



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:21 PM UTC

PDB ID : 5O5J / pdb_00005o5j
EMDB ID : EMD-3748
Title : Structure of the 30S small ribosomal subunit from Mycobacterium smegmatis
Authors : Hentschel, J.; Burnside, C.; Mignot, I.; Leibundgut, M.; Boehringer, D.; Ban, N.
Deposited on : 2017-06-02
Resolution : 3.45 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:

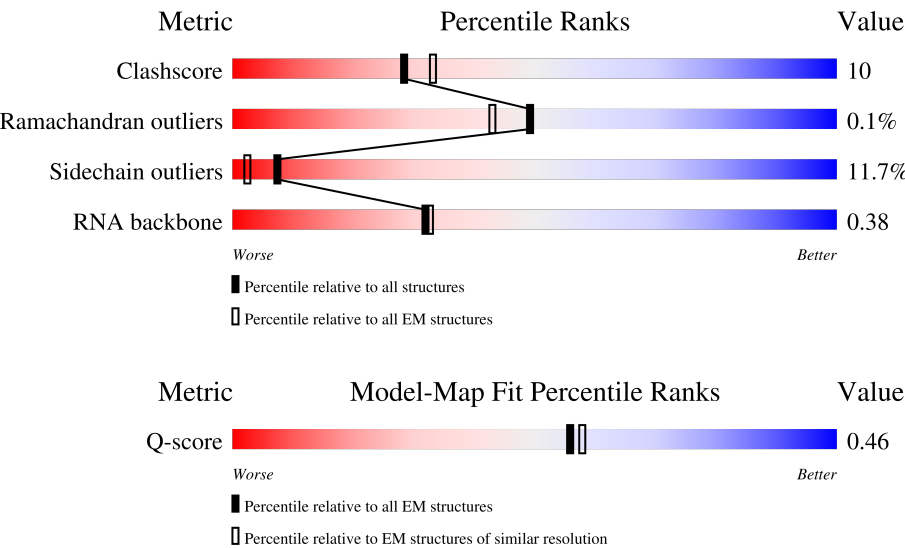
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.45 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	13836 (2.95 - 3.95)

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	1528	
2	B	33	
3	C	275	

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Mol	Chain	Length	Quality of chain
4	D	201	
5	E	214	
6	F	96	
7	G	156	
8	H	132	
9	I	150	
10	J	101	
11	K	138	
12	L	124	
13	M	124	
14	N	61	
15	O	89	
16	P	156	
17	Q	98	
18	R	84	
19	S	93	
20	T	86	
21	V	277	
22	W	19	
23	X	6	
24	g	75	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52163 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	1511	Total	C	N	O	P	0	0
			32439	14448	5930	10550	1511		

- Molecule 2 is a protein called Conserved domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	32	Total	C	N	O	S	0	0
			280	172	71	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	208	Total	C	N	O	S	0	0
			1660	1036	322	298	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	200	Total	C	N	O	S	0	0
			1641	1028	316	295	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	180	Total	C	N	O	S	0	0
			1296	812	245	235	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	96	Total	C	N	O	S	0	0
			771	486	138	145	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	155	Total	C	N	O	S	0	0
			1232	768	241	221	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	131	Total	C	N	O	S	0	0
			1010	633	189	187	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	126	Total	C	N	O	0	0
			994	630	194	170		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	99	Total	C	N	O	S	0	0
			788	495	146	144	3		

- 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
			855	528	170	156	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	122	Total	C	N	O	S	0	0
			958	594	197	165	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	116	Total	C	N	O	S	0	0
			935	572	191	169	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	60	Total	C	N	O	S	0	0
			477	302	97	73	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	88	Total	C	N	O		0	0
			720	449	147	124			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	113	Total	C	N	O		0	0
			891	570	162	159			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	94	Total	C	N	O	S	0	0
			748	469	142	135	2		

- Molecule 18 is a protein called 30S ribosomal protein S18 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	65	Total	C	N	O	S	0	0
			513	318	102	90	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	82	Total	C	N	O	S	0	0
			662	425	124	112	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	85	Total	C	N	O		0	0
			660	402	139	119			

- Molecule 21 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	228	Total	C	N	O	S	0	0
			1793	1132	322	330	9		

- Molecule 22 is a RNA chain called tRNA-Phe anticodon stem.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	19	Total	C	N	O	P	0	0
			410	183	78	130	19		

- Molecule 23 is a RNA chain called mRNA fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	6	Total	C	N	O	P	0	0
			117	54	13	45	5		

- Molecule 24 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	g	11	Total	C	N	O	0	0
			94	59	21	14		

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
25	A	215	Total	Mg	0
			215	215	
25	F	1	Total	Mg	0
			1	1	
25	R	1	Total	Mg	0
			1	1	

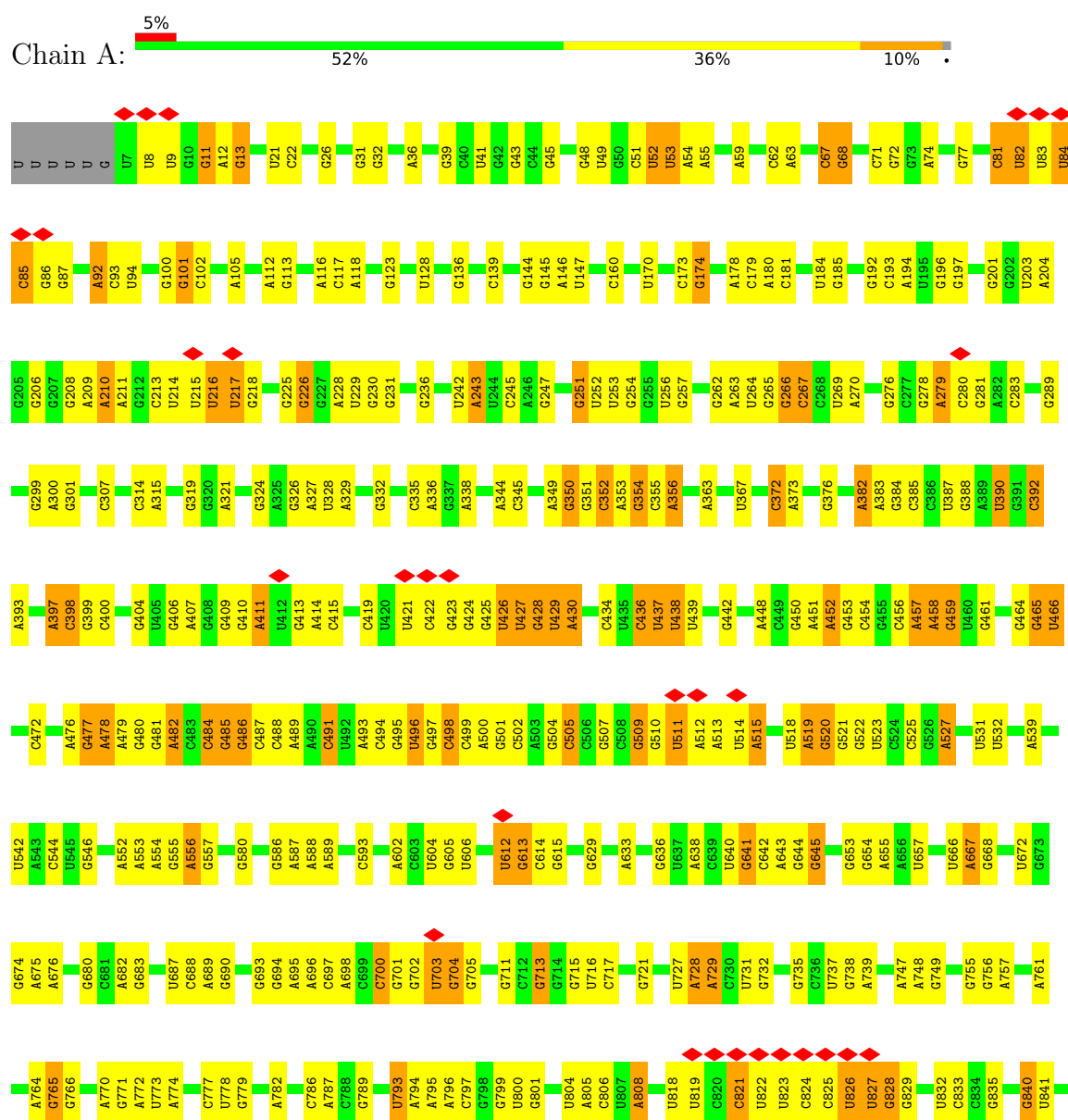
- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
26	N	1	Total	Zn	0
			1	1	
26	R	1	Total	Zn	0
			1	1	

3 Residue-property plots

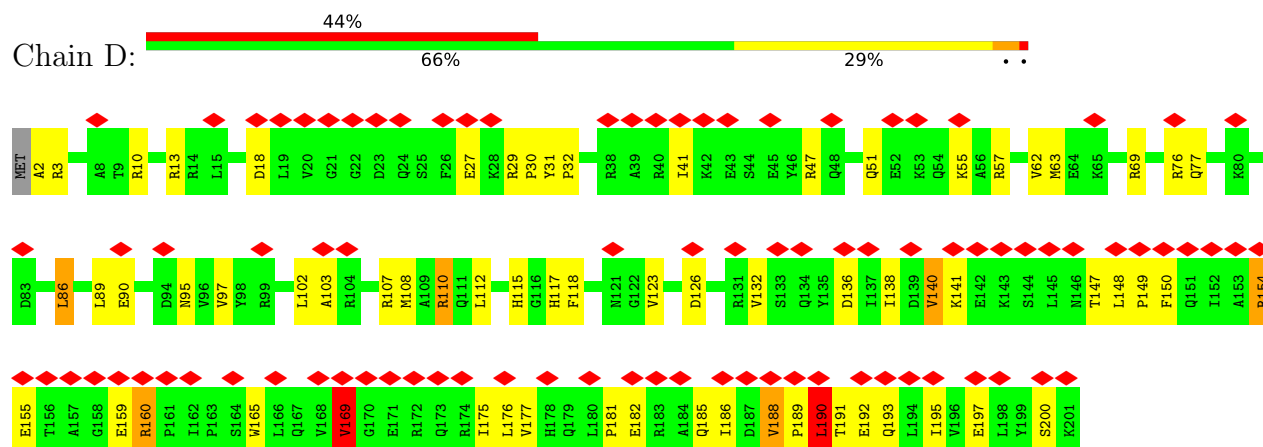
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA

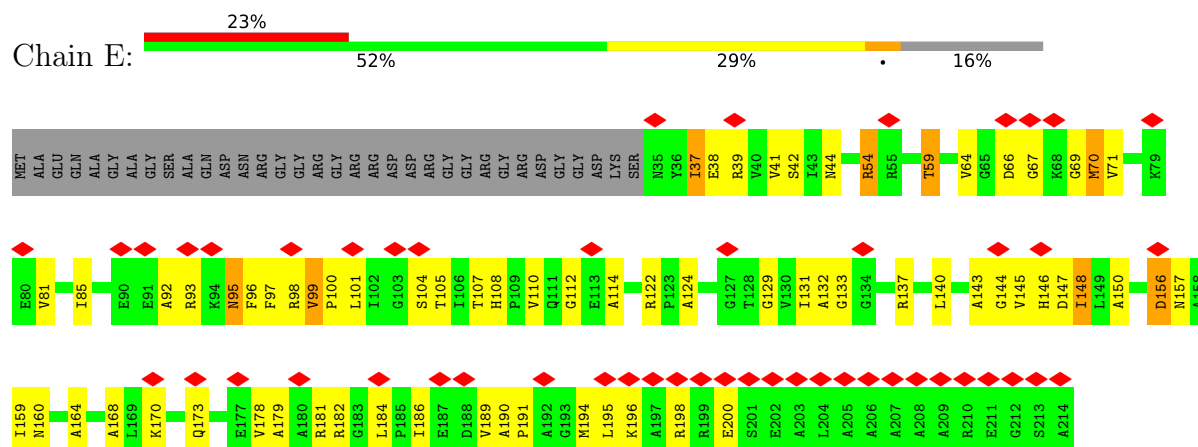




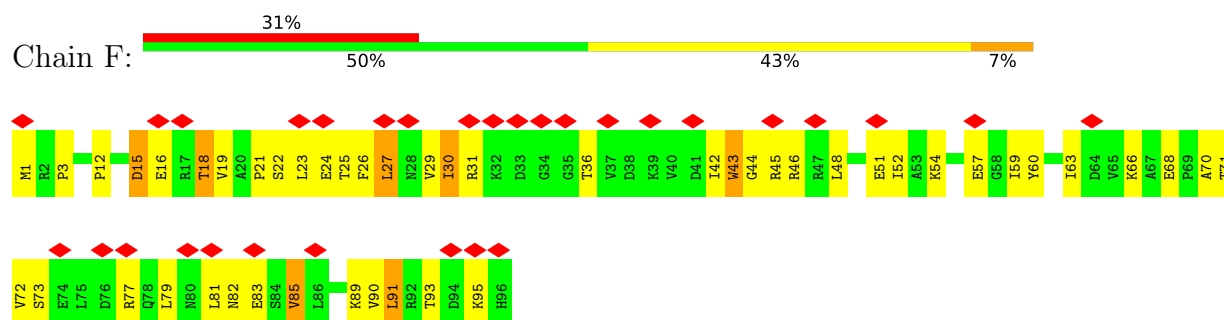
- Molecule 4: 30S ribosomal protein S4



- Molecule 5: 30S ribosomal protein S5

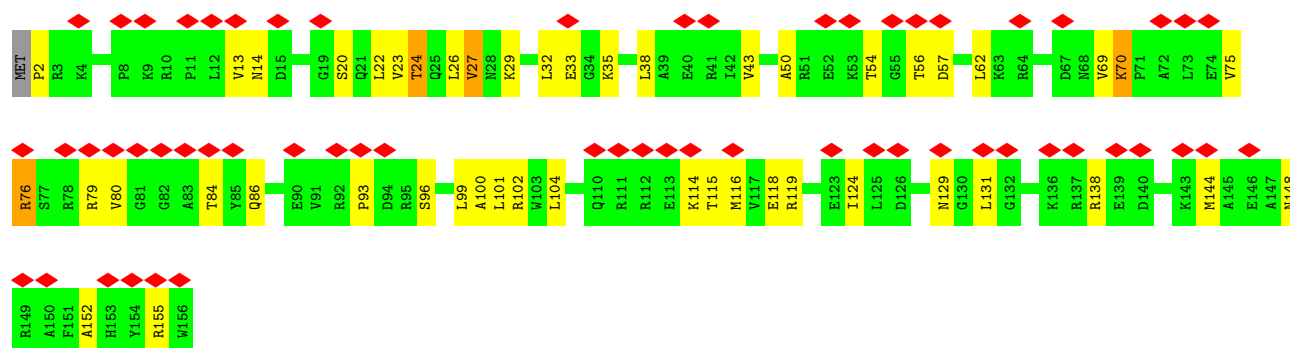


- Molecule 6: 30S ribosomal protein S6



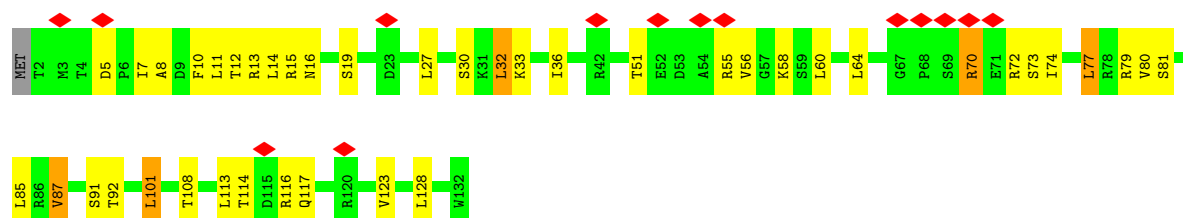
- Molecule 7: 30S ribosomal protein S7

Chain G: 



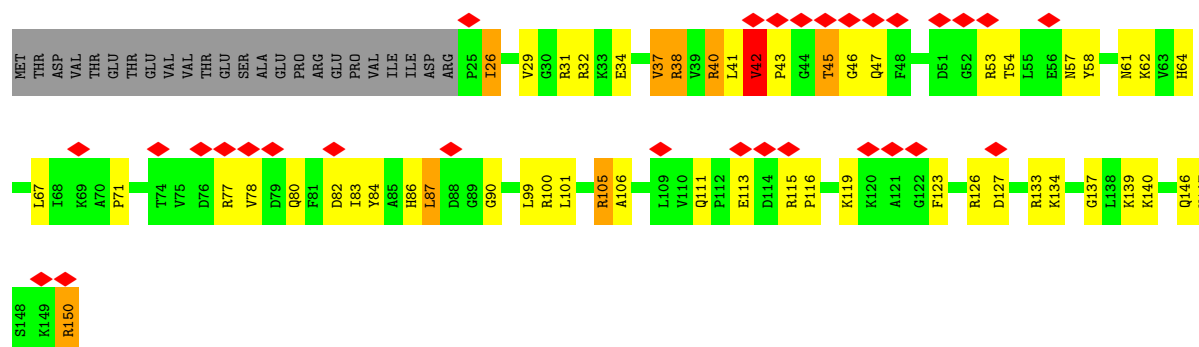
• Molecule 8: 30S ribosomal protein S8

Chain H: 



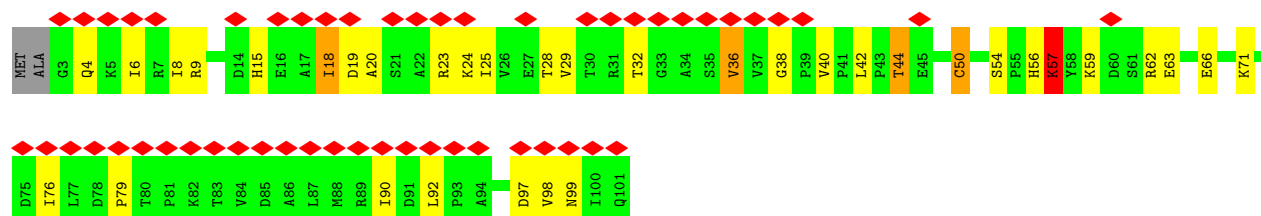
• Molecule 9: 30S ribosomal protein S9

Chain I: 

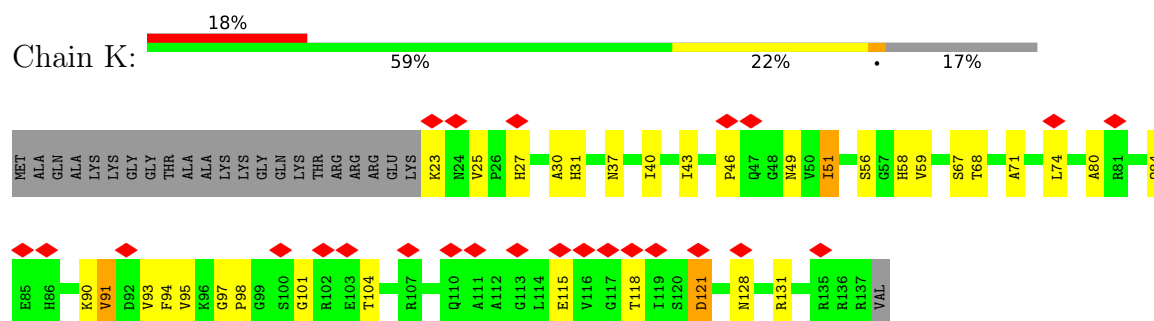


• Molecule 10: 30S ribosomal protein S10

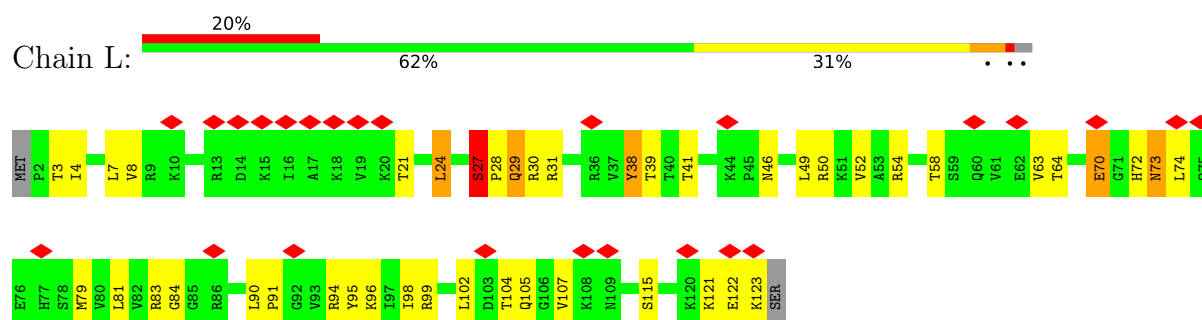
Chain J: 



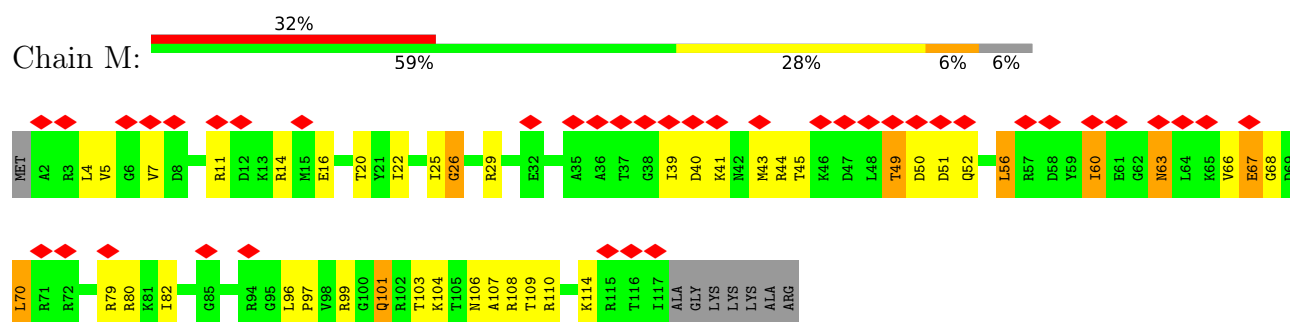
- Molecule 11: 30S ribosomal protein S11



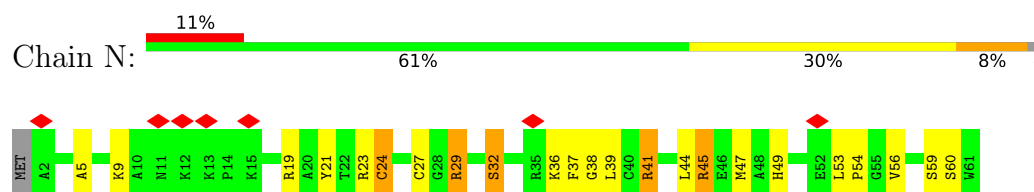
- Molecule 12: 30S ribosomal protein S12



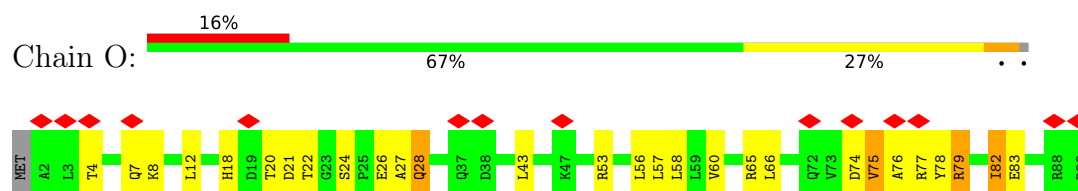
- Molecule 13: 30S ribosomal protein S13



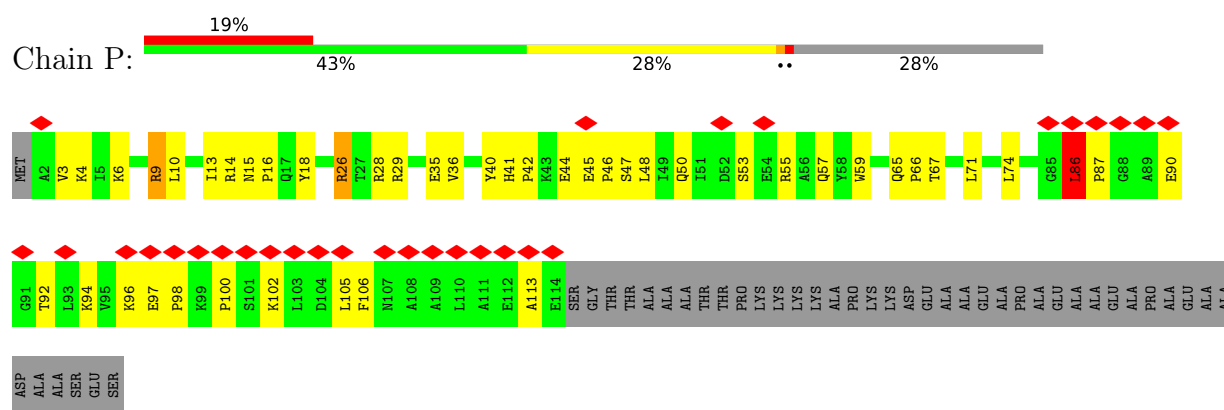
- Molecule 14: 30S ribosomal protein S14 type Z



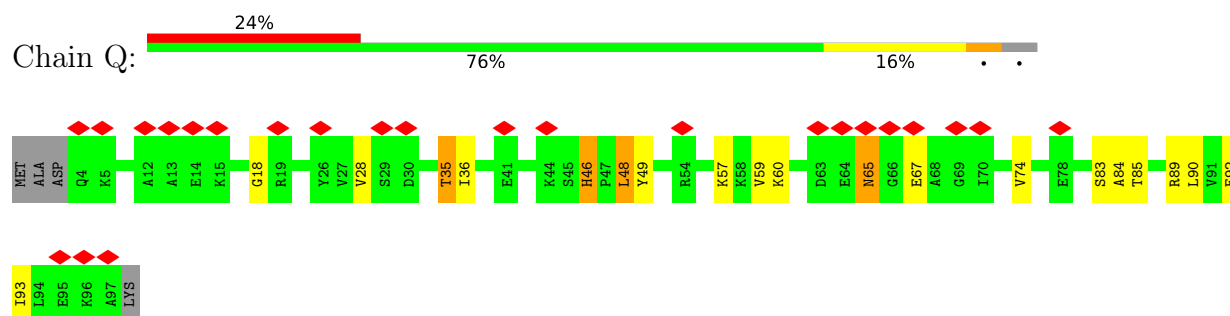
- Molecule 15: 30S ribosomal protein S15



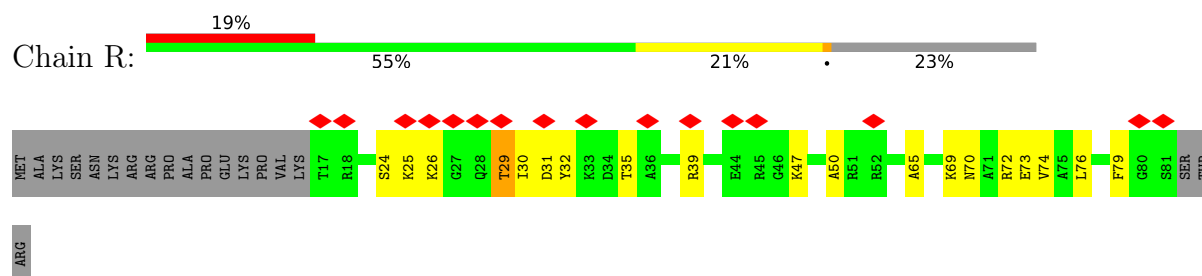
- Molecule 16: 30S ribosomal protein S16



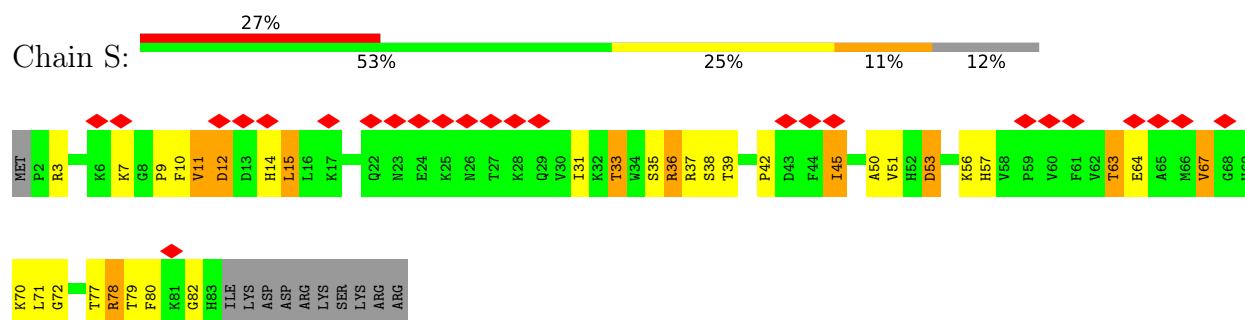
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18 2

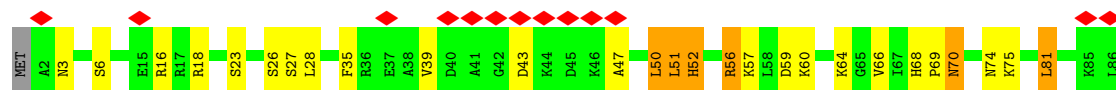


- Molecule 19: 30S ribosomal protein S19

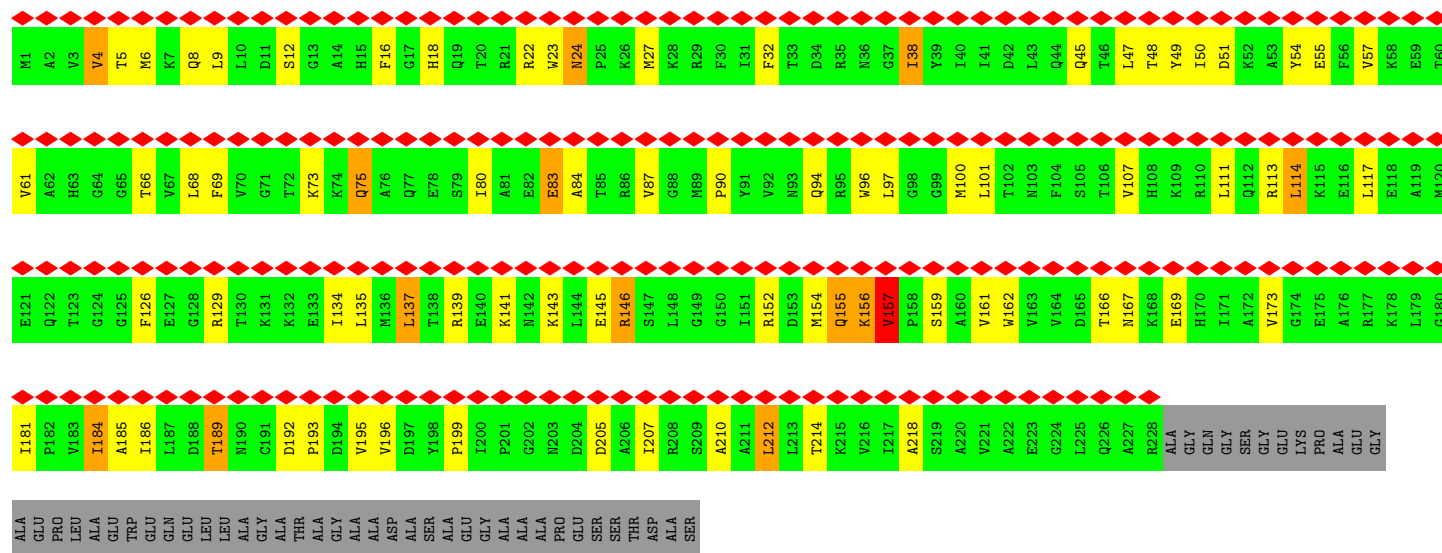
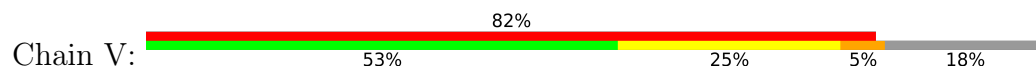


- Molecule 20: 30S ribosomal protein S20

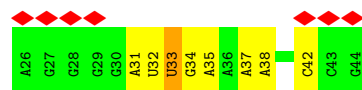




- Molecule 21: 30S ribosomal protein S2



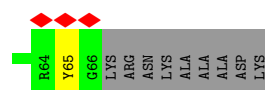
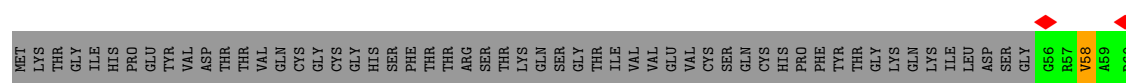
- Molecule 22: tRNA-Phe anticodon stem



- Molecule 23: mRNA fragment



- Molecule 24: 50S ribosomal protein L31



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	224584	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF correction in Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	100719	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.551	Depositor
Minimum map value	-0.237	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	300.24, 300.24, 300.24	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.39, 1.39, 1.39	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.39	0/36309	0.52	5/56657 (0.0%)
2	B	0.57	0/280	0.93	0/359
3	C	0.59	0/1684	0.99	5/2261 (0.2%)
4	D	0.51	0/1672	1.03	9/2251 (0.4%)
5	E	0.65	0/1312	1.09	5/1772 (0.3%)
6	F	0.57	0/782	1.02	0/1059
7	G	0.49	0/1252	0.92	2/1690 (0.1%)
8	H	0.68	0/1025	1.07	1/1385 (0.1%)
9	I	0.57	0/1012	0.96	3/1362 (0.2%)
10	J	0.62	0/802	1.04	6/1086 (0.6%)
11	K	0.63	0/873	1.05	3/1180 (0.3%)
12	L	0.66	0/969	1.03	2/1294 (0.2%)
13	M	0.47	0/942	0.90	2/1260 (0.2%)
14	N	0.64	0/488	1.07	5/650 (0.8%)
15	O	0.64	0/729	0.90	0/977
16	P	0.65	0/908	1.15	7/1226 (0.6%)
17	Q	0.58	0/759	1.04	2/1016 (0.2%)
18	R	0.70	0/518	0.98	1/693 (0.1%)
19	S	0.50	0/680	0.91	0/915
20	T	0.68	0/663	0.93	0/882
21	V	0.56	1/1822 (0.1%)	0.87	4/2457 (0.2%)
22	W	0.26	0/459	0.38	0/714
23	X	0.38	0/128	0.44	0/196
24	g	0.64	0/95	0.73	0/123
All	All	0.47	1/56163 (0.0%)	0.70	62/83465 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	V	157	VAL	CA-CB	5.01	1.60	1.54

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	97	GLY	CA-C-N	8.92	128.98	119.89
11	K	97	GLY	C-N-CA	8.92	128.98	119.89
10	J	57	LYS	CB-CA-C	-8.78	104.30	115.89
4	D	32	PRO	CA-C-N	7.45	127.41	120.03
4	D	32	PRO	C-N-CA	7.45	127.41	120.03
1	A	1482	U	P-O3'-C3'	7.30	131.16	120.20
5	E	99	VAL	CA-C-N	7.29	128.95	119.84
5	E	99	VAL	C-N-CA	7.29	128.95	119.84
4	D	190	LEU	CB-CA-C	-7.24	106.33	115.89
18	R	25	LYS	N-CA-C	-7.22	104.47	113.28
5	E	99	VAL	N-CA-C	6.93	116.23	108.05
14	N	53	LEU	CA-C-N	6.83	128.38	119.84
14	N	53	LEU	C-N-CA	6.83	128.38	119.84
16	P	41	HIS	CA-C-N	6.56	126.19	119.56
16	P	41	HIS	C-N-CA	6.56	126.19	119.56
14	N	29	ARG	CA-C-N	6.44	125.87	118.85
14	N	29	ARG	C-N-CA	6.44	125.87	118.85
7	G	57	ASP	CA-C-N	6.23	125.45	118.97
7	G	57	ASP	C-N-CA	6.23	125.45	118.97
16	P	92	THR	N-CA-C	-6.22	105.33	113.17
8	H	87	VAL	N-CA-C	6.09	116.97	107.28
13	M	67	GLU	CB-CA-C	-6.01	109.65	116.63
3	C	158	GLY	N-CA-C	-5.96	107.46	115.21
17	Q	46	HIS	CA-C-N	5.88	126.03	119.32
17	Q	46	HIS	C-N-CA	5.88	126.03	119.32
14	N	24	CYS	N-CA-C	5.78	118.45	110.35
12	L	27	SER	CA-C-N	5.71	125.07	118.85
12	L	27	SER	C-N-CA	5.71	125.07	118.85
21	V	192	ASP	CA-C-N	5.63	125.25	119.56
21	V	192	ASP	C-N-CA	5.63	125.25	119.56
5	E	107	THR	N-CA-C	5.56	117.03	110.97
3	C	77	GLY	N-CA-C	-5.54	104.00	111.54
16	P	45	GLU	CA-C-N	-5.54	114.11	119.87
16	P	45	GLU	C-N-CA	-5.54	114.11	119.87
10	J	57	LYS	N-CA-C	5.52	118.29	109.02
1	A	1482	U	C2'-C3'-O3'	5.51	117.76	109.50
16	P	86	LEU	CA-C-N	-5.50	112.96	119.84
16	P	86	LEU	C-N-CA	-5.50	112.96	119.84
4	D	77	GLN	CA-C-N	5.50	125.15	119.05
4	D	77	GLN	C-N-CA	5.50	125.15	119.05
10	J	38	GLY	CA-C-N	5.49	126.70	119.84
10	J	38	GLY	C-N-CA	5.49	126.70	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	42	VAL	CA-C-N	5.45	125.16	119.82
9	I	42	VAL	C-N-CA	5.45	125.16	119.82
3	C	12	LEU	N-CA-C	5.42	117.19	111.28
1	A	895	A	P-O3'-C3'	5.39	128.29	120.20
1	A	1171	G	P-O5'-C5'	-5.38	112.82	120.90
10	J	40	VAL	CA-C-N	5.32	125.48	119.90
10	J	40	VAL	C-N-CA	5.32	125.48	119.90
3	C	96	LYS	CB-CA-C	-5.25	110.09	117.23
5	E	81	VAL	CB-CA-C	-5.24	108.72	113.70
4	D	169	VAL	N-CA-C	5.21	117.98	112.83
4	D	190	LEU	N-CA-C	5.19	117.74	109.02
13	M	26	GLY	N-CA-C	-5.18	100.91	113.18
9	I	137	GLY	N-CA-C	-5.15	108.95	115.08
4	D	160	ARG	CA-C-N	5.14	125.42	119.92
4	D	160	ARG	C-N-CA	5.14	125.42	119.92
1	A	1482	U	C4'-C3'-O3'	5.11	117.06	109.40
3	C	162	MET	N-CA-C	-5.11	99.92	110.80
11	K	98	PRO	N-CA-C	5.03	119.11	111.11
21	V	24	ASN	CA-C-N	5.03	124.69	119.56
21	V	24	ASN	C-N-CA	5.03	124.69	119.56

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	32439	0	16320	388	0
2	B	280	0	342	9	0
3	C	1660	0	1707	40	0
4	D	1641	0	1668	49	0
5	E	1296	0	1360	42	0
6	F	771	0	797	35	0
7	G	1232	0	1282	26	0
8	H	1010	0	1046	34	0
9	I	994	0	1050	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	788	0	819	25	0
11	K	855	0	863	17	0
12	L	958	0	1045	34	0
13	M	935	0	986	28	0
14	N	477	0	499	15	0
15	O	720	0	760	16	0
16	P	891	0	935	34	0
17	Q	748	0	795	12	0
18	R	513	0	537	12	0
19	S	662	0	677	25	0
20	T	660	0	712	17	0
21	V	1793	0	1839	45	0
22	W	410	0	207	7	0
23	X	117	0	63	6	0
24	g	94	0	95	2	0
25	A	215	0	0	0	0
25	F	1	0	0	0	0
25	R	1	0	0	0	0
26	N	1	0	0	0	0
26	R	1	0	0	0	0
All	All	52163	0	36404	836	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 10.

All (836) 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)
10:J:66:GLU:HB2	14:N:59:SER:HB2	1.47	0.95
1:A:206:G:H4'	20:T:52:HIS:HE1	1.32	0.93
1:A:644:G:H22	1:A:721:G:H1	1.22	0.87
1:A:1300:A:OP1	19:S:3:ARG:NH2	2.13	0.82
6:F:30:ILE:HG22	6:F:36:THR:HG21	1.61	0.82
10:J:63:GLU:OE1	14:N:45:ARG:NH1	2.12	0.81
21:V:162:TRP:HH2	21:V:214:THR:HG22	1.44	0.81
1:A:206:G:H4'	20:T:52:HIS:CE1	2.16	0.80
12:L:54:ARG:HH11	12:L:64:THR:HG23	1.47	0.80
1:A:700:C:H5'	18:R:50:ALA:HA	1.64	0.79
1:A:208:G:OP1	20:T:56:ARG:NH2	2.15	0.78
1:A:1117:U:H1'	1:A:1118:A:H5''	1.65	0.78
1:A:808:A:H62	1:A:840:G:H21	1.30	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1350:U:H5'	10:J:62:ARG:NH1	2.00	0.77
13:M:14:ARG:NH1	13:M:16:GLU:OE2	2.18	0.77
1:A:986:G:N1	1:A:1016:G:O6	2.18	0.76
16:P:48:LEU:HB2	16:P:96:LYS:HE3	1.68	0.75
1:A:481:G:H2'	1:A:482:A:H8	1.51	0.75
13:M:4:LEU:HG	13:M:5:VAL:HG23	1.66	0.75
1:A:452:A:H62	16:P:94:LYS:H	1.34	0.74
1:A:1301:A:OP1	19:S:70:LYS:NZ	2.21	0.74
6:F:3:PRO:HB2	6:F:93:THR:HB	1.67	0.74
1:A:502:C:H41	12:L:50:ARG:HH12	1.35	0.74
13:M:97:PRO:HB2	13:M:101:GLN:HG3	1.68	0.74
1:A:1465:C:H2'	1:A:1466:G:H5'	1.68	0.73
3:C:11:ARG:NH2	3:C:175:LEU:O	2.21	0.73
17:Q:46:HIS:HD2	17:Q:49:TYR:H	1.36	0.73
20:T:35:PHE:HA	20:T:50:LEU:HD21	1.71	0.73
17:Q:65:ASN:HB2	17:Q:67:GLU:HG3	1.70	0.73
6:F:44:GLY:HA2	6:F:59:ILE:HG23	1.71	0.72
1:A:1267:U:H3'	1:A:1268:C:H5'	1.70	0.72
21:V:6:MET:HG2	21:V:47:LEU:HD11	1.72	0.72
1:A:1350:U:H5'	10:J:62:ARG:HH11	1.55	0.72
3:C:58:ARG:HG2	3:C:63:VAL:HG22	1.71	0.72
1:A:481:G:H2'	1:A:482:A:C8	2.24	0.71
16:P:46:PRO:HG3	16:P:96:LYS:HA	1.73	0.71
1:A:1177:A:O2'	1:A:1178:A:OP1	2.07	0.70
21:V:4:VAL:HG13	21:V:8:GLN:HB3	1.71	0.70
1:A:984:A:H61	1:A:1018:C:H42	1.39	0.70
6:F:89:LYS:HE3	6:F:91:LEU:HD21	1.72	0.70
13:M:5:VAL:HG21	13:M:60:ILE:HD11	1.74	0.70
22:W:32:U:H3	22:W:38:A:H61	1.40	0.70
12:L:81:LEU:HB3	12:L:98:ILE:HG22	1.74	0.69
4:D:147:THR:HG22	4:D:149:PRO:HD2	1.74	0.69
12:L:121:LYS:HG3	12:L:122:GLU:H	1.57	0.69
1:A:500:A:H62	1:A:509:G:H8	1.40	0.69
9:I:53:ARG:HB3	9:I:57:ASN:HD22	1.56	0.69
6:F:48:LEU:HD13	6:F:52:ILE:HD12	1.72	0.69
1:A:1099:C:OP2	9:I:31:ARG:NH2	2.26	0.69
17:Q:65:ASN:OD1	17:Q:65:ASN:N	2.26	0.69
6:F:12:PRO:O	6:F:45:ARG:NH1	2.25	0.69
1:A:1434:U:O2'	1:A:1435:U:H5''	1.92	0.68
1:A:1486:A:H2	1:A:1489:G:H1	1.41	0.68
1:A:448:A:OP2	1:A:465:G:N2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:132:ALA:O	5:E:137:ARG:NH1	2.27	0.68
1:A:924:G:H21	9:I:146:GLN:HE22	1.40	0.67
6:F:24:GLU:OE2	6:F:31:ARG:NH1	2.27	0.67
1:A:253:U:H2'	1:A:254:G:H8	1.60	0.67
1:A:315:A:N7	1:A:328:U:H5	1.92	0.67
1:A:193:C:N4	17:Q:18:GLY:O	2.25	0.67
1:A:411:A:C4	1:A:413:G:H1'	2.30	0.67
1:A:372:C:N4	1:A:388:G:OP2	2.28	0.66
16:P:35:GLU:OE1	16:P:59:TRP:NE1	2.20	0.66
1:A:1160:A:OP2	9:I:115:ARG:NH2	2.28	0.66
3:C:90:LEU:HD13	3:C:98:VAL:HG11	1.76	0.66
9:I:77:ARG:HH22	9:I:111:GLN:HG2	1.59	0.66
1:A:955:G:OP1	10:J:59:LYS:HE3	1.95	0.66
13:M:7:VAL:HG21	13:M:22:ILE:HG12	1.78	0.66
1:A:1199:C:H2'	1:A:1200:A:C8	2.31	0.65
1:A:299:G:H2'	1:A:300:A:C8	2.32	0.65
1:A:265:G:H2'	1:A:267:C:H5	1.61	0.65
1:A:1159:G:OP2	9:I:119:LYS:NZ	2.27	0.65
1:A:1289:U:H5''	13:M:101:GLN:HE22	1.61	0.65
21:V:117:LEU:HB3	21:V:141:LYS:HE3	1.79	0.65
12:L:79:MET:HE3	12:L:102:LEU:HB3	1.79	0.64
1:A:452:A:N6	16:P:94:LYS:H	1.93	0.64
1:A:480:G:H2'	1:A:481:G:H8	1.61	0.64
1:A:657:U:H3	1:A:693:G:H22	1.45	0.64
9:I:61:ASN:HD22	9:I:64:HIS:HD2	1.43	0.64
6:F:82:ASN:OD1	6:F:83:GLU:N	2.31	0.64
4:D:188:VAL:HG22	4:D:189:PRO:HD2	1.79	0.64
10:J:54:SER:O	14:N:41:ARG:NH2	2.31	0.64
1:A:253:U:H2'	1:A:254:G:C8	2.34	0.63
1:A:1287:G:HO2'	1:A:1288:A:H8	1.45	0.63
3:C:76:ILE:HG22	3:C:83:ALA:HB2	1.79	0.63
1:A:100:G:H2'	1:A:101:G:H5''	1.79	0.63
17:Q:83:SER:OG	17:Q:84:ALA:O	2.15	0.63
21:V:18:HIS:HB3	21:V:22:ARG:HD2	1.80	0.63
1:A:1018:C:H2'	1:A:1019:U:C6	2.34	0.62
16:P:44:GLU:HB3	16:P:47:SER:HA	1.79	0.62
1:A:1470:G:H2'	1:A:1471:G:O4'	1.99	0.62
4:D:126:ASP:OD1	4:D:126:ASP:N	2.32	0.62
1:A:1513:G:N7	2:B:7:LYS:HE3	2.15	0.62
3:C:6:ASN:HD22	14:N:49:HIS:HB3	1.65	0.62
1:A:987:A:H8	1:A:1007:U:H1'	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1382:C:H4'	1:A:1383:C:H5''	1.80	0.61
1:A:426:U:OP1	4:D:31:TYR:OH	2.17	0.61
7:G:69:VAL:HG23	7:G:100:ALA:HB1	1.82	0.61
1:A:777:C:H2'	1:A:778:U:C6	2.35	0.61
12:L:39:THR:HB	12:L:49:LEU:HG	1.81	0.61
21:V:111:LEU:HD21	21:V:152:ARG:HA	1.82	0.61
1:A:438:U:O2'	1:A:439:U:O2	2.18	0.61
1:A:1202:G:O3'	19:S:77:THR:HG21	2.00	0.61
1:A:1458:G:H2'	1:A:1459:G:O4'	2.01	0.61
16:P:40:TYR:CE2	16:P:42:PRO:HG3	2.36	0.61
19:S:33:THR:HG22	19:S:35:SER:H	1.65	0.61
20:T:35:PHE:CE1	20:T:51:LEU:HB2	2.35	0.61
14:N:32:SER:O	14:N:32:SER:OG	2.11	0.61
1:A:819:U:H3	1:A:829:G:H1	1.48	0.61
20:T:39:VAL:HG22	20:T:47:ALA:HB1	1.82	0.61
1:A:1338:G:H2'	1:A:1339:A:C8	2.36	0.60
4:D:103:ALA:HA	4:D:108:MET:HE2	1.83	0.60
7:G:26:LEU:HD13	7:G:101:LEU:HD22	1.84	0.60
1:A:519:A:H2'	1:A:520:G:C8	2.36	0.60
1:A:821:C:H42	1:A:826:U:H3	1.48	0.60
9:I:126:ARG:NH1	9:I:127:ASP:O	2.30	0.60
1:A:203:U:H2'	1:A:204:A:H8	1.67	0.60
1:A:480:G:H2'	1:A:481:G:C8	2.37	0.60
19:S:36:ARG:HD2	19:S:72:GLY:HA3	1.84	0.60
1:A:493:A:H2'	1:A:494:C:H6	1.66	0.60
1:A:1145:G:H1	1:A:1153:U:H3	1.49	0.60
1:A:1284:U:O4	13:M:14:ARG:HD3	2.01	0.60
1:A:858:A:H1'	8:H:12:THR:HG21	1.83	0.59
6:F:79:LEU:O	6:F:85:VAL:HG21	2.02	0.59
9:I:150:ARG:NH2	22:W:33:U:OP2	2.34	0.59
16:P:15:ASN:OD1	16:P:15:ASN:N	2.35	0.59
21:V:162:TRP:CH2	21:V:214:THR:HG22	2.30	0.59
1:A:436:C:H5''	4:D:148:LEU:HD12	1.84	0.59
1:A:924:G:H21	9:I:146:GLN:NE2	2.01	0.59
1:A:1358:A:O3'	7:G:29:LYS:NZ	2.34	0.59
13:M:20:THR:HG23	13:M:26:GLY:HA2	1.85	0.59
11:K:90:LYS:HG3	11:K:115:GLU:HB2	1.84	0.59
1:A:954:C:OP2	10:J:59:LYS:NZ	2.23	0.59
1:A:1229:A:H4'	9:I:53:ARG:HH22	1.68	0.59
1:A:987:A:C8	1:A:1007:U:H1'	2.38	0.59
1:A:1267:U:H3'	1:A:1268:C:C5'	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:C:H2'	1:A:174:G:H5''	1.85	0.58
9:I:37:VAL:HB	9:I:87:LEU:HD22	1.85	0.58
1:A:808:A:H62	1:A:840:G:N2	2.00	0.58
1:A:667:A:H5'	11:K:58:HIS:CE1	2.39	0.58
7:G:20:SER:HB2	7:G:23:VAL:HG23	1.86	0.57
21:V:9:LEU:HD23	21:V:212:LEU:HD13	1.86	0.57
1:A:882:A:H2'	1:A:883:A:C8	2.39	0.57
1:A:1171:G:OP1	3:C:5:ILE:HG12	2.04	0.57
1:A:372:C:H41	1:A:387:U:H2'	1.68	0.57
3:C:169:ARG:HH11	3:C:169:ARG:HB2	1.68	0.57
4:D:3:ARG:HG3	4:D:110:ARG:NH1	2.19	0.57
1:A:693:G:H2'	1:A:694:G:C8	2.39	0.57
3:C:14:ILE:HD12	3:C:178:LEU:HD22	1.85	0.57
9:I:101:LEU:HG	9:I:105:ARG:HD2	1.86	0.57
19:S:63:THR:HG22	19:S:64:GLU:H	1.70	0.57
1:A:1375:G:H21	1:A:1486:A:H8	1.51	0.57
1:A:1477:A:H4'	1:A:1478:G:OP1	2.03	0.57
16:P:100:PRO:HB2	16:P:105:LEU:HD21	1.87	0.57
1:A:438:U:OP1	4:D:117:HIS:NE2	2.34	0.56
1:A:728:A:H8	1:A:728:A:OP2	1.89	0.56
1:A:1261:A:OP2	10:J:71:LYS:NZ	2.37	0.56
4:D:169:VAL:HB	16:P:113:ALA:HB1	1.86	0.56
5:E:38:GLU:HG2	5:E:64:VAL:HG22	1.86	0.56
1:A:407:A:H5'	4:D:3:ARG:HH22	1.69	0.56
1:A:495:G:H2'	1:A:496:U:H6	1.70	0.56
5:E:104:SER:HA	5:E:146:HIS:HD2	1.69	0.56
18:R:65:ALA:O	18:R:69:LYS:HG3	2.04	0.56
1:A:236:G:H5''	17:Q:57:LYS:NZ	2.21	0.56
1:A:695:A:H2'	1:A:696:A:C8	2.41	0.56
12:L:122:GLU:HG2	12:L:123:LYS:H	1.69	0.56
13:M:79:ARG:O	13:M:82:ILE:HG22	2.06	0.56
5:E:156:ASP:OD1	5:E:156:ASP:N	2.39	0.56
13:M:39:ILE:HD12	13:M:56:LEU:HD13	1.86	0.56
1:A:254:G:H4'	17:Q:35:THR:HG21	1.86	0.56
4:D:181:PRO:HB2	4:D:186:ILE:HG12	1.88	0.56
10:J:50:CYS:SG	10:J:62:ARG:HD3	2.45	0.56
19:S:42:PRO:HA	19:S:45:ILE:HG13	1.86	0.56
1:A:972:U:H2'	1:A:973:U:C6	2.41	0.56
7:G:62:LEU:HD13	7:G:124:ILE:HD13	1.87	0.56
23:X:3:U:HO2'	23:X:4:U:H5	1.51	0.56
1:A:427:U:O2'	1:A:521:G:OP1	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:135:LEU:O	21:V:139:ARG:HG2	2.05	0.55
17:Q:46:HIS:CD2	17:Q:49:TYR:H	2.19	0.55
1:A:243:A:H4'	1:A:243:A:OP1	2.07	0.55
1:A:74:A:N7	1:A:92:A:N6	2.54	0.55
1:A:531:U:O2'	12:L:83:ARG:NH1	2.39	0.55
1:A:1461:U:H2'	1:A:1462:C:C6	2.41	0.55
1:A:1482:U:OP2	23:X:4:U:O2'	2.23	0.55
3:C:46:LEU:HD12	3:C:51:ILE:HD11	1.89	0.55
16:P:86:LEU:HB2	16:P:87:PRO:CD	2.37	0.55
3:C:87:ARG:O	3:C:91:GLU:HG2	2.06	0.55
1:A:393:A:OP1	16:P:14:ARG:NH2	2.33	0.55
1:A:489:A:C8	1:A:523:U:O2'	2.60	0.55
1:A:1312:U:H2'	1:A:1313:G:H5'	1.88	0.55
1:A:1465:C:C2'	1:A:1466:G:H5'	2.35	0.55
3:C:12:LEU:HA	3:C:16:THR:HG23	1.88	0.55
9:I:58:TYR:HE2	9:I:87:LEU:HD12	1.71	0.55
1:A:263:A:OP1	20:T:74:ASN:ND2	2.39	0.55
1:A:642:C:OP2	6:F:95:LYS:NZ	2.26	0.55
1:A:84:U:H4'	1:A:85:C:OP2	2.07	0.55
1:A:893:U:H2'	1:A:894:C:C6	2.42	0.55
5:E:70:MET:HE1	5:E:98:ARG:HG3	1.88	0.55
1:A:500:A:N6	1:A:509:G:H8	2.04	0.54
1:A:1261:A:P	10:J:9:ARG:HH22	2.30	0.54
7:G:50:ALA:O	7:G:54:THR:HG22	2.07	0.54
1:A:826:U:H2'	1:A:828:G:H5'	1.90	0.54
4:D:41:ILE:HG21	4:D:47:ARG:CZ	2.37	0.54
1:A:1290:C:OP2	13:M:99:ARG:HG3	2.07	0.54
4:D:55:LYS:CB	4:D:190:LEU:HD11	2.37	0.54
19:S:9:PRO:HD3	24:g:65:TYR:CD1	2.43	0.54
1:A:976:A:C8	1:A:1197:U:H4'	2.43	0.54
1:A:1297:U:O2'	1:A:1342:A:N3	2.33	0.54
12:L:121:LYS:HG3	12:L:122:GLU:N	2.22	0.54
14:N:21:TYR:HE1	14:N:23:ARG:HE	1.55	0.54
1:A:252:U:H2'	1:A:253:U:C6	2.43	0.54
9:I:54:THR:HG23	9:I:57:ASN:H	1.72	0.54
4:D:63:MET:HE2	4:D:63:MET:HA	1.90	0.54
17:Q:46:HIS:CD2	17:Q:48:LEU:H	2.26	0.54
8:H:114:THR:HG22	8:H:117:GLN:HG3	1.90	0.53
10:J:6:ILE:HB	10:J:76:ILE:HG23	1.90	0.53
1:A:184:U:H5''	20:T:81:LEU:HD13	1.90	0.53
1:A:1076:C:HO2'	1:A:1151:A:HO2'	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3:ARG:HG3	4:D:110:ARG:HH11	1.72	0.53
16:P:102:LYS:HA	16:P:105:LEU:HD12	1.90	0.53
12:L:72:HIS:HD2	12:L:74:LEU:HB2	1.73	0.53
12:L:83:ARG:HH21	12:L:96:LYS:HD2	1.74	0.53
1:A:216:U:O2'	1:A:217:U:H5'	2.09	0.53
1:A:399:G:H2'	1:A:400:C:C6	2.44	0.53
5:E:132:ALA:HB2	5:E:150:ALA:HB3	1.91	0.53
1:A:442:G:H1	1:A:472:C:H42	1.56	0.53
4:D:55:LYS:HB2	4:D:190:LEU:HD11	1.90	0.53
1:A:278:G:H5'	1:A:279:A:OP1	2.09	0.53
1:A:716:U:H2'	1:A:717:C:C6	2.43	0.53
1:A:819:U:H3	1:A:829:G:H22	1.57	0.53
1:A:236:G:H5''	17:Q:57:LYS:HZ2	1.74	0.53
1:A:457:A:O2'	1:A:458:A:O5'	2.18	0.53
16:P:53:SER:O	16:P:57:GLN:HG2	2.09	0.53
22:W:32:U:H3	22:W:38:A:N6	2.05	0.53
1:A:518:U:C2	1:A:519:A:C8	2.97	0.53
1:A:893:U:H2'	1:A:894:C:H6	1.74	0.53
1:A:909:G:O2'	1:A:1487:A:N7	2.40	0.53
3:C:94:THR:C	3:C:96:LYS:H	2.16	0.53
21:V:16:PHE:HA	21:V:38:ILE:HD11	1.90	0.53
1:A:279:A:H8	1:A:279:A:H5''	1.75	0.52
1:A:777:C:H2'	1:A:778:U:H6	1.73	0.52
1:A:827:U:O2'	1:A:829:G:OP2	2.27	0.52
5:E:44:ASN:HB3	5:E:59:THR:HG23	1.91	0.52
6:F:27:LEU:O	6:F:30:ILE:HG13	2.09	0.52
21:V:100:MET:HA	21:V:107:VAL:HG21	1.91	0.52
1:A:527:A:OP2	4:D:2:ALA:N	2.42	0.52
1:A:638:A:H1'	15:O:22:THR:HG21	1.91	0.52
1:A:957:A:N1	1:A:1349:C:O2'	2.41	0.52
1:A:1324:C:H2'	1:A:1325:G:C8	2.43	0.52
13:M:108:ARG:NH2	13:M:114:LYS:HA	2.25	0.52
21:V:126:PHE:O	21:V:134:ILE:HG13	2.09	0.52
1:A:694:G:H2'	1:A:695:A:C8	2.44	0.52
1:A:1132:U:H5''	10:J:44:THR:HG23	1.91	0.52
13:M:11:ARG:O	13:M:45:THR:HB	2.09	0.52
1:A:593:C:OP2	4:D:76:ARG:NH2	2.42	0.52
1:A:1514:G:H2'	1:A:1515:A:C8	2.44	0.52
6:F:51:GLU:OE1	6:F:51:GLU:N	2.37	0.52
15:O:8:LYS:O	15:O:12:LEU:HB2	2.09	0.52
19:S:80:PHE:CZ	19:S:82:GLY:HA2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:A:H2'	1:A:494:C:C6	2.43	0.52
1:A:502:C:H41	12:L:50:ARG:NH1	2.04	0.52
7:G:116:MET:HE2	7:G:119:ARG:HH21	1.74	0.52
9:I:61:ASN:HD22	9:I:64:HIS:CD2	2.25	0.52
14:N:32:SER:OG	14:N:41:ARG:HG2	2.10	0.52
1:A:687:U:H4'	11:K:31:HIS:ND1	2.25	0.52
1:A:390:U:H4'	16:P:29:ARG:NH2	2.25	0.52
6:F:19:VAL:HG11	6:F:42:ILE:HG21	1.92	0.52
6:F:70:ALA:O	6:F:73:SER:OG	2.26	0.52
13:M:49:THR:HG22	13:M:50:ASP:H	1.75	0.52
21:V:162:TRP:HD1	21:V:184:ILE:HB	1.74	0.52
1:A:146:A:H2'	1:A:147:U:C6	2.45	0.52
1:A:1515:A:H2'	1:A:1516:U:O4'	2.10	0.52
8:H:30:SER:HB2	8:H:33:LYS:HG3	1.91	0.51
1:A:363:A:N7	12:L:27:SER:OG	2.43	0.51
1:A:612:U:H5'	1:A:613:G:C8	2.45	0.51
8:H:79:ARG:NE	8:H:81:SER:O	2.36	0.51
13:M:25:ILE:HG23	13:M:29:ARG:HB2	1.92	0.51
21:V:161:VAL:HG23	21:V:181:ILE:HG21	1.92	0.51
1:A:934:U:O4	13:M:104:LYS:HE2	2.10	0.51
5:E:114:ALA:HB3	5:E:164:ALA:HA	1.92	0.51
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.92	0.51
3:C:109:GLU:HB2	3:C:143:GLN:NE2	2.26	0.51
7:G:129:ASN:HB2	7:G:131:LEU:HG	1.91	0.51
1:A:81:C:H3'	1:A:82:U:H5''	1.91	0.51
6:F:22:SER:O	6:F:25:THR:OG1	2.19	0.51
1:A:737:U:H2'	1:A:738:G:O4'	2.11	0.51
1:A:1374:U:H2'	1:A:1375:G:C8	2.46	0.51
11:K:80:ALA:O	11:K:84:GLN:HG2	2.10	0.51
19:S:42:PRO:HD3	19:S:67:VAL:HG21	1.93	0.51
22:W:34:G:H1	23:X:6:U:H3	1.59	0.51
1:A:884:G:H5'	2:B:18:ARG:NH1	2.26	0.51
1:A:1310:C:H2'	1:A:1311:G:O4'	2.11	0.51
12:L:21:THR:HG22	12:L:24:LEU:HG	1.92	0.51
16:P:9:ARG:O	16:P:10:LEU:HD23	2.10	0.51
1:A:392:C:OP1	16:P:9:ARG:NH2	2.41	0.50
1:A:1092:C:H1'	3:C:179:ARG:HD3	1.92	0.50
1:A:1152:C:H2'	1:A:1153:U:C6	2.47	0.50
1:A:1299:C:O2	19:S:37:ARG:NH2	2.42	0.50
1:A:1300:A:H5''	1:A:1301:A:OP2	2.11	0.50
1:A:41:U:O2'	1:A:480:G:H4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:C:O2'	1:A:865:C:H5'	2.10	0.50
3:C:109:GLU:HB2	3:C:143:GLN:HE22	1.76	0.50
5:E:97:PHE:CZ	5:E:170:LYS:HG2	2.46	0.50
10:J:92:LEU:HD13	10:J:98:VAL:HG21	1.93	0.50
11:K:43:ILE:O	11:K:51:ILE:HG13	2.12	0.50
15:O:43:LEU:HD13	15:O:53:ARG:HG2	1.92	0.50
1:A:495:G:H2'	1:A:496:U:C6	2.47	0.50
1:A:770:A:OP1	22:W:38:A:O2'	2.30	0.50
7:G:70:LYS:HD2	7:G:96:SER:HB3	1.93	0.50
13:M:40:ASP:HB3	13:M:43:MET:HG3	1.93	0.50
1:A:11:G:H1	5:E:122:ARG:HH11	1.59	0.50
1:A:556:A:N6	1:A:739:A:OP1	2.41	0.50
1:A:786:C:H2'	1:A:787:A:H8	1.76	0.50
7:G:54:THR:HG23	7:G:56:THR:H	1.76	0.50
4:D:90:GLU:O	4:D:95:ASN:ND2	2.44	0.50
1:A:1063:U:O2'	1:A:1082:A:OP2	2.29	0.50
5:E:67:GLY:O	5:E:144:GLY:HA3	2.11	0.50
9:I:45:THR:HG22	9:I:46:GLY:H	1.76	0.50
1:A:13:G:H5'	5:E:133:GLY:HA3	1.94	0.50
1:A:645:G:H3'	1:A:705:G:H21	1.76	0.50
1:A:690:G:H5''	6:F:54:LYS:HZ1	1.77	0.50
1:A:872:G:O2'	1:A:888:A:N6	2.45	0.50
11:K:59:VAL:HG11	11:K:74:LEU:HB3	1.93	0.50
1:A:688:C:H2'	1:A:689:A:H8	1.77	0.50
1:A:1177:A:HO2'	1:A:1178:A:P	2.31	0.50
2:B:5:ILE:O	2:B:9:ARG:HG3	2.12	0.50
8:H:8:ALA:O	8:H:12:THR:HG23	2.12	0.50
21:V:210:ALA:O	21:V:214:THR:HG23	2.12	0.50
1:A:793:U:H5''	1:A:796:A:N6	2.27	0.50
1:A:851:A:H5''	1:A:852:U:OP1	2.12	0.50
22:W:35:A:H61	23:X:5:C:H42	1.60	0.50
1:A:1324:C:H2'	1:A:1325:G:H8	1.76	0.49
3:C:75:VAL:HB	3:C:102:ILE:HD13	1.94	0.49
19:S:80:PHE:CE2	19:S:82:GLY:HA2	2.47	0.49
1:A:1461:U:H2'	1:A:1462:C:H6	1.77	0.49
20:T:27:SER:HB3	20:T:57:LYS:NZ	2.27	0.49
1:A:276:G:H4'	17:Q:60:LYS:NZ	2.27	0.49
1:A:458:A:H4'	1:A:459:G:O4'	2.13	0.49
1:A:793:U:O2	1:A:793:U:H2'	2.11	0.49
1:A:1304:C:OP1	19:S:78:ARG:NH2	2.46	0.49
12:L:95:TYR:N	12:L:95:TYR:CD1	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:A:H2'	1:A:676:A:C8	2.47	0.49
1:A:928:A:H2'	1:A:929:G:C8	2.47	0.49
21:V:18:HIS:HB2	21:V:189:THR:HG22	1.95	0.49
1:A:522:G:OP1	4:D:10:ARG:NH2	2.45	0.49
1:A:1197:U:H5''	14:N:5:ALA:HB2	1.94	0.49
5:E:190:ALA:C	8:H:116:ARG:HH22	2.21	0.49
9:I:77:ARG:O	9:I:80:GLN:HG2	2.12	0.49
1:A:1486:A:H2'	1:A:1488:G:C8	2.47	0.49
5:E:145:VAL:HG11	5:E:148:ILE:HD12	1.94	0.49
21:V:68:LEU:HD23	21:V:90:PRO:HB2	1.95	0.49
10:J:59:LYS:HE2	10:J:62:ARG:NH2	2.27	0.49
1:A:458:A:OP1	1:A:459:G:H1'	2.13	0.49
7:G:75:VAL:CG1	7:G:86:GLN:HB3	2.43	0.49
8:H:85:LEU:HB2	12:L:4:ILE:HD12	1.94	0.49
9:I:113:GLU:O	9:I:116:PRO:HD2	2.13	0.49
15:O:76:ALA:HA	15:O:79:ARG:HD2	1.95	0.49
1:A:173:C:H1'	1:A:1430:A:C2	2.48	0.49
4:D:191:THR:HG22	4:D:193:GLN:HG2	1.94	0.49
7:G:24:THR:O	7:G:27:VAL:HG22	2.13	0.49
1:A:251:G:C6	1:A:266:G:O6	2.66	0.48
5:E:157:ASN:ND2	5:E:160:ASN:H	2.11	0.48
1:A:230:G:H2'	1:A:231:G:O4'	2.13	0.48
1:A:919:A:O2'	7:G:76:ARG:NH2	2.46	0.48
18:R:24:SER:HB3	18:R:26:LYS:HG2	1.94	0.48
20:T:70:ASN:N	20:T:70:ASN:HD22	2.11	0.48
1:A:465:G:O2'	1:A:466:U:H5''	2.13	0.48
1:A:994:C:H2'	1:A:995:A:C8	2.47	0.48
1:A:1397:U:H2'	1:A:1398:G:H8	1.78	0.48
4:D:112:LEU:HB3	4:D:118:PHE:HE1	1.77	0.48
5:E:181:ARG:HD2	8:H:73:SER:O	2.13	0.48
19:S:10:PHE:O	19:S:39:THR:HG22	2.13	0.48
1:A:382:A:H2'	1:A:383:A:H8	1.77	0.48
1:A:546:G:H8	1:A:546:G:OP1	1.96	0.48
5:E:196:LYS:O	5:E:200:GLU:HG2	2.14	0.48
10:J:56:HIS:C	10:J:57:LYS:HG3	2.36	0.48
1:A:413:G:N2	1:A:428:G:H1'	2.28	0.48
19:S:12:ASP:OD1	19:S:38:SER:HB3	2.14	0.48
1:A:11:G:H1	5:E:122:ARG:NH1	2.11	0.48
1:A:382:A:H2'	1:A:383:A:C8	2.48	0.48
13:M:56:LEU:O	13:M:60:ILE:HG23	2.13	0.48
20:T:68:HIS:ND1	20:T:69:PRO:HD2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:66:ASP:OD1	5:E:70:MET:HB2	2.14	0.48
5:E:70:MET:HE1	5:E:98:ARG:CG	2.44	0.48
6:F:15:ASP:OD1	6:F:15:ASP:N	2.37	0.48
21:V:48:THR:O	21:V:51:ASP:HB3	2.13	0.48
1:A:1130:C:N4	1:A:1131:G:O6	2.47	0.48
5:E:105:THR:HG21	5:E:124:ALA:H	1.78	0.48
1:A:521:G:H2'	1:A:522:G:C8	2.49	0.48
1:A:690:G:H5''	6:F:54:LYS:NZ	2.29	0.48
1:A:1281:A:H2'	1:A:1281:A:N3	2.28	0.48
9:I:53:ARG:HB3	9:I:57:ASN:ND2	2.26	0.48
1:A:225:G:H2'	1:A:226:G:O4'	2.14	0.48
1:A:1236:G:H2'	1:A:1260:A:N6	2.29	0.48
3:C:151:VAL:HG22	3:C:200:VAL:HG13	1.95	0.48
6:F:23:LEU:HD13	6:F:63:ILE:HD11	1.95	0.48
7:G:79:ARG:HA	7:G:84:THR:HA	1.95	0.48
7:G:115:THR:HB	7:G:118:GLU:HG3	1.96	0.48
11:K:31:HIS:HD2	11:K:94:PHE:HB2	1.79	0.48
8:H:7:ILE:HB	8:H:79:ARG:NH1	2.28	0.47
21:V:12:SER:OG	21:V:212:LEU:HD12	2.14	0.47
1:A:510:G:N3	1:A:510:G:H2'	2.29	0.47
8:H:5:ASP:OD1	8:H:79:ARG:NH1	2.47	0.47
10:J:25:ILE:HD11	10:J:92:LEU:HD11	1.97	0.47
16:P:86:LEU:HB2	16:P:87:PRO:HD3	1.97	0.47
20:T:28:LEU:HD12	20:T:28:LEU:HA	1.72	0.47
1:A:749:G:H4'	1:A:1497:A:H4'	1.96	0.47
1:A:1193:U:O2'	1:A:1194:A:H5''	2.13	0.47
7:G:13:VAL:HG22	7:G:14:ASN:H	1.79	0.47
1:A:1200:A:H2'	1:A:1201:G:C8	2.49	0.47
3:C:22:TRP:CE2	14:N:54:PRO:HG3	2.50	0.47
6:F:21:PRO:O	6:F:24:GLU:HB3	2.14	0.47
8:H:81:SER:HB2	8:H:87:VAL:H	1.80	0.47
1:A:52:U:H3'	1:A:53:U:H5''	1.96	0.47
1:A:264:U:O4	1:A:265:G:C6	2.68	0.47
5:E:190:ALA:HB1	5:E:194:MET:HE2	1.96	0.47
6:F:46:ARG:HB3	6:F:60:TYR:CE2	2.49	0.47
19:S:15:LEU:HD23	19:S:33:THR:HG21	1.97	0.47
1:A:488:C:H1'	1:A:489:A:H2	1.79	0.47
1:A:1444:A:H2'	1:A:1445:G:O4'	2.14	0.47
8:H:14:LEU:HA	8:H:14:LEU:HD23	1.68	0.47
1:A:958:G:OP2	1:A:1340:U:O2'	2.30	0.47
1:A:1248:U:O2'	1:A:1249:G:O4'	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1486:A:H2	1:A:1489:G:N1	2.09	0.47
3:C:72:PRO:HD3	3:C:104:GLU:HB3	1.96	0.47
5:E:108:HIS:HE1	5:E:173:GLN:H	1.63	0.47
16:P:65:GLN:NE2	16:P:66:PRO:HD2	2.29	0.47
21:V:94:GLN:HG3	21:V:146:ARG:O	2.15	0.47
5:E:179:ALA:HA	5:E:189:VAL:HG21	1.96	0.47
9:I:111:GLN:HG3	9:I:113:GLU:HG2	1.97	0.47
1:A:997:A:H5'	19:S:14:HIS:CE1	2.48	0.47
1:A:1481:G:H2'	1:A:1482:U:H5'	1.97	0.47
5:E:194:MET:HE1	8:H:101:LEU:HD21	1.96	0.47
20:T:81:LEU:HD12	20:T:81:LEU:HA	1.56	0.47
1:A:399:G:H2'	1:A:400:C:H6	1.79	0.47
8:H:10:PHE:CD1	8:H:10:PHE:C	2.92	0.47
12:L:28:PRO:HB2	12:L:29:GLN:HE21	1.80	0.47
21:V:49:TYR:HB3	21:V:199:PRO:O	2.14	0.47
5:E:101:LEU:HD21	5:E:145:VAL:HG22	1.96	0.46
21:V:4:VAL:HG11	21:V:212:LEU:HD21	1.96	0.46
1:A:1287:G:O2'	1:A:1288:A:H8	1.97	0.46
1:A:1424:G:H8	1:A:1424:G:H5''	1.80	0.46
2:B:22:ARG:HD3	2:B:25:ARG:NH2	2.29	0.46
3:C:23:TYR:CD1	3:C:23:TYR:C	2.93	0.46
1:A:1323:U:H2'	1:A:1324:C:C6	2.51	0.46
3:C:123:LEU:HB3	3:C:196:ILE:HD11	1.96	0.46
6:F:43:TRP:CD1	6:F:43:TRP:N	2.83	0.46
4:D:138:ILE:HB	4:D:175:ILE:HB	1.96	0.46
5:E:69:GLY:C	5:E:70:MET:HE2	2.40	0.46
19:S:11:VAL:HG12	19:S:38:SER:HB2	1.97	0.46
1:A:519:A:H2'	1:A:520:G:H8	1.80	0.46
5:E:129:GLY:N	5:E:147:ASP:OD1	2.47	0.46
1:A:39:G:O2'	12:L:115:SER:O	2.26	0.46
8:H:12:THR:HA	8:H:15:ARG:NH1	2.31	0.46
15:O:18:HIS:CE1	15:O:21:ASP:HB3	2.50	0.46
15:O:75:VAL:O	15:O:78:TYR:HB3	2.14	0.46
1:A:49:U:H5''	1:A:307:C:O2'	2.16	0.46
1:A:1117:U:H4'	1:A:1118:A:OP1	2.15	0.46
1:A:1194:A:N7	1:A:1196:G:C5	2.84	0.46
12:L:38:TYR:HD1	12:L:38:TYR:N	2.13	0.46
12:L:81:LEU:HB3	12:L:98:ILE:CG2	2.43	0.46
1:A:731:U:C5	1:A:732:G:C5	3.03	0.46
6:F:27:LEU:HD11	6:F:63:ILE:HG21	1.98	0.46
10:J:4:GLN:O	10:J:79:PRO:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:C:H2'	1:A:643:A:C8	2.51	0.46
1:A:1122:U:H2'	1:A:1123:G:H8	1.81	0.46
4:D:165:TRP:CE3	4:D:181:PRO:HB3	2.50	0.46
5:E:41:VAL:HG23	5:E:42:SER:H	1.81	0.46
21:V:57:VAL:O	21:V:61:VAL:HG23	2.16	0.46
5:E:112:GLY:HA3	5:E:168:ALA:HB2	1.96	0.46
6:F:46:ARG:HB3	6:F:60:TYR:HE2	1.81	0.46
1:A:85:C:H4'	1:A:86:G:C8	2.51	0.45
1:A:210:A:H8	1:A:210:A:OP2	1.99	0.45
1:A:654:G:H2'	1:A:655:A:C8	2.50	0.45
1:A:1107:G:H1'	1:A:1261:A:C6	2.51	0.45
1:A:1232:A:H2'	1:A:1233:A:O4'	2.16	0.45
3:C:46:LEU:H	3:C:46:LEU:HG	1.64	0.45
4:D:13:ARG:HD3	4:D:29:ARG:O	2.16	0.45
8:H:108:THR:HG21	8:H:123:VAL:HG21	1.99	0.45
12:L:70:GLU:CD	12:L:70:GLU:H	2.24	0.45
1:A:429:U:O4'	1:A:430:A:H8	1.99	0.45
1:A:1036:U:OP1	3:C:163:SER:OG	2.32	0.45
12:L:38:TYR:N	12:L:38:TYR:CD1	2.83	0.45
21:V:114:LEU:HD21	21:V:145:GLU:HG3	1.98	0.45
1:A:185:G:H1	1:A:203:U:H3	1.64	0.45
1:A:376:G:H5''	16:P:6:LYS:HB3	1.98	0.45
1:A:1362:G:N7	7:G:2:PRO:HB2	2.32	0.45
7:G:86:GLN:HB2	7:G:148:ASN:ND2	2.31	0.45
8:H:74:ILE:HG21	8:H:77:LEU:HD22	1.98	0.45
10:J:24:LYS:HD2	10:J:92:LEU:HD23	1.97	0.45
12:L:73:ASN:ND2	12:L:105:GLN:H	2.14	0.45
16:P:86:LEU:H	16:P:86:LEU:HG	1.59	0.45
19:S:64:GLU:OE2	24:g:58:VAL:HB	2.16	0.45
1:A:1298:G:N7	19:S:7:LYS:NZ	2.64	0.45
1:A:928:A:O2'	1:A:1315:A:N3	2.47	0.45
1:A:1337:A:H2'	1:A:1338:G:C8	2.51	0.45
6:F:89:LYS:HG3	6:F:90:VAL:N	2.30	0.45
8:H:11:LEU:HD22	8:H:77:LEU:HG	1.97	0.45
9:I:150:ARG:HA	9:I:150:ARG:HD3	1.64	0.45
21:V:129:ARG:CZ	21:V:137:LEU:HD11	2.47	0.45
1:A:850:C:H2'	1:A:851:A:O4'	2.16	0.45
4:D:89:LEU:HD12	4:D:89:LEU:HA	1.68	0.45
4:D:176:LEU:HB3	16:P:106:PHE:CE1	2.52	0.45
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.56	0.45
20:T:64:LYS:HB2	20:T:66:VAL:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:83:GLU:HG2	21:V:84:ALA:N	2.32	0.45
1:A:71:C:H2'	1:A:72:G:C8	2.52	0.45
1:A:504:G:H2'	1:A:505:C:C6	2.51	0.45
1:A:965:A:H1'	1:A:1029:U:O2	2.17	0.45
1:A:1059:G:H2'	1:A:1060:A:C8	2.52	0.45
1:A:1333:U:H4'	7:G:33:GLU:CD	2.42	0.45
6:F:1:MET:HE3	6:F:66:LYS:HB3	1.98	0.45
12:L:90:LEU:HA	12:L:91:PRO:HD3	1.81	0.45
13:M:44:ARG:HA	13:M:44:ARG:HD3	1.80	0.45
1:A:256:U:H2'	1:A:257:G:H8	1.82	0.45
1:A:100:G:C2'	1:A:101:G:H5''	2.46	0.45
1:A:1323:U:H2'	1:A:1324:C:H6	1.82	0.45
1:A:1436:G:OP2	1:A:1436:G:H3'	2.17	0.45
8:H:79:ARG:HG2	8:H:80:VAL:H	1.82	0.45
16:P:9:ARG:CZ	16:P:16:PRO:HB3	2.46	0.45
1:A:67:C:H5'	1:A:68:G:OP2	2.17	0.45
4:D:192:GLU:HA	4:D:195:ILE:HD12	1.99	0.45
7:G:104:LEU:HD21	7:G:124:ILE:HG12	1.97	0.45
21:V:75:GLN:HG3	21:V:207:ILE:HB	1.99	0.45
1:A:976:A:N7	1:A:1197:U:H4'	2.31	0.44
1:A:1436:G:H3'	1:A:1436:G:P	2.56	0.44
4:D:165:TRP:HE3	4:D:185:GLN:HG3	1.82	0.44
1:A:1400:A:H5'	2:B:31:LEU:HD21	1.98	0.44
9:I:34:GLU:O	9:I:90:GLY:N	2.49	0.44
11:K:121:ASP:OD1	11:K:121:ASP:N	2.50	0.44
14:N:38:GLY:O	14:N:39:LEU:HD23	2.16	0.44
21:V:45:GLN:O	21:V:49:TYR:HD2	2.00	0.44
1:A:85:C:H4'	1:A:86:G:H8	1.82	0.44
1:A:419:C:C2	1:A:425:G:N2	2.85	0.44
1:A:1312:U:C2'	1:A:1313:G:H5'	2.46	0.44
9:I:41:LEU:HD22	9:I:106:ALA:HB1	2.00	0.44
21:V:166:THR:HG23	21:V:173:VAL:HG21	1.99	0.44
1:A:476:A:H5'	1:A:477:G:OP2	2.16	0.44
1:A:613:G:H2'	1:A:614:C:C6	2.53	0.44
1:A:698:A:C2	18:R:47:LYS:HE2	2.52	0.44
1:A:715:G:H1'	18:R:73:GLU:OE2	2.18	0.44
1:A:959:A:N6	1:A:1205:U:O5'	2.51	0.44
4:D:132:VAL:HG13	4:D:136:ASP:OD2	2.17	0.44
8:H:12:THR:O	8:H:15:ARG:N	2.50	0.44
9:I:62:LYS:HD2	9:I:62:LYS:HA	1.73	0.44
10:J:29:VAL:HG11	10:J:36:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:40:ASP:OD1	13:M:41:LYS:N	2.50	0.44
1:A:264:U:C4	1:A:265:G:C5	3.06	0.44
1:A:703:U:O2'	1:A:704:G:P	2.75	0.44
1:A:980:G:H1	1:A:1023:U:H3	1.65	0.44
1:A:1185:A:H2'	1:A:1186:U:O4'	2.16	0.44
3:C:7:PRO:HG2	3:C:184:TYR:CD1	2.52	0.44
3:C:49:ALA:HB2	3:C:74:ILE:HB	2.00	0.44
5:E:93:ARG:HA	5:E:96:PHE:CE2	2.53	0.44
15:O:58:LEU:HA	15:O:58:LEU:HD23	1.55	0.44
16:P:97:GLU:HA	16:P:98:PRO:HD3	1.86	0.44
1:A:144:G:H2'	1:A:145:G:C8	2.53	0.44
1:A:672:U:O2'	1:A:674:G:N7	2.40	0.44
13:M:96:LEU:HB3	13:M:97:PRO:HD2	1.99	0.44
6:F:89:LYS:NZ	18:R:70:ASN:OD1	2.49	0.44
14:N:47:MET:HE2	14:N:47:MET:HB3	1.90	0.44
1:A:495:G:C5	1:A:496:U:C5	3.06	0.44
1:A:613:G:H2'	1:A:614:C:H6	1.83	0.44
1:A:1250:A:HO2'	1:A:1307:C:HO2'	1.64	0.44
21:V:97:LEU:HG	21:V:100:MET:HE3	2.00	0.44
1:A:349:A:H2'	1:A:350:G:O4'	2.18	0.44
1:A:895:A:H4'	1:A:896:A:O5'	2.18	0.44
7:G:101:LEU:HD23	7:G:101:LEU:HA	1.71	0.44
21:V:111:LEU:HD12	21:V:111:LEU:HA	1.81	0.44
1:A:265:G:O2'	1:A:266:G:O5'	2.30	0.43
1:A:413:G:H2'	1:A:428:G:H21	1.83	0.43
1:A:452:A:H2	16:P:47:SER:HB2	1.83	0.43
1:A:1148:U:H2'	1:A:1148:U:OP1	2.18	0.43
3:C:111:GLN:O	3:C:115:VAL:HG23	2.18	0.43
10:J:92:LEU:CD1	10:J:98:VAL:HG21	2.48	0.43
13:M:49:THR:HB	13:M:52:GLN:HG3	2.00	0.43
1:A:31:G:H2'	1:A:32:G:O4'	2.17	0.43
1:A:397:A:H5'	1:A:398:C:OP1	2.18	0.43
1:A:409:G:H2'	1:A:410:G:O4'	2.18	0.43
1:A:1515:A:O5'	1:A:1515:A:H8	2.01	0.43
3:C:188:GLU:HG3	3:C:195:ARG:HB3	2.00	0.43
11:K:90:LYS:HG2	11:K:91:VAL:N	2.33	0.43
1:A:1152:C:H2'	1:A:1153:U:H6	1.81	0.43
1:A:1425:G:H5'	1:A:1426:C:C5	2.52	0.43
17:Q:36:ILE:HD13	17:Q:90:LEU:HD22	1.99	0.43
21:V:27:MET:HG2	21:V:193:PRO:HD3	2.00	0.43
1:A:251:G:N1	1:A:266:G:C6	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:140:VAL:HG21	4:D:150:PHE:CZ	2.54	0.43
1:A:644:G:N2	1:A:721:G:H1	2.02	0.43
1:A:965:A:H5'	1:A:966:C:OP2	2.18	0.43
3:C:12:LEU:HD21	3:C:18:TRP:NE1	2.33	0.43
3:C:149:ILE:HG13	3:C:202:ILE:HG12	1.99	0.43
5:E:182:ARG:HH21	5:E:189:VAL:HA	1.84	0.43
20:T:35:PHE:HE1	20:T:51:LEU:HB2	1.82	0.43
1:A:555:G:O2'	1:A:801:G:OP2	2.32	0.43
1:A:1168:G:O2'	9:I:133:ARG:NH1	2.52	0.43
1:A:1332:A:OP2	9:I:140:LYS:NZ	2.40	0.43
9:I:37:VAL:HG21	9:I:99:LEU:HA	2.00	0.43
13:M:106:ASN:O	13:M:107:ALA:HB3	2.19	0.43
1:A:352:C:O2	1:A:355:C:N4	2.49	0.43
1:A:1216:U:H2'	1:A:1217:A:O4'	2.19	0.43
9:I:134:LYS:HE3	9:I:139:LYS:O	2.19	0.43
23:X:3:U:O2'	23:X:4:U:H5	2.02	0.43
1:A:256:U:H2'	1:A:257:G:C8	2.54	0.43
1:A:588:A:C2	1:A:589:A:H1'	2.53	0.43
1:A:1472:G:H2'	1:A:1473:A:H8	1.84	0.43
3:C:21:ARG:HH21	3:C:55:GLU:CD	2.27	0.43
4:D:86:LEU:HD13	4:D:186:ILE:HG21	2.01	0.43
4:D:140:VAL:HG21	4:D:150:PHE:HZ	1.84	0.43
16:P:48:LEU:HD22	16:P:96:LYS:NZ	2.33	0.43
1:A:67:C:H5''	1:A:67:C:H6	1.84	0.43
4:D:154:ARG:HG2	4:D:155:GLU:HG3	1.99	0.43
1:A:203:U:H2'	1:A:204:A:C8	2.52	0.43
1:A:580:G:OP1	8:H:91:SER:N	2.51	0.43
1:A:806:C:H5'	8:H:13:ARG:HH21	1.84	0.43
1:A:905:A:H2'	1:A:906:C:O4'	2.19	0.43
5:E:99:VAL:HA	5:E:100:PRO:HD3	1.68	0.43
15:O:78:TYR:CZ	15:O:82:ILE:HD11	2.54	0.43
16:P:9:ARG:HB2	16:P:29:ARG:NH1	2.34	0.43
16:P:71:LEU:O	16:P:74:LEU:HB2	2.19	0.43
21:V:90:PRO:HG2	21:V:154:MET:HE2	2.01	0.43
1:A:636:G:O2'	15:O:28:GLN:NE2	2.52	0.42
1:A:755:G:H2'	1:A:756:G:O4'	2.19	0.42
1:A:1082:A:O2'	1:A:1083:C:H5'	2.19	0.42
1:A:1138:A:H62	1:A:1159:G:H21	1.67	0.42
1:A:1493:C:OP1	2:B:8:ARG:NH2	2.52	0.42
7:G:152:ALA:HB1	7:G:155:ARG:CZ	2.48	0.42
8:H:128:LEU:HA	8:H:128:LEU:HD23	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:54:ARG:NH1	12:L:64:THR:HG23	2.25	0.42
20:T:35:PHE:CZ	20:T:39:VAL:HG21	2.54	0.42
21:V:185:ALA:HB3	21:V:196:VAL:HG11	2.01	0.42
1:A:426:U:H5'	1:A:427:U:OP2	2.19	0.42
1:A:653:G:H1	1:A:697:C:H42	1.67	0.42
1:A:1408:A:H2'	1:A:1409:A:O4'	2.19	0.42
3:C:26:LYS:HD3	3:C:26:LYS:HA	1.71	0.42
5:E:140:LEU:HD23	5:E:140:LEU:HA	1.85	0.42
5:E:140:LEU:HD13	5:E:148:ILE:HG21	2.01	0.42
6:F:26:PHE:O	6:F:29:VAL:HG12	2.18	0.42
16:P:55:ARG:HD3	16:P:55:ARG:HA	1.46	0.42
4:D:197:GLU:O	4:D:200:SER:HB3	2.19	0.42
5:E:104:SER:HA	5:E:146:HIS:CD2	2.52	0.42
6:F:18:THR:C	6:F:21:PRO:HD2	2.44	0.42
11:K:101:GLY:O	11:K:104:THR:N	2.52	0.42
12:L:7:LEU:HD23	12:L:7:LEU:HA	1.78	0.42
13:M:25:ILE:HG23	13:M:29:ARG:CB	2.49	0.42
1:A:688:C:H2'	1:A:689:A:C8	2.54	0.42
1:A:1295:U:H2'	1:A:1296:C:C6	2.55	0.42
1:A:1452:A:H2'	1:A:1453:A:H8	1.84	0.42
9:I:42:VAL:HA	9:I:43:PRO:HD3	1.85	0.42
16:P:9:ARG:HG2	16:P:18:TYR:CE1	2.55	0.42
21:V:155:GLN:O	21:V:157:VAL:N	2.51	0.42
1:A:698:A:H5'	11:K:128:ASN:HB2	2.00	0.42
1:A:964:U:C2	1:A:965:A:C6	3.07	0.42
1:A:1135:G:H2'	1:A:1136:A:H8	1.85	0.42
1:A:1302:C:OP1	19:S:70:LYS:HE2	2.19	0.42
3:C:60:ARG:HA	3:C:60:ARG:HD3	1.89	0.42
6:F:68:GLU:O	6:F:71:THR:OG1	2.31	0.42
7:G:22:LEU:HD23	7:G:22:LEU:HA	1.81	0.42
21:V:111:LEU:CD2	21:V:152:ARG:HA	2.48	0.42
1:A:1130:C:H2'	1:A:1131:G:C8	2.54	0.42
3:C:32:VAL:HG21	14:N:37:PHE:O	2.20	0.42
5:E:191:PRO:O	5:E:195:LEU:HG	2.19	0.42
11:K:27:HIS:O	11:K:46:PRO:HD3	2.19	0.42
15:O:4:THR:OG1	15:O:7:GLN:HG3	2.20	0.42
21:V:69:PHE:HB3	21:V:80:ILE:HG23	2.02	0.42
1:A:485:G:C8	1:A:515:A:C4	3.08	0.42
1:A:640:U:H2'	1:A:641:G:O4'	2.20	0.42
1:A:1480:C:H2'	1:A:1481:G:O4'	2.20	0.42
3:C:175:LEU:HA	3:C:175:LEU:HD23	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:165:TRP:CE3	4:D:185:GLN:HG3	2.55	0.42
6:F:77:ARG:O	6:F:81:LEU:HG	2.20	0.42
10:J:42:LEU:HD23	10:J:42:LEU:HA	1.63	0.42
11:K:37:ASN:HA	11:K:67:SER:HB3	2.01	0.42
21:V:96:TRP:CH2	21:V:101:LEU:HD13	2.54	0.42
21:V:159:SER:O	21:V:181:ILE:HG23	2.19	0.42
1:A:105:A:C6	1:A:326:G:C6	3.08	0.42
1:A:1077:C:H5''	21:V:143:LYS:NZ	2.34	0.42
1:A:1110:A:H4'	9:I:40:ARG:NH1	2.35	0.42
2:B:11:ARG:HG2	2:B:11:ARG:HH11	1.84	0.42
4:D:97:VAL:HG21	4:D:118:PHE:CZ	2.55	0.42
6:F:82:ASN:HB3	6:F:85:VAL:HG22	2.01	0.42
1:A:1280:C:H2'	7:G:114:LYS:NZ	2.34	0.42
5:E:143:ALA:HB3	5:E:145:VAL:HG23	2.02	0.42
1:A:1258:C:H2'	1:A:1260:A:H8	1.85	0.42
4:D:182:GLU:O	4:D:186:ILE:HG13	2.19	0.42
5:E:37:ILE:H	5:E:37:ILE:HG13	1.74	0.42
6:F:16:GLU:HA	6:F:19:VAL:HG23	2.00	0.42
8:H:81:SER:CB	8:H:87:VAL:H	2.32	0.42
16:P:26:ARG:HE	16:P:26:ARG:HB2	1.33	0.42
19:S:53:ASP:OD1	19:S:56:LYS:HG2	2.20	0.42
21:V:134:ILE:HD13	21:V:134:ILE:HA	1.84	0.42
1:A:196:G:H2'	1:A:197:G:C8	2.55	0.41
1:A:269:U:H2'	1:A:270:A:C8	2.55	0.41
1:A:511:U:H4'	1:A:511:U:OP1	2.20	0.41
1:A:765:G:C6	1:A:766:G:N7	2.88	0.41
1:A:1271:A:H2'	1:A:1272:G:H5'	2.00	0.41
2:B:25:ARG:HD3	2:B:29:ARG:NH2	2.35	0.41
6:F:82:ASN:HB3	6:F:85:VAL:CG2	2.50	0.41
13:M:70:LEU:HA	13:M:70:LEU:HD23	1.75	0.41
19:S:71:LEU:HD23	19:S:71:LEU:HA	1.82	0.41
1:A:178:A:C2	1:A:209:A:C4	3.08	0.41
1:A:586:G:H5''	1:A:587:A:H5'	2.02	0.41
1:A:1019:U:H2'	1:A:1020:G:O4'	2.20	0.41
1:A:1417:A:H2'	1:A:1418:G:O4'	2.20	0.41
1:A:1494:C:H2'	1:A:1495:G:C8	2.54	0.41
4:D:86:LEU:HB3	4:D:186:ILE:HD13	2.02	0.41
8:H:10:PHE:HA	8:H:27:LEU:HD21	2.03	0.41
9:I:71:PRO:HG3	9:I:123:PHE:CD2	2.56	0.41
16:P:4:LYS:HE2	16:P:4:LYS:HB3	1.88	0.41
23:X:3:U:H6	23:X:3:U:H2'	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:U:H2'	1:A:22:C:C6	2.56	0.41
1:A:101:G:H2'	1:A:102:C:O4'	2.20	0.41
1:A:384:G:H2'	1:A:385:C:C6	2.54	0.41
1:A:498:C:H5	1:A:509:G:H3'	1.85	0.41
1:A:614:C:H2'	1:A:615:G:C8	2.54	0.41
1:A:847:A:H2'	1:A:848:C:C6	2.55	0.41
8:H:16:ASN:O	8:H:19:SER:N	2.52	0.41
8:H:70:ARG:HD2	8:H:70:ARG:HA	1.49	0.41
11:K:30:ALA:HB3	11:K:93:VAL:HG12	2.03	0.41
11:K:93:VAL:HG22	11:K:118:THR:O	2.20	0.41
21:V:23:TRP:HA	21:V:189:THR:HG23	2.02	0.41
21:V:87:VAL:HG21	21:V:218:ALA:HB1	2.01	0.41
1:A:747:A:H2'	1:A:748:A:O4'	2.20	0.41
4:D:27:GLU:O	4:D:30:PRO:HD3	2.21	0.41
5:E:92:ALA:O	5:E:95:ASN:N	2.52	0.41
9:I:47:GLN:HB2	9:I:82:ASP:OD1	2.20	0.41
11:K:56:SER:OG	11:K:71:ALA:HB1	2.21	0.41
12:L:94:ARG:HB2	12:L:95:TYR:CD1	2.55	0.41
15:O:57:LEU:HD23	15:O:57:LEU:HA	1.68	0.41
1:A:228:A:H2'	1:A:229:U:O4'	2.21	0.41
1:A:335:C:H2'	1:A:336:A:C8	2.54	0.41
1:A:437:U:HO2'	1:A:438:U:P	2.44	0.41
1:A:604:U:H2'	1:A:605:G:H8	1.85	0.41
1:A:832:U:H2'	1:A:833:C:C6	2.55	0.41
1:A:1248:U:O2'	1:A:1249:G:O5'	2.39	0.41
1:A:1322:G:O2'	22:W:31:A:O2'	2.27	0.41
1:A:1363:U:O2'	1:A:1364:U:OP2	2.37	0.41
8:H:101:LEU:HD23	8:H:101:LEU:HA	1.78	0.41
12:L:31:ARG:HE	12:L:31:ARG:HB3	1.69	0.41
21:V:156:LYS:O	21:V:157:VAL:HG22	2.21	0.41
1:A:251:G:C4	1:A:266:G:N7	2.89	0.41
1:A:509:G:H5'	1:A:510:G:OP2	2.20	0.41
1:A:532:U:H4'	12:L:84:GLY:O	2.20	0.41
1:A:602:A:H5'	4:D:69:ARG:HH22	1.86	0.41
1:A:1082:A:H2'	1:A:1083:C:C6	2.56	0.41
1:A:1194:A:N6	1:A:1196:G:N3	2.68	0.41
1:A:1199:C:H2'	1:A:1200:A:H8	1.79	0.41
1:A:1410:C:H2'	1:A:1411:A:C8	2.56	0.41
1:A:1435:U:H4'	1:A:1436:G:O5'	2.19	0.41
8:H:60:LEU:HD23	8:H:60:LEU:HA	1.77	0.41
10:J:18:ILE:HD12	10:J:18:ILE:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:C:C2	1:A:522:G:N2	2.88	0.41
4:D:51:GLN:HB3	4:D:55:LYS:HE3	2.03	0.41
8:H:7:ILE:HD11	8:H:32:LEU:CD2	2.50	0.41
8:H:77:LEU:HD12	8:H:77:LEU:HA	1.74	0.41
13:M:56:LEU:HD12	13:M:56:LEU:HA	1.86	0.41
13:M:63:ASN:OD1	13:M:63:ASN:N	2.52	0.41
1:A:804:U:H2'	1:A:805:A:C8	2.56	0.41
1:A:1197:U:H2'	1:A:1198:C:C6	2.55	0.41
1:A:1248:U:O2'	1:A:1249:G:C8	2.71	0.41
1:A:1380:C:OP2	5:E:54:ARG:NH2	2.52	0.41
1:A:1384:G:C6	1:A:1385:C:C2	3.09	0.41
9:I:26:ILE:HG22	9:I:41:LEU:H	1.85	0.41
10:J:19:ASP:O	10:J:23:ARG:HG2	2.21	0.41
12:L:99:ARG:HD3	12:L:99:ARG:HA	1.86	0.41
14:N:5:ALA:O	14:N:9:LYS:HB2	2.21	0.41
19:S:3:ARG:HH21	19:S:7:LYS:HD3	1.85	0.41
1:A:84:U:H3'	1:A:85:C:C5	2.55	0.41
1:A:355:C:H2'	1:A:356:A:O4'	2.21	0.41
1:A:404:G:O2'	1:A:478:A:N1	2.48	0.41
1:A:645:G:C8	1:A:713:G:C2	3.08	0.41
1:A:728:A:O2'	1:A:729:A:N7	2.50	0.41
1:A:859:C:H6	1:A:859:C:O5'	2.04	0.41
1:A:1452:A:H2'	1:A:1453:A:C8	2.56	0.41
3:C:141:MET:HE1	3:C:148:GLY:HA2	2.03	0.41
3:C:173:VAL:HA	3:C:174:PRO:HD3	1.87	0.41
6:F:60:TYR:CZ	18:R:76:LEU:HD21	2.56	0.41
7:G:75:VAL:HG11	7:G:86:GLN:HB3	2.02	0.41
9:I:38:ARG:HG3	9:I:86:HIS:HB2	2.02	0.41
9:I:40:ARG:HG2	9:I:84:TYR:HB2	2.02	0.41
9:I:71:PRO:HG3	9:I:123:PHE:HD2	1.86	0.41
1:A:439:U:O2	4:D:115:HIS:ND1	2.54	0.41
1:A:696:A:H1'	11:K:128:ASN:O	2.21	0.41
1:A:1270:A:C2	1:A:1271:A:C4	3.09	0.41
4:D:57:ARG:HB2	4:D:62:VAL:HG23	2.02	0.41
8:H:14:LEU:CD2	8:H:64:LEU:HD21	2.51	0.41
8:H:51:THR:HG21	8:H:58:LYS:HD3	2.03	0.41
12:L:31:ARG:HH21	12:L:58:THR:CG2	2.34	0.41
15:O:26:GLU:OE2	15:O:77:ARG:HD2	2.21	0.41
16:P:40:TYR:CZ	16:P:42:PRO:HG3	2.56	0.41
18:R:29:THR:HG22	18:R:30:ILE:H	1.86	0.41
1:A:867:G:O2'	1:A:896:A:N1	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:117:HIS:HA	4:D:141:LYS:HE2	2.02	0.40
4:D:159:GLU:HB3	4:D:160:ARG:H	1.80	0.40
9:I:67:LEU:HD23	9:I:67:LEU:HA	1.78	0.40
13:M:67:GLU:HB3	13:M:68:GLY:H	1.61	0.40
18:R:72:ARG:HB3	18:R:79:PHE:CE1	2.56	0.40
1:A:324:G:N1	1:A:327:A:OP2	2.51	0.40
1:A:486:G:H2'	1:A:487:C:C6	2.56	0.40
1:A:927:G:C2	1:A:928:A:C8	3.10	0.40
1:A:1163:G:H3'	1:A:1164:U:H5'	2.03	0.40
1:A:1423:U:H2'	1:A:1424:G:O4'	2.21	0.40
4:D:112:LEU:HB3	4:D:118:PHE:CE1	2.55	0.40
10:J:28:THR:HG21	10:J:90:ILE:HD11	2.03	0.40
12:L:27:SER:HA	12:L:28:PRO:HD3	1.93	0.40
18:R:35:THR:O	18:R:39:ARG:HG2	2.21	0.40
1:A:491:C:O2'	1:A:514:U:H1'	2.20	0.40
1:A:605:G:H2'	1:A:606:U:H6	1.86	0.40
1:A:940:A:N3	1:A:967:C:O2'	2.54	0.40
1:A:1488:G:OP1	1:A:1491:A:H4'	2.21	0.40
3:C:50:GLY:O	3:C:69:THR:HG23	2.20	0.40
3:C:66:ASP:HB3	3:C:103:LEU:HD11	2.02	0.40
5:E:178:VAL:HG21	8:H:101:LEU:HD13	2.04	0.40
10:J:20:ALA:O	10:J:24:LYS:HG3	2.21	0.40
12:L:30:ARG:HD2	12:L:30:ARG:HA	1.77	0.40
18:R:32:TYR:H	18:R:32:TYR:HD1	1.68	0.40
18:R:74:VAL:HG23	18:R:76:LEU:HG	2.04	0.40
21:V:50:ILE:O	21:V:54:TYR:HB2	2.20	0.40
1:A:407:A:OP1	4:D:107:ARG:NH1	2.52	0.40
1:A:501:G:O5'	12:L:70:GLU:HA	2.21	0.40
1:A:602:A:H5'	4:D:69:ARG:NH2	2.36	0.40
1:A:727:U:H2'	1:A:728:A:O4'	2.21	0.40
1:A:962:C:H1'	14:N:19:ARG:HG2	2.03	0.40
2:B:18:ARG:HA	2:B:18:ARG:HD3	1.89	0.40
3:C:75:VAL:O	3:C:82:GLU:HB3	2.21	0.40
7:G:93:PRO:O	7:G:96:SER:HB2	2.21	0.40
20:T:60:LYS:HE3	20:T:60:LYS:HB2	1.78	0.40
1:A:63:A:C2	1:A:354:G:C8	3.09	0.40
1:A:457:A:HO2'	1:A:458:A:C5'	2.31	0.40
1:A:498:C:C5	1:A:509:G:H3'	2.57	0.40
3:C:134:ARG:HD2	3:C:134:ARG:HA	1.84	0.40
15:O:24:SER:O	15:O:27:ALA:HB3	2.21	0.40
15:O:53:ARG:O	15:O:56:LEU:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:66:LEU:HA	15:O:66:LEU:HD23	1.64	0.40
15:O:74:ASP:CG	15:O:77:ARG:HB2	2.46	0.40
16:P:9:ARG:NE	16:P:16:PRO:HB3	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	30/33 (91%)	28 (93%)	2 (7%)	0	100	100
3	C	206/275 (75%)	191 (93%)	13 (6%)	2 (1%)	12	44
4	D	198/201 (98%)	185 (93%)	13 (7%)	0	100	100
5	E	178/214 (83%)	170 (96%)	8 (4%)	0	100	100
6	F	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
7	G	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
8	H	129/132 (98%)	125 (97%)	4 (3%)	0	100	100
9	I	124/150 (83%)	119 (96%)	5 (4%)	0	100	100
10	J	97/101 (96%)	92 (95%)	5 (5%)	0	100	100
11	K	113/138 (82%)	105 (93%)	8 (7%)	0	100	100
12	L	120/124 (97%)	112 (93%)	8 (7%)	0	100	100
13	M	114/124 (92%)	103 (90%)	11 (10%)	0	100	100
14	N	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	O	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
16	P	111/156 (71%)	107 (96%)	4 (4%)	0	100	100
17	Q	92/98 (94%)	87 (95%)	5 (5%)	0	100	100
18	R	63/84 (75%)	63 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	80/93 (86%)	77 (96%)	3 (4%)	0	100	100
20	T	83/86 (96%)	80 (96%)	3 (4%)	0	100	100
21	V	226/277 (82%)	207 (92%)	18 (8%)	1 (0%)	30	62
24	g	9/75 (12%)	8 (89%)	1 (11%)	0	100	100
All	All	2364/2763 (86%)	2233 (94%)	128 (5%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	125	ASN
21	V	156	LYS
3	C	162	MET

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	30/31 (97%)	23 (77%)	7 (23%)	1	5
3	C	170/212 (80%)	155 (91%)	15 (9%)	9	33
4	D	175/176 (99%)	164 (94%)	11 (6%)	16	44
5	E	127/147 (86%)	111 (87%)	16 (13%)	4	22
6	F	85/85 (100%)	76 (89%)	9 (11%)	6	27
7	G	131/132 (99%)	118 (90%)	13 (10%)	7	30
8	H	107/108 (99%)	97 (91%)	10 (9%)	8	32
9	I	102/125 (82%)	87 (85%)	15 (15%)	3	17
10	J	89/90 (99%)	79 (89%)	10 (11%)	6	26
11	K	89/105 (85%)	79 (89%)	10 (11%)	6	26
12	L	103/105 (98%)	89 (86%)	14 (14%)	3	20
13	M	99/104 (95%)	87 (88%)	12 (12%)	5	23
14	N	49/50 (98%)	41 (84%)	8 (16%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	76/77 (99%)	68 (90%)	8 (10%)	6	28
16	P	92/118 (78%)	82 (89%)	10 (11%)	6	27
17	Q	80/83 (96%)	70 (88%)	10 (12%)	4	22
18	R	55/72 (76%)	53 (96%)	2 (4%)	31	58
19	S	73/84 (87%)	60 (82%)	13 (18%)	2	10
20	T	69/70 (99%)	54 (78%)	15 (22%)	1	6
21	V	191/218 (88%)	167 (87%)	24 (13%)	4	22
24	g	8/63 (13%)	7 (88%)	1 (12%)	4	22
All	All	2000/2255 (89%)	1767 (88%)	233 (12%)	7	25

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	4	VAL
2	B	6	LYS
2	B	8	ARG
2	B	10	LYS
2	B	11	ARG
2	B	24	THR
2	B	30	LYS
3	C	21	ARG
3	C	36	VAL
3	C	46	LEU
3	C	58	ARG
3	C	66	ASP
3	C	75	VAL
3	C	76	ILE
3	C	82	GLU
3	C	103	LEU
3	C	149	ILE
3	C	166	GLU
3	C	167	PHE
3	C	169	ARG
3	C	182	ILE
3	C	191	THR
4	D	18	ASP
4	D	86	LEU
4	D	102	LEU
4	D	110	ARG

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Mol	Chain	Res	Type
4	D	123	VAL
4	D	140	VAL
4	D	154	ARG
4	D	169	VAL
4	D	177	VAL
4	D	188	VAL
4	D	190	LEU
5	E	37	ILE
5	E	39	ARG
5	E	54	ARG
5	E	59	THR
5	E	70	MET
5	E	71	VAL
5	E	85	ILE
5	E	95	ASN
5	E	110	VAL
5	E	131	ILE
5	E	148	ILE
5	E	156	ASP
5	E	159	ILE
5	E	184	LEU
5	E	186	ILE
5	E	198	ARG
6	F	15	ASP
6	F	18	THR
6	F	27	LEU
6	F	30	ILE
6	F	43	TRP
6	F	57	GLU
6	F	72	VAL
6	F	85	VAL
6	F	91	LEU
7	G	24	THR
7	G	27	VAL
7	G	32	LEU
7	G	35	LYS
7	G	38	LEU
7	G	43	VAL
7	G	70	LYS
7	G	76	ARG
7	G	80	VAL
7	G	99	LEU

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Mol	Chain	Res	Type
7	G	102	ARG
7	G	138	ARG
7	G	144	MET
8	H	32	LEU
8	H	36	ILE
8	H	55	ARG
8	H	56	VAL
8	H	70	ARG
8	H	72	ARG
8	H	77	LEU
8	H	92	THR
8	H	101	LEU
8	H	113	LEU
9	I	26	ILE
9	I	29	VAL
9	I	32	ARG
9	I	37	VAL
9	I	38	ARG
9	I	40	ARG
9	I	42	VAL
9	I	45	THR
9	I	78	VAL
9	I	83	ILE
9	I	87	LEU
9	I	100	ARG
9	I	105	ARG
9	I	147	TYR
9	I	150	ARG
10	J	8	ILE
10	J	15	HIS
10	J	18	ILE
10	J	32	THR
10	J	36	VAL
10	J	44	THR
10	J	50	CYS
10	J	57	LYS
10	J	97	ASP
10	J	99	ASN
11	K	23	LYS
11	K	25	VAL
11	K	40	ILE
11	K	49	ASN

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Mol	Chain	Res	Type
11	K	51	ILE
11	K	68	THR
11	K	91	VAL
11	K	95	VAL
11	K	121	ASP
11	K	131	ARG
12	L	3	THR
12	L	8	VAL
12	L	24	LEU
12	L	27	SER
12	L	29	GLN
12	L	38	TYR
12	L	41	THR
12	L	46	ASN
12	L	52	VAL
12	L	63	VAL
12	L	70	GLU
12	L	73	ASN
12	L	104	THR
12	L	107	VAL
13	M	49	THR
13	M	51	ASP
13	M	56	LEU
13	M	60	ILE
13	M	63	ASN
13	M	66	VAL
13	M	70	LEU
13	M	80	ARG
13	M	101	GLN
13	M	103	THR
13	M	109	THR
13	M	110	ARG
14	N	24	CYS
14	N	32	SER
14	N	36	LYS
14	N	41	ARG
14	N	44	LEU
14	N	45	ARG
14	N	56	VAL
14	N	60	SER
15	O	20	THR
15	O	28	GLN

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Mol	Chain	Res	Type
15	O	60	VAL
15	O	65	ARG
15	O	75	VAL
15	O	79	ARG
15	O	82	ILE
15	O	83	GLU
16	P	3	VAL
16	P	9	ARG
16	P	13	ILE
16	P	26	ARG
16	P	28	ARG
16	P	36	VAL
16	P	50	GLN
16	P	67	THR
16	P	86	LEU
16	P	90	GLU
17	Q	28	VAL
17	Q	35	THR
17	Q	48	LEU
17	Q	59	VAL
17	Q	65	ASN
17	Q	74	VAL
17	Q	85	THR
17	Q	89	ARG
17	Q	92	GLU
17	Q	93	ILE
18	R	29	THR
18	R	31	ASP
19	S	11	VAL
19	S	12	ASP
19	S	15	LEU
19	S	31	ILE
19	S	33	THR
19	S	36	ARG
19	S	45	ILE
19	S	51	VAL
19	S	53	ASP
19	S	63	THR
19	S	67	VAL
19	S	78	ARG
19	S	79	THR
20	T	3	ASN

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Mol	Chain	Res	Type
20	T	6	SER
20	T	16	ARG
20	T	18	ARG
20	T	23	SER
20	T	26	SER
20	T	43	ASP
20	T	50	LEU
20	T	51	LEU
20	T	52	HIS
20	T	56	ARG
20	T	59	ASP
20	T	70	ASN
20	T	75	LYS
20	T	81	LEU
21	V	4	VAL
21	V	5	THR
21	V	24	ASN
21	V	32	PHE
21	V	38	ILE
21	V	55	GLU
21	V	66	THR
21	V	73	LYS
21	V	75	GLN
21	V	83	GLU
21	V	113	ARG
21	V	114	LEU
21	V	137	LEU
21	V	146	ARG
21	V	155	GLN
21	V	157	VAL
21	V	167	ASN
21	V	169	GLU
21	V	184	ILE
21	V	186	ILE
21	V	189	THR
21	V	195	VAL
21	V	205	ASP
21	V	212	LEU
24	g	58	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	8	HIS
3	C	125	ASN
3	C	176	HIS
4	D	51	GLN
4	D	84	ASN
4	D	95	ASN
4	D	151	GLN
5	E	146	HIS
5	E	157	ASN
5	E	160	ASN
6	F	28	ASN
6	F	96	HIS
7	G	28	ASN
7	G	106	ASN
7	G	142	HIS
9	I	57	ASN
9	I	61	ASN
9	I	64	HIS
9	I	146	GLN
10	J	56	HIS
11	K	27	HIS
11	K	31	HIS
11	K	38	ASN
11	K	128	ASN
12	L	29	GLN
12	L	73	ASN
13	M	101	GLN
15	O	28	GLN
16	P	17	GLN
16	P	41	HIS
16	P	65	GLN
17	Q	46	HIS
17	Q	62	HIS
19	S	26	ASN
19	S	52	HIS
19	S	57	HIS
19	S	69	HIS
20	T	3	ASN
20	T	52	HIS
20	T	70	ASN
20	T	71	GLN
20	T	84	ASN
21	V	24	ASN

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Mol	Chain	Res	Type
21	V	108	HIS
21	V	167	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1528 (98%)	398 (26%)	17 (1%)
22	W	18/19 (94%)	3 (16%)	0
23	X	5/6 (83%)	2 (40%)	0
All	All	1533/1553 (98%)	403 (26%)	17 (1%)

All (403) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	U
1	A	9	U
1	A	11	G
1	A	12	A
1	A	13	G
1	A	26	G
1	A	36	A
1	A	43	G
1	A	45	G
1	A	48	G
1	A	51	C
1	A	52	U
1	A	53	U
1	A	54	A
1	A	55	A
1	A	59	A
1	A	62	C
1	A	67	C
1	A	68	G
1	A	77	G
1	A	81	C
1	A	82	U
1	A	83	U
1	A	85	C
1	A	87	G
1	A	92	A
1	A	93	C

Continued on next page...

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Mol	Chain	Res	Type
1	A	94	U
1	A	101	G
1	A	112	A
1	A	113	G
1	A	116	A
1	A	117	C
1	A	118	A
1	A	123	G
1	A	128	U
1	A	136	G
1	A	139	C
1	A	160	C
1	A	170	U
1	A	174	G
1	A	179	C
1	A	180	A
1	A	181	C
1	A	192	G
1	A	194	A
1	A	201	G
1	A	210	A
1	A	211	A
1	A	213	C
1	A	214	U
1	A	215	U
1	A	216	U
1	A	217	U
1	A	218	G
1	A	226	G
1	A	242	U
1	A	243	A
1	A	245	C
1	A	247	G
1	A	251	G
1	A	262	G
1	A	266	G
1	A	267	C
1	A	279	A
1	A	280	C
1	A	281	G
1	A	283	C
1	A	289	G

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Mol	Chain	Res	Type
1	A	301	G
1	A	314	C
1	A	319	G
1	A	321	A
1	A	329	A
1	A	332	G
1	A	338	A
1	A	344	A
1	A	345	C
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	367	U
1	A	372	C
1	A	373	A
1	A	382	A
1	A	390	U
1	A	392	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	411	A
1	A	414	A
1	A	415	C
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	426	U
1	A	427	U
1	A	428	G
1	A	429	U
1	A	430	A
1	A	434	C
1	A	436	C
1	A	438	U
1	A	450	G
1	A	451	A
1	A	452	A

Continued on next page...

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Mol	Chain	Res	Type
1	A	453	G
1	A	454	C
1	A	456	C
1	A	457	A
1	A	458	A
1	A	459	G
1	A	461	G
1	A	464	G
1	A	465	G
1	A	466	U
1	A	477	G
1	A	478	A
1	A	479	A
1	A	482	A
1	A	484	C
1	A	485	G
1	A	486	G
1	A	491	C
1	A	496	U
1	A	497	G
1	A	498	C
1	A	499	C
1	A	505	C
1	A	507	G
1	A	509	G
1	A	511	U
1	A	512	A
1	A	513	A
1	A	515	A
1	A	519	A
1	A	520	G
1	A	525	C
1	A	527	A
1	A	539	A
1	A	542	U
1	A	544	C
1	A	552	A
1	A	553	A
1	A	554	A
1	A	556	A
1	A	557	G
1	A	612	U

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Mol	Chain	Res	Type
1	A	613	G
1	A	629	G
1	A	633	A
1	A	641	G
1	A	645	G
1	A	666	U
1	A	667	A
1	A	668	G
1	A	680	G
1	A	682	A
1	A	683	G
1	A	700	C
1	A	701	G
1	A	702	G
1	A	703	U
1	A	704	G
1	A	711	G
1	A	713	G
1	A	728	A
1	A	729	A
1	A	735	G
1	A	757	A
1	A	761	A
1	A	764	A
1	A	765	G
1	A	771	G
1	A	772	A
1	A	773	U
1	A	774	A
1	A	779	G
1	A	782	A
1	A	789	G
1	A	793	U
1	A	794	A
1	A	795	A
1	A	797	C
1	A	799	G
1	A	800	U
1	A	808	A
1	A	818	U
1	A	821	C
1	A	822	U

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Mol	Chain	Res	Type
1	A	823	U
1	A	824	C
1	A	825	C
1	A	826	U
1	A	827	U
1	A	828	G
1	A	835	G
1	A	840	G
1	A	841	U
1	A	865	C
1	A	884	G
1	A	895	A
1	A	896	A
1	A	908	G
1	A	909	G
1	A	913	C
1	A	914	C
1	A	915	G
1	A	916	C
1	A	917	A
1	A	921	G
1	A	930	C
1	A	932	U
1	A	940	A
1	A	942	U
1	A	943	U
1	A	945	G
1	A	947	U
1	A	948	G
1	A	950	A
1	A	951	A
1	A	953	G
1	A	954	C
1	A	955	G
1	A	956	A
1	A	957	A
1	A	959	A
1	A	971	G
1	A	973	U
1	A	974	U
1	A	975	G
1	A	982	A

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Mol	Chain	Res	Type
1	A	984	A
1	A	986	G
1	A	987	A
1	A	988	C
1	A	992	G
1	A	996	G
1	A	999	A
1	A	1000	U
1	A	1003	C
1	A	1007	U
1	A	1008	C
1	A	1010	C
1	A	1011	U
1	A	1013	G
1	A	1014	U
1	A	1020	G
1	A	1021	U
1	A	1022	G
1	A	1024	G
1	A	1025	C
1	A	1028	G
1	A	1033	G
1	A	1034	C
1	A	1036	U
1	A	1045	U
1	A	1047	A
1	A	1048	G
1	A	1054	G
1	A	1064	G
1	A	1074	G
1	A	1075	U
1	A	1079	G
1	A	1081	A
1	A	1085	A
1	A	1104	G
1	A	1108	C
1	A	1110	A
1	A	1112	C
1	A	1115	G
1	A	1116	U
1	A	1117	U
1	A	1118	A

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Mol	Chain	Res	Type
1	A	1120	G
1	A	1123	G
1	A	1128	C
1	A	1129	U
1	A	1132	U
1	A	1133	G
1	A	1138	A
1	A	1140	U
1	A	1141	G
1	A	1147	G
1	A	1149	C
1	A	1150	A
1	A	1152	C
1	A	1162	G
1	A	1164	U
1	A	1165	G
1	A	1171	G
1	A	1172	A
1	A	1176	C
1	A	1177	A
1	A	1178	A
1	A	1181	C
1	A	1182	A
1	A	1183	U
1	A	1193	U
1	A	1194	A
1	A	1206	U
1	A	1207	C
1	A	1217	A
1	A	1219	A
1	A	1231	A
1	A	1233	A
1	A	1235	G
1	A	1238	U
1	A	1239	G
1	A	1241	G
1	A	1242	A
1	A	1248	U
1	A	1249	G
1	A	1251	G
1	A	1254	G
1	A	1255	G

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Mol	Chain	Res	Type
1	A	1261	A
1	A	1265	U
1	A	1266	U
1	A	1267	U
1	A	1268	C
1	A	1269	A
1	A	1272	G
1	A	1281	A
1	A	1282	G
1	A	1283	U
1	A	1284	U
1	A	1285	C
1	A	1287	G
1	A	1298	G
1	A	1299	C
1	A	1300	A
1	A	1301	A
1	A	1302	C
1	A	1305	G
1	A	1313	G
1	A	1320	G
1	A	1322	G
1	A	1327	U
1	A	1328	A
1	A	1329	G
1	A	1335	G
1	A	1343	G
1	A	1344	C
1	A	1345	A
1	A	1346	A
1	A	1347	C
1	A	1351	G
1	A	1353	G
1	A	1357	A
1	A	1363	U
1	A	1364	U
1	A	1381	A
1	A	1382	C
1	A	1383	C
1	A	1385	C
1	A	1389	U
1	A	1402	G

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Mol	Chain	Res	Type
1	A	1406	G
1	A	1407	U
1	A	1424	G
1	A	1425	G
1	A	1426	C
1	A	1429	A
1	A	1430	A
1	A	1434	U
1	A	1435	U
1	A	1436	G
1	A	1438	G
1	A	1459	G
1	A	1460	A
1	A	1466	G
1	A	1468	U
1	A	1471	G
1	A	1478	G
1	A	1481	G
1	A	1482	U
1	A	1483	A
1	A	1486	A
1	A	1487	A
1	A	1488	G
1	A	1490	U
1	A	1491	A
1	A	1492	G
1	A	1501	G
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1511	C
1	A	1512	U
1	A	1513	G
1	A	1514	G
1	A	1516	U
22	W	33	U
22	W	37	A
22	W	42	C
23	X	2	U
23	X	3	U

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	84	U
1	A	280	C
1	A	422	C
1	A	429	U
1	A	437	U
1	A	456	C
1	A	485	G
1	A	498	C
1	A	703	U
1	A	895	A
1	A	1007	U
1	A	1116	U
1	A	1117	U
1	A	1149	C
1	A	1171	G
1	A	1477	A
1	A	1482	U

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 219 ligands modelled in this entry, 219 are 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](#)

There are no chain breaks in this entry.

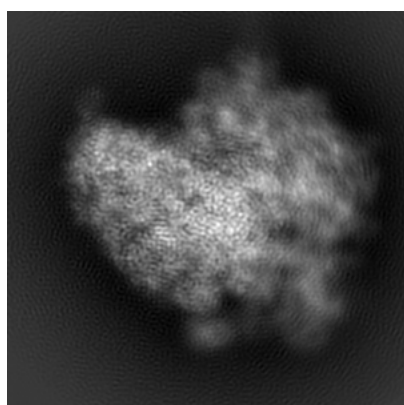
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3748. These allow visual inspection of the internal detail of the map and identification of artifacts.

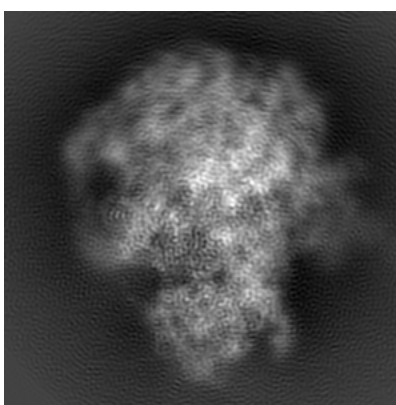
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

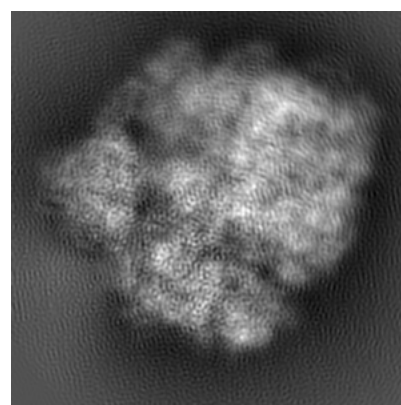
6.1.1 Primary map



X



Y

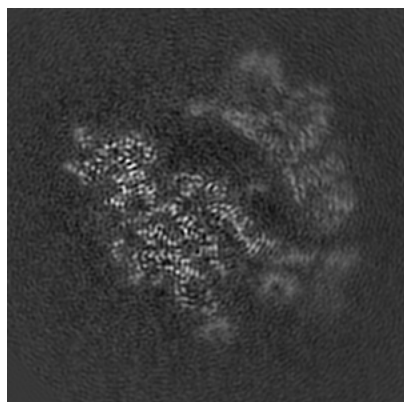


Z

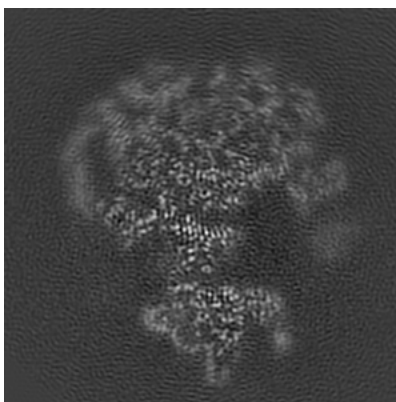
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

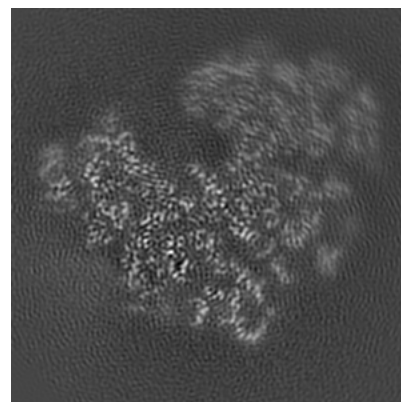
6.2.1 Primary map



X Index: 108



Y Index: 108

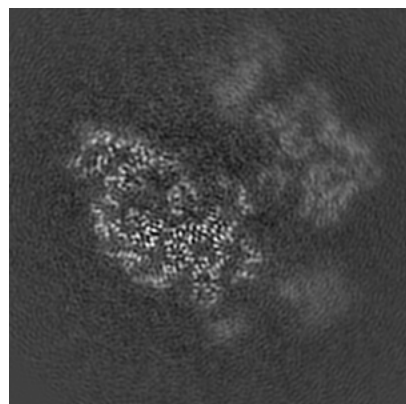


Z Index: 108

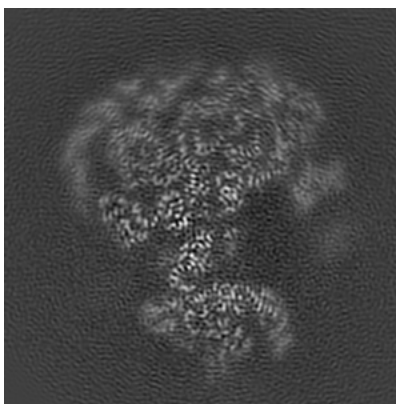
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

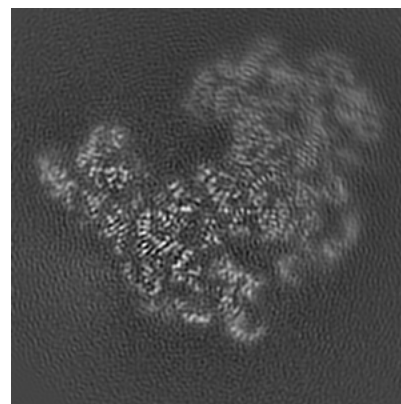
6.3.1 Primary map



X Index: 99



Y Index: 105

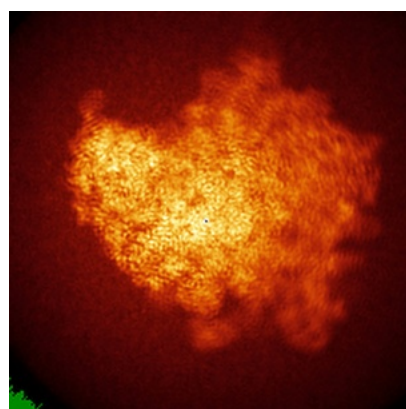


Z Index: 103

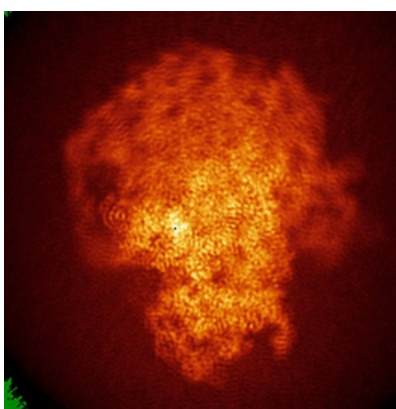
The images above show the largest variance slices of the map in three orthogonal directions.

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

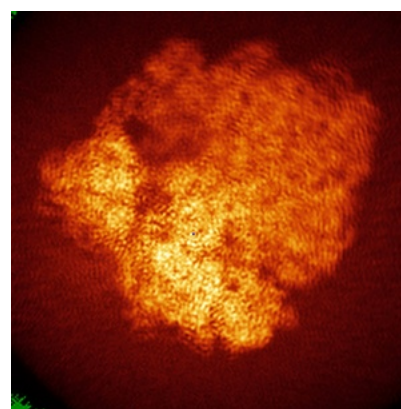
6.4.1 Primary map



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

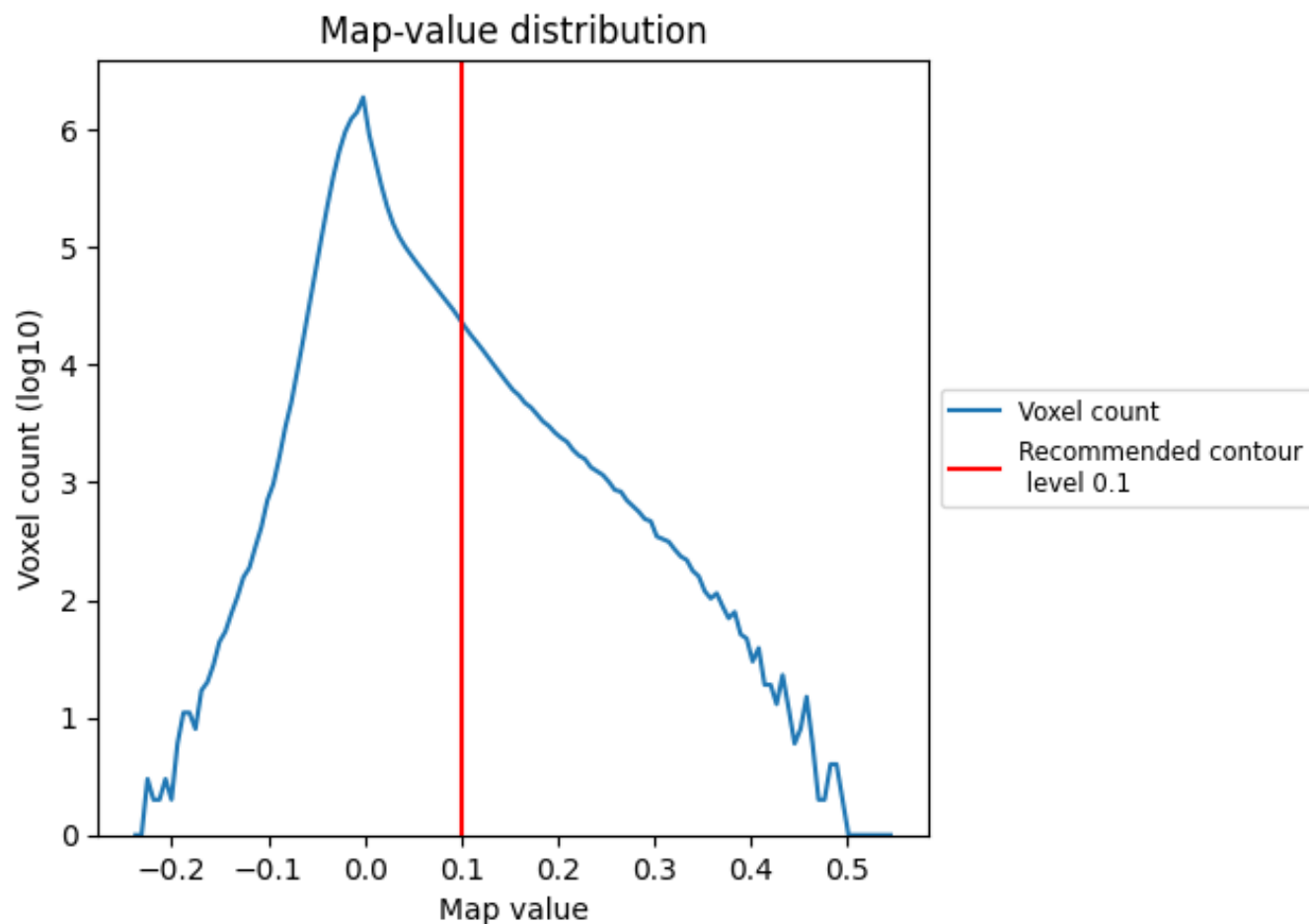
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

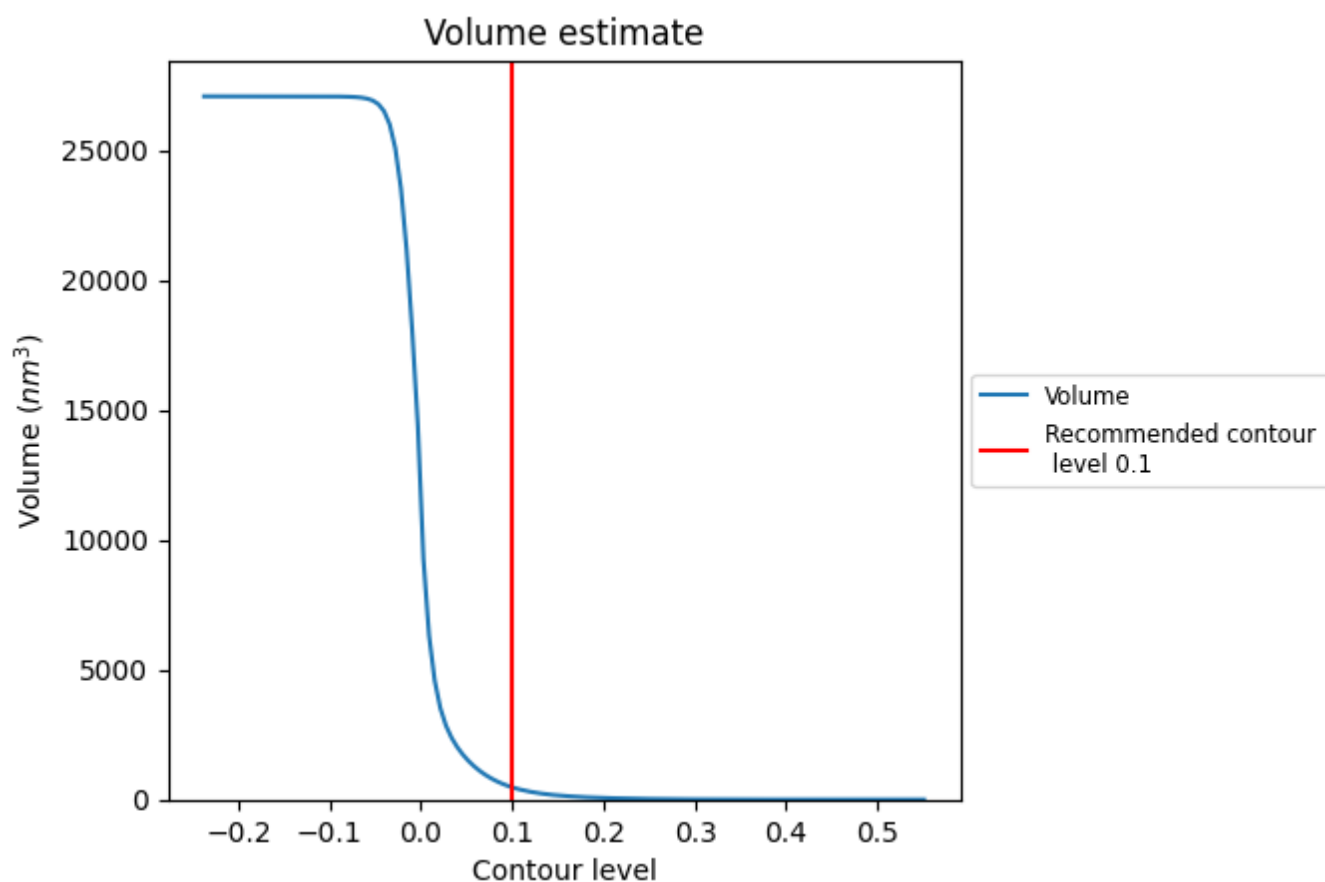
This section contains the results of statistical analysis of the map.

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.

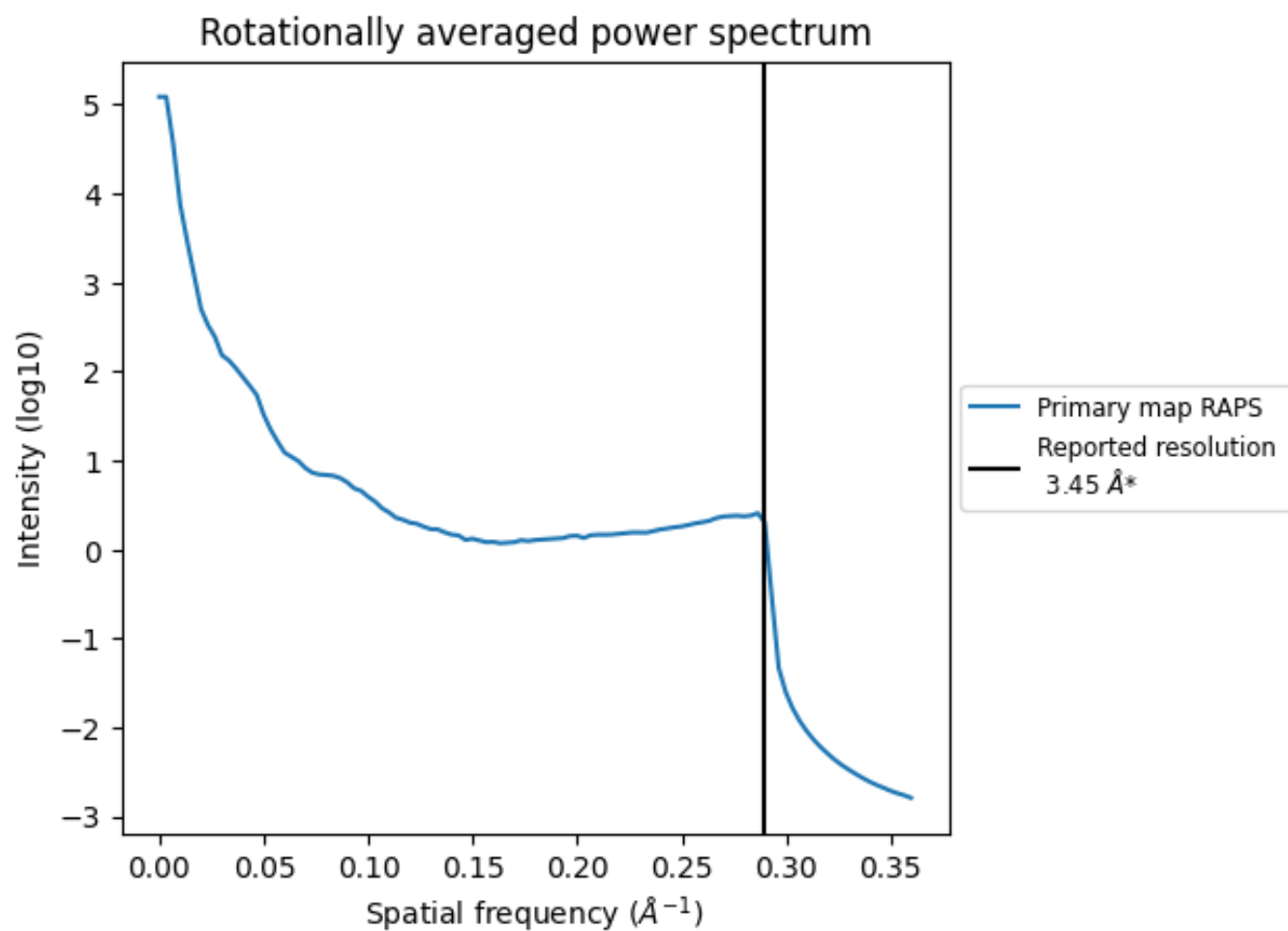
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 472 nm³; this corresponds to an approximate mass of 427 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 ⓘ

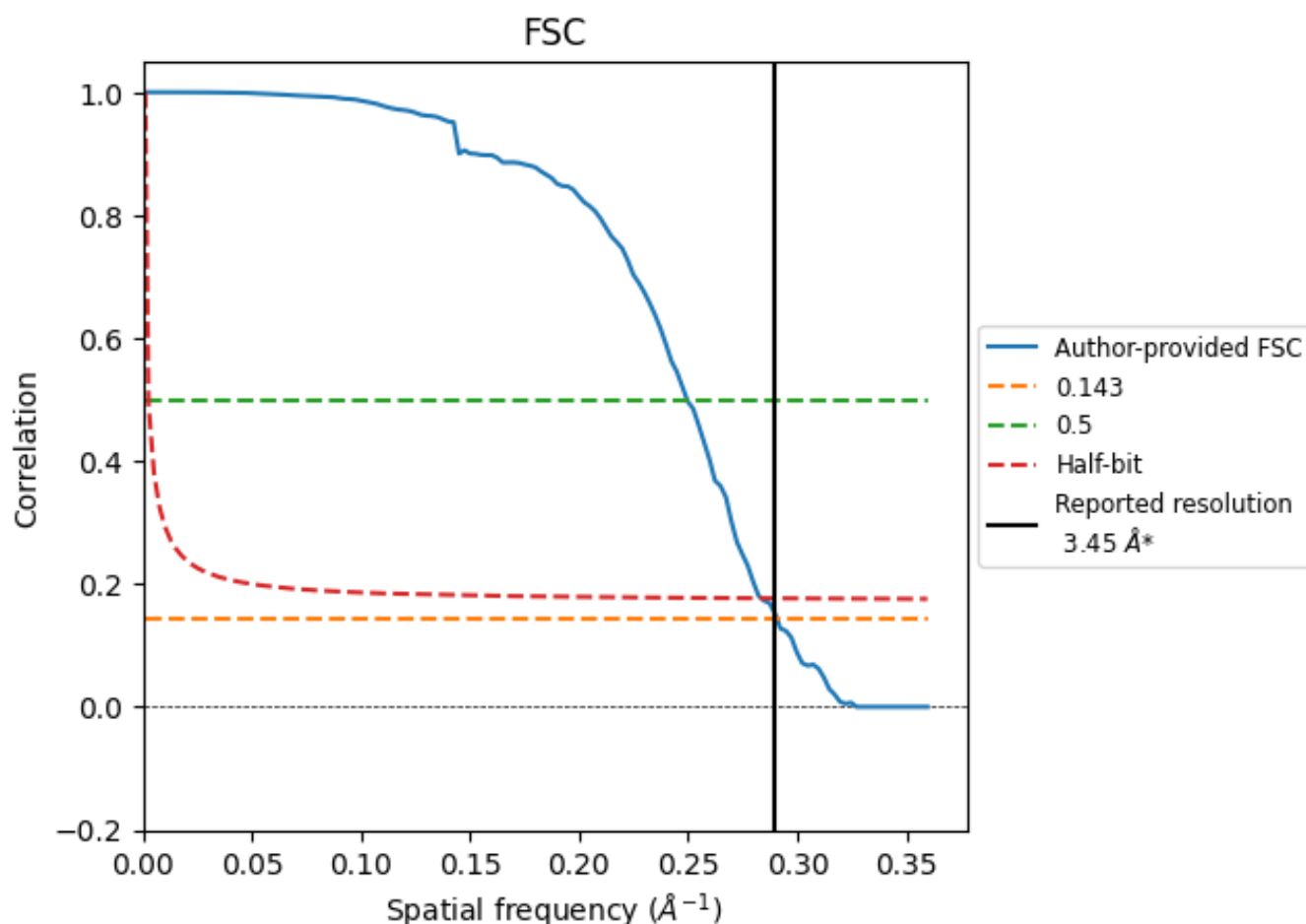


*Reported resolution corresponds to spatial frequency of 0.290 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.290 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

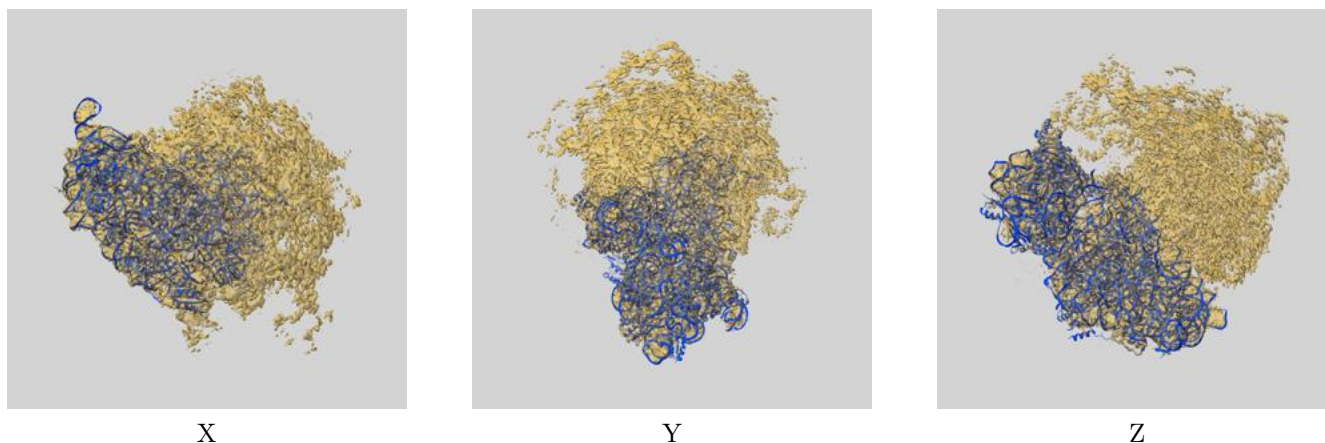
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	3.44	4.01	3.53
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

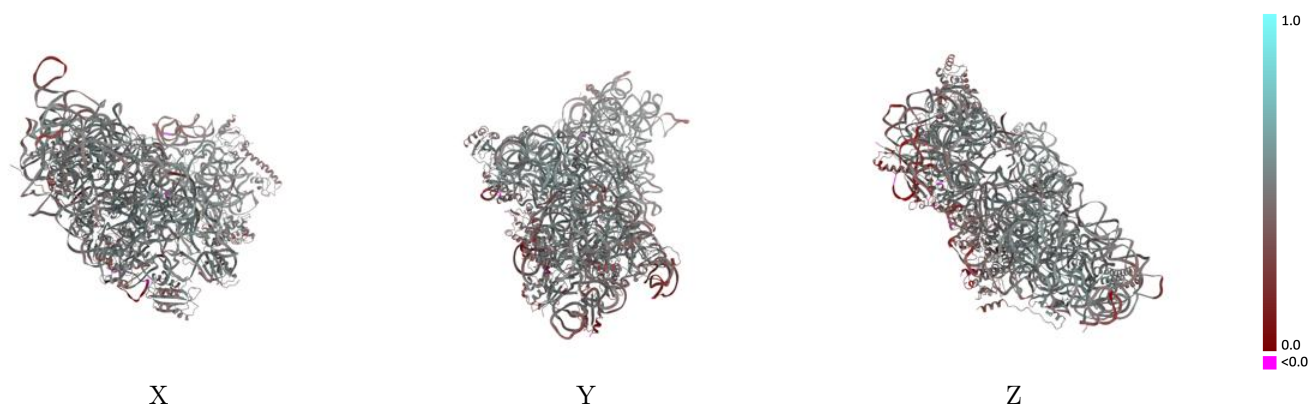
This section contains information regarding the fit between EMDB map EMD-3748 and PDB model 5O5J. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



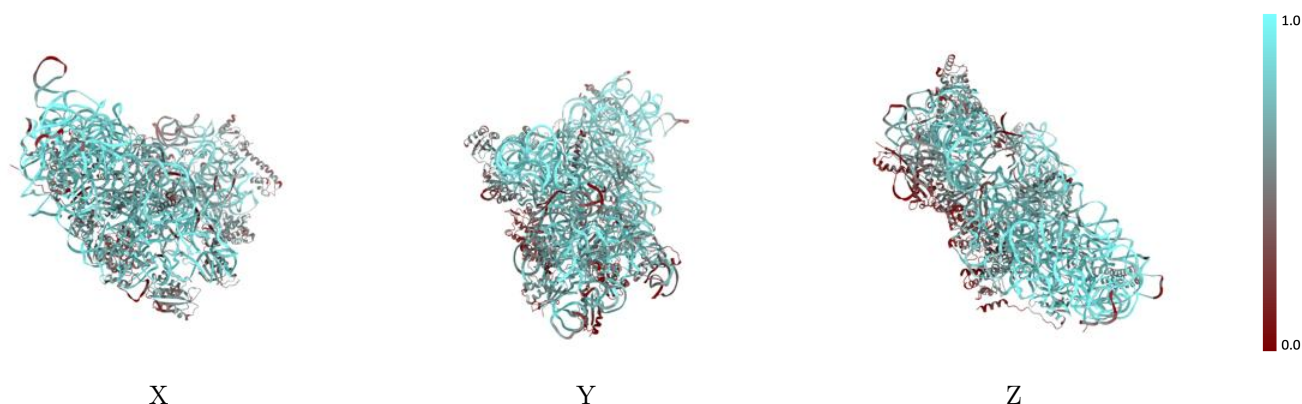
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



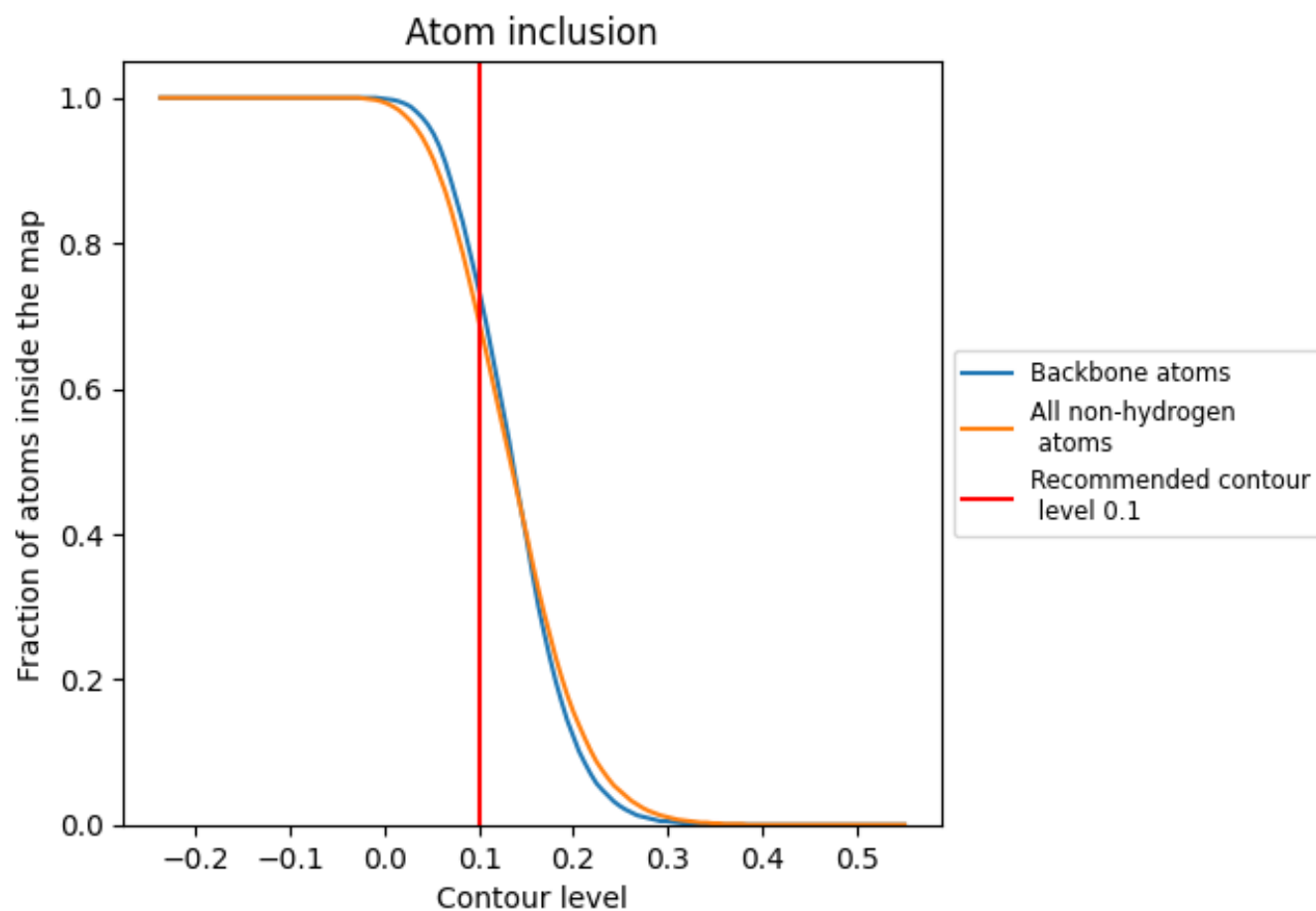
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 69% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6930	 0.4600
A	 0.8180	 0.4760
B	 0.3890	 0.4770
C	 0.4140	 0.4340
D	 0.4500	 0.4080
E	 0.5080	 0.4520
F	 0.4950	 0.4360
G	 0.4720	 0.4170
H	 0.6540	 0.4970
I	 0.5540	 0.4570
J	 0.4160	 0.3970
K	 0.5670	 0.4570
L	 0.6030	 0.4850
M	 0.4920	 0.4230
N	 0.6610	 0.5130
O	 0.6280	 0.4640
P	 0.6000	 0.4730
Q	 0.5720	 0.4620
R	 0.5800	 0.4490
S	 0.5500	 0.4520
T	 0.6190	 0.4430
V	 0.0320	 0.2930
W	 0.4440	 0.4530
X	 0.4020	 0.4180
g	 0.4370	 0.4280

