



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:08 PM UTC

PDB ID : 7K5I / pdb_00007k5i
EMDB ID : EMD-22681
Title : SARS-COV-2 nsp1 in complex with human 40S ribosome
Authors : Wang, L.; Shi, M.; Wu, H.
Deposited on : 2020-09-16
Resolution : 2.90 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:

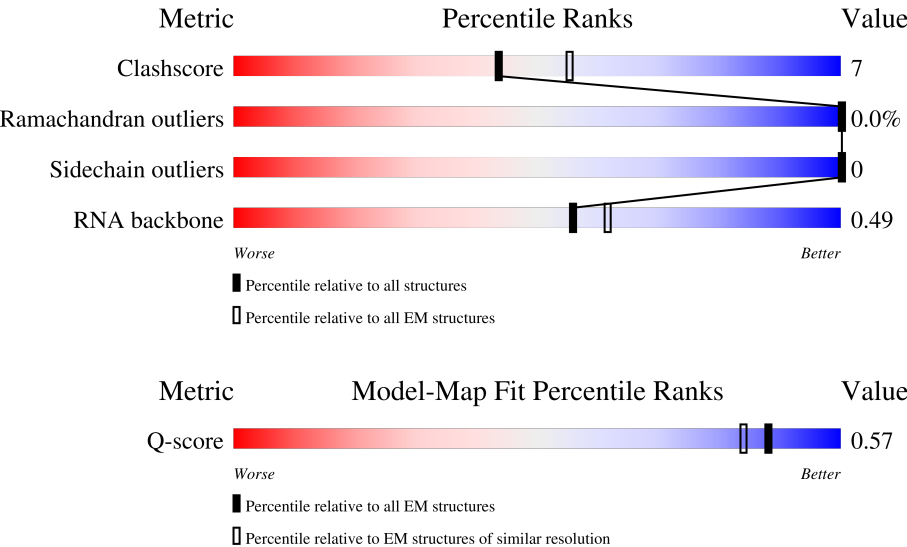
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.90 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.



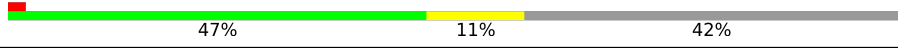
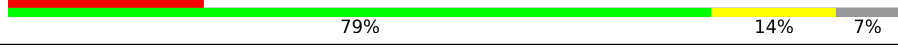
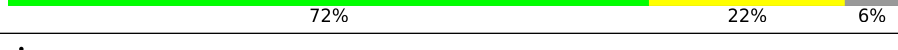
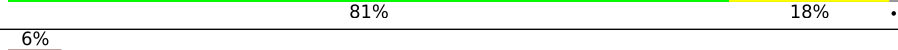
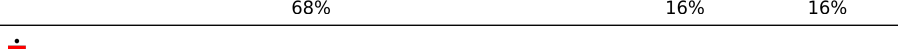
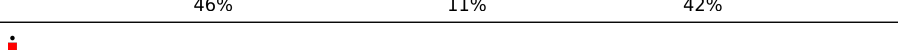
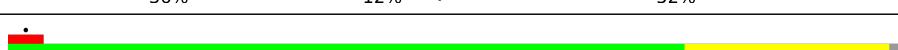
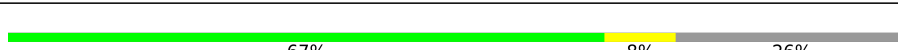
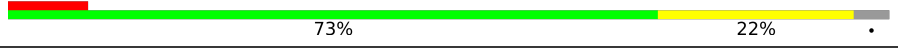
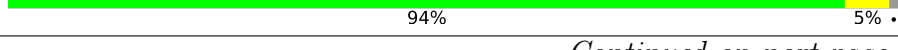
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	R	135	
2	2	1868	
3	d	56	

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Mol	Chain	Length	Quality of chain
4	D	243	
5	F	204	
6	K	165	
7	M	132	
8	P	145	
9	Q	146	
10	S	152	
11	T	145	
12	U	119	
13	Z	125	
14	c	69	
15	f	149	
16	g	317	
17	A	295	
18	B	264	
19	C	293	
20	E	263	
21	G	249	
22	H	194	
23	I	208	
24	J	194	
25	L	158	
26	N	151	
27	O	151	
28	V	83	

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Mol	Chain	Length	Quality of chain
29	W	130	89%10%
30	X	143	86%13%
31	Y	133	83%10%7%
32	a	102	85%14%
33	b	84	89%8%
34	e	59	71%14%15%
35	h	25	36%72%24%
36	1	180	11%6%83%

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 74540 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	132	Total	C	N	O	S	0	0
			1066	669	199	194	4		

- Molecule 2 is a RNA chain called 40S ribosomal rRNA18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1665	Total	C	N	O	P	0	0
			35552	15869	6385	11633	1665		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1772	C	G	conflict	GB 337376

- Molecule 3 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	54	Total	C	N	O	S	0	0
			455	284	93	73	5		

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	225	Total	C	N	O	S	0	0
			1748	1115	315	311	7		

- Molecule 5 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 6 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	95	Total	C	N	O	S	0	0
			800	522	142	131	5		

- Molecule 7 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 8 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	120	Total	C	N	O	S	0	0
			984	625	184	168	7		

- Molecule 9 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 10 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	143	Total	C	N	O	S	0	0
			1184	743	240	200	1		

- Molecule 11 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	T	144	Total	C	N	O	S	0	0
			1122	703	217	199	3		

- Molecule 12 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 13 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 14 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	c	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

- Molecule 15 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	72	Total	C	N	O	S	0	0
			585	366	114	97	8		

- Molecule 16 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 17 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	A	206	Total	C	N	O	S	0	0
			1624	1035	287	294	8		

- Molecule 18 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 19 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	C	218	Total	C	N	O	S	0	0
			1682	1090	289	293	10		

- Molecule 20 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 21 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 22 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 23 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 24 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 25 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 26 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 27 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	O	135	Total	C	N	O	S	0	0
			1006	616	198	186	6		

- Molecule 28 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 29 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 30 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 31 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 32 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 33 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	50	Total	C	N	O	S	0	0
			397	242	89	65	1		

- Molecule 35 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	24	Total	C	N	O	S	0	0
			231	140	63	26	2		

- Molecule 36 is a protein called Host translation inhibitor nsp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1	30	Total	C	N	O	S	0	0
			250	153	44	52	1		

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	2	1	Total	Mg	0
			1	1	

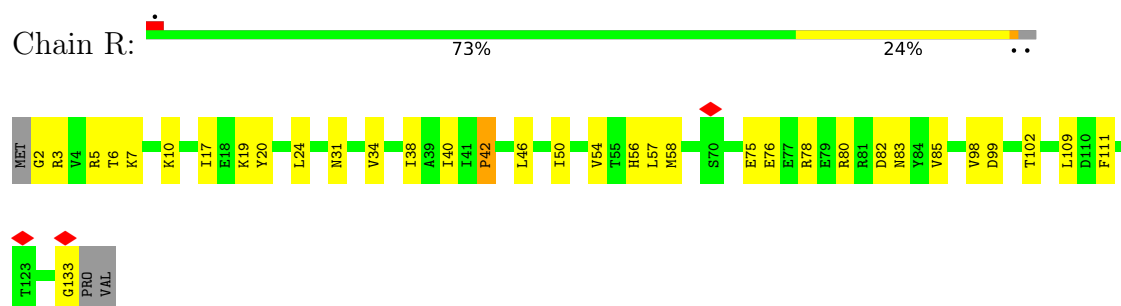
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	d	1	Total	Zn	0
			1	1	
38	f	1	Total	Zn	0
			1	1	
38	a	1	Total	Zn	0
			1	1	

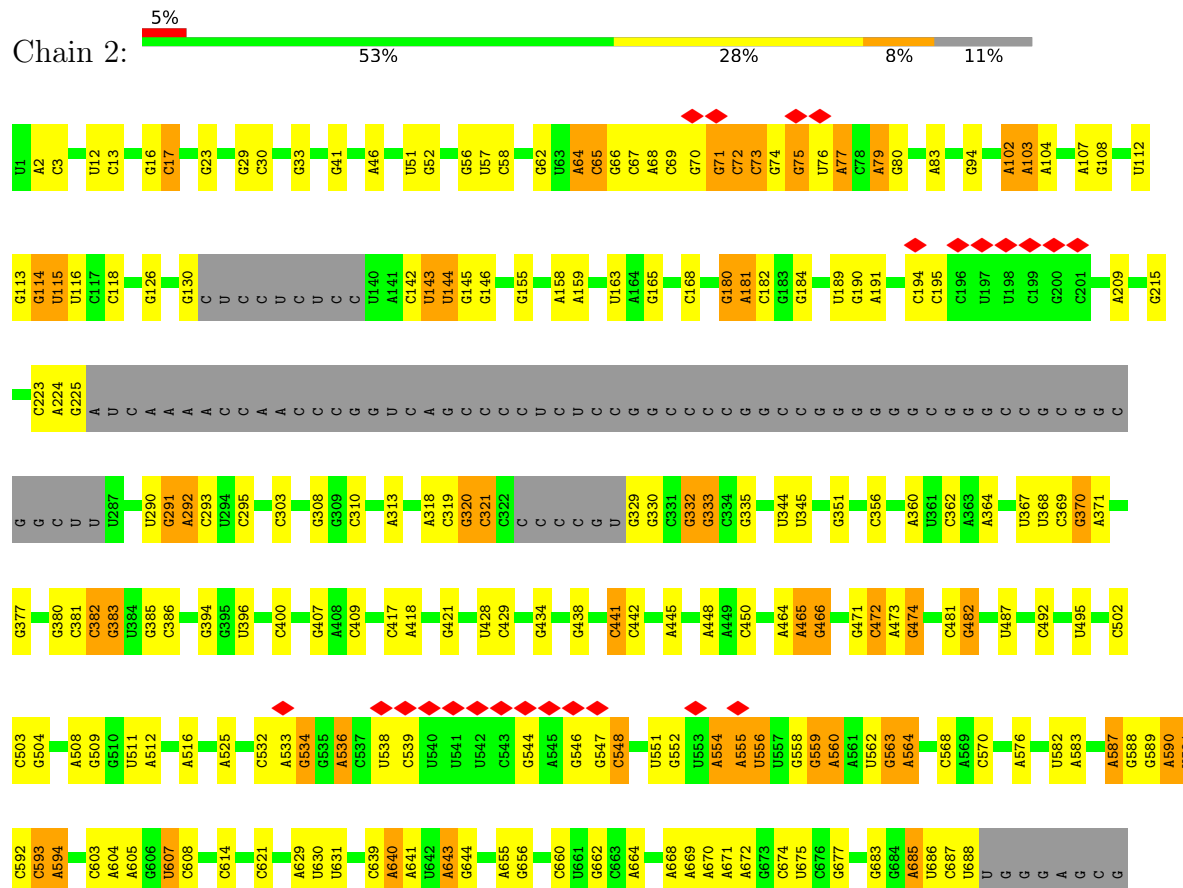
3 Residue-property plots

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: 40S ribosomal protein S17



• Molecule 2: 40S ribosomal rRNA18S



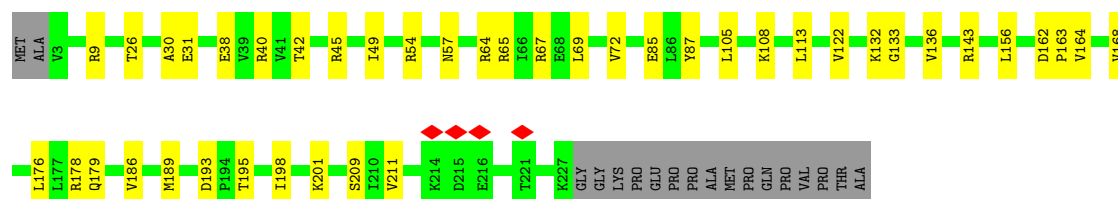


Chain d: 



- Molecule 4: 40S ribosomal protein S3

Chain D: 



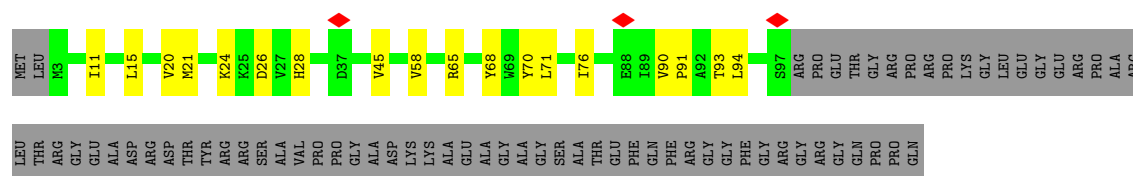
- Molecule 5: 40S ribosomal protein S5

Chain F: 



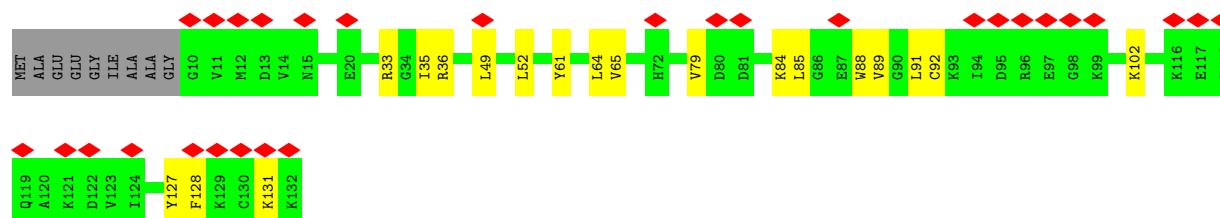
- Molecule 6: 40S ribosomal protein S10

Chain K: 



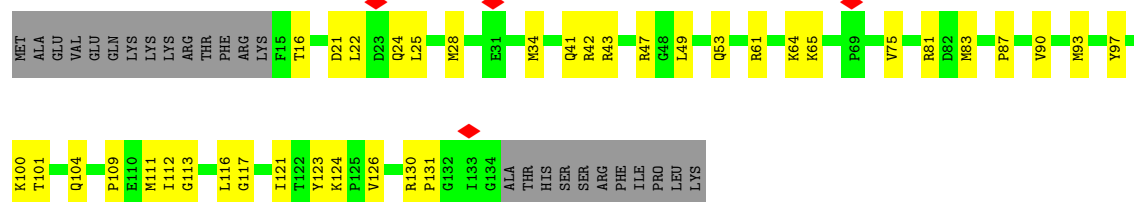
- Molecule 7: 40S ribosomal protein S12

Chain M: 



- Molecule 8: 40S ribosomal protein S15

Chain P: 



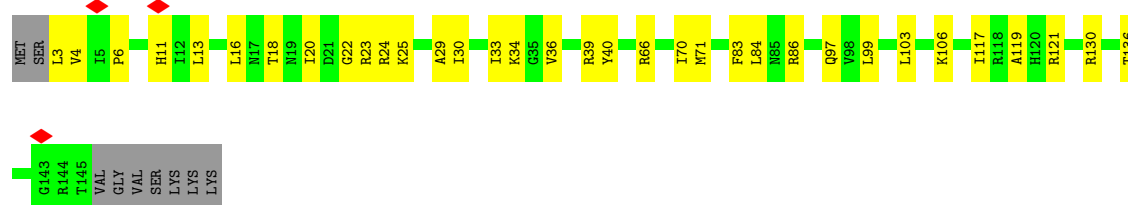
- Molecule 9: 40S ribosomal protein S16

Chain Q: 



- Molecule 10: 40S ribosomal protein S18

Chain S: 



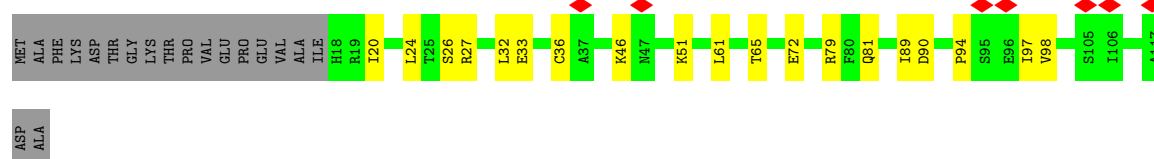
- Molecule 11: 40S ribosomal protein S19

Chain T: 

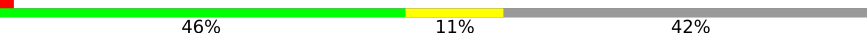


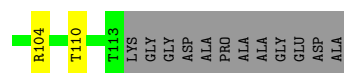
- Molecule 12: 40S ribosomal protein S20

Chain U: 



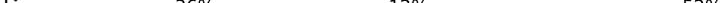
- Molecule 13: 40S ribosomal protein S25

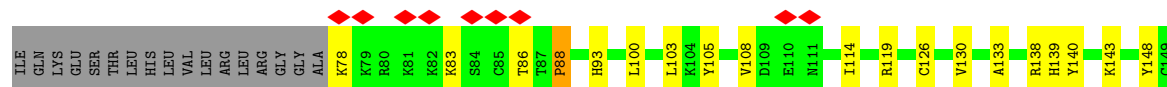
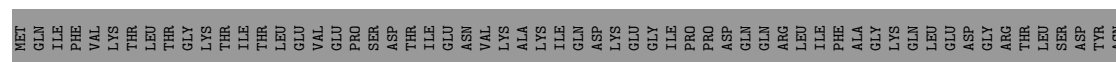
Chain Z: 



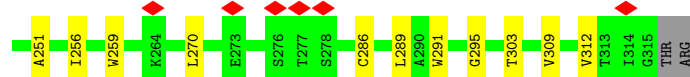
- Chain c: 67% 22% 12%

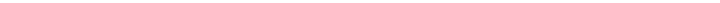


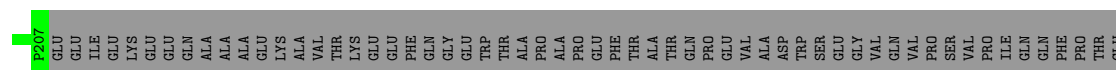
- Chain f:  6% 36% 12% 46%

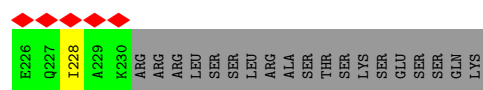


- Chain g: 76% 23%

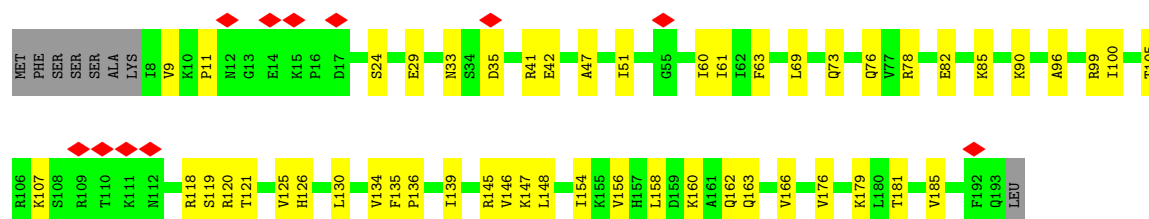


- Chain A:  59% 11% 30%

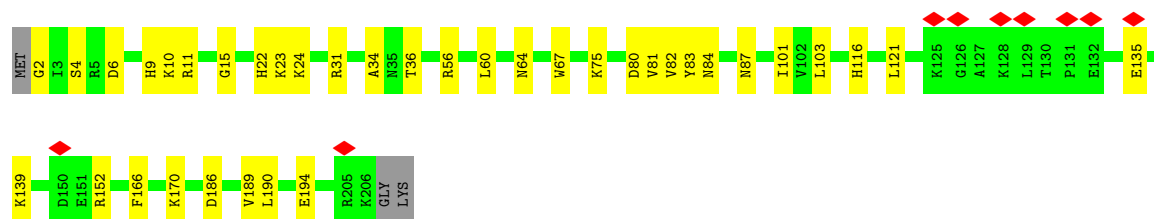
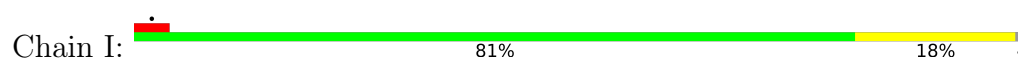




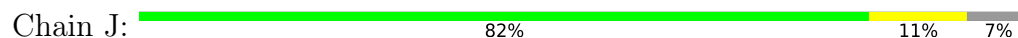
- Molecule 22: 40S ribosomal protein S7



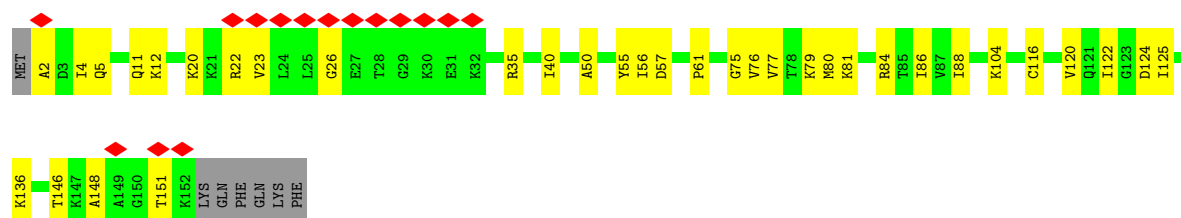
- Molecule 23: 40S ribosomal protein S8



- Molecule 24: 40S ribosomal protein S9

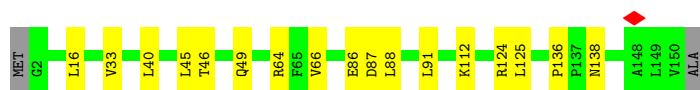


- Molecule 25: 40S ribosomal protein S11

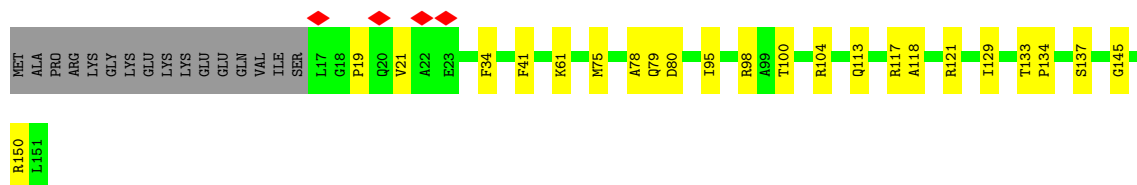


- Molecule 26: 40S ribosomal protein S13





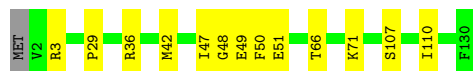
- Molecule 27: 40S ribosomal protein S14



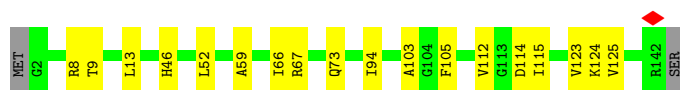
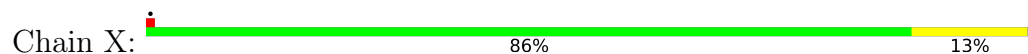
- Molecule 28: 40S ribosomal protein S21



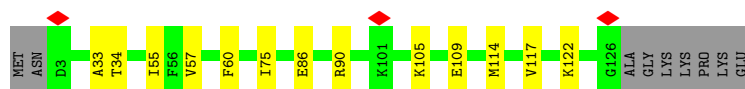
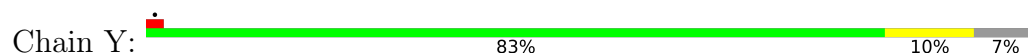
- Molecule 29: 40S ribosomal protein S15a



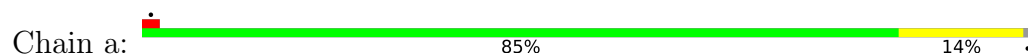
- Molecule 30: 40S ribosomal protein S23



- Molecule 31: 40S ribosomal protein S24



- Molecule 32: 40S ribosomal protein S26



- | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|
| VAL | LEU | LEU | ARG | LYS | ASN | GLY | ASN | LYS | GLY | ALA | GLY | GLY | HIS | SER | TYR | GLY | ALA | ASP | LEU | SER | PHE | ASP | GLY | ASP | GLU | L149 | F157 | M160 | H165 | S166 | V169 | T170 | R171 | E172 | L173 | M174 | L177 | M178 | GLY |
|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	794651	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	9.459	Depositor
Minimum map value	-5.531	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.199	Depositor
Recommended contour level	0.54	Depositor
Map size ($\text{\AA}$)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	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	R	0.17	0/1080	0.38	0/1449
2	2	0.19	0/39755	0.32	0/61954
3	d	0.17	0/466	0.43	0/618
4	D	0.15	0/1776	0.33	0/2392
5	F	0.17	0/1516	0.41	1/2037 (0.0%)
6	K	0.16	0/824	0.42	0/1112
7	M	0.13	0/963	0.34	0/1291
8	P	0.15	0/1003	0.36	0/1341
9	Q	0.17	0/1126	0.39	0/1506
10	S	0.15	0/1202	0.38	0/1610
11	T	0.15	0/1142	0.39	0/1530
12	U	0.16	0/805	0.34	0/1081
13	Z	0.16	0/580	0.37	0/780
14	c	0.18	0/481	0.36	0/643
15	f	0.14	0/595	0.38	0/785
16	g	0.16	0/2497	0.40	0/3399
17	A	0.16	0/1661	0.33	0/2259
18	B	0.16	0/1756	0.34	0/2350
19	C	0.18	0/1718	0.36	0/2322
20	E	0.16	0/2118	0.32	0/2849
21	G	0.13	0/1885	0.29	0/2510
22	H	0.15	0/1524	0.35	0/2042
23	I	0.16	0/1711	0.38	0/2282
24	J	0.16	0/1524	0.33	0/2035
25	L	0.17	0/1250	0.39	0/1673
26	N	0.15	0/1226	0.33	0/1649
27	O	0.17	0/1019	0.38	0/1367
28	V	0.16	0/631	0.33	0/844
29	W	0.18	0/1051	0.41	0/1406
30	X	0.18	0/1116	0.38	0/1490
31	Y	0.16	0/1031	0.32	0/1370
32	a	0.17	0/828	0.36	0/1109

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.16	0/653	0.36	0/876
34	e	0.16	0/399	0.37	0/520
35	h	0.11	0/232	0.29	0/295
36	1	0.17	0/255	0.27	0/344
All	All	0.17	0/79399	0.34	1/115120 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	R	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	171	GLU	N-CA-C	-5.03	107.80	114.04

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	42	PRO	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	R	1066	0	1116	28	0
2	2	35552	0	17948	368	0
3	d	455	0	445	11	0
4	D	1748	0	1844	29	0
5	F	1495	0	1549	27	0
6	K	800	0	818	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	953	0	990	14	0
8	P	984	0	1028	24	0
9	Q	1109	0	1174	17	0
10	S	1184	0	1244	29	0
11	T	1122	0	1153	20	0
12	U	795	0	862	14	0
13	Z	574	0	627	15	0
14	c	479	0	507	13	0
15	f	585	0	615	16	0
16	g	2440	0	2396	54	0
17	A	1624	0	1634	25	0
18	B	1729	0	1803	25	0
19	C	1682	0	1769	16	0
20	E	2076	0	2177	23	0
21	G	1862	0	2018	34	0
22	H	1501	0	1593	35	0
23	I	1682	0	1769	28	0
24	J	1499	0	1618	14	0
25	L	1229	0	1302	23	0
26	N	1202	0	1289	13	0
27	O	1006	0	1030	20	0
28	V	625	0	628	4	0
29	W	1034	0	1080	10	0
30	X	1098	0	1167	11	0
31	Y	1014	0	1082	8	0
32	a	814	0	863	12	0
33	b	640	0	663	4	0
34	e	397	0	438	6	0
35	h	231	0	277	4	0
36	1	250	0	226	8	0
37	2	1	0	0	0	0
38	a	1	0	0	0	0
38	d	1	0	0	0	0
38	f	1	0	0	0	0
All	All	74540	0	58742	855	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 7.

All (855) 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)
14:c:29:GLN:OE1	14:c:45:ASN:ND2	2.10	0.85
2:2:103:A:OP2	2:2:356:C:N4	2.10	0.84
16:g:113:PHE:HE2	16:g:117:ASN:HD22	1.26	0.84
2:2:1601:A:H5'	2:2:1636:G:H22	1.41	0.83
23:I:82:VAL:HG12	23:I:83:TYR:H	1.43	0.83
2:2:64:A:H2	2:2:83:A:H62	1.27	0.82
21:G:69:THR:HG22	21:G:71:GLY:H	1.48	0.78
22:H:73:GLN:HA	22:H:76:GLN:HB2	1.64	0.78
16:g:114:SER:OG	16:g:116:ASP:OD1	2.03	0.77
16:g:17:TRP:HB2	16:g:36:ARG:HD3	1.66	0.77
20:E:87:MET:HE2	20:E:123:LEU:HB2	1.66	0.76
35:h:17:ARG:HA	35:h:20:MET:HG2	1.68	0.76
2:2:1396:A:O2'	2:2:1398:G:N7	2.18	0.76
2:2:1402:A:H4'	12:U:51:LYS:HE2	1.67	0.75
16:g:5:MET:HE2	16:g:312:VAL:HG22	1.69	0.74
9:Q:27:ARG:NH1	9:Q:95:TYR:OH	2.22	0.73
25:L:4:ILE:HG23	25:L:5:GLN:HG2	1.71	0.73
16:g:174:VAL:HB	16:g:188:HIS:HB2	1.70	0.72
23:I:80:ASP:OD2	23:I:81:VAL:N	2.22	0.72
2:2:65:C:N4	21:G:134:GLY:O	2.22	0.72
16:g:87:LEU:HB3	16:g:101:PHE:HB2	1.72	0.72
2:2:1606:G:H5'	11:T:86:GLY:HA2	1.71	0.71
2:2:1551:U:OP1	4:D:9:ARG:NH1	2.23	0.71
1:R:99:ASP:OD2	17:A:42:LYS:NZ	2.20	0.70
9:Q:28:GLY:HA3	9:Q:67:ASP:HB2	1.73	0.70
27:O:117:ARG:HH21	27:O:121:ARG:HH21	1.36	0.70
19:C:165:VAL:HG21	19:C:217:ALA:HB1	1.73	0.70
2:2:981:A:H2'	2:2:982:G:C8	2.27	0.69
18:B:28:LYS:HD2	18:B:48:LEU:HD13	1.74	0.69
21:G:213:LEU:HG	21:G:217:MET:HE2	1.75	0.69
9:Q:16:LYS:HD3	9:Q:79:ALA:HA	1.73	0.69
12:U:51:LYS:HB3	12:U:90:ASP:HB2	1.74	0.69
2:2:551:U:H1'	34:e:44:ASN:HD22	1.58	0.69
2:2:190:G:O2'	2:2:209:A:N6	2.26	0.68
1:R:82:ASP:O	17:A:85:ARG:NH2	2.26	0.68
2:2:1354:G:H21	2:2:1356:G:H8	1.42	0.68
2:2:1239:U:H5''	8:P:124:LYS:HD3	1.76	0.67
5:F:124:ASP:OD2	14:c:47:LYS:NZ	2.19	0.67
14:c:43:ILE:HG22	14:c:65:ALA:HB3	1.76	0.67
2:2:1374:C:O2'	2:2:1464:C:O2	2.11	0.67
18:B:164:ILE:O	18:B:168:MET:HG3	1.94	0.67
8:P:81:ARG:NH1	8:P:97:TYR:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:942:G:H2'	2:2:943:U:C6	2.30	0.66
10:S:6:PRO:HD2	13:Z:49:LEU:HD13	1.77	0.66
2:2:1153:C:OP2	29:W:71:LYS:NZ	2.29	0.66
2:2:1507:G:N2	15:f:86:THR:OG1	2.28	0.66
1:R:17:ILE:HD12	1:R:57:LEU:HD23	1.78	0.66
2:2:1060:A:O2'	2:2:1062:A:N7	2.29	0.66
7:M:52:LEU:HD11	7:M:65:VAL:HG11	1.78	0.66
22:H:9:VAL:HG23	22:H:24:SER:HB2	1.79	0.65
2:2:532:C:N3	2:2:533:A:N6	2.45	0.65
2:2:808:A:O2'	2:2:809:A:H8	1.78	0.65
20:E:151:ASP:OD1	21:G:216:ARG:NH2	2.29	0.65
10:S:84:LEU:HD22	10:S:97:GLN:HB2	1.78	0.65
3:d:56:ASP:OXT	12:U:79:ARG:NH1	2.30	0.65
16:g:42:MET:HE1	16:g:92:LEU:HB3	1.79	0.65
4:D:45:ARG:HD3	4:D:85:GLU:HG3	1.79	0.65
9:Q:96:TYR:O	9:Q:97:GLN:HG3	1.98	0.64
20:E:97:GLU:OE2	20:E:113:ARG:NH1	2.28	0.64
1:R:109:LEU:HD21	17:A:52:LYS:HB2	1.79	0.64
9:Q:110:ASP:O	9:Q:114:GLN:HG2	1.97	0.64
2:2:1269:G:OP2	15:f:83:LYS:NZ	2.26	0.64
25:L:35:ARG:NH1	25:L:50:ALA:O	2.30	0.64
22:H:147:LYS:HA	29:W:49:GLU:HG2	1.78	0.64
2:2:1521:C:H5'	8:P:126:VAL:HB	1.79	0.64
24:J:71:LEU:O	24:J:75:ASN:ND2	2.32	0.63
2:2:1283:C:O2'	2:2:1286:G:O2'	2.15	0.63
2:2:1706:G:O2'	2:2:1850:A:O2'	2.14	0.63
2:2:640:A:H2'	2:2:641:A:C8	2.34	0.63
2:2:1629:C:OP1	10:S:39:ARG:NE	2.27	0.63
3:d:20:SER:OG	6:K:65:ARG:NH2	2.31	0.63
24:J:138:ARG:NH2	24:J:153:SER:OG	2.31	0.63
2:2:980:A:H2'	2:2:981:A:C8	2.33	0.63
18:B:107:ARG:NH1	27:O:133:THR:O	2.29	0.63
22:H:51:ILE:HG12	22:H:179:LYS:HD3	1.80	0.63
2:2:919:A:OP2	26:N:64:ARG:NH2	2.32	0.63
2:2:928:G:H2'	2:2:929:G:C8	2.33	0.63
18:B:143:THR:HB	18:B:205:TYR:CE2	2.34	0.62
15:f:119:ARG:HH22	15:f:148:TYR:HD2	1.45	0.62
2:2:1722:G:O6	2:2:1812:U:O2	2.18	0.62
11:T:108:GLU:OE2	11:T:121:ARG:NH1	2.31	0.62
2:2:380:G:P	23:I:56:ARG:HH22	2.22	0.62
10:S:16:LEU:HD21	10:S:99:LEU:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Q:58:LEU:HB3	9:Q:62:ARG:HD2	1.81	0.62
21:G:7:PHE:HB2	21:G:124:LEU:HD23	1.80	0.62
34:e:39:ASN:HA	34:e:43:VAL:HG22	1.81	0.62
2:2:1291:A:OP2	2:2:1302:G:O2'	2.17	0.62
2:2:145:G:H2'	2:2:146:G:C8	2.35	0.62
2:2:380:G:OP1	23:I:56:ARG:NH2	2.29	0.62
1:R:20:TYR:OH	4:D:211:VAL:O	2.16	0.61
2:2:1785:C:O2'	2:2:1786:U:O4'	2.19	0.61
2:2:165:G:OP2	2:2:165:G:N2	2.30	0.61
1:R:5:ARG:HB2	1:R:10:LYS:HE3	1.81	0.61
2:2:1228:A:H2'	2:2:1229:G:C8	2.35	0.61
4:D:67:ARG:NH1	6:K:93:THR:O	2.24	0.61
2:2:750:C:H2'	2:2:751:G:C8	2.36	0.61
2:2:1507:G:N2	15:f:88:PRO:O	2.34	0.61
2:2:1536:G:H2'	2:2:1537:A:C8	2.36	0.61
7:M:64:LEU:HA	15:f:108:VAL:HG21	1.83	0.61
16:g:73:SER:H	16:g:117:ASN:HD21	1.48	0.61
16:g:152:SER:OG	16:g:168:CYS:SG	2.57	0.61
2:2:590:A:O2'	2:2:593:C:N4	2.34	0.61
12:U:61:LEU:O	12:U:81:GLN:HA	2.01	0.61
4:D:108:LYS:HB3	4:D:113:LEU:HD12	1.83	0.61
8:P:41:GLN:NE2	8:P:113:GLY:O	2.34	0.61
20:E:129:ILE:HG12	20:E:139:LEU:HD23	1.82	0.61
2:2:1447:G:O2'	12:U:33:GLU:OE2	2.18	0.60
22:H:154:ILE:HB	22:H:185:VAL:HG22	1.83	0.60
17:A:77:ILE:HG12	17:A:99:ILE:HB	1.82	0.60
3:d:29:GLY:O	3:d:40:ARG:N	2.34	0.60
22:H:78:ARG:NE	22:H:82:GLU:OE2	2.34	0.60
2:2:107:A:H2'	2:2:108:G:C8	2.36	0.60
2:2:1289:U:H3	2:2:1310:U:H3	1.49	0.60
5:F:74:ASN:OD1	5:F:86:LYS:NZ	2.35	0.60
16:g:110:SER:HB2	16:g:153:CYS:HA	1.82	0.60
26:N:40:LEU:HB3	26:N:45:LEU:HD12	1.83	0.60
2:2:594:A:H61	2:2:643:A:H5''	1.67	0.60
9:Q:9:SER:HA	9:Q:25:CYS:O	2.02	0.60
21:G:85:ARG:O	21:G:87:ARG:NH1	2.35	0.60
2:2:536:A:H61	2:2:548:C:H42	1.49	0.60
19:C:200:ARG:O	24:J:54:ARG:NH2	2.34	0.60
22:H:47:ALA:HB3	22:H:63:PHE:HB2	1.84	0.60
2:2:70:G:O6	2:2:71:G:N2	2.35	0.59
2:2:818:A:OP1	24:J:80:ARG:NH2	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1464:C:O2'	2:2:1465:A:OP1	2.17	0.59
2:2:1757:G:O6	2:2:1775:U:O2	2.20	0.59
4:D:195:THR:HA	4:D:201:LYS:HE2	1.84	0.59
2:2:1284:A:C6	7:M:91:LEU:HD22	2.38	0.59
25:L:77:VAL:HG11	25:L:80:MET:HE3	1.84	0.59
2:2:69:C:H2'	2:2:70:G:C5	2.36	0.59
2:2:112:U:O2'	2:2:114:G:O2'	2.20	0.59
17:A:158:ASP:OD1	28:V:60:ARG:NH2	2.32	0.59
27:O:117:ARG:NH2	27:O:121:ARG:HH21	2.01	0.59
22:H:69:LEU:O	22:H:73:GLN:HG2	2.03	0.59
2:2:677:G:N1	2:2:1027:A:OP2	2.29	0.59
2:2:1259:A:N6	2:2:1519:U:OP1	2.35	0.59
2:2:1579:A:O2'	2:2:1581:C:OP2	2.20	0.59
15:f:108:VAL:HG22	15:f:114:ILE:HG22	1.84	0.59
2:2:913:A:H2	22:H:99:ARG:H	1.51	0.59
2:2:1588:A:H2'	2:2:1589:A:C8	2.37	0.59
2:2:1722:G:O6	2:2:1812:U:C2	2.56	0.59
4:D:57:ASN:O	4:D:65:ARG:NH1	2.36	0.59
2:2:75:G:H1	21:G:155:GLN:HG3	1.67	0.58
35:h:8:LYS:HE3	35:h:12:ARG:HH21	1.69	0.58
2:2:1276:A:H62	2:2:1321:G:H21	1.50	0.58
10:S:40:TYR:HA	10:S:83:PHE:HE2	1.69	0.58
2:2:1143:A:H5'	19:C:190:SER:HB2	1.86	0.58
2:2:686:U:O2	22:H:118:ARG:NH1	2.28	0.58
18:B:143:THR:HB	18:B:205:TYR:HE2	1.69	0.58
18:B:217:MET:HE2	18:B:220:LYS:HG2	1.85	0.58
27:O:78:ALA:HB3	27:O:118:ALA:HB3	1.84	0.58
2:2:607:U:OP1	36:1:171:ARG:NH2	2.35	0.58
2:2:1607:A:H61	2:2:1632:G:H1'	1.69	0.58
2:2:1599:U:H4'	2:2:1600:G:H5'	1.86	0.57
16:g:245:ARG:NH1	16:g:295:GLY:O	2.37	0.57
17:A:12:GLU:HA	17:A:15:VAL:HG12	1.86	0.57
15:f:126:CYS:HB3	15:f:143:LYS:HD2	1.85	0.57
7:M:36:ARG:NH2	15:f:105:TYR:OH	2.38	0.57
7:M:85:LEU:HA	7:M:88:TRP:HE3	1.68	0.57
2:2:1122:A:H4'	18:B:205:TYR:CD1	2.39	0.57
2:2:1217:A:H2'	2:2:1218:C:C6	2.39	0.57
2:2:1246:A:O2'	12:U:72:GLU:OE2	2.21	0.57
2:2:1438:A:O2'	2:2:1439:A:OP1	2.20	0.57
14:c:46:VAL:HG21	14:c:50:VAL:HG21	1.86	0.57
2:2:1473:G:N2	2:2:1476:A:OP2	2.27	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:111:PHE:HE2	17:A:10:MET:HE3	1.70	0.57
34:e:11:LYS:NZ	34:e:15:GLN:OE1	2.38	0.57
2:2:913:A:N6	22:H:119:SER:O	2.37	0.57
24:J:107:GLU:O	24:J:113:GLN:NE2	2.38	0.57
27:O:100:THR:HG21	27:O:104:ARG:HE	1.70	0.57
2:2:1281:G:H2'	2:2:1282:A:C8	2.39	0.56
2:2:1413:G:H2'	2:2:1414:A:H8	1.68	0.56
5:F:41:VAL:HG13	5:F:42:LYS:HG3	1.87	0.56
11:T:116:ASP:N	11:T:120:GLY:O	2.35	0.56
15:f:126:CYS:HB2	15:f:130:VAL:HG21	1.86	0.56
2:2:115:U:OP1	2:2:382:C:O2'	2.23	0.56
2:2:1644:C:H4'	9:Q:140:ARG:HB2	1.87	0.56
10:S:33:ILE:HD11	10:S:71:MET:HE1	1.87	0.56
18:B:25:PHE:HA	18:B:28:LYS:HG3	1.87	0.56
21:G:121:ILE:HB	21:G:124:LEU:HB2	1.87	0.56
2:2:75:G:H22	21:G:155:GLN:HA	1.70	0.56
2:2:143:U:H4'	2:2:144:U:H5'	1.86	0.56
2:2:1005:G:OP2	18:B:162:ARG:NH2	2.39	0.56
2:2:1797:U:H2'	2:2:1798:C:C6	2.41	0.56
27:O:75:MET:SD	27:O:79:GLN:NE2	2.77	0.56
31:Y:117:VAL:O	31:Y:122:LYS:NZ	2.37	0.56
22:H:119:SER:OG	22:H:120:ARG:NH1	2.38	0.56
8:P:24:GLN:O	8:P:28:MET:HG2	2.06	0.56
2:2:303:C:H5''	23:I:75:LYS:HD2	1.87	0.56
2:2:886:A:C2	2:2:887:U:H1'	2.41	0.56
6:K:91:PRO:HD2	6:K:94:LEU:HD12	1.86	0.56
16:g:165:ILE:HG12	16:g:177:TRP:HB2	1.88	0.56
27:O:145:GLY:O	32:a:22:ARG:NH2	2.38	0.56
33:b:34:ASP:OD1	33:b:43:ILE:HG22	2.06	0.56
18:B:122:GLU:HG2	18:B:140:VAL:HG23	1.87	0.56
4:D:164:VAL:O	4:D:168:VAL:HG22	2.06	0.56
21:G:121:ILE:HG22	21:G:123:GLY:H	1.70	0.56
2:2:142:C:OP2	21:G:188:LYS:NZ	2.39	0.55
2:2:798:G:O2'	22:H:105:THR:O	2.25	0.55
2:2:115:U:O2'	2:2:381:C:O2	2.21	0.55
2:2:750:C:O2'	2:2:751:G:OP1	2.23	0.55
2:2:1810:U:H2'	2:2:1811:C:C6	2.41	0.55
2:2:591:U:O2'	2:2:593:C:H5'	2.06	0.55
10:S:86:ARG:NH1	10:S:106:LYS:HG2	2.22	0.55
2:2:94:G:HO2'	2:2:508:A:HO2'	1.55	0.55
25:L:23:VAL:HG13	25:L:26:GLY:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:180:G:H2'	2:2:181:A:C8	2.41	0.55
2:2:1550:G:H3'	2:2:1579:A:H61	1.72	0.55
16:g:191:HIS:CD2	16:g:195:LEU:HD21	2.41	0.55
20:E:87:MET:HE1	20:E:236:ILE:HG21	1.89	0.55
2:2:1536:G:H2'	2:2:1537:A:H8	1.71	0.55
2:2:1798:C:H2'	2:2:1799:G:O4'	2.07	0.55
10:S:11:HIS:O	10:S:22:GLY:N	2.33	0.55
2:2:1614:A:OP2	8:P:42:ARG:NH1	2.40	0.54
13:Z:58:LEU:HD12	13:Z:62:VAL:HG21	1.88	0.54
2:2:291:G:H2'	2:2:292:A:C8	2.43	0.54
4:D:143:ARG:NH1	36:1:160:ASN:OD1	2.41	0.54
23:I:11:ARG:O	25:L:136:LYS:NZ	2.37	0.54
2:2:808:A:O2'	2:2:809:A:O5'	2.26	0.54
2:2:1310:U:OP2	7:M:36:ARG:NH2	2.41	0.54
2:2:1673:U:O2'	5:F:84:GLY:O	2.22	0.54
13:Z:47:LEU:HB2	13:Z:79:ILE:HG22	1.90	0.54
21:G:78:SER:OG	21:G:79:LYS:N	2.39	0.54
19:C:61:MET:HA	19:C:61:MET:HE2	1.89	0.54
21:G:5:ILE:HD12	21:G:16:ILE:HD12	1.89	0.54
10:S:16:LEU:HD23	10:S:33:ILE:HD12	1.90	0.54
16:g:212:LYS:HA	16:g:235:ILE:HG13	1.90	0.54
21:G:129:VAL:O	21:G:131:ARG:NH2	2.40	0.54
23:I:34:ALA:HB2	23:I:56:ARG:HD2	1.89	0.54
2:2:1464:C:HO2'	2:2:1465:A:P	2.31	0.54
16:g:242:SER:HB3	16:g:247:TRP:H	1.72	0.54
1:R:31:ASN:HA	1:R:34:VAL:HG12	1.91	0.53
1:R:83:ASN:HA	17:A:201:LEU:HD11	1.90	0.53
2:2:77:A:O2'	21:G:174:PRO:O	2.24	0.53
22:H:130:LEU:HD21	22:H:156:VAL:HG21	1.90	0.53
2:2:1138:C:OP1	17:A:155:ARG:NH2	2.30	0.53
2:2:1606:G:H5'	11:T:86:GLY:CA	2.38	0.53
10:S:30:ILE:O	10:S:33:ILE:HG12	2.08	0.53
2:2:570:C:O2'	31:Y:34:THR:O	2.21	0.53
21:G:159:ARG:NH2	21:G:171:THR:O	2.36	0.53
2:2:1714:U:H2'	2:2:1715:A:C8	2.43	0.53
7:M:127:TYR:O	7:M:131:LYS:NZ	2.42	0.53
17:A:132:GLN:NE2	17:A:136:GLU:OE1	2.42	0.53
1:R:98:VAL:HG13	1:R:102:THR:HB	1.91	0.53
6:K:24:LYS:HD3	6:K:26:ASP:HB2	1.89	0.53
31:Y:105:LYS:O	31:Y:109:GLU:HG3	2.08	0.53
8:P:64:LYS:NZ	8:P:90:VAL:O	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:36:VAL:HG21	10:S:71:MET:HE3	1.90	0.53
22:H:35:ASP:HB3	22:H:78:ARG:HH12	1.73	0.53
2:2:70:G:H1	2:2:80:G:N2	2.06	0.53
2:2:1007:C:H2'	2:2:1008:A:C8	2.44	0.53
2:2:1240:A:N3	2:2:1267:C:O2'	2.37	0.53
5:F:103:LEU:HD11	13:Z:67:LEU:HD22	1.90	0.53
29:W:3:ARG:NH1	29:W:29:PRO:HD3	2.24	0.53
8:P:111:MET:HE2	10:S:117:ILE:HG23	1.91	0.53
22:H:69:LEU:HD13	22:H:96:ALA:HB2	1.90	0.53
20:E:54:TYR:OH	20:E:97:GLU:OE1	2.22	0.53
23:I:11:ARG:NH1	23:I:15:GLY:O	2.42	0.53
2:2:72:C:N4	2:2:79:A:N7	2.57	0.52
5:F:34:SER:HA	14:c:55:VAL:HG13	1.91	0.52
16:g:72:SER:OG	16:g:74:ASP:O	2.26	0.52
16:g:87:LEU:HD21	16:g:120:ILE:HG21	1.90	0.52
18:B:129:THR:OG1	18:B:131:ASP:OD1	2.27	0.52
2:2:1292:C:N3	15:f:138:ARG:NH2	2.54	0.52
2:2:1607:A:N6	2:2:1632:G:H1'	2.24	0.52
2:2:1383:A:H4'	4:D:156:LEU:HD11	1.92	0.52
8:P:34:MET:HB3	8:P:42:ARG:HG3	1.91	0.52
16:g:17:TRP:CE2	16:g:303:THR:HG23	2.44	0.52
25:L:75:GLY:HA3	25:L:88:ILE:HD12	1.91	0.52
2:2:1431:G:O2'	2:2:1432:U:OP1	2.22	0.52
8:P:83:MET:HB3	8:P:116:LEU:HD12	1.91	0.52
16:g:226:HIS:NE2	16:g:228:TYR:O	2.41	0.52
19:C:183:LYS:HA	19:C:195:LEU:O	2.09	0.52
1:R:56:HIS:NE2	2:2:1465:A:OP2	2.35	0.52
2:2:816:A:OP2	24:J:10:ARG:NH2	2.35	0.52
2:2:1236:G:H21	2:2:1522:A:H62	1.57	0.52
8:P:22:LEU:HA	8:P:25:LEU:HB2	1.91	0.52
28:V:30:ALA:O	28:V:60:ARG:HD3	2.10	0.52
2:2:1010:G:H2'	2:2:1011:A:C8	2.45	0.52
12:U:24:LEU:HB3	12:U:32:LEU:HD11	1.92	0.52
24:J:32:ILE:HD13	34:e:34:ARG:HD3	1.91	0.52
2:2:562:U:H2'	2:2:563:G:C8	2.45	0.52
7:M:35:ILE:HD13	7:M:61:TYR:CZ	2.44	0.52
9:Q:31:LEU:HB3	9:Q:67:ASP:OD1	2.09	0.52
30:X:9:THR:HG22	30:X:13:LEU:HG	1.92	0.52
32:a:77:CYS:O	32:a:81:SER:OG	2.24	0.52
26:N:87:ASP:OD1	26:N:88:LEU:N	2.43	0.51
30:X:105:PHE:CE2	30:X:112:VAL:HB	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:115:U:H2'	2:2:116:U:C6	2.46	0.51
2:2:189:U:H2'	2:2:190:G:O4'	2.10	0.51
25:L:124:ASP:HB2	25:L:146:THR:O	2.10	0.51
8:P:81:ARG:HB3	8:P:117:GLY:HA3	1.91	0.51
10:S:4:VAL:HG12	10:S:6:PRO:HD3	1.91	0.51
16:g:156:PHE:HD1	16:g:165:ILE:HG22	1.75	0.51
2:2:1776:G:H5''	21:G:143:LYS:NZ	2.26	0.51
16:g:120:ILE:HB	16:g:132:TRP:HB2	1.92	0.51
20:E:182:MET:HB2	20:E:228:ILE:HD11	1.93	0.51
2:2:102:A:H5'	2:2:104:A:C4	2.45	0.51
2:2:1512:C:O2'	3:d:7:TYR:O	2.21	0.51
4:D:49:ILE:HD13	4:D:87:TYR:HB2	1.92	0.51
27:O:113:GLN:NE2	32:a:44:ILE:O	2.44	0.51
9:Q:53:GLU:OE1	9:Q:85:ARG:NH2	2.24	0.51
25:L:148:ALA:O	25:L:151:THR:OG1	2.29	0.51
2:2:798:G:H21	22:H:107:LYS:HG2	1.76	0.51
2:2:1779:G:H2'	2:2:1780:G:C8	2.46	0.51
2:2:1869:A:N6	18:B:114:VAL:O	2.43	0.51
22:H:100:ILE:HG12	22:H:125:VAL:HG21	1.93	0.51
2:2:1217:A:H2'	2:2:1218:C:H6	1.74	0.51
2:2:1569:A:O2'	2:2:1626:C:O2'	2.11	0.51
2:2:1729:U:H3	2:2:1805:G:H1	1.57	0.51
5:F:40:ALA:HB1	5:F:45:TYR:CG	2.45	0.51
27:O:95:ILE:HB	27:O:129:ILE:HG12	1.93	0.51
2:2:118:C:H1'	2:2:445:A:C5	2.46	0.51
2:2:1780:G:H2'	2:2:1781:A:C8	2.46	0.51
2:2:1781:A:H2'	2:2:1782:G:C8	2.46	0.51
5:F:34:SER:HA	14:c:55:VAL:CG1	2.40	0.51
15:f:119:ARG:HH21	15:f:139:HIS:HB2	1.76	0.51
33:b:45:THR:OG1	33:b:82:LYS:NZ	2.44	0.51
2:2:1142:G:N2	2:2:1145:A:OP2	2.32	0.51
2:2:1325:G:H1'	2:2:1510:G:H5''	1.93	0.50
8:P:61:ARG:O	8:P:65:LYS:HG2	2.11	0.50
10:S:24:ARG:HD2	10:S:29:ALA:HA	1.92	0.50
14:c:35:MET:HE2	14:c:55:VAL:HG21	1.92	0.50
2:2:532:C:H2'	2:2:533:A:C8	2.47	0.50
2:2:1809:A:H2'	2:2:1810:U:C6	2.45	0.50
7:M:85:LEU:O	7:M:89:VAL:HG22	2.11	0.50
17:A:137:ALA:HB1	17:A:142:LEU:HB2	1.92	0.50
35:h:14:LYS:HA	35:h:17:ARG:HG2	1.93	0.50
2:2:1286:G:N1	2:2:1312:G:N7	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1355:C:O2'	2:2:1356:G:O4'	2.28	0.50
4:D:162:ASP:N	4:D:163:PRO:HD2	2.26	0.50
8:P:75:VAL:HG12	8:P:93:MET:HG3	1.93	0.50
1:R:76:GLU:HG2	1:R:80:ARG:HE	1.77	0.50
2:2:590:A:HO2'	2:2:593:C:N4	2.09	0.50
16:g:156:PHE:CD1	16:g:165:ILE:HG22	2.47	0.50
2:2:1808:U:H2'	2:2:1809:A:C8	2.46	0.50
21:G:57:ASP:HA	21:G:106:LEU:HA	1.94	0.50
2:2:1098:C:H2'	2:2:1099:G:C8	2.47	0.50
2:2:1139:C:H5	2:2:1149:A:H62	1.59	0.50
24:J:93:LYS:HB2	24:J:96:TYR:CD1	2.47	0.50
2:2:1598:G:P	13:Z:80:ARG:HH21	2.35	0.50
22:H:41:ARG:NH1	22:H:42:GLU:OE2	2.45	0.50
2:2:895:G:H2'	2:2:896:U:C6	2.47	0.50
2:2:1342:U:H4'	2:2:1343:U:O5'	2.09	0.50
2:2:1629:C:O2'	10:S:83:PHE:O	2.25	0.50
5:F:102:LEU:HD22	13:Z:110:THR:HG21	1.94	0.50
2:2:1431:G:HO2'	2:2:1432:U:P	2.35	0.49
8:P:109:PRO:O	8:P:112:ILE:HG23	2.11	0.49
22:H:60:ILE:HD11	22:H:90:LYS:HE3	1.94	0.49
25:L:40:ILE:HG13	25:L:61:PRO:HB2	1.95	0.49
2:2:1679:A:OP1	14:c:20:ARG:NH2	2.37	0.49
3:d:6:LEU:HD12	3:d:6:LEU:O	2.12	0.49
5:F:120:GLY:O	5:F:146:ARG:NH1	2.44	0.49
18:B:105:LEU:HG	18:B:213:ARG:HA	1.94	0.49
20:E:139:LEU:HG	20:E:150:PRO:HG3	1.95	0.49
2:2:291:G:O2'	2:2:292:A:OP1	2.28	0.49
2:2:1025:U:OP1	2:2:1090:C:O2'	2.28	0.49
3:d:25:SER:O	3:d:25:SER:OG	2.28	0.49
23:I:101:ILE:HD12	23:I:190:LEU:HD11	1.92	0.49
2:2:75:G:N1	21:G:155:GLN:HG3	2.28	0.49
2:2:538:U:H2'	2:2:539:C:C6	2.48	0.49
10:S:34:LYS:HG2	10:S:103:LEU:HD23	1.94	0.49
16:g:130:LYS:HE2	16:g:141:THR:HG23	1.93	0.49
21:G:48:TYR:OH	21:G:119:LYS:O	2.22	0.49
2:2:988:C:H5'	18:B:116:LYS:HA	1.93	0.49
2:2:996:A:H2'	2:2:997:A:C8	2.47	0.49
2:2:1289:U:H2'	2:2:1290:G:C8	2.47	0.49
2:2:1776:G:H5''	21:G:143:LYS:HZ1	1.78	0.49
16:g:220:ASP:HB3	16:g:222:ASN:O	2.13	0.49
18:B:144:LYS:HB2	18:B:208:HIS:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:I:4:SER:HB3	23:I:24:LYS:HD3	1.95	0.49
25:L:35:ARG:NH2	25:L:55:TYR:O	2.45	0.49
2:2:1405:A:H2'	2:2:1406:G:O4'	2.12	0.49
2:2:1743:G:H21	2:2:1791:A:H62	1.59	0.49
2:2:677:G:P	26:N:124:ARG:HH21	2.35	0.49
2:2:1568:C:H2'	2:2:1569:A:C8	2.47	0.49
8:P:93:MET:SD	8:P:104:GLN:NE2	2.69	0.49
23:I:116:HIS:O	23:I:152:ARG:NH1	2.38	0.49
25:L:122:ILE:HG13	25:L:122:ILE:O	2.13	0.49
1:R:40:ILE:HB	4:D:209:SER:HB2	1.93	0.49
6:K:26:ASP:OD1	6:K:28:HIS:NE2	2.46	0.49
6:K:58:VAL:HG12	6:K:71:LEU:HA	1.94	0.49
15:f:133:ALA:N	15:f:140:TYR:O	2.40	0.49
30:X:123:VAL:HG12	30:X:124:LYS:HG3	1.94	0.49
2:2:17:C:O2'	2:2:1194:A:N1	2.38	0.49
2:2:587:A:H5'	2:2:592:C:H41	1.78	0.49
2:2:441:C:OP2	23:I:2:GLY:N	2.46	0.48
2:2:957:A:H3'	2:2:958:G:H21	1.78	0.48
2:2:1817:G:H2'	2:2:1818:A:C8	2.48	0.48
5:F:140:ASP:HB2	14:c:46:VAL:HG12	1.95	0.48
2:2:367:U:H4'	2:2:371:A:C8	2.48	0.48
2:2:980:A:H2'	2:2:981:A:H8	1.77	0.48
9:Q:97:GLN:HB2	9:Q:102:GLU:OE2	2.14	0.48
21:G:98:ARG:HG2	21:G:99:GLY:N	2.28	0.48
30:X:67:ARG:HG3	30:X:115:ILE:HG12	1.94	0.48
2:2:332:G:O2'	2:2:333:G:OP1	2.25	0.48
2:2:1304:U:H2'	2:2:1305:C:H6	1.78	0.48
2:2:1585:U:O2'	2:2:1586:U:O5'	2.30	0.48
4:D:133:GLY:HA3	4:D:156:LEU:O	2.13	0.48
2:2:748:C:N4	2:2:794:A:H61	2.11	0.48
5:F:40:ALA:HB1	5:F:45:TYR:CD1	2.49	0.48
17:A:5:LEU:HD21	28:V:41:LYS:HA	1.95	0.48
17:A:184:ARG:HE	17:A:191:ARG:HG2	1.79	0.48
17:A:188:THR:O	17:A:189:ILE:HD13	2.13	0.48
22:H:135:PHE:CG	22:H:136:PRO:HA	2.49	0.48
2:2:1341:C:H4'	2:2:1342:U:H5'	1.95	0.48
2:2:1597:C:H4'	2:2:1603:G:O6	2.13	0.48
2:2:1786:U:H2'	2:2:1787:G:H8	1.78	0.48
10:S:3:LEU:HD21	13:Z:55:TYR:HE1	1.77	0.48
14:c:62:GLU:HG2	27:O:121:ARG:HH22	1.78	0.48
2:2:29:G:H2'	2:2:30:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1228:A:H2'	2:2:1229:G:H8	1.78	0.48
2:2:1567:G:H2'	2:2:1568:C:O4'	2.13	0.48
2:2:822:U:H2'	2:2:824:C:OP2	2.13	0.48
2:2:1330:G:H4'	2:2:1331:C:O5'	2.12	0.48
2:2:1643:U:H2'	2:2:1644:C:C6	2.49	0.48
21:G:209:TYR:O	21:G:213:LEU:N	2.46	0.48
2:2:329:G:H2'	2:2:330:G:H8	1.78	0.48
2:2:1189:A:H2'	2:2:1190:A:C8	2.49	0.48
3:d:38:MET:HE1	3:d:46:TYR:HB2	1.95	0.48
8:P:130:ARG:HE	8:P:131:PRO:HD2	1.79	0.48
21:G:224:ARG:O	21:G:228:ILE:HG12	2.13	0.48
1:R:5:ARG:NH2	2:2:1455:A:OP1	2.47	0.48
8:P:100:LYS:HG2	8:P:101:THR:HG23	1.96	0.48
2:2:656:G:H5'	2:2:662:G:N2	2.28	0.48
8:P:87:PRO:HA	8:P:90:VAL:HG23	1.95	0.48
24:J:18:ARG:O	24:J:24:ARG:NH1	2.45	0.48
25:L:80:MET:HE1	25:L:120:VAL:HG22	1.95	0.48
2:2:472:C:O2'	2:2:474:G:OP1	2.26	0.47
2:2:1374:C:H2'	2:2:1375:G:O4'	2.14	0.47
4:D:132:LYS:HE3	4:D:189:MET:HE2	1.96	0.47
21:G:7:PHE:CE2	21:G:9:ALA:HB3	2.48	0.47
2:2:900:C:H2'	2:2:901:G:H8	1.79	0.47
2:2:1398:G:H22	2:2:1448:A:H2	1.62	0.47
15:f:100:LEU:HB3	15:f:103:LEU:HG	1.95	0.47
16:g:91:ASP:OD2	16:g:93:THR:OG1	2.30	0.47
18:B:30:TRP:CD2	27:O:19:PRO:HG3	2.48	0.47
30:X:59:ALA:HB1	30:X:114:ASP:HB3	1.95	0.47
36:1:157:PHE:HE2	36:1:170:THR:HG22	1.79	0.47
1:R:20:TYR:CE2	1:R:38:ILE:HG21	2.49	0.47
2:2:816:A:P	24:J:10:ARG:HH22	2.37	0.47
2:2:1538:C:O2	11:T:48:TYR:OH	2.23	0.47
2:2:1598:G:OP1	13:Z:80:ARG:NH2	2.47	0.47
8:P:43:ARG:O	8:P:47:ARG:HG3	2.13	0.47
11:T:108:GLU:N	11:T:108:GLU:OE1	2.47	0.47
5:F:73:THR:O	5:F:89:THR:HG21	2.15	0.47
2:2:1866:A:N6	32:a:84:VAL:HG13	2.30	0.47
16:g:85:GLY:O	16:g:86:THR:OG1	2.27	0.47
2:2:180:G:O2'	2:2:181:A:OP1	2.27	0.47
2:2:1305:C:OP2	15:f:93:HIS:ND1	2.45	0.47
10:S:18:THR:HB	10:S:33:ILE:HG22	1.97	0.47
14:c:16:LYS:NZ	14:c:31:ARG:HE	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:107:A:H2'	2:2:108:G:H8	1.80	0.47
2:2:630:U:O4	36:1:165:HIS:HA	2.14	0.47
2:2:808:A:H5''	20:E:219:ALA:O	2.14	0.47
2:2:932:G:O2'	2:2:934:G:OP2	2.23	0.47
2:2:1256:G:O6	12:U:65:THR:HG23	2.15	0.47
16:g:107:ASP:HB2	16:g:125:ARG:HH11	1.78	0.47
17:A:10:MET:HB2	17:A:55:TRP:CD2	2.49	0.47
2:2:441:C:H2'	2:2:442:C:C6	2.50	0.47
36:1:166:SER:HA	36:1:169:VAL:HG22	1.97	0.47
2:2:1310:U:H5'	15:f:130:VAL:HG22	1.97	0.47
2:2:1545:A:N3	2:2:1671:G:O2'	2.36	0.47
2:2:1736:G:H2'	2:2:1737:G:C8	2.50	0.47
2:2:1779:G:H2'	2:2:1780:G:H8	1.79	0.47
4:D:42:THR:HB	4:D:45:ARG:O	2.15	0.47
16:g:240:CYS:SG	16:g:291:TRP:HD1	2.38	0.47
23:I:36:THR:HG21	23:I:60:LEU:HD12	1.97	0.47
1:R:20:TYR:O	1:R:24:LEU:HD23	2.15	0.47
2:2:533:A:H8	2:2:533:A:O5'	1.98	0.47
2:2:57:U:OP1	2:2:504:G:O2'	2.31	0.46
2:2:860:G:N2	29:W:107:SER:OG	2.42	0.46
2:2:1726:G:H2'	2:2:1727:G:H8	1.78	0.46
16:g:251:ALA:HB1	16:g:286:CYS:HB3	1.96	0.46
2:2:1772:C:H2'	2:2:1773:C:C6	2.51	0.46
2:2:370:G:O2'	23:I:10:LYS:NZ	2.48	0.46
2:2:685:A:H62	2:2:917:U:H3	1.62	0.46
9:Q:16:LYS:HG2	9:Q:17:LYS:H	1.79	0.46
25:L:104:LYS:NZ	30:X:8:ARG:HD3	2.31	0.46
1:R:50:ILE:O	1:R:54:VAL:HG23	2.14	0.46
2:2:533:A:H3'	2:2:534:G:H5''	1.97	0.46
2:2:639:C:HO2'	2:2:640:A:H8	1.61	0.46
2:2:1594:A:OP2	13:Z:104:ARG:HG3	2.16	0.46
3:d:10:HIS:HB3	3:d:12:ARG:NH1	2.30	0.46
6:K:15:LEU:HD13	6:K:21:MET:HB2	1.97	0.46
22:H:134:VAL:HG11	22:H:158:LEU:HD22	1.97	0.46
26:N:33:VAL:HG21	26:N:66:VAL:HG11	1.97	0.46
27:O:34:PHE:HB3	27:O:41:PHE:HB2	1.97	0.46
29:W:36:ARG:NH2	29:W:110:ILE:O	2.48	0.46
11:T:105:GLN:C	11:T:107:LEU:H	2.23	0.46
18:B:120:MET:HE2	18:B:142:PHE:HE2	1.79	0.46
20:E:95:THR:OG1	20:E:97:GLU:HG3	2.14	0.46
20:E:100:ARG:NH1	20:E:118:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:I:121:LEU:HD21	23:I:166:PHE:CG	2.51	0.46
13:Z:42:ASP:OD1	13:Z:42:ASP:N	2.49	0.46
23:I:82:VAL:HG12	23:I:83:TYR:N	2.22	0.46
2:2:434:G:OP1	23:I:23:LYS:HG2	2.15	0.46
2:2:1137:U:O2'	2:2:1138:C:OP1	2.22	0.46
2:2:804:U:H2'	2:2:805:U:C6	2.51	0.46
8:P:121:ILE:HG22	8:P:123:TYR:H	1.81	0.46
16:g:163:PRO:HB3	16:g:179:LEU:HD12	1.97	0.46
16:g:230:LEU:HD23	16:g:259:TRP:CG	2.51	0.46
2:2:674:C:H2'	2:2:675:U:C6	2.51	0.46
2:2:1101:U:H2'	2:2:1102:G:C8	2.50	0.46
2:2:1354:G:O2'	2:2:1356:G:N1	2.47	0.46
25:L:20:LYS:HD3	25:L:22:ARG:NH2	2.31	0.46
2:2:886:A:N3	2:2:887:U:H1'	2.30	0.46
2:2:1440:C:H4'	2:2:1441:U:OP1	2.16	0.46
2:2:1597:C:H4'	2:2:1603:G:C6	2.51	0.46
18:B:23:ASP:O	18:B:26:SER:OG	2.32	0.46
30:X:52:LEU:HD11	30:X:73:GLN:HB2	1.97	0.46
2:2:924:G:H21	26:N:87:ASP:HB3	1.82	0.45
2:2:1273:C:O2'	2:2:1506:A:N1	2.42	0.45
2:2:1776:G:H2'	2:2:1777:G:C8	2.51	0.45
4:D:178:ARG:HG3	4:D:179:GLN:HG2	1.97	0.45
20:E:43:PRO:HD2	20:E:46:ILE:HD12	1.98	0.45
31:Y:86:GLU:OE2	31:Y:90:ARG:HD2	2.16	0.45
2:2:495:U:O2'	20:E:27:PHE:O	2.34	0.45
2:2:1438:A:HO2'	2:2:1439:A:P	2.39	0.45
2:2:1589:A:N3	2:2:1653:U:O2'	2.42	0.45
2:2:1606:G:H22	2:2:1632:G:H2'	1.82	0.45
2:2:1651:A:O2'	5:F:83:ASN:OD1	2.23	0.45
10:S:23:ARG:HB2	13:Z:48:VAL:HG21	1.96	0.45
17:A:30:LEU:HD21	17:A:35:GLU:HG2	1.99	0.45
2:2:891:G:N3	2:2:891:G:H2'	2.32	0.45
2:2:1749:G:H2'	2:2:1750:C:C6	2.51	0.45
11:T:73:GLY:O	11:T:94:ARG:NH2	2.50	0.45
11:T:144:LYS:HE2	11:T:145:HIS:CE1	2.51	0.45
21:G:2:LYS:HD2	21:G:15:LEU:HD21	1.98	0.45
36:1:171:ARG:NH2	36:1:172:GLU:OE2	2.47	0.45
1:R:19:LYS:HB2	1:R:19:LYS:HE3	1.72	0.45
2:2:502:C:H5'	20:E:66:MET:HE2	1.97	0.45
2:2:1534:C:H5'	2:2:1536:G:O4'	2.15	0.45
16:g:26:GLN:NE2	16:g:73:SER:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:g:220:ASP:OD2	16:g:227:LEU:HB2	2.17	0.45
17:A:103:PHE:CG	17:A:133:PRO:HG3	2.51	0.45
19:C:142:LYS:HB3	19:C:154:ALA:HB2	1.98	0.45
19:C:166:ARG:HB3	19:C:247:THR:HB	1.98	0.45
19:C:194:ARG:HD3	19:C:196:ILE:HD11	1.99	0.45
2:2:396:U:OP2	25:L:79:LYS:NZ	2.33	0.45
2:2:811:A:H2'	2:2:812:A:C8	2.51	0.45
11:T:144:LYS:HE2	11:T:145:HIS:HE1	1.81	0.45
30:X:94:ILE:HG12	30:X:125:VAL:HG21	1.99	0.45
2:2:508:A:H3'	2:2:509:G:H8	1.81	0.45
2:2:874:G:H2'	2:2:875:A:H8	1.81	0.45
2:2:1265:A:O2'	2:2:1327:G:OP2	2.32	0.45
13:Z:48:VAL:HG22	13:Z:80:ARG:HG3	1.98	0.45
18:B:127:VAL:HG21	18:B:173:THR:HA	1.98	0.45
1:R:85:VAL:HG12	17:A:200:ASP:HB2	1.98	0.45
2:2:1606:G:H5'	11:T:86:GLY:C	2.41	0.45
17:A:52:LYS:O	17:A:56:GLU:HG2	2.17	0.45
21:G:121:ILE:HD12	21:G:124:LEU:HD22	1.98	0.45
31:Y:114:MET:O	31:Y:122:LYS:NZ	2.48	0.45
21:G:121:ILE:HG21	21:G:124:LEU:HD13	1.99	0.45
2:2:511:U:H2'	2:2:512:A:C8	2.51	0.45
2:2:639:C:O2'	2:2:640:A:H8	2.00	0.45
7:M:79:VAL:HG21	7:M:85:LEU:HD21	1.98	0.45
16:g:153:CYS:SG	16:g:198:VAL:HG12	2.56	0.45
16:g:251:ALA:HB2	16:g:289:LEU:HD11	1.98	0.45
19:C:101:SER:HB3	19:C:132:ASP:HB2	1.99	0.45
22:H:29:GLU:O	22:H:33:ASN:ND2	2.41	0.45
2:2:465:A:H4'	2:2:466:G:O5'	2.16	0.45
2:2:750:C:H2'	2:2:751:G:H8	1.79	0.45
2:2:919:A:OP2	2:2:919:A:H8	2.00	0.45
2:2:975:G:OP1	27:O:98:ARG:NH1	2.49	0.45
2:2:1542:C:O2'	9:Q:43:GLU:OE1	2.28	0.45
9:Q:34:VAL:HG13	9:Q:70:VAL:HB	1.99	0.45
11:T:123:LEU:H	11:T:123:LEU:HD23	1.81	0.45
20:E:133:THR:HG22	20:E:134:LYS:HG3	1.98	0.45
23:I:22:HIS:ND1	23:I:23:LYS:O	2.47	0.45
33:b:36:LYS:HD2	33:b:37:CYS:N	2.31	0.45
2:2:382:C:H2'	2:2:383:G:H8	1.82	0.44
2:2:559:G:O2'	2:2:560:A:H8	1.99	0.44
2:2:1223:A:H2'	2:2:1224:G:O4'	2.17	0.44
16:g:195:LEU:HD23	16:g:211:GLY:HA3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:344:U:H2'	2:2:345:U:C6	2.51	0.44
2:2:380:G:OP1	23:I:31:ARG:HD2	2.17	0.44
17:A:84:GLN:HG2	17:A:100:ALA:HB1	1.99	0.44
23:I:103:LEU:HD13	23:I:170:LYS:HD3	1.98	0.44
32:a:24:THR:HG21	32:a:71:LEU:HD22	1.99	0.44
2:2:1164:G:O2'	2:2:1165:G:H5'	2.17	0.44
4:D:136:VAL:HG22	4:D:186:VAL:HG22	1.99	0.44
6:K:90:VAL:HG22	6:K:94:LEU:HB2	2.00	0.44
22:H:162:GLN:O	22:H:166:VAL:HG22	2.17	0.44
1:R:2:GLY:N	2:2:1369:A:OP1	2.51	0.44
2:2:70:G:O5'	2:2:70:G:H8	2.01	0.44
2:2:1088:U:H4'	2:2:1089:G:OP2	2.17	0.44
2:2:1521:C:O2'	10:S:136:THR:O	2.32	0.44
2:2:1653:U:H2'	2:2:1654:G:C8	2.53	0.44
5:F:74:ASN:HA	5:F:77:MET:HE2	2.00	0.44
16:g:73:SER:OG	16:g:117:ASN:OD1	2.25	0.44
22:H:160:LYS:HA	22:H:163:GLN:HB2	1.98	0.44
1:R:75:GLU:N	1:R:78:ARG:HH21	2.16	0.44
2:2:799:U:H2'	2:2:800:U:C6	2.52	0.44
16:g:110:SER:CB	16:g:153:CYS:HA	2.46	0.44
21:G:67:VAL:HB	21:G:99:GLY:HA2	1.99	0.44
22:H:139:ILE:HG23	22:H:156:VAL:HG13	1.99	0.44
25:L:11:GLN:HB3	25:L:56:ILE:HG21	1.99	0.44
2:2:929:G:H2'	2:2:930:C:O4'	2.17	0.44
2:2:952:G:H2'	2:2:953:C:C6	2.52	0.44
2:2:1354:G:N2	2:2:1356:G:C8	2.80	0.44
2:2:1686:G:H2'	2:2:1687:C:C6	2.52	0.44
2:2:1854:U:OP1	27:O:150:ARG:NH1	2.51	0.44
22:H:126:HIS:CE1	22:H:181:THR:HG23	2.53	0.44
25:L:76:VAL:HG22	25:L:125:ILE:HD13	1.99	0.44
2:2:1713:C:H2'	2:2:1714:U:C6	2.52	0.44
11:T:60:THR:HG23	11:T:75:MET:HE3	1.99	0.44
27:O:61:LYS:NZ	27:O:80:ASP:OD2	2.47	0.44
27:O:117:ARG:HD2	32:a:49:ALA:HB2	2.00	0.44
4:D:105:LEU:HD12	4:D:122:VAL:HG21	2.00	0.44
6:K:11:ILE:HG12	6:K:45:VAL:HG22	1.98	0.44
6:K:20:VAL:HG12	6:K:70:TYR:CD1	2.52	0.44
20:E:88:ASP:OD1	20:E:122:LYS:NZ	2.51	0.44
24:J:45:ARG:O	24:J:49:THR:HG23	2.18	0.44
26:N:91:LEU:HD12	26:N:125:LEU:HD12	1.98	0.44
2:2:1139:C:H2'	2:2:1140:G:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:33:ARG:H	7:M:33:ARG:HG2	1.55	0.44
20:E:173:ILE:HD11	20:E:235:TRP:CE2	2.53	0.44
22:H:9:VAL:HG12	22:H:11:PRO:HD3	2.00	0.44
36:1:174:MET:HE2	36:1:177:LEU:HD12	2.00	0.44
16:g:9:GLY:O	16:g:309:VAL:HG12	2.18	0.43
23:I:64:ASN:O	23:I:186:ASP:HA	2.18	0.43
23:I:67:TRP:HA	23:I:189:VAL:HG12	2.00	0.43
25:L:2:ALA:HB3	25:L:5:GLN:HB2	2.00	0.43
2:2:532:C:H2'	2:2:533:A:N7	2.32	0.43
19:C:70:VAL:HG21	19:C:93:ILE:HG23	2.00	0.43
19:C:183:LYS:HG2	19:C:196:ILE:HA	2.01	0.43
2:2:558:G:H2'	2:2:559:G:C8	2.53	0.43
2:2:1636:G:O2'	5:F:164:ARG:NH1	2.51	0.43
12:U:20:ILE:HG13	12:U:98:VAL:HG21	2.00	0.43
16:g:101:PHE:CD1	16:g:136:GLY:HA2	2.53	0.43
2:2:16:G:H2'	2:2:17:C:C6	2.53	0.43
2:2:1019:C:H2'	2:2:1020:A:O4'	2.18	0.43
2:2:1227:G:C2	2:2:1228:A:C8	3.07	0.43
12:U:26:SER:OG	12:U:27:ARG:N	2.52	0.43
16:g:114:SER:HA	16:g:156:PHE:CD2	2.53	0.43
1:R:3:ARG:CD	2:2:1454:A:H5''	2.48	0.43
2:2:1364:U:H2'	2:2:1365:G:H5'	2.00	0.43
2:2:1401:A:H2'	2:2:1402:A:C8	2.53	0.43
2:2:1412:C:C4	2:2:1413:G:N7	2.87	0.43
8:P:16:THR:HA	8:P:21:ASP:HA	2.00	0.43
23:I:6:ASP:OD1	23:I:9:HIS:ND1	2.52	0.43
2:2:329:G:H2'	2:2:330:G:C8	2.54	0.43
2:2:582:U:H1'	31:Y:33:ALA:HB2	2.00	0.43
2:2:1304:U:H2'	2:2:1305:C:C6	2.54	0.43
2:2:1679:A:H5''	2:2:1680:G:O5'	2.19	0.43
16:g:256:ILE:HB	16:g:270:LEU:HB2	2.00	0.43
24:J:26:ASP:O	24:J:30:LYS:HG3	2.18	0.43
1:R:42:PRO:HG2	1:R:46:LEU:HD23	2.01	0.43
1:R:58:MET:HE3	1:R:58:MET:HB3	1.84	0.43
1:R:111:PHE:CE1	17:A:12:GLU:HG2	2.53	0.43
2:2:194:C:H2'	2:2:195:C:C6	2.53	0.43
2:2:1407:U:H2'	2:2:1408:U:C6	2.54	0.43
2:2:1545:A:H2'	2:2:1546:G:C8	2.53	0.43
2:2:1667:U:H2'	2:2:1668:U:C6	2.54	0.43
4:D:69:LEU:HA	4:D:72:VAL:HG12	1.99	0.43
2:2:687:C:H4'	22:H:121:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:793:G:O2'	2:2:794:A:OP1	2.29	0.43
2:2:866:U:H2'	2:2:867:G:C8	2.54	0.43
2:2:1010:G:H2'	2:2:1011:A:H8	1.82	0.43
2:2:1535:U:O2	5:F:88:MET:HE3	2.19	0.43
2:2:1867:U:C5	32:a:98:PRO:HG2	2.54	0.43
7:M:84:LYS:HA	7:M:84:LYS:HD3	1.88	0.43
16:g:8:ARG:HB3	16:g:309:VAL:HG13	2.00	0.43
2:2:563:G:N7	24:J:172:ARG:NH2	2.55	0.43
2:2:813:A:OP1	20:E:16:LYS:NZ	2.32	0.43
2:2:944:A:H5''	27:O:134:PRO:HB3	2.01	0.43
2:2:1144:A:H2'	2:2:1145:A:C8	2.52	0.43
2:2:1395:C:O2'	2:2:1396:A:H5'	2.18	0.43
16:g:230:LEU:HD23	16:g:259:TRP:CD2	2.53	0.43
20:E:151:ASP:HB3	21:G:216:ARG:HH12	1.83	0.43
22:H:146:VAL:HG12	29:W:42:MET:HE1	1.99	0.43
23:I:84:ASN:HB3	23:I:87:ASN:O	2.18	0.43
25:L:55:TYR:OH	25:L:116:CYS:HB3	2.19	0.43
30:X:46:HIS:CD2	30:X:103:ALA:HB2	2.54	0.43
31:Y:57:VAL:HB	31:Y:60:PHE:HE2	1.83	0.43
2:2:811:A:O2'	2:2:812:A:OP1	2.37	0.43
2:2:1413:G:H2'	2:2:1414:A:C8	2.50	0.43
2:2:1636:G:H1'	5:F:164:ARG:HH12	1.84	0.43
2:2:1652:G:H1	2:2:1672:U:H3	1.67	0.43
3:d:25:SER:HA	6:K:65:ARG:HH21	1.84	0.43
11:T:39:LEU:HD13	11:T:47:PRO:HG3	2.00	0.43
2:2:158:A:H2'	2:2:159:A:O4'	2.19	0.42
2:2:1025:U:H2'	2:2:1026:C:O4'	2.19	0.42
2:2:1566:G:H4'	2:2:1566:G:OP1	2.19	0.42
2:2:1588:A:N3	2:2:1654:G:O2'	2.44	0.42
2:2:1713:C:H2'	2:2:1714:U:H6	1.84	0.42
32:a:98:PRO:HA	32:a:99:PRO:HD3	1.89	0.42
36:1:166:SER:O	36:1:170:THR:HG23	2.19	0.42
2:2:1539:U:OP1	11:T:44:GLU:N	2.52	0.42
2:2:1757:G:O6	2:2:1775:U:C2	2.72	0.42
5:F:179:ASN:ND2	5:F:186:ASN:O	2.38	0.42
7:M:92:CYS:HA	7:M:102:LYS:O	2.19	0.42
11:T:113:VAL:HG13	11:T:122:LYS:O	2.19	0.42
17:A:77:ILE:HD12	17:A:122:LEU:HD11	2.01	0.42
2:2:12:U:H2'	2:2:13:C:C6	2.55	0.42
2:2:554:A:H2'	2:2:556:U:C6	2.55	0.42
2:2:563:G:HO2'	2:2:564:A:H8	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1446:A:O2'	2:2:1447:G:H8	2.02	0.42
2:2:1491:G:H2'	2:2:1492:U:C6	2.54	0.42
4:D:38:GLU:OE2	4:D:40:ARG:NE	2.52	0.42
5:F:74:ASN:O	5:F:77:MET:HG2	2.19	0.42
22:H:145:ARG:HD3	29:W:50:PHE:O	2.20	0.42
2:2:293:C:O2	2:2:293:C:H2'	2.19	0.42
2:2:808:A:O2'	2:2:809:A:C8	2.67	0.42
2:2:986:G:C8	27:O:137:SER:O	2.73	0.42
2:2:1365:G:H2'	2:2:1366:G:C8	2.55	0.42
2:2:1533:A:H2	2:2:1536:G:N3	2.17	0.42
2:2:1566:G:O6	11:T:97:LYS:HB2	2.19	0.42
5:F:86:LYS:O	5:F:90:VAL:HG23	2.19	0.42
16:g:71:ILE:HG22	16:g:72:SER:O	2.19	0.42
17:A:5:LEU:O	17:A:9:GLN:HG2	2.19	0.42
17:A:10:MET:HB2	17:A:55:TRP:CE2	2.54	0.42
26:N:86:GLU:OE1	26:N:86:GLU:N	2.52	0.42
2:2:900:C:H2'	2:2:901:G:C8	2.55	0.42
2:2:1736:G:H2'	2:2:1737:G:H8	1.83	0.42
4:D:72:VAL:HG22	6:K:68:TYR:HD2	1.85	0.42
10:S:25:LYS:O	10:S:29:ALA:N	2.51	0.42
20:E:62:LYS:O	20:E:66:MET:HG2	2.19	0.42
23:I:82:VAL:CG1	23:I:83:TYR:H	2.23	0.42
29:W:47:ILE:O	29:W:66:THR:HG23	2.19	0.42
32:a:22:ARG:HA	32:a:22:ARG:HD2	1.83	0.42
32:a:64:LEU:HA	32:a:65:PRO:HD3	1.91	0.42
2:2:903:A:H2'	2:2:904:A:C8	2.54	0.42
18:B:139:CYS:SG	18:B:168:MET:HE2	2.58	0.42
19:C:196:ILE:HB	19:C:223:TYR:HB2	2.02	0.42
27:O:19:PRO:HB2	27:O:21:VAL:HG23	2.02	0.42
2:2:1130:G:OP2	2:2:1130:G:N2	2.38	0.42
3:d:10:HIS:HB3	3:d:12:ARG:HH11	1.83	0.42
4:D:201:LYS:HB2	4:D:201:LYS:HE3	1.73	0.42
7:M:49:LEU:HD21	7:M:128:PHE:CZ	2.55	0.42
10:S:66:ARG:HG2	10:S:70:ILE:CD1	2.50	0.42
12:U:26:SER:HB3	12:U:32:LEU:HB2	2.01	0.42
2:2:1472:C:H2'	2:2:1473:G:O4'	2.19	0.42
11:T:53:PHE:CE1	11:T:103:VAL:HG12	2.54	0.42
18:B:110:MET:O	18:B:114:VAL:HG23	2.19	0.42
2:2:893:U:N3	2:2:894:G:N7	2.68	0.42
8:P:53:GLN:HG3	8:P:83:MET:SD	2.60	0.42
16:g:8:ARG:HG2	16:g:52:TYR:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:g:218:LEU:HB2	16:g:228:TYR:HB2	2.00	0.42
19:C:104:ASP:OD1	19:C:104:ASP:N	2.52	0.42
2:2:1408:U:H2'	2:2:1409:A:C8	2.55	0.42
2:2:1520:G:O2'	2:2:1521:C:OP1	2.32	0.42
2:2:1776:G:H2'	2:2:1777:G:H8	1.84	0.42
19:C:85:SER:OG	28:V:25:GLY:O	2.28	0.42
21:G:14:LYS:NZ	21:G:123:GLY:HA3	2.34	0.42
26:N:136:PRO:HB2	26:N:138:ASN:OD1	2.20	0.42
31:Y:55:ILE:HG12	31:Y:75:ILE:HG12	2.01	0.42
2:2:65:C:C4	21:G:133:LEU:HB3	2.55	0.41
2:2:72:C:O2'	2:2:73:C:H5'	2.20	0.41
2:2:1798:C:O2'	23:I:2:GLY:HA2	2.20	0.41
4:D:31:GLU:O	4:D:54:ARG:NH2	2.53	0.41
16:g:227:LEU:HD23	16:g:228:TYR:CD1	2.55	0.41
21:G:2:LYS:O	21:G:108:VAL:HA	2.20	0.41
22:H:61:ILE:HD11	22:H:176:VAL:HG13	2.02	0.41
33:b:82:LYS:O	33:b:83:GLN:HG3	2.20	0.41
1:R:20:TYR:CZ	1:R:38:ILE:HG21	2.55	0.41
2:2:224:A:H2'	2:2:225:G:C8	2.55	0.41
2:2:750:C:HO2'	2:2:751:G:P	2.40	0.41
2:2:1203:G:H2'	2:2:1204:A:C8	2.54	0.41
2:2:1773:C:H2'	2:2:1774:C:C6	2.55	0.41
1:R:6:THR:HG22	1:R:7:LYS:N	2.35	0.41
2:2:481:C:H2'	2:2:482:G:O4'	2.20	0.41
2:2:1440:C:O2'	2:2:1441:U:O5'	2.28	0.41
4:D:26:THR:O	4:D:30:ALA:HB2	2.20	0.41
4:D:64:ARG:HD2	6:K:94:LEU:HD21	2.02	0.41
20:E:199:GLU:HG2	20:E:207:VAL:HB	2.02	0.41
2:2:291:G:HO2'	2:2:292:A:P	2.43	0.41
2:2:1031:A:H4'	26:N:112:LYS:NZ	2.35	0.41
2:2:1610:G:O2'	10:S:86:ARG:NH2	2.53	0.41
2:2:1733:U:H2'	2:2:1734:G:O4'	2.21	0.41
16:g:112:ALA:HB3	16:g:121:VAL:CG1	2.50	0.41
17:A:90:PHE:CD2	17:A:179:ALA:HB2	2.56	0.41
2:2:394:G:H5'	25:L:81:LYS:HB3	2.03	0.41
2:2:1243:U:H4'	15:f:78:LYS:HE3	2.02	0.41
5:F:122:ARG:HE	5:F:122:ARG:HB2	1.75	0.41
9:Q:62:ARG:HD3	9:Q:108:ILE:HD11	2.01	0.41
12:U:94:PRO:HG2	12:U:97:ILE:HG13	2.01	0.41
16:g:80:SER:O	16:g:87:LEU:HD12	2.21	0.41
16:g:212:LYS:HG3	16:g:235:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:C:200:ARG:HA	19:C:221:ASP:OD1	2.20	0.41
22:H:145:ARG:HE	29:W:51:GLU:HB2	1.86	0.41
30:X:9:THR:HG22	30:X:9:THR:O	2.20	0.41
30:X:66:ILE:HD13	34:e:4:GLY:HA3	2.02	0.41
2:2:51:U:H2'	2:2:52:G:C8	2.56	0.41
2:2:1648:G:H3'	9:Q:126:ARG:O	2.21	0.41
18:B:133:TYR:HD2	18:B:217:MET:HE3	1.85	0.41
10:S:13:LEU:HD23	10:S:20:ILE:O	2.21	0.41
12:U:36:CYS:SG	12:U:89:ILE:HD11	2.60	0.41
13:Z:49:LEU:HD23	13:Z:49:LEU:HA	1.79	0.41
2:2:344:U:H2'	2:2:345:U:H6	1.86	0.41
2:2:1347:U:H2'	2:2:1348:G:N3	2.35	0.41
2:2:1406:G:H2'	2:2:1407:U:C6	2.56	0.41
12:U:46:LYS:HE2	12:U:97:ILE:HG23	2.02	0.41
16:g:67:SER:HB3	16:g:83:TRP:CD1	2.56	0.41
24:J:131:ARG:NH1	24:J:143:ASN:O	2.53	0.41
2:2:511:U:H2'	2:2:512:A:H8	1.84	0.41
2:2:919:A:H5''	26:N:16:LEU:HD12	2.02	0.41
2:2:1499:U:H4'	4:D:176:LEU:HD13	2.02	0.41
2:2:1608:U:H4'	10:S:130:ARG:HH12	1.85	0.41
2:2:1808:U:H2'	2:2:1809:A:H8	1.84	0.41
4:D:193:ASP:OD2	4:D:198:ILE:HG12	2.21	0.41
5:F:78:MET:O	5:F:79:HIS:HB2	2.20	0.41
5:F:126:THR:CG2	14:c:26:GLN:HE21	2.33	0.41
9:Q:96:TYR:C	9:Q:98:LYS:H	2.29	0.41
18:B:124:HIS:HA	18:B:137:LEU:O	2.21	0.41
20:E:148:ARG:NH2	21:G:202:ASN:OD1	2.54	0.41
20:E:162:ILE:HD13	20:E:162:ILE:HA	1.90	0.41
22:H:82:GLU:HA	22:H:85:LYS:HE3	2.03	0.41
26:N:45:LEU:HD22	26:N:49:GLN:HB3	2.02	0.41
27:O:75:MET:HG2	27:O:118:ALA:HB2	2.03	0.41
2:2:807:G:O2'	2:2:808:A:H5'	2.21	0.41
2:2:884:C:H2'	2:2:885:U:O4'	2.21	0.41
2:2:1600:G:OP1	13:Z:44:LEU:N	2.54	0.41
2:2:1719:A:N6	2:2:1814:G:O2'	2.54	0.41
5:F:133:THR:HB	5:F:135:ARG:HH11	1.85	0.41
10:S:13:LEU:HD23	10:S:13:LEU:H	1.86	0.41
10:S:117:ILE:O	10:S:119:ALA:N	2.51	0.41
35:h:14:LYS:O	35:h:18:ARG:HG3	2.22	0.41
2:2:1277:C:H2'	2:2:1278:A:H8	1.86	0.40
2:2:1411:G:C6	2:2:1412:C:C4	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:127:ARG:CZ	5:F:134:VAL:HA	2.52	0.40
13:Z:46:ASN:HB3	13:Z:79:ILE:C	2.47	0.40
2:2:223:C:H2'	2:2:224:A:C8	2.56	0.40
2:2:320:G:H2'	2:2:321:C:C6	2.56	0.40
2:2:878:G:H3'	2:2:879:C:H5''	2.03	0.40
2:2:1321:G:O2'	2:2:1322:G:H5''	2.21	0.40
2:2:1365:G:H2'	2:2:1366:G:H8	1.86	0.40
2:2:1865:C:O2	32:a:92:ARG:HB3	2.21	0.40
4:D:195:THR:H	4:D:201:LYS:HG3	1.86	0.40
14:c:16:LYS:HE2	14:c:18:LEU:HD21	2.03	0.40
25:L:80:MET:HG2	25:L:86:ILE:HG22	2.02	0.40
34:e:53:LYS:HD3	34:e:53:LYS:HA	1.95	0.40
1:R:133:GLY:HA2	18:B:152:LYS:HD3	2.02	0.40
2:2:554:A:O2'	2:2:555:A:OP1	2.31	0.40
2:2:1171:G:O2'	2:2:1187:G:O6	2.38	0.40
2:2:1587:G:O6	11:T:67:ARG:HD2	2.21	0.40
16:g:165:ILE:CG1	16:g:177:TRP:HB2	2.50	0.40
19:C:147:VAL:O	19:C:151:ILE:HG13	2.20	0.40
23:I:135:GLU:O	23:I:139:LYS:HB3	2.20	0.40
5:F:30:ILE:HG21	5:F:36:GLN:HA	2.03	0.40
8:P:49:LEU:HD22	8:P:53:GLN:HG2	2.04	0.40
22:H:148:LEU:HD21	29:W:48:GLY:HA2	2.04	0.40
25:L:57:ASP:HB2	25:L:84:ARG:NH2	2.36	0.40
32:a:97:PRO:HA	32:a:98:PRO:HD3	1.99	0.40
2:2:1610:G:OP1	10:S:121:ARG:NH1	2.53	0.40
2:2:1807:C:H2'	2:2:1808:U:O4'	2.21	0.40
3:d:30:LEU:HA	3:d:39:CYS:HA	2.04	0.40
6:K:76:ILE:H	6:K:76:ILE:HD12	1.87	0.40
10:S:86:ARG:HH12	10:S:106:LYS:HG2	1.85	0.40
11:T:29:LYS:NZ	11:T:102:ARG:HH22	2.19	0.40
16:g:242:SER:HB2	16:g:247:TRP:HB2	2.03	0.40
18:B:106:THR:HG22	18:B:108:ASP:H	1.86	0.40
23:I:194:GLU:OE1	25:L:12:LYS:NZ	2.51	0.40
26:N:46:THR:HB	26:N:86:GLU:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	130/135 (96%)	125 (96%)	5 (4%)	0	100	100
3	d	52/56 (93%)	49 (94%)	3 (6%)	0	100	100
4	D	223/243 (92%)	216 (97%)	7 (3%)	0	100	100
5	F	187/204 (92%)	176 (94%)	11 (6%)	0	100	100
6	K	93/165 (56%)	92 (99%)	1 (1%)	0	100	100
7	M	121/132 (92%)	113 (93%)	8 (7%)	0	100	100
8	P	118/145 (81%)	114 (97%)	4 (3%)	0	100	100
9	Q	137/146 (94%)	124 (90%)	13 (10%)	0	100	100
10	S	141/152 (93%)	134 (95%)	7 (5%)	0	100	100
11	T	142/145 (98%)	137 (96%)	5 (4%)	0	100	100
12	U	98/119 (82%)	96 (98%)	2 (2%)	0	100	100
13	Z	70/125 (56%)	67 (96%)	3 (4%)	0	100	100
14	c	59/69 (86%)	58 (98%)	1 (2%)	0	100	100
15	f	70/149 (47%)	64 (91%)	5 (7%)	1 (1%)	9	30
16	g	312/317 (98%)	294 (94%)	18 (6%)	0	100	100
17	A	204/295 (69%)	198 (97%)	6 (3%)	0	100	100
18	B	211/264 (80%)	204 (97%)	7 (3%)	0	100	100
19	C	216/293 (74%)	209 (97%)	7 (3%)	0	100	100
20	E	260/263 (99%)	256 (98%)	4 (2%)	0	100	100
21	G	228/249 (92%)	222 (97%)	6 (3%)	0	100	100
22	H	184/194 (95%)	181 (98%)	3 (2%)	0	100	100
23	I	203/208 (98%)	195 (96%)	8 (4%)	0	100	100
24	J	178/194 (92%)	175 (98%)	3 (2%)	0	100	100
25	L	149/158 (94%)	136 (91%)	13 (9%)	0	100	100
26	N	147/151 (97%)	146 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	O	133/151 (88%)	126 (95%)	7 (5%)	0	100	100
28	V	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
29	W	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
30	X	139/143 (97%)	138 (99%)	1 (1%)	0	100	100
31	Y	122/133 (92%)	120 (98%)	2 (2%)	0	100	100
32	a	99/102 (97%)	98 (99%)	1 (1%)	0	100	100
33	b	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
34	e	46/59 (78%)	44 (96%)	2 (4%)	0	100	100
35	h	22/25 (88%)	22 (100%)	0	0	100	100
36	l	28/180 (16%)	27 (96%)	1 (4%)	0	100	100
All	All	4809/5661 (85%)	4631 (96%)	177 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	f	88	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	118/122 (97%)	118 (100%)	0	100	100
3	d	48/49 (98%)	48 (100%)	0	100	100
4	D	188/202 (93%)	188 (100%)	0	100	100
5	F	159/170 (94%)	159 (100%)	0	100	100
6	K	86/136 (63%)	86 (100%)	0	100	100
7	M	104/108 (96%)	104 (100%)	0	100	100
8	P	107/130 (82%)	107 (100%)	0	100	100
9	Q	115/121 (95%)	115 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	S	124/132 (94%)	124 (100%)	0	100	100
11	T	114/115 (99%)	114 (100%)	0	100	100
12	U	92/107 (86%)	92 (100%)	0	100	100
13	Z	64/103 (62%)	64 (100%)	0	100	100
14	c	54/62 (87%)	54 (100%)	0	100	100
15	f	65/133 (49%)	65 (100%)	0	100	100
16	g	272/275 (99%)	272 (100%)	0	100	100
17	A	172/243 (71%)	172 (100%)	0	100	100
18	B	194/231 (84%)	194 (100%)	0	100	100
19	C	182/225 (81%)	182 (100%)	0	100	100
20	E	224/225 (100%)	224 (100%)	0	100	100
21	G	200/218 (92%)	200 (100%)	0	100	100
22	H	167/174 (96%)	167 (100%)	0	100	100
23	I	178/180 (99%)	178 (100%)	0	100	100
24	J	160/168 (95%)	160 (100%)	0	100	100
25	L	135/142 (95%)	135 (100%)	0	100	100
26	N	130/131 (99%)	130 (100%)	0	100	100
27	O	104/119 (87%)	104 (100%)	0	100	100
28	V	66/67 (98%)	66 (100%)	0	100	100
29	W	112/113 (99%)	112 (100%)	0	100	100
30	X	113/115 (98%)	113 (100%)	0	100	100
31	Y	108/115 (94%)	108 (100%)	0	100	100
32	a	88/89 (99%)	88 (100%)	0	100	100
33	b	74/76 (97%)	74 (100%)	0	100	100
34	e	40/48 (83%)	40 (100%)	0	100	100
35	h	23/24 (96%)	23 (100%)	0	100	100
36	l	28/151 (18%)	28 (100%)	0	100	100
All	All	4208/4819 (87%)	4208 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
5	F	82	ASN
7	M	48	HIS
8	P	79	HIS
10	S	76	GLN
11	T	145	HIS
13	Z	64	ASN
16	g	191	HIS
16	g	272	GLN
16	g	311	GLN
17	A	141	ASN
20	E	112	HIS
21	G	13	GLN
22	H	157	HIS
22	H	165	ASN
23	I	116	HIS
26	N	58	HIS
26	N	62	GLN
27	O	20	GLN
27	O	79	GLN
29	W	15	ASN
29	W	56	HIS
30	X	26	GLN
31	Y	63	HIS
32	a	8	ASN
32	a	43	ASN
34	e	44	ASN
36	l	158	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	1655/1868 (88%)	365 (22%)	35 (2%)

All (365) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	2	A
2	2	3	C
2	2	17	C
2	2	23	G
2	2	33	G
2	2	41	G

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Mol	Chain	Res	Type
2	2	46	A
2	2	56	G
2	2	58	C
2	2	62	G
2	2	64	A
2	2	66	G
2	2	67	C
2	2	68	A
2	2	71	G
2	2	72	C
2	2	73	C
2	2	74	G
2	2	75	G
2	2	76	U
2	2	77	A
2	2	79	A
2	2	103	A
2	2	113	G
2	2	114	G
2	2	115	U
2	2	126	G
2	2	130	G
2	2	143	U
2	2	144	U
2	2	155	G
2	2	163	U
2	2	168	C
2	2	181	A
2	2	182	C
2	2	184	G
2	2	191	A
2	2	215	G
2	2	290	U
2	2	291	G
2	2	292	A
2	2	295	C
2	2	308	G
2	2	310	C
2	2	313	A
2	2	318	A
2	2	319	C
2	2	320	G

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Mol	Chain	Res	Type
2	2	321	C
2	2	332	G
2	2	333	G
2	2	335	G
2	2	351	G
2	2	360	A
2	2	362	C
2	2	364	A
2	2	368	U
2	2	369	C
2	2	370	G
2	2	377	G
2	2	383	G
2	2	385	G
2	2	386	C
2	2	400	C
2	2	407	G
2	2	409	C
2	2	418	A
2	2	421	G
2	2	428	U
2	2	429	C
2	2	438	G
2	2	441	C
2	2	448	A
2	2	450	C
2	2	464	A
2	2	465	A
2	2	466	G
2	2	471	G
2	2	472	C
2	2	473	A
2	2	474	G
2	2	482	G
2	2	487	U
2	2	492	C
2	2	503	C
2	2	516	A
2	2	525	A
2	2	534	G
2	2	536	A
2	2	544	G

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Mol	Chain	Res	Type
2	2	546	G
2	2	548	C
2	2	552	G
2	2	554	A
2	2	555	A
2	2	556	U
2	2	559	G
2	2	560	A
2	2	563	G
2	2	564	A
2	2	568	C
2	2	576	A
2	2	583	A
2	2	587	A
2	2	588	G
2	2	589	G
2	2	590	A
2	2	591	U
2	2	593	C
2	2	594	A
2	2	603	C
2	2	604	A
2	2	605	A
2	2	607	U
2	2	608	C
2	2	614	C
2	2	621	C
2	2	629	A
2	2	631	U
2	2	640	A
2	2	643	A
2	2	644	G
2	2	655	A
2	2	660	C
2	2	664	A
2	2	668	A
2	2	669	A
2	2	670	A
2	2	671	A
2	2	672	A
2	2	683	G
2	2	685	A

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Mol	Chain	Res	Type
2	2	688	U
2	2	748	C
2	2	749	U
2	2	750	C
2	2	751	G
2	2	792	C
2	2	793	G
2	2	794	A
2	2	795	A
2	2	797	C
2	2	798	G
2	2	809	A
2	2	810	A
2	2	811	A
2	2	812	A
2	2	821	G
2	2	822	U
2	2	823	U
2	2	824	C
2	2	830	A
2	2	842	C
2	2	847	A
2	2	852	G
2	2	869	A
2	2	870	A
2	2	871	U
2	2	872	A
2	2	873	G
2	2	878	G
2	2	879	C
2	2	880	G
2	2	887	U
2	2	890	U
2	2	891	G
2	2	892	U
2	2	898	U
2	2	913	A
2	2	914	U
2	2	920	A
2	2	924	G
2	2	926	A
2	2	930	C

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Mol	Chain	Res	Type
2	2	933	G
2	2	934	G
2	2	970	G
2	2	971	G
2	2	978	G
2	2	981	A
2	2	988	C
2	2	990	A
2	2	992	A
2	2	999	G
2	2	1001	A
2	2	1002	U
2	2	1017	U
2	2	1023	A
2	2	1028	A
2	2	1040	G
2	2	1049	A
2	2	1060	A
2	2	1061	U
2	2	1062	A
2	2	1067	C
2	2	1083	A
2	2	1085	C
2	2	1096	G
2	2	1114	U
2	2	1115	U
2	2	1116	C
2	2	1118	C
2	2	1119	A
2	2	1121	G
2	2	1126	G
2	2	1133	A
2	2	1138	C
2	2	1139	C
2	2	1143	A
2	2	1148	A
2	2	1153	C
2	2	1154	U
2	2	1157	G
2	2	1171	G
2	2	1195	A
2	2	1202	U

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Mol	Chain	Res	Type
2	2	1203	G
2	2	1204	A
2	2	1207	G
2	2	1208	A
2	2	1215	C
2	2	1217	A
2	2	1221	G
2	2	1224	G
2	2	1227	G
2	2	1232	U
2	2	1235	G
2	2	1236	G
2	2	1242	U
2	2	1243	U
2	2	1251	A
2	2	1257	G
2	2	1259	A
2	2	1260	A
2	2	1261	C
2	2	1269	G
2	2	1274	G
2	2	1275	G
2	2	1284	A
2	2	1285	G
2	2	1286	G
2	2	1289	U
2	2	1301	A
2	2	1302	G
2	2	1309	C
2	2	1313	A
2	2	1314	U
2	2	1315	U
2	2	1323	U
2	2	1329	U
2	2	1331	C
2	2	1341	C
2	2	1343	U
2	2	1348	G
2	2	1354	G
2	2	1355	C
2	2	1356	G
2	2	1366	G

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Mol	Chain	Res	Type
2	2	1371	U
2	2	1373	C
2	2	1378	A
2	2	1382	A
2	2	1404	U
2	2	1406	G
2	2	1425	G
2	2	1431	G
2	2	1432	U
2	2	1439	A
2	2	1441	U
2	2	1454	A
2	2	1455	A
2	2	1463	U
2	2	1464	C
2	2	1465	A
2	2	1466	G
2	2	1476	A
2	2	1477	U
2	2	1478	U
2	2	1487	A
2	2	1489	A
2	2	1490	G
2	2	1493	C
2	2	1494	U
2	2	1495	G
2	2	1497	G
2	2	1505	U
2	2	1507	G
2	2	1509	U
2	2	1510	G
2	2	1520	G
2	2	1521	C
2	2	1522	A
2	2	1528	G
2	2	1530	U
2	2	1531	A
2	2	1533	A
2	2	1548	G
2	2	1551	U
2	2	1559	C
2	2	1560	U

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Mol	Chain	Res	Type
2	2	1566	G
2	2	1570	G
2	2	1572	C
2	2	1574	C
2	2	1578	U
2	2	1580	A
2	2	1581	C
2	2	1585	U
2	2	1586	U
2	2	1588	A
2	2	1598	G
2	2	1599	U
2	2	1600	G
2	2	1601	A
2	2	1606	G
2	2	1612	G
2	2	1618	C
2	2	1621	U
2	2	1623	A
2	2	1625	U
2	2	1637	A
2	2	1641	A
2	2	1646	C
2	2	1647	A
2	2	1648	G
2	2	1649	U
2	2	1654	G
2	2	1663	A
2	2	1665	G
2	2	1671	G
2	2	1675	A
2	2	1678	A
2	2	1695	A
2	2	1697	A
2	2	1698	C
2	2	1699	A
2	2	1706	G
2	2	1722	G
2	2	1723	G
2	2	1729	U
2	2	1744	G
2	2	1756	C

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Mol	Chain	Res	Type
2	2	1778	C
2	2	1783	C
2	2	1786	U
2	2	1812	U
2	2	1826	G
2	2	1829	G
2	2	1831	A
2	2	1835	A
2	2	1836	G
2	2	1838	U
2	2	1849	G
2	2	1850	A
2	2	1851	A
2	2	1852	C
2	2	1855	G
2	2	1859	A
2	2	1861	G
2	2	1862	G
2	2	1863	A
2	2	1864	U
2	2	1865	C
2	2	1868	U
2	2	1869	A

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	65	C
2	2	102	A
2	2	114	G
2	2	143	U
2	2	180	G
2	2	291	G
2	2	332	G
2	2	382	C
2	2	417	C
2	2	465	A
2	2	547	G
2	2	554	A
2	2	590	A
2	2	604	A
2	2	749	U

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Mol	Chain	Res	Type
2	2	750	C
2	2	793	G
2	2	797	C
2	2	811	A
2	2	980	A
2	2	1137	U
2	2	1231	C
2	2	1288	U
2	2	1308	U
2	2	1330	G
2	2	1342	U
2	2	1403	C
2	2	1430	C
2	2	1431	G
2	2	1438	A
2	2	1440	C
2	2	1464	C
2	2	1494	U
2	2	1520	G
2	2	1648	G

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 4 ligands modelled in this entry, 4 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.

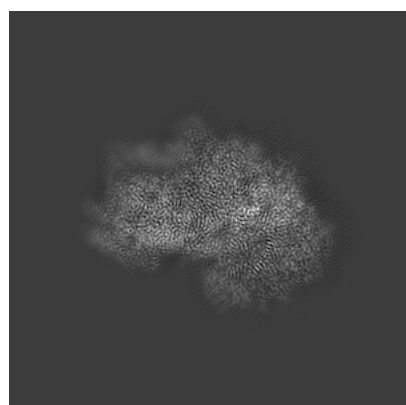
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22681. These allow visual inspection of the internal detail of the map and identification of artifacts.

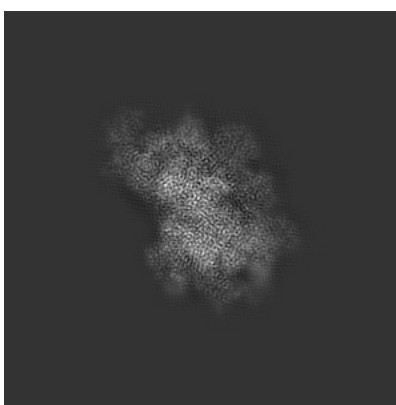
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

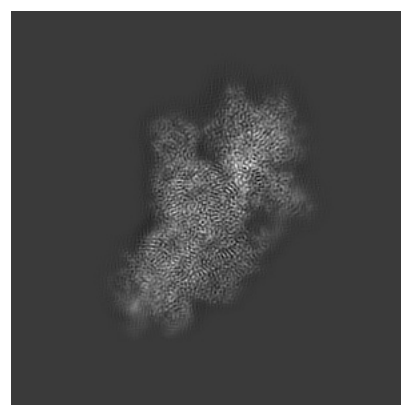
6.1.1 Primary map



X



Y

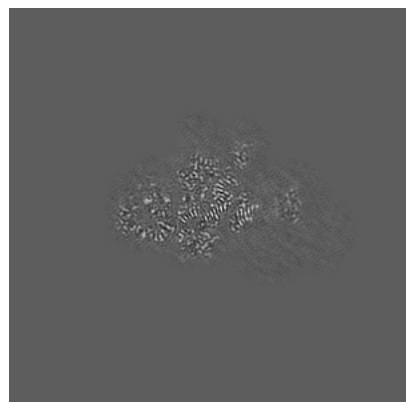


Z

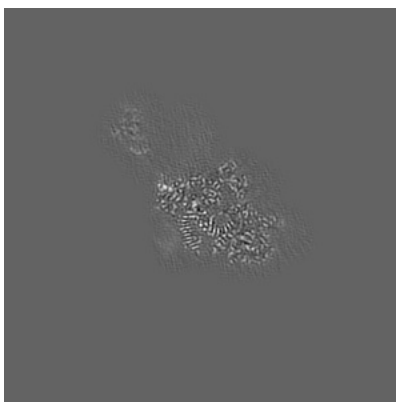
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

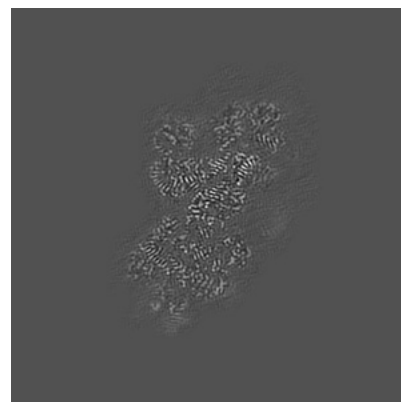
6.2.1 Primary map



X Index: 180



Y Index: 180

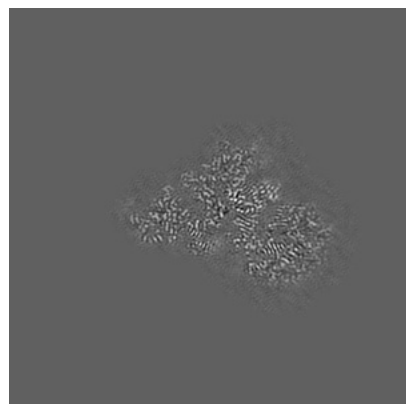


Z Index: 180

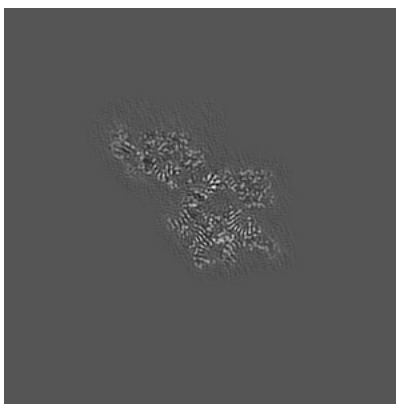
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

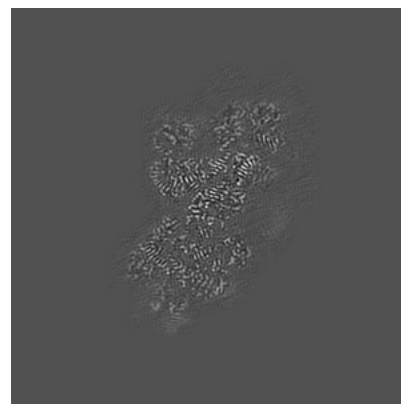
6.3.1 Primary map



X Index: 203



Y Index: 203

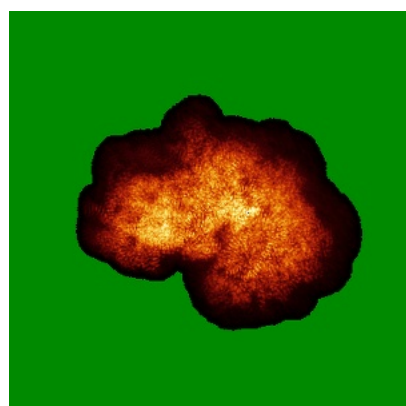


Z Index: 180

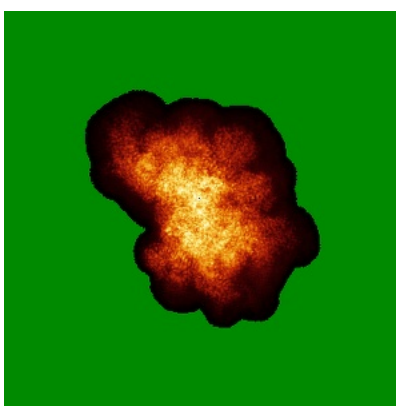
The images above show the largest variance slices of the map in three orthogonal directions.

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

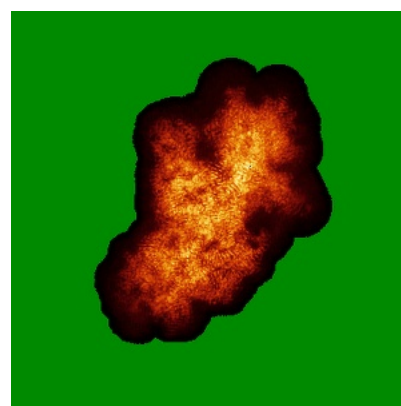
6.4.1 Primary map



X



Y

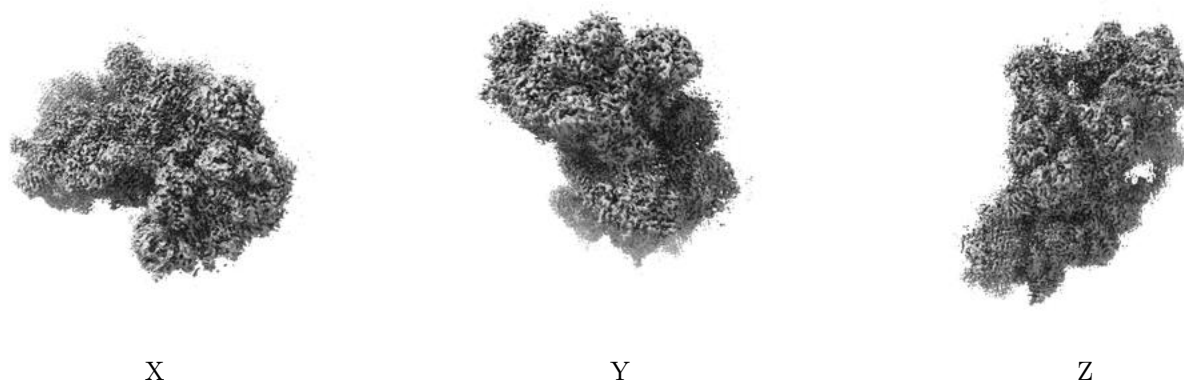


Z

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

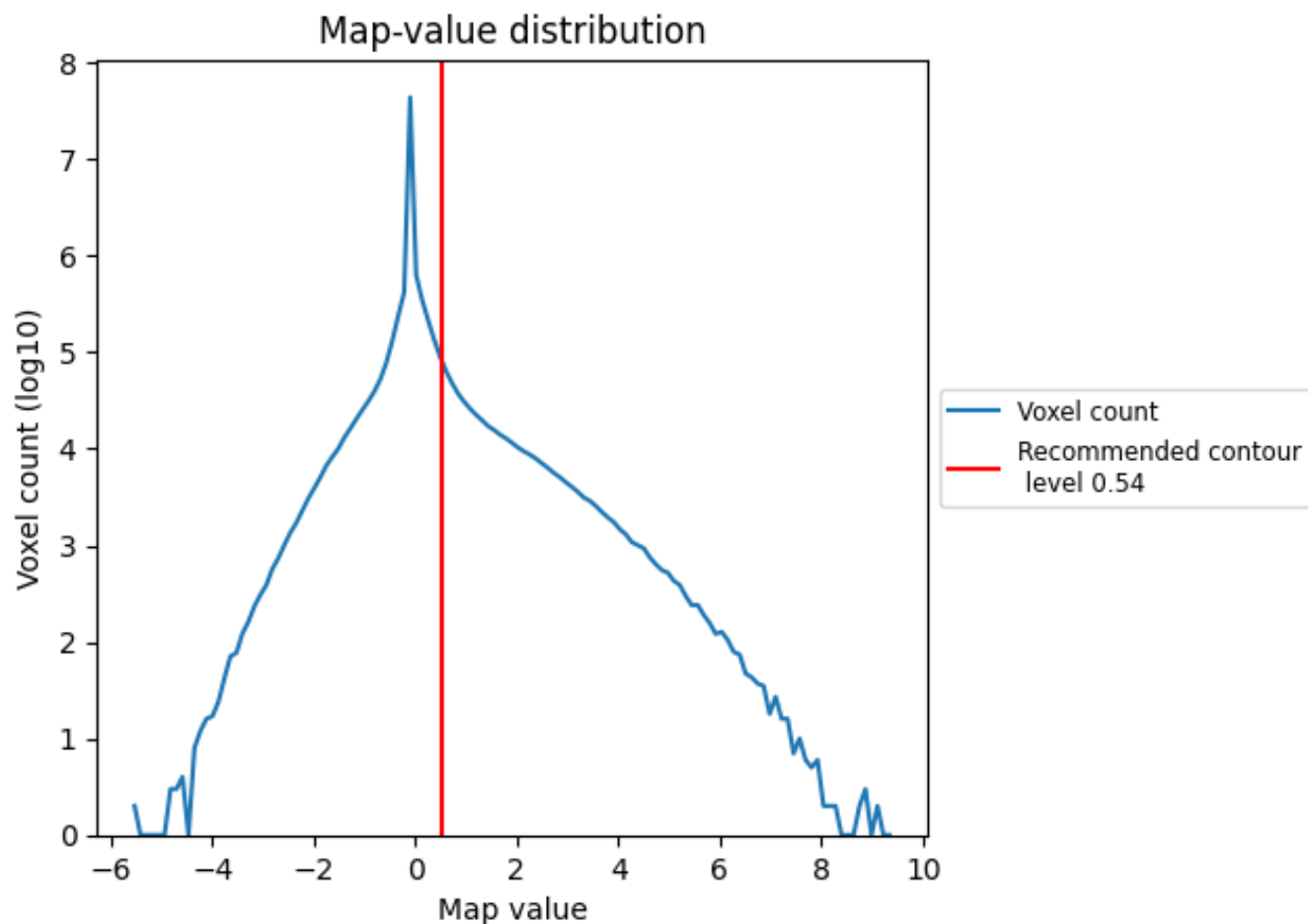
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

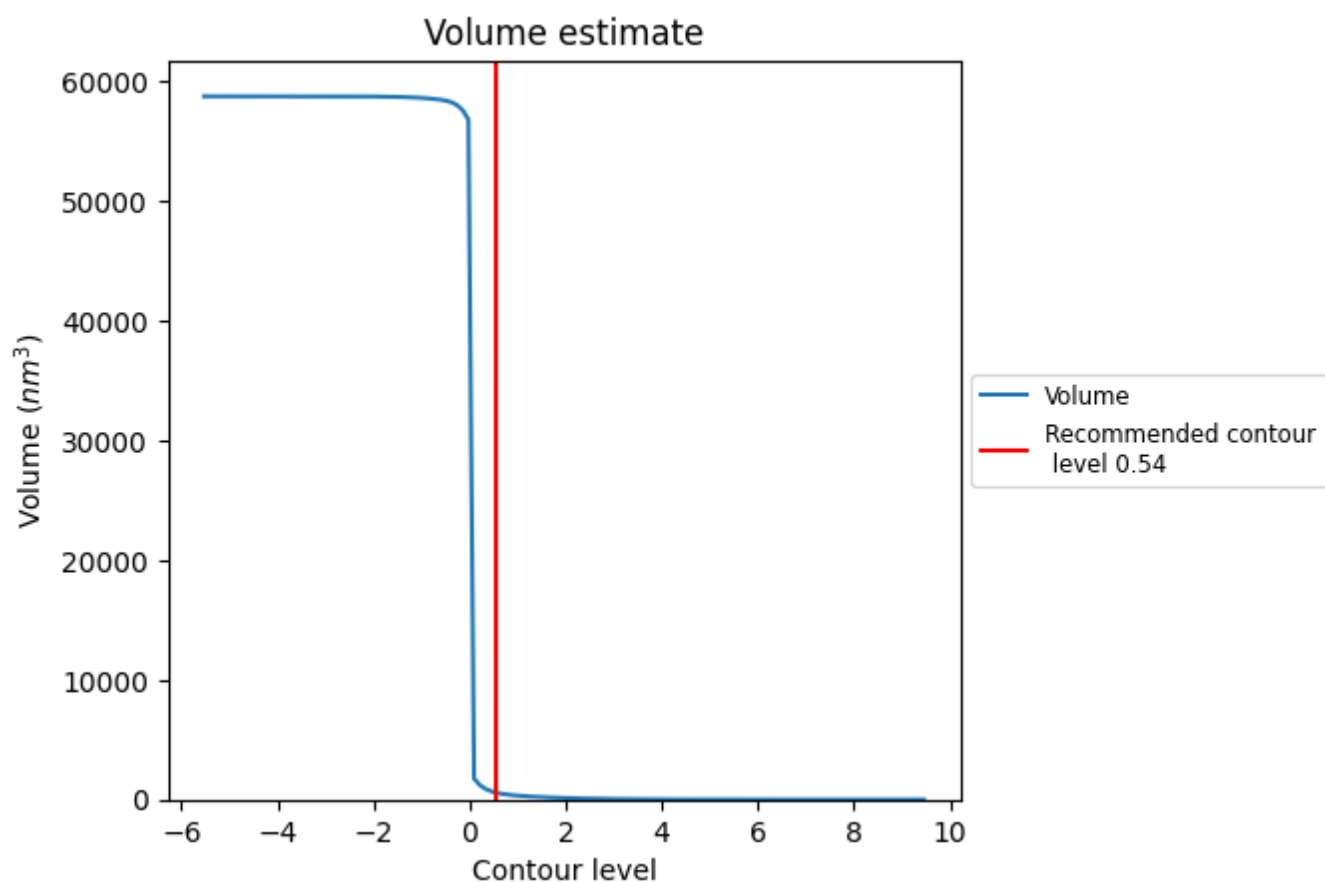
This section contains the results of statistical analysis of the map.

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.

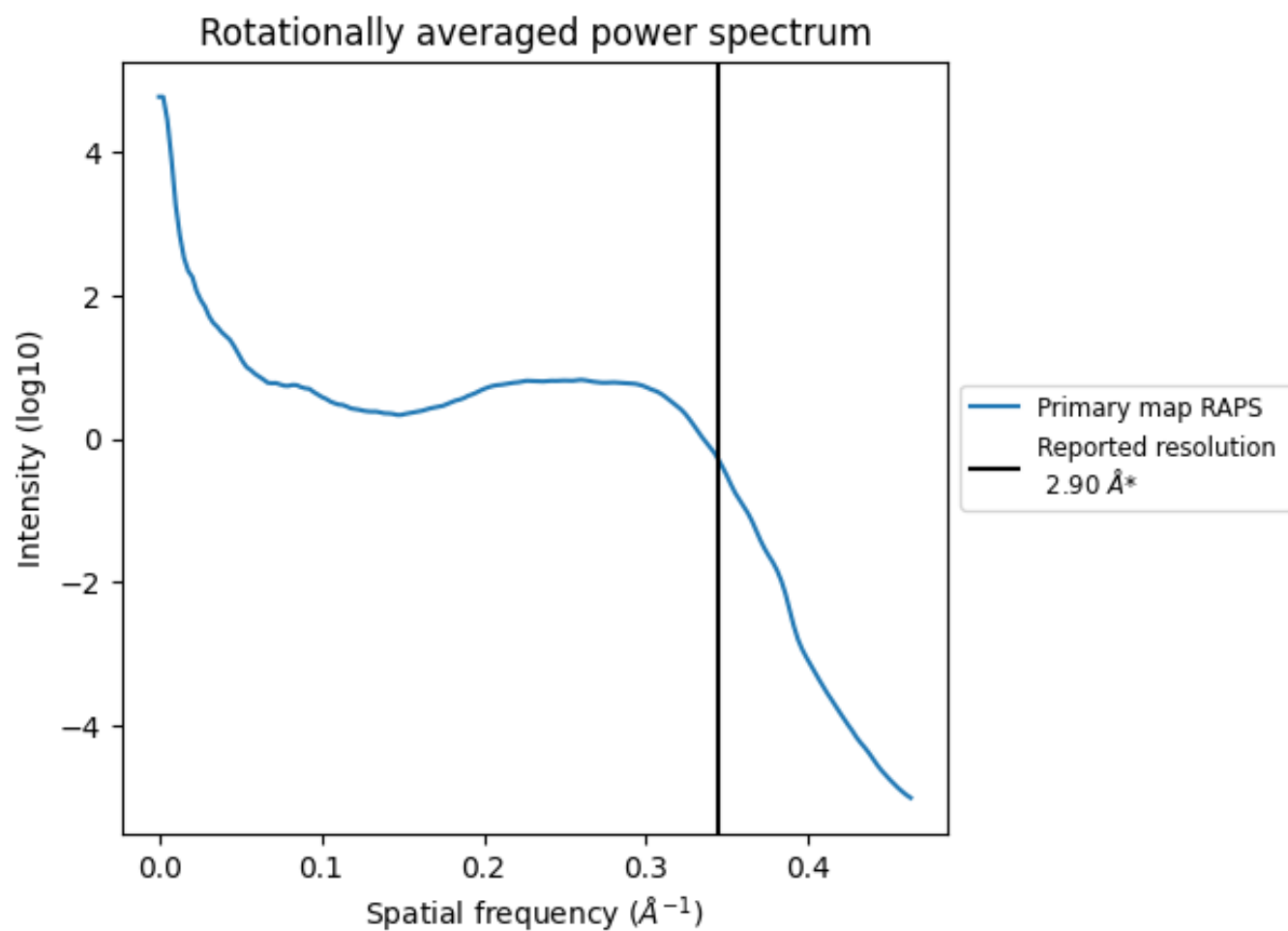
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 587 nm³; this corresponds to an approximate mass of 530 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 0.345 Å⁻¹

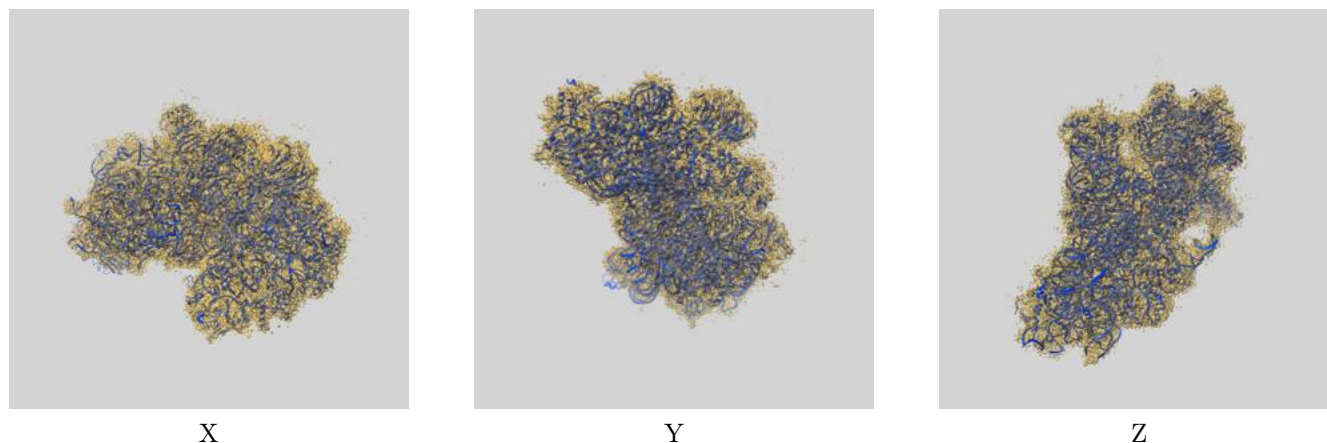
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

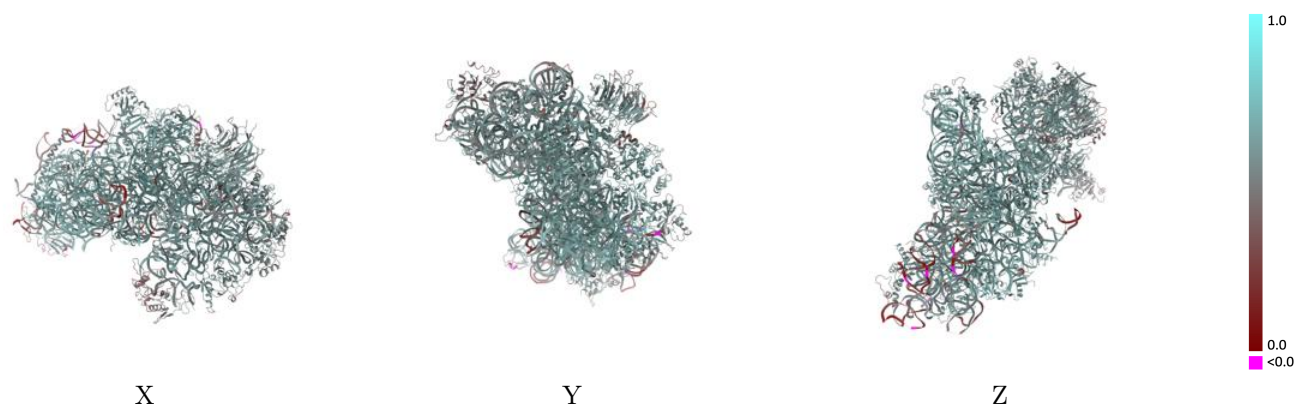
This section contains information regarding the fit between EMDB map EMD-22681 and PDB model 7K5I. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.54 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](#)

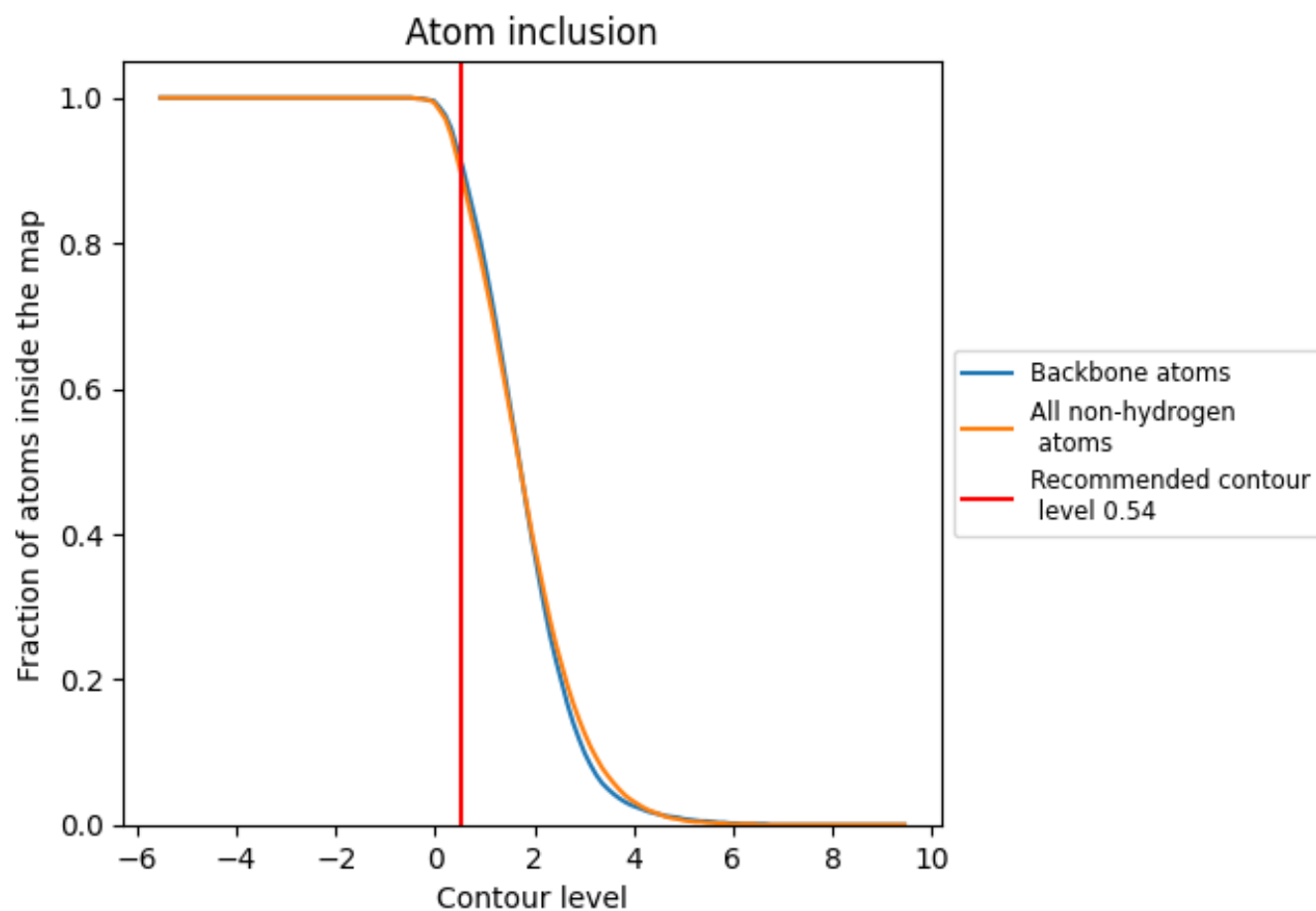


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 89% 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 (0.54) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8920	 0.5700
1	 0.9340	 0.5990
2	 0.9140	 0.5710
A	 0.9600	 0.6220
B	 0.8880	 0.5970
C	 0.9610	 0.6260
D	 0.8720	 0.5590
E	 0.9530	 0.6260
F	 0.8820	 0.5610
G	 0.6590	 0.4830
H	 0.8020	 0.5400
I	 0.8660	 0.5600
J	 0.9530	 0.6290
K	 0.8950	 0.5590
L	 0.8660	 0.5820
M	 0.5900	 0.4100
N	 0.9290	 0.5990
O	 0.9240	 0.5950
P	 0.8510	 0.5380
Q	 0.9250	 0.5750
R	 0.8550	 0.5300
S	 0.8240	 0.5150
T	 0.8600	 0.5440
U	 0.7980	 0.5160
V	 0.9200	 0.6170
W	 0.9760	 0.6410
X	 0.9570	 0.6320
Y	 0.9490	 0.6240
Z	 0.8070	 0.4980
a	 0.9410	 0.6090
b	 0.9040	 0.5960
c	 0.8610	 0.5590
d	 0.9340	 0.6100
e	 0.9320	 0.6050
f	 0.7050	 0.4690



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Chain	Atom inclusion	Q-score
g	 0.8360	 0.5260
h	 0.4710	 0.5010