



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 02:41 AM UTC

PDB ID : 6V92 / pdb_00006v92
EMDB ID : EMD-21114
Title : RSC-NCP
Authors : Patel, A.B.; Moore, C.M.; Greber, B.J.; Nogales, E.
Deposited on : 2019-12-13
Resolution : 20.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

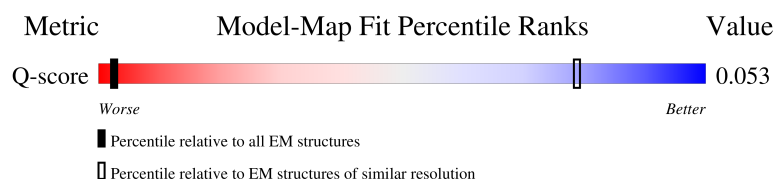
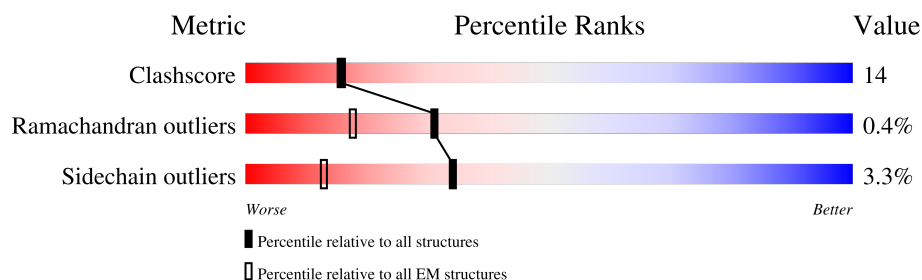
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	28 (19.50 - 20.50)

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

Mol	Chain	Length	Quality of chain
1	A	477	23% 52% 27% 16%
2	R	1359	18% 6% 76%
3	B	467	20% 61% 22% 15%
4	P	157	11% 19% 14% 66%

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Mol	Chain	Length	Quality of chain
5	C	78	
6	D	180	
7	E	435	
8	F	889	
9	G	885	
10	H	625	
11	I	557	
11	J	557	
11	K	557	
11	L	557	
12	M	483	
13	N	581	
14	O	502	
15	Q	426	
16	S	883	
17	2	28	
18	3	19	
18	4	19	
19	5	14	
20	6	15	
21	7	49	
22	i	146	
22	j	146	
23	a	136	
23	e	136	

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Mol	Chain	Length	Quality of chain
24	b	103	
24	f	103	
25	c	130	
25	g	130	
26	d	126	
26	h	126	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 44583 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Actin-related protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	399	Total	C	N	O	S	3	0
			3227	2081	528	603	15		

- Molecule 2 is a protein called Nuclear protein STH1/NPS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	325	Total	C	N	O	S	0	0
			2663	1668	487	504	4		

- Molecule 3 is a protein called Actin-like protein ARP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	396	Total	C	N	O	S	1	0
			3198	2053	523	615	7		

- Molecule 4 is a protein called Regulator of Ty1 transposition protein 102.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	54	Total	C	N	O	S	0	0
			490	313	84	92	1		

- Molecule 5 is a protein called High temperature lethal protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	60	Total	C	N	O	S	0	0
			493	301	92	96	4		

- Molecule 6 is a protein called Chromatin structure-remodeling complex protein RSC14.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	100	Total	C	N	O	S	0	0
			772	490	132	148	2		

- Molecule 7 is a protein called Chromatin structure-remodeling complex subunit RSC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	120	Total	C	N	O	S	0	0
			978	610	166	200	2		

- Molecule 8 is a protein called Chromatin structure-remodeling complex subunit RSC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	67	Total	C	N	O	S	0	0
			536	346	94	95	1		

- Molecule 9 is a protein called Chromatin structure-remodeling complex protein RSC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	53	Total	C	N	O	S	0	0
			422	270	71	79	2		

- Molecule 10 is a protein called Chromatin structure-remodeling complex subunit RSC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	131	Total	C	N	O	S	0	0
			1083	696	175	205	7		

- Molecule 11 is a protein called Chromatin structure-remodeling complex protein RSC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	293	Total	C	N	O	S	0	0
			2416	1537	423	448	8		
11	J	115	Total	C	N	O	S	0	0
			924	579	149	190	6		
11	K	109	Total	C	N	O	S	0	0
			878	554	139	179	6		
11	L	298	Total	C	N	O	S	0	0
			2445	1557	428	452	8		

- Molecule 12 is a protein called Chromatin structure-remodeling complex protein RSC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	310	Total	C	N	O	S	0	0
			2474	1558	414	496	6		

- Molecule 13 is a protein called Chromatin structure-remodeling complex subunit RSC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	412	Total	C	N	O	S	0	0
			3275	2105	540	612	18		

- Molecule 14 is a protein called Chromatin structure-remodeling complex protein RSC58.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	384	Total	C	N	O	S	0	0
			3145	2025	529	581	10		

- Molecule 15 is a protein called Chromatin structure-remodeling complex subunit SFH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	264	Total	C	N	O	S	0	0
			2137	1349	362	418	8		

- Molecule 16 is a protein called Chromatin structure-remodeling complex protein RSC30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	34	Total	C	N	O	S	0	0
			278	182	41	54	1		

- Molecule 17 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	2	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 18 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	3	19	Total	C	N	O	0	0
			95	57	19	19		
18	4	19	Total	C	N	O	0	0
			95	57	19	19		

- Molecule 19 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	5	14	Total	C	N	O	0	0
			70	42	14	14		

- Molecule 20 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	6	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 21 is a protein called Unknown Protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	7	49	Total	C	N	O	0	0
			245	147	49	49		

- Molecule 22 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	i	146	Total	C	N	O	P	0	0
			2990	1431	540	874	145		
22	j	146	Total	C	N	O	P	0	0
			2990	1431	540	874	145		

- Molecule 23 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	97	Total	C	N	O	S	0	0
			801	505	155	137	4		
23	e	99	Total	C	N	O	S	0	0
			816	514	158	140	4		

- Molecule 24 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	78	Total	C	N	O	S	0	0
			619	391	120	107	1		
24	f	85	Total	C	N	O	S	0	0
			683	430	136	116	1		

- Molecule 25 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	c	108	Total	C	N	O	0	0
			835	526	165	144		
25	g	104	Total	C	N	O	0	0
			805	508	157	140		

- Molecule 26 is a protein called Histone H2B type 1-K.

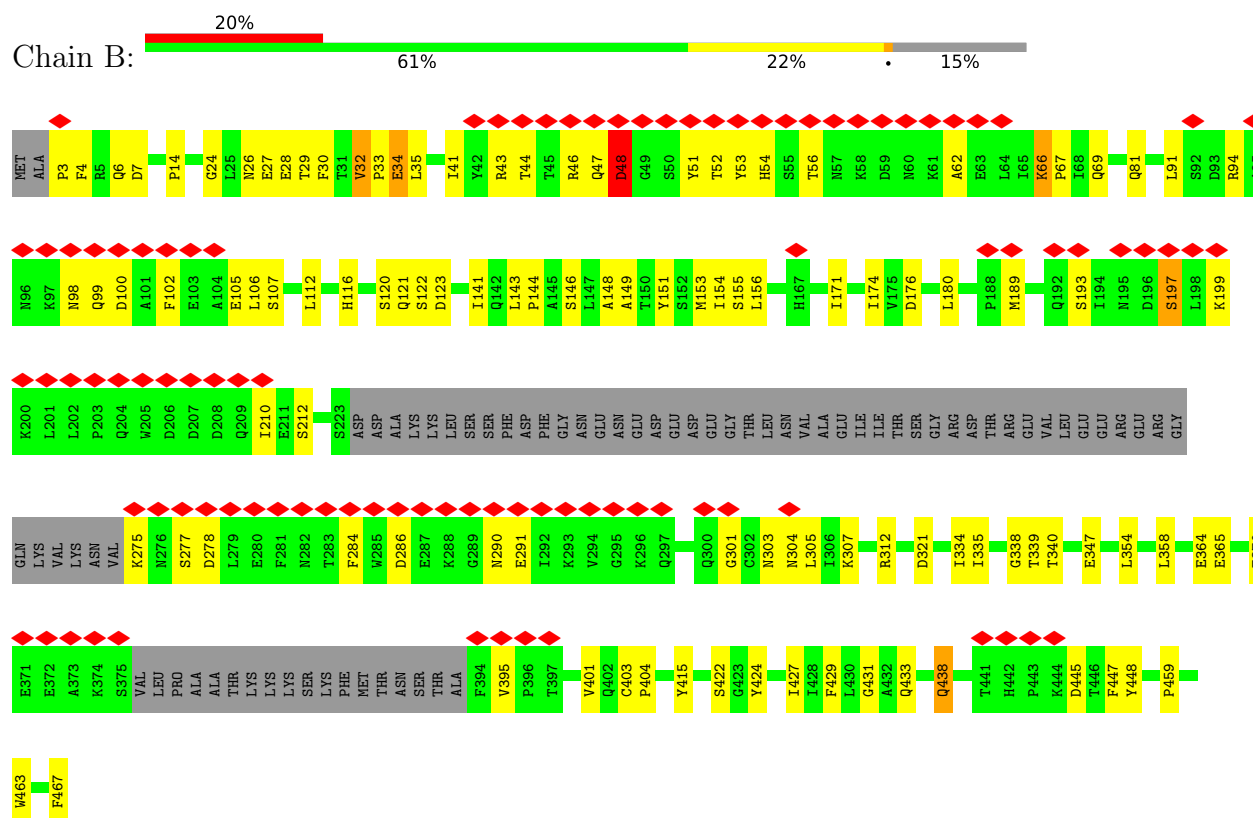
Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	96	Total	C	N	O	S	0	0
			754	473	138	141	2		
26	h	94	Total	C	N	O	S	0	0
			735	461	134	138	2		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

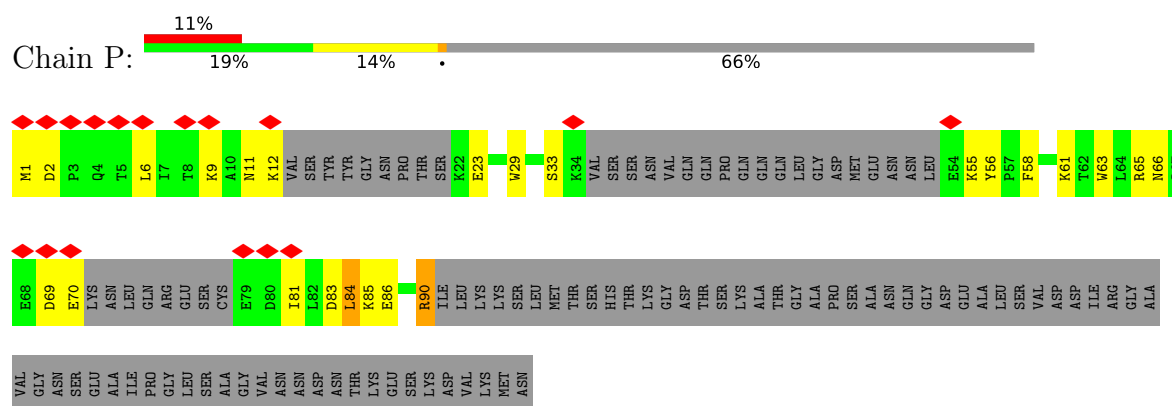
Mol	Chain	Residues	Atoms		AltConf
27	I	1	Total	Zn	0
			1	1	



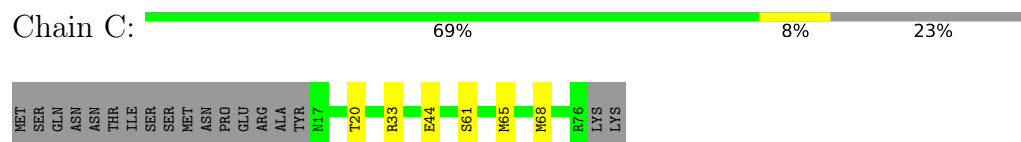
- Molecule 3: Actin-like protein ARP9



- Molecule 4: Regulator of Ty1 transposition protein 102

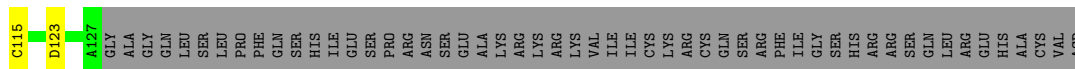


- Molecule 5: High temperature lethal protein 1

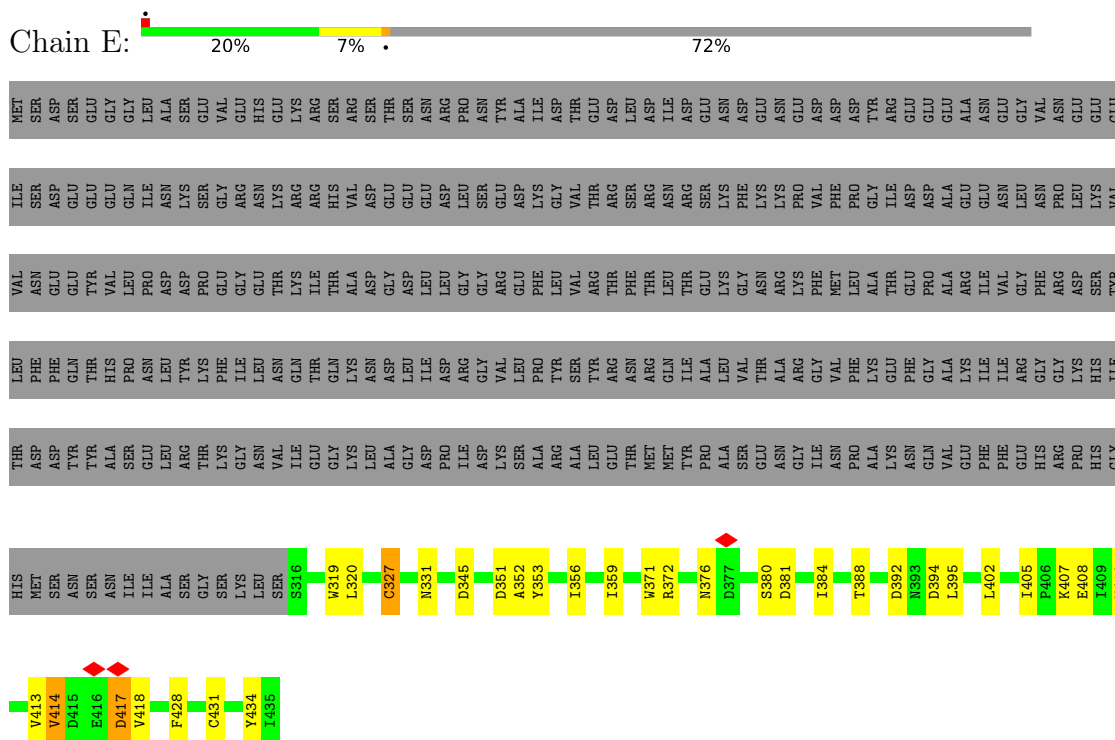


- Molecule 6: Chromatin structure-remodeling complex protein RSC14

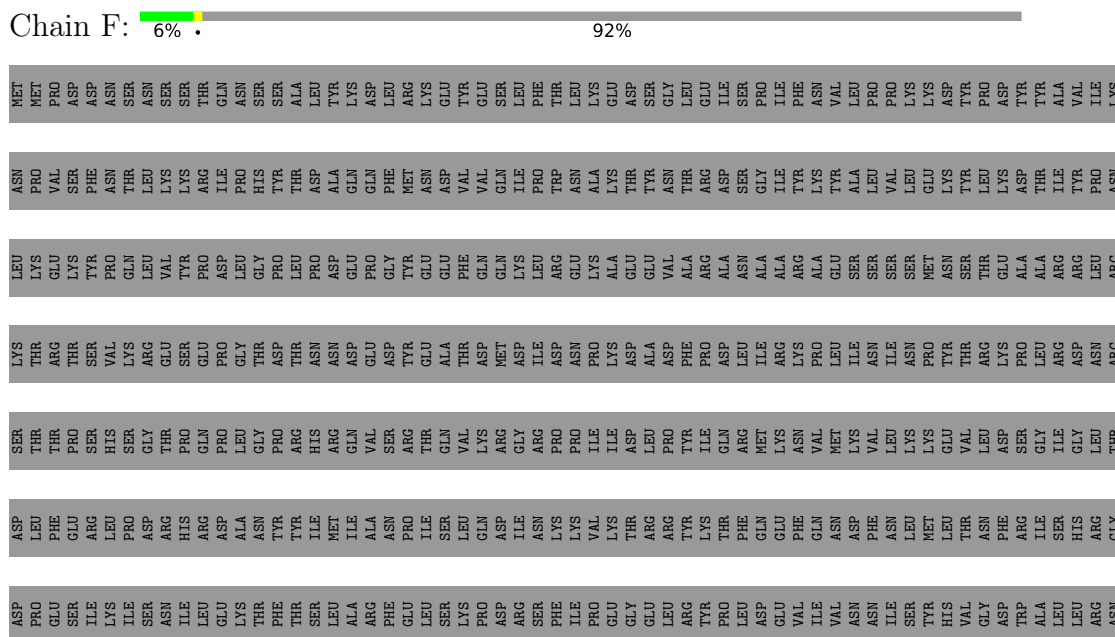




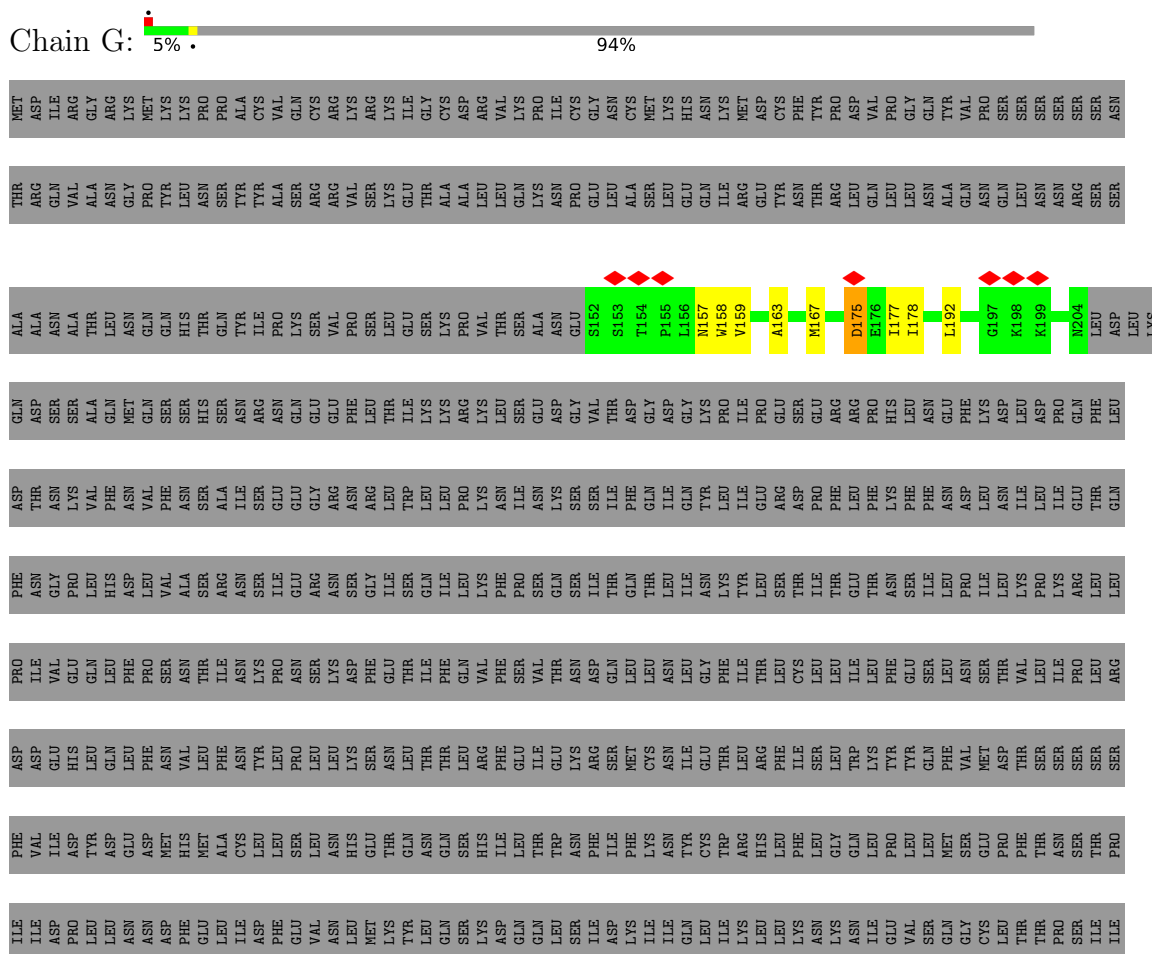
- Molecule 7: Chromatin structure-remodeling complex subunit RSC7



- Molecule 8: Chromatin structure-remodeling complex subunit RSC2

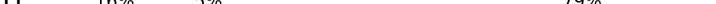


- Molecule 9: Chromatin structure-remodeling complex protein RSC3



PHE	ILE	LYS	ALA	ASN
GLY	ASN	ASN	GLY	ASN
LEU	ASN	VAL	HIS	ILE
THR	PHE	ILE	GLU	MET
GLU	LYS	HIS	PHE	ASP
ASN	SER	LEU	THR	SER
ASN	GLY	ILE	PHE	LEU
PHE	ILE	ILE	ILE	ILE
ASN	SER	ASN	ASN	TYR
GLU	ALA	LYS	LYS	ARG
VAL	GLU	ILE	SER	ASN
PHE	GLN	ALA	ILE	SER
GLU	LEU	MET	VAL	MET
ALA	ILE	LEU	VAL	LEU
ILE	LYS	LEU	LEU	TYR
ARG	LEU	SER	GLN	LEU
SER	ASN	ASP	THR	ASN
	HIS	TYR	LEU	PHE
	GLU	THR	VAL	TYR
	LEU	LYS	LEU	LEU
	SER	ASN	MET	LEU
	LYS	CYS	LEU	LEU
	ILE	LYS	LEU	GLN
	SER	LYS	ALA	PHE
	GLU	GLN	LEU	GLU
	SER	ASN	TYR	THR
	LEU	LYS	GLN	LEU
	ILE	LEU	ARG	LYS
	LYS	ILE	SER	ASN
	THR	GLU	PHE	TYR
	ASP	ASN	ASP	ALA
	PHE	LEU	SER	LYS
	TYR	ILE	SER	PHE
	GLU	ILE	LYS	ASN
	GLN	LYS	ARG	GLU
	ARG	ILE	THR	ILE
	LYS	LYS	ASN	LEU
	ASN	THR	ASP	GLU
	SER	ILE	ALA	GLU
	VAL	LYS	ASN	PHE
	THR	LYS	GLU	LEU
	SER	TYR	ILE	GLU
	ASN	ILE	SER	LEU
	GLY	LYS	GLU	LEU
	VAL	ASN	GLN	ARG
	LEU	LEU	THR	GLU
	GLY	GLU	ASP	THR
	ALA	GLU	ILE	LEU
	ALA	ASN	HIS	PHE
	ALA	LYS	SER	PHE
	PRO	VAL	ASN	ASN
	VAL	THR	ASN	PHE
	ASP	THR	ASP	SER
	SER	SER	ASN	ASN
	ASP	ALA	SER	LEU
	ALA	ASP	LYS	ALA
	ASN	SER	ARG	ASN
	SER	ASN	ILE	ILE
	ASP	TYR	LYS	PHE
	THR	SER	ASN	THR

- Molecule 10: Chromatin structure-remodeling complex subunit RSC4

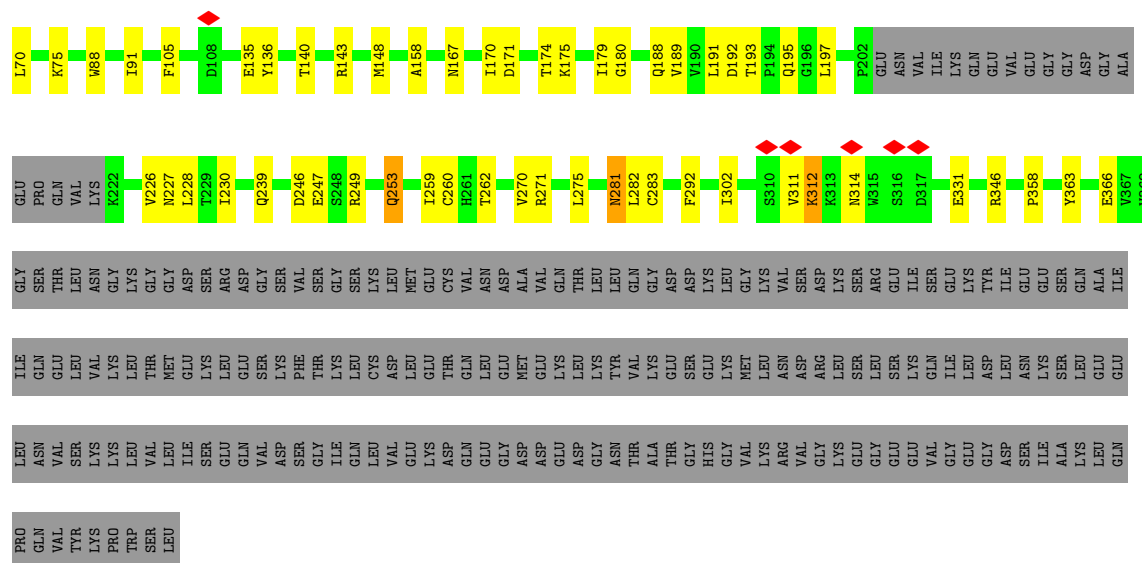
Chain H:  16% 5% 79%

[illegible]

- Molecule 11: Chromatin structure-remodeling complex protein RSC8

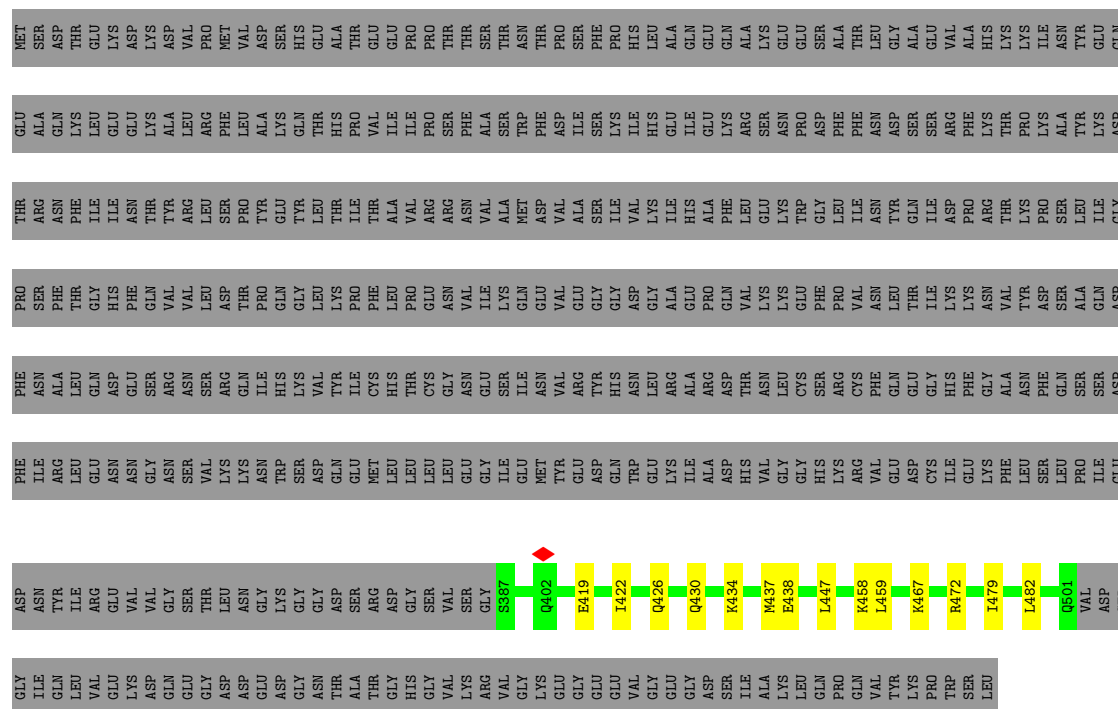
Chain I: 43% 9% 47%

MET	ASP	ASP	THR	GLU	LYS	ASP	LYS	ASP	VAL	PRO	MET	VAL	ASP	SER	HIS	ALA	THR	GLU	GLU	PRO	PRO	THR	THR	SER	THR	THR	THR	PRO	SER	PHE	PRO	PRO	HIS	LEU	ALA	ALA	GLN	GLU	GLN	ALA	ALA	LYS	GLU	GLU	GLU	GLY	ALA	VAL	VAL	ALA	ALA	HIS	THR	LYS	LYS	ILE	N57	ES9
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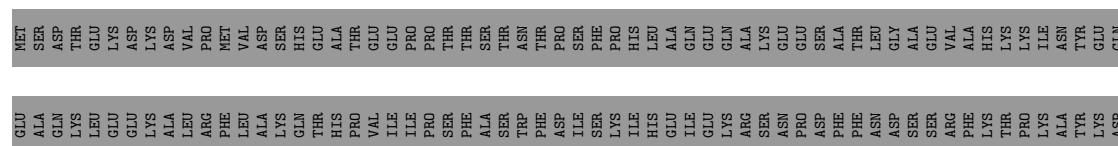
● Molecule 11: Chromatin structure-remodeling complex protein RSC8

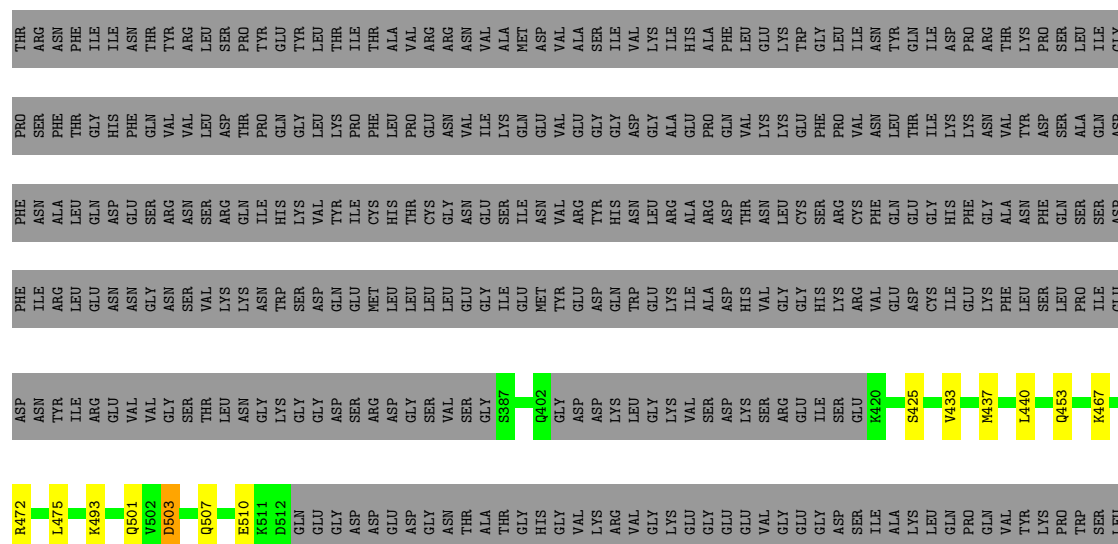
Chain J: 18% 79%



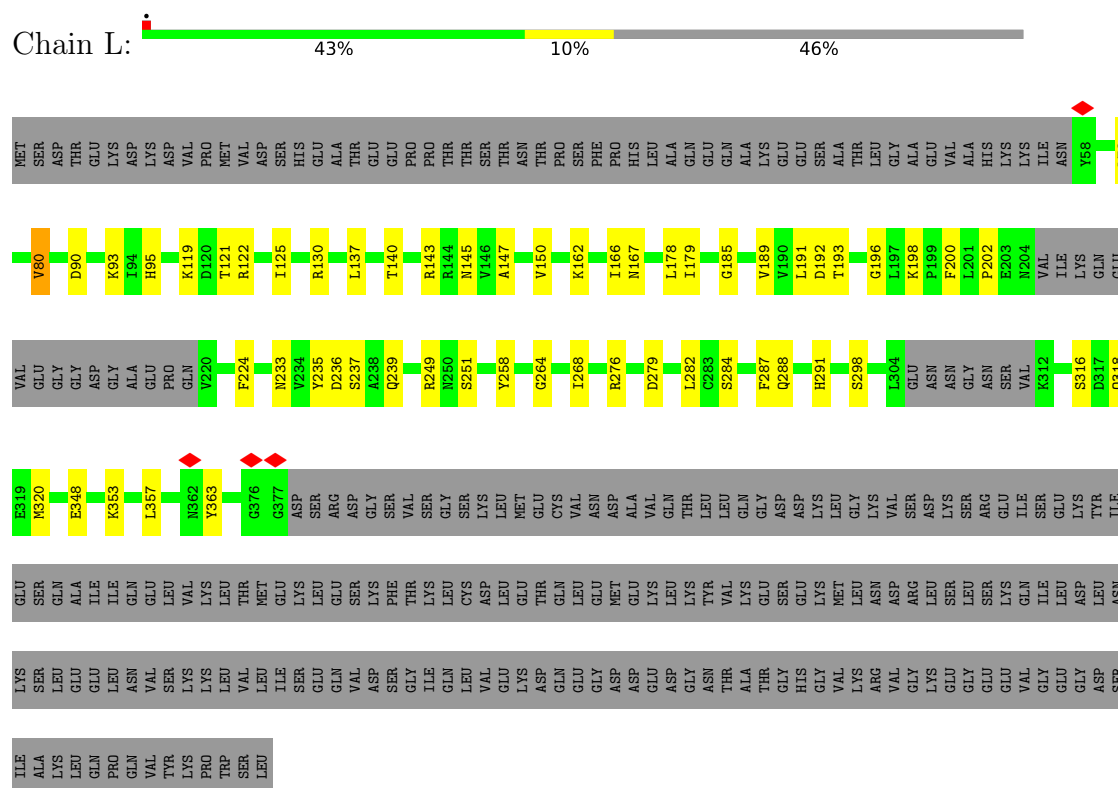
● Molecule 11: Chromatin structure-remodeling complex protein RSC8

Chain K: 17% 80%

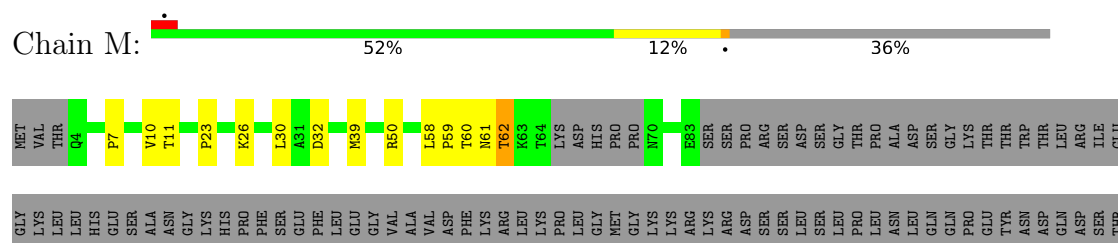


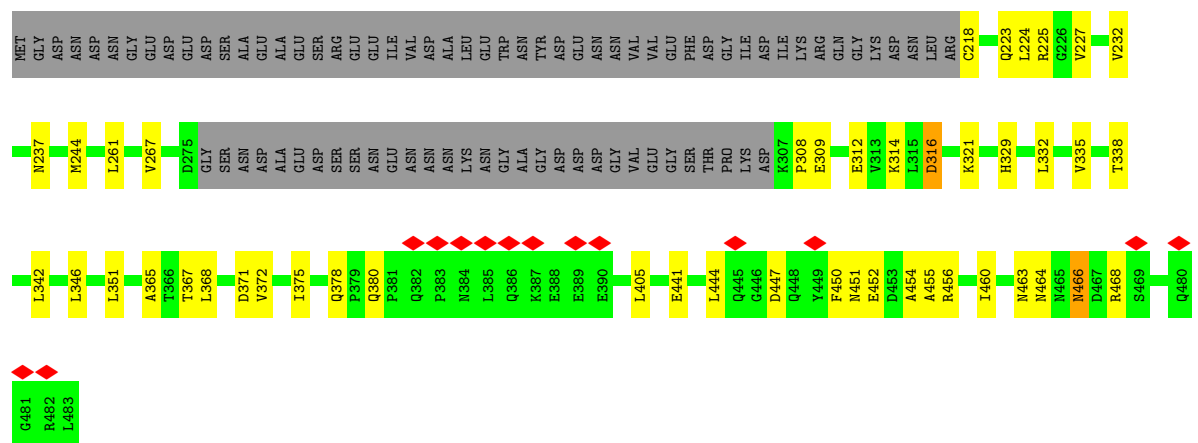


• Molecule 11: Chromatin structure-remodeling complex protein RSC8

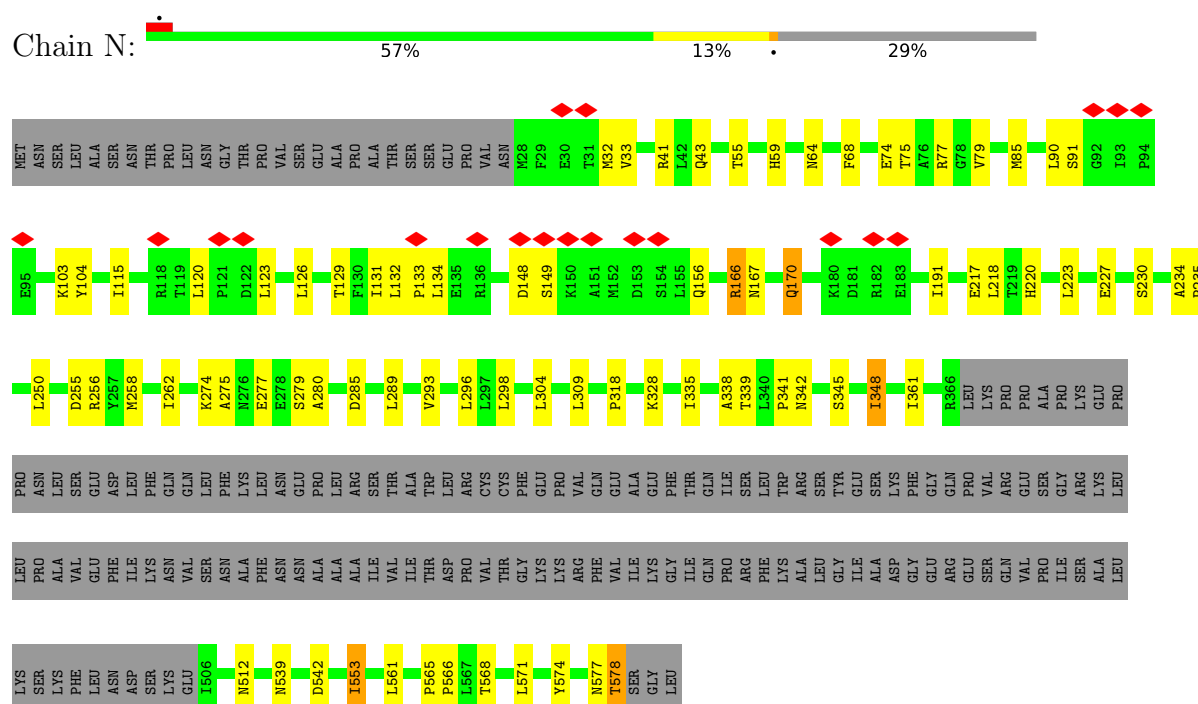


• Molecule 12: Chromatin structure-remodeling complex protein RSC6

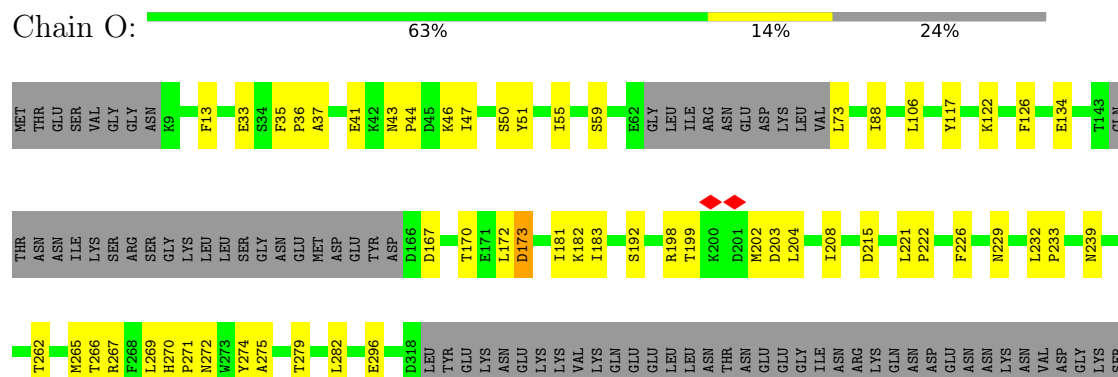


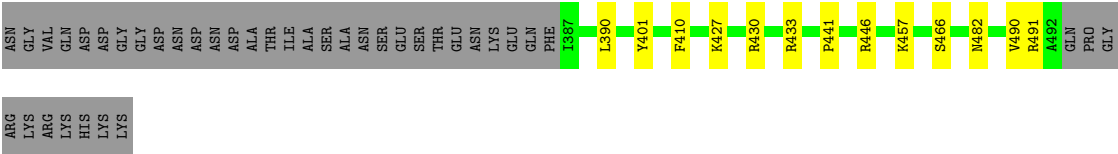


• Molecule 13: Chromatin structure-remodeling complex subunit RSC9

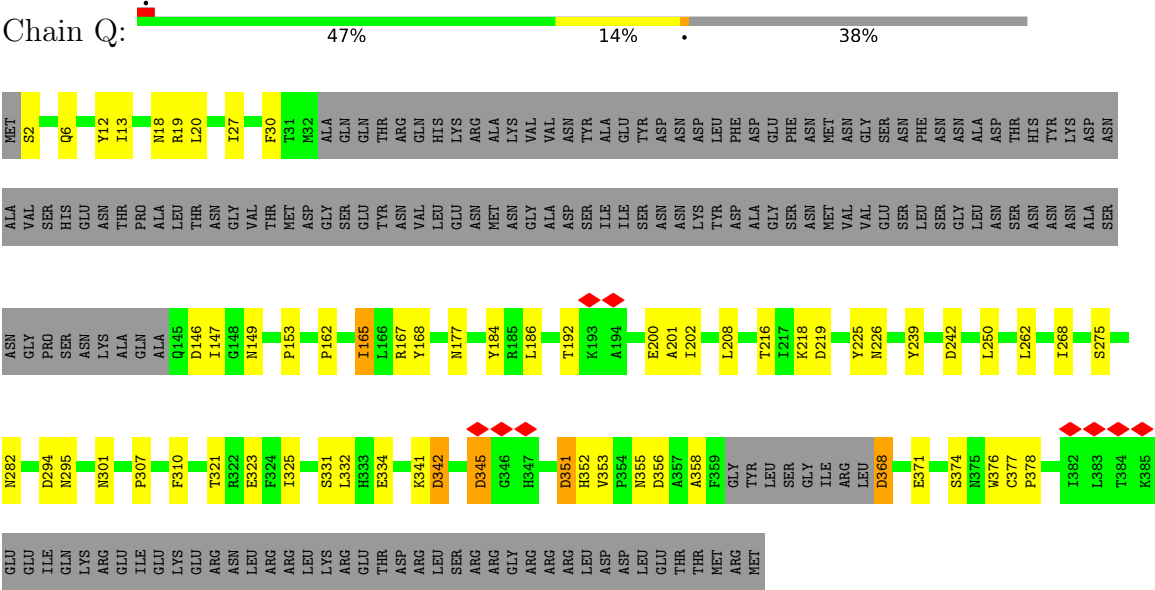


• Molecule 14: Chromatin structure-remodeling complex protein RSC58

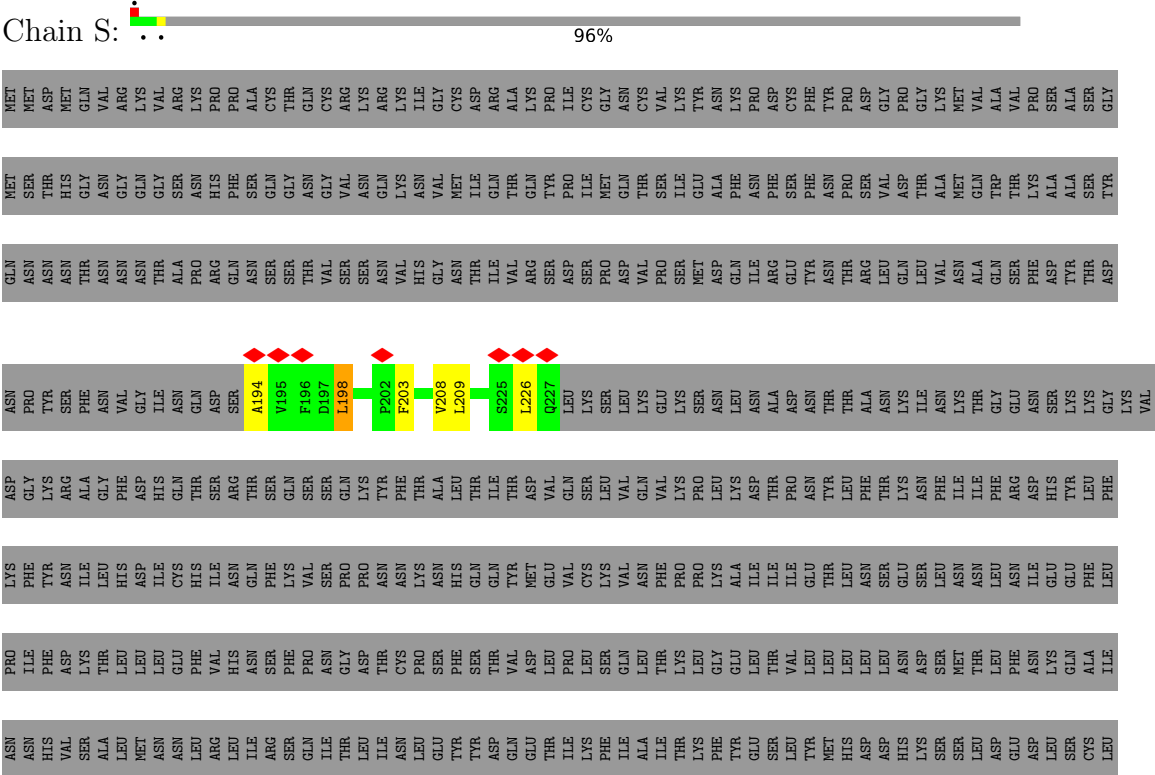




• Molecule 15: Chromatin structure-remodeling complex subunit SFH1



• Molecule 16: Chromatin structure-remodeling complex protein RSC30



[illegible]

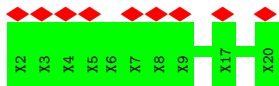
- Molecule 17: Unknown Protein

Chain 2: 93% 7%

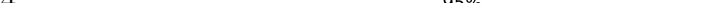


- Molecule 18: Unknown Protein

Chain 3:  47% 100%

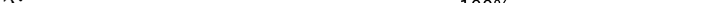


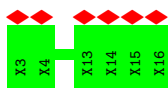
- Molecule 18: Unknown Protein

Chain 4:  95% 5%



- Molecule 19: Unknown Protein

Chain 5:  43% 100%

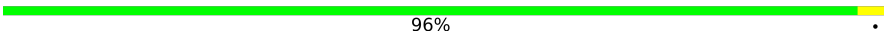


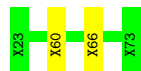
- Molecule 20: Unknown Protein

Chain 6: 100%

There are no outlier residues recorded for this chain.

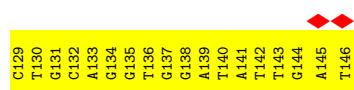
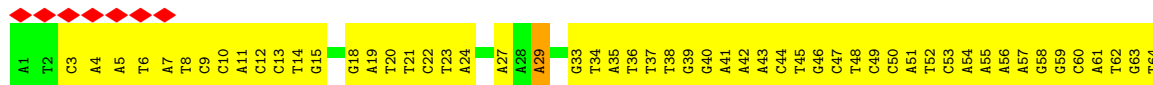
- Molecule 21: Unknown Protein

Chain 7:  96%



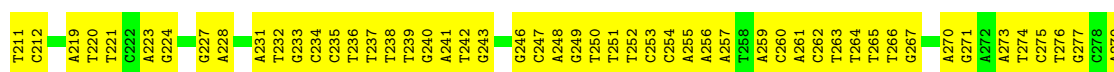
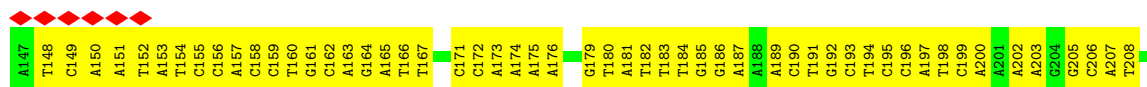
- Molecule 22: DNA (146-MER)

Chain i:  6% 16% 84%



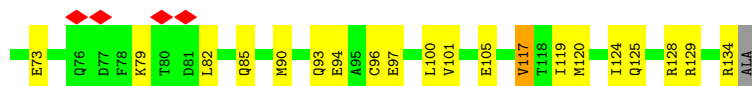
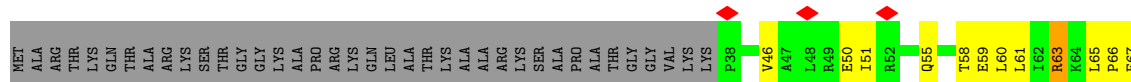
- Molecule 22: DNA (146-MER)

Chain j:  10% 20% 80%



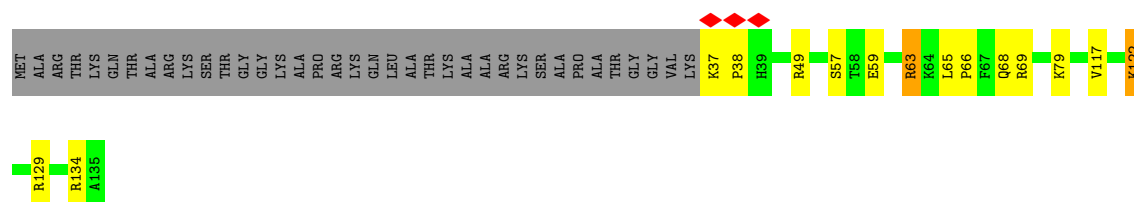
- Molecule 23: Histone H3.1

Chain a:  5% 48% 22% 29%



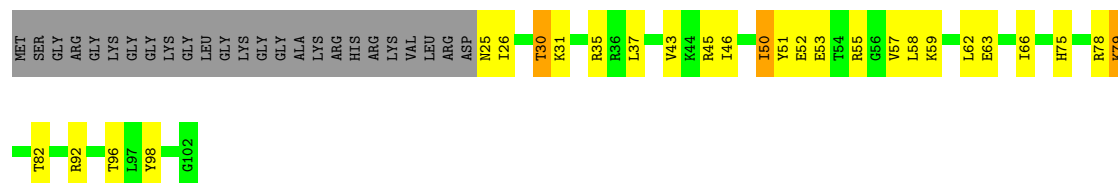
- Molecule 23: Histone H3.1

Chain e:  62% 10% 27%



- Molecule 24: Histone H4

Chain b: 50% 23% • 24%



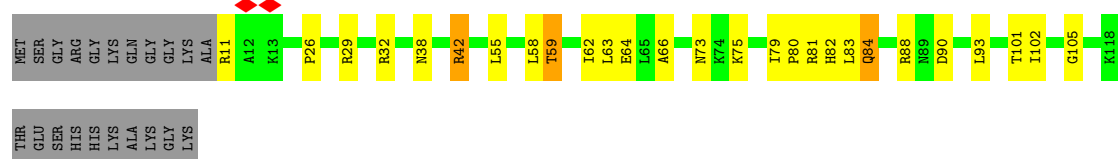
- Molecule 24: Histone H4

Chain f: 66% 14% • 17%



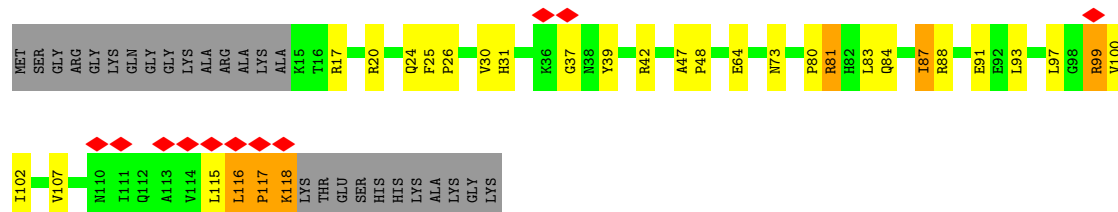
- Molecule 25: Histone H2A type 1-B/E

Chain c: 62% 18% • 17%



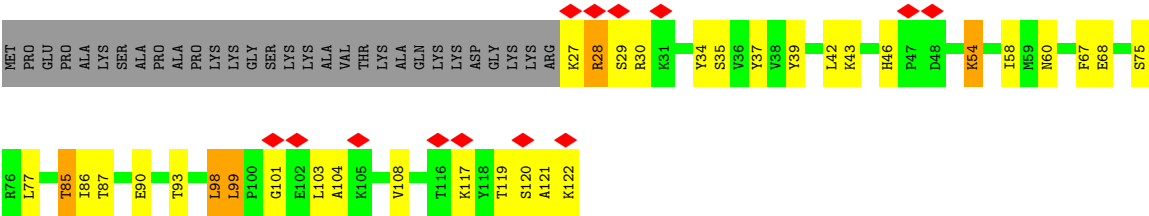
- Molecule 25: Histone H2A type 1-B/E

Chain g: 8% 55% 19% 5% 20%

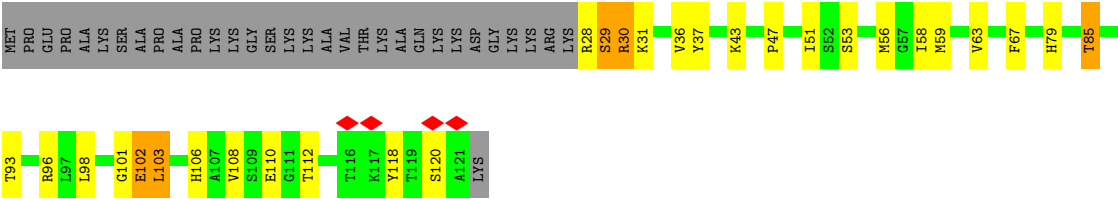


- Molecule 26: Histone H2B type 1-K

Chain d: 10% 49% 23% • 24%



• Molecule 26: Histone H2B type 1-K



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13337	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	437.76, 437.76, 437.76	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	3.42, 3.42, 3.42	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	A	0.56	1/3303 (0.0%)	0.90	6/4465 (0.1%)
2	R	0.44	2/2697 (0.1%)	0.67	7/3616 (0.2%)
3	B	0.58	0/3269	0.88	2/4432 (0.0%)
4	P	0.46	0/501	0.82	0/669
5	C	0.17	0/495	0.27	0/662
6	D	0.14	0/786	0.25	0/1062
7	E	0.17	0/997	0.31	0/1356
8	F	0.18	0/551	0.27	0/748
9	G	0.14	0/431	0.24	0/584
10	H	0.18	0/1108	0.35	0/1497
11	I	0.22	0/2474	0.31	0/3343
11	J	0.21	0/926	0.31	0/1233
11	K	0.17	0/879	0.25	0/1172
11	L	0.18	0/2502	0.29	0/3376
12	M	0.18	0/2515	0.29	0/3423
13	N	0.21	0/3334	0.34	0/4515
14	O	0.19	0/3216	0.32	0/4358
15	Q	0.18	0/2181	0.36	0/2964
16	S	0.10	0/281	0.17	0/378
22	i	0.30	0/3354	0.76	1/5175 (0.0%)
22	j	0.30	0/3354	0.76	0/5175
23	a	0.47	0/813	0.89	1/1090 (0.1%)
23	e	0.55	0/828	0.86	1/1109 (0.1%)
24	b	0.49	0/626	0.99	4/837 (0.5%)
24	f	0.58	0/691	0.94	2/923 (0.2%)
25	c	0.51	0/845	0.91	1/1139 (0.1%)
25	g	0.48	0/815	0.99	8/1100 (0.7%)
26	d	0.51	0/765	0.94	2/1025 (0.2%)
26	h	0.51	0/746	0.87	0/1003
All	All	0.36	3/45283 (0.0%)	0.63	35/62429 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	328	LYS	C-O	9.02	1.34	1.24
2	R	333	ILE	C-O	8.93	1.34	1.24
1	A	380	SER	C-N	5.22	1.40	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	333	ILE	N-CA-C	10.80	121.63	110.62
2	R	328	LYS	N-CA-C	9.98	122.16	111.28
2	R	333	ILE	CA-C-O	9.85	131.19	120.95
2	R	328	LYS	CA-C-O	9.68	130.81	120.55
24	b	50	ILE	N-CA-C	7.14	117.90	110.62
1	A	431	ASP	N-CA-C	6.99	121.43	112.34
25	g	24	GLN	N-CA-C	-6.93	104.82	113.55
25	g	87	ILE	N-CA-C	6.45	116.61	110.42
24	b	46	ILE	N-CA-C	6.31	117.20	108.12
23	a	117	VAL	N-CA-C	-6.26	107.19	113.20
26	d	99	LEU	N-CA-C	6.17	117.85	110.07
26	d	35	SER	N-CA-C	5.87	121.06	111.37
1	A	380	SER	CA-C-N	-5.64	113.10	118.97
1	A	380	SER	C-N-CA	-5.64	113.10	118.97
23	e	117	VAL	N-CA-C	-5.57	107.85	113.47
24	b	79	LYS	N-CA-C	-5.53	106.53	113.72
24	f	46	ILE	N-CA-C	5.49	115.90	107.77
2	R	333	ILE	O-C-N	-5.45	116.58	121.87
1	A	176	LYS	N-CA-C	5.42	117.19	111.28
25	g	73	ASN	N-CA-C	-5.37	106.11	113.30
1	A	215	LYS	N-CA-C	-5.29	106.76	113.43
25	g	116	LEU	CA-C-N	5.19	126.33	119.84
25	g	116	LEU	C-N-CA	5.19	126.33	119.84
25	c	42	ARG	N-CA-C	5.14	117.20	109.23
1	A	404	MET	N-CA-C	5.14	116.57	111.07
2	R	328	LYS	O-C-N	-5.11	116.70	122.12
2	R	334	ASP	N-CA-C	-5.11	105.79	111.36
24	b	30	THR	N-CA-C	5.11	116.69	110.41
22	i	29	DA	C5'-C4'-C3'	-5.09	107.26	114.90
25	g	25	PHE	CA-C-N	5.09	126.20	119.84
25	g	25	PHE	C-N-CA	5.09	126.20	119.84
24	f	28	GLY	N-CA-C	-5.08	108.02	114.16
3	B	66	LYS	CA-C-N	5.06	124.37	118.85
3	B	66	LYS	C-N-CA	5.06	124.37	118.85
25	g	91	GLU	N-CA-C	5.05	116.87	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3227	0	3251	154	0
2	R	2663	0	2746	164	0
3	B	3198	0	3187	138	0
4	P	490	0	467	19	0
5	C	493	0	507	5	0
6	D	772	0	754	11	0
7	E	978	0	935	27	0
8	F	536	0	533	13	0
9	G	422	0	423	9	0
10	H	1083	0	1062	22	0
11	I	2416	0	2358	40	0
11	J	924	0	976	12	0
11	K	878	0	930	12	0
11	L	2445	0	2402	49	0
12	M	2474	0	2465	48	0
13	N	3275	0	3373	50	0
14	O	3145	0	3168	53	0
15	Q	2137	0	2069	44	0
16	S	278	0	287	6	0
17	2	140	0	34	2	0
18	3	95	0	21	0	0
18	4	95	0	21	1	0
19	5	70	0	16	0	0
20	6	75	0	17	0	0
21	7	245	0	63	2	0
22	i	2990	0	1652	217	0
22	j	2990	0	1652	184	0
23	a	801	0	839	39	0
23	e	816	0	856	19	0
24	b	619	0	659	34	0
24	f	683	0	729	22	0
25	c	835	0	897	26	0
25	g	805	0	861	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	d	754	0	782	39	0
26	h	735	0	756	38	0
27	I	1	0	0	0	0
All	All	44583	0	41748	1250	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 (1250) 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)
2:R:353:PHE:CZ	3:B:447:PHE:CE2	2.05	1.45
2:R:353:PHE:CZ	3:B:447:PHE:HE2	1.34	1.41
2:R:353:PHE:CE1	3:B:447:PHE:HE2	1.47	1.33
2:R:365:GLU:HG2	3:B:415:TYR:CD2	1.65	1.32
2:R:353:PHE:CE2	3:B:447:PHE:CE2	2.21	1.29
2:R:349:ARG:O	2:R:353:PHE:CD2	1.84	1.28
1:A:76:LEU:CD2	1:A:108:MET:HE1	1.63	1.27
2:R:365:GLU:HG2	3:B:415:TYR:CE2	1.70	1.25
1:A:76:LEU:CD2	1:A:108:MET:CE	2.15	1.24
2:R:320:LYS:O	2:R:324:LEU:HG	1.34	1.20
2:R:364:MET:HE2	3:B:30:PHE:HE1	1.02	1.19
2:R:353:PHE:CE2	3:B:447:PHE:CZ	2.31	1.19
2:R:365:GLU:OE2	3:B:415:TYR:CE2	1.96	1.18
2:R:353:PHE:CE1	3:B:447:PHE:CE2	2.30	1.17
2:R:351:PHE:CE1	3:B:176:ASP:HB3	1.81	1.16
22:j:194:DT:H2''	22:j:195:DC:H5''	1.20	1.15
2:R:365:GLU:CG	3:B:415:TYR:CE2	2.28	1.14
3:B:189:MET:HE2	3:B:305:LEU:CA	1.80	1.11
1:A:343:SER:CB	1:A:344:ILE:HA	1.81	1.11
22:i:139:DA:H2''	22:i:140:DT:H5'	1.26	1.09
2:R:347:GLN:O	2:R:351:PHE:HD2	1.36	1.09
1:A:76:LEU:HD22	1:A:108:MET:HE1	1.11	1.08
3:B:189:MET:HE2	3:B:305:LEU:HA	1.21	1.08
22:i:51:DA:H2''	22:i:52:DT:H5''	1.29	1.08
1:A:150:GLY:HA2	2:R:336:ILE:HD11	1.31	1.08
22:j:155:DC:H2''	22:j:156:DC:H5'	1.35	1.07
1:A:343:SER:HB3	1:A:344:ILE:HA	1.09	1.07
22:j:157:DA:H2''	22:j:158:DC:H5'	1.37	1.06
1:A:114:LYS:HG3	1:A:115:PRO:HD3	1.37	1.06
2:R:336:ILE:HG22	2:R:339:ARG:NH2	1.70	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:63:ARG:HH11	23:a:63:ARG:HB2	0.91	1.05
2:R:320:LYS:O	2:R:324:LEU:CG	2.03	1.05
2:R:353:PHE:CE2	3:B:447:PHE:HE2	1.69	1.04
2:R:365:GLU:CG	3:B:415:TYR:CZ	2.39	1.04
22:i:46:DG:H2''	22:i:47:DC:H5''	1.39	1.03
2:R:347:GLN:O	2:R:351:PHE:CD2	2.11	1.03
2:R:364:MET:HE2	3:B:30:PHE:CE1	1.93	1.03
1:A:122:ARG:HH11	1:A:122:ARG:HG2	1.25	1.02
2:R:365:GLU:CD	3:B:415:TYR:CE2	2.37	1.02
22:i:4:DA:H2''	22:i:5:DA:H5'	1.41	1.02
23:a:63:ARG:HB2	23:a:63:ARG:NH1	1.75	1.01
23:e:63:ARG:HH11	23:e:63:ARG:HB2	1.23	1.01
1:A:216:ARG:HG2	1:A:216:ARG:HH11	1.17	1.00
22:i:39:DG:H2''	22:i:40:DG:H5''	1.43	1.00
22:i:101:DC:H2''	22:i:102:DA:H5'	1.39	1.00
25:c:84:GLN:HE22	25:c:88:ARG:HE	1.08	1.00
2:R:360:LEU:HD11	3:B:438:GLN:NE2	1.78	0.99
22:i:128:DT:H2''	22:i:129:DC:H5''	1.45	0.99
22:j:152:DT:H2''	22:j:153:DA:H5'	1.45	0.99
23:e:63:ARG:HB2	23:e:63:ARG:NH1	1.78	0.98
1:A:76:LEU:CD2	1:A:108:MET:HE3	1.93	0.98
1:A:47:PHE:CD1	1:A:85:MET:HE1	1.99	0.98
1:A:442:THR:HB	2:R:339:ARG:HE	1.26	0.97
2:R:360:LEU:CD1	3:B:438:GLN:HG2	1.94	0.97
1:A:76:LEU:HD21	1:A:108:MET:HE3	1.46	0.97
22:i:50:DC:H2''	22:i:51:DA:H5'	1.45	0.97
2:R:320:LYS:HB3	2:R:324:LEU:HD11	1.46	0.96
2:R:336:ILE:HG22	2:R:339:ARG:HH22	1.29	0.96
22:i:19:DA:H2''	22:i:20:DT:H5'	1.45	0.96
3:B:189:MET:CE	3:B:305:LEU:HA	1.94	0.96
1:A:150:GLY:CA	2:R:336:ILE:HD11	1.96	0.96
1:A:343:SER:HB3	1:A:344:ILE:CA	1.95	0.96
2:R:351:PHE:CZ	3:B:176:ASP:HB3	2.00	0.95
2:R:364:MET:CE	3:B:30:PHE:HE1	1.79	0.95
23:a:63:ARG:HH11	23:a:63:ARG:CB	1.79	0.94
22:i:58:DG:H2''	22:i:59:DG:H5'	1.50	0.94
22:i:128:DT:C2'	22:i:129:DC:H5''	1.97	0.94
22:i:133:DA:H2''	22:i:134:DG:H5''	1.47	0.94
26:d:34:TYR:H	26:d:60:ASN:HD21	1.16	0.94
22:j:194:DT:C2'	22:j:195:DC:H5''	1.97	0.93
24:f:19:ARG:CZ	24:f:19:ARG:HA	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:j:248:DA:H2''	22:j:249:DG:H5'	1.51	0.93
22:j:264:DT:H2''	22:j:265:DT:H5'	1.51	0.92
2:R:365:GLU:HG2	3:B:415:TYR:CG	2.05	0.92
2:R:349:ARG:O	2:R:353:PHE:HD2	1.36	0.92
22:i:139:DA:H2''	22:i:140:DT:C5'	2.00	0.91
22:j:238:DT:H2''	22:j:239:DT:H5'	1.51	0.91
2:R:353:PHE:CD2	3:B:447:PHE:CE2	2.58	0.91
1:A:76:LEU:HD22	1:A:108:MET:CE	1.86	0.91
22:j:241:DA:H2''	22:j:242:DT:H5'	1.50	0.90
22:i:8:DT:H1'	22:i:9:DC:H5''	1.53	0.90
2:R:365:GLU:OE2	3:B:415:TYR:HE2	1.52	0.90
26:d:28:ARG:HA	26:d:28:ARG:NE	1.87	0.90
22:i:23:DT:H2''	22:i:24:DA:H5'	1.53	0.89
22:j:264:DT:H2''	22:j:265:DT:C5'	2.03	0.89
22:j:192:DG:H2''	22:j:193:DC:H5'	1.53	0.89
22:j:282:DT:H2''	22:j:283:DG:H5''	1.53	0.88
1:A:84:GLU:OE2	1:A:88:ARG:NH1	2.05	0.88
22:i:64:DT:H2''	22:i:65:DT:H5'	1.56	0.88
25:g:17:ARG:HH12	25:g:31:HIS:HD2	1.18	0.88
2:R:353:PHE:CD1	3:B:447:PHE:HE2	1.91	0.87
22:i:52:DT:H2''	22:i:53:DC:H5'	1.54	0.87
22:i:9:DC:H2''	22:i:10:DC:H5'	1.53	0.87
1:A:148:SER:O	2:R:340:GLN:NE2	2.05	0.87
22:i:43:DA:H2''	22:i:44:DC:H5''	1.57	0.87
2:R:357:GLY:O	2:R:361:HIS:CD2	2.26	0.87
2:R:365:GLU:OE2	3:B:415:TYR:CZ	2.27	0.87
22:i:45:DT:H2''	22:i:46:DG:C8	2.11	0.86
2:R:353:PHE:CE2	3:B:447:PHE:HZ	1.90	0.86
22:i:51:DA:C2'	22:i:52:DT:H5''	2.03	0.86
2:R:353:PHE:CD2	3:B:447:PHE:CZ	2.64	0.86
3:B:303:ASN:HD21	3:B:307:LYS:HZ1	1.21	0.86
22:j:161:DG:H2''	22:j:162:DC:H5''	1.56	0.85
22:i:96:DT:H2''	22:i:97:DG:H5'	1.58	0.85
25:c:38:ASN:HD22	26:h:79:HIS:CE1	1.95	0.85
22:i:42:DA:H2''	22:i:43:DA:H5'	1.58	0.84
22:j:183:DT:H2''	22:j:184:DT:H5'	1.60	0.84
23:a:125:GLN:HG2	23:a:134:ARG:HH12	1.43	0.83
25:c:84:GLN:NE2	25:c:88:ARG:HE	1.76	0.83
2:R:369:GLN:O	2:R:373:GLU:HG3	1.79	0.83
22:i:60:DC:H5''	23:a:63:ARG:HH21	1.43	0.82
22:i:101:DC:H2''	22:i:102:DA:C5'	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:360:LEU:HD11	3:B:438:GLN:HE21	1.41	0.82
2:R:365:GLU:HG3	3:B:415:TYR:CZ	2.15	0.82
23:a:85:GLN:NE2	24:b:82:THR:HG22	1.95	0.82
1:A:150:GLY:HA2	2:R:336:ILE:CD1	2.11	0.81
25:c:42:ARG:HG3	26:d:85:THR:HB	1.63	0.81
1:A:147:LEU:CD2	1:A:443:MET:SD	2.68	0.81
22:i:36:DT:H2''	22:i:37:DT:H5'	1.62	0.81
2:R:351:PHE:CE1	3:B:176:ASP:CB	2.62	0.80
22:i:36:DT:H2''	22:i:37:DT:C5'	2.11	0.80
24:b:92:ARG:HH21	26:d:98:LEU:HD13	1.45	0.80
2:R:329:ILE:O	2:R:332:ILE:HG22	1.80	0.80
2:R:353:PHE:CD1	3:B:447:PHE:CE2	2.66	0.80
22:j:197:DA:H2''	22:j:198:DT:H5'	1.62	0.80
22:j:282:DT:H2''	22:j:283:DG:C5'	2.11	0.80
22:j:246:DG:H1'	22:j:247:DC:H5''	1.64	0.80
22:i:92:DT:H2''	22:i:93:DT:H5''	1.64	0.79
22:i:93:DT:H2''	22:i:94:DG:H5'	1.65	0.79
22:i:128:DT:C3'	22:i:129:DC:H5''	2.10	0.79
22:i:91:DT:H2''	22:i:92:DT:H5'	1.63	0.79
24:f:92:ARG:NH1	24:f:92:ARG:HB3	1.98	0.79
3:B:459:PRO:HG2	4:P:63:TRP:CD2	2.18	0.79
22:i:118:DT:H1'	22:i:119:DT:H5'	1.63	0.78
22:j:262:DC:H2''	22:j:263:DT:H5''	1.65	0.78
22:j:149:DC:H2''	22:j:150:DA:H5'	1.65	0.78
25:g:87:ILE:HD12	25:g:102:ILE:HD11	1.65	0.78
2:R:360:LEU:HD11	3:B:438:GLN:CG	2.14	0.78
22:i:64:DT:H2''	22:i:65:DT:C5'	2.13	0.78
22:j:239:DT:H4'	22:j:240:DG:OP1	1.84	0.78
1:A:159:ILE:HD11	1:A:408:ILE:HD11	1.65	0.78
2:R:365:GLU:HG2	3:B:415:TYR:CZ	2.12	0.78
22:j:148:DT:H2''	22:j:149:DC:C5'	2.14	0.78
3:B:189:MET:CE	3:B:305:LEU:CA	2.59	0.78
26:d:120:SER:HB2	26:d:122:LYS:HG3	1.65	0.78
22:i:43:DA:C2'	22:i:44:DC:H5''	2.14	0.78
2:R:360:LEU:HD13	3:B:438:GLN:HG2	1.63	0.77
22:i:51:DA:H2''	22:i:52:DT:C5'	2.12	0.77
1:A:114:LYS:HG3	1:A:115:PRO:CD	2.14	0.77
2:R:371:ARG:O	2:R:375:THR:HG23	1.84	0.77
2:R:320:LYS:HB3	2:R:324:LEU:CD1	2.15	0.76
2:R:360:LEU:CD1	3:B:438:GLN:CG	2.62	0.76
22:i:46:DG:C2'	22:i:47:DC:H5''	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:349:ARG:HB3	2:R:353:PHE:HE2	1.50	0.76
22:i:40:DG:H2''	22:i:41:DA:C8	2.21	0.76
1:A:100:GLU:HG2	1:A:132:ASN:HB3	1.68	0.75
22:j:194:DT:H2''	22:j:195:DC:C5'	2.09	0.75
2:R:349:ARG:O	2:R:353:PHE:CE2	2.38	0.75
2:R:373:GLU:O	2:R:377:LYS:HG3	1.86	0.75
26:d:34:TYR:H	26:d:60:ASN:ND2	1.84	0.75
22:j:254:DC:H2''	22:j:255:DA:N7	2.01	0.75
3:B:303:ASN:HD21	3:B:307:LYS:NZ	1.85	0.75
25:g:118:LYS:HE2	25:g:118:LYS:O	1.86	0.75
1:A:122:ARG:HH11	1:A:122:ARG:CG	1.99	0.75
22:i:89:DC:H2''	22:i:90:DT:H71	1.68	0.74
22:j:290:DG:H2''	22:j:291:DA:OP2	1.86	0.74
15:Q:282:ASN:OD1	15:Q:295:ASN:ND2	2.20	0.74
1:A:147:LEU:HD22	1:A:443:MET:SD	2.28	0.74
22:i:92:DT:H2''	22:i:93:DT:C5'	2.17	0.74
22:j:282:DT:C2'	22:j:283:DG:H5''	2.16	0.74
24:b:75:HIS:CD2	26:d:93:THR:HG21	2.21	0.74
24:f:92:ARG:HB3	24:f:92:ARG:HH11	1.51	0.74
2:R:360:LEU:CD1	3:B:438:GLN:HE21	2.00	0.74
22:i:96:DT:H2''	22:i:97:DG:C5'	2.18	0.73
22:j:262:DC:H2''	22:j:263:DT:C5'	2.17	0.73
2:R:360:LEU:HD11	3:B:438:GLN:CD	2.12	0.73
25:g:42:ARG:HB2	26:h:85:THR:HB	1.69	0.73
2:R:287:ARG:NH1	13:N:217:GLU:OE1	2.21	0.73
22:i:74:DT:H2''	22:i:75:DT:H5'	1.68	0.73
1:A:216:ARG:HG2	1:A:216:ARG:NH1	1.94	0.73
25:g:102:ILE:HG23	26:h:58:ILE:HD13	1.70	0.73
22:i:38:DT:H2''	22:i:39:DG:C8	2.24	0.73
4:P:84:LEU:O	4:P:85:LYS:HB2	1.89	0.73
22:i:140:DT:H2''	22:i:141:DA:H5''	1.68	0.72
22:j:189:DA:H2''	22:j:190:DC:O5'	1.89	0.72
2:R:348:GLU:O	2:R:352:GLN:HG3	1.88	0.72
3:B:14:PRO:O	3:B:116[B]:HIS:HE1	1.72	0.72
25:g:87:ILE:HD13	25:g:97:LEU:HD12	1.70	0.72
22:j:162:DC:H2''	22:j:163:DA:N7	2.05	0.72
1:A:108:MET:HE2	1:A:119:ILE:HG21	1.71	0.72
22:j:274:DT:H2''	22:j:275:DC:H5'	1.72	0.72
22:j:275:DC:H2''	22:j:276:DT:H5'	1.70	0.72
22:i:140:DT:C2'	22:i:141:DA:H5''	2.20	0.72
1:A:76:LEU:HD21	1:A:108:MET:CE	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:340:GLN:O	2:R:344:TRP:HD1	1.72	0.71
2:R:320:LYS:C	2:R:324:LEU:HG	2.14	0.71
22:j:240:DG:H2''	22:j:241:DA:O5'	1.91	0.71
22:j:252:DT:H2''	22:j:253:DC:O5'	1.91	0.71
10:H:527:THR:C	10:H:529:ASN:H	1.97	0.71
22:j:291:DA:H4'	23:e:37:LYS:NZ	2.06	0.71
25:c:55:LEU:O	25:c:59:THR:HG23	1.91	0.71
1:A:183:LYS:O	1:A:183:LYS:HG2	1.91	0.71
22:j:219:DA:H2''	22:j:220:DT:H5'	1.73	0.71
24:f:92:ARG:HH21	26:h:98:LEU:HD23	1.56	0.71
6:D:96:GLN:NE2	18:4:15:UNK:O	2.22	0.70
22:i:60:DC:H5''	23:a:63:ARG:NH2	2.05	0.70
22:i:141:DA:H2''	22:i:142:DT:H5'	1.71	0.70
8:F:813:LEU:HD11	14:O:183:ILE:HD12	1.73	0.70
10:H:443:MET:HE2	14:O:221:LEU:HD11	1.72	0.70
25:c:84:GLN:HE22	25:c:88:ARG:NE	1.88	0.70
22:i:134:DG:H2''	22:i:135:DG:H5'	1.71	0.70
11:L:268:ILE:HD11	14:O:232:LEU:HD22	1.73	0.70
2:R:353:PHE:CG	3:B:447:PHE:CE2	2.80	0.70
22:i:135:DG:H2''	22:i:136:DT:O5'	1.90	0.70
22:i:133:DA:C2'	22:i:134:DG:H5''	2.20	0.69
23:a:125:GLN:CG	23:a:134:ARG:HH12	2.05	0.69
24:f:19:ARG:HA	24:f:19:ARG:NE	2.05	0.69
22:j:233:DG:H2''	22:j:234:DC:OP2	1.91	0.69
3:B:189:MET:HE2	3:B:305:LEU:CB	2.23	0.69
1:A:344:ILE:HG23	1:A:344:ILE:O	1.92	0.69
11:I:136:TYR:O	11:I:167:ASN:ND2	2.26	0.69
13:N:345:SER:HA	13:N:348:ILE:HD11	1.75	0.69
14:O:35:PHE:O	14:O:73:LEU:N	2.26	0.69
22:i:40:DG:H2''	22:i:41:DA:N7	2.07	0.69
3:B:98:ASN:O	3:B:99:GLN:HG2	1.93	0.69
5:C:20:THR:HG22	14:O:275:ALA:H	1.58	0.69
2:R:320:LYS:O	2:R:324:LEU:CB	2.41	0.69
24:b:75:HIS:HD2	26:d:93:THR:HG21	1.58	0.69
1:A:14:SER:HA	1:A:71:VAL:HB	1.74	0.68
11:I:135:GLU:OE2	15:Q:19:ARG:NH2	2.27	0.68
13:N:220:HIS:NE2	14:O:296:GLU:O	2.27	0.68
2:R:365:GLU:CG	3:B:415:TYR:CD2	2.58	0.68
11:L:178:LEU:HD21	15:Q:325:ILE:HD11	1.76	0.68
22:j:148:DT:H2''	22:j:149:DC:H5''	1.75	0.68
22:j:165:DA:H2''	22:j:166:DT:C5'	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LEU:HD23	1:A:108:MET:CE	2.23	0.68
2:R:365:GLU:HG3	3:B:415:TYR:CE1	2.28	0.68
2:R:365:GLU:CD	3:B:415:TYR:CZ	2.69	0.67
1:A:392:VAL:HB	1:A:423:THR:HG22	1.75	0.67
3:B:107:SER:O	4:P:11:ASN:HA	1.95	0.67
3:B:275:LYS:HB3	3:B:278:ASP:OD2	1.94	0.67
7:E:376:ASN:ND2	7:E:381:ASP:O	2.27	0.67
12:M:218:CYS:SG	21:7:60:UNK:N	2.68	0.67
22:j:262:DC:C2'	22:j:263:DT:H5''	2.24	0.67
1:A:311:GLU:OE2	1:A:407:ARG:NH2	2.28	0.67
3:B:189:MET:HE1	3:B:304:ASN:C	2.19	0.67
3:B:303:ASN:ND2	3:B:307:LYS:NZ	2.43	0.67
22:i:95:DA:H2''	22:i:96:DT:H5''	1.77	0.67
23:e:122:LYS:HB2	23:e:122:LYS:NZ	2.10	0.67
1:A:76:LEU:HD23	1:A:108:MET:HE1	1.73	0.67
2:R:231:SER:HB3	2:R:234:MET:HG2	1.75	0.67
2:R:226:THR:HG22	14:O:126:PHE:HB2	1.78	0.66
22:j:148:DT:H2''	22:j:149:DC:H5'	1.75	0.66
22:j:238:DT:C2'	22:j:239:DT:H5'	2.23	0.66
2:R:353:PHE:CD2	3:B:447:PHE:HE2	2.08	0.66
12:M:456:ARG:NH2	14:O:262:THR:O	2.28	0.66
22:i:39:DG:C2'	22:i:40:DG:H5''	2.24	0.66
2:R:365:GLU:OE2	3:B:415:TYR:OH	2.14	0.66
22:i:37:DT:H1'	22:i:38:DT:H5''	1.78	0.66
22:j:279:DA:H2''	22:j:280:DG:H5'	1.78	0.66
13:N:55:THR:O	13:N:64:ASN:ND2	2.28	0.66
22:j:162:DC:H2''	22:j:163:DA:C8	2.31	0.66
1:A:382:GLU:CD	1:A:382:GLU:H	2.03	0.65
25:c:38:ASN:HD22	26:h:79:HIS:HE1	1.44	0.65
8:F:813:LEU:HD22	11:L:276:ARG:HH21	1.62	0.65
1:A:343:SER:CB	1:A:344:ILE:CA	2.66	0.65
2:R:365:GLU:CG	3:B:415:TYR:CE1	2.79	0.65
1:A:458:GLU:HG2	1:A:459:ASP:N	2.10	0.65
22:j:186:DG:OP1	26:h:85:THR:HG23	1.96	0.65
3:B:303:ASN:ND2	3:B:307:LYS:HZ1	1.95	0.65
22:i:95:DA:H2''	22:i:96:DT:C5'	2.27	0.65
22:j:271:DG:P	26:d:28:ARG:HH12	2.19	0.65
15:Q:18:ASN:ND2	15:Q:177:ASN:O	2.29	0.65
23:e:37:LYS:HB2	23:e:38:PRO:C	2.22	0.65
22:i:93:DT:H2''	22:i:94:DG:C5'	2.26	0.65
22:j:248:DA:H2''	22:j:249:DG:C5'	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:501:GLN:HG2	12:M:244:MET:HB3	1.79	0.65
1:A:180:VAL:HG11	1:A:332:LEU:HG	1.78	0.65
1:A:446:LEU:HD23	2:R:339:ARG:HH12	1.62	0.65
11:J:426:GLN:NE2	12:M:26:LYS:O	2.30	0.65
23:e:122:LYS:HB2	23:e:122:LYS:HZ2	1.62	0.65
14:O:33:GLU:HG3	14:O:106:LEU:HD11	1.79	0.65
22:i:50:DC:H2''	22:i:51:DA:C5'	2.25	0.65
22:j:161:DG:C2'	22:j:162:DC:H5''	2.26	0.65
13:N:75:THR:HG1	15:Q:12:TYR:HH	1.42	0.64
2:R:351:PHE:HE1	3:B:176:ASP:HB3	1.57	0.64
22:i:111:DA:H4'	25:g:42:ARG:CZ	2.28	0.64
22:i:120:DT:H5'	22:i:120:DT:H6	1.62	0.64
2:R:116:ASN:ND2	11:L:363:TYR:OH	2.29	0.64
26:h:28:ARG:HG3	26:h:30:ARG:HG2	1.80	0.64
22:i:92:DT:C2'	22:i:93:DT:H5''	2.28	0.64
23:e:49:ARG:HG3	23:e:49:ARG:HH11	1.61	0.64
15:Q:184:TYR:OH	15:Q:242:ASP:OD1	2.15	0.64
22:j:207:DA:H1'	22:j:208:DT:H5'	1.80	0.64
22:j:266:DT:H2''	22:j:267:DG:C8	2.31	0.64
14:O:41:GLU:OE2	14:O:50:SER:OG	2.16	0.64
22:i:130:DT:H2''	22:i:131:DG:C8	2.32	0.64
1:A:150:GLY:CA	2:R:336:ILE:CD1	2.72	0.63
1:A:442:THR:HB	2:R:339:ARG:NE	2.05	0.63
1:A:446:LEU:HD11	2:R:332:ILE:HD11	1.80	0.63
22:j:195:DC:H2''	22:j:196:DC:C6	2.33	0.63
25:g:87:ILE:HD12	25:g:102:ILE:CD1	2.28	0.63
1:A:148:SER:HB2	1:A:442:THR:HG21	1.79	0.63
7:E:392:ASP:HB3	11:I:226:VAL:HB	1.80	0.63
24:b:58:LEU:HD23	24:b:58:LEU:C	2.22	0.63
25:c:84:GLN:HG3	25:c:105:GLY:HA3	1.81	0.63
1:A:121:GLU:O	1:A:125:GLU:HG3	1.98	0.63
22:i:23:DT:H2''	22:i:24:DA:C5'	2.27	0.63
2:R:221:CYS:HB3	8:F:875:THR:HG22	1.81	0.63
2:R:375:THR:O	2:R:379:ARG:HG3	1.98	0.63
22:i:99:DA:H2''	22:i:100:DG:H5'	1.79	0.63
23:e:129:ARG:HD3	23:e:134:ARG:O	1.98	0.62
22:j:165:DA:H2''	22:j:166:DT:H5'	1.81	0.62
1:A:446:LEU:CD2	2:R:332:ILE:HG13	2.29	0.62
22:j:242:DT:H1'	22:j:243:DG:H5''	1.81	0.62
22:i:128:DT:H2''	22:i:129:DC:C5'	2.26	0.62
1:A:153:SER:HA	1:A:169:ILE:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:i:8:DT:C1'	22:i:9:DC:H5''	2.28	0.62
22:j:205:DG:H1'	22:j:206:DC:H5''	1.82	0.62
1:A:149:MET:HA	2:R:340:GLN:HE22	1.64	0.62
22:i:44:DC:H2''	22:i:45:DT:O5'	2.00	0.62
3:B:47:GLN:O	3:B:48:ASP:HB3	2.00	0.62
22:i:37:DT:H2''	22:i:38:DT:H5'	1.81	0.62
22:j:259:DA:H2''	22:j:260:DC:H5'	1.80	0.62
2:R:48:LYS:NZ	14:O:401:TYR:OH	2.21	0.61
1:A:203:GLU:O	1:A:204:GLU:HB2	2.00	0.61
10:H:527:THR:O	10:H:529:ASN:N	2.33	0.61
22:i:139:DA:C2'	22:i:140:DT:H5'	2.17	0.61
10:H:449:LYS:O	10:H:516:THR:OG1	2.16	0.61
11:I:260:CYS:HB2	11:I:283:CYS:SG	2.40	0.61
22:j:256:DA:H2''	22:j:257:DA:OP2	1.99	0.61
1:A:256:ILE:O	1:A:260:GLN:HB2	2.00	0.61
3:B:14:PRO:O	3:B:116[B]:HIS:CE1	2.53	0.61
23:a:58:THR:HG21	25:g:81:ARG:HG2	1.82	0.61
11:I:282:LEU:HD21	11:I:292:PHE:HB3	1.83	0.61
22:i:140:DT:H2''	22:i:141:DA:C5'	2.31	0.61
11:I:312:LYS:H	11:I:312:LYS:HD3	1.66	0.60
12:M:463:ASN:HA	12:M:468:ARG:HH21	1.66	0.60
1:A:47:PHE:CG	1:A:85:MET:HE1	2.36	0.60
1:A:442:THR:O	2:R:339:ARG:CZ	2.49	0.60
2:R:351:PHE:HE1	3:B:176:ASP:CB	2.10	0.60
7:E:405:ILE:HD11	11:L:162:LYS:HD3	1.82	0.60
6:D:64:HIS:HD2	6:D:66:TYR:H	1.47	0.60
15:Q:2:SER:N	15:Q:6:GLN:OE1	2.35	0.60
23:e:63:ARG:HH11	23:e:63:ARG:CB	2.08	0.60
3:B:53:TYR:CD1	3:B:81:GLN:HG3	2.37	0.60
1:A:389:LEU:HB3	1:A:421:LEU:HD23	1.84	0.60
2:R:353:PHE:CE1	3:B:447:PHE:CD2	2.90	0.60
3:B:44:THR:OG1	3:B:62:ALA:HB2	2.02	0.60
22:i:19:DA:H2''	22:i:20:DT:C5'	2.26	0.60
2:R:329:ILE:O	2:R:332:ILE:CG2	2.49	0.60
22:i:85:DA:H1'	22:i:86:DT:H5''	1.83	0.60
22:j:264:DT:H2''	22:j:265:DT:H5''	1.80	0.60
24:b:75:HIS:HD2	26:d:93:THR:CG2	2.14	0.60
22:j:279:DA:H2''	22:j:280:DG:C5'	2.31	0.60
1:A:108:MET:CE	1:A:119:ILE:HG21	2.31	0.60
11:I:239:GLN:OE1	11:I:346:ARG:NH1	2.35	0.60
22:j:265:DT:H2''	22:j:266:DT:O5'	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:h:96:ARG:CZ	26:h:108:VAL:HG21	2.32	0.59
11:L:288:GLN:HB2	11:L:291:HIS:CE1	2.37	0.59
13:N:296:LEU:HD21	13:N:309:LEU:HG	1.83	0.59
22:i:108:DC:H2''	22:i:109:DA:N7	2.17	0.59
1:A:399:SER:HA	1:A:404:MET:HG2	1.85	0.59
3:B:199:LYS:HD2	3:B:210:ILE:HD13	1.85	0.59
7:E:408:GLU:N	7:E:408:GLU:OE1	2.35	0.59
26:h:28:ARG:NH1	26:h:29:SER:HB2	2.17	0.59
11:L:95:HIS:O	11:L:95:HIS:ND1	2.34	0.59
22:j:249:DG:H1'	22:j:250:DT:H5''	1.84	0.59
22:j:288:DT:H1'	22:j:289:DT:H5''	1.84	0.59
11:L:237:SER:OG	11:L:249:ARG:NH1	2.35	0.59
22:i:120:DT:H5'	22:i:120:DT:C6	2.38	0.59
1:A:380:SER:O	1:A:383:GLN:HB2	2.03	0.59
3:B:35:LEU:HD11	4:P:84:LEU:HD13	1.84	0.59
22:j:180:DT:H1'	22:j:181:DA:H5'	1.84	0.59
1:A:334:ALA:HB2	1:A:415:ARG:HD3	1.85	0.58
2:R:262:ILE:HD13	14:O:265:MET:HE3	1.83	0.58
12:M:378:GLN:OE1	12:M:380:GLN:NE2	2.36	0.58
22:j:248:DA:H5'	24:b:78:ARG:CD	2.33	0.58
22:j:275:DC:H2''	22:j:276:DT:C5'	2.33	0.58
1:A:418:GLN:HG3	1:A:418:GLN:O	2.03	0.58
23:a:61:LEU:HD12	24:b:37:LEU:HD23	1.85	0.58
1:A:159:ILE:HG23	1:A:164:CYS:SG	2.44	0.58
14:O:167:ASP:OD2	14:O:182:LYS:NZ	2.36	0.58
22:i:115:DA:H2''	22:i:116:DC:H5''	1.84	0.58
25:c:79:ILE:HG12	25:c:82:HIS:CE1	2.39	0.58
1:A:400:LEU:HD12	1:A:433:LYS:HE2	1.84	0.58
2:R:353:PHE:CG	3:B:447:PHE:HE2	2.19	0.58
14:O:170:THR:HG22	14:O:172:LEU:H	1.68	0.58
15:Q:351:ASP:OD1	15:Q:351:ASP:N	2.35	0.58
15:Q:368:ASP:OD1	15:Q:368:ASP:N	2.35	0.58
23:a:60:LEU:HD13	23:a:93:GLN:CD	2.29	0.58
7:E:380:SER:HB2	12:M:464:ASN:HA	1.86	0.58
22:j:271:DG:H4'	22:j:271:DG:OP1	2.02	0.58
22:j:291:DA:H4'	23:e:37:LYS:HZ1	1.67	0.58
25:c:93:LEU:HD23	26:d:103:LEU:HD21	1.86	0.58
3:B:141:ILE:HG12	3:B:448:TYR:HB3	1.85	0.58
22:i:46:DG:H2''	22:i:47:DC:H6	1.68	0.58
2:R:130:ASP:OD1	14:O:430:ARG:NH2	2.31	0.58
22:i:115:DA:C2'	22:i:116:DC:H5''	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:29:TRP:CD2	4:P:61:LYS:HD3	2.38	0.58
11:J:434:LYS:NZ	11:J:438:GLU:OE2	2.37	0.58
22:i:35:DA:H2''	22:i:36:DT:O5'	2.03	0.58
22:i:37:DT:H2''	22:i:38:DT:C5'	2.34	0.58
22:i:141:DA:H2''	22:i:142:DT:C5'	2.33	0.58
22:i:145:DA:H1'	22:i:146:DT:H5''	1.86	0.58
23:a:46:VAL:O	23:a:50:GLU:HG3	2.04	0.58
22:j:246:DG:H2''	22:j:247:DC:H5'	1.86	0.57
22:j:285:DA:H1'	22:j:286:DT:H5''	1.86	0.57
23:e:37:LYS:N	23:e:38:PRO:HA	2.18	0.57
13:N:574:TYR:O	13:N:578:THR:OG1	2.21	0.57
1:A:241:LYS:NZ	1:A:245:GLU:HB3	2.19	0.57
22:j:227:DG:H2''	22:j:228:DA:OP2	2.04	0.57
23:a:67:PHE:CD2	23:a:93:GLN:HG3	2.40	0.57
2:R:340:GLN:O	2:R:344:TRP:CD1	2.54	0.57
22:j:158:DC:H2''	22:j:159:DC:OP2	2.04	0.57
1:A:44:GLU:O	1:A:44:GLU:HG2	2.05	0.57
8:F:852:ASP:OD1	8:F:853:VAL:N	2.36	0.57
11:I:57:ASN:N	11:I:59:GLU:OE1	2.38	0.57
11:I:271:ARG:HD2	11:I:281:ASN:HD22	1.68	0.57
22:j:286:DT:H2''	22:j:287:DA:O5'	2.04	0.57
2:R:287:ARG:NH2	13:N:156:GLN:OE1	2.38	0.57
22:i:113:DA:H2''	22:i:114:DC:O5'	2.04	0.57
1:A:216:ARG:NE	1:A:216:ARG:HA	2.20	0.57
2:R:365:GLU:HG2	3:B:415:TYR:CD1	2.40	0.57
5:C:33:ARG:NH2	12:M:441:GLU:OE2	2.36	0.57
22:j:227:DG:H4'	24:b:45:ARG:CZ	2.34	0.57
23:a:51:ILE:O	23:a:55:GLN:HG3	2.04	0.57
22:i:36:DT:H2''	22:i:37:DT:H5''	1.84	0.57
22:i:53:DC:H2''	22:i:54:DA:H5'	1.87	0.57
23:a:117:VAL:HG12	23:a:117:VAL:O	2.04	0.57
1:A:381:PRO:C	1:A:383:GLN:H	2.11	0.57
26:d:34:TYR:N	26:d:60:ASN:HD21	1.93	0.57
9:G:167:MET:HE1	9:G:177:ILE:HA	1.86	0.56
14:O:266:THR:HG23	14:O:267:ARG:HG3	1.87	0.56
1:A:381:PRO:HG2	1:A:382:GLU:OE2	2.04	0.56
22:i:104:DT:OP1	26:d:27:LYS:N	2.38	0.56
22:j:194:DT:C3'	22:j:195:DC:H5''	2.36	0.56
3:B:34:GLU:CD	3:B:34:GLU:H	2.13	0.56
26:d:54:LYS:O	26:d:58:ILE:HD12	2.06	0.56
5:C:68:MET:HE1	11:J:437:MET:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:i:62:DT:H2''	22:i:63:DG:C8	2.41	0.56
24:b:58:LEU:HD23	24:b:58:LEU:O	2.05	0.56
25:g:17:ARG:HH12	25:g:31:HIS:CD2	2.11	0.56
1:A:72:ASP:OD1	1:A:74:GLN:HB2	2.05	0.56
1:A:426:ASN:O	1:A:432:ARG:NE	2.35	0.56
1:A:446:LEU:HD22	2:R:332:ILE:HG13	1.88	0.56
8:F:814:PRO:O	11:L:276:ARG:NH2	2.39	0.56
22:j:186:DG:OP1	26:h:85:THR:CG2	2.54	0.56
24:f:89:ALA:O	24:f:93:GLN:HG2	2.05	0.56
22:i:33:DG:H2''	22:i:34:DT:O5'	2.06	0.56
22:j:193:DC:H1'	22:j:194:DT:C5	2.41	0.56
22:i:5:DA:H1'	22:i:6:DT:H5''	1.88	0.55
22:i:73:DA:H1'	22:i:74:DT:H5''	1.88	0.55
22:i:61:DA:H1'	22:i:62:DT:H5''	1.86	0.55
1:A:26:LEU:HB3	1:A:27:PRO:HD2	1.88	0.55
1:A:196:ARG:NH2	1:A:312:TYR:OH	2.39	0.55
15:Q:202:ILE:HG12	15:Q:226:ASN:HB2	1.87	0.55
22:j:281:DG:H2''	22:j:282:DT:H5'	1.87	0.55
2:R:356:LEU:O	2:R:359:SER:OG	2.22	0.55
11:L:268:ILE:HD12	14:O:233:PRO:HD2	1.88	0.55
1:A:194:HIS:NE2	1:A:203:GLU:OE1	2.39	0.55
1:A:426:ASN:HB3	1:A:432:ARG:HG2	1.88	0.55
10:H:513:SER:O	10:H:588:THR:HA	2.07	0.55
14:O:35:PHE:HB2	14:O:36:PRO:HD2	1.89	0.55
22:i:43:DA:H2''	22:i:44:DC:C5'	2.32	0.55
25:g:102:ILE:CG2	26:h:58:ILE:HD13	2.34	0.55
1:A:122:ARG:HG2	1:A:122:ARG:NH1	2.06	0.55
25:c:55:LEU:O	25:c:59:THR:CG2	2.55	0.55
26:d:28:ARG:HA	26:d:28:ARG:HE	1.68	0.55
26:d:104:ALA:O	26:d:108:VAL:HG23	2.07	0.55
25:g:47:ALA:N	25:g:48:PRO:HD2	2.21	0.55
2:R:239:ILE:HG12	11:I:302:ILE:HD11	1.89	0.55
7:E:372:ARG:HB2	11:I:188:GLN:HB2	1.89	0.55
11:I:226:VAL:HG13	11:I:228:LEU:HG	1.88	0.55
11:L:179:ILE:HD11	15:Q:321:THR:HA	1.89	0.55
22:i:5:DA:H2''	22:i:6:DT:C5'	2.37	0.55
22:i:128:DT:H2''	22:i:129:DC:O4'	2.07	0.55
12:M:227:VAL:HG12	13:N:361:ILE:HD12	1.88	0.55
22:i:34:DT:H2''	22:i:35:DA:C8	2.42	0.55
14:O:167:ASP:HB3	14:O:173:ASP:HB3	1.89	0.54
22:i:9:DC:C2'	22:i:10:DC:H5'	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:i:77:DA:C2'	22:i:78:DG:H5''	2.36	0.54
22:i:119:DT:H1'	22:i:120:DT:H5''	1.88	0.54
22:j:283:DG:H2''	22:j:284:DG:C8	2.42	0.54
24:b:92:ARG:HB3	24:b:92:ARG:NH1	2.23	0.54
22:i:77:DA:H2''	22:i:78:DG:C5'	2.37	0.54
22:i:29:DA:OP1	25:c:32:ARG:NH1	2.39	0.54
22:i:80:DT:H4'	24:f:45:ARG:CZ	2.37	0.54
22:i:94:DG:H2''	22:i:95:DA:OP2	2.06	0.54
22:j:165:DA:H2''	22:j:166:DT:H5''	1.90	0.54
26:h:28:ARG:HH12	26:h:29:SER:HB2	1.71	0.54
26:h:108:VAL:O	26:h:112:THR:HG23	2.07	0.54
14:O:198:ARG:NH2	14:O:199:THR:O	2.41	0.54
22:j:291:DA:H2''	22:j:292:DT:H5''	1.89	0.54
22:i:20:DT:H1'	22:i:21:DT:H5''	1.90	0.54
4:P:69:ASP:O	4:P:70:GLU:HG3	2.06	0.54
12:M:351:LEU:HD11	12:M:368:LEU:HD11	1.90	0.54
15:Q:147:ILE:HD11	15:Q:167:ARG:HB3	1.90	0.54
22:i:99:DA:H1'	22:i:100:DG:H5'	1.90	0.54
22:j:151:DA:H2''	22:j:152:DT:O5'	2.06	0.54
22:j:246:DG:H2''	22:j:247:DC:C5'	2.38	0.54
22:j:280:DG:H2''	22:j:281:DG:H5'	1.89	0.54
2:R:105:ASP:OD1	2:R:106:LYS:N	2.40	0.54
10:H:489:ASN:O	10:H:490:GLU:HG2	2.06	0.54
12:M:225:ARG:HB3	21:7:66:UNK:HA	1.90	0.54
22:i:48:DT:H2''	22:i:49:DC:H5'	1.90	0.54
23:e:65:LEU:HB3	23:e:66:PRO:HD3	1.89	0.54
25:g:26:PRO:HD3	26:h:37:TYR:CD1	2.43	0.54
3:B:43:ARG:HG3	3:B:53:TYR:CE2	2.42	0.54
3:B:189:MET:HE2	3:B:305:LEU:HB2	1.90	0.54
3:B:275:LYS:HE3	3:B:277:SER:H	1.73	0.54
22:i:114:DC:H2''	22:i:115:DA:C8	2.43	0.54
2:R:295:VAL:HG12	13:N:170:GLN:HG3	1.90	0.54
11:L:191:LEU:HG	11:L:200:PHE:HB2	1.90	0.54
22:j:281:DG:H1'	22:j:282:DT:H5''	1.88	0.54
11:K:433:VAL:HG21	12:M:32:ASP:HB3	1.90	0.54
11:L:235:TYR:O	14:O:446:ARG:NH1	2.41	0.54
12:M:267:VAL:HG22	12:M:314:LYS:HE3	1.89	0.54
22:i:95:DA:C2'	22:i:96:DT:H5''	2.37	0.54
8:F:813:LEU:HD23	8:F:814:PRO:HD2	1.89	0.53
22:i:77:DA:H2''	22:i:78:DG:H5''	1.89	0.53
24:b:51:TYR:O	24:b:55:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:192:GLU:OE2	12:M:456:ARG:NH1	2.42	0.53
2:R:349:ARG:HB3	2:R:353:PHE:CE2	2.37	0.53
2:R:349:ARG:C	2:R:353:PHE:CD2	2.80	0.53
22:i:131:DG:H2''	22:i:132:DC:H5'	1.89	0.53
22:j:155:DC:C2'	22:j:156:DC:H5'	2.24	0.53
22:j:273:DA:H2''	22:j:274:DT:H5''	1.90	0.53
22:i:93:DT:H1'	22:i:94:DG:H5''	1.90	0.53
22:i:118:DT:C1'	22:i:119:DT:H5'	2.37	0.53
22:j:172:DC:H2''	22:j:173:DA:C8	2.43	0.53
22:j:275:DC:H1'	22:j:276:DT:H5''	1.89	0.53
1:A:241:LYS:O	1:A:242:ASP:C	2.52	0.53
2:R:57:GLN:NE2	11:L:251:SER:OG	2.41	0.53
11:I:70:LEU:O	11:I:75:LYS:NZ	2.39	0.53
3:B:189:MET:HG2	3:B:305:LEU:HD13	1.90	0.53
10:H:448:TYR:HA	10:H:493:GLN:HE21	1.73	0.53
1:A:25:GLU:OE1	2:R:346:ARG:NH1	2.42	0.53
7:E:431:CYS:HA	7:E:434:TYR:HD2	1.72	0.53
10:H:453:GLN:HA	10:H:486:PHE:O	2.09	0.53
12:M:451:ASN:OD1	12:M:451:ASN:N	2.42	0.53
14:O:491:ARG:HG2	17:2:358:UNK:HA	1.91	0.53
22:j:270:DA:H2''	22:j:271:DG:O5'	2.09	0.53
25:c:90:ASP:OD2	25:c:93:LEU:HG	2.09	0.53
1:A:438:LEU:O	1:A:442:THR:HG23	2.08	0.53
13:N:285:ASP:OD1	13:N:285:ASP:N	2.36	0.53
22:j:280:DG:H1'	22:j:281:DG:H5''	1.90	0.53
11:L:80:VAL:HG21	11:L:130:ARG:HG2	1.91	0.53
22:i:108:DC:H2''	22:i:109:DA:C5	2.43	0.53
1:A:261:GLN:HB2	1:A:262:GLU:OE1	2.09	0.53
2:R:253:LYS:HE3	2:R:257:ILE:HD11	1.89	0.53
2:R:350:CYS:SG	3:B:467:PHE:C	2.92	0.53
6:D:66:TYR:OH	11:I:331:GLU:OE2	2.20	0.53
22:j:181:DA:H1'	22:j:182:DT:H5''	1.91	0.53
2:R:126:GLU:OE2	11:L:233:ASN:ND2	2.42	0.53
7:E:380:SER:OG	12:M:463:ASN:ND2	2.43	0.53
22:j:247:DC:H2''	22:j:248:DA:C8	2.43	0.53
23:e:122:LYS:NZ	23:e:122:LYS:CB	2.72	0.53
2:R:62:TYR:HB2	2:R:79:ILE:HG21	1.91	0.52
7:E:327:CYS:SG	11:L:145:ASN:ND2	2.82	0.52
11:I:363:TYR:HA	11:I:366:GLU:HG2	1.91	0.52
11:L:193:THR:OG1	11:L:196:GLY:O	2.26	0.52
22:j:157:DA:C2'	22:j:158:DC:H5'	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:j:197:DA:C2'	22:j:198:DT:H5'	2.36	0.52
23:a:63:ARG:O	23:a:66:PRO:HD2	2.09	0.52
2:R:361:HIS:CE1	3:B:151:TYR:O	2.62	0.52
15:Q:275:SER:O	15:Q:301:ASN:ND2	2.41	0.52
15:Q:345:ASP:OD1	15:Q:345:ASP:N	2.43	0.52
22:i:22:DC:H1'	22:i:23:DT:H5''	1.90	0.52
22:j:291:DA:H2''	22:j:292:DT:C5'	2.38	0.52
22:i:109:DA:H1'	22:i:110:DA:H5'	1.92	0.52
2:R:351:PHE:HE1	3:B:176:ASP:CG	2.18	0.52
3:B:43:ARG:HD3	3:B:51:TYR:CD1	2.44	0.52
3:B:189:MET:CE	3:B:305:LEU:N	2.72	0.52
22:i:134:DG:H2''	22:i:135:DG:C5'	2.39	0.52
26:d:120:SER:CB	26:d:122:LYS:HG3	2.35	0.52
1:A:6:LYS:HE3	3:B:121:GLN:OE1	2.09	0.52
1:A:80:TRP:NE1	1:A:122:ARG:HD3	2.24	0.52
1:A:147:LEU:HD23	1:A:443:MET:SD	2.47	0.52
9:G:159:VAL:HG11	16:S:208:VAL:HG21	1.91	0.52
22:i:49:DC:OP1	23:a:85:GLN:HG2	2.10	0.52
22:i:52:DT:C2'	22:i:53:DC:H5'	2.34	0.52
22:j:190:DC:H4'	22:j:190:DC:OP1	2.09	0.52
2:R:364:MET:CE	3:B:30:PHE:CE1	2.72	0.52
11:I:91:ILE:HD12	11:L:185:GLY:HA2	1.91	0.52
22:i:21:DT:H6	22:i:21:DT:H5'	1.75	0.52
24:b:59:LYS:O	24:b:63:GLU:HG3	2.10	0.52
1:A:399:SER:OG	1:A:432:ARG:NH1	2.42	0.52
4:P:83:ASP:C	4:P:84:LEU:O	2.52	0.52
7:E:319:TRP:H	7:E:319:TRP:CD1	2.27	0.52
22:i:4:DA:H2''	22:i:5:DA:C5'	2.28	0.52
22:j:149:DC:C2'	22:j:150:DA:H5'	2.37	0.52
22:j:198:DT:OP1	24:f:18:HIS:N	2.43	0.52
7:E:353:TYR:OH	15:Q:323:GLU:OE2	2.24	0.52
11:J:458:LYS:NZ	11:K:453:GLN:OE1	2.42	0.52
22:i:115:DA:H1'	22:i:116:DC:H5''	1.92	0.52
1:A:133:VAL:HG13	1:A:134:PRO:HD2	1.91	0.52
1:A:197:LEU:HD11	1:A:231:PHE:CZ	2.45	0.52
12:M:466:ASN:OD1	12:M:466:ASN:N	2.42	0.52
22:i:133:DA:H2''	22:i:134:DG:C5'	2.31	0.52
22:i:145:DA:H2''	22:i:146:DT:C5'	2.40	0.52
26:h:102:GLU:OE1	26:h:102:GLU:HA	2.09	0.52
1:A:152:SER:OG	2:R:333:ILE:HD11	2.10	0.51
8:F:798:ILE:HD11	14:O:192:SER:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:175:ASP:OD1	9:G:175:ASP:N	2.43	0.51
11:J:467:LYS:NZ	12:M:62:THR:O	2.42	0.51
22:i:5:DA:H2''	22:i:6:DT:H5'	1.91	0.51
22:j:251:DT:H2''	22:j:252:DT:H5'	1.92	0.51
25:c:26:PRO:HD3	26:d:37:TYR:CD1	2.46	0.51
23:a:117:VAL:HG13	25:g:115:LEU:CD2	2.40	0.51
15:Q:342:ASP:N	15:Q:342:ASP:OD1	2.42	0.51
22:i:104:DT:H2''	22:i:105:DT:H5'	1.93	0.51
11:I:249:ARG:NH2	11:I:253:GLN:HE21	2.09	0.51
11:J:430:GLN:NE2	11:K:425:SER:OG	2.41	0.51
22:j:179:DG:C2'	22:j:180:DT:H5''	2.41	0.51
22:j:231:DA:H1'	22:j:232:DT:H5''	1.93	0.51
22:j:261:DA:H1'	22:j:262:DC:H5''	1.92	0.51
23:a:60:LEU:HD13	23:a:93:GLN:NE2	2.25	0.51
11:L:348:GLU:HB3	14:O:457:LYS:HE3	1.92	0.51
13:N:227:GLU:O	13:N:230:SER:OG	2.15	0.51
22:i:129:DC:H2''	22:i:130:DT:C6	2.45	0.51
10:H:497:ALA:HB3	14:O:229:ASN:HA	1.92	0.51
22:j:166:DT:OP2	26:h:53:SER:HB2	2.10	0.51
22:j:183:DT:C2'	22:j:184:DT:H5'	2.36	0.51
1:A:201:ILE:O	1:A:202:LYS:HB2	2.11	0.51
1:A:418:GLN:HG2	1:A:419:TYR:CE1	2.46	0.51
3:B:32:VAL:HG23	3:B:33:PRO:HD2	1.92	0.51
22:j:247:DC:H2''	22:j:248:DA:N7	2.25	0.51
22:j:174:DA:H2''	22:j:175:DA:OP2	2.11	0.51
7:E:402:LEU:HD12	7:E:405:ILE:HD13	1.92	0.51
13:N:255:ASP:OD1	13:N:256:ARG:N	2.44	0.51
22:i:139:DA:C2'	22:i:140:DT:C5'	2.84	0.51
22:j:166:DT:H2'	22:j:167:DT:H72	1.93	0.51
2:R:371:ARG:HH12	3:B:28:GLU:C	2.19	0.51
3:B:335:ILE:HG22	3:B:340:THR:HG21	1.93	0.51
22:i:12:DC:H2''	22:i:13:DC:H5'	1.93	0.51
22:i:99:DA:C2'	22:i:100:DG:H5'	2.40	0.51
22:j:153:DA:H1'	22:j:154:DT:H5''	1.93	0.51
22:j:251:DT:H2'	22:j:252:DT:H71	1.93	0.51
1:A:47:PHE:HB2	1:A:85:MET:CE	2.41	0.50
25:c:64:GLU:O	26:d:46:HIS:HE1	1.94	0.50
2:R:111:ASP:OD1	2:R:111:ASP:N	2.38	0.50
22:j:248:DA:H5'	24:b:78:ARG:HD2	1.93	0.50
24:b:31:LYS:HE3	24:b:51:TYR:CE2	2.46	0.50
2:R:365:GLU:HG2	3:B:415:TYR:CE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:85:LYS:O	4:P:90:ARG:NH1	2.44	0.50
11:L:147:ALA:HB1	15:Q:355:ASN:HD22	1.76	0.50
12:M:454:ALA:HB1	12:M:460:ILE:HG21	1.93	0.50
15:Q:30:PHE:HA	15:Q:216:THR:O	2.11	0.50
15:Q:358:ALA:H	15:Q:371:GLU:HB2	1.75	0.50
2:R:351:PHE:CZ	3:B:176:ASP:CB	2.83	0.50
3:B:171:ILE:HD13	3:B:312:ARG:CG	2.42	0.50
2:R:226:THR:HG21	14:O:122:LYS:HG3	1.93	0.50
10:H:511:LEU:HD23	10:H:525:LEU:HD11	1.94	0.50
12:M:60:THR:O	12:M:61:ASN:ND2	2.44	0.50
3:B:47:GLN:O	3:B:48:ASP:CB	2.59	0.50
15:Q:268:ILE:HD13	15:Q:341:LYS:HG2	1.93	0.50
22:j:171:DC:H2''	22:j:172:DC:O5'	2.12	0.50
3:B:102:PHE:HZ	4:P:6:LEU:CD2	2.25	0.50
22:i:3:DC:H2''	22:i:4:DA:N7	2.26	0.50
22:i:20:DT:C2'	22:i:21:DT:H71	2.42	0.50
22:i:138:DG:H2''	22:i:139:DA:OP2	2.12	0.50
22:j:179:DG:H1'	22:j:180:DT:H5''	1.92	0.50
22:j:291:DA:H1'	22:j:292:DT:H5''	1.94	0.50
23:a:63:ARG:C	23:a:66:PRO:HD2	2.37	0.50
13:N:250:LEU:HB2	13:N:262:ILE:HG21	1.92	0.50
22:i:129:DC:H2''	22:i:130:DT:H71	1.93	0.50
22:j:199:DC:H2''	22:j:200:DA:OP2	2.11	0.50
23:a:128:ARG:NH1	23:a:134:ARG:HD2	2.26	0.50
1:A:460:TYR:CZ	1:A:464:LYS:HE3	2.47	0.50
7:E:417:ASP:N	7:E:417:ASP:OD1	2.42	0.50
11:I:105:PHE:HE1	11:I:148:MET:HE1	1.77	0.50
22:i:43:DA:H1'	22:i:44:DC:H5''	1.94	0.50
22:j:193:DC:H2''	22:j:194:DT:H71	1.93	0.50
23:a:125:GLN:HG2	23:a:134:ARG:NH1	2.21	0.50
1:A:22:SER:HA	1:A:441:LEU:CD1	2.42	0.49
22:i:125:DG:H2''	22:i:126:DA:C8	2.47	0.49
22:j:235:DC:H2''	22:j:236:DT:C7	2.42	0.49
22:j:239:DT:H1'	22:j:240:DG:H5'	1.94	0.49
25:c:73:ASN:ND2	25:c:75:LYS:HG3	2.26	0.49
14:O:270:HIS:HD2	14:O:272:ASN:HB2	1.77	0.49
15:Q:200:GLU:HG3	15:Q:201:ALA:H	1.76	0.49
22:i:92:DT:H2''	22:i:93:DT:H5'	1.93	0.49
22:j:232:DT:H2''	22:j:233:DG:C8	2.48	0.49
22:j:291:DA:C2'	22:j:292:DT:H5''	2.41	0.49
25:c:59:THR:HA	25:c:62:ILE:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:g:93:LEU:HD23	26:h:103:LEU:HD21	1.94	0.49
3:B:153:MET:HG3	3:B:334:ILE:HD13	1.94	0.49
22:j:284:DG:H2''	22:j:285:DA:H8	1.77	0.49
24:f:75:HIS:HD2	26:h:93:THR:OG1	1.94	0.49
6:D:62:ALA:HB3	6:D:71:VAL:HG23	1.94	0.49
8:F:869:ARG:H	11:L:318:GLN:NE2	2.09	0.49
22:i:7:DA:O3'	23:e:49:ARG:HD3	2.13	0.49
22:i:27:DA:H4'	26:d:30:ARG:HD3	1.93	0.49
22:i:56:DA:H2''	22:i:57:DA:N7	2.27	0.49
22:i:8:DT:C2'	22:i:9:DC:H5''	2.42	0.49
22:i:145:DA:H2''	22:i:146:DT:H5'	1.94	0.49
24:b:92:ARG:HH21	26:d:98:LEU:CD1	2.18	0.49
11:L:282:LEU:HD22	11:L:291:HIS:CD2	2.48	0.49
22:i:144:DG:H2''	22:i:145:DA:OP2	2.11	0.49
22:j:219:DA:H1'	22:j:220:DT:H5''	1.94	0.49
25:c:102:ILE:HG23	26:d:58:ILE:HG12	1.95	0.49
2:R:352:GLN:O	2:R:356:LEU:HG	2.13	0.49
2:R:357:GLY:C	2:R:361:HIS:CD2	2.90	0.49
7:E:345:ASP:O	15:Q:149:ASN:ND2	2.45	0.49
22:i:38:DT:H5'	22:i:38:DT:H6	1.77	0.49
25:g:26:PRO:HD3	26:h:37:TYR:CG	2.48	0.49
25:g:87:ILE:CD1	25:g:102:ILE:HD11	2.40	0.49
22:j:197:DA:H1'	22:j:198:DT:H5''	1.95	0.49
1:A:389:LEU:O	1:A:421:LEU:HA	2.13	0.49
1:A:407:ARG:O	1:A:411:GLU:HB2	2.12	0.49
2:R:351:PHE:CE1	3:B:176:ASP:CG	2.91	0.49
7:E:331:ASN:HD21	11:L:137:LEU:HA	1.78	0.49
11:I:192:ASP:OD1	11:I:193:THR:N	2.45	0.49
15:Q:153:PRO:HB3	15:Q:168:TYR:CE2	2.47	0.49
22:j:154:DT:H6	22:j:154:DT:H5'	1.78	0.49
22:j:159:DC:H2''	22:j:160:DT:H71	1.95	0.49
26:h:36:VAL:HG23	26:h:37:TYR:N	2.28	0.49
12:M:308:PRO:HB3	12:M:329:HIS:CD2	2.48	0.48
22:i:18:DG:H2''	22:i:19:DA:OP2	2.12	0.48
22:i:63:DG:H1'	22:i:64:DT:H5''	1.95	0.48
22:i:111:DA:C8	22:i:112:DT:H72	2.48	0.48
1:A:15:HIS:ND1	1:A:16[B]:ARG:HG2	2.28	0.48
9:G:163:ALA:HB1	16:S:194:ALA:HB1	1.94	0.48
13:N:341:PRO:HD3	13:N:553:ILE:HD11	1.95	0.48
1:A:141:GLU:HB3	1:A:142:PRO:HD3	1.94	0.48
11:L:320:MET:HE3	11:L:357:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:i:83:DA:H2''	22:i:84:DC:H5'	1.95	0.48
22:i:129:DC:H2''	22:i:130:DT:C5	2.48	0.48
1:A:458:GLU:O	1:A:459:ASP:C	2.57	0.48
22:i:7:DA:H2''	22:i:8:DT:OP2	2.13	0.48
22:i:111:DA:H2''	22:i:112:DT:OP2	2.13	0.48
22:j:198:DT:OP2	24:f:18:HIS:HA	2.13	0.48
22:j:276:DT:H2''	22:j:277:DG:N7	2.28	0.48
11:L:236:ASP:OD2	11:L:239:GLN:NE2	2.45	0.48
1:A:170:ILE:O	1:A:173:ILE:HG22	2.13	0.48
1:A:183:LYS:O	1:A:183:LYS:CG	2.61	0.48
11:L:284:SER:HB2	14:O:181:ILE:HD11	1.95	0.48
13:N:126:LEU:O	13:N:129:THR:OG1	2.25	0.48
22:j:175:DA:H2''	22:j:176:DA:C8	2.49	0.48
1:A:381:PRO:HG2	1:A:382:GLU:CD	2.39	0.48
3:B:286:ASP:HB3	3:B:290:ASN:H	1.79	0.48
22:i:77:DA:H1'	22:i:78:DG:H5''	1.95	0.48
22:j:285:DA:H2''	22:j:286:DT:H5'	1.95	0.48
1:A:381:PRO:C	1:A:383:GLN:N	2.72	0.48
11:L:140:THR:HG22	11:L:143:ARG:HH22	1.79	0.48
13:N:191:ILE:HD12	13:N:218:LEU:HD21	1.96	0.48
22:i:143:DT:H2''	22:i:144:DG:OP2	2.13	0.48
22:j:287:DA:H2'	22:j:288:DT:C7	2.43	0.48
23:e:49:ARG:HH11	23:e:49:ARG:CG	2.26	0.48
26:h:28:ARG:CG	26:h:30:ARG:HG2	2.44	0.48
2:R:215:THR:HG21	2:R:237:PHE:H	1.79	0.48
3:B:364:GLU:HG2	3:B:365:GLU:N	2.29	0.48
22:j:179:DG:H2''	22:j:180:DT:H5''	1.96	0.48
22:j:191:DT:H2''	22:j:192:DG:OP2	2.14	0.48
24:b:75:HIS:HB2	26:d:93:THR:HG21	1.96	0.48
1:A:438:LEU:HD23	1:A:438:LEU:HA	1.67	0.47
15:Q:202:ILE:HB	15:Q:225:TYR:HB3	1.96	0.47
15:Q:294:ASP:OD1	15:Q:295:ASN:N	2.46	0.47
22:i:46:DG:H2''	22:i:47:DC:C6	2.48	0.47
22:i:78:DG:H2''	22:i:79:DC:C5	2.48	0.47
22:j:264:DT:H1'	25:c:11:ARG:NH2	2.29	0.47
24:f:31:LYS:HB3	24:f:32:PRO:CD	2.44	0.47
25:g:37:GLY:HA3	25:g:39:TYR:CE2	2.49	0.47
26:h:29:SER:O	26:h:31:LYS:N	2.47	0.47
2:R:372:ILE:O	2:R:375:THR:OG1	2.30	0.47
9:G:175:ASP:O	9:G:178:ILE:HG22	2.14	0.47
11:I:311:VAL:HB	11:I:314:ASN:HD22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:208:LEU:O	15:Q:218:LYS:HA	2.13	0.47
24:b:52:GLU:OE2	24:b:55:ARG:NH1	2.48	0.47
13:N:68:PHE:CZ	15:Q:13:ILE:HD11	2.49	0.47
15:Q:356:ASP:O	15:Q:374:SER:N	2.37	0.47
22:j:197:DA:H2''	22:j:198:DT:C5'	2.40	0.47
22:j:251:DT:C2'	22:j:252:DT:H71	2.44	0.47
24:b:92:ARG:HB3	24:b:92:ARG:CZ	2.44	0.47
23:e:57:SER:HB2	23:e:59:GLU:OE2	2.14	0.47
1:A:337:VAL:O	1:A:340:ALA:HB3	2.15	0.47
1:A:458:GLU:O	1:A:461:GLU:N	2.47	0.47
2:R:338:GLU:O	2:R:342:GLU:HG3	2.13	0.47
3:B:286:ASP:HB2	3:B:290:ASN:HB2	1.95	0.47
11:I:358:PRO:HB2	11:L:224:PHE:HB2	1.94	0.47
22:i:3:DC:H2''	22:i:4:DA:C8	2.49	0.47
2:R:353:PHE:CD2	3:B:447:PHE:HZ	2.20	0.47
3:B:148:ALA:O	3:B:431:GLY:HA3	2.14	0.47
3:B:370:GLU:HG3	3:B:395:VAL:HG21	1.97	0.47
11:I:195:GLN:C	11:I:197:LEU:H	2.23	0.47
11:J:419:GLU:O	11:J:422:ILE:HG12	2.13	0.47
22:j:266:DT:H2''	22:j:267:DG:N7	2.30	0.47
1:A:259:LYS:HD2	1:A:259:LYS:O	2.14	0.47
1:A:325:PRO:O	1:A:331:PRO:HG2	2.15	0.47
2:R:217:SER:OG	2:R:220:ASP:OD1	2.32	0.47
3:B:30:PHE:HB3	3:B:433:GLN:OE1	2.14	0.47
4:P:9:LYS:HD2	4:P:12:LYS:HE2	1.97	0.47
10:H:444:GLU:HG2	10:H:445:TYR:H	1.80	0.47
12:M:237:ASN:ND2	12:M:321:LYS:O	2.47	0.47
22:i:4:DA:C2'	22:i:5:DA:H5'	2.30	0.47
22:i:101:DC:H5'	24:f:78:ARG:CD	2.45	0.47
22:i:108:DC:H2''	22:i:109:DA:C8	2.50	0.47
24:b:92:ARG:NH2	26:d:98:LEU:HD13	2.22	0.47
3:B:403:CYS:HB2	3:B:404:PRO:HA	1.97	0.47
10:H:524:THR:HG23	10:H:605:ARG:HB3	1.97	0.47
22:i:59:DG:H2''	22:i:60:DC:OP2	2.14	0.47
22:i:90:DT:OP2	23:e:69:ARG:NH2	2.47	0.47
22:j:254:DC:H2''	22:j:255:DA:C8	2.50	0.47
3:B:26:ASN:O	3:B:27:GLU:HB2	2.15	0.47
11:I:249:ARG:HH21	11:I:253:GLN:HE21	1.61	0.47
22:j:197:DA:H1'	22:j:198:DT:C5'	2.45	0.47
26:h:51:ILE:HG21	26:h:56:MET:HE2	1.97	0.47
2:R:212:ASN:OD1	2:R:212:ASN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:120:SER:HB2	3:B:123:ASP:H	1.79	0.47
11:K:472:ARG:NH2	11:K:503:ASP:OD2	2.37	0.47
13:N:279:SER:OG	13:N:280:ALA:N	2.48	0.47
14:O:198:ARG:HD3	14:O:203:ASP:OD1	2.14	0.47
22:i:43:DA:C1'	22:i:44:DC:H5''	2.45	0.47
25:g:84:GLN:O	25:g:88:ARG:HG2	2.15	0.47
7:E:372:ARG:HH12	11:I:227:ASN:HD21	1.62	0.46
22:i:11:DA:H2''	22:i:12:DC:OP2	2.14	0.46
22:j:282:DT:H2''	22:j:283:DG:H5'	1.95	0.46
15:Q:331:SER:O	15:Q:334:GLU:HB2	2.15	0.46
22:i:70:DT:H2''	22:i:71:DG:H5'	1.97	0.46
24:b:96:THR:O	25:g:101:THR:HG23	2.14	0.46
26:h:43:LYS:O	26:h:47:PRO:HG3	2.16	0.46
2:R:369:GLN:O	2:R:373:GLU:CG	2.59	0.46
12:M:23:PRO:HB2	12:M:26:LYS:HG2	1.97	0.46
22:j:270:DA:O3'	26:d:28:ARG:NH1	2.47	0.46
26:h:28:ARG:HH11	26:h:29:SER:H	1.64	0.46
1:A:447:PRO:HG3	2:R:335:PHE:CG	2.49	0.46
8:F:818:TRP:HA	11:L:287:PHE:CD1	2.51	0.46
13:N:115:ILE:HA	13:N:120:LEU:HD12	1.96	0.46
13:N:335:ILE:O	13:N:339:THR:OG1	2.24	0.46
22:i:116:DC:H2'	22:i:117:DT:H72	1.97	0.46
23:a:124:ILE:O	23:a:128:ARG:HG3	2.15	0.46
26:d:28:ARG:NE	26:d:28:ARG:CA	2.71	0.46
25:g:80:PRO:HG3	26:h:58:ILE:HD12	1.97	0.46
1:A:188:PHE:HZ	1:A:319:ILE:HD13	1.80	0.46
1:A:216:ARG:NH1	1:A:216:ARG:CG	2.69	0.46
3:B:189:MET:HG2	3:B:305:LEU:CD1	2.45	0.46
10:H:525:LEU:O	10:H:532:PRO:HD2	2.16	0.46
12:M:452:GLU:HA	12:M:455:ALA:HB3	1.98	0.46
13:N:223:LEU:HD12	13:N:258:MET:HE2	1.97	0.46
22:i:73:DA:H2''	22:i:74:DT:C5'	2.46	0.46
22:i:89:DC:H2''	22:i:90:DT:C7	2.41	0.46
22:j:179:DG:H2''	22:j:180:DT:C5'	2.45	0.46
23:a:90:MET:O	23:a:94:GLU:HG2	2.15	0.46
26:d:87:THR:OG1	26:d:90:GLU:OE2	2.33	0.46
10:H:490:GLU:HG3	11:L:264:GLY:O	2.15	0.46
12:M:309:GLU:N	12:M:312:GLU:OE1	2.47	0.46
22:i:46:DG:C3'	22:i:47:DC:H5''	2.45	0.46
22:i:84:DC:H2''	22:i:85:DA:C8	2.51	0.46
22:i:132:DC:H2''	22:i:133:DA:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:j:262:DC:H1'	22:j:263:DT:H5''	1.96	0.46
7:E:331:ASN:ND2	11:L:137:LEU:HA	2.31	0.46
11:J:472:ARG:HH22	11:K:467:LYS:HB2	1.81	0.46
22:j:211:DT:H2''	22:j:212:DC:H5'	1.98	0.46
1:A:236:LEU:HD22	1:A:309:PHE:CD2	2.51	0.46
2:R:136:LEU:C	2:R:139:PRO:HD2	2.40	0.46
7:E:372:ARG:HH22	11:I:227:ASN:HD21	1.64	0.46
1:A:150:GLY:N	2:R:336:ILE:HD13	2.30	0.46
1:A:419:TYR:N	1:A:419:TYR:CD1	2.84	0.46
2:R:208:ARG:NH1	6:D:85:HIS:O	2.49	0.46
3:B:212:SER:HB3	3:B:284:PHE:HE2	1.81	0.46
4:P:56:TYR:HB3	4:P:58:PHE:CE2	2.51	0.46
6:D:64:HIS:CD2	6:D:66:TYR:H	2.30	0.46
7:E:388:THR:HG23	11:I:230:ILE:HB	1.98	0.46
22:i:106:DT:H2''	22:i:107:DC:H5'	1.98	0.46
25:c:63:LEU:HD13	26:d:42:LEU:HB2	1.98	0.46
26:d:28:ARG:O	26:d:29:SER:HB2	2.16	0.46
26:d:119:THR:C	26:d:121:ALA:H	2.24	0.46
1:A:6:LYS:HD2	1:A:23:ASN:ND2	2.30	0.46
15:Q:162:PRO:O	15:Q:165:ILE:HB	2.16	0.46
22:i:115:DA:H2''	22:i:116:DC:C5'	2.45	0.46
23:a:119:ILE:HD13	24:b:43:VAL:HG11	1.97	0.46
22:i:140:DT:H1'	22:i:141:DA:H5''	1.98	0.45
1:A:282:ASN:O	1:A:285:VAL:HG22	2.16	0.45
3:B:102:PHE:HZ	4:P:6:LEU:HD23	1.82	0.45
3:B:189:MET:HE1	3:B:305:LEU:N	2.32	0.45
3:B:424:TYR:CD1	3:B:427:ILE:HD12	2.51	0.45
6:D:98:GLU:OE2	13:N:41:ARG:NH2	2.29	0.45
7:E:414:VAL:HG22	7:E:418:VAL:HB	1.98	0.45
12:M:372:VAL:HG12	12:M:375:ILE:HB	1.98	0.45
22:j:262:DC:H2''	22:j:263:DT:H5'	1.94	0.45
10:H:608:ASP:O	10:H:609:LYS:HG2	2.16	0.45
13:N:561:LEU:HD21	13:N:571:LEU:HD12	1.98	0.45
1:A:164:CYS:HB2	1:A:182:SER:HB3	1.98	0.45
1:A:232:LYS:HA	1:A:236:LEU:HG	1.99	0.45
1:A:320:SER:OG	1:A:322:LYS:N	2.38	0.45
9:G:192:LEU:HD11	16:S:209:LEU:HD22	1.97	0.45
11:J:482:LEU:HD11	11:K:507:GLN:HA	1.99	0.45
22:i:99:DA:H1'	22:i:100:DG:C5'	2.46	0.45
22:i:137:DG:H2''	22:i:138:DG:OP2	2.15	0.45
25:g:81:ARG:NH2	25:g:107:VAL:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:23:GLU:OE2	4:P:65:ARG:HD3	2.16	0.45
11:K:493:LYS:HE2	11:K:510:GLU:HG2	1.97	0.45
11:L:150:VAL:HG11	15:Q:310:PHE:CE1	2.51	0.45
15:Q:307:PRO:HB3	15:Q:332:LEU:HD23	1.97	0.45
26:d:117:LYS:O	26:d:122:LYS:HB2	2.17	0.45
3:B:143:LEU:HD12	3:B:144:PRO:HD2	1.98	0.45
11:L:166:ILE:HG22	11:L:167:ASN:CG	2.42	0.45
11:L:298:SER:HB3	14:O:390:LEU:HG	1.98	0.45
22:i:73:DA:C2'	22:i:74:DT:H5''	2.46	0.45
22:j:149:DC:H1'	22:j:150:DA:C5'	2.47	0.45
25:g:99:ARG:HG3	25:g:99:ARG:HH11	1.82	0.45
1:A:47:PHE:HD1	1:A:85:MET:HE1	1.70	0.45
3:B:3:PRO:HA	3:B:4:PHE:HA	1.67	0.45
4:P:33:SER:HB3	4:P:55:LYS:CD	2.46	0.45
9:G:157:ASN:ND2	16:S:203:PHE:O	2.46	0.45
11:L:147:ALA:HB3	15:Q:371:GLU:H	1.80	0.45
22:i:136:DT:H4'	22:i:136:DT:OP1	2.17	0.45
24:f:18:HIS:N	24:f:18:HIS:CD2	2.84	0.45
24:f:51:TYR:O	24:f:55:ARG:HG3	2.16	0.45
3:B:121:GLN:HG2	3:B:463:TRP:CH2	2.52	0.45
11:L:258:TYR:OH	14:O:173:ASP:OD1	2.33	0.45
22:i:91:DT:C2'	22:i:92:DT:H5'	2.40	0.45
22:j:172:DC:H4'	22:j:172:DC:OP1	2.16	0.45
22:j:274:DT:H2''	22:j:275:DC:C5'	2.43	0.45
1:A:412:LEU:HD12	1:A:412:LEU:HA	1.76	0.45
2:R:133:ASP:HA	14:O:427:LYS:HZ1	1.82	0.45
6:D:64:HIS:CD2	6:D:66:TYR:HB2	2.52	0.45
11:K:433:VAL:O	11:K:437:MET:HG2	2.17	0.45
26:d:75:SER:HA	26:d:86:ILE:HD11	1.97	0.45
13:N:77:ARG:NH1	16:S:198:LEU:H	2.15	0.45
22:j:186:DG:H1'	22:j:187:DA:C8	2.51	0.45
1:A:344:ILE:O	1:A:344:ILE:CG2	2.64	0.44
3:B:197:SER:HB3	3:B:301:GLY:HA2	1.99	0.44
3:B:286:ASP:CB	3:B:290:ASN:H	2.29	0.44
6:D:64:HIS:HD2	6:D:66:TYR:HB2	1.81	0.44
10:H:487:ASN:ND2	10:H:490:GLU:OE2	2.43	0.44
12:M:372:VAL:HG13	12:M:375:ILE:HD12	1.99	0.44
22:i:61:DA:H2''	22:i:62:DT:H5'	1.99	0.44
23:a:63:ARG:HH22	24:b:30:THR:CG2	2.30	0.44
26:h:43:LYS:HA	26:h:43:LYS:HD3	1.63	0.44
4:P:66:ASN:HB3	4:P:70:GLU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:447:ASP:HB3	14:O:270:HIS:CD2	2.52	0.44
15:Q:20:LEU:HA	15:Q:27:ILE:HD12	1.99	0.44
22:j:175:DA:H2"	22:j:176:DA:H8	1.82	0.44
3:B:30:PHE:CD1	3:B:30:PHE:N	2.84	0.44
11:I:180:GLY:HA3	11:L:198:LYS:HE3	2.00	0.44
25:c:73:ASN:O	25:c:73:ASN:CG	2.61	0.44
1:A:25:GLU:OE1	2:R:346:ARG:HD2	2.18	0.44
1:A:147:LEU:C	1:A:149:MET:H	2.26	0.44
2:R:177:LYS:HG2	12:M:444:LEU:HD13	1.98	0.44
4:P:33:SER:HB3	4:P:55:LYS:HD3	1.98	0.44
6:D:123:ASP:OD2	10:H:474:ARG:NH2	2.50	0.44
11:I:59:GLU:H	11:I:59:GLU:CD	2.25	0.44
22:i:4:DA:C2	22:j:290:DG:N2	2.85	0.44
22:i:37:DT:C1'	22:i:38:DT:H5"	2.45	0.44
25:c:66:ALA:HB2	25:c:83:LEU:HD23	1.99	0.44
2:R:157:LYS:HD3	5:C:44:GLU:HB2	1.98	0.44
2:R:248:LEU:O	14:O:257:PRO:HG2	2.18	0.44
11:I:171:ASP:O	11:I:174:THR:HG22	2.17	0.44
11:I:281:ASN:OD1	11:I:281:ASN:N	2.50	0.44
12:M:450:PHE:HA	14:O:265:MET:HE1	1.98	0.44
13:N:32:MET:HE2	17:2:345:UNK:HA	1.99	0.44
3:B:180:LEU:HA	3:B:180:LEU:HD23	1.69	0.44
7:E:392:ASP:OD2	7:E:395:LEU:HD13	2.16	0.44
11:I:88:TRP:CD1	11:I:88:TRP:H	2.34	0.44
11:I:239:GLN:H	11:I:239:GLN:HG3	1.60	0.44
12:M:59:PRO:HB2	12:M:244:MET:HE1	1.99	0.44
2:R:367:ASP:O	2:R:371:ARG:HG3	2.17	0.44
3:B:354:LEU:HD22	3:B:358:LEU:HD22	1.98	0.44
4:P:1:MET:HG2	4:P:2:ASP:N	2.33	0.44
26:d:43:LYS:HE2	26:d:43:LYS:HA	1.99	0.44
1:A:145:ILE:O	1:A:149:MET:HG2	2.17	0.44
2:R:320:LYS:C	2:R:324:LEU:CD1	2.90	0.44
2:R:320:LYS:C	2:R:324:LEU:CG	2.83	0.44
2:R:351:PHE:O	2:R:355:ARG:HG3	2.17	0.44
3:B:146:SER:HB2	3:B:174:ILE:HD11	1.99	0.44
11:I:246:ASP:OD1	11:I:247:GLU:N	2.49	0.44
14:O:202:MET:HG3	14:O:204:LEU:HD11	2.00	0.44
1:A:282:ASN:HA	1:A:283:PRO:HD2	1.90	0.44
22:i:80:DT:H2"	22:i:81:DG:OP2	2.18	0.44
23:a:90:MET:HA	23:a:90:MET:HE2	1.99	0.44
25:g:42:ARG:CB	26:h:85:THR:HB	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:MET:HA	2:R:340:GLN:NE2	2.33	0.43
13:N:234:ALA:HB3	13:N:235:PRO:HD3	1.99	0.43
22:j:159:DC:H2''	22:j:160:DT:OP2	2.17	0.43
22:j:220:DT:C2'	22:j:221:DT:H71	2.48	0.43
22:j:250:DT:H2''	22:j:251:DT:H5'	1.99	0.43
22:j:263:DT:H2''	22:j:264:DT:O5'	2.17	0.43
1:A:320:SER:OG	1:A:321:ASP:N	2.49	0.43
1:A:334:ALA:CB	1:A:415:ARG:HD3	2.46	0.43
12:M:227:VAL:HG13	12:M:346:LEU:HD12	1.99	0.43
13:N:539:ASN:OD1	13:N:577:ASN:ND2	2.51	0.43
22:i:21:DT:H5'	22:i:21:DT:C6	2.53	0.43
22:j:261:DA:H2''	22:j:262:DC:H5'	1.99	0.43
24:b:53:GLU:O	24:b:57:VAL:HG23	2.18	0.43
3:B:189:MET:HG3	3:B:193:SER:OG	2.19	0.43
23:a:93:GLN:O	23:a:97:GLU:HG3	2.17	0.43
25:c:26:PRO:HD3	26:d:37:TYR:CG	2.52	0.43
2:R:320:LYS:C	2:R:324:LEU:HD12	2.43	0.43
2:R:383:LEU:HB3	2:R:384:LYS:HA	1.99	0.43
7:E:371:TRP:CD2	11:L:202:PRO:HG3	2.53	0.43
14:O:51:TYR:CE2	14:O:55:ILE:HD11	2.53	0.43
22:i:10:DC:H6	22:i:10:DC:H2'	1.65	0.43
22:i:34:DT:H2''	22:i:35:DA:H8	1.83	0.43
22:j:152:DT:H2''	22:j:153:DA:C5'	2.31	0.43
22:j:248:DA:OP1	24:b:79:LYS:HB2	2.18	0.43
1:A:446:LEU:CD1	2:R:332:ILE:CD1	2.97	0.43
2:R:112:GLU:OE2	14:O:466:SER:OG	2.29	0.43
12:M:10:VAL:HG22	12:M:11:THR:H	1.84	0.43
22:i:11:DA:H1'	22:i:12:DC:H5'	2.00	0.43
23:a:117:VAL:O	23:a:117:VAL:CG1	2.66	0.43
9:G:178:ILE:HD12	16:S:226:LEU:HD23	2.01	0.43
22:i:36:DT:C2'	22:i:37:DT:H5''	2.48	0.43
22:i:84:DC:H6	22:i:84:DC:H2'	1.73	0.43
26:d:34:TYR:HB2	26:d:60:ASN:ND2	2.33	0.43
26:d:67:PHE:CD1	26:d:67:PHE:C	2.97	0.43
1:A:431:ASP:O	1:A:435:GLN:HB2	2.19	0.43
9:G:158:TRP:CD1	13:N:74:GLU:HG3	2.54	0.43
12:M:335:VAL:O	12:M:338:THR:OG1	2.31	0.43
22:i:64:DT:H2''	22:i:65:DT:H5''	1.96	0.43
22:i:101:DC:H5'	24:f:78:ARG:HD3	1.99	0.43
22:i:101:DC:C2'	22:i:102:DA:C5'	2.91	0.43
22:j:280:DG:H1'	22:j:281:DG:C5'	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:j:284:DG:H2''	22:j:285:DA:C8	2.53	0.43
23:a:73:GLU:CD	24:b:25:ASN:HD22	2.25	0.43
25:c:79:ILE:HB	25:c:80:PRO:HD2	2.00	0.43
25:g:83:LEU:O	25:g:87:ILE:HG13	2.18	0.43
26:h:106:HIS:O	26:h:110:GLU:HG2	2.17	0.43
2:R:349:ARG:C	2:R:353:PHE:CE2	2.97	0.43
3:B:338:GLY:O	3:B:339:THR:C	2.59	0.43
11:I:140:THR:HG23	11:I:143:ARG:HH21	1.83	0.43
13:N:59:HIS:O	13:N:59:HIS:ND1	2.49	0.43
13:N:75:THR:OG1	15:Q:12:TYR:OH	2.20	0.43
15:Q:20:LEU:HD23	15:Q:27:ILE:HG21	2.01	0.43
1:A:32:PRO:C	1:A:34:SER:H	2.26	0.43
1:A:47:PHE:HB2	1:A:85:MET:HE1	1.99	0.43
1:A:129:ASP:OD2	1:A:460:TYR:HE2	2.01	0.43
1:A:180:VAL:CG1	1:A:332:LEU:HG	2.48	0.43
1:A:261:GLN:HB2	1:A:262:GLU:CD	2.43	0.43
3:B:46:ARG:O	3:B:47:GLN:C	2.62	0.43
12:M:378:GLN:HG2	12:M:380:GLN:HG3	2.00	0.43
13:N:132:LEU:N	13:N:133:PRO:HD2	2.33	0.43
22:i:39:DG:H1'	22:i:40:DG:O4'	2.18	0.43
22:j:148:DT:C2'	22:j:149:DC:H5''	2.46	0.43
22:j:205:DG:H1'	22:j:206:DC:C5'	2.49	0.43
3:B:286:ASP:HB2	3:B:290:ASN:O	2.18	0.43
12:M:261:LEU:HD23	12:M:261:LEU:HA	1.88	0.43
13:N:542:ASP:OD1	13:N:542:ASP:N	2.50	0.43
23:a:117:VAL:HG13	25:g:115:LEU:HD22	2.01	0.43
25:c:38:ASN:ND2	26:h:79:HIS:HE1	2.14	0.43
1:A:80:TRP:CE2	1:A:122:ARG:HD3	2.53	0.42
1:A:147:LEU:HG	2:R:336:ILE:HG21	2.00	0.42
1:A:151:LYS:HE3	1:A:424:PHE:CE1	2.53	0.42
3:B:156:LEU:HD23	3:B:156:LEU:HA	1.76	0.42
8:F:808:ASP:OD1	8:F:809:PRO:HD2	2.19	0.42
14:O:55:ILE:O	14:O:59:SER:N	2.48	0.42
14:O:433:ARG:NH1	14:O:441:PRO:HB3	2.34	0.42
22:i:136:DT:H2''	22:i:137:DG:C8	2.54	0.42
22:j:202:DA:H2''	22:j:203:DA:OP2	2.18	0.42
22:j:237:DT:H1'	22:j:238:DT:H5''	2.01	0.42
23:a:58:THR:CG2	25:g:81:ARG:HG2	2.47	0.42
26:h:59:MET:O	26:h:63:VAL:HG23	2.19	0.42
1:A:198:ALA:N	1:A:199:PRO:HD2	2.34	0.42
2:R:344:TRP:O	2:R:348:GLU:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:66:LYS:HA	3:B:67:PRO:HD3	1.78	0.42
7:E:394:ASP:HB2	7:E:428:PHE:HE1	1.84	0.42
13:N:166:ARG:HG3	13:N:167:ASN:N	2.34	0.42
13:N:223:LEU:HD23	13:N:223:LEU:HA	1.82	0.42
15:Q:219:ASP:OD2	15:Q:239:TYR:OH	2.30	0.42
22:j:287:DA:H2'	22:j:288:DT:H72	2.01	0.42
24:f:35:ARG:O	24:f:39:ARG:HG2	2.19	0.42
24:f:75:HIS:CD2	26:h:93:THR:OG1	2.71	0.42
1:A:314:PHE:CZ	1:A:407:ARG:HG3	2.54	0.42
11:J:482:LEU:HD23	11:J:482:LEU:HA	1.91	0.42
15:Q:376:TRP:CG	15:Q:377:CYS:H	2.37	0.42
22:i:91:DT:H2''	22:i:92:DT:C5'	2.43	0.42
3:B:445:ASP:HA	3:B:448:TYR:CE1	2.55	0.42
4:P:83:ASP:O	4:P:86:GLU:HG3	2.18	0.42
22:j:182:DT:H2''	22:j:183:DT:OP2	2.18	0.42
23:a:63:ARG:HH22	24:b:30:THR:HG21	1.84	0.42
24:f:19:ARG:HA	24:f:19:ARG:NH1	2.32	0.42
1:A:122:ARG:CG	1:A:122:ARG:NH1	2.66	0.42
11:I:158:ALA:HB2	15:Q:186:LEU:HD12	2.01	0.42
11:J:479:ILE:HD11	11:K:475:LEU:HD21	2.01	0.42
13:N:85:MET:SD	13:N:103:LYS:HB3	2.59	0.42
15:Q:146:ASP:OD1	15:Q:147:ILE:N	2.52	0.42
22:i:64:DT:C2'	22:i:65:DT:H5''	2.50	0.42
22:i:131:DG:H2''	22:i:132:DC:C6	2.55	0.42
25:c:58:LEU:HD11	26:d:99:LEU:HD11	2.01	0.42
26:d:120:SER:C	26:d:122:LYS:N	2.77	0.42
11:L:121:THR:O	11:L:125:ILE:HG13	2.20	0.42
12:M:30:LEU:HA	12:M:30:LEU:HD23	1.86	0.42
13:N:148:ASP:OD1	13:N:149:SER:N	2.50	0.42
14:O:13:PHE:CE1	14:O:134:GLU:HB3	2.55	0.42
14:O:44:PRO:HA	14:O:47:ILE:HG13	2.00	0.42
22:i:136:DT:C2'	22:i:137:DG:C8	3.02	0.42
22:j:192:DG:H2''	22:j:193:DC:C5'	2.38	0.42
26:h:67:PHE:CD1	26:h:67:PHE:C	2.97	0.42
1:A:300:THR:C	1:A:301:LEU:HD23	2.44	0.42
3:B:275:LYS:HA	3:B:275:LYS:HD2	1.91	0.42
10:H:523:GLU:HG2	10:H:606:CYS:SG	2.59	0.42
11:I:135:GLU:HG2	11:I:136:TYR:H	1.84	0.42
11:L:90:ASP:HB3	11:L:93:LYS:HB2	2.02	0.42
11:L:119:LYS:HG3	11:L:122:ARG:NH2	2.34	0.42
15:Q:356:ASP:N	15:Q:374:SER:HA	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:i:120:DT:H2''	22:i:121:DG:C8	2.55	0.42
22:j:238:DT:H1'	22:j:239:DT:H5'	2.01	0.42
1:A:197:LEU:HD11	1:A:231:PHE:CE1	2.55	0.42
7:E:320:LEU:HB3	11:L:73:LEU:HD11	2.02	0.42
8:F:818:TRP:HA	11:L:287:PHE:HD1	1.85	0.42
12:M:332:LEU:HD23	13:N:565:PRO:HB3	2.00	0.42
12:M:371:ASP:OD1	12:M:371:ASP:N	2.53	0.42
23:a:101:VAL:O	23:a:105:GLU:HG3	2.19	0.42
3:B:6:GLN:O	3:B:24:GLY:HA2	2.19	0.42
12:M:7:PRO:HB2	14:O:282:LEU:HB3	2.02	0.42
13:N:328:LYS:HE2	13:N:328:LYS:HB3	1.87	0.42
13:N:338:ALA:O	13:N:342:ASN:ND2	2.52	0.42
14:O:173:ASP:OD1	14:O:173:ASP:N	2.48	0.42
22:j:185:DG:C5	22:j:186:DG:C6	3.08	0.42
1:A:381:PRO:O	1:A:383:GLN:N	2.53	0.42
3:B:429:PHE:HE1	3:B:433:GLN:HE21	1.68	0.42
4:P:9:LYS:HD2	4:P:12:LYS:NZ	2.34	0.42
13:N:298:LEU:HD12	13:N:304:LEU:HD23	2.01	0.42
14:O:270:HIS:ND1	14:O:271:PRO:HD2	2.34	0.42
22:j:246:DG:C1'	22:j:247:DC:H5''	2.43	0.42
1:A:442:THR:O	2:R:339:ARG:NH2	2.53	0.41
1:A:451:LEU:HA	1:A:451:LEU:HD23	1.81	0.41
2:R:133:ASP:HA	14:O:427:LYS:NZ	2.34	0.41
11:K:493:LYS:HG3	11:K:510:GLU:HG2	2.02	0.41
13:N:274:LYS:HB2	13:N:277:GLU:HB3	2.02	0.41
22:i:64:DT:H1'	22:i:65:DT:H5''	2.02	0.41
22:i:100:DG:H1'	22:i:101:DC:C5	2.55	0.41
22:i:129:DC:H2''	22:i:130:DT:C7	2.49	0.41
22:j:149:DC:H1'	22:j:150:DA:H5''	2.02	0.41
22:j:154:DT:H5'	22:j:154:DT:C6	2.55	0.41
25:g:116:LEU:HA	25:g:117:PRO:HD3	1.78	0.41
1:A:150:GLY:N	2:R:336:ILE:CD1	2.83	0.41
2:R:63:ARG:HH21	11:L:287:PHE:HA	1.85	0.41
3:B:26:ASN:HB3	3:B:29:THR:O	2.20	0.41
11:I:260:CYS:SG	11:I:262:THR:OG1	2.76	0.41
14:O:222:PRO:HG2	14:O:226:PHE:CE2	2.55	0.41
22:j:219:DA:H2''	22:j:220:DT:C5'	2.46	0.41
24:b:35:ARG:HD3	24:b:51:TYR:OH	2.20	0.41
23:e:37:LYS:N	23:e:38:PRO:CA	2.83	0.41
1:A:235:MET:SD	3:B:401:VAL:HG21	2.61	0.41
1:A:235:MET:HE1	1:A:288:LYS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:248:LEU:HD23	2:R:248:LEU:HA	1.85	0.41
2:R:360:LEU:HD21	3:B:438:GLN:NE2	2.35	0.41
6:D:110:HIS:NE2	6:D:115:CYS:SG	2.93	0.41
11:J:447:LEU:HD23	11:J:447:LEU:HA	1.91	0.41
13:N:90:LEU:HD23	13:N:90:LEU:HA	1.93	0.41
14:O:239:ASN:ND2	14:O:482:ASN:O	2.53	0.41
22:j:164:DG:H1'	22:j:165:DA:C8	2.56	0.41
22:j:185:DG:H4'	25:g:42:ARG:CZ	2.50	0.41
1:A:446:LEU:HD11	2:R:332:ILE:CD1	2.47	0.41
2:R:184:THR:HG21	12:M:451:ASN:O	2.21	0.41
10:H:457:PHE:HB3	10:H:483:GLU:HG3	2.03	0.41
22:i:101:DC:OP1	24:f:79:LYS:HB2	2.20	0.41
22:j:249:DG:H2''	22:j:250:DT:H5'	2.02	0.41
7:E:407:LYS:HA	7:E:410:TYR:CZ	2.55	0.41
8:F:807:GLY:O	11:L:316:SER:HB2	2.21	0.41
22:i:55:DA:H2''	22:i:56:DA:O5'	2.20	0.41
22:i:62:DT:H2''	22:i:63:DG:H8	1.84	0.41
22:i:73:DA:H2''	22:i:74:DT:H5''	2.02	0.41
22:i:95:DA:H2''	22:i:96:DT:H5'	2.00	0.41
22:j:165:DA:C2'	22:j:166:DT:H5''	2.51	0.41
22:j:235:DC:H2''	22:j:236:DT:H71	2.01	0.41
23:a:100:LEU:HD11	24:b:58:LEU:HD12	2.01	0.41
24:f:31:LYS:N	24:f:32:PRO:HD2	2.35	0.41
3:B:91:LEU:CD2	3:B:106:LEU:HD22	2.50	0.41
11:I:259:ILE:HD12	13:N:43:GLN:HG2	2.02	0.41
13:N:361:ILE:HA	13:N:512:ASN:HD21	1.86	0.41
22:i:101:DC:OP1	24:f:79:LYS:N	2.42	0.41
22:i:123:DT:OP1	26:h:30:ARG:HB2	2.20	0.41
22:j:205:DG:H2''	22:j:206:DC:H5'	2.02	0.41
23:a:79:LYS:HB3	23:a:82:LEU:HD11	2.02	0.41
25:g:20:ARG:O	26:h:118:TYR:HA	2.20	0.41
1:A:139:VAL:HG11	1:A:443:MET:HG3	2.03	0.41
3:B:112:LEU:HD12	3:B:141:ILE:HD12	2.02	0.41
5:C:61:SER:O	5:C:65:MET:HG2	2.20	0.41
12:M:223:GLN:HG3	12:M:224:LEU:H	1.85	0.41
13:N:561:LEU:HD22	13:N:568:THR:HA	2.03	0.41
22:i:37:DT:C2'	22:i:38:DT:H5''	2.51	0.41
22:j:207:DA:H2''	22:j:208:DT:H5'	2.02	0.41
22:j:285:DA:H2''	22:j:286:DT:C5'	2.51	0.41
2:R:62:TYR:O	2:R:66:GLN:HG3	2.21	0.41
14:O:37:ALA:HB3	14:O:73:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:43:ASN:HD21	14:O:46:LYS:HD2	1.86	0.41
22:i:90:DT:P	23:e:69:ARG:HH22	2.43	0.41
26:d:39:TYR:O	26:d:43:LYS:HG2	2.20	0.41
1:A:418:GLN:HG2	1:A:419:TYR:CD1	2.55	0.41
2:R:360:LEU:HD21	3:B:438:GLN:HE21	1.86	0.41
2:R:365:GLU:O	2:R:369:GLN:HG3	2.21	0.41
3:B:154:ILE:O	3:B:154:ILE:HG22	2.21	0.41
7:E:352:ALA:O	15:Q:19:ARG:HD2	2.21	0.41
8:F:862:GLY:HA3	8:F:864:PHE:CE2	2.56	0.41
11:K:440:LEU:HD13	12:M:39:MET:HE2	2.02	0.41
12:M:316:ASP:N	12:M:316:ASP:OD1	2.53	0.41
12:M:338:THR:O	12:M:342:LEU:HG	2.21	0.41
12:M:365:ALA:O	12:M:367:THR:HG23	2.21	0.41
13:N:275:ALA:HB2	13:N:318:PRO:O	2.20	0.41
15:Q:377:CYS:HB2	15:Q:378:PRO:HD2	2.03	0.41
22:i:13:DC:H2''	22:i:14:DT:C6	2.56	0.41
22:i:64:DT:C2'	22:i:65:DT:C5'	2.92	0.41
22:i:85:DA:H2''	22:i:86:DT:C5'	2.51	0.41
22:i:116:DC:C2'	22:i:117:DT:H72	2.51	0.41
22:i:118:DT:H5'	22:i:118:DT:H6	1.86	0.41
22:i:140:DT:C1'	22:i:141:DA:H5''	2.51	0.41
22:j:207:DA:H1'	22:j:208:DT:C5'	2.49	0.41
22:j:236:DT:H2''	22:j:237:DT:OP2	2.20	0.41
22:j:242:DT:H6	22:j:242:DT:H2'	1.78	0.41
23:a:65:LEU:HB3	23:a:66:PRO:HD3	2.03	0.41
26:h:96:ARG:NH1	26:h:108:VAL:HG21	2.35	0.41
1:A:442:THR:CB	2:R:339:ARG:HH21	2.34	0.41
1:A:458:GLU:O	1:A:460:TYR:N	2.53	0.41
12:M:405:LEU:HD12	12:M:405:LEU:HA	1.92	0.41
22:i:123:DT:H2''	22:i:124:DA:C8	2.56	0.41
22:j:174:DA:H1'	22:j:175:DA:C5'	2.50	0.41
23:a:120:MET:C	24:b:50:ILE:HD11	2.46	0.41
26:h:36:VAL:CG2	26:h:37:TYR:N	2.84	0.41
1:A:153:SER:HG	1:A:171:ASP:H	1.66	0.40
14:O:117:TYR:OH	14:O:215:ASP:OD2	2.30	0.40
22:i:9:DC:H6	22:i:9:DC:H5'	1.86	0.40
22:i:15:DG:N2	22:j:279:DA:C2	2.89	0.40
22:i:118:DT:H5'	22:i:118:DT:C6	2.56	0.40
22:i:125:DG:H2''	22:i:126:DA:H8	1.85	0.40
1:A:108:MET:SD	1:A:123:TYR:HE2	2.43	0.40
2:R:360:LEU:CD2	3:B:438:GLN:HE21	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:312:ARG:HA	3:B:312:ARG:HD3	1.79	0.40
10:H:502:LEU:HD11	10:H:509:LEU:HD11	2.03	0.40
11:I:148:MET:HE2	11:I:148:MET:HB3	1.95	0.40
13:N:565:PRO:N	13:N:566:PRO:HD2	2.36	0.40
15:Q:358:ALA:H	15:Q:371:GLU:CB	2.32	0.40
22:i:129:DC:C2'	22:i:130:DT:H71	2.51	0.40
24:f:35:ARG:HG2	24:f:35:ARG:HH11	1.86	0.40
26:h:103:LEU:HD12	26:h:103:LEU:HA	1.85	0.40
1:A:389:LEU:HD22	1:A:421:LEU:CD2	2.52	0.40
2:R:365:GLU:CG	3:B:415:TYR:CD1	3.03	0.40
13:N:131:ILE:O	13:N:134:LEU:HB3	2.21	0.40
14:O:170:THR:HG22	14:O:172:LEU:N	2.36	0.40
22:j:220:DT:H2'	22:j:221:DT:H71	2.04	0.40
22:j:262:DC:C1'	22:j:263:DT:H5''	2.51	0.40
3:B:146:SER:O	3:B:149:ALA:HB3	2.21	0.40
11:I:175:LYS:HE2	11:L:192:ASP:OD1	2.21	0.40
13:N:289:LEU:O	13:N:293:VAL:HG23	2.21	0.40
22:j:223:DA:H1'	22:j:224:DG:C8	2.57	0.40
23:a:96:CYS:SG	24:b:62:LEU:HD21	2.62	0.40
24:b:26:ILE:O	24:b:55:ARG:HD3	2.21	0.40
24:b:62:LEU:O	24:b:66:ILE:HG13	2.21	0.40
1:A:381:PRO:HG2	1:A:382:GLU:H	1.86	0.40
2:R:104:ILE:HG23	14:O:410:PHE:HD1	1.87	0.40
2:R:329:ILE:C	2:R:332:ILE:HG22	2.44	0.40
7:E:331:ASN:HD22	11:L:137:LEU:HD12	1.87	0.40
10:H:489:ASN:OD1	10:H:489:ASN:N	2.54	0.40
10:H:515:LEU:HD11	10:H:523:GLU:CD	2.47	0.40
11:L:320:MET:HE1	11:L:353:LYS:HE3	2.03	0.40
12:M:50:ARG:HA	12:M:50:ARG:HD3	1.78	0.40
24:b:98:TYR:CZ	25:g:100:VAL:HG11	2.57	0.40
25:g:26:PRO:O	25:g:30:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/477 (82%)	369 (94%)	18 (5%)	5 (1%)	9	42
2	R	319/1359 (24%)	296 (93%)	23 (7%)	0	100	100
3	B	391/467 (84%)	368 (94%)	21 (5%)	2 (0%)	24	63
4	P	46/157 (29%)	43 (94%)	2 (4%)	1 (2%)	5	29
5	C	58/78 (74%)	56 (97%)	2 (3%)	0	100	100
6	D	96/180 (53%)	90 (94%)	6 (6%)	0	100	100
7	E	118/435 (27%)	108 (92%)	10 (8%)	0	100	100
8	F	63/889 (7%)	56 (89%)	7 (11%)	0	100	100
9	G	51/885 (6%)	49 (96%)	2 (4%)	0	100	100
10	H	127/625 (20%)	114 (90%)	10 (8%)	3 (2%)	4	27
11	I	289/557 (52%)	274 (95%)	15 (5%)	0	100	100
11	J	113/557 (20%)	109 (96%)	4 (4%)	0	100	100
11	K	105/557 (19%)	101 (96%)	4 (4%)	0	100	100
11	L	292/557 (52%)	277 (95%)	15 (5%)	0	100	100
12	M	302/483 (62%)	281 (93%)	21 (7%)	0	100	100
13	N	408/581 (70%)	380 (93%)	28 (7%)	0	100	100
14	O	376/502 (75%)	352 (94%)	24 (6%)	0	100	100
15	Q	258/426 (61%)	224 (87%)	34 (13%)	0	100	100
16	S	32/883 (4%)	32 (100%)	0	0	100	100
23	a	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
23	e	97/136 (71%)	95 (98%)	2 (2%)	0	100	100
24	b	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
24	f	83/103 (81%)	80 (96%)	3 (4%)	0	100	100
25	c	106/130 (82%)	101 (95%)	5 (5%)	0	100	100
25	g	102/130 (78%)	98 (96%)	3 (3%)	1 (1%)	12	49
26	d	94/126 (75%)	89 (95%)	4 (4%)	1 (1%)	11	46
26	h	92/126 (73%)	88 (96%)	0	4 (4%)	2	17
All	All	4581/11645 (39%)	4297 (94%)	267 (6%)	17 (0%)	31	67

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	48	ASP
10	H	528	ILE
26	h	120	SER
1	A	343	SER
26	d	101	GLY
26	h	29	SER
26	h	30	ARG
26	h	101	GLY
1	A	382	GLU
1	A	459	ASP
4	P	84	LEU
10	H	529	ASN
1	A	431	ASP
1	A	458	GLU
3	B	155	SER
10	H	527	THR
25	g	117	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	357/420 (85%)	331 (93%)	26 (7%)	13	34
2	R	297/1228 (24%)	292 (98%)	5 (2%)	53	69
3	B	363/423 (86%)	344 (95%)	19 (5%)	21	42
4	P	53/140 (38%)	51 (96%)	2 (4%)	29	50
5	C	58/75 (77%)	58 (100%)	0	100	100
6	D	82/151 (54%)	82 (100%)	0	100	100
7	E	113/388 (29%)	105 (93%)	8 (7%)	13	35
8	F	60/810 (7%)	60 (100%)	0	100	100
9	G	48/832 (6%)	47 (98%)	1 (2%)	47	65
10	H	126/578 (22%)	123 (98%)	3 (2%)	43	64
11	I	268/500 (54%)	259 (97%)	9 (3%)	32	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	J	111/500 (22%)	110 (99%)	1 (1%)	70	79
11	K	106/500 (21%)	105 (99%)	1 (1%)	70	79
11	L	270/500 (54%)	267 (99%)	3 (1%)	65	76
12	M	286/435 (66%)	281 (98%)	5 (2%)	53	69
13	N	374/521 (72%)	364 (97%)	10 (3%)	39	61
14	O	358/462 (78%)	351 (98%)	7 (2%)	48	66
15	Q	243/384 (63%)	233 (96%)	10 (4%)	27	49
16	S	33/824 (4%)	32 (97%)	1 (3%)	36	57
23	a	85/111 (77%)	82 (96%)	3 (4%)	32	53
23	e	86/111 (78%)	82 (95%)	4 (5%)	23	45
24	b	63/79 (80%)	63 (100%)	0	100	100
24	f	70/79 (89%)	67 (96%)	3 (4%)	26	47
25	c	85/100 (85%)	80 (94%)	5 (6%)	18	39
25	g	83/100 (83%)	78 (94%)	5 (6%)	17	39
26	d	82/105 (78%)	76 (93%)	6 (7%)	13	34
26	h	80/105 (76%)	77 (96%)	3 (4%)	29	50
All	All	4240/10461 (40%)	4100 (97%)	140 (3%)	34	55

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

Mol	Chain	Res	Type
1	A	2	THR
1	A	36	ILE
1	A	88	ARG
1	A	122	ARG
1	A	135	VAL
1	A	159	ILE
1	A	195	GLU
1	A	216	ARG
1	A	218	THR
1	A	230	GLN
1	A	246	LEU
1	A	251	LYS
1	A	262	GLU
1	A	301	LEU
1	A	319	ILE

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Mol	Chain	Res	Type
1	A	321	ASP
1	A	343	SER
1	A	380	SER
1	A	382	GLU
1	A	386	SER
1	A	397	SER
1	A	414	ILE
1	A	418	GLN
1	A	432	ARG
1	A	442	THR
1	A	462	THR
2	R	215	THR
2	R	262	ILE
2	R	265	VAL
2	R	295	VAL
2	R	297	VAL
3	B	7	ASP
3	B	32	VAL
3	B	34	GLU
3	B	41	ILE
3	B	48	ASP
3	B	52	THR
3	B	54	HIS
3	B	56	THR
3	B	69	GLN
3	B	94	ARG
3	B	100	ASP
3	B	105	GLU
3	B	122	SER
3	B	197	SER
3	B	291	GLU
3	B	321	ASP
3	B	347	GLU
3	B	422	SER
3	B	438	GLN
4	P	81	ILE
4	P	90	ARG
7	E	327	CYS
7	E	351	ASP
7	E	356	ILE
7	E	359	ILE
7	E	384	ILE

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Mol	Chain	Res	Type
7	E	413	VAL
7	E	414	VAL
7	E	417	ASP
9	G	175	ASP
10	H	510	THR
10	H	527	THR
10	H	528	ILE
11	I	170	ILE
11	I	179	ILE
11	I	189	VAL
11	I	191	LEU
11	I	253	GLN
11	I	270	VAL
11	I	275	LEU
11	I	281	ASN
11	I	312	LYS
11	J	459	LEU
11	K	503	ASP
11	L	80	VAL
11	L	189	VAL
11	L	279	ASP
12	M	58	LEU
12	M	62	THR
12	M	232	VAL
12	M	316	ASP
12	M	466	ASN
13	N	33	VAL
13	N	79	VAL
13	N	91	SER
13	N	104	TYR
13	N	123	LEU
13	N	166	ARG
13	N	170	GLN
13	N	348	ILE
13	N	553	ILE
13	N	578	THR
14	O	88	ILE
14	O	173	ASP
14	O	208	ILE
14	O	269	LEU
14	O	274	TYR
14	O	279	THR

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Mol	Chain	Res	Type
14	O	490	VAL
15	Q	165	ILE
15	Q	192	THR
15	Q	250	LEU
15	Q	262	LEU
15	Q	342	ASP
15	Q	345	ASP
15	Q	351	ASP
15	Q	352	HIS
15	Q	353	VAL
15	Q	368	ASP
16	S	198	LEU
23	a	59	GLU
23	a	63	ARG
23	a	129	ARG
25	c	29	ARG
25	c	59	THR
25	c	81	ARG
25	c	84	GLN
25	c	101	THR
26	d	28	ARG
26	d	54	LYS
26	d	68	GLU
26	d	77	LEU
26	d	85	THR
26	d	98	LEU
23	e	63	ARG
23	e	68	GLN
23	e	79	LYS
23	e	122	LYS
24	f	19	ARG
24	f	92	ARG
24	f	93	GLN
25	g	64	GLU
25	g	81	ARG
25	g	99	ARG
25	g	101	THR
25	g	118	LYS
26	h	85	THR
26	h	102	GLU
26	h	103	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	137	GLN
2	R	57	GLN
2	R	72	ASN
2	R	116	ASN
2	R	201	ASN
2	R	270	HIS
2	R	290	GLN
2	R	340	GLN
2	R	361	HIS
3	B	167	HIS
3	B	303	ASN
3	B	304	ASN
3	B	433	GLN
3	B	438	GLN
6	D	64	HIS
6	D	108	HIS
7	E	331	ASN
7	E	376	ASN
7	E	396	ASN
8	F	800	ASN
8	F	877	HIS
10	H	465	GLN
10	H	478	ASN
10	H	493	GLN
10	H	506	GLN
10	H	512	GLN
10	H	601	HIS
10	H	622	ASN
11	I	60	GLN
11	I	63	GLN
11	I	167	ASN
11	I	227	ASN
11	I	253	GLN
11	I	314	ASN
11	J	430	GLN
11	J	478	GLN
11	K	426	GLN
11	K	501	GLN
11	L	145	ASN
11	L	188	GLN
11	L	291	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	L	318	GLN
12	M	61	ASN
12	M	233	GLN
12	M	329	HIS
12	M	340	ASN
12	M	378	GLN
12	M	380	GLN
13	N	43	GLN
13	N	512	ASN
13	N	559	HIS
13	N	577	ASN
14	O	22	ASN
14	O	97	HIS
14	O	270	HIS
14	O	272	ASN
14	O	391	GLN
14	O	484	ASN
15	Q	3	HIS
15	Q	158	GLN
15	Q	164	ASN
15	Q	261	GLN
23	a	76	GLN
23	a	85	GLN
23	a	113	HIS
24	b	75	HIS
25	c	31	HIS
25	c	38	ASN
25	c	73	ASN
25	c	84	GLN
25	c	112	GLN
26	d	60	ASN
24	f	75	HIS
24	f	93	GLN
25	g	24	GLN
25	g	31	HIS
25	g	73	ASN
26	h	44	GLN
26	h	79	HIS
26	h	92	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	7	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	7	57:UNK	C	60:UNK	N	4.98

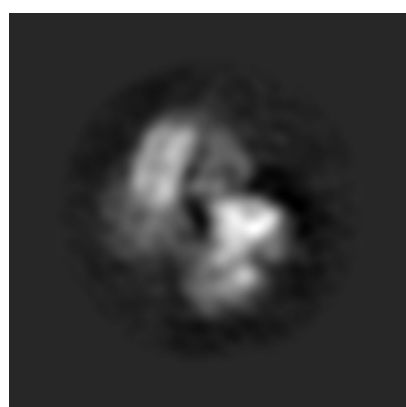
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21114. 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

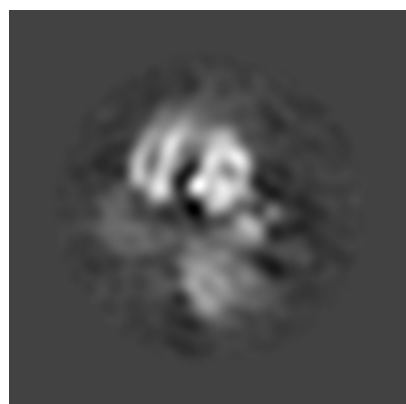


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 64



Y Index: 64



Z Index: 64

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

6.3 Largest variance slices [i](#)

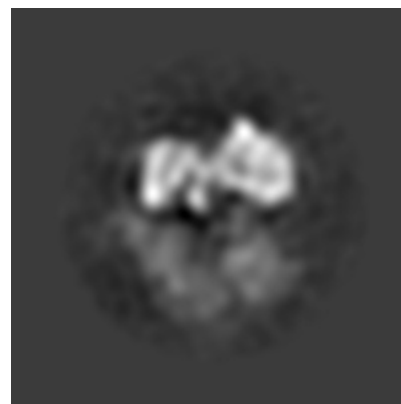
6.3.1 Primary map



X Index: 68



Y Index: 71

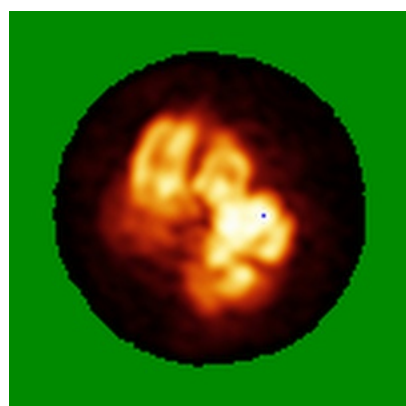


Z Index: 59

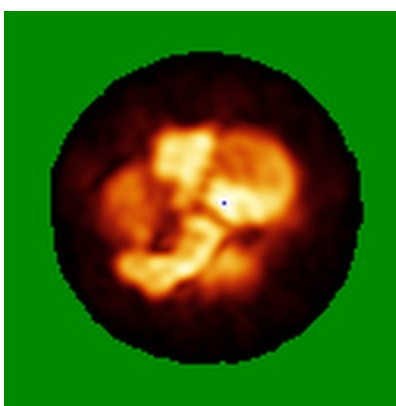
The images above show the largest variance slices of the map in three orthogonal directions.

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

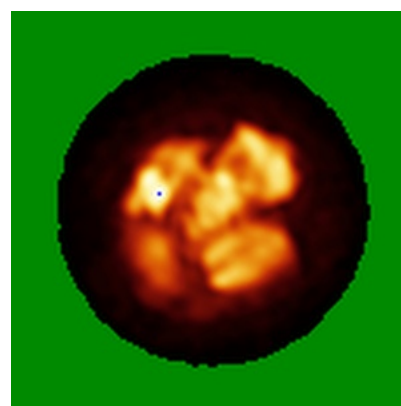
6.4.1 Primary map



X



Y



Z

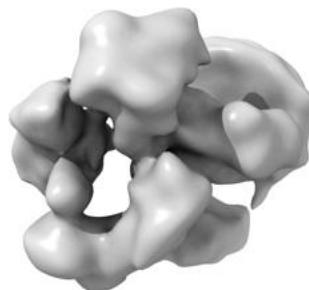
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

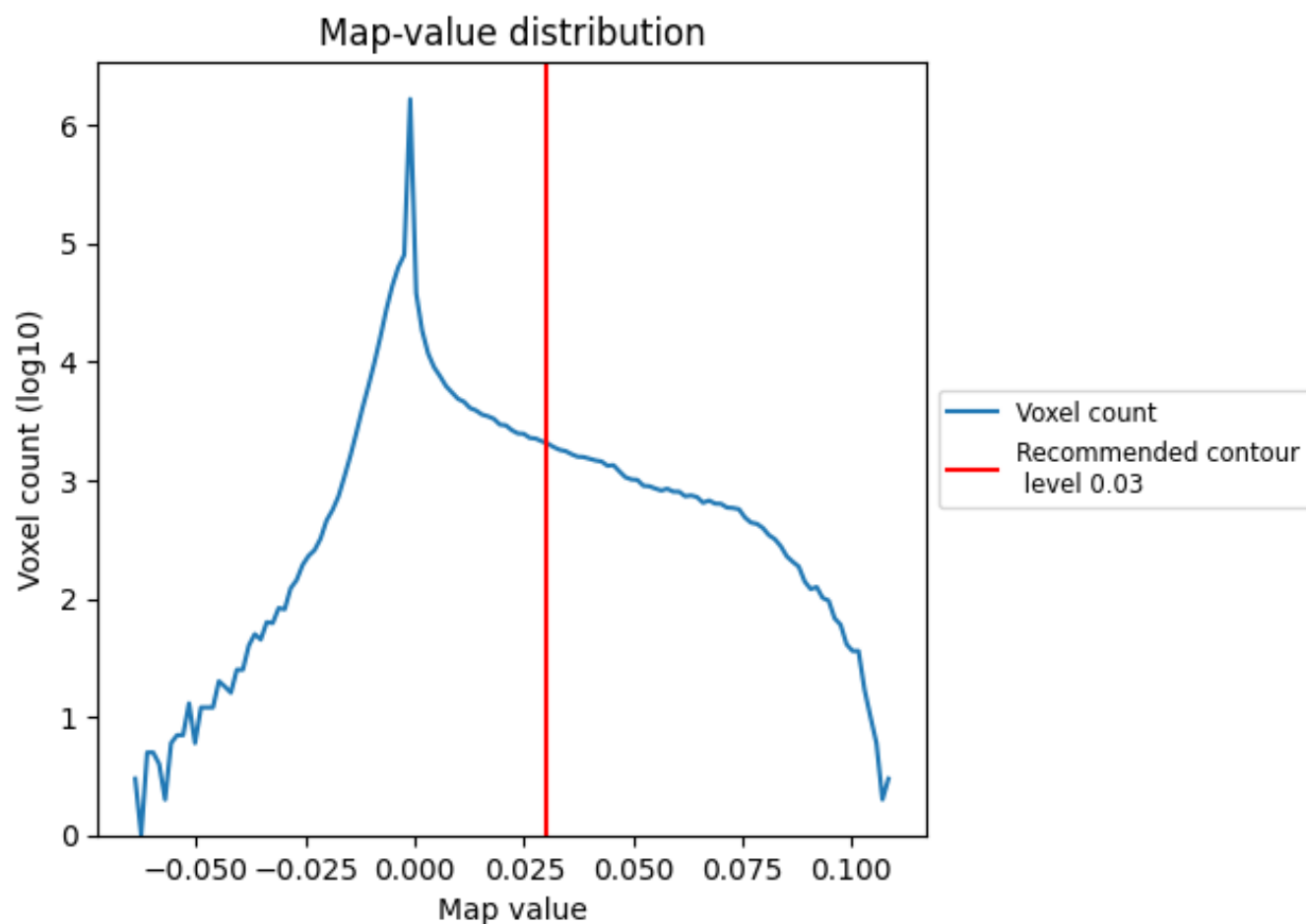
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

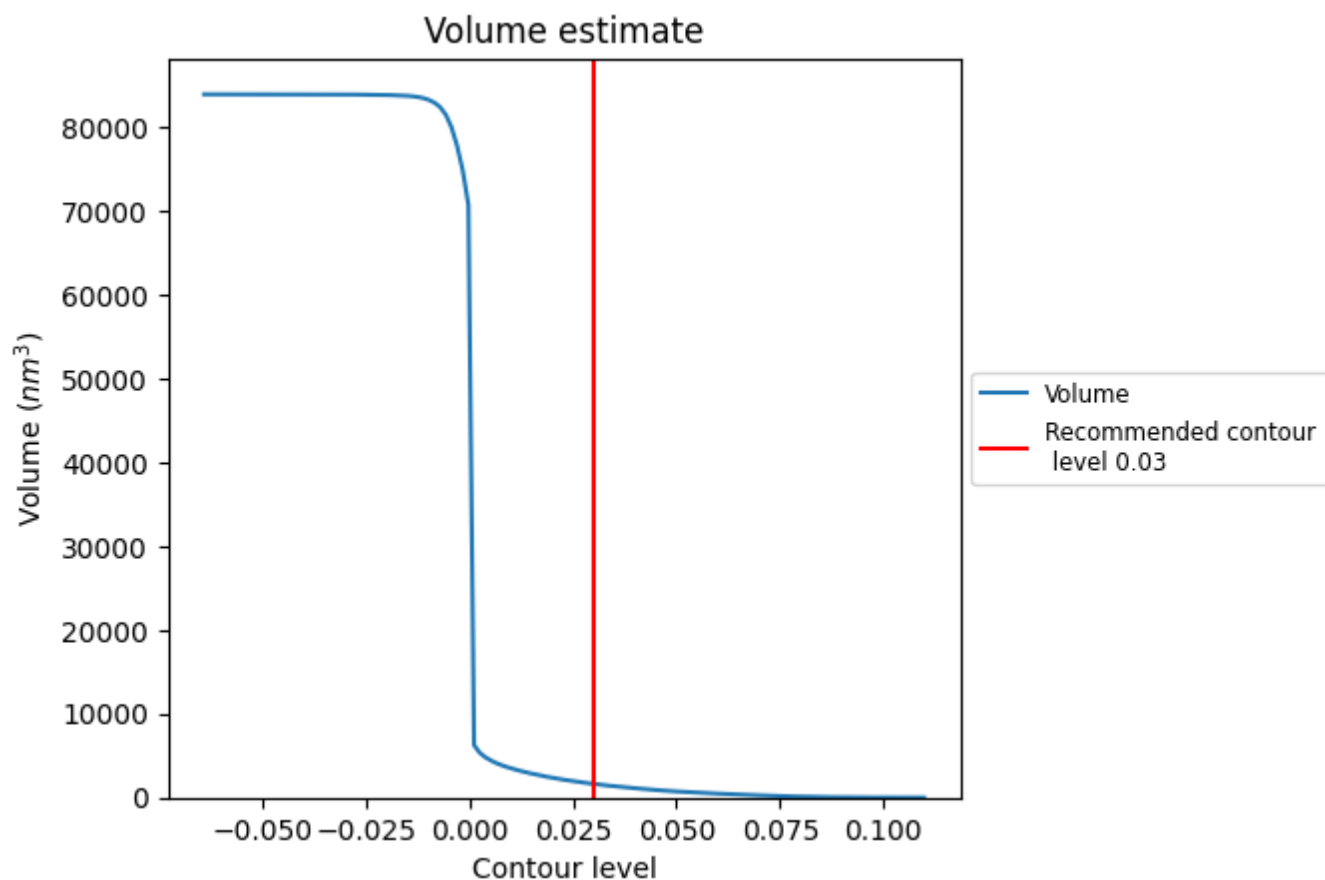
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

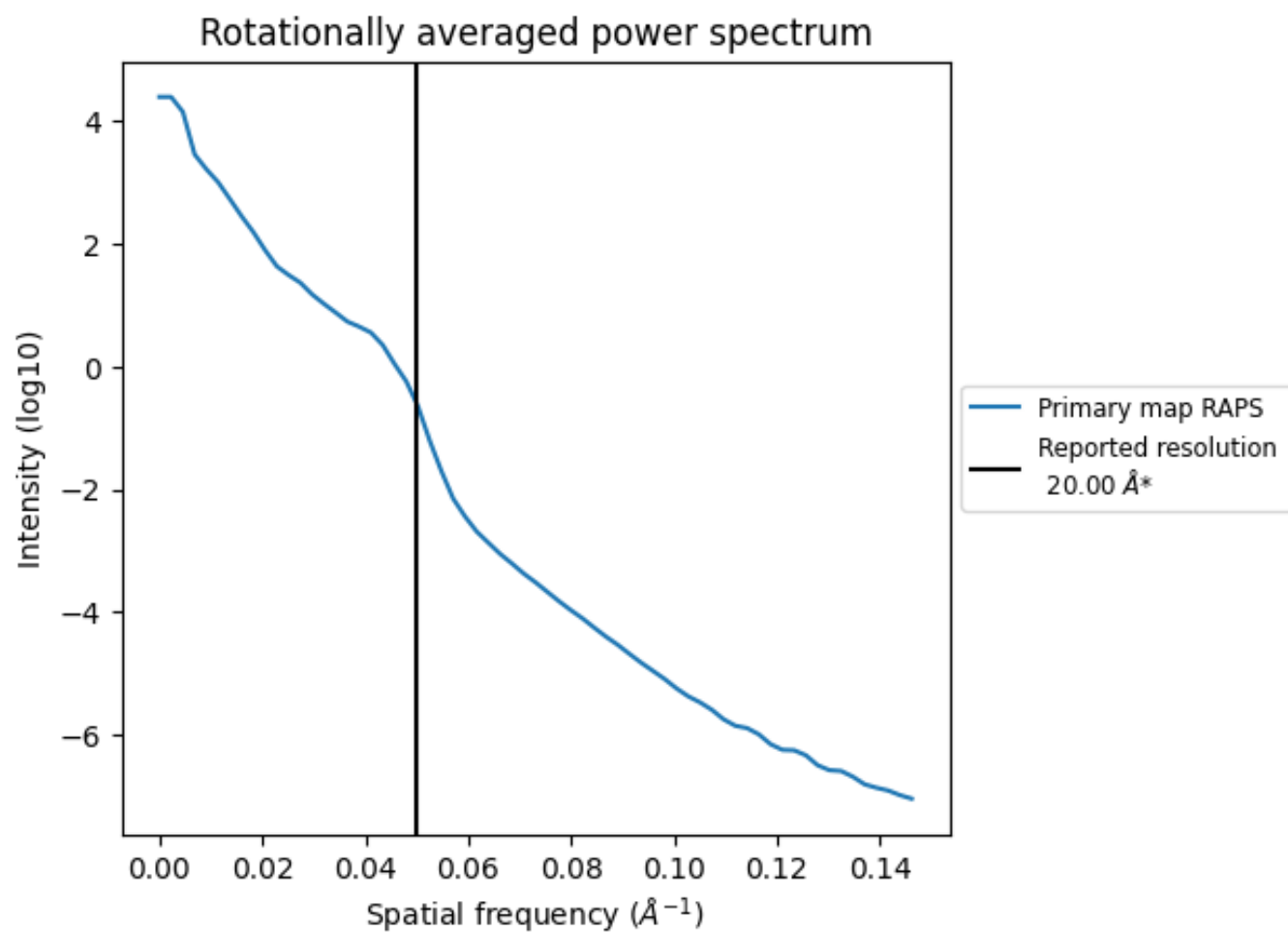
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1633 nm³; this corresponds to an approximate mass of 1475 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 0.050 Å⁻¹

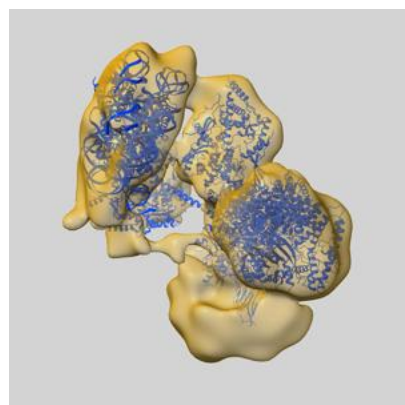
8 Fourier-Shell correlation ⓘ

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

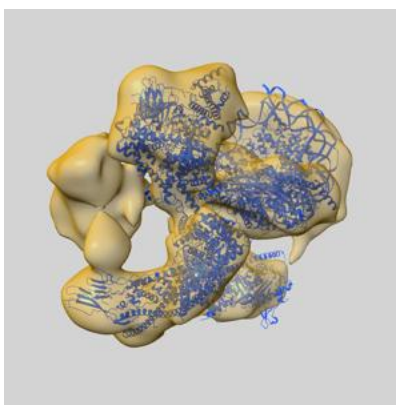
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21114 and PDB model 6V92. Per-residue inclusion information can be found in section [3](#) on page [10](#).

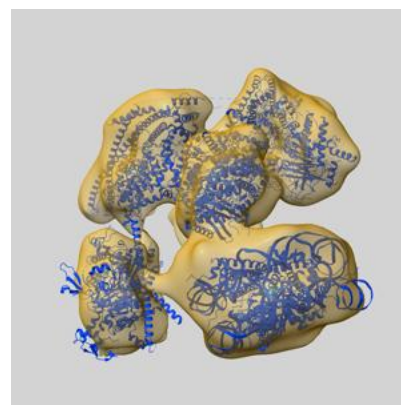
9.1 Map-model overlay [i](#)



X



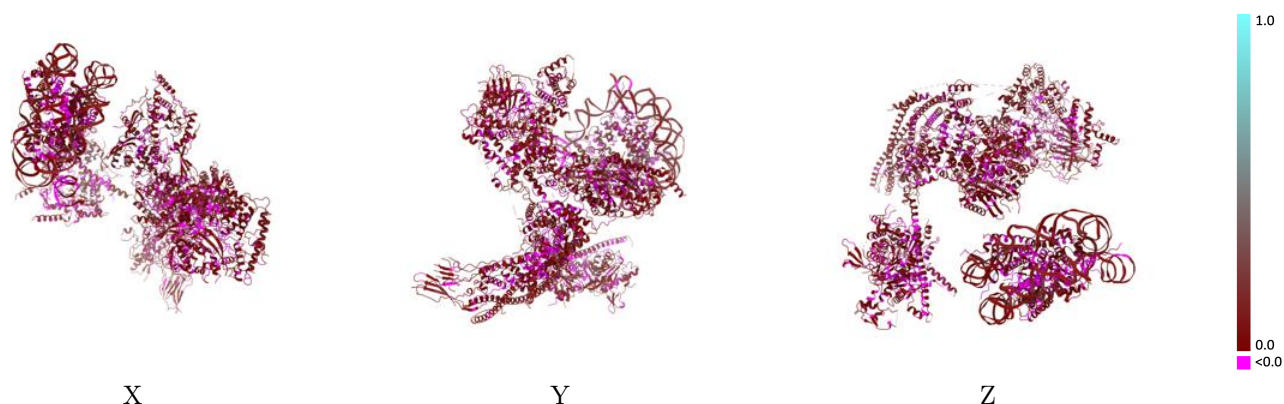
Y



Z

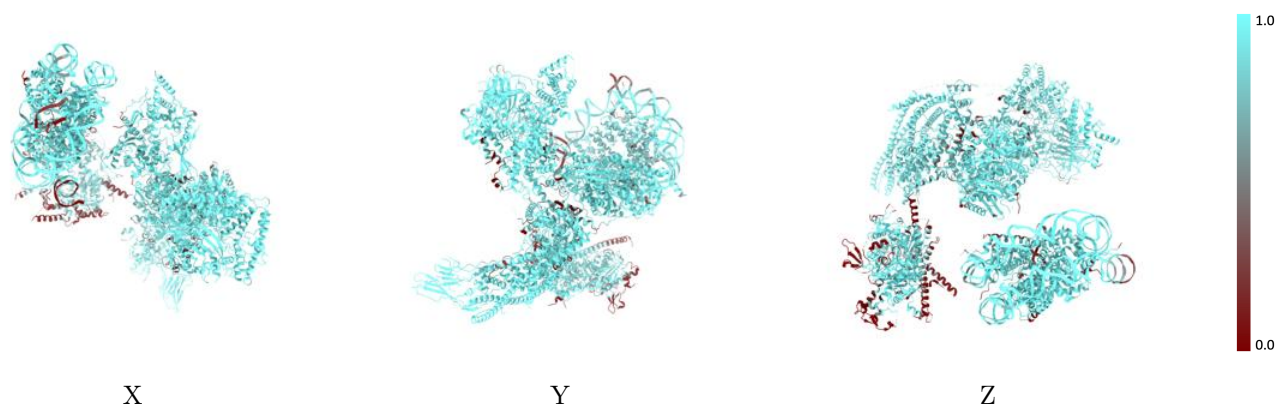
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



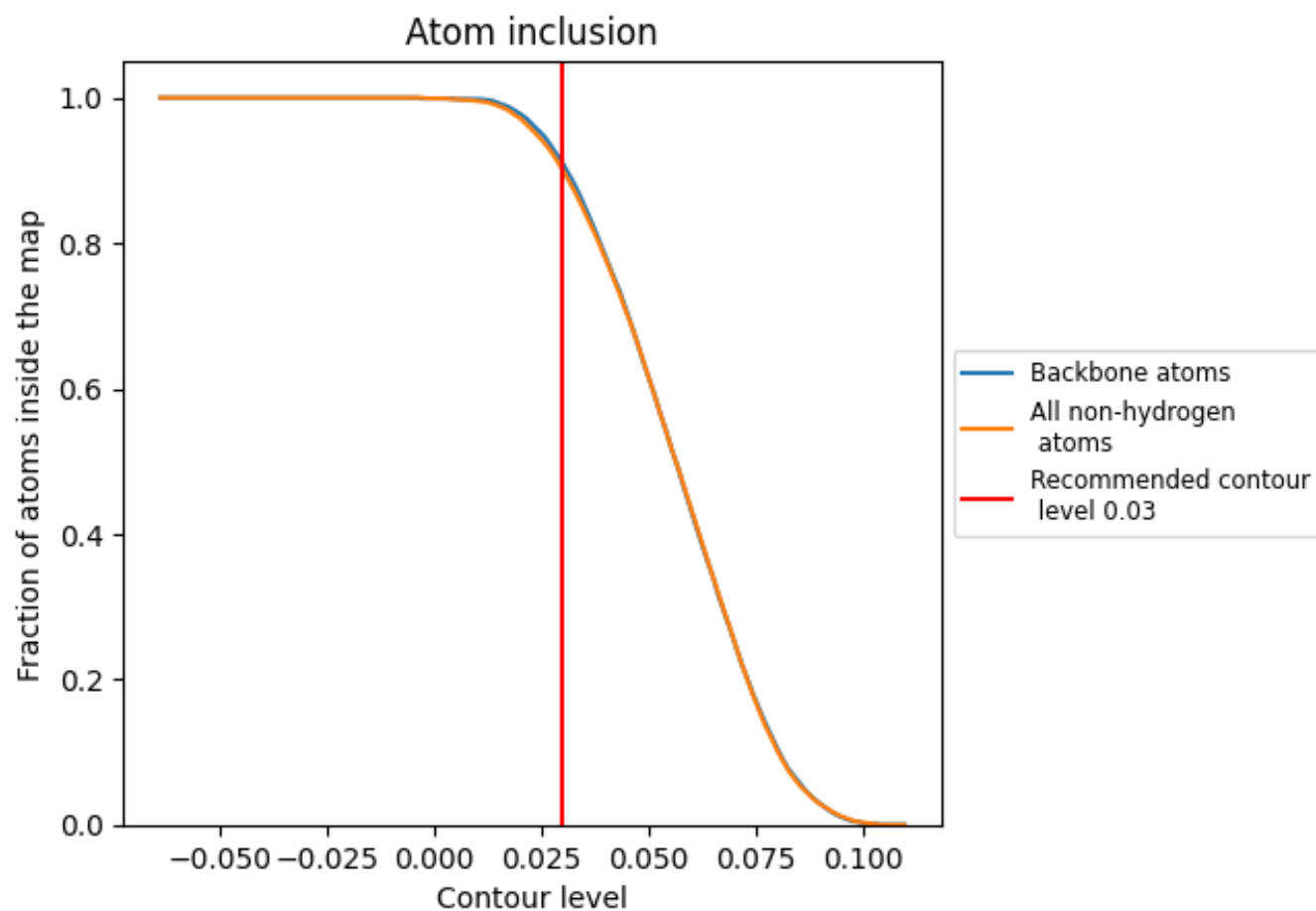
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 90% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9000	 0.0530
2	 1.0000	 0.0480
3	 0.5790	 0.0250
4	 0.9900	 0.0580
5	 0.5710	 0.0050
6	 1.0000	 0.0500
7	 0.9880	 0.0500
A	 0.6960	 0.0330
B	 0.7390	 0.0370
C	 0.9920	 0.0650
D	 0.8760	 0.0380
E	 0.9690	 0.0740
F	 1.0000	 0.0290
G	 0.8230	 0.0470
H	 0.9570	 0.0530
I	 0.9710	 0.0510
J	 0.9720	 0.0800
K	 0.9690	 0.0810
L	 0.9720	 0.0510
M	 0.9430	 0.0480
N	 0.9370	 0.0490
O	 0.9940	 0.0650
P	 0.6980	 0.0590
Q	 0.9560	 0.0660
R	 0.8230	 0.0410
S	 0.7630	 0.0680
a	 0.9360	 0.0280
b	 0.9900	 0.0440
c	 0.9580	 0.0380
d	 0.8560	 0.0200
e	 0.9550	 0.0430
f	 0.9950	 0.0050
g	 0.8830	 0.0110
h	 0.9370	 0.0120
i	 0.8990	 0.0860
j	 0.8970	 0.0930

