



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 04:32 AM UTC

PDB ID : 6SPC / pdb_00006spc
EMDB ID : EMD-10281
Title : Pseudomonas aeruginosa 30s ribosome from an aminoglycoside resistant clinical isolate
Authors : Halfon, Y.; Jimenez-Fernande, A.; La Ros, R.; Espinos, R.; Krogh Johansen, H.; Matzov, D.; Eyal, Z.; Bashan, A.; Zimmerman, E.; Belousoff, M.; Molin, S.; Yonath, A.
Deposited on : 2019-09-01
Resolution : 2.95 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:

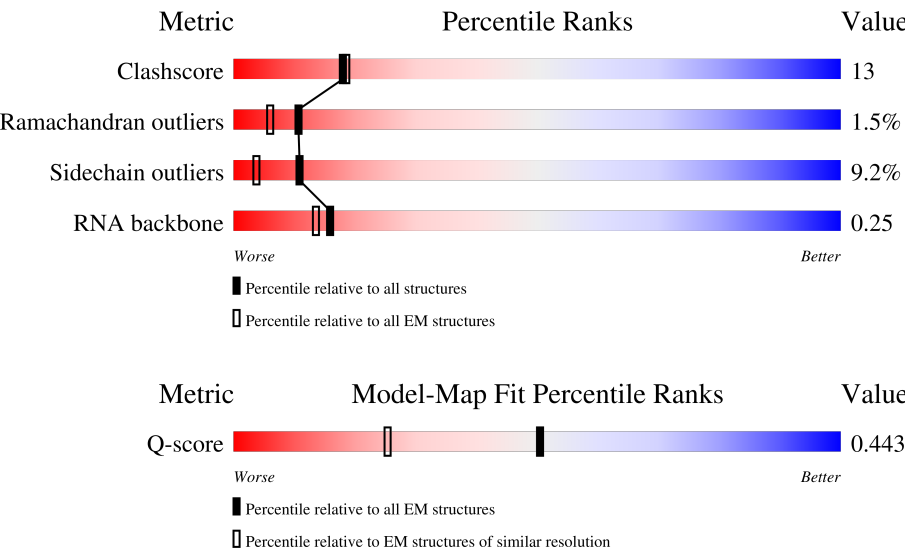
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.95 Å.

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



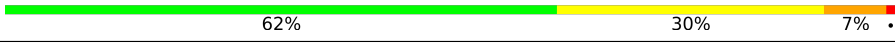
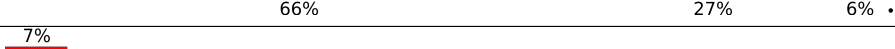
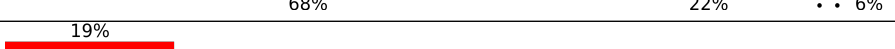
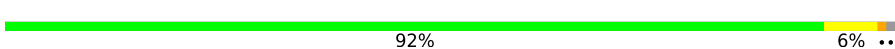
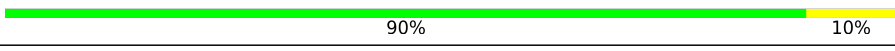
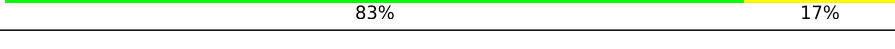
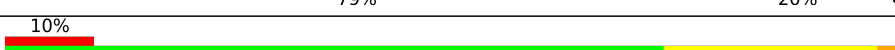
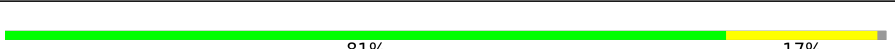
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13114 (2.45 - 3.45)

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	1519	
2	b	221	
3	c	203	

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Mol	Chain	Length	Quality of chain
4	d	205	
5	e	149	
6	f	100	
7	g	154	
8	h	125	
9	i	126	
10	j	96	
11	k	115	
12	l	120	
13	m	109	
14	n	98	
15	o	87	
16	p	78	
17	q	76	
18	r	56	
19	s	80	
20	t	86	
21	u	34	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 50569 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1519	Total	C	N	O	P	0	0
			32595	14540	5985	10552	1518		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	2	A	-	conflict	GB 1359201046
a	?	-	C	deletion	GB 1359201046
a	?	-	G	deletion	GB 1359201046
a	72	A	G	conflict	GB 1359201046
a	101	A	G	conflict	GB 1359201046

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	221	Total	C	N	O	S	0	0
			1728	1088	316	314	10		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	?	-	THR	deletion	UNP A0A072ZPV8
b	?	-	PHE	deletion	UNP A0A072ZPV8
b	?	-	ASP	deletion	UNP A0A072ZPV8
b	?	-	LYS	deletion	UNP A0A072ZPV8
b	?	-	LEU	deletion	UNP A0A072ZPV8

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	203	Total	C	N	O	S	0	0
			1609	1017	303	284	5		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	205	Total	C	N	O	S	0	0
			1600	991	310	294	5		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	149	Total	C	N	O	S	0	0
			1092	687	202	197	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	?	-	ALA	deletion	UNP A0A241XG65

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	100	Total	C	N	O	S	0	0
			802	497	152	149	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	80	ALA	TYR	conflict	UNP A0A069Q263

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	154	Total	C	N	O	S	0	0
			1190	747	227	211	5		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	123	Total	C	N	O	S	0	0
			915	575	161	174	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	94	ALA	LYS	conflict	UNP E2RXT9
h	129	VAL	LEU	conflict	UNP E2RXT9

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	126	Total	C	N	O	S	0	0
			994	616	198	179	1		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	96	Total	C	N	O	S	0	0
			763	479	143	140	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	115	Total	C	N	O	S	0	0
			828	511	159	156	2		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	113	Total	C	N	O	S	0	0
			893	547	184	158	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	109	Total	C	N	O	S	0	0
			847	515	173	155	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	?	-	TYR	deletion	UNP E2RXU3

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	98	Total	C	N	O	S	0	0
			776	479	163	131	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	86	Total	C	N	O	S	0	0
			686	425	134	126	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	78	Total	C	N	O		0	0
			606	379	120	107			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	76	Total	C	N	O	S	0	0
			619	387	120	110	2		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	56	Total	C	N	O		0	0
			443	283	79	81			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	80	Total	C	N	O	S	0	0
			635	405	121	106	3		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			653	404	135	112	2		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	u	34	Total	C	N	O	0	0
			295	178	70	47		

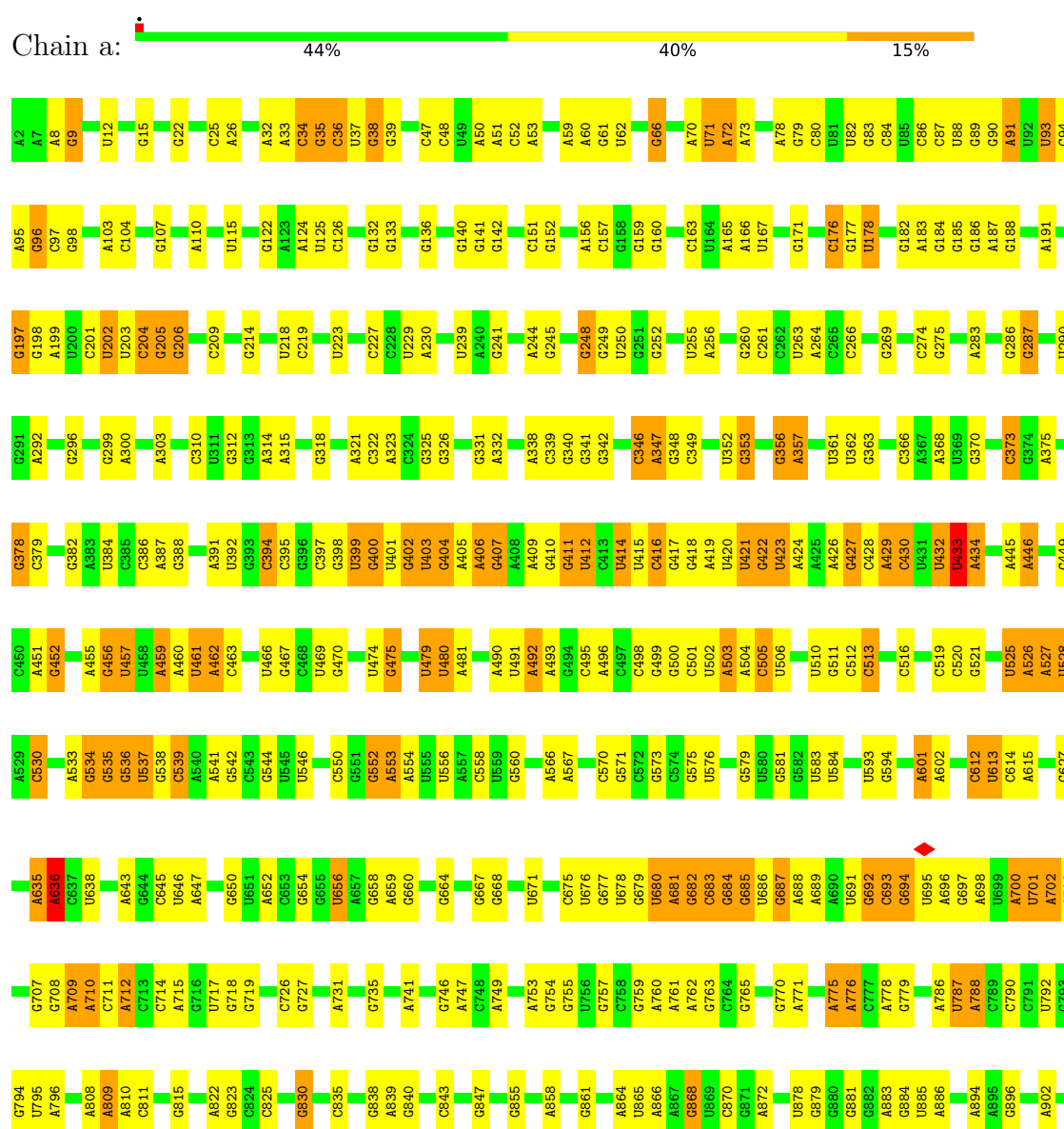
There is a discrepancy between the modelled and reference sequences:

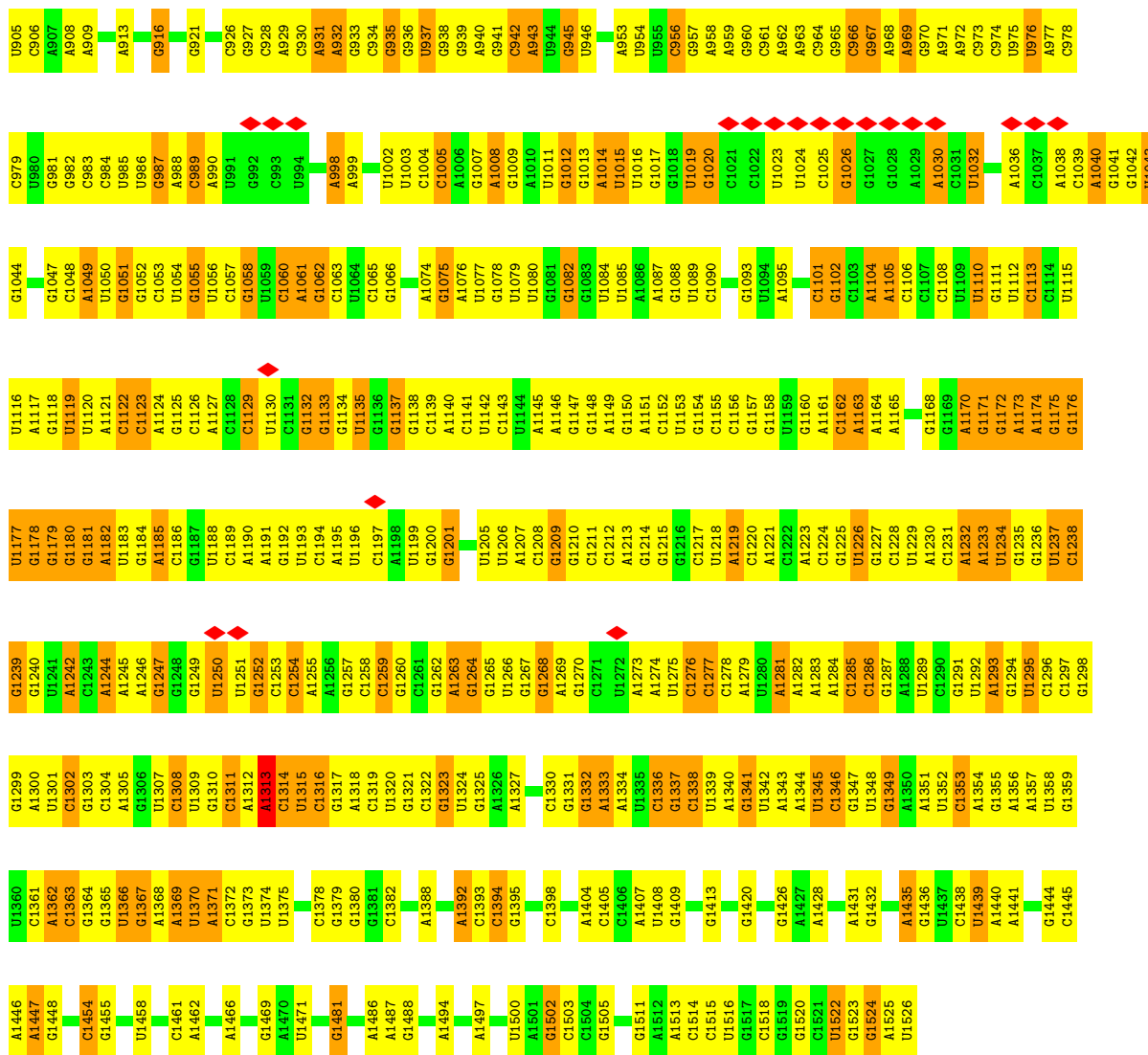
Chain	Residue	Modelled	Actual	Comment	Reference
u	46	ARG	LYS	conflict	UNP A0A069QC99

3 Residue-property plots

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

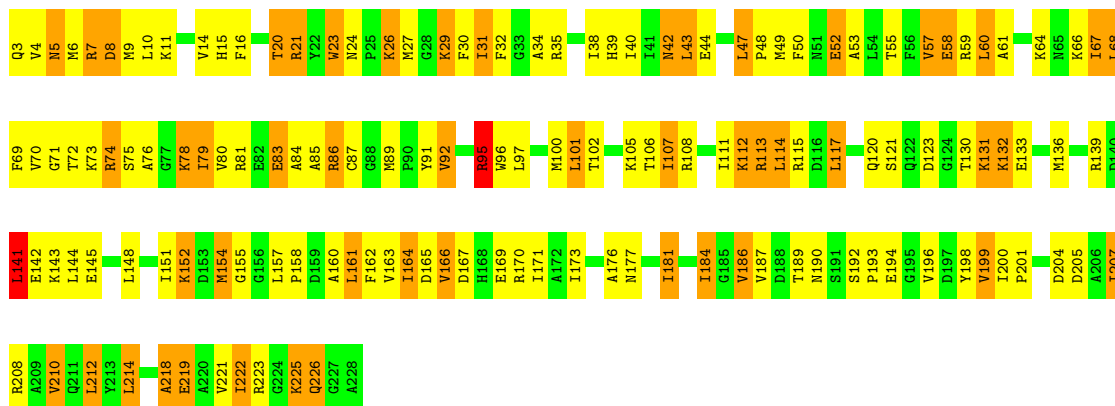
• Molecule 1: 16S rRNA



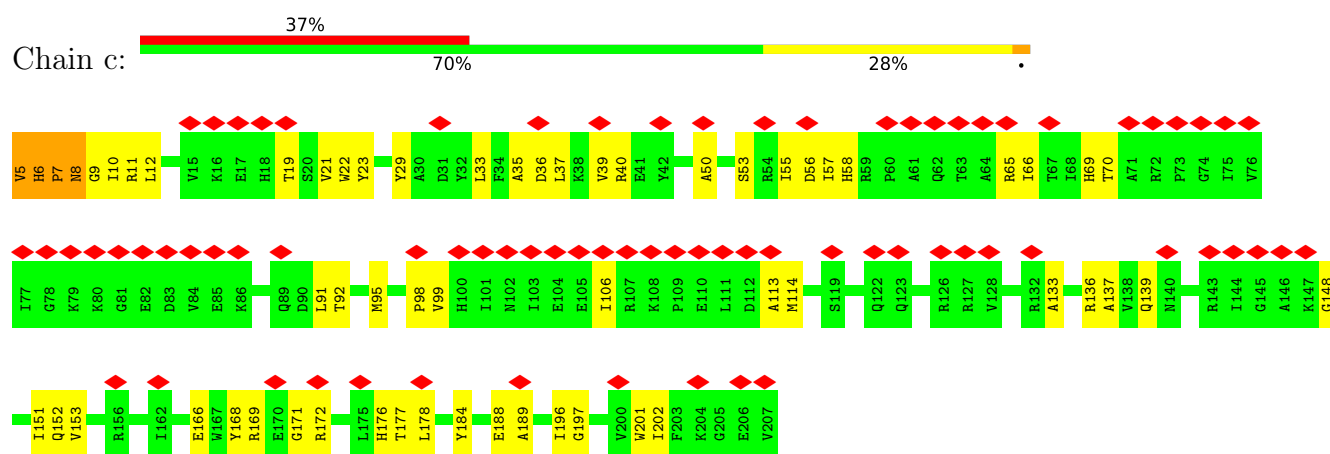


• Molecule 2: 30S ribosomal protein S2

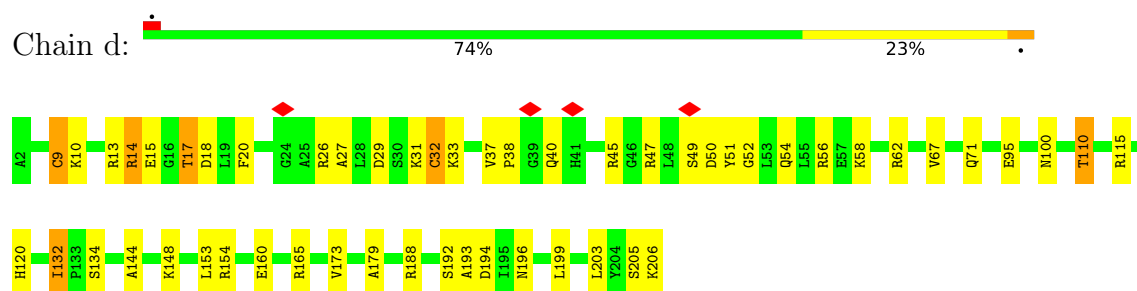
Chain b: 34% 42% 23%



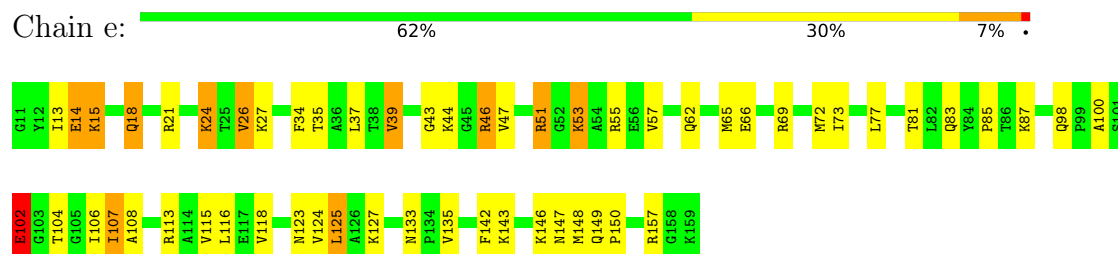
• Molecule 3: 30S ribosomal protein S3



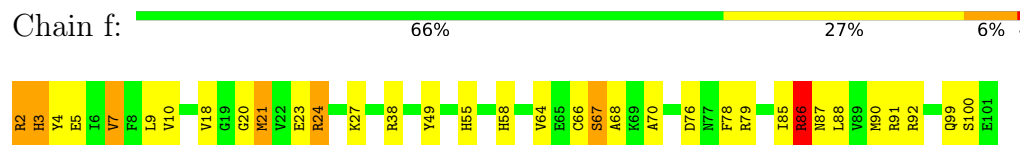
• Molecule 4: 30S ribosomal protein S4



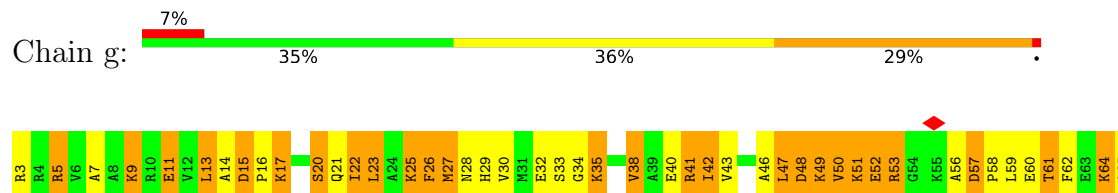
• Molecule 5: 30S ribosomal protein S5

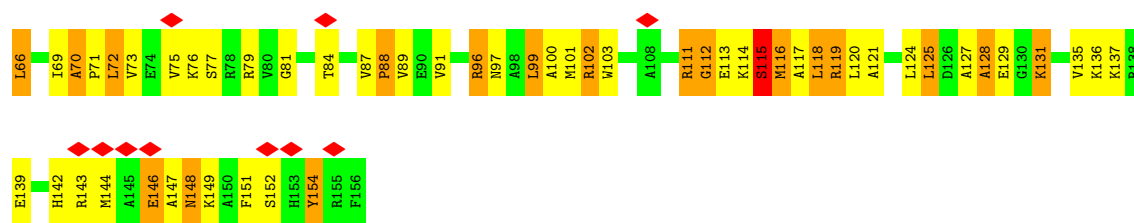


• Molecule 6: 30S ribosomal protein S6

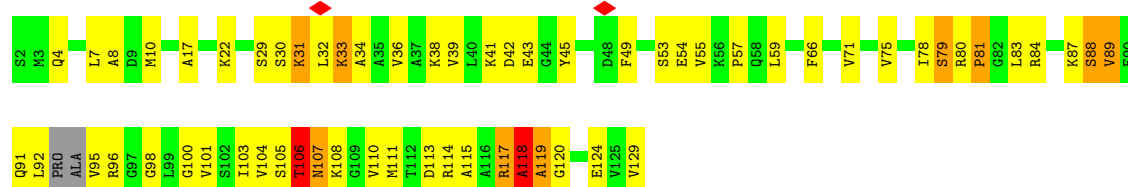


• Molecule 7: 30S ribosomal protein S7





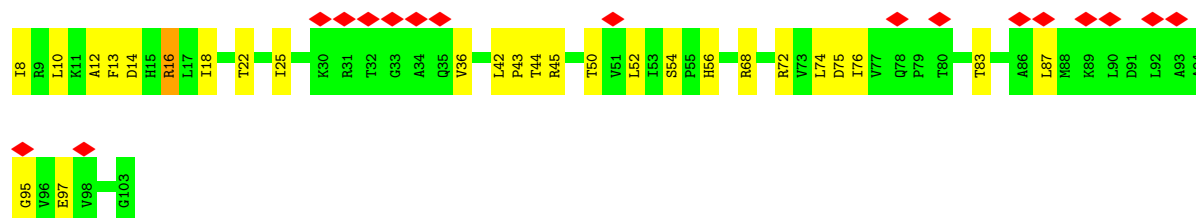
• Molecule 8: 30S ribosomal protein S8



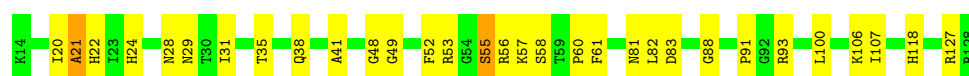
• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

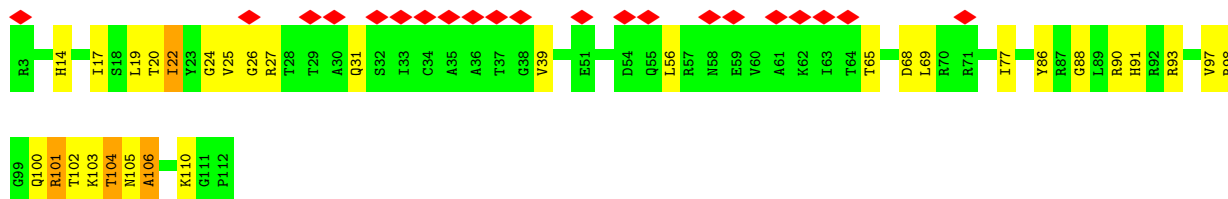


• Molecule 12: 30S ribosomal protein S12

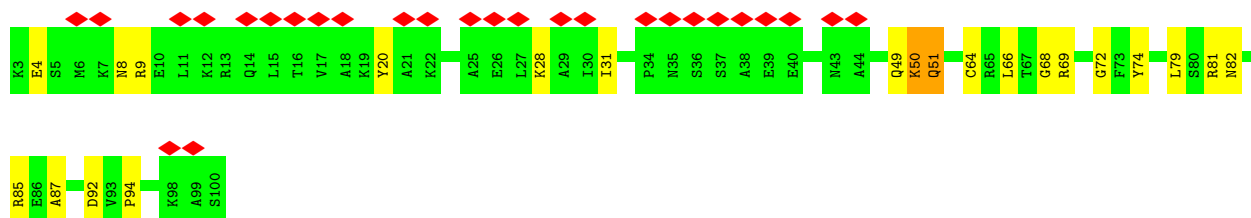
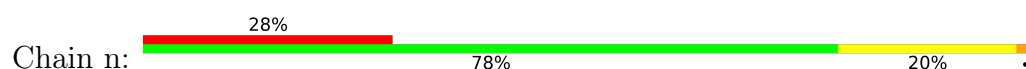




- Molecule 13: 30S ribosomal protein S13



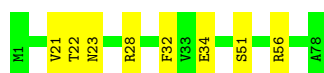
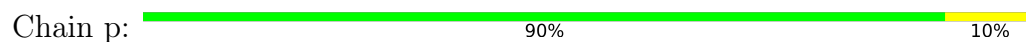
- Molecule 14: 30S ribosomal protein S14



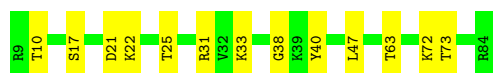
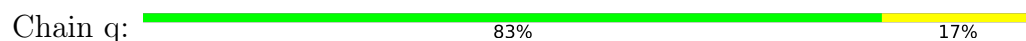
- Molecule 15: 30S ribosomal protein S15



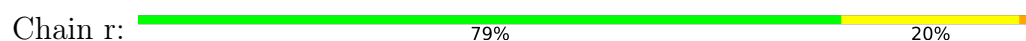
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

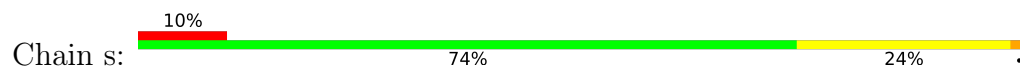


- Molecule 18: 30S ribosomal protein S18

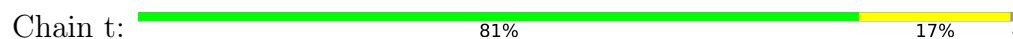




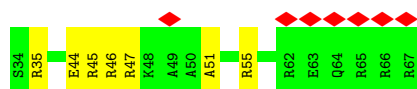
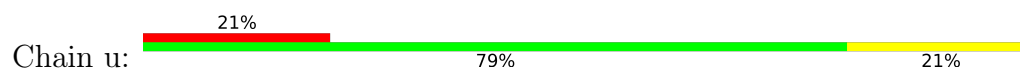
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	319022	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.603	Depositor
Minimum map value	-0.352	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.00936	Depositor
Map size ($\text{\AA}$)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality i

5.1 Standard geometry i

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	0.64	11/36497 (0.0%)	0.64	25/56927 (0.0%)
2	b	0.52	0/1754	0.97	4/2355 (0.2%)
3	c	0.26	0/1638	0.64	0/2209
4	d	0.46	0/1619	0.90	2/2168 (0.1%)
5	e	0.53	0/1106	0.83	0/1488
6	f	0.47	0/815	0.80	1/1098 (0.1%)
7	g	0.35	0/1207	0.94	3/1616 (0.2%)
8	h	0.79	0/924	1.38	8/1243 (0.6%)
9	i	0.30	0/1006	0.79	0/1347
10	j	0.29	0/773	0.71	0/1045
11	k	0.51	1/844 (0.1%)	0.74	0/1148
12	l	0.54	0/906	1.01	5/1215 (0.4%)
13	m	0.32	0/853	0.83	3/1144 (0.3%)
14	n	0.28	0/786	0.74	0/1047
15	o	0.62	0/693	0.85	2/926 (0.2%)
16	p	0.75	0/617	0.97	0/832
17	q	0.56	0/627	0.72	0/844
18	r	0.60	0/450	0.88	0/608
19	s	4.26	1/649 (0.2%)	0.79	2/874 (0.2%)
20	t	0.60	0/660	0.73	0/880
21	u	0.41	0/298	0.71	0/391
All	All	0.75	13/54722 (0.0%)	0.72	55/81405 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	c	0	2
4	d	0	2
8	h	0	15
11	k	0	2

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	l	0	6
13	m	0	4
14	n	0	2
16	p	0	1
All	All	0	34

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	s	3	ARG	CB-CG	108.12	4.76	1.52
1	a	1313	A	C6-N1	18.15	1.71	1.35
1	a	1313	A	N3-C4	17.31	1.69	1.34
1	a	1313	A	N1-C2	17.09	1.68	1.34
1	a	1313	A	C2-N3	16.59	1.66	1.33
1	a	1313	A	C5-C6	15.91	1.72	1.41
1	a	1313	A	C5-C4	14.53	1.67	1.38
1	a	1219	A	N9-C4	13.23	1.64	1.37
1	a	1219	A	N9-C8	-10.59	1.16	1.37
1	a	1219	A	N3-C4	6.16	1.47	1.34
11	k	21	ALA	CA-CB	-5.79	1.44	1.53
1	a	1219	A	C8-N7	5.08	1.41	1.31
1	a	636	A	C1'-N9	5.01	1.54	1.47

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1219	A	N7-C8-N9	-24.13	41.41	113.80
1	a	1219	A	C4-C5-N7	-22.85	42.15	110.70
1	a	1219	A	C8-N9-C4	-17.78	52.46	105.80
1	a	1219	A	C8-N9-C1'	-9.99	97.72	127.70
1	a	1219	A	C5-N7-C8	9.54	132.53	103.90
1	a	1219	A	C6-C5-N7	8.95	159.14	132.30
1	a	1219	A	C4-N9-C1'	7.96	150.19	126.30
8	h	118	ALA	N-CA-C	7.30	126.36	110.80
1	a	479	U	N1-C1'-C2'	7.07	124.61	114.00
1	a	636	A	N9-C1'-C2'	6.99	124.48	114.00
4	d	148	LYS	N-CA-C	-6.88	105.82	114.56
1	a	356	G	C4'-C3'-O3'	6.63	122.95	113.00
2	b	81	ARG	N-CA-C	-6.45	104.61	113.18
8	h	119	ALA	CA-C-N	6.28	133.72	121.41
8	h	119	ALA	C-N-CA	6.28	133.72	121.41
12	l	24	LEU	CA-CB-CG	6.12	137.73	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	117	ARG	CA-C-N	6.03	133.06	121.54
8	h	117	ARG	C-N-CA	6.03	133.06	121.54
2	b	141	LEU	N-CA-C	-5.95	105.11	112.90
1	a	1313	A	N1-C2-N3	-5.91	111.57	129.30
1	a	1061	A	N9-C1'-C2'	5.88	122.82	114.00
19	s	68	GLY	N-CA-C	5.79	126.90	113.18
4	d	32	CYS	CA-CB-SG	5.78	127.70	114.40
12	l	116	TYR	N-CA-C	5.72	117.30	110.44
6	f	3	HIS	N-CA-C	5.72	118.64	110.24
8	h	107	ASN	N-CA-C	5.70	119.41	112.23
1	a	1439	U	P-O3'-C3'	5.63	128.64	120.20
1	a	636	A	C3'-C2'-O2'	-5.52	106.32	114.60
1	a	1219	A	N3-C4-N9	5.47	143.81	127.40
12	l	111	LYS	CA-C-N	5.46	131.97	121.54
12	l	111	LYS	C-N-CA	5.46	131.97	121.54
12	l	107	VAL	N-CA-C	-5.45	108.19	113.53
7	g	70	ALA	CA-C-N	5.44	125.44	119.89
7	g	70	ALA	C-N-CA	5.44	125.44	119.89
1	a	762	A	C2'-C3'-O3'	5.42	121.83	113.70
8	h	106	THR	N-CA-C	5.31	122.10	110.80
1	a	636	A	O4'-C1'-N9	5.30	116.16	108.20
1	a	536	G	P-O3'-C3'	5.23	128.04	120.20
1	a	378	G	C2'-C3'-O3'	5.23	121.54	113.70
1	a	479	U	P-O3'-C3'	5.23	128.04	120.20
1	a	613	U	C2'-C3'-O3'	5.19	121.48	113.70
19	s	3	ARG	CB-CG-CD	5.19	123.23	111.30
15	o	15	TYR	CA-C-N	5.18	127.99	120.79
15	o	15	TYR	C-N-CA	5.18	127.99	120.79
1	a	433	U	P-O3'-C3'	5.18	127.97	120.20
2	b	218	ALA	N-CA-C	-5.18	105.72	111.36
7	g	26	PHE	N-CA-C	5.17	119.08	112.87
1	a	394	C	C2'-C3'-O3'	5.17	121.45	113.70
13	m	24	GLY	N-CA-C	5.10	125.27	113.18
2	b	166	VAL	N-CA-C	5.04	118.12	111.17
1	a	159	G	P-O3'-C3'	5.03	127.75	120.20
1	a	1313	A	C2-N3-C4	5.01	125.64	110.60
8	h	119	ALA	N-CA-C	5.01	117.14	110.53
13	m	104	THR	CA-C-N	5.00	131.10	121.54
13	m	104	THR	C-N-CA	5.00	131.10	121.54

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	c	12	LEU	Peptide
3	c	176	HIS	Peptide
4	d	205	SER	Peptide
4	d	49	SER	Peptide
8	h	100	GLY	Peptide
8	h	104	VAL	Peptide
8	h	29	SER	Peptide
8	h	31	LYS	Peptide
8	h	33	LYS	Peptide
8	h	34	ALA	Peptide
8	h	41	LYS	Peptide
8	h	43	GLU	Peptide
8	h	49	PHE	Peptide
8	h	66	PHE	Peptide
8	h	75	VAL	Peptide
8	h	79	SER	Peptide
8	h	80	ARG	Peptide
8	h	83	LEU	Peptide
8	h	88	SER	Peptide
11	k	118	HIS	Peptide
11	k	55	SER	Peptide
12	l	104	THR	Peptide
12	l	107	VAL	Peptide
12	l	110	ARG	Peptide
12	l	111	LYS	Peptide
12	l	113	ARG	Peptide
12	l	115	LYS	Peptide
13	m	101	ARG	Peptide
13	m	106	ALA	Peptide
13	m	22	ILE	Peptide
13	m	26	GLY	Peptide
14	n	50	LYS	Peptide
14	n	51	GLN	Peptide
16	p	51	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	32595	0	16400	423	0
2	b	1728	0	1766	184	0
3	c	1609	0	1636	55	0
4	d	1600	0	1620	77	0
5	e	1092	0	1139	69	0
6	f	802	0	769	45	0
7	g	1190	0	1227	195	0
8	h	915	0	952	38	0
9	i	994	0	1031	122	0
10	j	763	0	801	20	0
11	k	828	0	808	29	0
12	l	893	0	932	25	0
13	m	847	0	888	28	0
14	n	776	0	818	20	0
15	o	686	0	709	3	0
16	p	606	0	606	3	0
17	q	619	0	659	9	0
18	r	443	0	460	12	0
19	s	635	0	662	29	0
20	t	653	0	699	10	0
21	u	295	0	313	6	0
All	All	50569	0	34895	1070	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 13.

All (1070) 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)
1:a:1313:A:N1	1:a:1313:A:C2	1.68	1.58
1:a:1313:A:C4	1:a:1313:A:N3	1.69	1.57
1:a:1313:A:N1	1:a:1313:A:C6	1.71	1.56
2:b:113:ARG:HG3	2:b:144:LEU:CD1	1.31	1.53
7:g:16:PRO:HB2	9:i:46:MET:CB	1.38	1.51
2:b:207:ILE:HD13	2:b:208:ARG:N	1.25	1.49
7:g:16:PRO:HB3	9:i:46:MET:C	1.42	1.40
7:g:16:PRO:CB	9:i:46:MET:HB2	1.50	1.39
7:g:146:GLU:O	11:k:61:PHE:CE1	1.76	1.39
2:b:113:ARG:CG	2:b:144:LEU:CD1	1.99	1.37
7:g:16:PRO:CB	9:i:46:MET:CB	2.01	1.35
2:b:73:LYS:NZ	2:b:165:ASP:OD2	1.57	1.35
1:a:1182:A:N1	3:c:6:HIS:HB2	1.38	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:58:GLU:CD	2:b:223:ARG:NH2	1.86	1.33
2:b:113:ARG:CG	2:b:144:LEU:HD13	1.57	1.31
2:b:58:GLU:OE1	2:b:223:ARG:NH2	1.60	1.29
2:b:207:ILE:CD1	2:b:208:ARG:H	1.45	1.29
4:d:14:ARG:NH1	4:d:38:PRO:HB2	1.48	1.29
1:a:1182:A:N1	3:c:6:HIS:CB	1.97	1.26
4:d:20:PHE:CD2	4:d:165:ARG:NH1	2.05	1.25
1:a:1173:A:C8	9:i:104:VAL:HB	1.71	1.25
2:b:113:ARG:HG2	2:b:144:LEU:CB	1.67	1.23
6:f:20:GLY:O	6:f:24:ARG:HG2	1.36	1.20
1:a:1182:A:C6	3:c:6:HIS:HB2	1.78	1.19
1:a:1336:C:O2'	9:i:127:TYR:O	1.58	1.18
1:a:1182:A:C2	3:c:6:HIS:HB2	1.76	1.18
1:a:1336:C:O3'	9:i:128:SER:HA	1.43	1.16
5:e:98:GLN:HE21	5:e:125:LEU:HD13	1.05	1.16
7:g:16:PRO:HG3	9:i:47:VAL:HG23	1.19	1.13
2:b:113:ARG:HG3	2:b:144:LEU:HD12	1.24	1.11
1:a:1286:C:H5''	7:g:41:ARG:NH1	1.64	1.11
1:a:1283:A:C5	7:g:35:LYS:HB3	1.85	1.10
1:a:1182:A:C6	3:c:6:HIS:CB	2.34	1.10
2:b:117:LEU:HD13	2:b:121:SER:HB3	1.28	1.10
4:d:20:PHE:HE2	4:d:165:ARG:HD2	1.13	1.09
5:e:98:GLN:NE2	5:e:125:LEU:HD13	1.67	1.09
4:d:14:ARG:HH11	4:d:38:PRO:CB	1.65	1.09
5:e:35:THR:HG22	5:e:53:LYS:CD	1.82	1.08
1:a:8:A:O4'	5:e:108:ALA:O	1.72	1.07
5:e:98:GLN:HE21	5:e:125:LEU:CD1	1.66	1.07
7:g:16:PRO:CB	9:i:46:MET:C	2.27	1.07
5:e:35:THR:CG2	5:e:53:LYS:HD3	1.83	1.07
7:g:17:LYS:CE	9:i:43:THR:HA	1.85	1.06
3:c:7:PRO:O	3:c:10:ILE:N	1.87	1.06
4:d:15:GLU:OE1	4:d:56:ARG:HD3	1.53	1.05
4:d:20:PHE:CE2	4:d:165:ARG:NH1	2.23	1.05
5:e:14:GLU:OE1	5:e:69:ARG:NH2	1.89	1.05
2:b:131:LYS:HE3	2:b:131:LYS:HA	1.35	1.04
4:d:20:PHE:CE2	4:d:165:ARG:HD2	1.92	1.04
7:g:17:LYS:HE3	9:i:43:THR:CA	1.86	1.04
1:a:931:A:H1'	7:g:76:LYS:NZ	1.70	1.04
2:b:47:LEU:HB3	2:b:48:PRO:HD3	1.34	1.04
7:g:16:PRO:HB2	9:i:46:MET:CA	1.87	1.03
7:g:16:PRO:CB	9:i:46:MET:CA	2.36	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:20:PHE:HE2	4:d:165:ARG:CD	1.72	1.03
1:a:1286:C:H5'	7:g:41:ARG:HH11	1.19	1.02
4:d:14:ARG:HH12	4:d:38:PRO:C	1.65	1.02
4:d:20:PHE:CE2	4:d:165:ARG:CZ	2.42	1.02
7:g:40:GLU:HG3	9:i:42:GLU:HA	1.41	1.02
2:b:15:HIS:NE2	2:b:16:PHE:CE1	2.28	1.01
4:d:20:PHE:HD2	4:d:165:ARG:NH1	1.49	1.01
7:g:146:GLU:O	11:k:61:PHE:CZ	2.12	1.01
4:d:14:ARG:NH1	4:d:38:PRO:O	1.94	1.00
7:g:17:LYS:HE3	9:i:43:THR:O	1.60	1.00
7:g:17:LYS:HE3	9:i:43:THR:C	1.86	0.99
5:e:35:THR:HG22	5:e:53:LYS:HD3	1.01	0.98
7:g:147:ALA:HB1	11:k:56:ARG:NH2	1.77	0.97
1:a:1371:A:N6	7:g:7:ALA:HB2	1.80	0.97
2:b:95:ARG:NH1	2:b:97:LEU:HD23	1.79	0.95
2:b:117:LEU:HD21	2:b:120:GLN:HB3	1.47	0.95
2:b:6:MET:HE2	2:b:6:MET:HA	1.49	0.95
1:a:931:A:H1'	7:g:76:LYS:HZ2	1.22	0.95
4:d:15:GLU:CD	4:d:56:ARG:HD3	1.91	0.95
4:d:15:GLU:OE1	4:d:56:ARG:CD	2.14	0.95
5:e:106:ILE:HD12	5:e:116:LEU:O	1.67	0.95
7:g:146:GLU:O	11:k:61:PHE:HE1	1.37	0.94
2:b:207:ILE:CD1	2:b:208:ARG:N	2.17	0.94
2:b:58:GLU:OE2	2:b:223:ARG:NH2	2.00	0.94
2:b:113:ARG:HG2	2:b:144:LEU:HB2	1.47	0.94
1:a:1337:G:P	9:i:128:SER:HA	2.08	0.93
2:b:113:ARG:HG3	2:b:144:LEU:HD13	0.94	0.92
7:g:17:LYS:HE3	9:i:43:THR:HA	1.48	0.92
1:a:1286:C:C5'	7:g:41:ARG:HH11	1.81	0.92
2:b:113:ARG:HG2	2:b:144:LEU:HB3	1.50	0.92
7:g:16:PRO:HG3	9:i:47:VAL:CG2	1.99	0.92
7:g:50:VAL:HG23	7:g:121:ALA:HB1	1.52	0.91
6:f:20:GLY:O	6:f:24:ARG:CG	2.19	0.91
2:b:113:ARG:CG	2:b:144:LEU:HD12	1.79	0.91
7:g:41:ARG:HG3	9:i:41:ARG:NH2	1.86	0.91
1:a:1336:C:O2'	9:i:128:SER:OG	1.89	0.91
2:b:47:LEU:HB3	2:b:48:PRO:CD	2.00	0.90
1:a:1369:A:H4'	7:g:22:ILE:HG22	1.54	0.89
1:a:1173:A:N7	9:i:104:VAL:HB	1.85	0.89
1:a:1065:C:OP1	5:e:55:ARG:NH2	2.05	0.89
1:a:1173:A:H61	9:i:85:ARG:HB2	1.36	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1362:A:OP1	9:i:114:LYS:NZ	2.06	0.88
2:b:84:ALA:HB2	2:b:218:ALA:HA	1.54	0.88
1:a:1182:A:N1	3:c:6:HIS:HB3	1.88	0.88
2:b:112:LYS:CG	2:b:115:ARG:HD3	2.03	0.88
5:e:39:VAL:CG1	5:e:118:VAL:HG21	2.03	0.88
1:a:1286:C:C5'	7:g:41:ARG:NH1	2.35	0.87
3:c:7:PRO:O	3:c:9:GLY:N	2.08	0.87
6:f:85:ILE:O	6:f:86:ARG:O	1.91	0.87
4:d:14:ARG:NH1	4:d:38:PRO:C	2.32	0.87
5:e:43:GLY:O	5:e:44:LYS:HD3	1.75	0.86
2:b:95:ARG:NH1	2:b:97:LEU:CD2	2.38	0.86
4:d:14:ARG:HH11	4:d:38:PRO:HB2	0.75	0.86
7:g:16:PRO:HB3	9:i:46:MET:CA	2.01	0.85
4:d:17:THR:OG1	4:d:18:ASP:N	2.02	0.85
7:g:9:LYS:NZ	7:g:9:LYS:HB3	1.90	0.85
4:d:14:ARG:NH1	4:d:38:PRO:CB	2.31	0.85
5:e:106:ILE:CD1	5:e:116:LEU:O	2.25	0.85
7:g:41:ARG:CG	9:i:41:ARG:NH2	2.40	0.85
2:b:131:LYS:HE3	2:b:131:LYS:CA	2.00	0.84
7:g:50:VAL:HG21	7:g:124:LEU:HB2	1.60	0.84
4:d:20:PHE:HD2	4:d:165:ARG:HH12	1.25	0.84
7:g:41:ARG:CD	9:i:41:ARG:NH2	2.41	0.84
2:b:141:LEU:O	2:b:141:LEU:HD22	1.77	0.84
1:a:1341:G:N7	9:i:109:ARG:HD2	1.94	0.83
2:b:47:LEU:CB	2:b:48:PRO:CD	2.57	0.83
2:b:47:LEU:CB	2:b:48:PRO:HD3	2.08	0.83
4:d:20:PHE:CE2	4:d:165:ARG:CD	2.59	0.82
7:g:16:PRO:CA	9:i:46:MET:HB2	2.10	0.81
1:a:1284:A:H5''	7:g:38:VAL:HG23	1.62	0.81
1:a:667:G:O3'	6:f:86:ARG:NH1	2.14	0.81
1:a:1341:G:O6	9:i:109:ARG:NH1	2.14	0.81
1:a:537:U:OP2	4:d:14:ARG:NH1	2.14	0.81
2:b:6:MET:HE2	2:b:6:MET:CA	2.11	0.81
7:g:121:ALA:HA	7:g:124:LEU:HG	1.63	0.81
7:g:118:LEU:HD12	7:g:118:LEU:O	1.80	0.80
6:f:2:ARG:O	6:f:4:TYR:CD2	2.33	0.80
1:a:1182:A:H2	3:c:6:HIS:HD1	1.29	0.80
1:a:176:C:H42	1:a:188:G:H1	1.29	0.80
2:b:184:ILE:HD12	2:b:198:TYR:HB2	1.64	0.79
4:d:20:PHE:CD2	4:d:165:ARG:CZ	2.64	0.79
1:a:1286:C:OP2	7:g:41:ARG:HD3	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:16:PRO:CG	9:i:47:VAL:HG23	2.10	0.79
1:a:761:A:H8	1:a:1505:G:H21	1.31	0.78
6:f:2:ARG:O	6:f:4:TYR:CE2	2.36	0.78
7:g:16:PRO:HG2	7:g:17:LYS:HE2	1.64	0.78
1:a:1283:A:C8	7:g:35:LYS:HG2	2.18	0.78
1:a:9:G:O2'	4:d:206:LYS:NZ	2.16	0.77
7:g:42:ILE:HD12	7:g:117:ALA:HB2	1.66	0.77
7:g:66:LEU:HD23	7:g:97:ASN:HB3	1.66	0.77
4:d:20:PHE:HE2	4:d:165:ARG:CZ	1.96	0.77
1:a:1173:A:O3'	9:i:99:ARG:NH1	2.18	0.77
1:a:1371:A:H61	7:g:7:ALA:HB2	1.47	0.77
6:f:49:TYR:OH	6:f:86:ARG:NH2	2.18	0.77
7:g:16:PRO:HB3	9:i:47:VAL:N	2.00	0.77
1:a:1173:A:C8	9:i:104:VAL:CB	2.64	0.76
1:a:1371:A:N6	7:g:7:ALA:CB	2.48	0.76
7:g:59:LEU:H	7:g:59:LEU:HD23	1.48	0.76
2:b:113:ARG:CG	2:b:144:LEU:CB	2.59	0.76
7:g:15:ASP:OD1	7:g:16:PRO:HD2	1.85	0.76
7:g:16:PRO:CA	9:i:46:MET:CB	2.63	0.76
2:b:199:VAL:HG13	2:b:201:PRO:HD3	1.66	0.76
7:g:16:PRO:CB	9:i:46:MET:HB3	2.11	0.76
7:g:41:ARG:CG	9:i:41:ARG:HH22	1.99	0.76
1:a:423:U:H4'	4:d:32:CYS:HB2	1.67	0.76
1:a:636:A:N3	8:h:108:LYS:N	2.29	0.76
5:e:43:GLY:C	5:e:44:LYS:HD3	2.11	0.75
7:g:30:VAL:HB	7:g:43:VAL:HG22	1.68	0.75
2:b:161:LEU:HD13	2:b:181:ILE:HD11	1.67	0.75
2:b:113:ARG:HG2	2:b:144:LEU:CG	2.16	0.75
2:b:112:LYS:HG2	2:b:115:ARG:HD3	1.66	0.75
1:a:1173:A:H3'	9:i:104:VAL:CG1	2.17	0.75
2:b:8:ASP:OD1	2:b:8:ASP:N	2.10	0.74
2:b:113:ARG:CD	2:b:144:LEU:HD13	2.17	0.74
7:g:143:ARG:HE	7:g:143:ARG:HA	1.53	0.74
2:b:83:GLU:N	2:b:83:GLU:OE1	2.17	0.74
2:b:70:VAL:HA	2:b:92:VAL:HG13	1.70	0.74
1:a:1182:A:C6	3:c:6:HIS:HB3	2.17	0.74
1:a:1371:A:C6	7:g:7:ALA:HB2	2.23	0.73
1:a:1182:A:C2	3:c:6:HIS:CB	2.58	0.73
6:f:88:LEU:HD21	18:r:65:LEU:HD22	1.69	0.73
4:d:20:PHE:HE2	4:d:165:ARG:NE	1.85	0.73
1:a:1341:G:H2'	9:i:109:ARG:HB3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:52:GLU:O	7:g:52:GLU:HG2	1.86	0.73
7:g:99:LEU:N	7:g:99:LEU:HD23	2.04	0.73
1:a:668:G:OP1	6:f:86:ARG:NH1	2.22	0.73
2:b:21:ARG:HH11	2:b:21:ARG:HB2	1.53	0.73
7:g:16:PRO:HB2	9:i:46:MET:HB2	0.75	0.72
4:d:20:PHE:CE2	4:d:165:ARG:NE	2.56	0.72
7:g:59:LEU:HA	7:g:62:PHE:HB3	1.71	0.72
7:g:96:ARG:NH1	7:g:96:ARG:HB2	2.05	0.72
7:g:96:ARG:HB2	7:g:96:ARG:HH11	1.55	0.72
1:a:668:G:P	6:f:86:ARG:HH12	2.13	0.72
1:a:1234:U:H3	7:g:115:SER:HA	1.55	0.71
7:g:16:PRO:HB3	9:i:46:MET:O	1.89	0.71
7:g:35:LYS:HD2	7:g:35:LYS:O	1.90	0.71
4:d:20:PHE:HE2	4:d:165:ARG:NH1	1.89	0.71
1:a:1065:C:H5''	5:e:55:ARG:NH2	2.06	0.71
2:b:152:LYS:HB2	2:b:152:LYS:NZ	2.04	0.71
8:h:105:SER:H	8:h:120:GLY:HA3	1.56	0.70
7:g:143:ARG:HA	7:g:143:ARG:NE	2.07	0.70
1:a:682:G:H5'	11:k:49:GLY:HA2	1.74	0.70
5:e:98:GLN:NE2	5:e:125:LEU:CD1	2.39	0.70
8:h:89:VAL:HG23	8:h:117:ARG:HG2	1.74	0.70
1:a:1283:A:C4	7:g:35:LYS:HB3	2.27	0.70
1:a:1283:A:C5	7:g:35:LYS:CB	2.70	0.70
7:g:15:ASP:C	9:i:50:GLN:NE2	2.49	0.70
2:b:27:MET:HG2	2:b:193:PRO:HD3	1.73	0.69
7:g:35:LYS:HD3	7:g:38:VAL:HB	1.74	0.69
1:a:1173:A:H3'	9:i:104:VAL:HG11	1.72	0.69
7:g:17:LYS:CE	9:i:43:THR:O	2.38	0.69
7:g:17:LYS:CE	9:i:43:THR:CA	2.56	0.69
2:b:58:GLU:CD	2:b:223:ARG:CZ	2.63	0.69
12:l:27:CYS:SG	12:l:30:ARG:NH2	2.66	0.69
7:g:15:ASP:CA	9:i:50:GLN:HE22	2.05	0.69
7:g:15:ASP:N	9:i:50:GLN:HE22	1.90	0.69
1:a:1182:A:C2	3:c:6:HIS:ND1	2.61	0.69
2:b:5:ASN:OD1	2:b:5:ASN:N	2.23	0.68
7:g:30:VAL:HG11	7:g:43:VAL:HA	1.74	0.68
7:g:57:ASP:N	7:g:57:ASP:OD1	2.23	0.68
1:a:719:G:H1	1:a:726:C:H5	1.41	0.68
5:e:35:THR:CG2	5:e:53:LYS:CD	2.58	0.68
1:a:8:A:C1'	5:e:108:ALA:O	2.41	0.68
1:a:1337:G:OP1	9:i:127:TYR:CD2	2.47	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1343:A:P	9:i:123:LYS:HG3	2.32	0.68
8:h:84:ARG:HH22	17:q:33:LYS:HE3	1.57	0.68
1:a:452:G:H1	1:a:469:U:H3	1.41	0.68
1:a:1283:A:N9	7:g:35:LYS:HG2	2.09	0.68
2:b:113:ARG:H	2:b:113:ARG:HE	1.40	0.68
2:b:113:ARG:HG2	2:b:144:LEU:CD1	1.94	0.68
1:a:1173:A:N7	9:i:104:VAL:CB	2.57	0.67
7:g:16:PRO:HD3	9:i:47:VAL:HG22	1.76	0.67
2:b:21:ARG:HH11	2:b:21:ARG:CB	2.07	0.67
9:i:46:MET:HG3	9:i:49:ARG:HD2	1.74	0.67
1:a:1174:A:OP1	9:i:104:VAL:HG12	1.92	0.67
7:g:17:LYS:CD	9:i:43:THR:HA	2.24	0.67
7:g:9:LYS:HB3	7:g:9:LYS:HZ3	1.59	0.67
1:a:34:C:H5	1:a:544:G:H1	1.42	0.67
1:a:872:A:H5''	8:h:81:PRO:HD2	1.77	0.67
2:b:95:ARG:HH12	2:b:97:LEU:CD2	2.07	0.67
12:l:72:HIS:HD2	12:l:74:LEU:H	1.41	0.67
1:a:1341:G:C8	9:i:109:ARG:HD2	2.29	0.67
1:a:62:U:H3	1:a:98:G:H1	1.43	0.66
1:a:823:G:O3'	2:b:23:TRP:HZ3	1.78	0.66
4:d:15:GLU:OE2	4:d:56:ARG:HD3	1.94	0.66
5:e:107:ILE:HG13	5:e:125:LEU:HA	1.77	0.66
7:g:51:LYS:HG3	7:g:58:PRO:HD3	1.78	0.66
2:b:79:ILE:HG22	2:b:214:LEU:HD23	1.77	0.66
7:g:9:LYS:HA	7:g:9:LYS:HE2	1.78	0.66
1:a:1505:G:H1	1:a:1518:C:H5	1.43	0.66
5:e:47:VAL:HG12	5:e:142:PHE:HE1	1.60	0.66
1:a:1249:G:N2	1:a:1253:C:O2	2.28	0.65
4:d:14:ARG:HD2	4:d:38:PRO:HG2	1.77	0.65
1:a:1284:A:C5'	7:g:38:VAL:HG23	2.26	0.65
1:a:1015:U:H5''	1:a:1016:U:H5'	1.79	0.65
1:a:1286:C:OP2	7:g:41:ARG:CD	2.44	0.65
3:c:21:VAL:HG12	10:j:95:GLY:HA3	1.78	0.65
5:e:39:VAL:HG21	5:e:115:VAL:HG22	1.77	0.65
1:a:916:G:H21	1:a:1392:A:H8	1.44	0.65
2:b:117:LEU:CD1	2:b:121:SER:HB3	2.18	0.65
3:c:148:GLY:HA3	3:c:172:ARG:H	1.61	0.65
2:b:89:MET:HE2	2:b:221:VAL:HG21	1.77	0.65
2:b:219:GLU:HA	2:b:222:ILE:HB	1.79	0.65
17:q:72:LYS:HG2	17:q:73:THR:HG23	1.79	0.65
1:a:422:G:OP2	4:d:10:LYS:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:23:LEU:HG	7:g:23:LEU:O	1.95	0.64
1:a:935:G:N2	1:a:936:G:N7	2.46	0.64
2:b:117:LEU:HD13	2:b:117:LEU:O	1.97	0.64
1:a:1179:G:N2	1:a:1181:G:O6	2.27	0.64
1:a:1269:A:H61	1:a:1277:C:H5'	1.62	0.64
1:a:686:U:H3	11:k:55:SER:HG	1.42	0.64
1:a:1346:C:N4	1:a:1363:C:O2	2.30	0.64
1:a:407:G:H22	4:d:32:CYS:HA	1.61	0.64
2:b:184:ILE:HD13	2:b:184:ILE:N	2.11	0.64
2:b:154:MET:SD	2:b:154:MET:N	2.70	0.64
7:g:50:VAL:HG22	7:g:125:LEU:HD23	1.79	0.64
1:a:70:A:H2	1:a:93:U:H3	1.45	0.64
1:a:1082:G:H21	1:a:1161:A:H61	1.46	0.64
2:b:117:LEU:HD22	2:b:117:LEU:C	2.22	0.64
11:k:20:ILE:HG22	11:k:83:ASP:HB2	1.78	0.64
2:b:113:ARG:CG	2:b:144:LEU:HB3	2.25	0.64
5:e:73:ILE:HG13	5:e:146:LYS:HE2	1.79	0.63
7:g:66:LEU:HD12	7:g:66:LEU:H	1.63	0.63
2:b:117:LEU:O	2:b:117:LEU:HD22	1.98	0.63
13:m:90:ARG:NH2	13:m:97:VAL:O	2.31	0.63
1:a:9:G:H1'	4:d:206:LYS:NZ	2.13	0.63
1:a:1337:G:OP1	9:i:127:TYR:C	2.41	0.63
1:a:931:A:H1'	7:g:76:LYS:HZ3	1.63	0.63
2:b:4:VAL:HG12	2:b:47:LEU:HG	1.79	0.63
2:b:80:VAL:HG13	2:b:80:VAL:O	1.98	0.63
2:b:152:LYS:HB2	2:b:152:LYS:HZ1	1.62	0.63
7:g:15:ASP:C	9:i:50:GLN:HE21	2.05	0.63
7:g:15:ASP:CA	9:i:50:GLN:NE2	2.62	0.63
1:a:398:G:O2'	1:a:492:A:N6	2.32	0.63
1:a:636:A:N6	8:h:118:ALA:O	2.31	0.63
13:m:20:THR:O	13:m:22:ILE:N	2.32	0.63
7:g:17:LYS:CE	9:i:43:THR:C	2.67	0.62
1:a:1426:G:O2'	1:a:1462:A:N6	2.32	0.62
2:b:112:LYS:HG2	2:b:115:ARG:CD	2.30	0.62
2:b:85:ALA:HA	2:b:89:MET:HB2	1.82	0.62
2:b:166:VAL:HG13	2:b:173:ILE:HD13	1.82	0.62
7:g:69:ILE:HG22	7:g:69:ILE:O	1.99	0.62
8:h:54:GLU:HG2	8:h:55:VAL:HG22	1.81	0.62
5:e:66:GLU:OE2	5:e:66:GLU:HA	1.99	0.62
2:b:6:MET:HA	2:b:6:MET:CE	2.26	0.62
2:b:112:LYS:CG	2:b:115:ARG:CD	2.75	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:12:ARG:HH12	9:i:13:LYS:HE3	1.63	0.62
2:b:73:LYS:HZ2	2:b:165:ASP:CG	2.01	0.62
5:e:14:GLU:OE1	5:e:69:ARG:CZ	2.47	0.62
1:a:1003:U:H5	1:a:1014:A:H61	1.47	0.61
1:a:255:U:OP2	20:t:74:ARG:NH2	2.34	0.61
2:b:133:GLU:OE1	2:b:133:GLU:N	2.30	0.61
1:a:932:A:N6	1:a:1338:C:N3	2.48	0.61
1:a:1065:C:C5'	5:e:55:ARG:NH2	2.62	0.61
1:a:1393:C:H4'	1:a:1394:C:H5'	1.82	0.61
6:f:5:GLU:OE2	18:r:24:LYS:NZ	2.32	0.61
7:g:139:GLU:HA	7:g:139:GLU:OE2	1.98	0.61
12:l:99:ARG:NE	12:l:113:ARG:O	2.32	0.61
7:g:17:LYS:NZ	9:i:43:THR:HA	2.14	0.61
7:g:41:ARG:HD3	9:i:41:ARG:NH2	2.15	0.61
1:a:1369:A:H61	7:g:29:HIS:HB2	1.66	0.61
3:c:151:ILE:HB	3:c:168:TYR:HB2	1.82	0.61
14:n:64:CYS:HB3	14:n:68:GLY:H	1.63	0.61
7:g:65:ALA:HA	7:g:127:ALA:HB1	1.82	0.61
3:c:58:HIS:HB2	3:c:65:ARG:HB3	1.83	0.61
7:g:15:ASP:OD1	7:g:16:PRO:CD	2.49	0.61
12:l:51:LYS:HG2	12:l:72:HIS:HE1	1.66	0.61
1:a:1341:G:C6	9:i:109:ARG:NH1	2.69	0.61
2:b:6:MET:HE2	2:b:6:MET:N	2.15	0.61
7:g:135:VAL:O	7:g:135:VAL:HG12	1.99	0.61
10:j:44:THR:HG23	10:j:68:ARG:HE	1.66	0.61
2:b:58:GLU:O	2:b:58:GLU:HG2	1.99	0.60
11:k:60:PRO:HD3	11:k:91:PRO:HB2	1.83	0.60
1:a:1283:A:C8	7:g:35:LYS:CG	2.85	0.60
1:a:1371:A:C6	7:g:7:ALA:CB	2.84	0.60
7:g:35:LYS:HD2	7:g:35:LYS:N	2.15	0.60
1:a:36:C:H1'	12:l:112:GLN:HE21	1.66	0.60
1:a:1343:A:OP1	9:i:123:LYS:HG3	2.01	0.60
3:c:7:PRO:C	3:c:9:GLY:N	2.59	0.60
7:g:16:PRO:HB2	9:i:46:MET:N	2.16	0.60
1:a:668:G:P	6:f:86:ARG:NH1	2.74	0.60
1:a:1293:A:HO2'	1:a:1295:U:H3	1.50	0.60
7:g:16:PRO:CA	9:i:46:MET:HB3	2.31	0.60
1:a:1215:G:H2'	19:s:53:ASN:HB3	1.83	0.60
2:b:15:HIS:NE2	2:b:16:PHE:CD1	2.69	0.60
3:c:7:PRO:HA	3:c:10:ILE:HD12	1.84	0.60
1:a:1316:C:OP2	19:s:69:HIS:ND1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:423:U:O2	4:d:31:LYS:N	2.35	0.60
1:a:1283:A:C8	7:g:35:LYS:CB	2.85	0.60
1:a:1311:C:H5'	14:n:49:GLN:HG3	1.84	0.60
8:h:87:LYS:H	8:h:119:ALA:HB3	1.66	0.59
1:a:503:A:H8	4:d:52:GLY:H	1.49	0.59
7:g:16:PRO:C	9:i:46:MET:HB2	2.26	0.59
7:g:27:MET:HE2	7:g:43:VAL:HG11	1.84	0.59
2:b:151:ILE:O	2:b:151:ILE:HG22	2.00	0.59
1:a:1283:A:N7	7:g:35:LYS:CB	2.65	0.59
2:b:15:HIS:CD2	2:b:16:PHE:CE1	2.90	0.59
6:f:2:ARG:HG3	6:f:2:ARG:HH11	1.66	0.59
7:g:146:GLU:OE2	7:g:146:GLU:HA	2.01	0.59
13:m:65:THR:H	13:m:68:ASP:HB2	1.67	0.59
1:a:399:U:OP2	4:d:115:ARG:NH1	2.35	0.59
2:b:112:LYS:HB3	2:b:115:ARG:HD3	1.85	0.59
2:b:112:LYS:CB	2:b:115:ARG:HD3	2.32	0.59
1:a:1283:A:N9	7:g:35:LYS:CG	2.66	0.58
1:a:594:G:H5''	8:h:117:ARG:HD2	1.83	0.58
1:a:1524:G:O6	21:u:46:ARG:NH1	2.36	0.58
1:a:1250:U:H5''	1:a:1353:C:H42	1.69	0.58
14:n:87:ALA:HB1	14:n:92:ASP:HB2	1.86	0.58
2:b:181:ILE:O	2:b:181:ILE:HG12	2.03	0.58
1:a:683:C:OP2	11:k:29:ASN:ND2	2.35	0.58
1:a:404:G:O2'	1:a:406:A:N6	2.35	0.58
3:c:29:TYR:OH	14:n:94:PRO:O	2.22	0.58
2:b:50:PHE:O	2:b:53:ALA:HB3	2.03	0.58
7:g:15:ASP:N	9:i:50:GLN:NE2	2.51	0.58
1:a:931:A:N3	7:g:76:LYS:HD3	2.17	0.58
1:a:1122:C:O2	1:a:1138:G:N1	2.37	0.58
7:g:61:THR:HG23	7:g:128:ALA:HB2	1.86	0.58
1:a:423:U:H1'	4:d:31:LYS:HG2	1.84	0.57
1:a:1102:G:N2	1:a:1179:G:O6	2.37	0.57
2:b:114:LEU:O	2:b:114:LEU:HG	1.98	0.57
5:e:143:LYS:O	5:e:147:ASN:ND2	2.36	0.57
6:f:2:ARG:HH11	6:f:2:ARG:CG	2.16	0.57
2:b:57:VAL:HG22	2:b:67:ILE:HD12	1.85	0.57
2:b:200:ILE:HG22	2:b:200:ILE:O	2.03	0.57
1:a:1074:A:OP1	5:e:51:ARG:NH2	2.37	0.57
10:j:12:ALA:HB3	10:j:18:ILE:HD12	1.86	0.57
2:b:113:ARG:H	2:b:113:ARG:NE	2.03	0.57
2:b:164:ILE:O	2:b:164:ILE:HG13	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:18:VAL:HA	6:f:21:MET:HB2	1.85	0.57
7:g:16:PRO:O	9:i:46:MET:HB2	2.04	0.57
1:a:397:C:OP2	4:d:71:GLN:NE2	2.37	0.57
1:a:1160:G:OP2	1:a:1162:C:N4	2.37	0.57
2:b:187:VAL:HG23	2:b:187:VAL:O	2.03	0.57
1:a:1220:C:N4	13:m:104:THR:OG1	2.38	0.57
7:g:35:LYS:HD2	7:g:35:LYS:H	1.70	0.57
8:h:78:ILE:HG12	8:h:79:SER:H	1.69	0.57
20:t:32:ILE:HG23	20:t:79:LEU:HD11	1.86	0.57
1:a:1520:G:OP1	21:u:45:ARG:NH2	2.38	0.57
7:g:41:ARG:HG3	9:i:41:ARG:CZ	2.33	0.57
7:g:46:ALA:HB1	7:g:121:ALA:HB2	1.87	0.57
1:a:402:G:O2'	4:d:165:ARG:NH2	2.37	0.57
1:a:635:A:H4'	8:h:108:LYS:HA	1.86	0.57
8:h:84:ARG:NH2	17:q:38:GLY:O	2.38	0.57
14:n:20:TYR:HE2	14:n:51:GLN:HB3	1.70	0.57
5:e:102:GLU:OE2	5:e:102:GLU:HA	2.04	0.56
10:j:10:LEU:HD13	10:j:72:ARG:HB3	1.86	0.56
8:h:39:VAL:HG21	8:h:110:VAL:HG12	1.86	0.56
13:m:88:GLY:HA2	13:m:91:HIS:HB3	1.87	0.56
1:a:403:U:O2'	4:d:26:ARG:NH1	2.38	0.56
1:a:658:G:H22	1:a:735:G:H1	1.51	0.56
1:a:1055:G:OP1	10:j:54:SER:OG	2.23	0.56
2:b:15:HIS:CD2	2:b:16:PHE:CD1	2.93	0.56
3:c:11:ARG:NH2	3:c:177:THR:O	2.39	0.56
1:a:1173:A:C5	9:i:104:VAL:HB	2.39	0.56
2:b:141:LEU:HD22	2:b:141:LEU:C	2.31	0.56
1:a:1058:G:N2	1:a:1060:C:O4'	2.38	0.56
1:a:1242:A:H61	9:i:72:VAL:HG22	1.71	0.56
3:c:169:ARG:NH2	3:c:171:GLY:O	2.38	0.56
12:l:99:ARG:HB3	12:l:113:ARG:HB2	1.88	0.56
1:a:1019:U:H1'	1:a:1020:G:H8	1.71	0.56
1:a:1119:U:O4	10:j:8:ILE:N	2.38	0.56
1:a:553:A:H4'	1:a:554:A:H3'	1.88	0.56
1:a:855:G:HO2'	1:a:868:G:HO2'	1.52	0.56
1:a:1075:G:H21	5:e:53:LYS:NZ	2.04	0.56
7:g:147:ALA:CB	11:k:56:ARG:NH2	2.62	0.56
9:i:24:GLY:HA3	9:i:62:ASP:HB2	1.88	0.56
7:g:72:LEU:HD13	7:g:96:ARG:HH21	1.71	0.56
1:a:786:A:H4'	1:a:787:U:H5'	1.87	0.56
3:c:7:PRO:O	3:c:8:ASN:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:136:ARG:HA	3:c:139:GLN:HB2	1.88	0.55
6:f:88:LEU:HD12	6:f:90:MET:CG	2.36	0.55
8:h:92:LEU:HD13	8:h:96:ARG:H	1.70	0.55
1:a:671:U:H3	1:a:707:G:H22	1.53	0.55
1:a:1173:A:N6	9:i:85:ARG:HB2	2.15	0.55
2:b:40:ILE:O	2:b:40:ILE:HG22	2.06	0.55
2:b:111:ILE:O	2:b:111:ILE:HG22	2.07	0.55
1:a:1160:G:N2	1:a:1163:A:O2'	2.38	0.55
7:g:146:GLU:C	11:k:61:PHE:CZ	2.83	0.55
1:a:79:G:N1	1:a:84:C:O2	2.40	0.55
4:d:15:GLU:OE1	4:d:56:ARG:HD2	2.05	0.55
7:g:41:ARG:CD	9:i:41:ARG:HH21	2.19	0.55
9:i:30:ILE:HG13	9:i:66:THR:HA	1.89	0.55
9:i:45:ARG:NH1	9:i:46:MET:SD	2.80	0.55
10:j:50:THR:O	14:n:74:TYR:OH	2.24	0.55
1:a:209:C:O2'	1:a:459:A:N7	2.39	0.55
1:a:1061:A:H1'	1:a:1062:G:C8	2.42	0.55
1:a:1170:A:N6	1:a:1175:G:O2'	2.39	0.55
5:e:157:ARG:NH2	8:h:42:ASP:O	2.40	0.55
10:j:36:VAL:HG22	10:j:76:ILE:HG22	1.88	0.55
5:e:104:THR:HG21	5:e:107:ILE:HD11	1.89	0.55
12:l:42:PRO:HB3	12:l:89:ASP:HB3	1.87	0.55
13:m:100:GLN:O	13:m:102:THR:OG1	2.22	0.55
1:a:687:G:OP1	11:k:127:ARG:NH1	2.40	0.55
1:a:1337:G:OP1	9:i:127:TYR:CG	2.60	0.55
1:a:1343:A:OP2	9:i:123:LYS:CG	2.55	0.55
2:b:113:ARG:HE	2:b:113:ARG:N	2.05	0.55
1:a:693:C:N3	1:a:694:G:N2	2.55	0.54
4:d:15:GLU:OE2	4:d:56:ARG:O	2.25	0.54
7:g:5:ARG:O	7:g:5:ARG:HD3	2.06	0.54
1:a:1242:A:N6	9:i:72:VAL:HG22	2.21	0.54
1:a:1336:C:O3'	9:i:128:SER:CA	2.36	0.54
1:a:809:A:N7	1:a:1503:C:O2'	2.37	0.54
1:a:825:C:H5'	2:b:21:ARG:HD3	1.90	0.54
1:a:686:U:N3	11:k:55:SER:OG	2.37	0.54
1:a:1173:A:H3'	9:i:104:VAL:HG12	1.90	0.54
2:b:117:LEU:HD13	2:b:121:SER:CB	2.20	0.54
7:g:154:TYR:CD1	7:g:154:TYR:N	2.75	0.54
1:a:1173:A:C5	9:i:104:VAL:CG2	2.90	0.54
5:e:100:ALA:HB3	5:e:123:ASN:HB3	1.89	0.54
9:i:40:GLY:HA2	9:i:45:ARG:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:73:ASN:OD1	12:l:73:ASN:N	2.38	0.54
1:a:1270:G:H1'	1:a:1276:C:H1'	1.90	0.54
2:b:221:VAL:HG22	2:b:225:LYS:HG3	1.89	0.54
1:a:681:A:H62	1:a:697:G:H21	1.56	0.54
1:a:966:C:OP2	10:j:56:HIS:NE2	2.41	0.54
17:q:10:THR:HG23	17:q:63:THR:HG23	1.90	0.54
1:a:404:G:H1	1:a:427:G:H1	1.54	0.54
1:a:414:U:O2'	1:a:416:C:OP2	2.26	0.54
1:a:1085:U:O2'	1:a:1087:A:N7	2.39	0.54
1:a:1341:G:O2'	1:a:1367:G:O6	2.25	0.54
1:a:1080:U:H3	1:a:1093:G:H22	1.54	0.53
1:a:1129:C:HO2'	1:a:1132:G:H1	1.53	0.53
1:a:1171:G:O6	1:a:1174:A:O2'	2.26	0.53
1:a:1176:G:H2'	1:a:1177:U:H4'	1.90	0.53
1:a:1313:A:C6	19:s:3:ARG:CG	2.91	0.53
2:b:20:THR:HG22	2:b:39:HIS:CE1	2.43	0.53
2:b:76:ALA:HB2	2:b:164:ILE:HD11	1.90	0.53
1:a:1369:A:C8	7:g:102:ARG:HG3	2.43	0.53
2:b:196:VAL:HG21	2:b:199:VAL:HG23	1.90	0.53
4:d:188:ARG:NH2	4:d:192:SER:O	2.41	0.53
1:a:503:A:N7	4:d:51:TYR:N	2.56	0.53
1:a:1182:A:C2	3:c:6:HIS:CG	2.95	0.53
3:c:188:GLU:HA	3:c:197:GLY:HA2	1.89	0.53
7:g:41:ARG:HG3	9:i:41:ARG:HH22	1.60	0.53
2:b:50:PHE:HA	2:b:200:ILE:CD1	2.38	0.53
3:c:22:TRP:HZ2	3:c:33:LEU:HG	1.72	0.53
1:a:423:U:H5''	4:d:29:ASP:HA	1.91	0.53
1:a:775:A:O2'	1:a:1516:U:O2	2.26	0.53
6:f:78:PHE:CE1	6:f:87:ASN:ND2	2.76	0.53
2:b:30:PHE:CZ	2:b:49:MET:HE1	2.44	0.53
1:a:197:G:O2'	1:a:462:A:N7	2.42	0.53
1:a:786:A:O2'	1:a:788:A:N7	2.40	0.53
1:a:1215:G:OP2	19:s:54:GLY:N	2.38	0.53
2:b:117:LEU:HD21	2:b:120:GLN:CB	2.31	0.53
1:a:1110:U:O2'	1:a:1113:C:N4	2.42	0.53
1:a:1247:G:O6	1:a:1278:C:N4	2.42	0.53
1:a:1283:A:N7	7:g:35:LYS:HB3	2.20	0.53
3:c:23:TYR:HD2	10:j:97:GLU:HB2	1.74	0.53
1:a:1084:U:HO2'	1:a:1165:A:HO2'	1.51	0.53
1:a:1313:A:C4	19:s:3:ARG:CB	2.92	0.53
1:a:51:A:H2	1:a:353:G:H22	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:318:G:N2	1:a:321:A:OP2	2.43	0.52
1:a:1182:A:C5	3:c:6:HIS:N	2.75	0.52
1:a:1370:U:H5	7:g:11:GLU:HB2	1.73	0.52
10:j:45:ARG:HB3	10:j:68:ARG:HA	1.92	0.52
11:k:81:ASN:ND2	11:k:106:LYS:O	2.42	0.52
12:l:72:HIS:CD2	12:l:74:LEU:H	2.23	0.52
2:b:120:GLN:HA	2:b:123:ASP:HB3	1.91	0.52
7:g:112:GLY:HA2	7:g:119:ARG:HG3	1.92	0.52
8:h:17:ALA:HB1	8:h:22:LYS:HB2	1.91	0.52
1:a:1065:C:P	5:e:55:ARG:NH2	2.83	0.52
4:d:54:GLN:HB3	4:d:203:LEU:HB2	1.90	0.52
1:a:66:G:H1	1:a:96:G:N2	2.07	0.52
1:a:656:U:O2'	1:a:830:G:OP1	2.27	0.52
4:d:188:ARG:HH22	4:d:193:ALA:HA	1.75	0.52
15:o:16:LYS:HE3	15:o:19:GLU:HA	1.90	0.52
1:a:942:C:O2'	13:m:105:ASN:N	2.41	0.52
2:b:6:MET:CA	2:b:6:MET:CE	2.85	0.52
2:b:21:ARG:CB	2:b:21:ARG:NH1	2.73	0.52
6:f:88:LEU:CD1	6:f:90:MET:SD	2.98	0.52
8:h:31:LYS:O	8:h:33:LYS:N	2.42	0.52
1:a:1323:G:O5'	13:m:25:VAL:N	2.43	0.52
7:g:40:GLU:CG	9:i:42:GLU:HA	2.27	0.52
8:h:36:VAL:HG13	8:h:103:ILE:HG21	1.91	0.52
21:u:51:ALA:HB1	21:u:55:ARG:HH21	1.75	0.52
1:a:1065:C:P	5:e:55:ARG:HH22	2.28	0.52
7:g:41:ARG:HD3	9:i:41:ARG:HH21	1.75	0.52
7:g:41:ARG:NE	9:i:41:ARG:NH2	2.58	0.52
2:b:186:VAL:HG11	2:b:204:ASP:HB3	1.91	0.52
13:m:77:ILE:HG23	13:m:91:HIS:HE1	1.75	0.52
2:b:196:VAL:HG23	2:b:196:VAL:O	2.09	0.51
6:f:10:VAL:HG22	6:f:58:HIS:HB3	1.91	0.51
14:n:64:CYS:H	14:n:69:ARG:H	1.57	0.51
1:a:942:C:H3'	13:m:110:LYS:HD3	1.91	0.51
7:g:118:LEU:HD12	7:g:118:LEU:C	2.35	0.51
16:p:34:GLU:OE2	16:p:56:ARG:NH2	2.38	0.51
1:a:945:G:N2	1:a:1224:C:O2	2.36	0.51
1:a:976:U:OP1	14:n:9:ARG:NH1	2.40	0.51
4:d:132:ILE:HG22	4:d:134:SER:H	1.75	0.51
5:e:125:LEU:HD22	5:e:125:LEU:O	2.10	0.51
12:l:105:SER:OG	12:l:106:GLY:N	2.43	0.51
1:a:87:C:H2'	1:a:89:G:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1343:A:OP2	9:i:123:LYS:HG3	2.09	0.51
4:d:196:ASN:HB3	4:d:199:LEU:HD13	1.92	0.51
9:i:59:GLU:HG2	9:i:60:LYS:HG3	1.92	0.51
1:a:12:U:H4'	1:a:520:C:H4'	1.93	0.51
1:a:1313:A:C4	19:s:3:ARG:CG	2.94	0.51
1:a:1408:U:H2'	1:a:1409:G:H8	1.76	0.51
7:g:99:LEU:HB3	7:g:103:TRP:CD2	2.45	0.51
7:g:124:LEU:HD23	7:g:124:LEU:N	2.25	0.51
7:g:143:ARG:NE	7:g:143:ARG:CA	2.73	0.51
2:b:207:ILE:CD1	2:b:207:ILE:N	2.73	0.51
1:a:407:G:N1	4:d:31:LYS:O	2.43	0.51
1:a:1061:A:H5'	1:a:1087:A:H4'	1.92	0.51
1:a:1315:U:OP1	19:s:69:HIS:ND1	2.43	0.51
10:j:8:ILE:HD11	10:j:76:ILE:HG23	1.92	0.51
1:a:930:C:O2	1:a:931:A:N6	2.44	0.51
1:a:1332:G:N1	1:a:1333:A:N3	2.53	0.51
2:b:112:LYS:N	2:b:112:LYS:CD	2.73	0.51
7:g:17:LYS:HZ2	9:i:43:THR:HA	1.76	0.51
20:t:68:HIS:CD2	20:t:70:ASN:H	2.28	0.51
1:a:584:U:OP1	8:h:31:LYS:N	2.44	0.51
1:a:905:U:OP2	12:l:94:ARG:NH2	2.44	0.51
2:b:86:ARG:NH1	2:b:87:CYS:SG	2.84	0.51
3:c:153:VAL:HB	3:c:166:GLU:HB2	1.93	0.51
4:d:15:GLU:OE1	4:d:15:GLU:HA	2.11	0.51
7:g:35:LYS:HD2	7:g:35:LYS:C	2.33	0.51
7:g:99:LEU:HD13	7:g:103:TRP:CH2	2.46	0.51
1:a:1182:A:C5	3:c:6:HIS:HB2	2.40	0.51
1:a:1156:C:H42	1:a:1168:G:H1	1.59	0.50
2:b:15:HIS:NE2	2:b:16:PHE:HE1	2.04	0.50
2:b:34:ALA:HB2	2:b:39:HIS:HD2	1.74	0.50
2:b:67:ILE:HD13	2:b:160:ALA:HB3	1.91	0.50
6:f:24:ARG:CG	6:f:24:ARG:NH2	2.73	0.50
1:a:346:C:O2	1:a:349:C:N4	2.44	0.50
1:a:461:U:H5''	1:a:462:A:H5''	1.93	0.50
1:a:989:C:O2'	14:n:8:ASN:ND2	2.44	0.50
2:b:68:LEU:HD23	2:b:158:PRO:HG3	1.92	0.50
5:e:85:PRO:HA	5:e:98:GLN:HA	1.92	0.50
7:g:96:ARG:NH1	7:g:96:ARG:CB	2.73	0.50
8:h:111:MET:HE1	8:h:114:ARG:H	1.76	0.50
14:n:28:LYS:HA	14:n:31:ILE:HD12	1.94	0.50
1:a:37:U:O2'	1:a:38:G:O4'	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:107:ILE:HD12	2:b:148:LEU:HD11	1.93	0.50
2:b:113:ARG:NE	2:b:113:ARG:N	2.60	0.50
3:c:69:HIS:HB3	3:c:106:ILE:HD11	1.94	0.50
6:f:76:ASP:HA	6:f:79:ARG:HB3	1.93	0.50
7:g:16:PRO:CB	9:i:47:VAL:N	2.68	0.50
7:g:116:MET:SD	7:g:119:ARG:NH1	2.85	0.50
1:a:422:G:H4'	4:d:9:CYS:HB3	1.92	0.50
1:a:1042:G:H4'	1:a:1043:U:H2'	1.92	0.50
1:a:1182:A:N6	3:c:6:HIS:HB3	2.26	0.50
4:d:14:ARG:NH1	4:d:38:PRO:CA	2.74	0.50
20:t:43:ASP:OD2	20:t:46:LYS:NZ	2.44	0.50
1:a:36:C:O2	12:l:112:GLN:NE2	2.43	0.50
1:a:499:G:H5'	1:a:528:U:H2'	1.93	0.50
2:b:223:ARG:HD2	2:b:223:ARG:O	2.12	0.50
6:f:2:ARG:CG	6:f:2:ARG:NH1	2.73	0.50
1:a:71:U:H2'	1:a:72:A:H4'	1.93	0.50
1:a:770:G:N2	1:a:796:A:OP2	2.34	0.50
1:a:1101:C:O2	1:a:1185:A:O2'	2.28	0.50
2:b:154:MET:SD	2:b:155:GLY:N	2.85	0.50
6:f:85:ILE:C	6:f:86:ARG:O	2.55	0.50
10:j:52:LEU:H	14:n:81:ARG:HD2	1.75	0.50
1:a:412:U:O2'	1:a:534:G:N2	2.45	0.50
1:a:429:A:H1'	4:d:153:LEU:HD21	1.94	0.50
2:b:152:LYS:NZ	2:b:152:LYS:CB	2.73	0.50
3:c:113:ALA:HA	3:c:202:ILE:HD12	1.94	0.50
6:f:7:VAL:O	6:f:87:ASN:HA	2.11	0.50
6:f:88:LEU:CD2	18:r:65:LEU:HD22	2.40	0.50
1:a:1369:A:N1	7:g:29:HIS:ND1	2.60	0.50
3:c:7:PRO:C	3:c:9:GLY:H	2.20	0.50
3:c:8:ASN:OD1	3:c:11:ARG:NH1	2.44	0.50
5:e:15:LYS:HB2	5:e:15:LYS:NZ	2.26	0.50
5:e:81:THR:HG22	5:e:123:ASN:HB2	1.93	0.50
7:g:35:LYS:N	7:g:35:LYS:CD	2.73	0.50
11:k:88:GLY:O	11:k:93:ARG:NH1	2.45	0.50
1:a:583:U:H5''	8:h:30:SER:HB3	1.93	0.49
9:i:30:ILE:HD13	9:i:39:PHE:HE2	1.77	0.49
1:a:1124:A:N6	1:a:1138:G:O2'	2.45	0.49
2:b:207:ILE:CG1	2:b:208:ARG:N	2.76	0.49
1:a:1178:G:N2	1:a:1180:G:O6	2.45	0.49
2:b:113:ARG:HD2	2:b:144:LEU:HB3	1.95	0.49
3:c:57:ILE:HG12	3:c:66:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:27:ARG:O	13:m:31:GLN:N	2.45	0.49
1:a:467:G:OP2	1:a:467:G:N2	2.32	0.49
1:a:1314:C:H2'	19:s:66:MET:HE2	1.95	0.49
2:b:29:LYS:HE2	2:b:30:PHE:CE1	2.48	0.49
1:a:357:A:OP1	12:l:30:ARG:NE	2.44	0.49
1:a:612:C:N4	1:a:615:A:OP2	2.40	0.49
1:a:1313:A:C6	19:s:3:ARG:CB	2.95	0.49
2:b:132:LYS:HG3	2:b:133:GLU:CD	2.37	0.49
5:e:39:VAL:HG13	5:e:118:VAL:HG21	1.92	0.49
8:h:8:ALA:HB2	8:h:78:ILE:HG21	1.95	0.49
1:a:204:C:OP2	1:a:205:G:N2	2.46	0.49
1:a:1313:A:C2	19:s:3:ARG:CG	2.96	0.49
2:b:163:VAL:HG11	2:b:169:GLU:HB2	1.93	0.49
1:a:432:U:H5''	4:d:120:HIS:HB3	1.94	0.49
5:e:106:ILE:HA	5:e:124:VAL:CG2	2.42	0.49
1:a:652:A:H5''	15:o:8:LYS:HD3	1.94	0.49
1:a:731:A:OP1	6:f:91:ARG:N	2.45	0.49
2:b:95:ARG:HB3	2:b:95:ARG:HH11	1.77	0.49
7:g:48:ASP:OD1	7:g:48:ASP:N	2.45	0.49
7:g:99:LEU:HB3	7:g:103:TRP:CE2	2.48	0.49
17:q:17:SER:HB3	17:q:25:THR:HB	1.94	0.49
1:a:411:G:N2	1:a:535:G:OP2	2.42	0.49
2:b:43:LEU:HD23	2:b:43:LEU:C	2.38	0.49
5:e:125:LEU:C	5:e:125:LEU:CD2	2.86	0.49
10:j:22:THR:HG22	10:j:25:ILE:HD12	1.93	0.49
1:a:1012:G:OP2	1:a:1032:U:O2'	2.31	0.49
1:a:1313:A:C5	19:s:3:ARG:CB	2.96	0.49
3:c:40:ARG:HG2	3:c:55:ILE:HG21	1.93	0.49
5:e:46:ARG:HG2	5:e:72:MET:HE2	1.95	0.49
5:e:104:THR:CG2	5:e:107:ILE:CD1	2.91	0.49
1:a:1311:C:H42	14:n:50:LYS:HE2	1.77	0.48
4:d:15:GLU:OE2	4:d:56:ARG:CA	2.60	0.48
6:f:88:LEU:HD21	18:r:65:LEU:CD2	2.42	0.48
1:a:202:U:O2'	1:a:203:U:O2	2.29	0.48
1:a:1133:G:OP2	1:a:1133:G:N2	2.44	0.48
1:a:1313:A:C2	19:s:3:ARG:CB	2.95	0.48
1:a:1238:C:O2'	13:m:27:ARG:NH1	2.36	0.48
1:a:1286:C:O5'	7:g:41:ARG:NH1	2.46	0.48
1:a:581:G:H4'	8:h:4:GLN:HB2	1.93	0.48
10:j:8:ILE:HB	10:j:74:LEU:HB2	1.95	0.48
12:l:50:ARG:NH1	12:l:89:ASP:OD2	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:709:A:H2'	1:a:710:A:C8	2.47	0.48
1:a:712:A:O2'	21:u:35:ARG:NH1	2.47	0.48
1:a:1337:G:P	9:i:128:SER:CA	2.95	0.48
1:a:1343:A:OP2	9:i:123:LYS:HB2	2.14	0.48
3:c:36:ASP:HB3	3:c:40:ARG:HH12	1.77	0.48
1:a:9:G:H1'	4:d:206:LYS:HZ1	1.78	0.48
1:a:263:U:H2'	1:a:264:A:C8	2.48	0.48
1:a:1182:A:C8	3:c:5:VAL:HA	2.49	0.48
7:g:16:PRO:HG3	9:i:47:VAL:N	2.28	0.48
9:i:49:ARG:HA	9:i:52:LEU:HB3	1.96	0.48
10:j:75:ASP:OD1	10:j:75:ASP:N	2.47	0.48
13:m:20:THR:HG21	13:m:27:ARG:HB2	1.96	0.48
21:u:44:GLU:OE2	21:u:47:ARG:NH1	2.47	0.48
1:a:1173:A:C5	9:i:104:VAL:HG23	2.49	0.48
7:g:11:GLU:HG3	7:g:13:LEU:HG	1.96	0.48
1:a:1008:A:H4'	19:s:15:LEU:HD12	1.95	0.48
2:b:69:PHE:CZ	2:b:84:ALA:HB3	2.49	0.48
4:d:18:ASP:OD2	4:d:20:PHE:CE1	2.67	0.48
18:r:23:TYR:HA	18:r:29:LEU:HD11	1.95	0.48
1:a:503:A:H1'	4:d:47:ARG:HG3	1.96	0.48
1:a:937:U:HO2'	1:a:1226:U:HO2'	1.53	0.48
5:e:39:VAL:HG11	5:e:118:VAL:HG21	1.92	0.48
8:h:124:GLU:HG3	8:h:129:VAL:N	2.28	0.48
1:a:248:G:O2'	17:q:21:ASP:O	2.30	0.47
1:a:420:U:O2'	1:a:535:G:OP2	2.32	0.47
1:a:702:A:N1	11:k:38:GLN:NE2	2.62	0.47
1:a:989:C:H4'	14:n:8:ASN:HD21	1.78	0.47
1:a:1123:C:N3	1:a:1137:G:N1	2.62	0.47
2:b:96:TRP:CD1	2:b:96:TRP:C	2.91	0.47
1:a:1065:C:H5''	5:e:55:ARG:CZ	2.44	0.47
1:a:1407:A:H2	1:a:1481:G:H22	1.62	0.47
6:f:66:CYS:HB2	6:f:70:ALA:HB3	1.96	0.47
1:a:1232:A:N6	1:a:1295:U:O2'	2.45	0.47
2:b:132:LYS:HG3	2:b:133:GLU:N	2.29	0.47
2:b:222:ILE:O	2:b:226:GLN:HG3	2.13	0.47
3:c:39:VAL:HG13	3:c:91:LEU:HD22	1.96	0.47
1:a:422:G:H3'	4:d:13:ARG:HE	1.79	0.47
5:e:37:LEU:HD22	5:e:135:VAL:HG12	1.96	0.47
2:b:83:GLU:N	2:b:83:GLU:CD	2.72	0.47
2:b:117:LEU:O	2:b:121:SER:HB3	2.15	0.47
5:e:106:ILE:HD11	5:e:116:LEU:O	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:67:SER:OG	6:f:68:ALA:N	2.48	0.47
7:g:16:PRO:CG	9:i:47:VAL:CG2	2.81	0.47
7:g:23:LEU:HD21	7:g:47:LEU:HD21	1.97	0.47
13:m:86:TYR:OH	19:s:78:ARG:NH2	2.40	0.47
1:a:526:A:O4'	1:a:1049:A:N6	2.48	0.47
1:a:1075:G:H21	5:e:53:LYS:HZ3	1.61	0.47
1:a:1254:C:O2'	1:a:1268:G:N2	2.45	0.47
2:b:31:ILE:HD13	2:b:39:HIS:HB3	1.97	0.47
2:b:101:LEU:HA	2:b:157:LEU:HD21	1.96	0.47
2:b:133:GLU:N	2:b:133:GLU:CD	2.73	0.47
6:f:88:LEU:HD22	18:r:65:LEU:HD13	1.97	0.47
7:g:111:ARG:HE	7:g:111:ARG:HB2	1.44	0.47
10:j:54:SER:OG	10:j:56:HIS:O	2.21	0.47
11:k:35:THR:HG22	11:k:41:ALA:HA	1.96	0.47
11:k:48:GLY:HA2	11:k:52:PHE:HB2	1.97	0.47
1:a:244:A:N6	1:a:269:G:O6	2.48	0.47
1:a:1182:A:N1	3:c:6:HIS:CG	2.80	0.47
1:a:1215:G:O4'	19:s:55:ARG:N	2.44	0.47
1:a:1313:A:C5	19:s:3:ARG:CG	2.98	0.47
2:b:84:ALA:HB1	2:b:221:VAL:HG11	1.96	0.47
5:e:13:ILE:O	5:e:14:GLU:O	2.33	0.47
7:g:51:LYS:HG2	7:g:51:LYS:O	2.14	0.47
7:g:56:ALA:HB1	7:g:60:GLU:HG2	1.95	0.47
7:g:70:ALA:HA	7:g:71:PRO:HD2	1.77	0.47
7:g:25:LYS:HD3	7:g:25:LYS:HA	1.52	0.47
3:c:152:GLN:HB3	3:c:201:TRP:CH2	2.49	0.47
13:m:86:TYR:HB3	19:s:73:GLU:HG2	1.97	0.47
1:a:72:A:H62	1:a:86:C:H5''	1.80	0.46
1:a:1024:U:N3	1:a:1026:G:N7	2.61	0.46
1:a:165:A:H2'	1:a:166:A:C8	2.50	0.46
1:a:525:U:O2	1:a:1201:G:O2'	2.31	0.46
1:a:1104:A:H5''	1:a:1105:A:C8	2.50	0.46
1:a:1242:A:C2	9:i:38:PHE:CD1	3.02	0.46
2:b:117:LEU:CD2	2:b:120:GLN:HB3	2.33	0.46
6:f:88:LEU:HD12	6:f:90:MET:SD	2.55	0.46
1:a:987:G:N7	1:a:1209:G:N2	2.63	0.46
1:a:1259:C:O2'	1:a:1263:A:N6	2.48	0.46
7:g:14:ALA:C	9:i:50:GLN:HE22	2.24	0.46
19:s:58:VAL:HG11	19:s:75:ALA:HB2	1.96	0.46
1:a:1238:C:H2'	1:a:1239:G:C8	2.50	0.46
4:d:15:GLU:OE2	4:d:56:ARG:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:50:GLN:HA	9:i:53:GLU:HG2	1.98	0.46
1:a:187:A:O2'	20:t:59:ASP:OD2	2.32	0.46
1:a:495:C:H2'	1:a:496:A:C8	2.51	0.46
1:a:1315:U:H5'	19:s:67:VAL:H	1.81	0.46
1:a:1349:G:N1	1:a:1362:A:N7	2.63	0.46
2:b:34:ALA:HB2	2:b:39:HIS:CD2	2.50	0.46
2:b:86:ARG:HD2	2:b:86:ARG:C	2.40	0.46
5:e:83:GLN:NE2	5:e:150:PRO:HB3	2.30	0.46
7:g:16:PRO:O	9:i:46:MET:CE	2.63	0.46
7:g:72:LEU:HB2	7:g:142:HIS:NE2	2.30	0.46
11:k:21:ALA:HB2	11:k:82:LEU:HD23	1.97	0.46
1:a:223:U:O2'	16:p:23:ASN:OD1	2.34	0.46
1:a:230:A:H5''	17:q:47:LEU:HD21	1.98	0.46
1:a:534:G:H5''	1:a:535:G:C8	2.51	0.46
5:e:34:PHE:N	5:e:34:PHE:CD1	2.84	0.46
7:g:53:ARG:O	7:g:53:ARG:HD3	2.16	0.46
9:i:23:PRO:HA	9:i:61:PHE:HA	1.97	0.46
1:a:107:G:H21	1:a:347:A:H8	1.63	0.46
1:a:1336:C:H4'	9:i:128:SER:OG	2.16	0.46
2:b:26:LYS:HD3	2:b:194:GLU:HG3	1.98	0.46
4:d:14:ARG:HD2	4:d:38:PRO:CG	2.44	0.46
1:a:931:A:C2	7:g:76:LYS:HD3	2.51	0.46
1:a:433:U:O2'	1:a:434:A:O5'	2.33	0.46
1:a:1051:G:N2	1:a:1193:U:O2	2.49	0.46
1:a:296:G:O2'	12:l:14:ARG:NH1	2.48	0.46
1:a:1249:G:N3	1:a:1252:G:N2	2.61	0.46
4:d:62:ARG:HG2	4:d:67:VAL:HG23	1.98	0.46
7:g:16:PRO:O	9:i:46:MET:CB	2.64	0.46
1:a:456:G:O2'	1:a:457:U:O5'	2.32	0.45
1:a:511:G:N1	1:a:527:A:OP2	2.41	0.45
1:a:646:U:O4	1:a:746:G:O2'	2.31	0.45
1:a:1215:G:OP2	19:s:53:ASN:N	2.48	0.45
2:b:170:ARG:O	2:b:170:ARG:HD3	2.16	0.45
3:c:189:ALA:N	3:c:196:ILE:O	2.49	0.45
5:e:106:ILE:HA	5:e:124:VAL:HG22	1.98	0.45
7:g:64:LYS:HE3	7:g:128:ALA:HA	1.99	0.45
1:a:1062:G:N2	1:a:1186:C:O2	2.49	0.45
2:b:186:VAL:CG1	2:b:204:ASP:HB3	2.45	0.45
9:i:30:ILE:HD11	9:i:67:VAL:HG12	1.97	0.45
1:a:505:C:H4'	4:d:40:GLN:HB3	1.99	0.45
1:a:1076:A:OP1	5:e:24:LYS:NZ	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:1180:G:H21	9:i:115:LYS:HE3	1.81	0.45
7:g:16:PRO:O	9:i:46:MET:HE2	2.17	0.45
7:g:23:LEU:HD21	7:g:47:LEU:HD11	1.99	0.45
7:g:49:LYS:HE3	7:g:117:ALA:HB3	1.96	0.45
7:g:66:LEU:HD12	7:g:66:LEU:N	2.30	0.45
9:i:20:PHE:HB2	9:i:64:PHE:HB3	1.99	0.45
1:a:103:A:H2	1:a:318:G:H21	1.63	0.45
1:a:776:A:H62	1:a:794:G:H21	1.65	0.45
1:a:1005:C:OP1	19:s:17:LYS:NZ	2.49	0.45
5:e:124:VAL:HG23	5:e:125:LEU:H	1.80	0.45
6:f:88:LEU:CD2	18:r:65:LEU:HD13	2.47	0.45
7:g:16:PRO:HA	9:i:46:MET:HB3	1.98	0.45
8:h:106:THR:HB	8:h:107:ASN:H	1.49	0.45
10:j:83:THR:HG23	10:j:87:LEU:HD12	1.97	0.45
1:a:1345:U:C4	7:g:33:SER:O	2.70	0.45
2:b:161:LEU:HD22	2:b:176:ALA:HB2	1.98	0.45
6:f:23:GLU:OE2	6:f:27:LYS:HD2	2.17	0.45
11:k:81:ASN:ND2	11:k:106:LYS:HG3	2.31	0.45
18:r:36:THR:HA	18:r:72:ASP:HB3	1.98	0.45
2:b:113:ARG:CD	2:b:113:ARG:N	2.80	0.45
2:b:173:ILE:O	2:b:173:ILE:HG22	2.16	0.45
4:d:17:THR:HG21	4:d:194:ASP:OD2	2.16	0.45
5:e:47:VAL:HG22	5:e:118:VAL:HG23	1.99	0.45
1:a:1242:A:H61	9:i:72:VAL:CG2	2.29	0.45
2:b:164:ILE:HD12	2:b:210:VAL:HG22	1.99	0.45
2:b:166:VAL:HG21	2:b:196:VAL:HG11	1.99	0.45
4:d:14:ARG:CZ	4:d:38:PRO:O	2.60	0.45
5:e:14:GLU:OE2	5:e:65:MET:SD	2.75	0.45
6:f:90:MET:HE2	6:f:90:MET:HB3	1.79	0.45
15:o:82:ILE:HD11	15:o:88:ARG:HB2	1.97	0.45
19:s:60:VAL:HG22	19:s:74:PHE:HB3	1.98	0.45
1:a:90:G:H5'	1:a:91:A:H5'	1.98	0.45
1:a:510:U:O2'	1:a:513:C:N3	2.41	0.45
19:s:19:VAL:HG11	19:s:40:ILE:HG21	1.97	0.45
20:t:30:THR:HG22	20:t:33:LYS:HE2	1.98	0.45
1:a:430:C:O2	4:d:154:ARG:NH1	2.49	0.45
3:c:19:THR:HB	3:c:56:ASP:HA	1.98	0.45
5:e:87:LYS:HE2	5:e:87:LYS:HB2	1.71	0.45
6:f:2:ARG:HD3	6:f:2:ARG:HA	1.55	0.45
6:f:64:VAL:HG12	6:f:66:CYS:H	1.82	0.45
7:g:27:MET:HG3	7:g:43:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:47:LEU:HD12	7:g:47:LEU:HA	1.66	0.45
1:a:9:G:OP2	5:e:127:LYS:NZ	2.36	0.44
1:a:593:U:H4'	8:h:118:ALA:HA	1.98	0.44
1:a:1233:A:H2'	1:a:1234:U:H4'	1.99	0.44
1:a:1283:A:N6	1:a:1366:U:OP1	2.50	0.44
3:c:37:LEU:HD13	14:n:66:LEU:HG	1.98	0.44
5:e:15:LYS:HB2	5:e:15:LYS:HZ3	1.81	0.44
6:f:21:MET:HG2	6:f:24:ARG:NH1	2.32	0.44
7:g:22:ILE:HB	7:g:101:MET:HE1	1.98	0.44
7:g:131:LYS:H	7:g:131:LYS:HG3	1.65	0.44
12:l:98:VAL:HB	12:l:113:ARG:HH11	1.82	0.44
2:b:96:TRP:CD1	2:b:96:TRP:O	2.70	0.44
1:a:1182:A:H2'	14:n:85:ARG:HH21	1.82	0.44
2:b:61:ALA:CB	2:b:221:VAL:HG23	2.47	0.44
4:d:15:GLU:OE2	4:d:56:ARG:CB	2.65	0.44
1:a:229:U:H2'	1:a:230:A:C8	2.53	0.44
2:b:50:PHE:HA	2:b:200:ILE:HD13	1.99	0.44
2:b:84:ALA:HA	2:b:87:CYS:HB2	1.98	0.44
5:e:18:GLN:HE21	5:e:18:GLN:HB3	1.49	0.44
5:e:104:THR:CG2	5:e:107:ILE:HD13	2.48	0.44
1:a:1173:A:C8	9:i:104:VAL:N	2.86	0.44
1:a:1283:A:C6	7:g:35:LYS:HB3	2.46	0.44
2:b:35:ARG:HG2	2:b:40:ILE:CD1	2.48	0.44
2:b:162:PHE:HD1	2:b:184:ILE:HB	1.83	0.44
1:a:400:G:N7	1:a:430:C:N4	2.65	0.44
1:a:402:G:O5'	4:d:110:THR:OG1	2.34	0.44
1:a:682:G:H22	1:a:692:G:H1	1.66	0.44
1:a:1156:C:N4	1:a:1157:G:O6	2.51	0.44
3:c:53:SER:HA	3:c:114:MET:HB2	2.00	0.44
11:k:82:LEU:HB2	11:k:107:ILE:HG22	1.98	0.44
14:n:72:GLY:HA3	14:n:81:ARG:HB2	1.99	0.44
1:a:402:G:H22	4:d:160:GLU:HB2	1.82	0.44
5:e:47:VAL:HG12	5:e:142:PHE:CE1	2.46	0.44
12:l:30:ARG:NH1	12:l:59:ASN:HD21	2.16	0.44
1:a:34:C:H2'	1:a:35:G:C8	2.53	0.44
1:a:1263:A:OP2	1:a:1264:G:N2	2.50	0.44
6:f:2:ARG:HB3	6:f:3:HIS:H	1.66	0.44
13:m:19:LEU:HD11	13:m:56:LEU:HD22	1.99	0.44
13:m:65:THR:O	13:m:69:LEU:N	2.39	0.44
1:a:8:A:C2	4:d:206:LYS:HD2	2.53	0.43
1:a:943:A:H5''	13:m:104:THR:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:998:A:H1'	1:a:1030:A:C6	2.52	0.43
2:b:142:GLU:HA	2:b:145:GLU:HB3	2.00	0.43
2:b:162:PHE:CD2	2:b:162:PHE:O	2.70	0.43
6:f:88:LEU:HD12	6:f:90:MET:HG3	1.98	0.43
1:a:398:G:H21	1:a:492:A:H8	1.65	0.43
2:b:43:LEU:HD23	2:b:44:GLU:HG2	2.00	0.43
2:b:43:LEU:HD23	2:b:44:GLU:N	2.33	0.43
4:d:95:GLU:HA	4:d:100:ASN:ND2	2.33	0.43
7:g:20:SER:HB2	7:g:21:GLN:H	1.51	0.43
1:a:141:G:H2'	1:a:142:G:C8	2.53	0.43
1:a:684:G:O2'	11:k:57:LYS:N	2.52	0.43
1:a:1336:C:C2'	9:i:127:TYR:O	2.59	0.43
2:b:212:LEU:HD22	2:b:212:LEU:HA	1.71	0.43
7:g:51:LYS:CG	7:g:58:PRO:HD3	2.48	0.43
4:d:37:VAL:HG22	4:d:45:ARG:HH21	1.83	0.43
7:g:99:LEU:HD13	7:g:103:TRP:CZ2	2.53	0.43
8:h:95:VAL:O	8:h:98:GLY:N	2.51	0.43
1:a:579:G:O2'	12:l:5:ASN:OD1	2.28	0.43
2:b:60:LEU:HD22	2:b:60:LEU:HA	1.88	0.43
5:e:83:GLN:HB3	5:e:148:MET:HE2	1.99	0.43
6:f:5:GLU:OE1	6:f:92:ARG:NE	2.49	0.43
9:i:11:ARG:HG2	9:i:15:ALA:HB3	2.00	0.43
1:a:1308:C:C2	19:s:6:LYS:HE3	2.53	0.43
7:g:59:LEU:H	7:g:59:LEU:CD2	2.24	0.43
7:g:66:LEU:HB3	7:g:97:ASN:ND2	2.33	0.43
1:a:80:C:O2	1:a:83:G:N1	2.51	0.43
1:a:1444:G:H21	1:a:1447:A:H2	1.66	0.43
2:b:53:ALA:CB	2:b:200:ILE:HD11	2.48	0.43
2:b:113:ARG:CD	2:b:144:LEU:HB3	2.49	0.43
2:b:164:ILE:CD1	2:b:210:VAL:HG22	2.48	0.43
1:a:498:C:H5	1:a:535:G:H22	1.67	0.43
1:a:926:C:H2'	1:a:927:G:C8	2.53	0.43
2:b:107:ILE:O	2:b:107:ILE:HG23	2.18	0.43
2:b:107:ILE:HD13	2:b:107:ILE:HA	1.57	0.43
3:c:92:THR:HB	3:c:98:PRO:HA	2.01	0.43
9:i:19:VAL:HG22	9:i:65:VAL:HG22	2.00	0.43
1:a:1302:C:OP2	13:m:98:ARG:NH2	2.42	0.43
1:a:1370:U:C5	7:g:11:GLU:HB2	2.54	0.43
2:b:42:ASN:HD22	2:b:42:ASN:HA	1.59	0.43
2:b:207:ILE:N	2:b:207:ILE:HD12	2.34	0.43
4:d:144:ALA:HA	4:d:179:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:106:ILE:HG23	5:e:124:VAL:HG21	1.99	0.43
7:g:69:ILE:CG2	7:g:100:ALA:HA	2.48	0.43
9:i:29:SER:OG	9:i:33:ARG:O	2.22	0.43
1:a:1244:A:H1'	1:a:1281:A:C6	2.54	0.43
7:g:16:PRO:HG2	7:g:17:LYS:CE	2.43	0.43
7:g:57:ASP:HB3	7:g:58:PRO:HD2	2.01	0.43
1:a:36:C:H4'	12:l:116:TYR:CE1	2.54	0.42
1:a:1285:C:H5'	7:g:41:ARG:NH1	2.34	0.42
2:b:32:PHE:O	2:b:32:PHE:CG	2.70	0.42
9:i:49:ARG:O	9:i:53:GLU:N	2.48	0.42
12:l:112:GLN:H	12:l:112:GLN:HG3	1.68	0.42
13:m:14:HIS:HB2	13:m:17:ILE:HB	2.01	0.42
1:a:700:A:H4'	1:a:701:U:H5'	2.00	0.42
1:a:9:G:N7	1:a:552:G:O2'	2.44	0.42
1:a:66:G:H1	1:a:96:G:H22	1.67	0.42
1:a:70:A:O2'	1:a:71:U:O4'	2.37	0.42
1:a:1060:C:H41	1:a:1185:A:H62	1.65	0.42
1:a:1157:G:H2'	1:a:1158:G:C8	2.54	0.42
2:b:79:ILE:HG21	2:b:210:VAL:HG12	2.01	0.42
7:g:23:LEU:HD13	7:g:62:PHE:CZ	2.54	0.42
7:g:41:ARG:CB	9:i:41:ARG:HH22	2.33	0.42
8:h:38:LYS:O	8:h:42:ASP:N	2.51	0.42
8:h:117:ARG:HB3	8:h:118:ALA:H	1.68	0.42
1:a:61:G:O2'	1:a:373:C:O2	2.37	0.42
1:a:421:U:OP2	4:d:13:ARG:NH2	2.43	0.42
1:a:1237:U:C2	13:m:17:ILE:HD11	2.55	0.42
1:a:1313:A:C2	1:a:1313:A:C4	2.98	0.42
5:e:13:ILE:O	5:e:14:GLU:C	2.62	0.42
7:g:23:LEU:HB2	7:g:62:PHE:CZ	2.54	0.42
1:a:204:C:O2'	1:a:206:G:O6	2.32	0.42
1:a:480:U:H2'	1:a:481:A:H8	1.84	0.42
1:a:645:C:N4	1:a:747:A:OP2	2.48	0.42
1:a:1060:C:H2'	1:a:1061:A:H4'	2.01	0.42
1:a:1172:G:H1'	9:i:99:ARG:NH2	2.34	0.42
1:a:1253:C:H41	1:a:1268:G:H1	1.67	0.42
2:b:4:VAL:CG1	2:b:47:LEU:HG	2.47	0.42
1:a:36:C:H4'	12:l:116:TYR:CZ	2.55	0.42
1:a:680:U:O2'	1:a:681:A:N7	2.44	0.42
2:b:27:MET:HE3	2:b:27:MET:HB3	1.85	0.42
3:c:37:LEU:HD11	14:n:79:LEU:HD21	2.02	0.42
8:h:54:GLU:OE1	8:h:54:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:331:G:H2'	1:a:332:A:C8	2.54	0.42
1:a:638:U:O4	8:h:84:ARG:HG3	2.19	0.42
1:a:1122:C:N4	1:a:1135:U:H3'	2.34	0.42
1:a:290:U:O2'	1:a:550:C:O2	2.36	0.42
1:a:1215:G:P	19:s:54:GLY:H	2.43	0.42
1:a:1494:A:H5''	1:a:1502:G:H5'	2.01	0.42
2:b:27:MET:HE2	2:b:189:THR:HA	2.00	0.42
3:c:50:ALA:HB1	3:c:70:THR:HB	2.01	0.42
6:f:55:HIS:HD2	18:r:74:HIS:CE1	2.38	0.42
7:g:112:GLY:HA2	7:g:119:ARG:CG	2.49	0.42
1:a:1522:U:O4	21:u:46:ARG:NH2	2.52	0.42
8:h:33:LYS:HA	8:h:36:VAL:HG23	2.02	0.42
10:j:14:ASP:OD2	10:j:16:ARG:NE	2.51	0.42
1:a:249:G:H4'	17:q:22:LYS:HD2	2.01	0.42
1:a:368:A:H5''	1:a:446:A:C2	2.54	0.42
1:a:1065:C:H2'	1:a:1066:G:C8	2.55	0.42
1:a:1283:A:C4	7:g:35:LYS:CG	3.03	0.42
1:a:1283:A:N7	7:g:35:LYS:HB2	2.34	0.42
7:g:3:ARG:O	7:g:3:ARG:HD3	2.20	0.42
1:a:103:A:H5'	1:a:104:C:C5	2.55	0.41
1:a:516:C:H1'	1:a:530:C:H5''	2.01	0.41
1:a:684:G:H5''	11:k:53:ARG:H	1.85	0.41
1:a:684:G:C8	11:k:52:PHE:HB3	2.55	0.41
1:a:969:A:C6	14:n:82:ASN:HB3	2.55	0.41
1:a:1308:C:C6	19:s:6:LYS:HG3	2.55	0.41
2:b:7:ARG:HG2	2:b:11:LYS:HD2	2.01	0.41
3:c:133:ALA:O	3:c:137:ALA:N	2.53	0.41
12:l:108:LYS:HB3	12:l:114:SER:HB2	2.01	0.41
1:a:1336:C:H3'	1:a:1337:G:C8	2.55	0.41
2:b:49:MET:O	2:b:50:PHE:C	2.63	0.41
2:b:68:LEU:HD23	2:b:158:PRO:CG	2.50	0.41
12:l:29:GLN:HB3	12:l:81:LEU:HD22	2.01	0.41
1:a:178:U:O2	1:a:188:G:N2	2.53	0.41
1:a:1242:A:C2	9:i:38:PHE:CE1	3.07	0.41
1:a:1322:C:H3'	13:m:20:THR:HG23	2.01	0.41
1:a:1435:A:H62	1:a:1454:C:H42	1.67	0.41
3:c:35:ALA:HB1	3:c:95:MET:HG3	2.01	0.41
12:l:112:GLN:HA	12:l:113:ARG:HA	1.67	0.41
1:a:1040:A:O2'	14:n:4:GLU:OE1	2.33	0.41
4:d:50:ASP:O	4:d:54:GLN:N	2.43	0.41
5:e:39:VAL:CG1	5:e:118:VAL:CG2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:t:30:THR:HA	20:t:33:LYS:HE2	2.02	0.41
1:a:1315:U:OP1	19:s:69:HIS:N	2.39	0.41
2:b:73:LYS:O	2:b:74:ARG:C	2.63	0.41
2:b:132:LYS:HE2	2:b:132:LYS:HB2	1.94	0.41
6:f:38:ARG:HH12	18:r:24:LYS:HE2	1.86	0.41
11:k:24:HIS:HB3	11:k:31:ILE:HB	2.02	0.41
13:m:90:ARG:HA	13:m:93:ARG:HB3	2.01	0.41
1:a:667:G:H4'	6:f:86:ARG:NH1	2.35	0.41
1:a:1238:C:HO2'	13:m:27:ARG:HH12	1.60	0.41
1:a:218:U:H2'	1:a:219:C:C6	2.56	0.41
5:e:34:PHE:CD2	5:e:57:VAL:HG22	2.55	0.41
10:j:42:LEU:HA	10:j:43:PRO:HD3	1.81	0.41
1:a:303:A:O2'	1:a:601:A:N1	2.46	0.41
2:b:72:THR:O	2:b:72:THR:OG1	2.37	0.41
5:e:34:PHE:N	5:e:34:PHE:HD1	2.19	0.41
6:f:9:LEU:HD13	6:f:9:LEU:HA	1.89	0.41
6:f:99:GLN:HG3	6:f:100:SER:H	1.85	0.41
7:g:9:LYS:HE2	7:g:9:LYS:CA	2.44	0.41
8:h:10:MET:HE2	8:h:10:MET:HB3	1.75	0.41
13:m:39:VAL:HG11	13:m:56:LEU:HD11	2.02	0.41
16:p:22:THR:HG22	16:p:32:PHE:HA	2.01	0.41
1:a:286:G:C5	1:a:287:G:H1'	2.56	0.41
1:a:685:G:H4'	11:k:28:ASN:HA	2.03	0.41
1:a:1313:A:N1	19:s:3:ARG:CG	2.84	0.41
2:b:32:PHE:HB2	2:b:42:ASN:ND2	2.35	0.41
2:b:79:ILE:HG22	2:b:79:ILE:O	2.21	0.41
7:g:22:ILE:H	7:g:22:ILE:HG12	1.67	0.41
8:h:45:TYR:HE1	8:h:71:VAL:HG11	1.86	0.41
12:l:68:GLY:O	12:l:99:ARG:NH1	2.54	0.41
17:q:31:ARG:NH2	17:q:40:TYR:O	2.54	0.41
1:a:594:G:OP1	8:h:88:SER:OG	2.32	0.41
1:a:943:A:H5'	13:m:103:LYS:N	2.36	0.41
1:a:943:A:H5'	13:m:102:THR:C	2.46	0.41
1:a:1182:A:C6	3:c:6:HIS:N	2.89	0.41
2:b:112:LYS:HG3	2:b:115:ARG:CD	2.50	0.41
2:b:120:GLN:O	2:b:120:GLN:HG3	2.21	0.41
7:g:73:VAL:CG1	7:g:88:PRO:HB2	2.51	0.41
7:g:148:ASN:HA	7:g:151:PHE:CD2	2.56	0.41
1:a:455:A:H2	1:a:466:U:H3	1.69	0.40
1:a:474:U:H2'	1:a:475:G:C8	2.55	0.40
2:b:52:GLU:N	2:b:52:GLU:OE1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:11:ARG:HH21	3:c:178:LEU:HA	1.84	0.40
5:e:26:VAL:HG12	5:e:27:LYS:H	1.86	0.40
1:a:998:A:H3'	1:a:999:A:C8	2.57	0.40
1:a:1041:G:O2'	1:a:1043:U:N3	2.55	0.40
1:a:1129:C:O2'	1:a:1132:G:N1	2.47	0.40
1:a:1431:A:H5''	20:t:29:ARG:HH12	1.87	0.40
2:b:83:GLU:OE1	2:b:83:GLU:CA	2.69	0.40
3:c:92:THR:HG22	3:c:99:VAL:HG23	2.04	0.40
8:h:53:SER:HB3	8:h:57:PRO:HA	2.02	0.40
11:k:28:ASN:O	11:k:58:SER:OG	2.28	0.40
20:t:64:LYS:HG3	20:t:66:ILE:HG12	2.02	0.40
1:a:25:C:H2'	1:a:26:A:C8	2.56	0.40
1:a:151:C:H2'	1:a:152:G:H8	1.87	0.40
1:a:702:A:OP1	11:k:22:HIS:NE2	2.54	0.40
1:a:1283:A:C1'	7:g:35:LYS:HG2	2.51	0.40
2:b:85:ALA:CB	2:b:91:TYR:HB3	2.51	0.40
2:b:196:VAL:O	2:b:196:VAL:CG2	2.69	0.40
13:m:101:ARG:HE	13:m:106:ALA:HB2	1.86	0.40
20:t:25:ARG:HG3	20:t:66:ILE:HG22	2.03	0.40
1:a:636:A:O2'	8:h:110:VAL:HG23	2.20	0.40
1:a:790:C:O3'	11:k:127:ARG:NH2	2.54	0.40
1:a:956:C:O2	1:a:967:G:N2	2.54	0.40
1:a:1147:G:H2'	1:a:1148:G:C8	2.57	0.40
1:a:1311:C:OP1	14:n:49:GLN:NE2	2.44	0.40
1:a:1341:G:O2'	9:i:109:ARG:O	2.40	0.40
8:h:89:VAL:HG22	8:h:91:GLN:HE21	1.85	0.40
18:r:63:ARG:HG2	18:r:70:TYR:CD1	2.56	0.40
19:s:41:LEU:HB2	19:s:44:MET:HE2	2.02	0.40
1:a:539:C:OP1	4:d:58:LYS:NZ	2.54	0.40
1:a:1053:C:O2	3:c:184:TYR:OH	2.24	0.40
1:a:1084:U:O2'	1:a:1165:A:O2'	2.25	0.40
18:r:40:VAL:HA	18:r:41:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	217/221 (98%)	179 (82%)	34 (16%)	4 (2%)	6	19
3	c	201/203 (99%)	170 (85%)	29 (14%)	2 (1%)	12	32
4	d	203/205 (99%)	161 (79%)	39 (19%)	3 (2%)	8	23
5	e	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	9	24
6	f	98/100 (98%)	86 (88%)	10 (10%)	2 (2%)	6	16
7	g	152/154 (99%)	115 (76%)	27 (18%)	10 (7%)	1	1
8	h	121/125 (97%)	84 (69%)	29 (24%)	8 (7%)	1	1
9	i	124/126 (98%)	104 (84%)	20 (16%)	0	100	100
10	j	94/96 (98%)	82 (87%)	12 (13%)	0	100	100
11	k	113/115 (98%)	93 (82%)	20 (18%)	0	100	100
12	l	111/120 (92%)	91 (82%)	18 (16%)	2 (2%)	6	19
13	m	105/109 (96%)	86 (82%)	19 (18%)	0	100	100
14	n	96/98 (98%)	80 (83%)	16 (17%)	0	100	100
15	o	84/87 (97%)	79 (94%)	4 (5%)	1 (1%)	10	28
16	p	76/78 (97%)	64 (84%)	12 (16%)	0	100	100
17	q	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
18	r	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
19	s	78/80 (98%)	63 (81%)	15 (19%)	0	100	100
20	t	83/86 (96%)	83 (100%)	0	0	100	100
21	u	32/34 (94%)	25 (78%)	7 (22%)	0	100	100
All	All	2263/2318 (98%)	1898 (84%)	331 (15%)	34 (2%)	11	23

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	c	8	ASN
4	d	14	ARG
4	d	33	LYS
5	e	14	GLU
6	f	86	ARG
7	g	32	GLU
8	h	32	LEU

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Mol	Chain	Res	Type
8	h	106	THR
12	l	111	LYS
8	h	89	VAL
12	l	112	GLN
2	b	14	VAL
3	c	7	PRO
7	g	81	GLY
7	g	112	GLY
15	o	19	GLU
2	b	78	LYS
4	d	27	ALA
5	e	102	GLU
6	f	67	SER
7	g	27	MET
7	g	28	ASN
7	g	88	PRO
7	g	115	SER
7	g	128	ALA
8	h	118	ALA
8	h	113	ASP
8	h	115	ALA
2	b	71	GLY
2	b	95	ARG
7	g	34	GLY
7	g	152	SER
8	h	101	VAL
8	h	81	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
2	b	182/183 (100%)	107 (59%)	75 (41%)	0 0
3	c	163/169 (96%)	161 (99%)	2 (1%)	63 79
4	d	166/173 (96%)	161 (97%)	5 (3%)	36 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	108/109 (99%)	91 (84%)	17 (16%)	2	8
6	f	81/85 (95%)	76 (94%)	5 (6%)	16	39
7	g	116/120 (97%)	61 (53%)	55 (47%)	0	0
8	h	98/103 (95%)	95 (97%)	3 (3%)	35	59
9	i	102/102 (100%)	102 (100%)	0	100	100
10	j	85/85 (100%)	83 (98%)	2 (2%)	43	67
11	k	82/87 (94%)	81 (99%)	1 (1%)	63	79
12	l	100/104 (96%)	100 (100%)	0	100	100
13	m	91/91 (100%)	91 (100%)	0	100	100
14	n	78/80 (98%)	78 (100%)	0	100	100
15	o	73/73 (100%)	73 (100%)	0	100	100
16	p	60/63 (95%)	58 (97%)	2 (3%)	33	58
17	q	70/70 (100%)	70 (100%)	0	100	100
18	r	46/48 (96%)	44 (96%)	2 (4%)	26	52
19	s	69/71 (97%)	68 (99%)	1 (1%)	59	77
20	t	67/68 (98%)	66 (98%)	1 (2%)	57	76
21	u	28/28 (100%)	28 (100%)	0	100	100
All	All	1865/1912 (98%)	1694 (91%)	171 (9%)	11	23

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	3	GLN
2	b	5	ASN
2	b	7	ARG
2	b	8	ASP
2	b	9	MET
2	b	10	LEU
2	b	20	THR
2	b	21	ARG
2	b	23	TRP
2	b	24	ASN
2	b	26	LYS
2	b	29	LYS
2	b	31	ILE
2	b	38	ILE

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Mol	Chain	Res	Type
2	b	42	ASN
2	b	43	LEU
2	b	47	LEU
2	b	52	GLU
2	b	55	THR
2	b	57	VAL
2	b	58	GLU
2	b	59	ARG
2	b	60	LEU
2	b	64	LYS
2	b	66	LYS
2	b	67	ILE
2	b	68	LEU
2	b	74	ARG
2	b	75	SER
2	b	78	LYS
2	b	79	ILE
2	b	83	GLU
2	b	86	ARG
2	b	92	VAL
2	b	95	ARG
2	b	100	MET
2	b	101	LEU
2	b	102	THR
2	b	105	LYS
2	b	106	THR
2	b	107	ILE
2	b	108	ARG
2	b	112	LYS
2	b	113	ARG
2	b	114	LEU
2	b	117	LEU
2	b	130	THR
2	b	131	LYS
2	b	132	LYS
2	b	136	MET
2	b	139	ARG
2	b	141	LEU
2	b	143	LYS
2	b	152	LYS
2	b	154	MET
2	b	161	LEU

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Mol	Chain	Res	Type
2	b	164	ILE
2	b	167	ASP
2	b	171	ILE
2	b	177	ASN
2	b	181	ILE
2	b	184	ILE
2	b	186	VAL
2	b	190	ASN
2	b	192	SER
2	b	199	VAL
2	b	205	ASP
2	b	207	ILE
2	b	210	VAL
2	b	212	LEU
2	b	214	LEU
2	b	219	GLU
2	b	222	ILE
2	b	225	LYS
2	b	226	GLN
3	c	5	VAL
3	c	6	HIS
4	d	9	CYS
4	d	17	THR
4	d	110	THR
4	d	132	ILE
4	d	173	VAL
5	e	15	LYS
5	e	18	GLN
5	e	21	ARG
5	e	24	LYS
5	e	26	VAL
5	e	39	VAL
5	e	46	ARG
5	e	51	ARG
5	e	53	LYS
5	e	62	GLN
5	e	77	LEU
5	e	102	GLU
5	e	107	ILE
5	e	113	ARG
5	e	125	LEU
5	e	133	ASN

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Mol	Chain	Res	Type
5	e	149	GLN
6	f	2	ARG
6	f	7	VAL
6	f	21	MET
6	f	24	ARG
6	f	86	ARG
7	g	5	ARG
7	g	9	LYS
7	g	11	GLU
7	g	13	LEU
7	g	15	ASP
7	g	17	LYS
7	g	20	SER
7	g	22	ILE
7	g	23	LEU
7	g	25	LYS
7	g	26	PHE
7	g	35	LYS
7	g	38	VAL
7	g	41	ARG
7	g	42	ILE
7	g	47	LEU
7	g	48	ASP
7	g	49	LYS
7	g	50	VAL
7	g	51	LYS
7	g	52	GLU
7	g	53	ARG
7	g	57	ASP
7	g	61	THR
7	g	64	LYS
7	g	66	LEU
7	g	72	LEU
7	g	75	VAL
7	g	77	SER
7	g	79	ARG
7	g	84	THR
7	g	87	VAL
7	g	89	VAL
7	g	91	VAL
7	g	96	ARG
7	g	99	LEU

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Mol	Chain	Res	Type
7	g	102	ARG
7	g	111	ARG
7	g	113	GLU
7	g	114	LYS
7	g	115	SER
7	g	116	MET
7	g	118	LEU
7	g	119	ARG
7	g	120	LEU
7	g	125	LEU
7	g	129	GLU
7	g	131	LYS
7	g	136	LYS
7	g	137	LYS
7	g	144	MET
7	g	146	GLU
7	g	148	ASN
7	g	149	LYS
7	g	154	TYR
8	h	7	LEU
8	h	59	LEU
8	h	106	THR
10	j	13	PHE
10	j	16	ARG
11	k	100	LEU
16	p	21	VAL
16	p	28	ARG
18	r	55	LEU
18	r	70	TYR
19	s	55	ARG
20	t	27	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	19	GLN
2	b	36	ASN
2	b	39	HIS
2	b	42	ASN
2	b	65	ASN
2	b	177	ASN
2	b	215	ASN

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Mol	Chain	Res	Type
4	d	36	ASN
5	e	18	GLN
5	e	20	ASN
5	e	74	GLN
5	e	90	HIS
5	e	123	ASN
5	e	133	ASN
6	f	3	HIS
6	f	52	ASN
6	f	55	HIS
6	f	63	ASN
6	f	77	ASN
6	f	99	GLN
7	g	97	ASN
8	h	4	GLN
9	i	50	GLN
11	k	38	GLN
11	k	81	ASN
12	l	25	GLN
12	l	59	ASN
12	l	72	HIS
13	m	40	ASN
13	m	76	ASN
13	m	91	HIS
13	m	105	ASN
14	n	8	ASN
14	n	45	GLN
14	n	51	GLN
14	n	71	HIS
15	o	42	HIS
16	p	18	HIS
16	p	66	GLN
17	q	54	ASN
19	s	14	HIS
20	t	68	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1516/1519 (99%)	678 (44%)	0

All (678) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	9	G
1	a	15	G
1	a	22	G
1	a	32	A
1	a	33	A
1	a	34	C
1	a	35	G
1	a	36	C
1	a	38	G
1	a	39	G
1	a	47	C
1	a	48	C
1	a	50	A
1	a	52	C
1	a	53	A
1	a	59	A
1	a	60	A
1	a	66	G
1	a	71	U
1	a	72	A
1	a	73	A
1	a	78	A
1	a	82	U
1	a	88	U
1	a	91	A
1	a	93	U
1	a	94	C
1	a	95	A
1	a	96	G
1	a	97	C
1	a	110	A
1	a	115	U
1	a	122	G
1	a	124	A
1	a	125	U
1	a	126	C
1	a	132	G
1	a	133	G
1	a	136	G
1	a	140	G
1	a	156	A
1	a	157	C
1	a	160	G

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Mol	Chain	Res	Type
1	a	163	C
1	a	167	U
1	a	171	G
1	a	176	C
1	a	177	G
1	a	178	U
1	a	182	G
1	a	183	A
1	a	184	G
1	a	185	G
1	a	186	G
1	a	191	A
1	a	197	G
1	a	198	G
1	a	199	A
1	a	201	C
1	a	202	U
1	a	204	C
1	a	205	G
1	a	206	G
1	a	214	G
1	a	227	C
1	a	239	U
1	a	241	G
1	a	245	G
1	a	248	G
1	a	250	U
1	a	252	G
1	a	256	A
1	a	260	G
1	a	261	C
1	a	266	C
1	a	274	C
1	a	275	G
1	a	283	A
1	a	287	G
1	a	292	A
1	a	299	G
1	a	300	A
1	a	310	C
1	a	312	G
1	a	314	A

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Mol	Chain	Res	Type
1	a	315	A
1	a	322	C
1	a	323	A
1	a	325	G
1	a	326	G
1	a	338	A
1	a	339	C
1	a	340	G
1	a	341	G
1	a	342	G
1	a	346	C
1	a	347	A
1	a	348	G
1	a	352	U
1	a	353	G
1	a	356	G
1	a	357	A
1	a	361	U
1	a	362	U
1	a	363	G
1	a	366	C
1	a	370	G
1	a	373	C
1	a	375	A
1	a	378	G
1	a	379	C
1	a	382	G
1	a	384	U
1	a	386	C
1	a	387	A
1	a	388	G
1	a	391	A
1	a	392	U
1	a	394	C
1	a	395	C
1	a	399	U
1	a	400	G
1	a	401	U
1	a	402	G
1	a	403	U
1	a	404	G
1	a	405	A

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Mol	Chain	Res	Type
1	a	406	A
1	a	407	G
1	a	409	A
1	a	410	G
1	a	411	G
1	a	412	U
1	a	414	U
1	a	415	U
1	a	416	C
1	a	417	G
1	a	418	G
1	a	419	A
1	a	421	U
1	a	422	G
1	a	423	U
1	a	424	A
1	a	426	A
1	a	427	G
1	a	428	C
1	a	429	A
1	a	430	C
1	a	432	U
1	a	433	U
1	a	434	A
1	a	445	A
1	a	446	A
1	a	449	G
1	a	451	A
1	a	452	G
1	a	456	G
1	a	457	U
1	a	459	A
1	a	460	A
1	a	461	U
1	a	462	A
1	a	463	C
1	a	470	G
1	a	475	G
1	a	479	U
1	a	480	U
1	a	490	A
1	a	491	U

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Mol	Chain	Res	Type
1	a	492	A
1	a	493	A
1	a	500	G
1	a	501	C
1	a	502	U
1	a	503	A
1	a	504	A
1	a	505	C
1	a	506	U
1	a	512	C
1	a	513	C
1	a	519	C
1	a	521	G
1	a	525	U
1	a	526	A
1	a	527	A
1	a	528	U
1	a	530	C
1	a	533	A
1	a	534	G
1	a	535	G
1	a	536	G
1	a	537	U
1	a	538	G
1	a	539	C
1	a	541	A
1	a	542	G
1	a	546	U
1	a	552	G
1	a	553	A
1	a	556	U
1	a	558	C
1	a	560	G
1	a	566	A
1	a	567	A
1	a	570	C
1	a	571	G
1	a	573	G
1	a	575	G
1	a	576	U
1	a	601	A
1	a	602	A

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Mol	Chain	Res	Type
1	a	612	C
1	a	613	U
1	a	614	C
1	a	627	G
1	a	635	A
1	a	636	A
1	a	643	A
1	a	647	A
1	a	650	G
1	a	654	G
1	a	656	U
1	a	659	A
1	a	660	G
1	a	664	G
1	a	675	C
1	a	676	U
1	a	677	G
1	a	678	U
1	a	679	G
1	a	680	U
1	a	681	A
1	a	682	G
1	a	683	C
1	a	684	G
1	a	685	G
1	a	687	G
1	a	688	A
1	a	689	A
1	a	691	U
1	a	692	G
1	a	693	C
1	a	694	G
1	a	695	U
1	a	696	A
1	a	698	A
1	a	700	A
1	a	701	U
1	a	702	A
1	a	703	G
1	a	708	G
1	a	709	A
1	a	710	A

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Mol	Chain	Res	Type
1	a	711	C
1	a	712	A
1	a	714	C
1	a	715	A
1	a	717	U
1	a	718	G
1	a	727	G
1	a	741	A
1	a	749	A
1	a	753	A
1	a	754	G
1	a	755	G
1	a	757	G
1	a	759	G
1	a	760	A
1	a	763	G
1	a	765	G
1	a	771	A
1	a	775	A
1	a	776	A
1	a	778	A
1	a	779	G
1	a	787	U
1	a	788	A
1	a	792	U
1	a	795	U
1	a	808	A
1	a	809	A
1	a	810	A
1	a	811	C
1	a	815	G
1	a	822	A
1	a	830	G
1	a	835	C
1	a	838	G
1	a	839	A
1	a	840	G
1	a	843	C
1	a	847	G
1	a	858	A
1	a	861	G
1	a	864	A

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Mol	Chain	Res	Type
1	a	865	U
1	a	866	A
1	a	868	G
1	a	870	C
1	a	878	U
1	a	879	G
1	a	881	G
1	a	883	A
1	a	884	G
1	a	885	U
1	a	886	A
1	a	894	A
1	a	896	G
1	a	902	A
1	a	906	C
1	a	908	A
1	a	909	A
1	a	913	A
1	a	916	G
1	a	921	G
1	a	928	C
1	a	929	A
1	a	931	A
1	a	932	A
1	a	933	G
1	a	934	C
1	a	935	G
1	a	937	U
1	a	938	G
1	a	939	G
1	a	940	A
1	a	941	G
1	a	942	C
1	a	943	A
1	a	945	G
1	a	946	U
1	a	953	A
1	a	954	U
1	a	956	C
1	a	957	G
1	a	958	A
1	a	959	A

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Mol	Chain	Res	Type
1	a	960	G
1	a	961	C
1	a	962	A
1	a	963	A
1	a	964	C
1	a	965	G
1	a	966	C
1	a	967	G
1	a	968	A
1	a	969	A
1	a	970	G
1	a	971	A
1	a	972	A
1	a	973	C
1	a	974	C
1	a	975	U
1	a	976	U
1	a	977	A
1	a	978	C
1	a	979	C
1	a	981	G
1	a	982	G
1	a	983	C
1	a	984	C
1	a	985	U
1	a	986	U
1	a	987	G
1	a	988	A
1	a	989	C
1	a	990	A
1	a	998	A
1	a	1002	U
1	a	1004	C
1	a	1005	C
1	a	1007	G
1	a	1008	A
1	a	1009	G
1	a	1011	U
1	a	1012	G
1	a	1013	G
1	a	1014	A
1	a	1015	U

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Mol	Chain	Res	Type
1	a	1017	G
1	a	1019	U
1	a	1020	G
1	a	1023	U
1	a	1025	C
1	a	1026	G
1	a	1030	A
1	a	1032	U
1	a	1036	A
1	a	1038	A
1	a	1039	C
1	a	1040	A
1	a	1043	U
1	a	1044	G
1	a	1047	G
1	a	1048	C
1	a	1049	A
1	a	1050	U
1	a	1051	G
1	a	1052	G
1	a	1054	U
1	a	1055	G
1	a	1056	U
1	a	1057	C
1	a	1058	G
1	a	1060	C
1	a	1062	G
1	a	1063	C
1	a	1075	G
1	a	1077	U
1	a	1078	G
1	a	1079	U
1	a	1082	G
1	a	1088	G
1	a	1089	U
1	a	1090	C
1	a	1095	A
1	a	1101	C
1	a	1102	G
1	a	1104	A
1	a	1105	A
1	a	1106	C

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Mol	Chain	Res	Type
1	a	1108	C
1	a	1110	U
1	a	1111	G
1	a	1112	U
1	a	1113	C
1	a	1115	U
1	a	1116	U
1	a	1117	A
1	a	1118	G
1	a	1119	U
1	a	1120	U
1	a	1121	A
1	a	1122	C
1	a	1123	C
1	a	1125	G
1	a	1126	C
1	a	1127	A
1	a	1129	C
1	a	1130	U
1	a	1132	G
1	a	1133	G
1	a	1134	G
1	a	1135	U
1	a	1137	G
1	a	1139	C
1	a	1140	A
1	a	1141	C
1	a	1142	U
1	a	1143	C
1	a	1145	A
1	a	1146	A
1	a	1149	A
1	a	1150	G
1	a	1151	A
1	a	1152	C
1	a	1153	U
1	a	1154	G
1	a	1155	C
1	a	1162	C
1	a	1163	A
1	a	1164	A
1	a	1170	A

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Mol	Chain	Res	Type
1	a	1171	G
1	a	1172	G
1	a	1173	A
1	a	1174	A
1	a	1175	G
1	a	1176	G
1	a	1177	U
1	a	1178	G
1	a	1179	G
1	a	1180	G
1	a	1181	G
1	a	1182	A
1	a	1183	U
1	a	1184	G
1	a	1185	A
1	a	1188	U
1	a	1189	C
1	a	1190	A
1	a	1191	A
1	a	1192	G
1	a	1194	C
1	a	1195	A
1	a	1196	U
1	a	1197	C
1	a	1199	U
1	a	1200	G
1	a	1201	G
1	a	1205	U
1	a	1206	U
1	a	1207	A
1	a	1208	C
1	a	1209	G
1	a	1210	G
1	a	1211	C
1	a	1212	C
1	a	1213	A
1	a	1214	G
1	a	1217	C
1	a	1218	U
1	a	1219	A
1	a	1221	A
1	a	1223	A

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Mol	Chain	Res	Type
1	a	1225	G
1	a	1226	U
1	a	1227	G
1	a	1228	C
1	a	1229	U
1	a	1230	A
1	a	1231	C
1	a	1232	A
1	a	1233	A
1	a	1234	U
1	a	1235	G
1	a	1236	G
1	a	1237	U
1	a	1238	C
1	a	1239	G
1	a	1240	G
1	a	1242	A
1	a	1244	A
1	a	1245	A
1	a	1246	A
1	a	1247	G
1	a	1250	U
1	a	1251	U
1	a	1252	G
1	a	1254	C
1	a	1255	A
1	a	1257	G
1	a	1258	C
1	a	1259	C
1	a	1260	G
1	a	1262	G
1	a	1263	A
1	a	1264	G
1	a	1265	G
1	a	1266	U
1	a	1267	G
1	a	1268	G
1	a	1273	A
1	a	1274	A
1	a	1275	U
1	a	1276	C
1	a	1277	C

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Mol	Chain	Res	Type
1	a	1279	A
1	a	1281	A
1	a	1282	A
1	a	1285	C
1	a	1286	C
1	a	1287	G
1	a	1289	U
1	a	1291	G
1	a	1292	U
1	a	1293	A
1	a	1294	G
1	a	1295	U
1	a	1296	C
1	a	1297	C
1	a	1298	G
1	a	1299	G
1	a	1300	A
1	a	1301	U
1	a	1302	C
1	a	1303	G
1	a	1304	C
1	a	1305	A
1	a	1307	U
1	a	1308	C
1	a	1309	U
1	a	1310	G
1	a	1311	C
1	a	1312	A
1	a	1313	A
1	a	1314	C
1	a	1315	U
1	a	1316	C
1	a	1317	G
1	a	1318	A
1	a	1319	C
1	a	1320	U
1	a	1321	G
1	a	1323	G
1	a	1324	U
1	a	1325	G
1	a	1327	A
1	a	1330	C

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Mol	Chain	Res	Type
1	a	1331	G
1	a	1332	G
1	a	1333	A
1	a	1334	A
1	a	1336	C
1	a	1337	G
1	a	1338	C
1	a	1339	U
1	a	1340	A
1	a	1341	G
1	a	1342	U
1	a	1344	A
1	a	1345	U
1	a	1346	C
1	a	1347	G
1	a	1348	U
1	a	1349	G
1	a	1351	A
1	a	1352	U
1	a	1353	C
1	a	1354	A
1	a	1355	G
1	a	1356	A
1	a	1357	A
1	a	1358	U
1	a	1359	G
1	a	1361	C
1	a	1362	A
1	a	1363	C
1	a	1364	G
1	a	1365	G
1	a	1366	U
1	a	1367	G
1	a	1368	A
1	a	1369	A
1	a	1370	U
1	a	1371	A
1	a	1372	C
1	a	1373	G
1	a	1374	U
1	a	1375	U
1	a	1378	C

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Mol	Chain	Res	Type
1	a	1379	G
1	a	1380	G
1	a	1382	C
1	a	1388	A
1	a	1392	A
1	a	1394	C
1	a	1395	G
1	a	1398	C
1	a	1404	A
1	a	1405	C
1	a	1413	G
1	a	1420	G
1	a	1428	A
1	a	1432	G
1	a	1435	A
1	a	1436	G
1	a	1438	C
1	a	1439	U
1	a	1440	A
1	a	1441	A
1	a	1445	C
1	a	1446	A
1	a	1447	A
1	a	1448	G
1	a	1454	C
1	a	1455	G
1	a	1458	U
1	a	1461	C
1	a	1466	A
1	a	1469	G
1	a	1471	U
1	a	1481	G
1	a	1486	A
1	a	1487	A
1	a	1488	G
1	a	1497	A
1	a	1500	U
1	a	1502	G
1	a	1511	G
1	a	1513	A
1	a	1514	C
1	a	1515	C

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Mol	Chain	Res	Type
1	a	1522	U
1	a	1523	G
1	a	1524	G
1	a	1525	A
1	a	1526	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	a	4
2	b	1
13	m	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	2:A	O3'	7:A	P	21.37
1	a	63:C	O3'	65:A	P	7.46

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	124:GLY	C	130:THR	N	5.42
1	m	20:THR	C	22:ILE	N	3.27
1	a	1376:C	O3'	1377:C	P	3.24
1	a	53:A	O3'	55:A	P	3.13

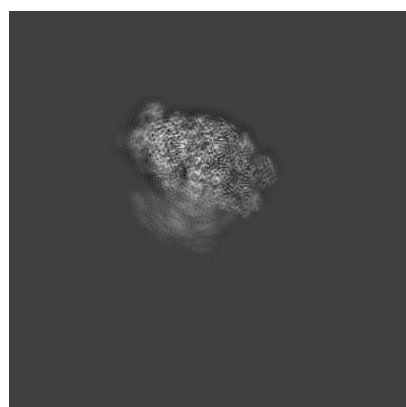
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10281. These allow visual inspection of the internal detail of the map and identification of artifacts.

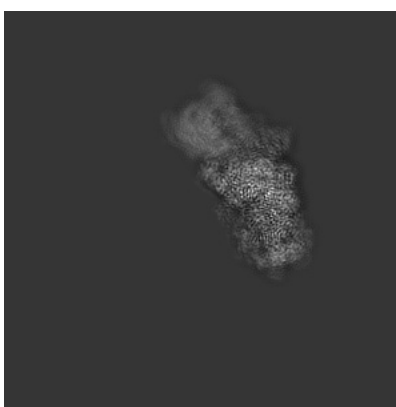
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

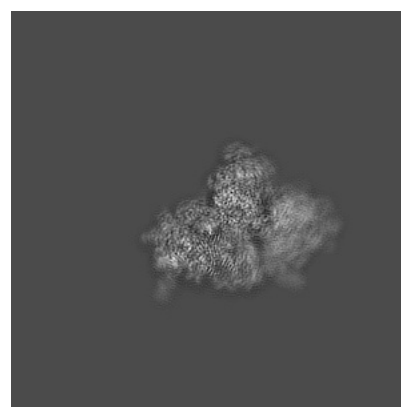
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

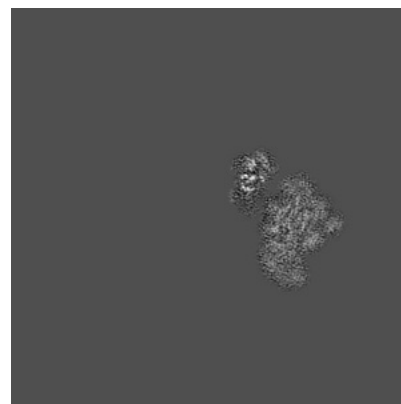
6.2.1 Primary map



X Index: 200



Y Index: 200

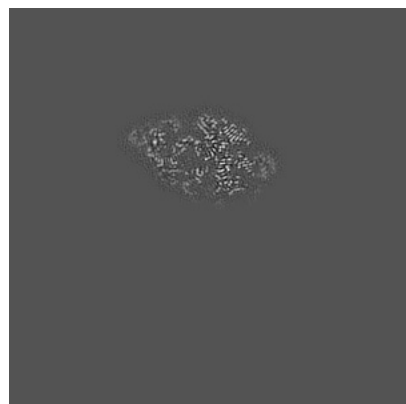


Z Index: 200

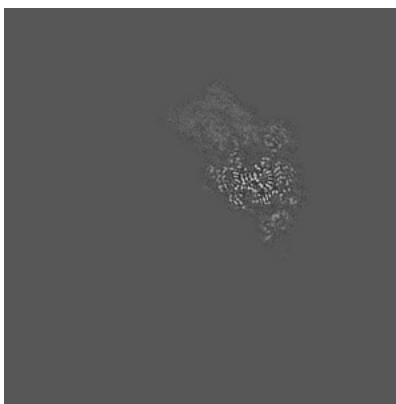
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

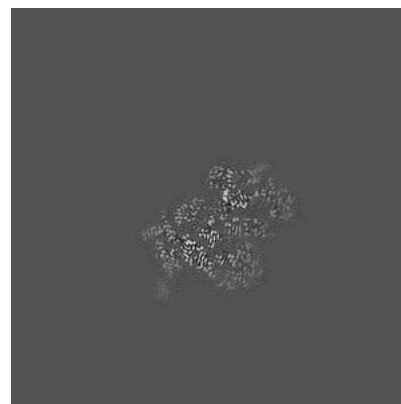
6.3.1 Primary map



X Index: 218



Y Index: 207

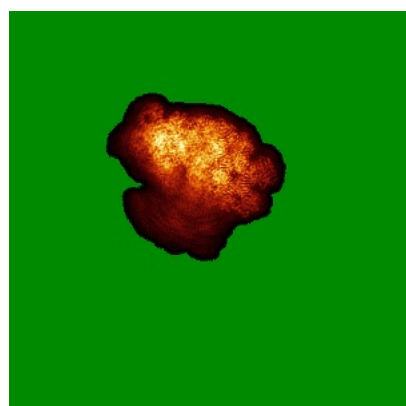


Z Index: 268

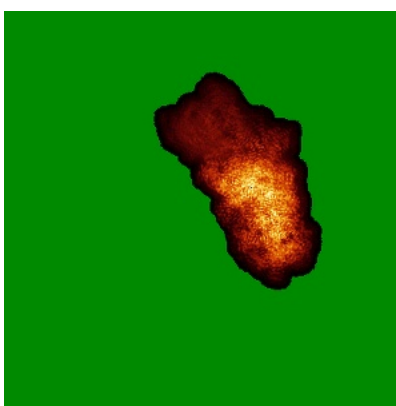
The images above show the largest variance slices of the map in three orthogonal directions.

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

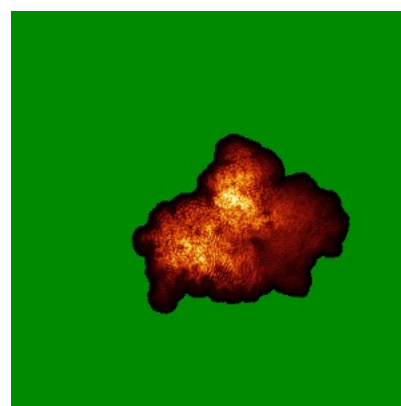
6.4.1 Primary map



X



Y

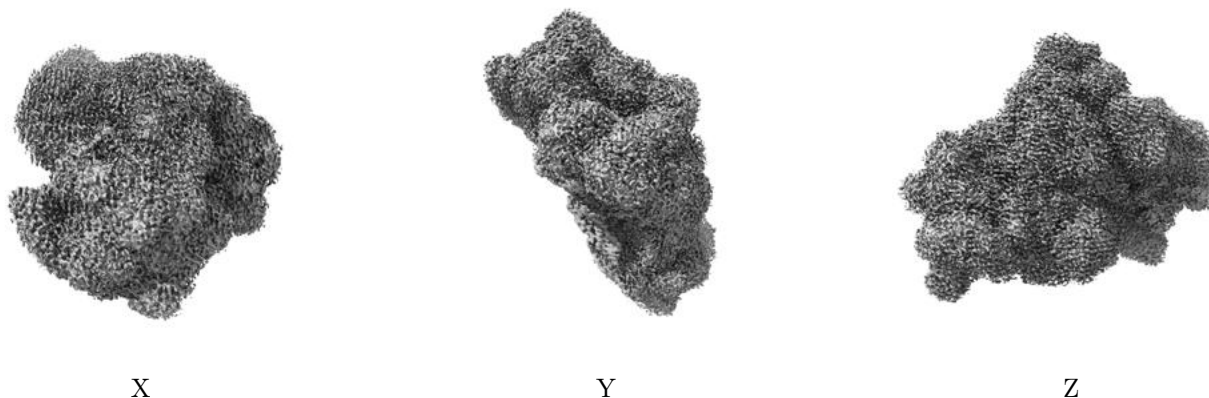


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00936. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

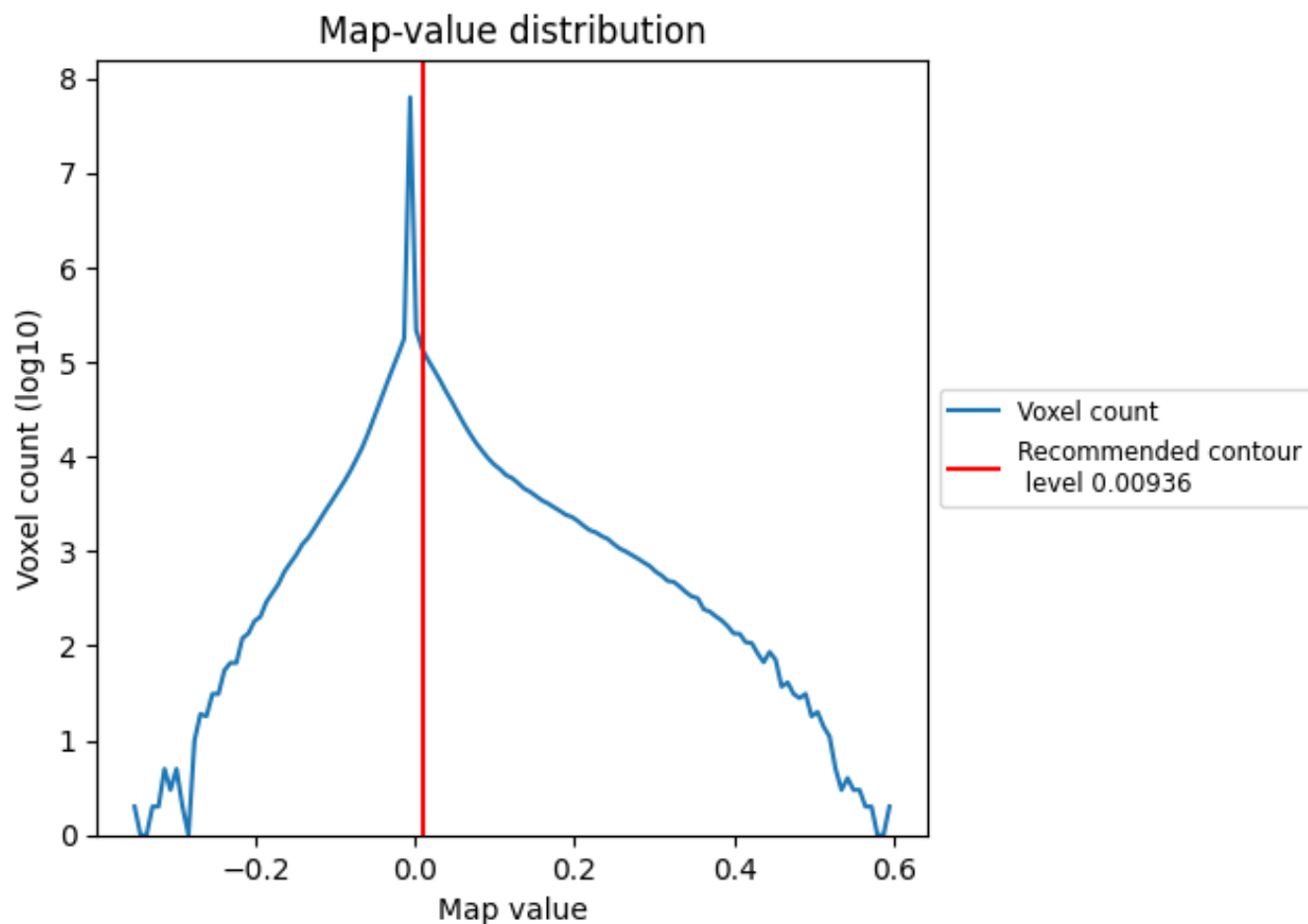
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

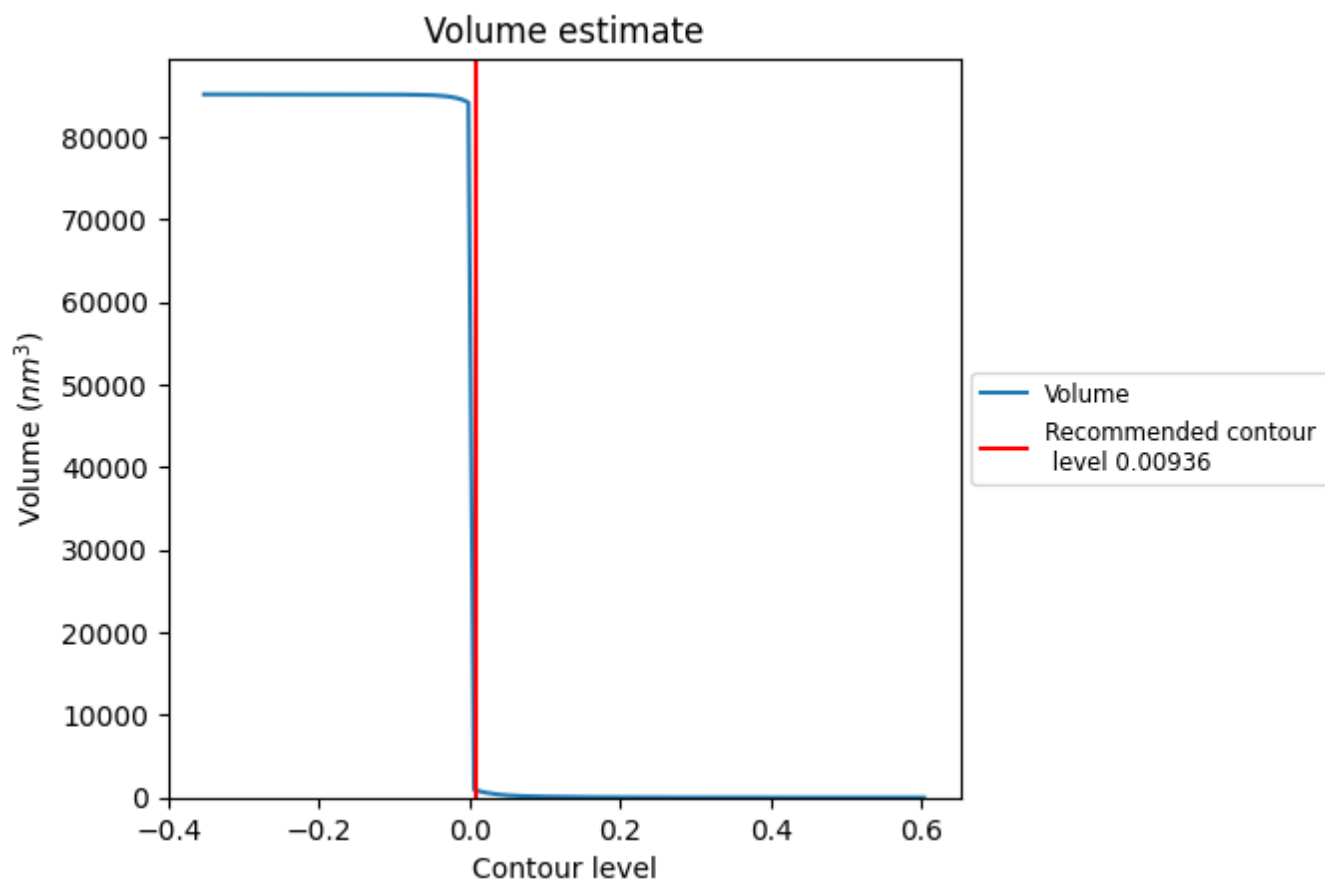
This section contains the results of statistical analysis of the map.

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.

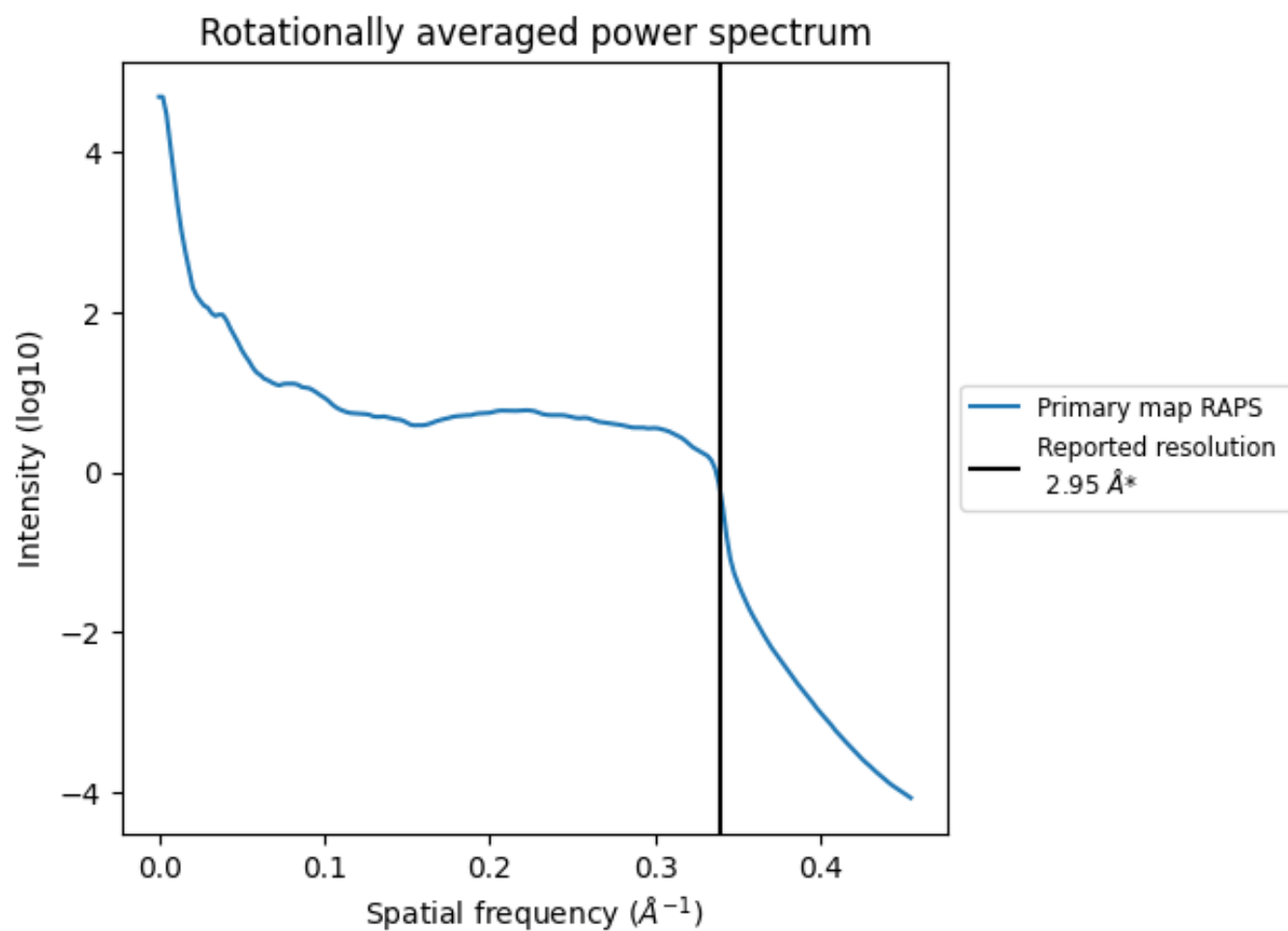
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 868 nm³; this corresponds to an approximate mass of 784 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 0.339 Å⁻¹

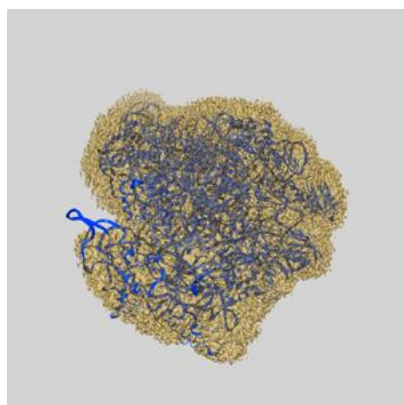
8 Fourier-Shell correlation

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

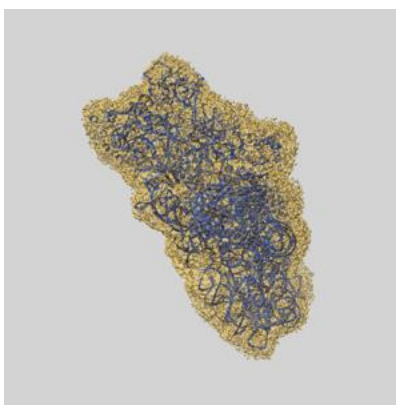
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10281 and PDB model 6SPC. Per-residue inclusion information can be found in section [3](#) on page [9](#).

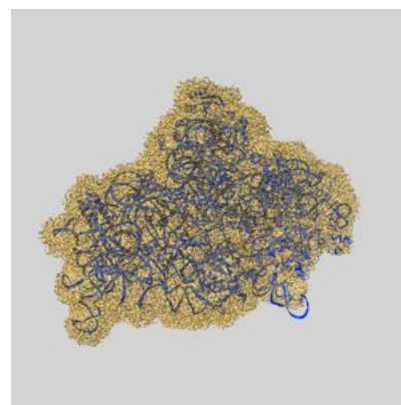
9.1 Map-model overlay [i](#)



X



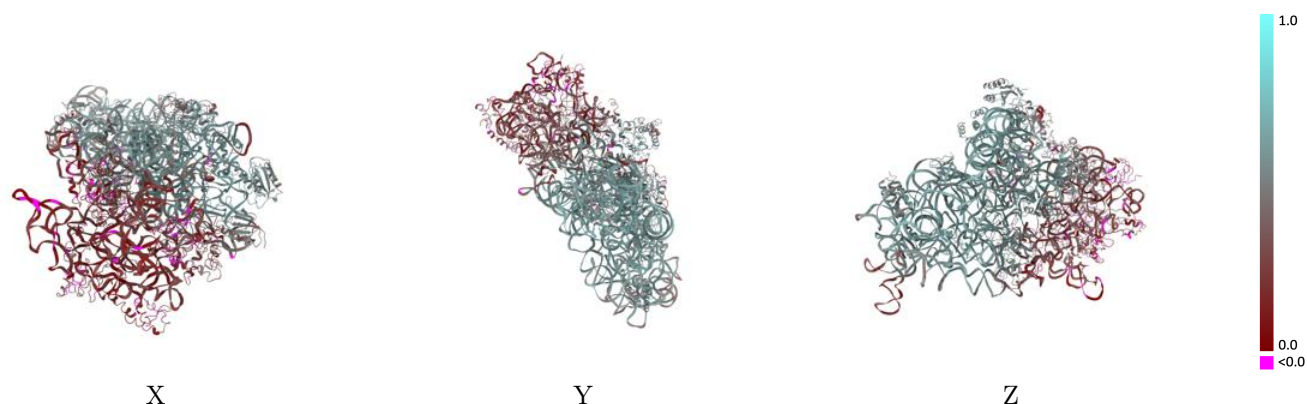
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00936 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](#)



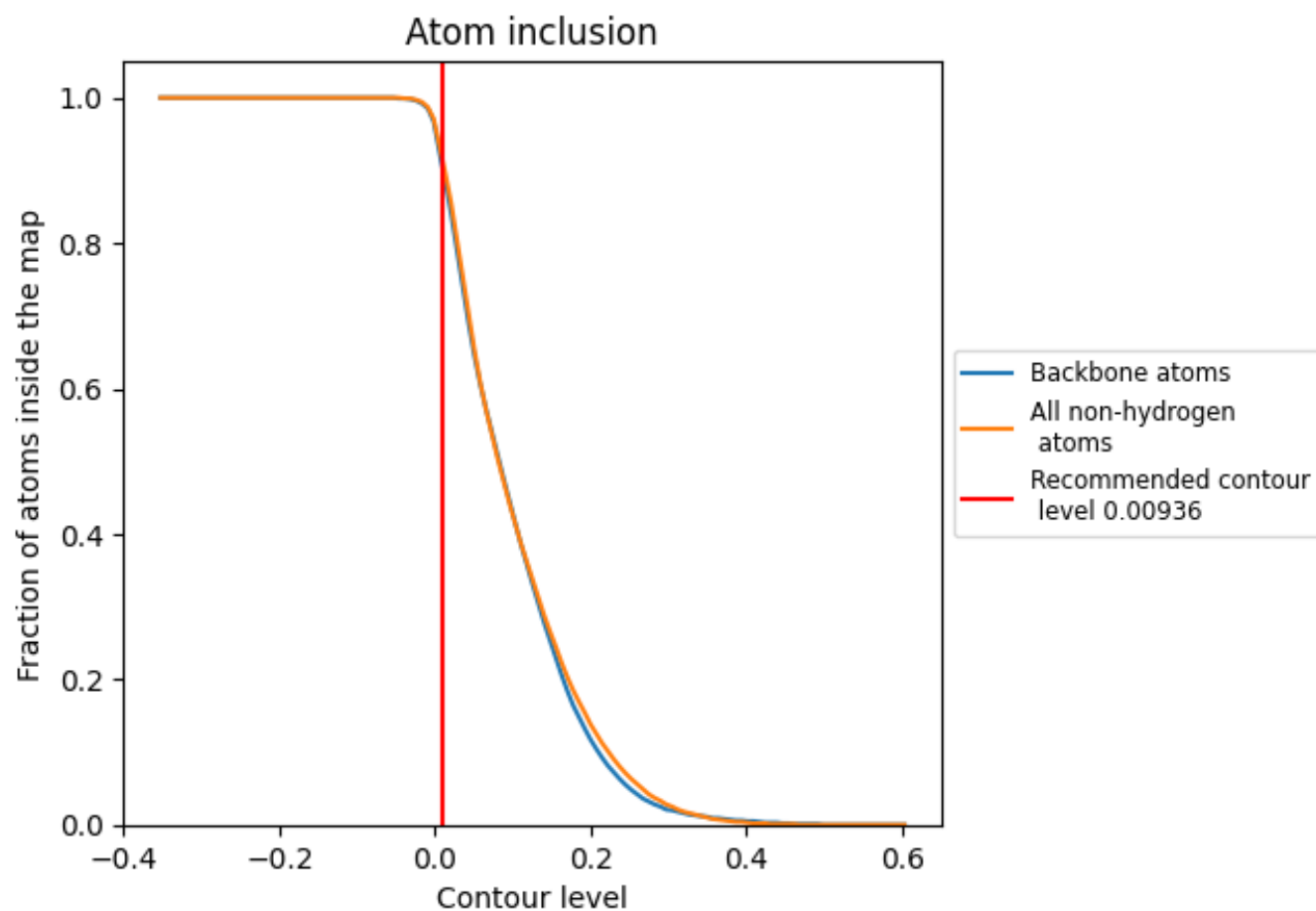
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00936).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 92% 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 (0.00936) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9150	 0.4430
a	 0.9450	 0.4710
b	 0.9770	 0.5140
c	 0.5420	 0.1890
d	 0.9280	 0.4220
e	 0.9730	 0.5630
f	 0.9820	 0.5190
g	 0.8150	 0.3130
h	 0.8830	 0.4250
i	 0.8250	 0.1150
j	 0.7150	 0.2080
k	 0.9680	 0.4590
l	 0.9410	 0.5120
m	 0.7200	 0.1780
n	 0.6120	 0.2090
o	 0.9960	 0.5860
p	 0.9880	 0.5980
q	 0.9770	 0.5740
r	 0.9860	 0.5670
s	 0.7620	 0.2050
t	 0.9890	 0.5810
u	 0.7280	 0.4130

