	9:H:145:ARG:HG2	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:52:VAL:O	14:M:56:CYS:CB	2.47	0.61
10:I:111:GLN:HG3	10:I:112:TRP:N	2.14	0.61
12:K:60:TRP:O	12:K:61:SER:HB3	1.99	0.61
19:R:97:LEU:CD1	19:R:98:VAL:N	2.55	0.61
24:W:104:LEU:HD13	24:W:106:THR:HG23	1.79	0.61
11:J:117:ALA:CB	11:J:126:LEU:HD12	2.30	0.61
17:P:85:LEU:HD12	17:P:88:PHE:CE2	2.35	0.61
20:S:49:ARG:HH21	21:T:43:LEU:HD21	1.65	0.61
33:g:194:TRP:NE1	33:g:202:LEU:HB3	2.14	0.61
2:A:187:LEU:HD11	2:A:193:TRP:HB3	1.83	0.61
12:K:11:ILE:HG21	12:K:44:ILE:HD11	1.82	0.61
15:N:26:LEU:O	15:N:27:GLN:HG3	2.00	0.61
22:U:53:GLU:O	22:U:95:PHE:CB	2.48	0.61
1:2:521:G:H5'	25:X:107:GLY:CA	2.31	0.61
18:Q:34:ASN:OD1	21:T:4:GLY:N	2.30	0.61
30:c:45:VAL:CG1	30:c:55:LEU:CD2	2.78	0.61
31:d:42:ARG:HG3	31:d:42:ARG:NH1	2.14	0.61
1:2:13:C:OP1	4:C:179:SER:CB	2.46	0.61
3:B:74:LEU:O	3:B:75:SER:CB	2.48	0.61
16:O:63:ARG:NH2	16:O:68:ILE:CG2	2.59	0.61
17:P:84:ILE:HG22	17:P:88:PHE:HE1	1.62	0.61
33:g:49:VAL:CG1	33:g:58:LEU:O	2.47	0.61
6:E:202:MET:HE2	6:E:202:MET:CA	2.27	0.60
12:K:11:ILE:HD11	12:K:34:LEU:CD1	2.30	0.60
15:N:20:ARG:H	15:N:20:ARG:NE	1.98	0.60
16:O:63:ARG:NE	16:O:68:ILE:CG2	2.60	0.60
18:Q:52:ILE:CD1	18:Q:106:LEU:HD11	2.29	0.60
18:Q:80:GLN:NE2	18:Q:116:ALA:CB	2.63	0.60
22:U:55:ARG:HD2	22:U:94:ASP:OD2	2.00	0.60
2:A:208:GLU:O	2:A:211:ILE:N	2.33	0.60
4:C:174:THR:HG23	4:C:183:ARG:HG3	1.83	0.60
11:J:120:VAL:HG23	11:J:121:HIS:N	2.16	0.60
25:X:60:ALA:HB1	25:X:115:ASP:HB3	1.83	0.60
25:X:130:SER:O	25:X:134:LEU:HG	2.01	0.60
30:c:55:LEU:N	30:c:55:LEU:HD12	2.16	0.60
34:n:20:VAL:O	34:n:23:ARG:HB2	2.01	0.60
1:2:522:C:H1'	25:X:46:SER:HB2	1.83	0.60
4:C:197:THR:O	4:C:201:LYS:HG2	2.00	0.60
4:C:206:ALA:HB1	4:C:208:PHE:CE2	2.33	0.60
7:F:25:VAL:O	7:F:26:ASP:HB2	2.00	0.60
16:O:28:VAL:HG12	16:O:28:VAL:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:101:A:O2'	1:2:102:G:O4'	2.18	0.60
1:2:988:C:O3'	17:P:128:SER:O	2.18	0.60
4:C:52:ARG:HG3	4:C:79:GLU:OE2	1.98	0.60
6:E:65:VAL:HG11	6:E:80:TYR:HB3	1.83	0.60
6:E:92:LEU:O	6:E:96:ASN:HA	2.01	0.60
9:H:165:VAL:HG12	9:H:165:VAL:O	2.01	0.60
16:O:48:THR:H	16:O:65:THR:HG22	1.65	0.60
27:Z:24:VAL:HG12	27:Z:24:VAL:O	2.01	0.60
5:D:43:THR:HB	5:D:46:ARG:O	2.01	0.60
6:E:95:SER:CB	26:Y:15:LYS:HG3	2.31	0.60
11:J:58:LEU:HD13	11:J:91:LEU:CD1	2.31	0.60
25:X:39:LYS:N	25:X:39:LYS:HD2	2.16	0.60
1:2:1244:G:H22	12:K:56:LYS:HZ1	1.47	0.60
1:2:98:C:O2'	1:2:99:U:H6	1.85	0.60
3:B:83:TRP:CE3	3:B:96:PHE:HA	2.37	0.60
10:I:10:LYS:HZ2	10:I:10:LYS:HB2	1.66	0.60
14:M:11:GLN:O	14:M:15:SER:N	2.35	0.60
17:P:85:LEU:C	17:P:111:ILE:HD11	2.25	0.60
30:c:37:SER:O	30:c:38:ASN:HB2	2.00	0.60
6:E:201:GLN:OE1	6:E:201:GLN:HA	2.00	0.60
28:a:18:THR:HG21	28:a:33:ASP:OD2	2.02	0.60
4:C:67:ILE:CG2	4:C:71:PHE:CE2	2.85	0.59
4:C:174:THR:HA	4:C:182:MET:O	2.02	0.59
14:M:39:LEU:O	14:M:65:ALA:HB1	2.01	0.59
16:O:42:TYR:CD1	16:O:106:ARG:CD	2.84	0.59
20:S:81:ILE:CG2	20:S:82:PRO:HD2	2.28	0.59
33:g:62:LEU:HD23	33:g:70:ALA:HB2	1.83	0.59
11:J:110:GLN:OE1	11:J:113:LYS:HE3	2.01	0.59
14:M:72:LEU:CB	14:M:93:CYS:CB	2.80	0.59
33:g:54:ASP:C	33:g:55:LYS:HG3	2.27	0.59
29:b:62:THR:HG23	29:b:63:PRO:HD2	1.83	0.59
30:c:38:ASN:O	30:c:39:ARG:HG2	2.01	0.59
1:2:1393:A:N3	7:F:72:THR:HG23	2.17	0.59
7:F:15:VAL:O	7:F:15:VAL:HG12	2.03	0.59
18:Q:34:ASN:CG	21:T:4:GLY:H	2.10	0.59
17:P:85:LEU:CD1	17:P:88:PHE:CE2	2.85	0.59
30:c:33:PHE:CE2	30:c:39:ARG:CD	2.86	0.59
17:P:61:ARG:NH1	17:P:87:GLU:O	2.36	0.59
20:S:82:PRO:C	20:S:83:VAL:HG13	2.27	0.59
28:a:23:CYS:CB	28:a:74:CYS:SG	2.90	0.59
16:O:34:ILE:CD1	16:O:36:MET:HG3	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:10:ARG:HG2	28:a:12:LYS:HG2	1.83	0.59
30:c:9:LYS:CE	30:c:35:ASP:CG	2.76	0.59
9:H:68:GLN:HG2	9:H:145:ARG:HG2	1.84	0.58
33:g:109:LEU:HD23	33:g:109:LEU:O	2.01	0.58
12:K:76:ARG:NH2	12:K:83:ALA:CB	2.65	0.58
28:a:10:ARG:HD2	28:a:33:ASP:HB2	1.85	0.58
2:A:72:VAL:CG1	2:A:117:PRO:CB	2.70	0.58
26:Y:28:HIS:CE1	26:Y:67:HIS:N	2.72	0.58
29:b:48:PHE:HE2	29:b:50:HIS:HB2	1.68	0.58
33:g:54:ASP:O	33:g:55:LYS:HG3	2.04	0.58
2:A:73:LEU:HD12	2:A:121:ILE:HG23	1.85	0.58
4:C:63:LYS:HE3	4:C:261:TRP:CG	2.38	0.58
7:F:67:SER:HB3	7:F:68:ARG:HB3	1.84	0.58
11:J:57:LEU:HD11	11:J:70:GLU:CG	2.33	0.58
16:O:52:VAL:HG21	16:O:61:LEU:HD11	1.86	0.58
2:A:62:MET:HE3	23:V:34:ILE:CG2	2.33	0.58
3:B:79:ARG:HD2	3:B:99:MET:SD	2.43	0.58
28:a:74:CYS:SG	28:a:77:CYS:SG	3.02	0.58
1:2:678:G:H4'	9:H:93:ASN:HD22	1.69	0.58
6:E:95:SER:OG	26:Y:15:LYS:CG	2.52	0.58
7:F:25:VAL:O	7:F:25:VAL:HG13	2.03	0.58
31:d:24:ILE:CD1	31:d:24:ILE:H	2.17	0.58
3:B:79:ARG:CZ	3:B:99:MET:CE	2.78	0.58
4:C:67:ILE:HD12	4:C:67:ILE:N	2.03	0.58
20:S:77:THR:HG23	20:S:78:GLU:N	2.19	0.58
25:X:42:LEU:HG	25:X:121:PHE:HE1	1.67	0.58
4:C:64:ILE:O	4:C:64:ILE:HG13	2.04	0.57
4:C:171:ASN:C	4:C:171:ASN:HD22	2.07	0.57
23:V:38:LYS:NZ	23:V:50:GLU:OE2	2.32	0.57
1:2:1414:U:OP1	18:Q:12:THR:HG22	2.04	0.57
2:A:73:LEU:CG	2:A:88:PHE:CD2	2.86	0.57
4:C:167:HIS:HB2	4:C:209:GLU:HB3	1.85	0.57
16:O:47:ASP:HA	16:O:65:THR:HG21	1.85	0.57
1:2:755:G:N7	28:a:15:ARG:NH2	2.52	0.57
11:J:131:HIS:CD2	11:J:159:THR:OG1	2.57	0.57
25:X:42:LEU:HD22	25:X:45:THR:O	2.04	0.57
14:M:52:VAL:O	14:M:56:CYS:CA	2.52	0.57
17:P:85:LEU:HD12	17:P:88:PHE:CZ	2.39	0.57
28:a:21:VAL:HG11	28:a:72:TYR:CD2	2.39	0.57
30:c:57:LEU:HD12	30:c:57:LEU:N	2.19	0.57
12:K:51:LYS:HB2	12:K:53:PHE:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:106:LEU:CD2	3:B:110:MET:HE3	2.35	0.57
12:K:34:LEU:HD12	12:K:34:LEU:C	2.29	0.57
16:O:106:ARG:NH2	16:O:142:PRO:CD	2.68	0.57
6:E:91:GLY:C	6:E:92:LEU:HD12	2.30	0.57
9:H:84:HIS:CD2	9:H:85:GLY:N	2.73	0.57
17:P:85:LEU:N	17:P:88:PHE:CE1	2.73	0.57
2:A:68:GLU:CD	2:A:184:ARG:HH21	2.11	0.57
19:R:97:LEU:HD13	19:R:97:LEU:C	2.28	0.57
4:C:208:PHE:H	4:C:208:PHE:HD2	1.53	0.57
23:V:11:MET:O	23:V:12:LEU:HG	2.05	0.57
33:g:53:ARG:HG3	33:g:82:PHE:CG	2.39	0.57
1:2:13:C:O5'	4:C:179:SER:HB2	2.05	0.57
1:2:1007:G:OP2	31:d:41:ARG:NH2	2.38	0.57
6:E:114:ILE:HD12	6:E:119:ALA:HB2	1.87	0.56
16:O:63:ARG:NH2	16:O:68:ILE:CB	2.34	0.56
16:O:100:GLY:CA	16:O:133:LYS:O	2.53	0.56
28:a:23:CYS:SG	28:a:26:CYS:CB	2.92	0.56
33:g:212:ARG:NH2	33:g:212:ARG:HB2	2.20	0.56
33:g:194:TRP:CD1	33:g:202:LEU:HB3	2.40	0.56
1:2:1052:G:O2'	1:2:1054:G:N2	2.37	0.56
3:B:35:THR:CG2	3:B:71:VAL:HG12	2.21	0.56
4:C:197:THR:HG22	4:C:201:LYS:HE3	1.88	0.56
11:J:119:SER:HB3	11:J:122:HIS:HB2	1.86	0.56
15:N:25:TRP:CD2	15:N:26:LEU:N	2.73	0.56
30:c:9:LYS:CE	30:c:35:ASP:OD2	2.52	0.56
30:c:45:VAL:HG12	30:c:55:LEU:HD23	1.87	0.56
33:g:174:ALA:HB1	33:g:178:SER:HB3	1.88	0.56
1:2:97:G:C4	1:2:239:G:C2	2.93	0.56
10:I:8:ASP:O	10:I:18:GLN:NE2	2.39	0.56
15:N:28:LEU:HD23	15:N:66:VAL:CG2	2.36	0.56
21:T:41:ALA:C	21:T:42:ASP:CG	2.73	0.56
4:C:181:ARG:HB2	4:C:216:LEU:HB3	1.86	0.56
1:2:98:C:C2'	1:2:99:U:H6	2.18	0.56
1:2:267:A:O3'	10:I:10:LYS:HE2	2.05	0.56
1:2:1242:G:N9	31:d:42:ARG:HD2	2.20	0.56
3:B:115:THR:HG21	3:B:152:ALA:HB3	1.88	0.56
24:W:8:ALA:HA	24:W:74:ALA:HB3	1.87	0.56
4:C:176:LYS:CB	4:C:181:ARG:HD3	2.34	0.56
16:O:61:LEU:HD21	16:O:89:VAL:HG23	0.60	0.56
16:O:65:THR:OG1	16:O:76:GLU:HA	2.06	0.56
16:O:93:LEU:O	16:O:97:GLY:CA	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:124:VAL:O	17:P:125:VAL:HG12	2.05	0.56
19:R:93:VAL:HG13	19:R:96:ILE:HG12	1.86	0.56
20:S:54:PRO:HG2	20:S:55:LEU:HD22	1.88	0.56
23:V:14:PRO:HG2	23:V:23:LEU:HD22	1.87	0.56
28:a:18:THR:OG1	28:a:33:ASP:OD2	2.22	0.56
33:g:175:ASP:O	33:g:176:GLU:HB3	2.04	0.56
7:F:22:PRO:O	7:F:23:ALA:HB3	2.06	0.56
32:e:30:VAL:HG23	32:e:30:VAL:O	2.06	0.56
4:C:172:THR:HA	4:C:184:LEU:O	2.06	0.56
10:I:8:ASP:OD1	10:I:9:LEU:N	2.38	0.56
12:K:51:LYS:CB	12:K:53:PHE:CE2	2.89	0.56
3:B:149:HIS:O	3:B:149:HIS:ND1	2.39	0.56
4:C:61:SER:CB	4:C:261:TRP:CZ2	2.87	0.56
2:A:87:LYS:HB2	2:A:200:PHE:CE1	2.41	0.55
3:B:36:GLY:HA2	3:B:37:LYS:CB	2.27	0.55
16:O:52:VAL:CG2	16:O:61:LEU:CD1	2.84	0.55
17:P:85:LEU:N	17:P:88:PHE:CZ	2.73	0.55
31:d:22:CYS:SG	31:d:25:CYS:CB	2.93	0.55
1:2:98:C:H2'	1:2:99:U:C6	2.40	0.55
3:B:160:VAL:HG21	3:B:203:ILE:HD11	1.89	0.55
4:C:51:PRO:HD3	4:C:60:LYS:HG3	1.88	0.55
6:E:64:ILE:HG22	26:Y:17:LEU:HD11	1.88	0.55
9:H:116:VAL:HG23	9:H:135:ASP:HA	1.88	0.55
16:O:68:ILE:HG12	16:O:68:ILE:O	2.06	0.55
15:N:25:TRP:CE3	15:N:26:LEU:HA	2.41	0.55
31:d:24:ILE:HG21	31:d:47:ARG:NH1	2.21	0.55
7:F:14:ASP:C	7:F:15:VAL:HG23	2.31	0.55
18:Q:115:VAL:O	18:Q:116:ALA:HB3	2.06	0.55
28:a:10:ARG:HG3	28:a:12:LYS:HG2	1.87	0.55
30:c:33:PHE:CE1	30:c:60:THR:HG22	2.41	0.55
2:A:83:ARG:CZ	2:A:87:LYS:NZ	2.70	0.55
30:c:67:LEU:HD13	30:c:67:LEU:O	2.07	0.55
3:B:79:ARG:CZ	3:B:99:MET:HE3	2.37	0.55
9:H:113:THR:HA	9:H:138:ASP:CG	2.31	0.55
12:K:27:GLN:HB3	12:K:39:ILE:HG22	1.89	0.55
15:N:20:ARG:H	15:N:20:ARG:HD3	1.69	0.55
7:F:23:ALA:HA	30:c:54:ILE:HD12	1.89	0.55
11:J:114:ARG:O	11:J:115:ALA:HB3	2.06	0.55
11:J:146:VAL:HG11	11:J:151:GLU:HA	1.89	0.55
12:K:79:PHE:C	12:K:81:LEU:HD12	2.32	0.55
23:V:38:LYS:NZ	23:V:49:PHE:C	2.64	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1038:G:O6	14:M:21:GLY:HA3	2.07	0.55
3:B:140:LYS:HG2	3:B:202:GLN:HB2	1.89	0.55
21:T:41:ALA:O	21:T:42:ASP:CB	2.55	0.55
27:Z:80:HIS:O	27:Z:81:ASP:CB	2.55	0.55
1:2:1283:U:N1	7:F:71:ASN:ND2	2.55	0.54
7:F:23:ALA:O	7:F:24:LEU:HB2	2.06	0.54
10:I:9:LEU:HD13	10:I:9:LEU:C	2.32	0.54
10:I:11:HIS:O	13:L:131:LYS:NZ	2.40	0.54
20:S:29:TYR:CE1	21:T:52:MET:HE1	2.43	0.54
16:O:53:THR:HG22	16:O:59:GLU:CA	2.36	0.54
21:T:46:THR:CG2	21:T:50:LYS:HG3	2.35	0.54
24:W:104:LEU:HB3	24:W:125:ILE:HG22	1.88	0.54
25:X:106:MET:HB3	25:X:113:VAL:CG2	2.36	0.54
28:a:34:LYS:O	28:a:34:LYS:HG2	2.07	0.54
3:B:34:PHE:HE1	3:B:70:MET:HE1	1.73	0.54
9:H:98:LEU:HD12	9:H:98:LEU:C	2.31	0.54
33:g:212:ARG:HB2	33:g:212:ARG:HH21	1.72	0.54
1:2:812:A:O2'	1:2:1565:U:O2	2.24	0.54
6:E:19:LEU:HD11	6:E:108:ARG:HD2	1.89	0.54
18:Q:57:TRP:HH2	21:T:2:ILE:HG21	1.72	0.54
20:S:85:MET:O	20:S:85:MET:HG2	2.07	0.54
22:U:55:ARG:HD3	22:U:94:ASP:OD1	2.07	0.54
11:J:114:ARG:CG	11:J:116:LEU:CD1	2.85	0.54
12:K:37:LEU:HD21	31:d:6:VAL:CG2	2.38	0.54
12:K:48:PHE:HB3	12:K:54:CYS:SG	2.48	0.54
22:U:39:VAL:HG22	22:U:109:ALA:HB1	1.90	0.54
24:W:106:THR:OG1	24:W:111:MET:HE3	2.08	0.54
32:e:13:LYS:CG	32:e:14:VAL:N	2.71	0.54
33:g:173:MET:O	33:g:174:ALA:CB	2.56	0.54
33:g:173:MET:HE1	33:g:175:ASP:CB	2.37	0.54
11:J:53:ALA:O	11:J:57:LEU:HG	2.08	0.54
15:N:21:SER:O	15:N:22:ALA:HB3	2.07	0.54
22:U:44:MET:HE2	22:U:54:VAL:HG21	1.89	0.54
2:A:153:ASP:O	2:A:154:TYR:HB2	2.07	0.54
1:2:719:G:O5'	16:O:67:GLY:HA2	2.08	0.54
3:B:75:SER:C	3:B:76:HIS:CD2	2.86	0.54
7:F:21:ASP:HB2	7:F:22:PRO:CD	2.38	0.54
7:F:101:PHE:HA	7:F:166:LEU:HD21	1.90	0.54
20:S:50:ALA:O	20:S:68:LEU:HD21	2.08	0.54
29:b:48:PHE:CE2	29:b:50:HIS:HB2	2.42	0.54
1:2:100:C:C2'	1:2:101:A:C5'	2.83	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:5:LYS:CB	7:F:10:TYR:O	2.53	0.54
7:F:96:ASN:HD21	7:F:99:VAL:HG23	1.72	0.54
9:H:82:PRO:CG	9:H:88:PHE:CZ	2.85	0.54
16:O:61:LEU:CD2	16:O:89:VAL:CG2	2.32	0.54
33:g:209:HIS:HE1	33:g:228:GLY:CA	1.87	0.54
1:2:97:G:C8	1:2:98:C:C5	2.97	0.53
1:2:101:A:C2	1:2:235:G:C6	2.96	0.53
5:D:17:LEU:HD21	31:d:23:ARG:HH21	1.64	0.53
9:H:83:GLU:O	9:H:84:HIS:CB	2.56	0.53
3:B:34:PHE:N	3:B:34:PHE:CD2	2.73	0.53
1:2:97:G:C8	1:2:98:C:H5	2.25	0.53
5:D:43:THR:CG2	5:D:44:PRO:CD	2.85	0.53
12:K:25:ASP:OD2	12:K:58:TYR:CE1	2.61	0.53
12:K:25:ASP:HB2	12:K:58:TYR:HE1	1.73	0.53
16:O:96:LEU:N	16:O:97:GLY:HA2	2.22	0.53
19:R:93:VAL:CG1	19:R:96:ILE:CG1	2.85	0.53
3:B:40:ILE:HG21	3:B:65:LEU:HD13	1.88	0.53
3:B:103:HIS:CE1	3:B:107:ASP:OD2	2.61	0.53
9:H:68:GLN:HE21	9:H:145:ARG:CG	2.15	0.53
12:K:76:ARG:CZ	12:K:84:ASN:H	2.22	0.53
20:S:92:ARG:HH11	20:S:115:ARG:HH22	1.56	0.53
27:Z:77:ILE:HG22	27:Z:79:GLY:H	1.73	0.53
11:J:108:GLN:CD	11:J:124:ARG:HD3	2.34	0.53
25:X:106:MET:HG2	25:X:121:PHE:N	2.22	0.53
3:B:61:ARG:CD	16:O:56:SER:HG	1.94	0.53
6:E:87:MET:HE1	6:E:236:ILE:HD12	1.91	0.53
14:M:15:SER:N	14:M:16:GLY:CA	2.72	0.53
24:W:104:LEU:HD12	24:W:104:LEU:C	2.34	0.53
1:2:911:G:C5'	24:W:4:THR:HG21	2.38	0.53
2:A:152:LEU:HD11	2:A:158:VAL:HG21	1.89	0.53
3:B:79:ARG:HH12	3:B:99:MET:HE1	1.66	0.53
4:C:169:VAL:CG2	4:C:211:LEU:HD21	2.39	0.53
7:F:71:ASN:N	7:F:71:ASN:OD1	2.41	0.53
12:K:76:ARG:NH1	12:K:84:ASN:H	2.05	0.53
13:L:18:LEU:O	13:L:19:ALA:HB3	2.09	0.53
15:N:23:PRO:HB2	15:N:25:TRP:NE1	2.24	0.53
33:g:82:PHE:O	33:g:99:SER:OG	2.24	0.53
1:2:98:C:H2'	1:2:99:U:H6	1.73	0.53
1:2:101:A:C2	1:2:235:G:C5	2.96	0.53
3:B:198:LYS:HD2	3:B:202:GLN:OE1	2.08	0.53
17:P:15:ARG:NE	20:S:90:PHE:CE2	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:g:206:PHE:CD1	33:g:208:ALA:HB2	2.43	0.53
1:2:1337:U:C5	27:Z:80:HIS:CD2	2.96	0.52
33:g:55:LYS:HA	33:g:83:VAL:HG23	1.91	0.52
3:B:33:TYR:HB3	3:B:34:PHE:HD2	1.74	0.52
3:B:35:THR:HG22	3:B:36:GLY:H	1.74	0.52
3:B:37:LYS:O	3:B:37:LYS:HG3	2.09	0.52
12:K:80:GLY:N	12:K:81:LEU:HD12	2.24	0.52
15:N:23:PRO:CB	15:N:25:TRP:CD1	2.85	0.52
19:R:93:VAL:CG1	19:R:96:ILE:H	2.22	0.52
20:S:82:PRO:CB	20:S:84:TRP:NE1	2.72	0.52
28:a:23:CYS:SG	28:a:74:CYS:SG	3.08	0.52
3:B:37:LYS:HG2	3:B:70:MET:O	2.10	0.52
6:E:201:GLN:CG	6:E:206:ASP:HA	2.39	0.52
12:K:55:ILE:N	12:K:55:ILE:CD1	2.73	0.52
33:g:140:VAL:HG21	33:g:165:VAL:HG11	1.90	0.52
16:O:42:TYR:HD1	16:O:106:ARG:HD3	1.74	0.52
20:S:55:LEU:HD22	20:S:55:LEU:N	2.25	0.52
24:W:104:LEU:HD11	24:W:106:THR:HG23	1.92	0.52
7:F:10:TYR:OH	7:F:86:PHE:O	2.26	0.52
9:H:40:ILE:HD12	9:H:69:ILE:HG23	1.92	0.52
20:S:81:ILE:HG23	20:S:82:PRO:CD	2.28	0.52
20:S:87:ASN:N	20:S:99:HIS:HB2	2.23	0.52
21:T:41:ALA:O	21:T:42:ASP:CG	2.53	0.52
30:c:11:ALA:O	30:c:54:ILE:HG23	2.09	0.52
30:c:35:ASP:O	30:c:36:ASP:HB2	2.09	0.52
1:2:1242:G:C8	31:d:42:ARG:HD2	2.44	0.52
11:J:116:LEU:CD1	11:J:116:LEU:N	2.73	0.52
17:P:125:VAL:CG1	17:P:126:LYS:H	2.20	0.52
24:W:36:ALA:CB	24:W:110:ILE:HD11	2.40	0.52
28:a:23:CYS:CB	28:a:73:TYR:C	2.82	0.52
4:C:211:LEU:HD12	4:C:212:PHE:O	2.10	0.52
12:K:58:TYR:CZ	12:K:61:SER:HA	2.45	0.52
20:S:89:ARG:HA	20:S:97:ASN:CB	2.39	0.52
21:T:2:ILE:N	21:T:2:ILE:CD1	2.73	0.52
30:c:41:LEU:HD21	30:c:60:THR:O	2.09	0.52
33:g:113:THR:HG23	33:g:113:THR:O	2.09	0.52
11:J:117:ALA:HB2	11:J:123:ALA:HA	1.91	0.52
19:R:93:VAL:CG1	19:R:96:ILE:N	2.73	0.52
1:2:203:A:H62	10:I:175:ARG:HH11	1.55	0.52
30:c:45:VAL:HG12	30:c:55:LEU:CD2	2.39	0.52
3:B:27:HIS:CE1	16:O:30:ARG:HD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:37:LYS:HE2	3:B:39:ASP:O	2.09	0.52
7:F:31:HIS:CD2	7:F:31:HIS:N	2.78	0.52
7:F:32:GLU:CA	7:F:35:HIS:CD2	2.85	0.52
10:I:109:PHE:CD2	10:I:180:ILE:HD11	2.44	0.52
11:J:116:LEU:N	11:J:116:LEU:HD12	2.25	0.52
20:S:50:ALA:N	20:S:51:GLY:CA	2.73	0.52
28:a:7:ASN:O	28:a:8:HIS:HB2	2.10	0.52
31:d:22:CYS:CB	31:d:25:CYS:CB	2.86	0.52
31:d:24:ILE:CD1	31:d:24:ILE:N	2.73	0.52
1:2:103:A:P	1:2:103:A:C3'	2.93	0.51
1:2:268:C:C5'	10:I:10:LYS:CD	2.88	0.51
1:2:644:G:H5'	6:E:201:GLN:HE22	1.75	0.51
1:2:644:G:C5'	6:E:201:GLN:HE22	2.23	0.51
3:B:88:ALA:HB1	3:B:91:GLU:O	2.09	0.51
7:F:22:PRO:HG2	30:c:10:LEU:HD21	1.91	0.51
10:I:10:LYS:CB	10:I:10:LYS:NZ	2.73	0.51
1:2:644:G:H4'	6:E:201:GLN:NE2	2.22	0.51
4:C:170:PRO:HD2	4:C:236:THR:CG2	2.41	0.51
16:O:42:TYR:HB3	16:O:49:PHE:HB2	1.92	0.51
20:S:50:ALA:O	20:S:68:LEU:CD2	2.58	0.51
30:c:57:LEU:N	30:c:57:LEU:CD1	2.73	0.51
3:B:86:ILE:HG23	3:B:87:ALA:N	2.25	0.51
4:C:68:GLU:OE2	23:V:12:LEU:CA	2.54	0.51
16:O:70:VAL:CG1	16:O:71:ARG:N	2.72	0.51
28:a:74:CYS:SG	28:a:77:CYS:HB2	2.50	0.51
33:g:112:ARG:HD3	33:g:112:ARG:N	2.24	0.51
1:2:633:A:C6	6:E:19:LEU:HD13	2.45	0.51
5:D:209:ILE:HD11	19:R:12:ALA:HB2	1.91	0.51
12:K:48:PHE:CB	12:K:54:CYS:SG	2.99	0.51
23:V:9:VAL:CG1	23:V:10:ASP:N	2.73	0.51
3:B:29:MET:SD	3:B:39:ASP:CA	2.98	0.51
4:C:168:THR:CG2	4:C:169:VAL:N	2.72	0.51
4:C:208:PHE:CD2	4:C:208:PHE:N	2.79	0.51
16:O:61:LEU:CD1	16:O:61:LEU:N	2.73	0.51
16:O:64:CYS:C	16:O:69:ALA:HB2	2.35	0.51
19:R:93:VAL:HG13	19:R:96:ILE:HG13	1.92	0.51
28:a:37:THR:HG21	28:a:70:LYS:NZ	2.25	0.51
2:A:184:ARG:CG	2:A:184:ARG:NH1	2.73	0.51
3:B:35:THR:HG22	3:B:36:GLY:N	2.26	0.51
5:D:13:ILE:HD13	31:d:35:TYR:HB3	1.92	0.51
11:J:117:ALA:CA	11:J:126:LEU:CD1	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:10:ARG:HG3	28:a:12:LYS:H	1.76	0.51
30:c:33:PHE:CD2	30:c:39:ARG:CG	2.93	0.51
33:g:191:VAL:HG11	33:g:227:THR:HG21	1.93	0.51
3:B:36:GLY:HA2	3:B:37:LYS:C	2.35	0.51
6:E:199:GLU:CD	6:E:209:HIS:HE2	2.04	0.51
15:N:23:PRO:CB	15:N:25:TRP:NE1	2.74	0.51
20:S:47:VAL:O	20:S:51:GLY:HA2	2.11	0.51
2:A:208:GLU:O	2:A:209:ALA:C	2.54	0.51
4:C:58:LEU:O	4:C:61:SER:OG	2.20	0.51
7:F:91:LEU:HD13	27:Z:76:VAL:CG1	2.41	0.51
22:U:67:ILE:HD12	31:d:53:PHE:CE2	2.45	0.51
33:g:74:THR:HG22	33:g:112:ARG:NE	2.26	0.51
1:2:1025:A:N3	1:2:1025:A:H2'	2.26	0.51
7:F:111:ARG:O	7:F:112:GLU:HB2	2.11	0.51
12:K:27:GLN:HA	12:K:27:GLN:NE2	2.14	0.51
17:P:125:VAL:CG1	17:P:126:LYS:N	2.73	0.51
28:a:23:CYS:CA	28:a:73:TYR:O	2.57	0.51
30:c:54:ILE:C	30:c:55:LEU:HD12	2.35	0.51
2:A:70:LYS:HE3	2:A:70:LYS:CA	2.22	0.51
14:M:19:ALA:CB	14:M:97:ALA:CB	2.64	0.51
17:P:85:LEU:CD1	17:P:88:PHE:CD2	2.94	0.51
25:X:110:GLY:O	25:X:111:ARG:HB2	2.10	0.51
4:C:120:GLY:HA3	4:C:205:MET:HB3	1.93	0.50
4:C:169:VAL:HG22	4:C:208:PHE:CE1	2.46	0.50
11:J:117:ALA:O	11:J:118:ASN:CB	2.57	0.50
16:O:65:THR:HG23	16:O:66:GLY:N	2.26	0.50
1:2:1390:G:H5''	18:Q:119:ARG:HB2	1.92	0.50
7:F:22:PRO:HG2	30:c:10:LEU:CD2	2.41	0.50
33:g:226:ILE:HD13	33:g:226:ILE:N	2.25	0.50
1:2:178:C:H4'	10:I:177:ASP:OD2	2.11	0.50
2:A:152:LEU:HD11	2:A:158:VAL:HG22	1.93	0.50
6:E:94:LYS:HE3	6:E:94:LYS:N	2.26	0.50
3:B:34:PHE:CE1	3:B:70:MET:HE1	2.46	0.50
12:K:81:LEU:CD1	12:K:81:LEU:N	2.73	0.50
33:g:204:LYS:HG3	33:g:205:GLU:N	2.27	0.50
1:2:1393:A:N3	7:F:72:THR:CG2	2.74	0.50
6:E:91:GLY:O	6:E:92:LEU:HD12	2.10	0.50
7:F:24:LEU:HD11	7:F:135:ARG:CZ	2.41	0.50
7:F:88:ILE:HD11	27:Z:84:CYS:SG	2.51	0.50
11:J:58:LEU:HD11	11:J:91:LEU:CD1	2.38	0.50
15:N:20:ARG:CD	15:N:20:ARG:N	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:b:31:SER:HB3	29:b:50:HIS:CE1	2.46	0.50
3:B:79:ARG:HD2	3:B:99:MET:HE3	1.94	0.50
16:O:51:HIS:CD2	16:O:59:GLU:HG3	2.44	0.50
2:A:64:TYR:HE1	2:A:184:ARG:HB3	1.77	0.50
2:A:73:LEU:HD12	2:A:121:ILE:CG2	2.41	0.50
2:A:203:ARG:NE	2:A:211:ILE:CD1	2.74	0.50
3:B:138:PHE:O	3:B:203:ILE:HA	2.12	0.50
10:I:112:TRP:CZ2	10:I:116:GLN:OE1	2.65	0.50
13:L:13:GLN:HE22	13:L:59:THR:HG22	1.77	0.50
1:2:1082:C:O2	1:2:1082:C:C2'	2.59	0.50
6:E:102:ILE:HD12	6:E:236:ILE:HD11	1.93	0.50
9:H:98:LEU:HD11	9:H:102:ASN:ND2	2.27	0.50
10:I:104:ILE:O	10:I:161:ARG:HA	2.11	0.50
17:P:128:SER:HB3	17:P:129:LYS:HB2	1.94	0.50
24:W:75:ILE:HD11	24:W:125:ILE:HD11	1.94	0.50
31:d:40:CYS:HB3	31:d:43:CYS:SG	2.52	0.50
1:2:97:G:C5	1:2:98:C:C4	3.00	0.50
2:A:86:HIS:O	2:A:90:GLU:HG2	2.12	0.50
5:D:45:THR:O	5:D:84:SER:HB3	2.11	0.50
22:U:52:LEU:HD13	22:U:95:PHE:CE1	2.47	0.49
12:K:58:TYR:HH	12:K:61:SER:HA	1.74	0.49
15:N:25:TRP:CE3	15:N:26:LEU:N	2.80	0.49
20:S:92:ARG:NH1	20:S:115:ARG:NH2	2.58	0.49
2:A:146:CYS:SG	2:A:158:VAL:HG13	2.52	0.49
4:C:154:VAL:HG11	4:C:208:PHE:HZ	1.76	0.49
7:F:65:LEU:HA	7:F:144:THR:HG21	1.94	0.49
10:I:165:VAL:O	10:I:178:GLY:HA3	2.11	0.49
21:T:43:LEU:N	21:T:43:LEU:CD1	2.73	0.49
1:2:97:G:H2'	1:2:98:C:C5	2.47	0.49
3:B:106:LEU:C	3:B:106:LEU:CD2	2.86	0.49
5:D:121:TYR:HA	5:D:124:ILE:HG22	1.93	0.49
11:J:131:HIS:O	11:J:157:ALA:CB	2.60	0.49
12:K:79:PHE:HB2	12:K:81:LEU:HD13	1.94	0.49
20:S:47:VAL:HG12	20:S:52:LEU:HD12	1.95	0.49
1:2:1153:U:O2'	1:2:1154:A:O5'	2.26	0.49
4:C:168:THR:HG22	4:C:169:VAL:H	1.78	0.49
11:J:120:VAL:CG2	11:J:121:HIS:N	2.75	0.49
16:O:34:ILE:CD1	16:O:36:MET:CG	2.91	0.49
1:2:1051:C:H1'	17:P:49:LYS:NZ	2.28	0.49
3:B:36:GLY:CA	3:B:37:LYS:C	2.85	0.49
17:P:86:PRO:HA	17:P:111:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:7:LEU:HD13	24:W:74:ALA:HB1	1.95	0.49
33:g:209:HIS:NE2	33:g:228:GLY:N	2.61	0.49
1:2:101:A:C2	1:2:235:G:C4	3.01	0.49
1:2:268:C:H5'	10:I:10:LYS:CD	2.40	0.49
3:B:34:PHE:HE1	3:B:70:MET:CE	2.26	0.49
7:F:27:TYR:N	7:F:27:TYR:CD2	2.80	0.49
3:B:42:VAL:HG23	3:B:42:VAL:O	2.13	0.49
10:I:10:LYS:HB2	10:I:10:LYS:NZ	2.26	0.49
17:P:46:PHE:O	17:P:50:HIS:CD2	2.65	0.49
33:g:49:VAL:HG22	33:g:59:VAL:HG12	1.95	0.49
33:g:203:ILE:HG23	33:g:204:LYS:N	2.28	0.49
1:2:1050:U:O2	1:2:1050:U:O4'	2.30	0.49
16:O:46:ASN:ND2	16:O:46:ASN:N	2.60	0.49
20:S:119:MET:HE1	20:S:121:MET:HE3	1.93	0.49
21:T:42:ASP:HB2	21:T:43:LEU:HD12	1.94	0.49
25:X:88:ARG:HB3	25:X:135:TRP:NE1	2.28	0.49
30:c:45:VAL:HG21	30:c:49:VAL:HG11	1.94	0.49
2:A:59:ALA:O	2:A:63:ILE:CD1	2.60	0.49
4:C:172:THR:HG22	4:C:185:ILE:HA	1.95	0.49
14:M:43:CYS:HA	14:M:44:GLU:HA	1.58	0.49
34:n:5:TRP:HA	34:n:5:TRP:CE3	2.48	0.49
2:A:72:VAL:HG12	2:A:117:PRO:HB2	1.92	0.48
25:X:37:ILE:C	25:X:40:THR:HG23	2.36	0.48
30:c:14:LYS:HD2	30:c:32:GLU:CG	2.43	0.48
2:A:37:PHE:CD2	2:A:38:THR:HG22	2.48	0.48
4:C:72:TYR:C	4:C:72:TYR:CD2	2.90	0.48
10:I:81:VAL:HG22	10:I:102:VAL:CG1	2.43	0.48
25:X:24:TRP:HZ2	25:X:33:LEU:HD21	1.69	0.48
26:Y:37:ASP:OD1	26:Y:37:ASP:N	2.45	0.48
33:g:55:LYS:HB3	33:g:81:HIS:O	2.12	0.48
1:2:911:G:C4'	24:W:4:THR:HG21	2.43	0.48
17:P:46:PHE:O	17:P:50:HIS:HB2	2.13	0.48
25:X:42:LEU:CG	25:X:121:PHE:HE1	2.26	0.48
5:D:17:LEU:HD11	31:d:39:ILE:HD11	1.94	0.48
7:F:108:CYS:SG	7:F:178:ALA:HB1	2.53	0.48
9:H:136:LYS:HG3	9:H:136:LYS:O	2.13	0.48
12:K:79:PHE:C	12:K:81:LEU:CD1	2.87	0.48
22:U:52:LEU:HD13	22:U:95:PHE:CD1	2.48	0.48
33:g:173:MET:SD	33:g:173:MET:C	2.96	0.48
11:J:110:GLN:HA	11:J:113:LYS:HE3	1.95	0.48
6:E:95:SER:CB	26:Y:15:LYS:HB3	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:c:17:ILE:CG1	30:c:67:LEU:HD21	2.42	0.48
20:S:89:ARG:HA	20:S:97:ASN:CA	2.41	0.48
30:c:66:ARG:CG	30:c:66:ARG:NH1	2.72	0.48
33:g:194:TRP:CD1	33:g:202:LEU:CA	2.97	0.48
29:b:31:SER:HB3	29:b:50:HIS:HE1	1.77	0.48
30:c:41:LEU:CD2	30:c:60:THR:O	2.62	0.48
33:g:206:PHE:CE1	33:g:208:ALA:CB	2.89	0.48
34:n:5:TRP:HA	34:n:5:TRP:HE3	1.78	0.48
16:O:27:PRO:O	16:O:28:VAL:HB	2.13	0.48
25:X:106:MET:HG2	25:X:120:ARG:O	2.11	0.48
3:B:75:SER:C	3:B:76:HIS:HD2	2.20	0.47
3:B:79:ARG:CD	3:B:99:MET:HE3	2.44	0.47
6:E:201:GLN:HB2	6:E:206:ASP:HA	1.96	0.47
21:T:71:ILE:HG12	21:T:77:ALA:HB3	1.96	0.47
34:n:22:ALA:C	34:n:24:SER:H	2.21	0.47
1:2:871:U:O4'	1:2:871:U:O2	2.30	0.47
4:C:169:VAL:HG23	4:C:211:LEU:HD21	1.96	0.47
12:K:11:ILE:HD11	12:K:34:LEU:HD13	1.94	0.47
12:K:27:GLN:HB3	12:K:39:ILE:CG2	2.44	0.47
19:R:93:VAL:CG1	19:R:96:ILE:CA	2.91	0.47
25:X:42:LEU:O	25:X:45:THR:OG1	2.32	0.47
28:a:18:THR:CG2	28:a:33:ASP:OD2	2.62	0.47
1:2:103:A:C2	1:2:190:A:N9	2.82	0.47
1:2:560:U:O3'	9:H:92:ARG:NH1	2.48	0.47
1:2:1346:U:C5	20:S:30:LEU:HD11	2.50	0.47
9:H:22:LEU:HB3	9:H:50:PHE:CE2	2.49	0.47
11:J:59:THR:HG22	24:W:87:GLU:HG2	1.95	0.47
15:N:18:TYR:CD2	15:N:18:TYR:C	2.92	0.47
17:P:15:ARG:NH1	20:S:90:PHE:CE2	2.82	0.47
21:T:68:ILE:HD11	21:T:114:LEU:CD2	2.44	0.47
33:g:109:LEU:C	33:g:109:LEU:CD2	2.85	0.47
34:n:13:LEU:HD11	34:n:17:ARG:CZ	2.44	0.47
1:2:1414:U:C5	18:Q:121:MET:CE	2.97	0.47
19:R:97:LEU:CD1	19:R:97:LEU:C	2.85	0.47
20:S:91:ASP:O	20:S:95:GLY:N	2.46	0.47
26:Y:30:GLY:O	26:Y:31:ALA:HB3	2.14	0.47
12:K:76:ARG:HH22	12:K:83:ALA:HB1	1.79	0.47
16:O:42:TYR:CD1	16:O:106:ARG:CG	2.96	0.47
21:T:68:ILE:HD11	21:T:114:LEU:HD22	1.97	0.47
1:2:97:G:C2'	1:2:98:C:C6	2.85	0.47
1:2:899:C:OP1	28:a:6:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:78:TYR:CD1	3:B:79:ARG:N	2.83	0.47
4:C:52:ARG:C	4:C:53:THR:HG1	2.07	0.47
9:H:68:GLN:HG3	9:H:145:ARG:HD3	1.89	0.47
16:O:69:ALA:C	16:O:70:VAL:CG2	2.87	0.47
18:Q:66:VAL:HG11	18:Q:74:GLN:HG3	1.96	0.47
33:g:99:SER:OG	33:g:100:TRP:N	2.48	0.47
1:2:750:G:C2	3:B:110:MET:HE2	2.39	0.47
1:2:1038:G:N1	14:M:21:GLY:CA	2.68	0.47
15:N:16:CYS:HG	15:N:62:MET:CE	2.27	0.47
33:g:111:THR:C	33:g:112:ARG:HG2	2.39	0.47
4:C:169:VAL:HG22	4:C:208:PHE:HE1	1.79	0.47
6:E:96:ASN:C	6:E:96:ASN:HD22	2.22	0.47
7:F:23:ALA:O	7:F:25:VAL:N	2.41	0.47
12:K:52:GLY:C	12:K:53:PHE:HD2	2.23	0.47
15:N:25:TRP:CE3	15:N:26:LEU:CA	2.97	0.47
16:O:69:ALA:C	16:O:70:VAL:HG23	2.40	0.47
19:R:93:VAL:HG22	19:R:96:ILE:H	1.75	0.47
1:2:1414:U:C4	18:Q:121:MET:HE1	2.50	0.47
7:F:17:PHE:CD1	7:F:18:SER:N	2.83	0.47
7:F:111:ARG:CD	30:c:58:LEU:HD21	2.42	0.47
24:W:75:ILE:HD11	24:W:125:ILE:CD1	2.45	0.47
30:c:67:LEU:C	30:c:67:LEU:CD1	2.85	0.47
11:J:117:ALA:CB	11:J:123:ALA:HA	2.44	0.47
16:O:34:ILE:HD12	16:O:36:MET:HG3	1.98	0.47
16:O:61:LEU:HD13	16:O:61:LEU:N	2.30	0.47
16:O:63:ARG:CZ	16:O:68:ILE:CG2	2.93	0.47
19:R:93:VAL:HG11	19:R:96:ILE:N	2.30	0.47
20:S:57:ARG:HH22	27:Z:58:THR:HG21	1.80	0.47
1:2:98:C:C2'	1:2:99:U:C6	2.98	0.46
1:2:684:U:O4'	1:2:684:U:O2	2.32	0.46
12:K:34:LEU:HD12	12:K:36:CYS:SG	2.51	0.46
23:V:9:VAL:HG12	23:V:10:ASP:H	1.79	0.46
4:C:51:PRO:CD	4:C:60:LYS:HE2	2.43	0.46
4:C:68:GLU:HG3	23:V:12:LEU:HB2	1.92	0.46
6:E:175:PHE:CZ	6:E:222:ILE:HD11	2.50	0.46
7:F:88:ILE:HD13	27:Z:43:VAL:HG11	1.97	0.46
9:H:116:VAL:CG2	9:H:135:ASP:HA	2.44	0.46
11:J:108:GLN:HG3	11:J:124:ARG:HG2	1.97	0.46
20:S:77:THR:CG2	20:S:78:GLU:N	2.78	0.46
21:T:42:ASP:N	21:T:42:ASP:OD1	2.49	0.46
29:b:41:CYS:SG	29:b:60:CYS:SG	3.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:17:LEU:CD2	31:d:23:ARG:HH21	2.21	0.46
6:E:96:ASN:C	6:E:96:ASN:ND2	2.72	0.46
27:Z:79:GLY:O	27:Z:82:LEU:O	2.33	0.46
30:c:17:ILE:HD11	30:c:67:LEU:HD21	1.92	0.46
1:2:101:A:C2	1:2:235:G:C2	3.04	0.46
5:D:41:ARG:HB2	5:D:41:ARG:NH1	2.30	0.46
17:P:85:LEU:HD11	17:P:88:PHE:CE2	2.51	0.46
20:S:54:PRO:HG2	20:S:55:LEU:HD23	1.98	0.46
33:g:191:VAL:HG21	33:g:208:ALA:HB1	1.85	0.46
2:A:114:PHE:CE2	4:C:53:THR:HG22	2.51	0.46
3:B:88:ALA:CB	3:B:91:GLU:O	2.63	0.46
3:B:110:MET:HA	3:B:138:PHE:CZ	2.50	0.46
11:J:116:LEU:CD1	11:J:116:LEU:H	2.27	0.46
12:K:32:GLU:N	12:K:32:GLU:CD	2.73	0.46
28:a:26:CYS:SG	28:a:74:CYS:SG	3.12	0.46
5:D:209:ILE:HD11	19:R:12:ALA:CB	2.46	0.46
12:K:57:THR:OG1	12:K:64:TYR:HB2	2.16	0.46
17:P:15:ARG:NH1	20:S:90:PHE:O	2.49	0.46
24:W:36:ALA:CB	24:W:110:ILE:CD1	2.93	0.46
2:A:88:PHE:CE1	2:A:92:LEU:CD1	2.93	0.46
2:A:89:ALA:CB	2:A:94:ALA:O	2.63	0.46
16:O:63:ARG:CZ	16:O:68:ILE:HG21	2.44	0.46
16:O:65:THR:OG1	16:O:76:GLU:CA	2.64	0.46
21:T:38:PRO:HG2	21:T:41:ALA:HB3	1.98	0.46
1:2:203:A:H62	10:I:175:ARG:NH1	2.00	0.46
15:N:26:LEU:CG	15:N:27:GLN:H	2.18	0.46
33:g:74:THR:CG2	33:g:112:ARG:NE	2.79	0.46
1:2:1283:U:O2	1:2:1283:U:H2'	2.15	0.46
1:2:1414:U:H5	18:Q:121:MET:CE	2.27	0.46
2:A:72:VAL:HG11	2:A:117:PRO:HG3	1.98	0.46
9:H:96:ARG:HA	9:H:96:ARG:HD3	1.66	0.46
16:O:64:CYS:O	16:O:69:ALA:CB	2.62	0.46
33:g:49:VAL:HG13	33:g:59:VAL:HG12	1.97	0.46
33:g:194:TRP:CD1	33:g:202:LEU:CB	2.99	0.46
2:A:124:ASP:HB3	2:A:127:THR:HG22	1.97	0.45
3:B:64:GLU:HG2	3:B:80:LEU:HD13	1.97	0.45
16:O:48:THR:H	16:O:65:THR:CG2	2.28	0.45
25:X:42:LEU:O	25:X:43:GLU:CB	2.62	0.45
31:d:41:ARG:HH22	31:d:42:ARG:NH2	2.14	0.45
33:g:53:ARG:HA	33:g:82:PHE:HB3	1.98	0.45
33:g:88:LEU:HD23	33:g:95:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:n:9:ARG:NH1	34:n:9:ARG:CG	2.73	0.45
4:C:153:PRO:O	4:C:237:PHE:HE2	2.00	0.45
18:Q:57:TRP:CZ2	21:T:2:ILE:HG21	2.52	0.45
24:W:105:SER:HA	24:W:110:ILE:HA	1.98	0.45
30:c:17:ILE:HG12	30:c:67:LEU:HD21	1.98	0.45
1:2:26:A:C2	25:X:47:MET:CE	2.98	0.45
1:2:297:G:C6	1:2:298:U:C5	3.04	0.45
1:2:456:U:H5'	26:Y:31:ALA:O	2.16	0.45
1:2:750:G:N2	3:B:110:MET:CE	2.43	0.45
13:L:92:ILE:HD12	25:X:12:ALA:HB1	1.98	0.45
3:B:66:SER:HA	3:B:80:LEU:HD23	1.98	0.45
4:C:154:VAL:CG1	4:C:208:PHE:CZ	2.99	0.45
11:J:117:ALA:HB1	11:J:123:ALA:N	2.31	0.45
28:a:23:CYS:HA	28:a:72:TYR:O	2.16	0.45
32:e:13:LYS:HG2	32:e:14:VAL:H	1.81	0.45
1:2:103:A:OP1	1:2:103:A:H8	1.99	0.45
1:2:716:C:H1'	16:O:59:GLU:OE1	2.16	0.45
1:2:1390:G:O2'	18:Q:121:MET:HG2	2.17	0.45
1:2:1553:G:OP2	34:n:2:ARG:NH1	2.29	0.45
3:B:28:VAL:CB	3:B:41:GLY:O	2.65	0.45
15:N:15:THR:HG21	29:b:21:LYS:HG2	1.98	0.45
15:N:25:TRP:CE3	15:N:25:TRP:C	2.95	0.45
18:Q:80:GLN:CD	18:Q:116:ALA:HB2	2.41	0.45
20:S:87:ASN:C	20:S:87:ASN:ND2	2.73	0.45
26:Y:28:HIS:O	26:Y:66:GLY:CA	2.63	0.45
33:g:98:SER:OG	33:g:125:VAL:HB	2.15	0.45
4:C:211:LEU:CD1	4:C:212:PHE:N	2.73	0.45
10:I:56:ARG:HA	10:I:171:GLY:O	2.16	0.45
20:S:91:ASP:OD2	20:S:92:ARG:N	2.50	0.45
4:C:171:ASN:O	4:C:173:VAL:HG13	2.16	0.45
1:2:1417:A:O2'	7:F:66:MET:HE2	2.17	0.45
4:C:116:ILE:HG12	4:C:130:ILE:HG22	1.98	0.45
16:O:130:ALA:N	16:O:131:GLY:HA2	2.31	0.45
23:V:9:VAL:CG1	23:V:10:ASP:H	2.30	0.45
2:A:72:VAL:CG1	2:A:117:PRO:HG3	2.47	0.45
7:F:27:TYR:N	7:F:27:TYR:HD2	2.14	0.45
10:I:180:ILE:HG22	10:I:181:LEU:N	2.32	0.45
1:2:456:U:P	26:Y:31:ALA:HB1	2.56	0.45
11:J:110:GLN:HE22	11:J:151:GLU:CD	2.24	0.45
20:S:119:MET:CE	20:S:121:MET:HE3	2.46	0.45
1:2:1157:U:N3	22:U:60:MET:HE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:71:ASP:OD2	2:A:72:VAL:N	2.50	0.44
3:B:29:MET:HE1	3:B:39:ASP:CA	2.47	0.44
29:b:55:VAL:O	29:b:63:PRO:HA	2.17	0.44
33:g:100:TRP:HA	33:g:124:ASP:HB2	1.98	0.44
1:2:103:A:OP1	1:2:103:A:C8	2.70	0.44
1:2:522:C:OP2	25:X:107:GLY:HA2	2.17	0.44
1:2:719:G:H5'	16:O:67:GLY:HA2	1.96	0.44
3:B:75:SER:OG	3:B:76:HIS:HD2	1.99	0.44
3:B:87:ALA:CB	3:B:219:LEU:HD11	2.44	0.44
4:C:153:PRO:O	4:C:237:PHE:CE2	2.70	0.44
6:E:95:SER:HB3	26:Y:15:LYS:CB	2.14	0.44
7:F:14:ASP:O	7:F:15:VAL:HG23	2.18	0.44
15:N:24:HIS:ND1	15:N:25:TRP:N	2.65	0.44
29:b:51:SER:OG	29:b:53:VAL:O	2.33	0.44
30:c:33:PHE:CD2	30:c:39:ARG:HD2	2.52	0.44
32:e:8:LEU:HD12	32:e:8:LEU:C	2.41	0.44
33:g:39:ILE:HD11	33:g:48:LEU:HD13	1.98	0.44
1:2:103:A:H4'	1:2:104:A:OP2	2.12	0.44
1:2:927:G:P	34:n:21:ARG:HH12	2.41	0.44
6:E:201:GLN:HG2	6:E:206:ASP:HA	1.98	0.44
7:F:23:ALA:HB2	30:c:54:ILE:HG21	1.98	0.44
10:I:107:ALA:N	10:I:108:PRO:CD	2.81	0.44
10:I:112:TRP:O	10:I:112:TRP:CE3	2.71	0.44
16:O:30:ARG:O	16:O:31:ASP:HB2	2.17	0.44
22:U:65:LEU:HD11	22:U:88:ILE:HD11	1.99	0.44
1:2:179:U:OP1	10:I:167:THR:HG21	2.17	0.44
1:2:1575:U:C5	28:a:75:VAL:HG21	2.52	0.44
3:B:84:ARG:HH21	3:B:84:ARG:CB	2.25	0.44
4:C:154:VAL:HG11	4:C:208:PHE:CE2	2.52	0.44
10:I:53:LEU:HD13	10:I:55:MET:HE2	2.00	0.44
25:X:42:LEU:CD1	25:X:121:PHE:HE1	2.29	0.44
28:a:5:ARG:HB2	28:a:8:HIS:H	1.82	0.44
30:c:33:PHE:CD2	30:c:39:ARG:CD	3.00	0.44
4:C:206:ALA:CB	4:C:208:PHE:CE2	3.01	0.44
5:D:41:ARG:HB2	5:D:41:ARG:HH11	1.82	0.44
17:P:52:HIS:NE2	17:P:56:LYS:HE2	2.33	0.44
25:X:35:THR:HG22	25:X:37:ILE:HG22	1.99	0.44
25:X:35:THR:CA	25:X:36:SER:HB3	2.47	0.44
2:A:58:LEU:HB2	23:V:78:LEU:HD21	2.00	0.44
3:B:28:VAL:HG23	3:B:41:GLY:C	2.35	0.44
18:Q:32:PRO:HB2	21:T:4:GLY:HA3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:50:ALA:HB3	20:S:51:GLY:HA2	1.99	0.44
23:V:40:ASN:HB2	23:V:44:LEU:O	2.18	0.44
30:c:14:LYS:HD2	30:c:32:GLU:HG3	1.99	0.44
1:2:251:U:OP1	10:I:11:HIS:HE1	2.01	0.44
3:B:34:PHE:CE1	3:B:70:MET:CE	3.01	0.44
3:B:133:LEU:HB2	3:B:168:LEU:HD21	2.00	0.44
4:C:167:HIS:CD2	4:C:210:ASP:OD2	2.63	0.44
11:J:114:ARG:NE	11:J:114:ARG:HA	2.32	0.44
12:K:31:HIS:CE1	12:K:32:GLU:O	2.70	0.44
16:O:52:VAL:C	16:O:53:THR:HG23	2.43	0.44
20:S:81:ILE:CG2	20:S:82:PRO:CD	2.94	0.44
25:X:57:ALA:HB1	25:X:67:ILE:CG2	2.48	0.44
5:D:71:ARG:HG3	5:D:87:ILE:HD12	2.00	0.44
6:E:128:GLN:HB3	6:E:140:VAL:HG22	1.99	0.44
9:H:138:ASP:O	9:H:140:THR:HB	2.18	0.44
12:K:52:GLY:C	12:K:53:PHE:CD2	2.95	0.44
17:P:30:PHE:CZ	17:P:86:PRO:HD3	2.52	0.44
25:X:35:THR:O	25:X:38:TYR:CD1	2.70	0.44
1:2:1337:U:H5	27:Z:80:HIS:CD2	2.35	0.43
3:B:75:SER:OG	3:B:76:HIS:CD2	2.70	0.43
11:J:110:GLN:OE1	11:J:113:LYS:CE	2.65	0.43
16:O:46:ASN:N	16:O:46:ASN:HD22	2.15	0.43
1:2:13:C:O5'	4:C:179:SER:CB	2.66	0.43
1:2:13:C:C5'	4:C:179:SER:HB2	2.48	0.43
1:2:1346:U:C6	20:S:30:LEU:HD11	2.53	0.43
9:H:88:PHE:O	9:H:88:PHE:CD2	2.70	0.43
20:S:92:ARG:HG3	20:S:93:ALA:N	2.34	0.43
33:g:55:LYS:CB	33:g:81:HIS:O	2.66	0.43
34:n:10:THR:O	34:n:11:ARG:C	2.60	0.43
1:2:98:C:O2	1:2:99:U:C6	2.70	0.43
1:2:1038:G:C6	14:M:21:GLY:CA	2.96	0.43
1:2:1244:G:N2	12:K:56:LYS:HZ3	2.11	0.43
3:B:69:ASP:OD1	3:B:70:MET:HE2	2.18	0.43
4:C:171:ASN:C	4:C:171:ASN:ND2	2.73	0.43
10:I:103:SER:HA	10:I:162:LEU:O	2.18	0.43
25:X:132:LEU:HD23	25:X:132:LEU:HA	1.86	0.43
33:g:203:ILE:CG2	33:g:204:LYS:N	2.81	0.43
1:2:1028:U:H5''	12:K:51:LYS:NZ	2.34	0.43
2:A:143:ILE:HG22	2:A:157:CYS:HB3	2.00	0.43
29:b:57:CYS:HB3	29:b:64:LEU:HD11	2.00	0.43
33:g:180:LEU:HB2	33:g:196:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:97:G:N9	1:2:98:C:C5	2.86	0.43
1:2:1153:U:H4'	1:2:1153:U:OP1	2.19	0.43
4:C:168:THR:CG2	4:C:169:VAL:H	2.32	0.43
11:J:122:HIS:O	11:J:125:THR:OG1	2.30	0.43
17:P:113:HIS:CE1	20:S:121:MET:HE1	2.53	0.43
21:T:41:ALA:C	21:T:42:ASP:OD1	2.62	0.43
1:2:98:C:C2	1:2:99:U:C6	3.07	0.43
1:2:800:G:H4'	1:2:1556:A:H4'	2.00	0.43
7:F:31:HIS:O	7:F:32:GLU:HB2	2.19	0.43
10:I:54:LYS:NZ	10:I:172:GLN:CG	2.82	0.43
11:J:147:TRP:O	11:J:149:GLU:N	2.52	0.43
12:K:48:PHE:HB2	12:K:54:CYS:SG	2.58	0.43
15:N:123:HIS:HA	15:N:126:THR:HG22	2.00	0.43
18:Q:117:ASP:HB2	18:Q:119:ARG:HD3	2.01	0.43
1:2:1242:G:C8	31:d:42:ARG:CD	3.02	0.43
9:H:113:THR:CA	9:H:138:ASP:OD2	2.49	0.43
16:O:61:LEU:HB3	16:O:92:ARG:NE	2.32	0.43
6:E:126:VAL:HG13	6:E:139:VAL:HG13	2.01	0.43
10:I:108:PRO:O	10:I:111:GLN:HG2	2.19	0.43
13:L:84:ILE:HG22	13:L:85:ARG:N	2.33	0.43
14:M:29:ILE:CB	14:M:59:HIS:CB	2.97	0.43
17:P:85:LEU:HD12	17:P:88:PHE:CD2	2.53	0.43
1:2:1460:G:H5''	34:n:24:SER:CB	2.48	0.43
3:B:44:VAL:O	3:B:44:VAL:HG13	2.18	0.43
4:C:126:ILE:CD1	4:C:202:LEU:HD22	2.30	0.43
20:S:49:ARG:HH22	21:T:43:LEU:HD11	1.84	0.43
26:Y:28:HIS:HE1	26:Y:67:HIS:C	2.26	0.43
31:d:22:CYS:SG	31:d:43:CYS:CB	3.06	0.43
3:B:33:TYR:HH	3:B:177:VAL:HG13	1.77	0.43
5:D:26:LEU:HD13	5:D:51:ILE:HD12	2.01	0.43
11:J:59:THR:CG2	24:W:87:GLU:HG2	2.49	0.43
20:S:47:VAL:HA	20:S:50:ALA:HB2	2.01	0.43
3:B:36:GLY:CA	3:B:37:LYS:HB3	2.39	0.42
3:B:55:MET:HE1	3:B:85:SER:O	2.18	0.42
7:F:23:ALA:C	7:F:25:VAL:N	2.77	0.42
10:I:81:VAL:HG22	10:I:102:VAL:HG12	2.01	0.42
34:n:22:ALA:C	34:n:24:SER:N	2.77	0.42
1:2:325:C:N3	1:2:335:G:N2	2.66	0.42
1:2:865:U:OP1	3:B:149:HIS:CE1	2.56	0.42
4:C:54:LYS:O	4:C:58:LEU:CD1	2.67	0.42
7:F:67:SER:HB3	7:F:68:ARG:CA	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:65:THR:OG1	16:O:76:GLU:C	2.62	0.42
26:Y:34:PRO:HG2	26:Y:39:ILE:HD11	2.01	0.42
30:c:63:GLU:C	30:c:64:ALA:O	2.61	0.42
31:d:22:CYS:HG	31:d:43:CYS:CB	2.27	0.42
1:2:1266:C:H3'	1:2:1267:U:H5''	2.02	0.42
1:2:1460:G:H5''	34:n:24:SER:OG	2.19	0.42
3:B:29:MET:SD	3:B:38:HIS:C	3.02	0.42
4:C:163:ILE:HG23	4:C:164:GLY:N	2.35	0.42
12:K:11:ILE:HD11	12:K:34:LEU:HD11	2.02	0.42
24:W:47:ILE:HD11	24:W:63:ILE:HG21	2.02	0.42
30:c:38:ASN:C	30:c:39:ARG:HG2	2.43	0.42
31:d:22:CYS:CB	31:d:40:CYS:CB	2.93	0.42
33:g:55:LYS:HG2	33:g:81:HIS:O	2.19	0.42
4:C:67:ILE:H	4:C:67:ILE:CD1	1.95	0.42
10:I:54:LYS:NZ	10:I:172:GLN:HG3	2.33	0.42
12:K:84:ASN:HA	12:K:85:ALA:C	2.45	0.42
16:O:101:VAL:HG23	16:O:101:VAL:O	2.20	0.42
21:T:5:LYS:O	21:T:5:LYS:HG3	2.19	0.42
1:2:268:C:H5''	10:I:10:LYS:CD	2.48	0.42
1:2:521:G:H2'	25:X:46:SER:OG	2.20	0.42
1:2:974:G:OP1	7:F:68:ARG:CB	2.67	0.42
1:2:1268:G:H2'	1:2:1268:G:N3	2.35	0.42
3:B:29:MET:CE	3:B:39:ASP:CB	2.88	0.42
16:O:29:LYS:HG2	16:O:33:GLU:OE1	2.20	0.42
29:b:51:SER:OG	29:b:52:ASN:N	2.51	0.42
29:b:65:ALA:HB1	29:b:72:ILE:HB	2.01	0.42
30:c:14:LYS:CD	30:c:32:GLU:HG3	2.50	0.42
30:c:55:LEU:N	30:c:55:LEU:CD1	2.81	0.42
12:K:15:LEU:HD11	12:K:67:LEU:HD13	2.02	0.42
15:N:20:ARG:CZ	15:N:20:ARG:HB2	2.49	0.42
20:S:43:ALA:O	20:S:47:VAL:HG23	2.20	0.42
30:c:20:THR:HG23	30:c:26:VAL:HG23	1.99	0.42
3:B:63:TRP:CE3	16:O:55:LEU:HB2	2.55	0.42
3:B:75:SER:O	3:B:76:HIS:HB2	2.19	0.42
4:C:153:PRO:CD	23:V:26:PRO:HG3	2.49	0.42
19:R:93:VAL:N	19:R:94:PRO:CA	2.72	0.42
20:S:55:LEU:CD2	20:S:55:LEU:N	2.82	0.42
20:S:85:MET:O	20:S:86:LEU:CD1	2.67	0.42
33:g:209:HIS:NE2	33:g:227:THR:C	2.78	0.42
34:n:7:LYS:CE	34:n:11:ARG:CZ	2.98	0.42
2:A:83:ARG:HE	2:A:203:ARG:NH1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:203:ARG:HE	2:A:211:ILE:HD12	1.84	0.42
6:E:90:ILE:CG2	6:E:92:LEU:HD11	2.44	0.42
15:N:4:LEU:HD12	15:N:5:HIS:CE1	2.53	0.42
15:N:19:ARG:HH21	15:N:22:ALA:HB1	1.85	0.42
16:O:35:VAL:O	16:O:99:ASP:HB3	2.19	0.42
33:g:188:ASP:O	33:g:211:GLY:O	2.38	0.42
33:g:225:VAL:HG22	33:g:226:ILE:N	2.34	0.42
2:A:62:MET:HE2	2:A:62:MET:HB3	1.90	0.42
4:C:173:VAL:HB	4:C:235:GLU:OE1	2.20	0.42
7:F:23:ALA:C	7:F:25:VAL:H	2.25	0.42
1:2:101:A:N1	1:2:235:G:C5	2.88	0.42
1:2:1576:C:OP1	28:a:87:ARG:NH2	2.53	0.42
10:I:55:MET:O	10:I:174:GLY:CA	2.68	0.42
18:Q:25:LEU:CD2	21:T:5:LYS:HE2	2.50	0.42
1:2:678:G:C4'	9:H:93:ASN:HD22	2.31	0.41
2:A:70:LYS:CE	2:A:70:LYS:CA	2.86	0.41
4:C:172:THR:CG2	4:C:186:PRO:CD	2.91	0.41
11:J:159:THR:O	11:J:163:THR:N	2.52	0.41
12:K:51:LYS:HB3	12:K:53:PHE:CE2	2.56	0.41
28:a:37:THR:HG21	28:a:70:LYS:HZ2	1.85	0.41
17:P:84:ILE:CA	17:P:88:PHE:CE1	3.00	0.41
20:S:84:TRP:O	20:S:89:ARG:NH1	2.53	0.41
1:2:97:G:C4	1:2:98:C:C6	3.09	0.41
1:2:101:A:C6	1:2:235:G:C6	3.08	0.41
10:I:9:LEU:C	10:I:9:LEU:CD1	2.93	0.41
12:K:27:GLN:OE1	12:K:42:TYR:CD2	2.72	0.41
15:N:20:ARG:O	15:N:65:ALA:CB	2.68	0.41
17:P:46:PHE:CA	17:P:50:HIS:HD2	2.29	0.41
20:S:28:LEU:HB2	20:S:56:ARG:O	2.21	0.41
20:S:82:PRO:HG3	20:S:84:TRP:CE2	2.54	0.41
2:A:28:LEU:HD23	2:A:45:HIS:CE1	2.55	0.41
4:C:163:ILE:HG23	4:C:164:GLY:H	1.85	0.41
10:I:112:TRP:CH2	10:I:116:GLN:OE1	2.74	0.41
22:U:103:LYS:O	22:U:107:GLN:HG3	2.19	0.41
4:C:167:HIS:HD2	4:C:210:ASP:CG	2.28	0.41
7:F:44:ARG:HH12	18:Q:119:ARG:CD	2.33	0.41
11:J:114:ARG:CB	11:J:116:LEU:CD1	2.97	0.41
16:O:83:MET:HG3	16:O:126:ALA:HB2	2.01	0.41
19:R:21:TYR:CD1	19:R:58:MET:HE1	2.56	0.41
20:S:57:ARG:HH21	27:Z:58:THR:HG21	1.81	0.41
34:n:7:LYS:HE3	34:n:11:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:30:VAL:HG22	7:F:30:VAL:O	2.21	0.41
12:K:53:PHE:CD2	12:K:53:PHE:N	2.88	0.41
13:L:144:ALA:HA	13:L:145:VAL:HA	1.85	0.41
24:W:41:MET:HE1	24:W:72:CYS:SG	2.61	0.41
24:W:47:ILE:HD11	24:W:63:ILE:CG2	2.50	0.41
4:C:177:CYS:SG	4:C:224:ASN:ND2	2.93	0.41
9:H:18:GLU:H	9:H:18:GLU:HG3	1.73	0.41
16:O:69:ALA:O	16:O:70:VAL:HG22	2.20	0.41
29:b:62:THR:CG2	29:b:63:PRO:HD2	2.49	0.41
1:2:404:C:O2'	11:J:141:GLN:NE2	2.45	0.41
6:E:201:GLN:HB2	6:E:206:ASP:CA	2.50	0.41
17:P:124:VAL:O	17:P:125:VAL:CB	2.68	0.41
1:2:720:U:OP1	16:O:66:GLY:CA	2.67	0.41
3:B:86:ILE:CG2	3:B:87:ALA:N	2.84	0.41
3:B:130:ILE:HD12	3:B:215:LYS:HD3	2.03	0.41
6:E:96:ASN:C	6:E:97:GLU:HG3	2.46	0.41
10:I:180:ILE:CG2	10:I:181:LEU:N	2.84	0.41
16:O:29:LYS:HE2	16:O:35:VAL:HG23	2.02	0.41
21:T:46:THR:O	21:T:103:SER:HB3	2.20	0.41
24:W:36:ALA:HB1	24:W:110:ILE:HD11	2.01	0.41
25:X:106:MET:CG	25:X:120:ARG:HA	2.48	0.41
26:Y:28:HIS:HE1	26:Y:67:HIS:O	2.04	0.41
26:Y:32:LYS:HE3	26:Y:32:LYS:HB3	1.88	0.41
28:a:73:TYR:O	28:a:74:CYS:SG	2.78	0.41
33:g:191:VAL:CG2	33:g:208:ALA:HB2	2.34	0.41
1:2:522:C:P	25:X:107:GLY:HA2	2.61	0.41
2:A:68:GLU:OE1	2:A:184:ARG:CZ	2.61	0.41
4:C:213:THR:HG22	4:C:214:SER:N	2.35	0.41
5:D:123:ILE:O	5:D:127:VAL:HG23	2.21	0.41
9:H:72:ILE:HD11	9:H:105:ILE:HG23	2.02	0.41
17:P:15:ARG:NH1	20:S:90:PHE:HD2	2.17	0.41
24:W:36:ALA:HB1	24:W:110:ILE:CD1	2.50	0.41
24:W:73:VAL:HG12	24:W:74:ALA:N	2.35	0.41
25:X:42:LEU:HD23	25:X:42:LEU:HA	1.97	0.41
2:A:33:LYS:N	2:A:34:PRO:CD	2.84	0.40
3:B:140:LYS:HB3	3:B:204:GLU:HB3	2.03	0.40
16:O:41:ILE:HA	16:O:49:PHE:O	2.21	0.40
16:O:51:HIS:NE2	16:O:53:THR:CG2	2.84	0.40
25:X:35:THR:N	25:X:36:SER:CB	2.71	0.40
33:g:101:ASP:O	33:g:102:SER:HB2	2.21	0.40
33:g:212:ARG:HB2	33:g:230:SER:OG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:102:G:C2	1:2:234:U:N3	2.89	0.40
1:2:435:U:OP2	11:J:166:LYS:O	2.39	0.40
2:A:49:LEU:HA	2:A:52:THR:HG22	2.04	0.40
2:A:63:ILE:HD11	2:A:143:ILE:CD1	2.51	0.40
3:B:33:TYR:CE2	3:B:178:GLU:HA	2.56	0.40
4:C:65:LYS:O	4:C:66:SER:CB	2.69	0.40
11:J:158:ASP:O	11:J:162:MET:N	2.48	0.40
16:O:62:ALA:C	16:O:63:ARG:HG2	2.46	0.40
33:g:105:ARG:HB3	33:g:107:TRP:NE1	2.36	0.40
33:g:112:ARG:N	33:g:112:ARG:CD	2.81	0.40
1:2:1407:A:N7	21:T:95:MET:HE2	2.36	0.40
2:A:70:LYS:CD	4:C:54:LYS:HZ1	2.34	0.40
2:A:88:PHE:CZ	2:A:92:LEU:HD12	2.55	0.40
3:B:87:ALA:O	3:B:88:ALA:CB	2.68	0.40
7:F:22:PRO:O	7:F:23:ALA:CB	2.69	0.40
11:J:159:THR:O	11:J:163:THR:CB	2.69	0.40
13:L:84:ILE:HD11	13:L:123:VAL:HG11	2.03	0.40
15:N:23:PRO:CG	15:N:25:TRP:NE1	2.84	0.40
22:U:54:VAL:O	22:U:54:VAL:HG13	2.21	0.40
30:c:38:ASN:O	30:c:39:ARG:CB	2.69	0.40
30:c:63:GLU:O	30:c:64:ALA:O	2.39	0.40
33:g:173:MET:HE1	33:g:175:ASP:CA	2.51	0.40
1:2:990:U:H5''	17:P:123:LYS:HD2	2.03	0.40
1:2:1244:G:H2'	12:K:58:TYR:HE2	1.86	0.40
3:B:34:PHE:CE1	3:B:70:MET:SD	3.14	0.40
3:B:139:THR:HG22	3:B:201:CYS:SG	2.62	0.40
4:C:55:LEU:HA	4:C:55:LEU:HD12	1.88	0.40
7:F:12:TYR:CB	7:F:35:HIS:ND1	2.67	0.40
12:K:84:ASN:H	12:K:85:ALA:HB3	1.80	0.40
15:N:21:SER:O	15:N:22:ALA:CB	2.69	0.40
17:P:86:PRO:HA	17:P:111:ILE:CD1	2.51	0.40
24:W:3:ARG:HE	24:W:3:ARG:HB3	1.65	0.40
28:a:31:PRO:HG2	28:a:34:LYS:HB3	2.04	0.40
28:a:73:TYR:O	28:a:74:CYS:CB	2.69	0.40
1:2:971:A:N6	1:2:972:G:C6	2.90	0.40
1:2:1007:G:P	31:d:41:ARG:HH22	2.44	0.40
6:E:84:THR:HG21	6:E:90:ILE:HD11	2.04	0.40
11:J:117:ALA:CB	11:J:126:LEU:CD1	2.99	0.40
11:J:157:ALA:O	11:J:158:ASP:CB	2.69	0.40
16:O:30:ARG:O	16:O:31:ASP:CB	2.70	0.40
17:P:128:SER:HA	17:P:129:LYS:HA	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:34:ILE:HG22	23:V:35:GLN:N	2.36	0.40
24:W:27:ILE:HD12	24:W:27:ILE:N	2.36	0.40
25:X:110:GLY:O	25:X:111:ARG:CB	2.69	0.40
26:Y:14:ASN:HD21	26:Y:17:LEU:HD23	1.86	0.40
33:g:92:ALA:C	33:g:109:LEU:HD12	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	196/256 (77%)	180 (92%)	11 (6%)	5 (3%)	4	20
3	B	215/247 (87%)	195 (91%)	11 (5%)	9 (4%)	2	13
4	C	213/272 (78%)	193 (91%)	15 (7%)	5 (2%)	5	22
5	D	204/216 (94%)	188 (92%)	15 (7%)	1 (0%)	24	52
6	E	242/255 (95%)	210 (87%)	26 (11%)	6 (2%)	4	20
7	F	182/193 (94%)	158 (87%)	16 (9%)	8 (4%)	2	12
8	G	29/216 (13%)	29 (100%)	0	0	100	100
9	H	159/168 (95%)	146 (92%)	10 (6%)	3 (2%)	6	25
10	I	162/197 (82%)	147 (91%)	10 (6%)	5 (3%)	3	17
11	J	160/185 (86%)	138 (86%)	16 (10%)	6 (4%)	2	14
12	K	86/141 (61%)	80 (93%)	6 (7%)	0	100	100
13	L	136/155 (88%)	121 (89%)	14 (10%)	1 (1%)	18	46
14	M	97/124 (78%)	84 (87%)	12 (12%)	1 (1%)	12	38
15	N	148/151 (98%)	128 (86%)	14 (10%)	6 (4%)	2	14
16	O	133/159 (84%)	104 (78%)	21 (16%)	8 (6%)	1	7
17	P	114/144 (79%)	102 (90%)	10 (9%)	2 (2%)	6	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	Q	127/140 (91%)	108 (85%)	14 (11%)	5 (4%)	2	14
19	R	116/129 (90%)	101 (87%)	11 (10%)	4 (3%)	3	16
20	S	133/155 (86%)	119 (90%)	10 (8%)	4 (3%)	3	18
21	T	144/148 (97%)	133 (92%)	9 (6%)	2 (1%)	9	30
22	U	91/123 (74%)	84 (92%)	6 (7%)	1 (1%)	11	36
23	V	85/89 (96%)	73 (86%)	9 (11%)	3 (4%)	3	16
24	W	124/130 (95%)	113 (91%)	10 (8%)	1 (1%)	16	44
25	X	138/144 (96%)	124 (90%)	10 (7%)	4 (3%)	3	18
26	Y	99/140 (71%)	84 (85%)	13 (13%)	2 (2%)	6	24
27	Z	71/115 (62%)	66 (93%)	2 (3%)	3 (4%)	2	13
28	a	96/118 (81%)	84 (88%)	6 (6%)	6 (6%)	1	7
29	b	80/86 (93%)	71 (89%)	6 (8%)	3 (4%)	2	14
30	c	59/68 (87%)	51 (86%)	3 (5%)	5 (8%)	0	4
31	d	50/57 (88%)	48 (96%)	2 (4%)	0	100	100
32	e	40/62 (64%)	38 (95%)	2 (5%)	0	100	100
33	g	299/335 (89%)	263 (88%)	30 (10%)	6 (2%)	6	24
34	n	22/25 (88%)	20 (91%)	2 (9%)	0	100	100
All	All	4250/5143 (83%)	3783 (89%)	352 (8%)	115 (3%)	6	20

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	42	ASP
3	B	88	ALA
7	F	15	VAL
7	F	26	ASP
10	I	149	VAL
11	J	63	ASN
11	J	158	ASP
11	J	159	THR
14	M	61	VAL
15	N	26	LEU
15	N	27	GLN
16	O	31	ASP
16	O	70	VAL
16	O	98	VAL

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Mol	Chain	Res	Type
16	O	99	ASP
17	P	125	VAL
18	Q	136	GLN
20	S	83	VAL
26	Y	18	ASP
27	Z	81	ASP
28	a	74	CYS
29	b	60	CYS
30	c	39	ARG
30	c	62	ARG
33	g	197	GLU
3	B	60	ASN
3	B	89	GLY
3	B	209	THR
6	E	232	GLU
7	F	16	ASP
9	H	33	GLU
10	I	40	GLU
10	I	148	VAL
11	J	96	SER
15	N	138	ASN
18	Q	139	TYR
19	R	63	ARG
20	S	61	LEU
20	S	89	ARG
25	X	130	SER
26	Y	94	GLY
28	a	46	ASP
28	a	47	ALA
30	c	64	ALA
33	g	113	THR
3	B	33	TYR
3	B	75	SER
3	B	143	ALA
4	C	66	SER
4	C	89	GLU
6	E	80	TYR
9	H	137	HIS
10	I	59	ARG
13	L	53	ASP
16	O	73	GLN
20	S	28	LEU

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Mol	Chain	Res	Type
21	T	39	GLU
21	T	75	HIS
22	U	23	LYS
23	V	4	ASP
23	V	10	ASP
25	X	61	LYS
27	Z	22	TRP
29	b	52	ASN
29	b	61	GLN
33	g	44	GLU
33	g	46	ASN
33	g	66	GLN
2	A	38	THR
2	A	123	CYS
3	B	203	ILE
4	C	163	ILE
4	C	165	LEU
4	C	260	ASP
5	D	144	ARG
6	E	94	LYS
6	E	133	ALA
6	E	245	ARG
9	H	84	HIS
10	I	86	ALA
11	J	97	LEU
11	J	145	LEU
15	N	22	ALA
16	O	71	ARG
17	P	126	LYS
18	Q	11	LYS
18	Q	38	SER
18	Q	39	GLU
19	R	88	THR
28	a	59	TYR
28	a	94	ASN
30	c	38	ASN
2	A	102	THR
2	A	157	CYS
3	B	206	VAL
6	E	195	ILE
7	F	21	ASP
7	F	22	PRO

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Mol	Chain	Res	Type
15	N	108	ASP
19	R	96	ILE
19	R	119	VAL
25	X	88	ARG
7	F	4	VAL
7	F	112	GLU
16	O	26	GLY
25	X	113	VAL
27	Z	73	ILE
28	a	45	VAL
30	c	8	VAL
33	g	78	GLY
7	F	96	ASN
15	N	59	GLY
16	O	67	GLY
24	W	95	PRO
23	V	81	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	172/211 (82%)	159 (92%)	13 (8%)	12	38
3	B	192/216 (89%)	185 (96%)	7 (4%)	31	56
4	C	174/216 (81%)	165 (95%)	9 (5%)	21	48
5	D	176/182 (97%)	173 (98%)	3 (2%)	53	67
6	E	209/217 (96%)	199 (95%)	10 (5%)	23	49
7	F	161/165 (98%)	154 (96%)	7 (4%)	26	52
9	H	137/141 (97%)	132 (96%)	5 (4%)	31	56
10	I	131/158 (83%)	126 (96%)	5 (4%)	29	55
11	J	141/168 (84%)	133 (94%)	8 (6%)	18	46
12	K	77/116 (66%)	71 (92%)	6 (8%)	11	37
13	L	124/137 (90%)	118 (95%)	6 (5%)	23	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	M	1/101 (1%)	1 (100%)	0	100	100
15	N	125/126 (99%)	118 (94%)	7 (6%)	19	46
16	O	99/115 (86%)	93 (94%)	6 (6%)	17	44
17	P	105/124 (85%)	101 (96%)	4 (4%)	29	55
18	Q	108/114 (95%)	104 (96%)	4 (4%)	30	55
19	R	104/111 (94%)	97 (93%)	7 (7%)	15	41
20	S	112/128 (88%)	102 (91%)	10 (9%)	9	31
21	T	120/122 (98%)	114 (95%)	6 (5%)	22	49
22	U	87/110 (79%)	84 (97%)	3 (3%)	32	58
23	V	72/74 (97%)	68 (94%)	4 (6%)	19	46
24	W	107/109 (98%)	98 (92%)	9 (8%)	10	34
25	X	112/115 (97%)	110 (98%)	2 (2%)	51	66
26	Y	77/118 (65%)	74 (96%)	3 (4%)	28	54
27	Z	60/93 (64%)	58 (97%)	2 (3%)	33	58
28	a	91/107 (85%)	81 (89%)	10 (11%)	6	22
29	b	76/79 (96%)	75 (99%)	1 (1%)	61	70
30	c	52/59 (88%)	48 (92%)	4 (8%)	12	37
31	d	46/51 (90%)	45 (98%)	1 (2%)	45	63
32	e	35/51 (69%)	30 (86%)	5 (14%)	3	13
33	g	256/282 (91%)	246 (96%)	10 (4%)	28	54
34	n	22/23 (96%)	16 (73%)	6 (27%)	0	1
All	All	3561/4139 (86%)	3378 (95%)	183 (5%)	23	48

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	32	MET
2	A	44	THR
2	A	54	GLU
2	A	55	LYS
2	A	70	LYS
2	A	73	LEU
2	A	102	THR
2	A	116	GLU
2	A	121	ILE

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Mol	Chain	Res	Type
2	A	142	CYS
2	A	153	ASP
2	A	176	LEU
2	A	184	ARG
3	B	34	PHE
3	B	53	VAL
3	B	58	VAL
3	B	80	LEU
3	B	150	THR
3	B	211	VAL
3	B	238	LEU
4	C	67	ILE
4	C	94	GLU
4	C	105	THR
4	C	116	ILE
4	C	171	ASN
4	C	208	PHE
4	C	210	ASP
4	C	211	LEU
4	C	235	GLU
5	D	83	ASP
5	D	101	ASN
5	D	170	THR
6	E	4	CYS
6	E	20	LEU
6	E	38	LEU
6	E	94	LYS
6	E	96	ASN
6	E	118	GLU
6	E	164	ILE
6	E	169	VAL
6	E	172	VAL
6	E	211	LYS
7	F	14	ASP
7	F	16	ASP
7	F	31	HIS
7	F	71	ASN
7	F	96	ASN
7	F	137	ASP
7	F	173	ASP
9	H	61	LEU
9	H	81	THR

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Mol	Chain	Res	Type
9	H	88	PHE
9	H	98	LEU
9	H	143	GLU
10	I	9	LEU
10	I	10	LYS
10	I	73	THR
10	I	149	VAL
10	I	181	LEU
11	J	20	GLU
11	J	58	LEU
11	J	91	LEU
11	J	98	THR
11	J	114	ARG
11	J	116	LEU
11	J	149	GLU
11	J	154	ILE
12	K	3	MET
12	K	23	VAL
12	K	27	GLN
12	K	35	ASP
12	K	55	ILE
12	K	81	LEU
13	L	29	LYS
13	L	97	ARG
13	L	109	ILE
13	L	119	ASP
13	L	120	LEU
13	L	132	THR
15	N	4	LEU
15	N	11	ILE
15	N	13	SER
15	N	15	THR
15	N	20	ARG
15	N	80	LEU
15	N	103	GLU
16	O	34	ILE
16	O	46	ASN
16	O	61	LEU
16	O	95	GLU
16	O	108	GLU
16	O	159	LEU
17	P	78	HIS

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Mol	Chain	Res	Type
17	P	82	MET
17	P	85	LEU
17	P	88	PHE
18	Q	31	THR
18	Q	44	LYS
18	Q	98	THR
18	Q	119	ARG
19	R	18	GLU
19	R	55	THR
19	R	88	THR
19	R	92	ASN
19	R	93	VAL
19	R	97	LEU
19	R	105	MET
20	S	28	LEU
20	S	52	LEU
20	S	60	THR
20	S	61	LEU
20	S	83	VAL
20	S	99	HIS
20	S	101	VAL
20	S	103	THR
20	S	112	GLU
20	S	116	MET
21	T	2	ILE
21	T	42	ASP
21	T	43	LEU
21	T	45	LYS
21	T	129	LEU
21	T	130	THR
22	U	21	VAL
22	U	44	MET
22	U	82	ASP
23	V	7	GLU
23	V	12	LEU
23	V	42	ASP
23	V	48	GLU
24	W	7	LEU
24	W	24	GLN
24	W	31	SER
24	W	66	LEU
24	W	71	LYS

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Mol	Chain	Res	Type
24	W	76	CYS
24	W	85	ASP
24	W	87	GLU
24	W	94	LEU
25	X	35	THR
25	X	89	ASP
26	Y	37	ASP
26	Y	78	LEU
26	Y	81	LEU
27	Z	80	HIS
27	Z	82	LEU
28	a	5	ARG
28	a	10	ARG
28	a	21	VAL
28	a	25	ASN
28	a	26	CYS
28	a	29	GLN
28	a	30	VAL
28	a	57	CYS
28	a	84	VAL
28	a	100	LEU
29	b	35	SER
30	c	27	THR
30	c	57	LEU
30	c	66	ARG
30	c	67	LEU
31	d	24	ILE
32	e	18	THR
32	e	29	GLU
32	e	31	ARG
32	e	36	LEU
32	e	48	ASN
33	g	40	GLU
33	g	67	GLU
33	g	95	LEU
33	g	101	ASP
33	g	117	LEU
33	g	173	MET
33	g	226	ILE
33	g	254	VAL
33	g	303	THR
33	g	306	CYS

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Mol	Chain	Res	Type
34	n	2	ARG
34	n	9	ARG
34	n	13	LEU
34	n	16	LYS
34	n	19	LYS
34	n	20	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	126	ASN
2	A	130	GLN
2	A	165	ASN
2	A	167	ASN
3	B	27	HIS
3	B	46	ASN
3	B	59	ASN
3	B	76	HIS
3	B	103	HIS
3	B	149	HIS
4	C	167	HIS
4	C	224	ASN
5	D	23	ASN
5	D	101	ASN
6	E	8	HIS
6	E	79	ASN
6	E	96	ASN
6	E	128	GLN
6	E	201	GLN
7	F	96	ASN
7	F	106	GLN
7	F	157	ASN
7	F	174	GLN
9	H	10	ASN
9	H	84	HIS
9	H	125	ASN
9	H	154	ASN
10	I	11	HIS
10	I	18	GLN
10	I	44	HIS
10	I	94	ASN
10	I	116	GLN

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Mol	Chain	Res	Type
11	J	27	GLN
11	J	89	GLN
11	J	112	HIS
11	J	121	HIS
11	J	131	HIS
11	J	136	ASN
11	J	141	GLN
11	J	153	ASN
12	K	27	GLN
13	L	13	GLN
13	L	90	GLN
15	N	5	HIS
15	N	58	ASN
16	O	46	ASN
16	O	73	GLN
17	P	50	HIS
18	Q	80	GLN
19	R	83	ASN
20	S	75	ASN
20	S	79	HIS
21	T	23	ASN
21	T	32	ASN
21	T	70	GLN
23	V	84	ASN
24	W	24	GLN
24	W	56	HIS
24	W	64	ASN
24	W	90	GLN
24	W	98	GLN
25	X	62	GLN
26	Y	14	ASN
26	Y	28	HIS
27	Z	78	ASN
27	Z	80	HIS
28	a	94	ASN
29	b	18	HIS
29	b	50	HIS
30	c	28	GLN
31	d	38	ASN
33	g	32	HIS
33	g	79	HIS
33	g	121	HIS

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Mol	Chain	Res	Type
33	g	155	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1472/1577 (93%)	410 (27%)	47 (3%)

All (410) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	U
1	2	4	U
1	2	16	C
1	2	18	A
1	2	24	G
1	2	25	C
1	2	38	U
1	2	40	G
1	2	43	U
1	2	45	A
1	2	46	G
1	2	50	U
1	2	55	G
1	2	57	G
1	2	58	U
1	2	59	U
1	2	61	G
1	2	75	A
1	2	82	A
1	2	89	A
1	2	91	U
1	2	93	A
1	2	94	U
1	2	95	A
1	2	97	G
1	2	98	C
1	2	99	U
1	2	100	C
1	2	101	A
1	2	102	G
1	2	103	A

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Mol	Chain	Res	Type
1	2	104	A
1	2	105	U
1	2	115	G
1	2	138	A
1	2	141	G
1	2	142	C
1	2	148	C
1	2	149	A
1	2	151	C
1	2	153	C
1	2	154	U
1	2	157	U
1	2	159	C
1	2	161	A
1	2	163	U
1	2	166	A
1	2	168	G
1	2	169	C
1	2	182	A
1	2	183	G
1	2	184	A
1	2	185	U
1	2	186	G
1	2	192	U
1	2	199	G
1	2	200	A
1	2	202	A
1	2	203	A
1	2	204	G
1	2	205	U
1	2	206	U
1	2	207	G
1	2	208	A
1	2	209	C
1	2	210	C
1	2	219	G
1	2	222	A
1	2	227	A
1	2	231	G
1	2	234	U
1	2	238	U
1	2	239	G

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Mol	Chain	Res	Type
1	2	241	C
1	2	242	C
1	2	246	C
1	2	248	G
1	2	251	U
1	2	252	G
1	2	254	A
1	2	255	C
1	2	259	G
1	2	263	C
1	2	264	U
1	2	266	U
1	2	267	A
1	2	268	C
1	2	274	U
1	2	277	G
1	2	280	A
1	2	282	C
1	2	289	A
1	2	290	A
1	2	291	C
1	2	292	G
1	2	299	U
1	2	300	A
1	2	308	A
1	2	311	G
1	2	312	C
1	2	315	G
1	2	318	A
1	2	321	G
1	2	331	G
1	2	332	A
1	2	333	U
1	2	335	G
1	2	347	A
1	2	349	G
1	2	350	G
1	2	351	G
1	2	354	G
1	2	355	C
1	2	356	A
1	2	357	G

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Mol	Chain	Res	Type
1	2	359	A
1	2	366	A
1	2	370	U
1	2	375	C
1	2	379	C
1	2	395	G
1	2	398	A
1	2	400	U
1	2	408	U
1	2	413	U
1	2	414	G
1	2	427	A
1	2	428	C
1	2	431	U
1	2	433	G
1	2	436	A
1	2	438	G
1	2	455	G
1	2	461	A
1	2	466	U
1	2	467	A
1	2	468	G
1	2	471	G
1	2	473	G
1	2	479	G
1	2	480	U
1	2	481	C
1	2	485	U
1	2	487	C
1	2	489	A
1	2	490	G
1	2	494	C
1	2	497	C
1	2	501	A
1	2	502	A
1	2	503	U
1	2	504	U
1	2	508	G
1	2	510	U
1	2	516	A
1	2	517	G
1	2	533	U

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Mol	Chain	Res	Type
1	2	541	A
1	2	542	A
1	2	545	C
1	2	546	G
1	2	547	C
1	2	556	U
1	2	561	U
1	2	562	G
1	2	566	A
1	2	567	G
1	2	569	A
1	2	571	U
1	2	574	U
1	2	579	C
1	2	580	G
1	2	582	A
1	2	589	C
1	2	591	U
1	2	592	U
1	2	593	C
1	2	613	G
1	2	614	C
1	2	615	U
1	2	616	U
1	2	622	A
1	2	623	U
1	2	626	C
1	2	627	C
1	2	628	A
1	2	634	A
1	2	639	U
1	2	649	A
1	2	656	C
1	2	658	U
1	2	659	U
1	2	662	U
1	2	676	A
1	2	677	A
1	2	682	A
1	2	683	A
1	2	696	G
1	2	697	G

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Mol	Chain	Res	Type
1	2	703	A
1	2	706	U
1	2	718	A
1	2	725	G
1	2	732	U
1	2	733	U
1	2	734	G
1	2	735	A
1	2	736	C
1	2	737	U
1	2	748	A
1	2	751	C
1	2	752	U
1	2	753	G
1	2	755	G
1	2	762	G
1	2	763	C
1	2	779	U
1	2	780	U
1	2	786	G
1	2	790	A
1	2	794	G
1	2	811	C
1	2	812	A
1	2	824	G
1	2	825	A
1	2	831	G
1	2	834	G
1	2	841	C
1	2	845	A
1	2	846	A
1	2	848	C
1	2	852	G
1	2	859	G
1	2	860	G
1	2	872	U
1	2	874	U
1	2	875	U
1	2	881	C
1	2	885	A
1	2	889	U
1	2	890	U

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Mol	Chain	Res	Type
1	2	895	A
1	2	900	A
1	2	901	U
1	2	905	U
1	2	906	C
1	2	908	U
1	2	909	G
1	2	912	C
1	2	917	G
1	2	918	G
1	2	920	G
1	2	923	A
1	2	924	U
1	2	928	A
1	2	947	A
1	2	959	G
1	2	964	G
1	2	965	C
1	2	967	C
1	2	968	A
1	2	972	G
1	2	983	U
1	2	986	G
1	2	993	U
1	2	995	U
1	2	996	G
1	2	999	U
1	2	1002	A
1	2	1004	A
1	2	1007	G
1	2	1008	G
1	2	1010	A
1	2	1025	A
1	2	1026	G
1	2	1027	A
1	2	1028	U
1	2	1029	G
1	2	1036	A
1	2	1037	U
1	2	1038	G
1	2	1039	A
1	2	1050	U

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Mol	Chain	Res	Type
1	2	1052	G
1	2	1053	G
1	2	1054	G
1	2	1059	U
1	2	1062	G
1	2	1064	A
1	2	1065	U
1	2	1066	A
1	2	1081	G
1	2	1093	G
1	2	1095	G
1	2	1099	C
1	2	1109	C
1	2	1114	C
1	2	1122	G
1	2	1124	U
1	2	1125	U
1	2	1128	G
1	2	1131	A
1	2	1145	U
1	2	1150	A
1	2	1151	A
1	2	1153	U
1	2	1154	A
1	2	1155	U
1	2	1156	U
1	2	1157	U
1	2	1158	A
1	2	1159	C
1	2	1170	U
1	2	1171	C
1	2	1172	C
1	2	1180	A
1	2	1181	A
1	2	1182	A
1	2	1185	U
1	2	1186	C
1	2	1197	U
1	2	1223	G
1	2	1224	G
1	2	1234	A
1	2	1235	C

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Mol	Chain	Res	Type
1	2	1236	A
1	2	1237	G
1	2	1241	C
1	2	1242	G
1	2	1244	G
1	2	1245	A
1	2	1251	U
1	2	1253	U
1	2	1254	A
1	2	1255	G
1	2	1256	A
1	2	1267	U
1	2	1268	G
1	2	1269	C
1	2	1270	A
1	2	1273	C
1	2	1279	A
1	2	1281	A
1	2	1284	G
1	2	1296	A
1	2	1304	G
1	2	1314	G
1	2	1318	G
1	2	1321	C
1	2	1322	U
1	2	1324	C
1	2	1325	U
1	2	1326	C
1	2	1329	A
1	2	1330	U
1	2	1331	A
1	2	1338	A
1	2	1343	A
1	2	1344	G
1	2	1345	U
1	2	1354	A
1	2	1362	A
1	2	1364	U
1	2	1365	C
1	2	1366	A
1	2	1372	A
1	2	1374	G

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Mol	Chain	Res	Type
1	2	1375	A
1	2	1377	C
1	2	1378	C
1	2	1379	A
1	2	1380	G
1	2	1390	G
1	2	1394	A
1	2	1396	G
1	2	1398	G
1	2	1407	A
1	2	1413	G
1	2	1418	A
1	2	1420	A
1	2	1422	G
1	2	1437	A
1	2	1438	C
1	2	1441	A
1	2	1444	G
1	2	1445	C
1	2	1457	A
1	2	1463	U
1	2	1464	G
1	2	1476	G
1	2	1479	A
1	2	1483	C
1	2	1484	C
1	2	1487	A
1	2	1510	A
1	2	1516	C
1	2	1536	A
1	2	1537	G
1	2	1538	U
1	2	1546	A
1	2	1549	U
1	2	1551	A
1	2	1553	G
1	2	1560	G
1	2	1562	A
1	2	1563	C
1	2	1572	G
1	2	1573	G
1	2	1574	A

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Mol	Chain	Res	Type
1	2	1576	C

All (47) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	23	A
1	2	24	G
1	2	57	G
1	2	92	A
1	2	94	U
1	2	97	G
1	2	98	C
1	2	101	A
1	2	102	G
1	2	103	A
1	2	183	G
1	2	203	A
1	2	208	A
1	2	238	U
1	2	251	U
1	2	299	U
1	2	311	G
1	2	331	G
1	2	348	C
1	2	427	A
1	2	466	U
1	2	480	U
1	2	560	U
1	2	627	C
1	2	676	A
1	2	779	U
1	2	848	C
1	2	908	U
1	2	917	G
1	2	966	A
1	2	1026	G
1	2	1052	G
1	2	1059	U
1	2	1150	A
1	2	1153	U
1	2	1154	A
1	2	1235	C

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Mol	Chain	Res	Type
1	2	1244	G
1	2	1254	A
1	2	1325	U
1	2	1342	U
1	2	1364	U
1	2	1374	G
1	2	1378	C
1	2	1379	A
1	2	1406	A
1	2	1515	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

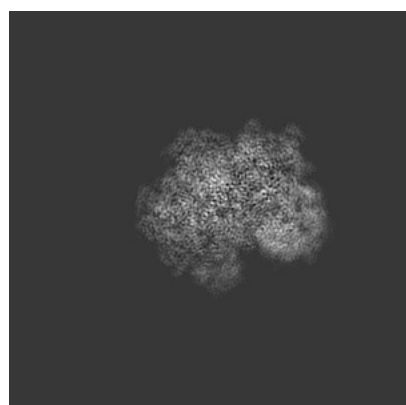
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6788. These allow visual inspection of the internal detail of the map and identification of artifacts.

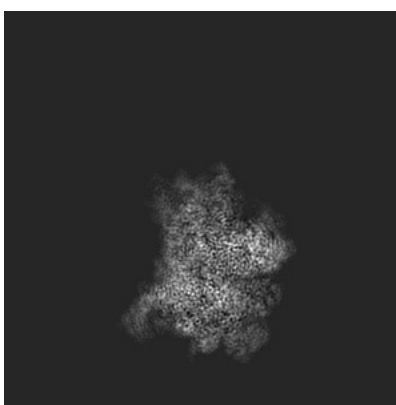
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

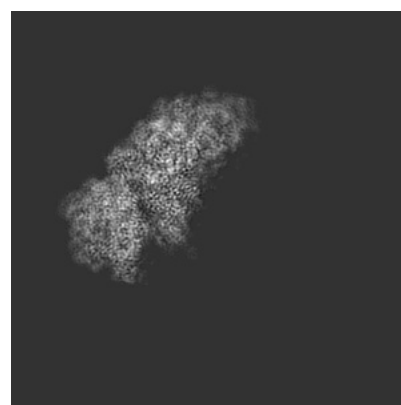
6.1.1 Primary map



X



Y

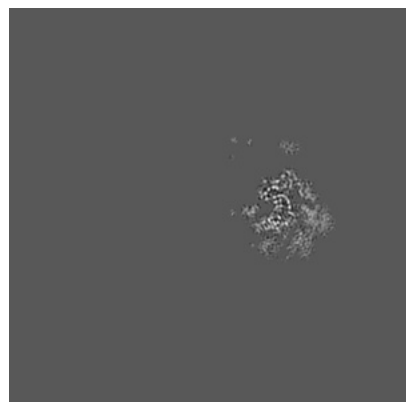


Z

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

6.2 Central slices [i](#)

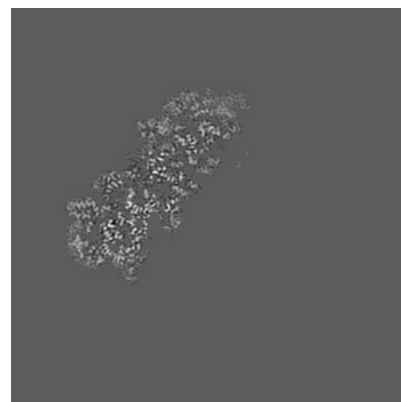
6.2.1 Primary map



X Index: 160



Y Index: 160

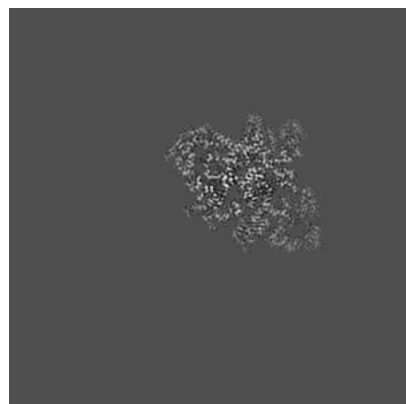


Z Index: 160

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: 128



Y Index: 167

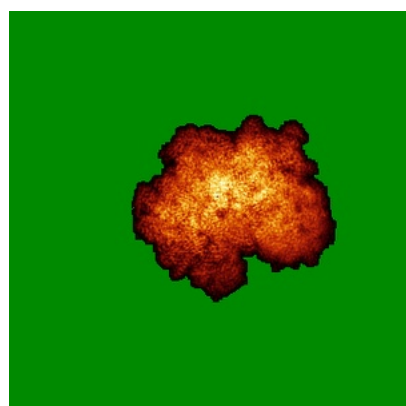


Z Index: 173

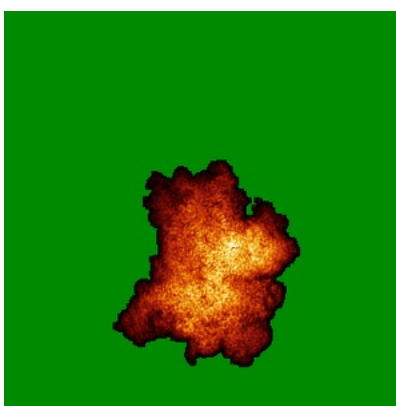
The images above show the largest variance slices of the map in three orthogonal directions.

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

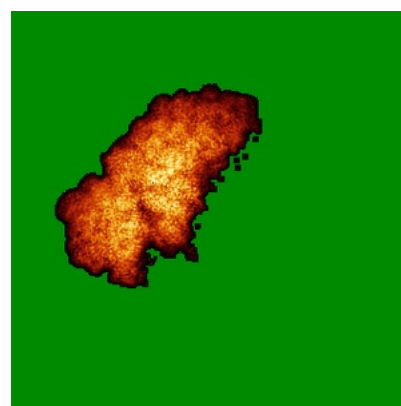
6.4.1 Primary map



X



Y

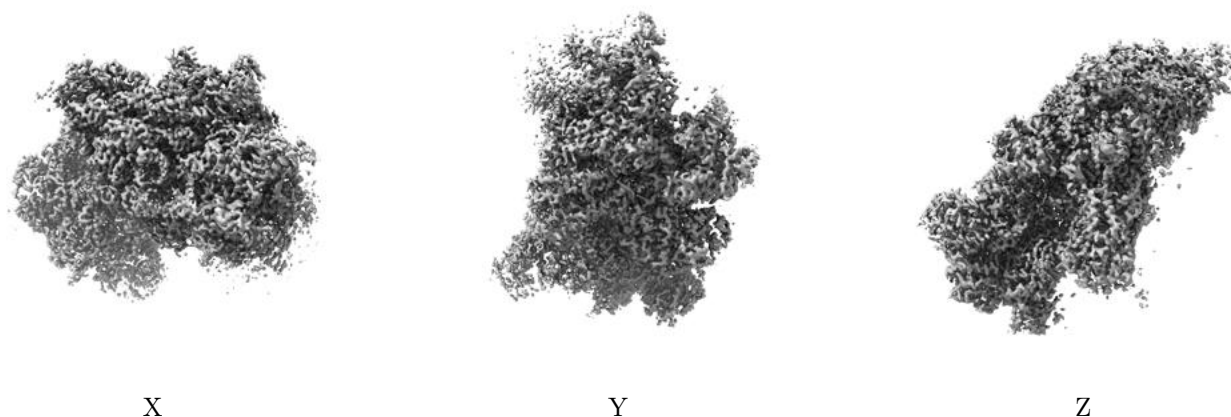


Z

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 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

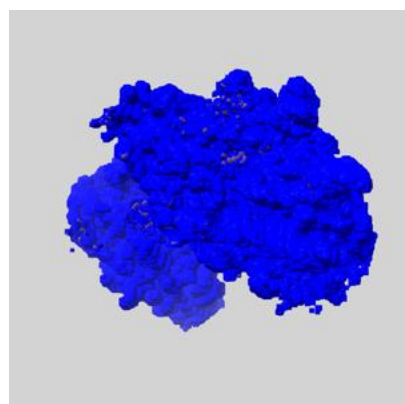
6.6 Mask visualisation [i](#)

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

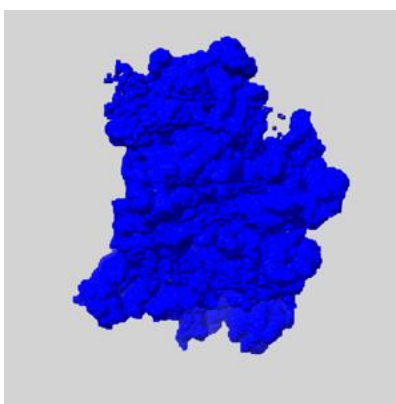
A mask typically either:

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

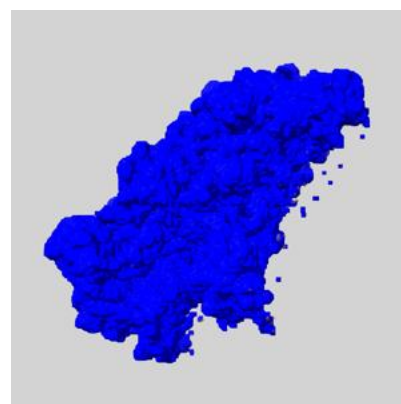
6.6.1 emd_6788_msk_1.map [i](#)



X



Y

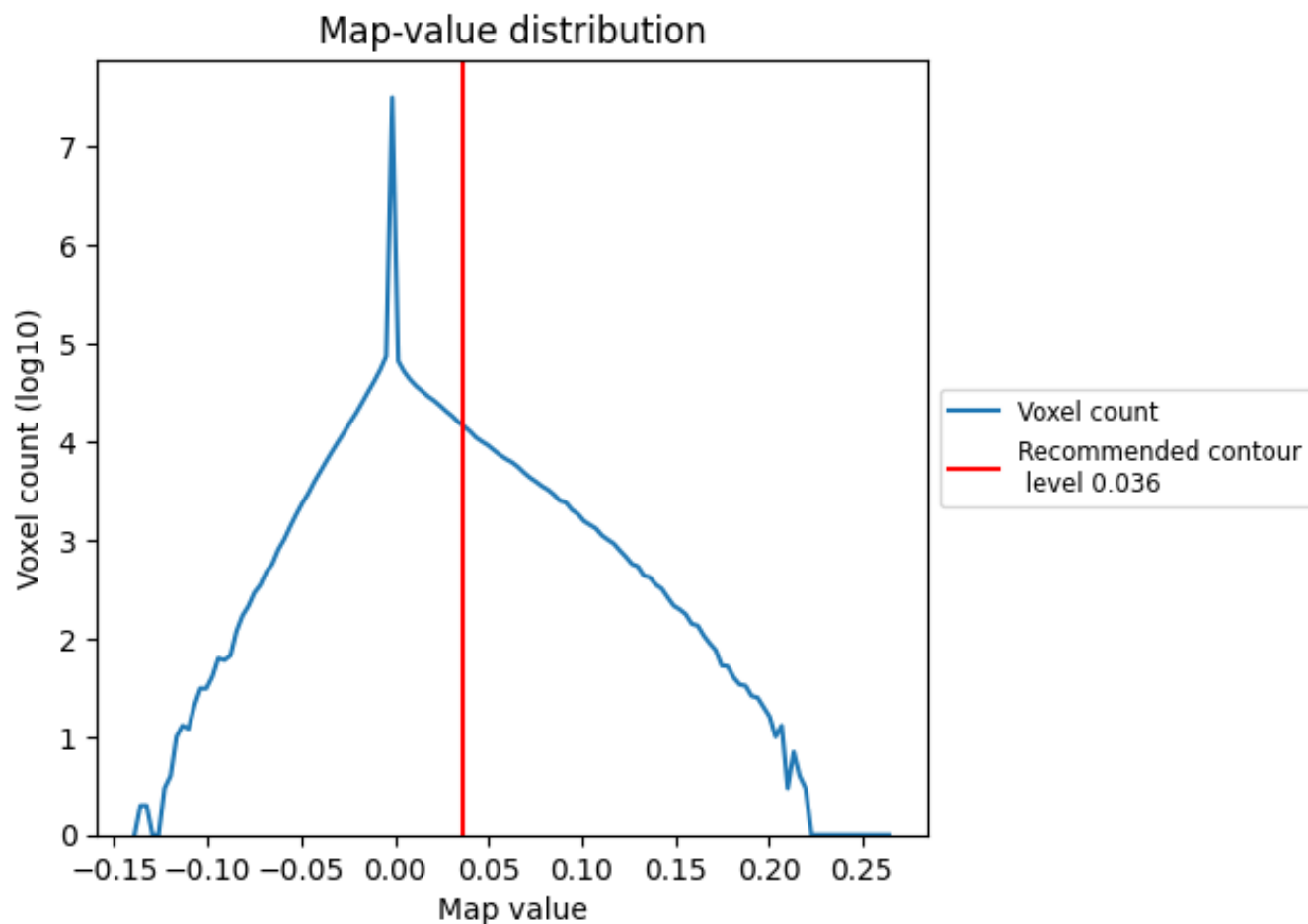


Z

7 Map analysis [i](#)

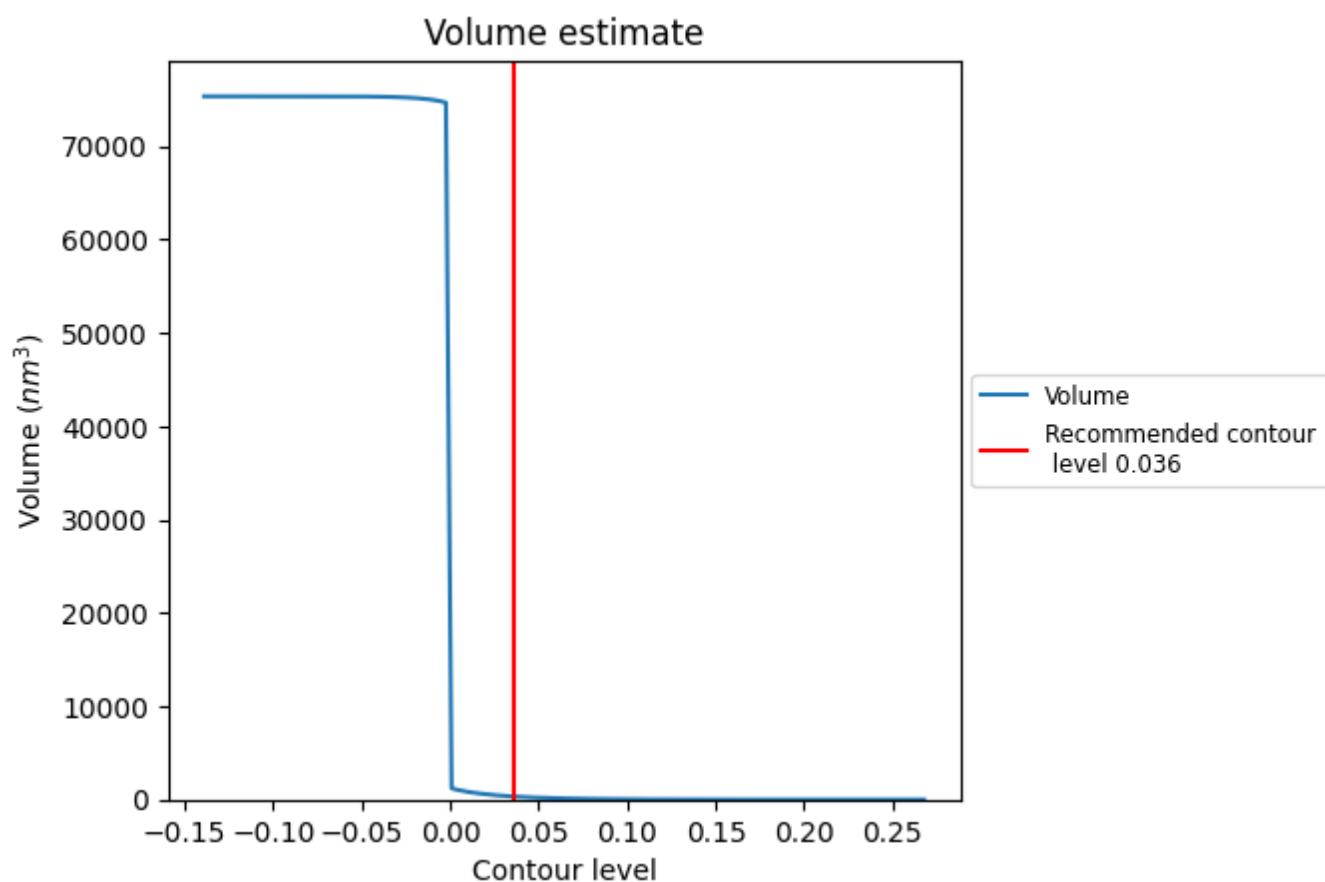
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

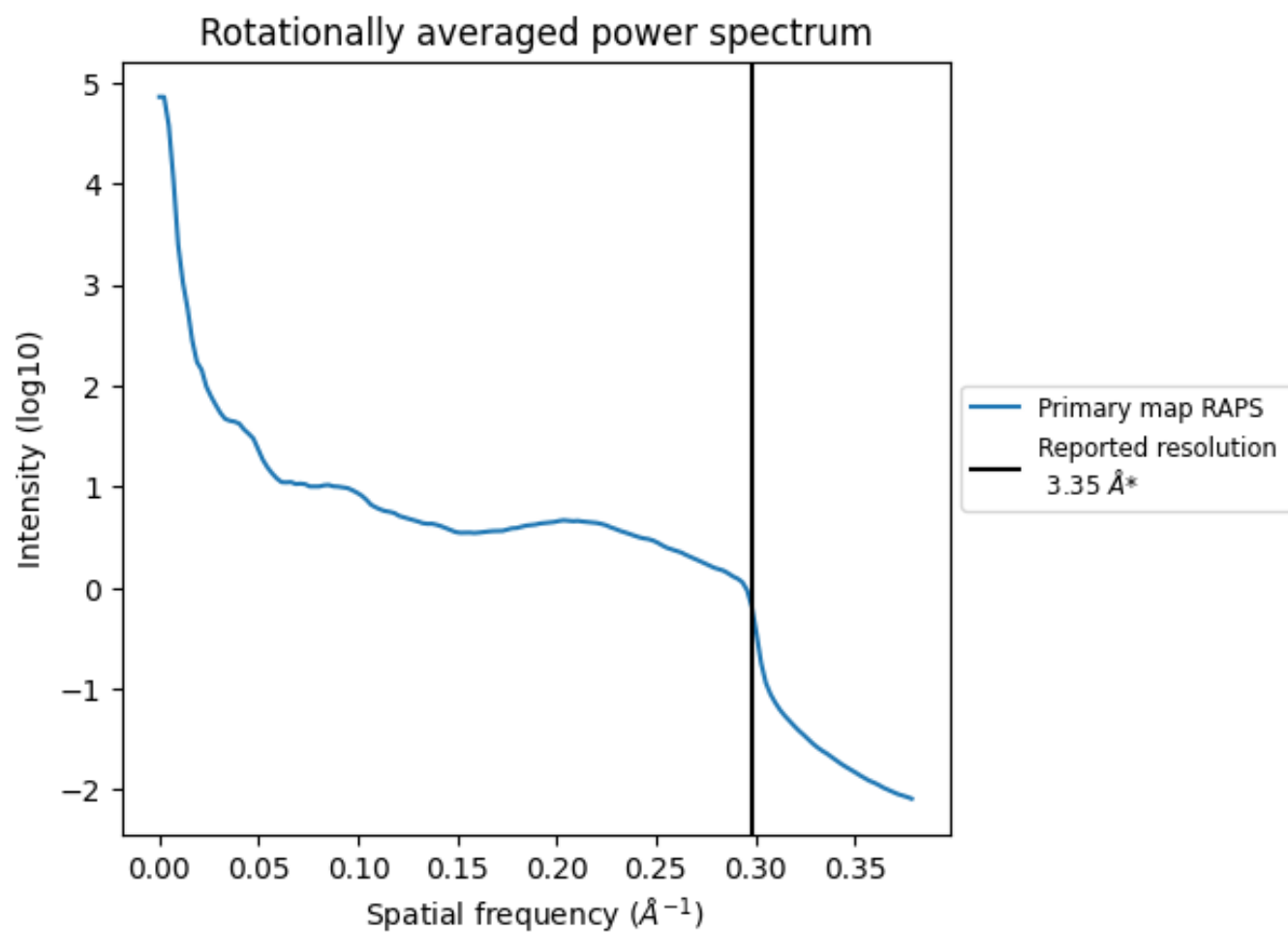
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 325 nm^3 ; this corresponds to an approximate mass of 294 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 ⓘ

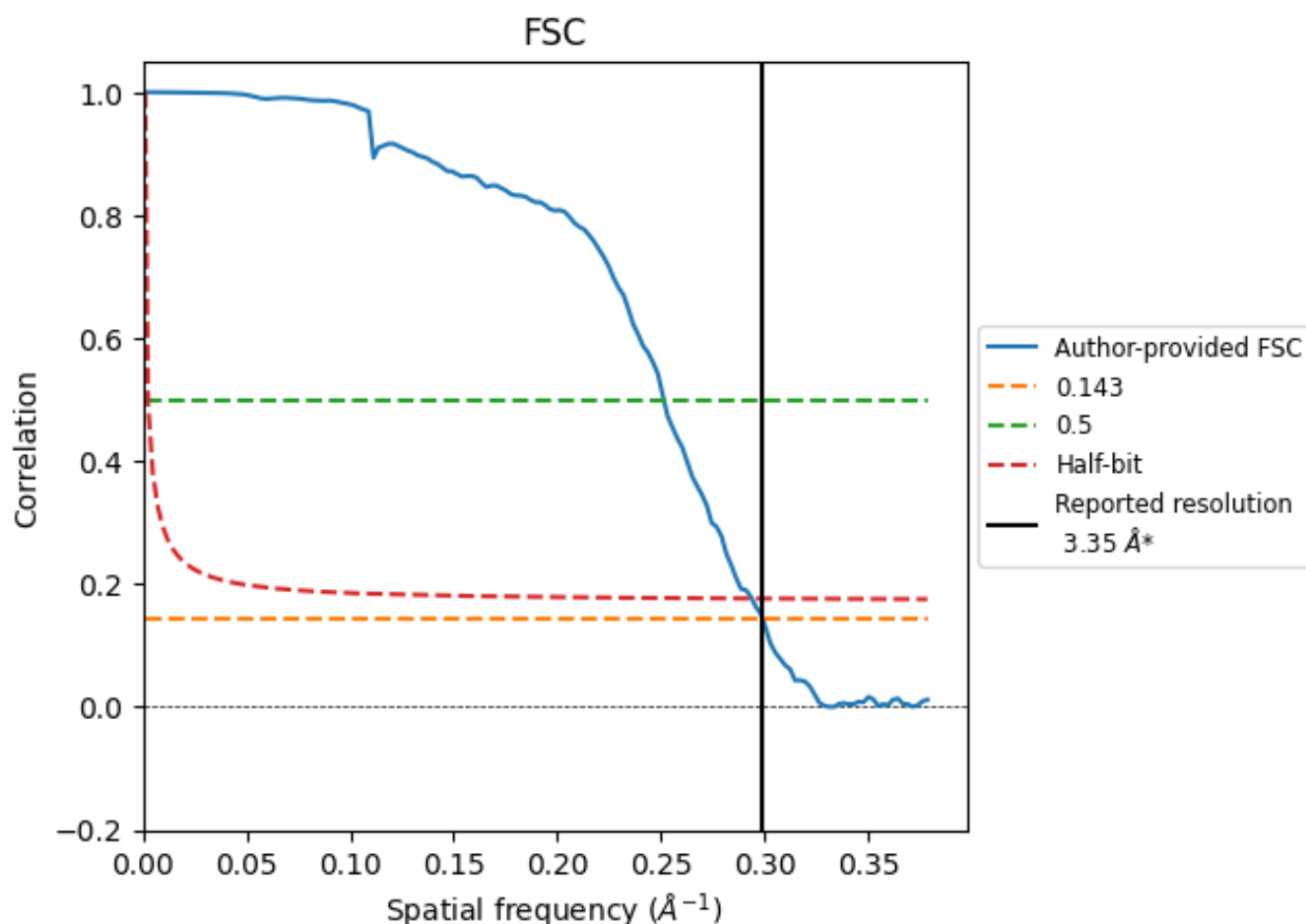


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.299 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

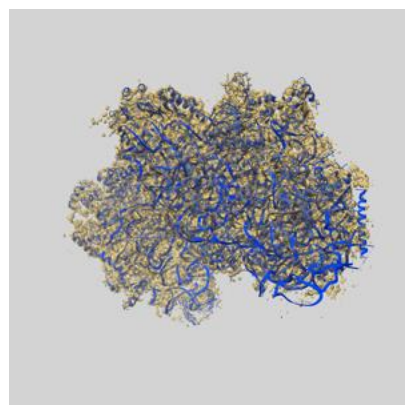
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.34	3.98	3.40
Unmasked-calculated*	-	-	-

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

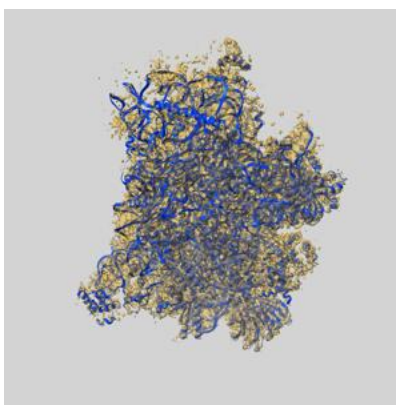
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6788 and PDB model 5XYI. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

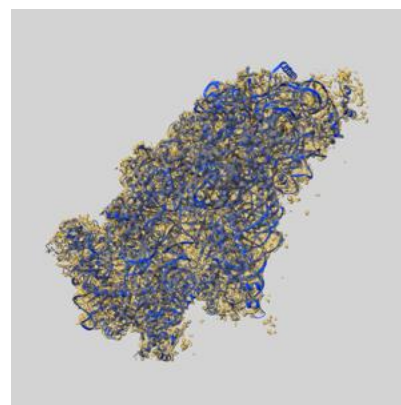
9.1 Map-model overlay [i](#)



X



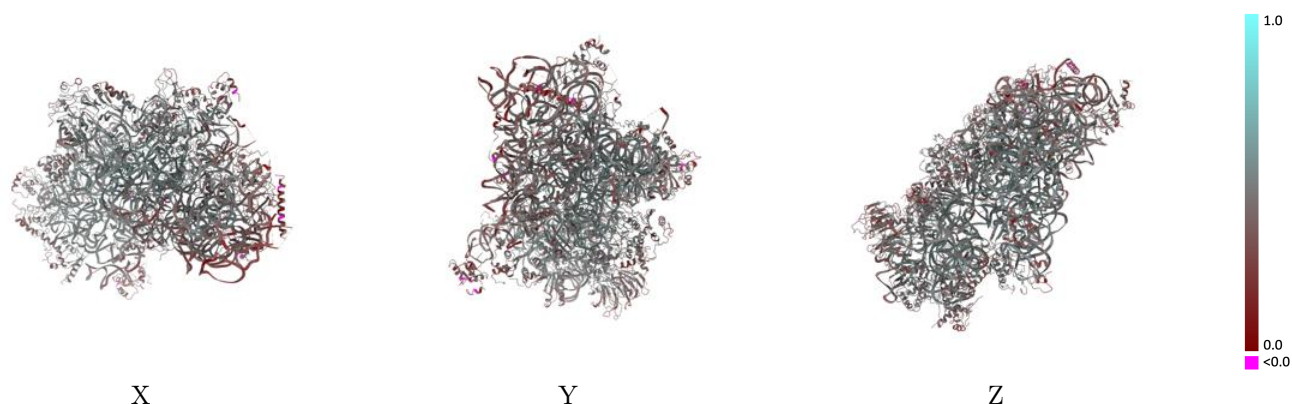
Y



Z

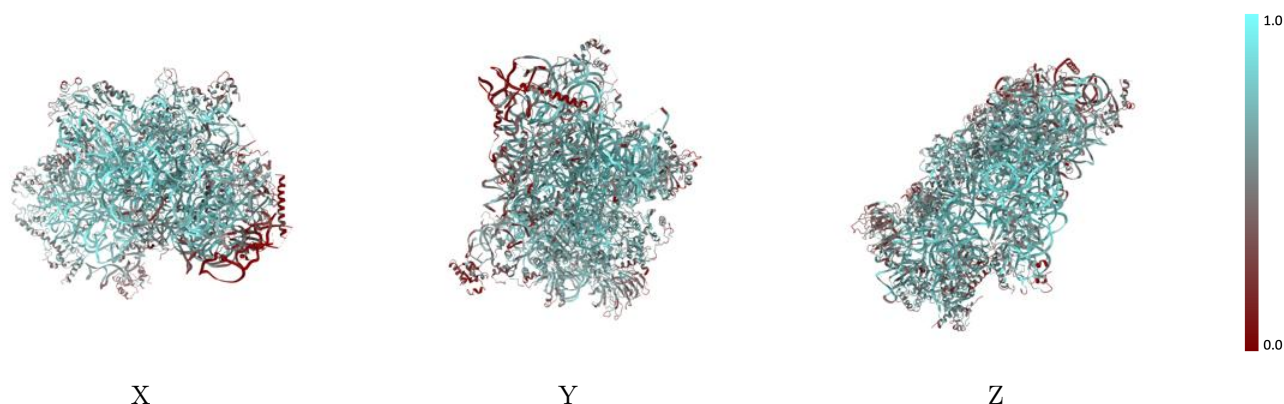
The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



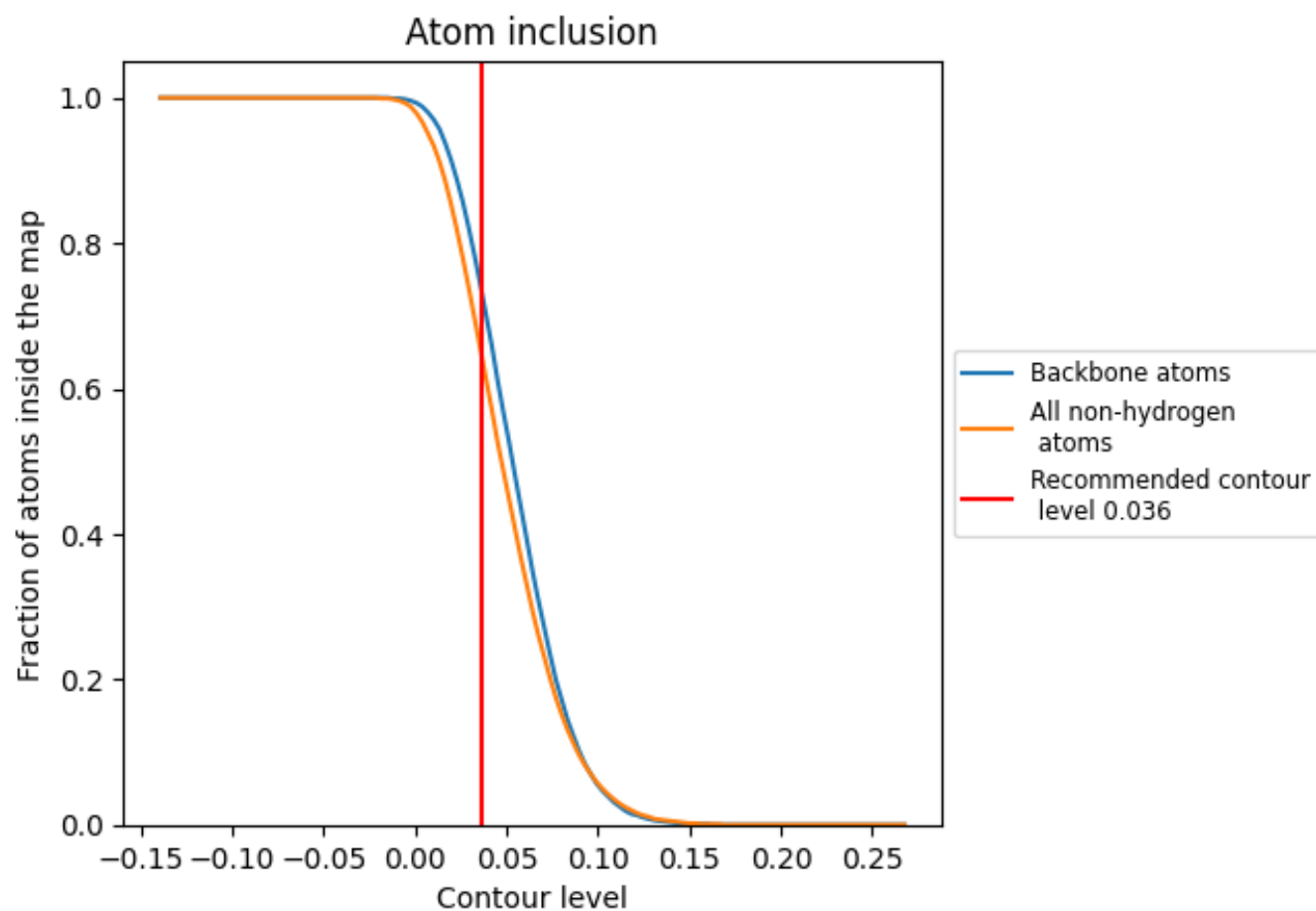
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.036).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 65% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6530	 0.4480
2	 0.7470	 0.4670
A	 0.6390	 0.4370
B	 0.5600	 0.4280
C	 0.7060	 0.4920
D	 0.5580	 0.4360
E	 0.4870	 0.4080
F	 0.5390	 0.4280
G	 0.0970	 0.2080
H	 0.5350	 0.4150
I	 0.5290	 0.4220
J	 0.5000	 0.4110
K	 0.5310	 0.4070
L	 0.5810	 0.4420
M	 0.2060	 0.2850
N	 0.6140	 0.4490
O	 0.6340	 0.4640
P	 0.5560	 0.4240
Q	 0.6600	 0.4790
R	 0.5680	 0.3970
S	 0.6140	 0.4540
T	 0.6450	 0.4630
U	 0.6080	 0.4500
V	 0.6440	 0.4520
W	 0.7240	 0.4880
X	 0.5390	 0.4380
Y	 0.3530	 0.3540
Z	 0.5210	 0.3970
a	 0.7020	 0.4960
b	 0.5590	 0.4200
c	 0.4400	 0.4370
d	 0.6860	 0.4860
e	 0.4290	 0.3820
g	 0.4660	 0.3860
n	 0.5740	 0.4270

