Full wwPDB EM Validation Report (i)

May 18, 2024 – 09:50 pm BST

PDB ID	:	6TMF
EMDB ID	:	EMD-10519
Title	:	Structure of an archaeal ABCE1-bound ribosomal post-splitting complex
Authors	:	Kratzat, H.; Becker, T.; Tampe, R.; Beckmann, R.
Deposited on	:	2019-12-04
Resolution	:	2.80 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 (i) 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 (1)) were used in the production of this report:

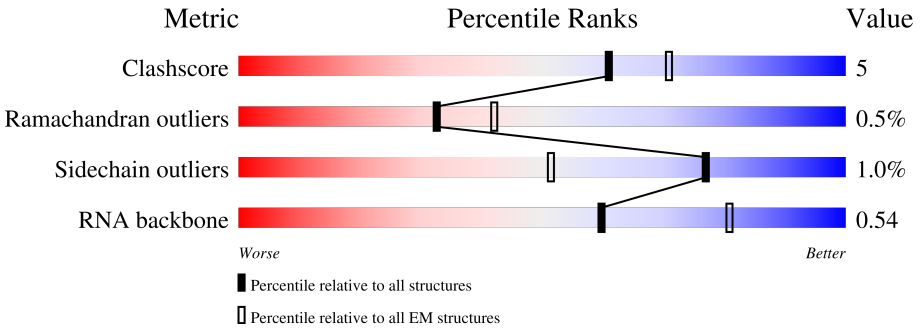
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	1485	64% 28% 7% •
2	B	195	89% 11%
3	C	193	92% 8%
4	D	184	85% 14% •
5	E	178	87% 11% ••
6	F	241	83% 17%
7	G	220	87% 12% •

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Mol	Chain	Length	Quality of chain
8	H	125	6% 87% 13%
9	I	214	78% 22%
10	J	129	92% 8%
11	K	126	88% 11%
12	L	132	80% 19%
13	M	102	97%
14	N	133	10% 86% 14%
15	O	144	84% 15%
16	P	136	85% 15%
17	Q	56	14% 79% 20%
18	R	151	91% 7%
19	S	111	5% 91% 9%
20	T	64	92% 8%
21	U	115	76% 24%
22	V	149	77% 21%
23	W	56	89% 9%
24	X	97	81% 19%
25	Y	63	8% 87% 13%
26	Z	50	98% 92% 8%
27	a	66	8% 95% 5%
28	b	123	89% 100%
29	c	37	8% 89% 11%
30	d	594	96%

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 65449 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1485	31920	14202	5912	10321	1485	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	195	1571	1014	271	282	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	193	1526	970	284	268	4	0	0

- Molecule 4 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	184	1520	976	272	268	4	0	0

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	178	1476	923	291	260	2	0	0

- Molecule 6 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	241	1963	1257	362	339	5	0	0

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	220	1721	1083	322	308	8	0	0

- Molecule 8 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	125	961	601	185	172	3	0	0

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	214	1704	1067	326	303	8	0	0

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	129	1022	661	176	182	3	0	0

- Molecule 11 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	K	126	997	625	199	173	0	0

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	132	1040	648	202	184	6	0	0

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	102	819	507	155	153	4	0	0

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	133	1005	621	200	181	3	0	0

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	144	1131	718	218	193	2	0	0

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	136	1109	700	217	188	4	0	0

- Molecule 17 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	56	459	291	94	68	6	0	0

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	151	1225	776	235	208	6	0	0

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	111	913	576	179	154	4	0	0

- Molecule 20 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	64	540	339	101	97	3	0	0

- Molecule 21 is a protein called 30S ribosomal protein S19P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	U	115	949	610	174	161	4	0	0

- Molecule 22 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	V	149	1218	786	217	215	0	0

- Molecule 23 is a protein called RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	W	56	435	275	76	76	8	0	0

- Molecule 24 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	X	97	799	509	138	148	4	0	0

- Molecule 25 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	63	475	303	82	85	5	0	0

- Molecule 26 is a protein called 30S ribosomal protein S27ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Z	50	417	264	83	64	6	0	0

- Molecule 27 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	a	66	514	316	101	96	1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	b	123	936	594	157	182	3	0	0

- Molecule 29 is a protein called LSU ribosomal protein L41E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	c	37	351	224	85	40	2	0	0

- Molecule 30 is a protein called ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	d	582	4622	2959	784	863	16	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	238	ALA	GLU	engineered mutation	UNP A0A0E3MFT8
d	485	ALA	GLU	engineered mutation	UNP A0A0E3MFT8

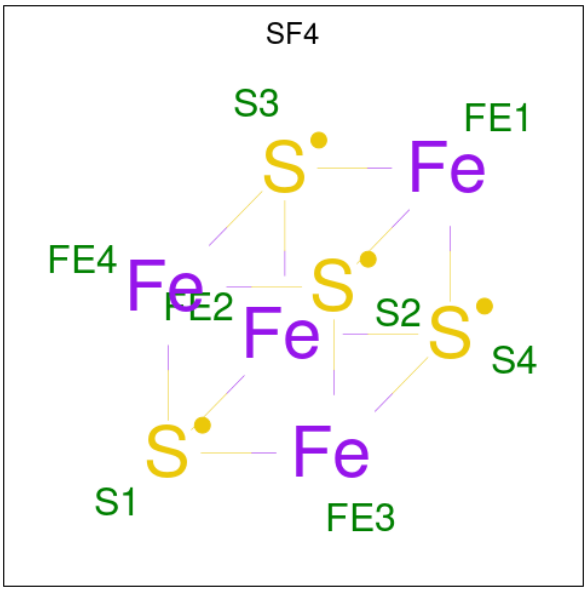
- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
31	A	27	27	27	0
31	d	2	2	2	0

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

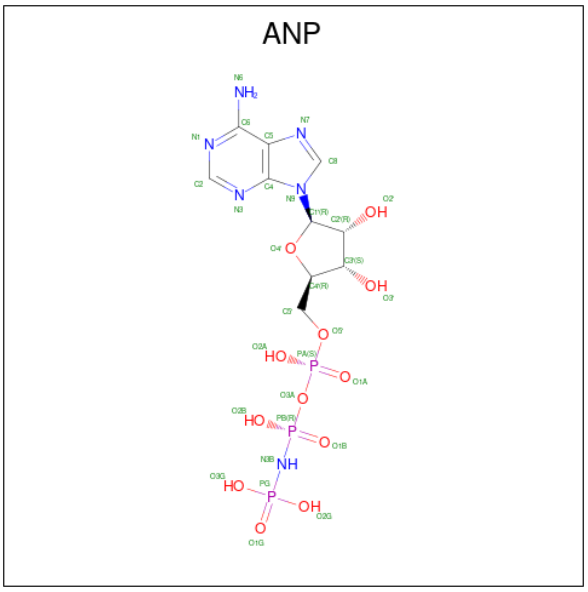
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
32	Q	1	1	1	0
32	W	2	2	2	0
32	Y	1	1	1	0

- Molecule 33 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
33	d	1	8	4	4	0
			Total	Fe	S	
33	d	1	8	4	4	0

- Molecule 34 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
34	d	1	31	10	6	12	3	0

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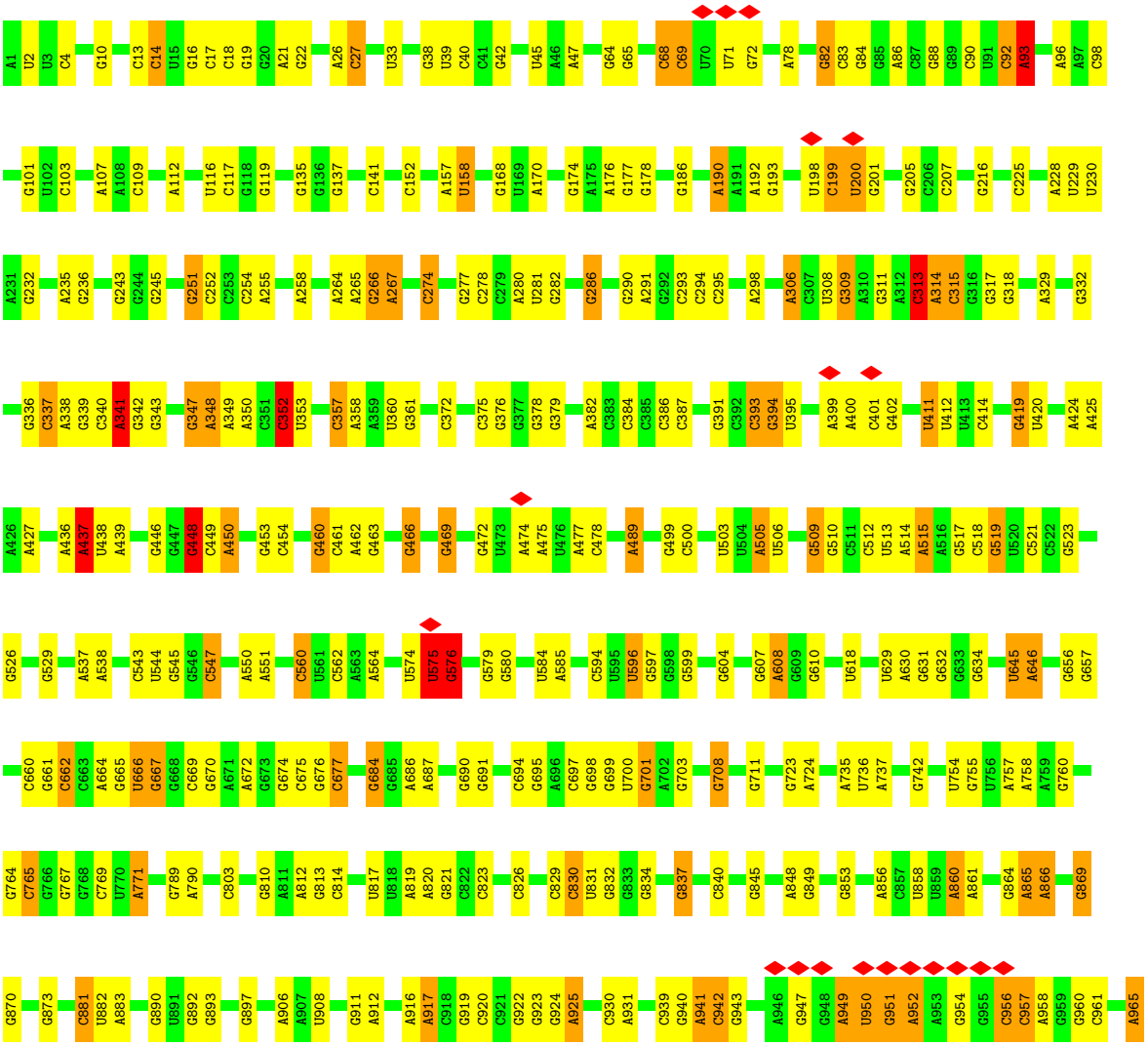
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
34	d	1	31	10	6	12	3	0

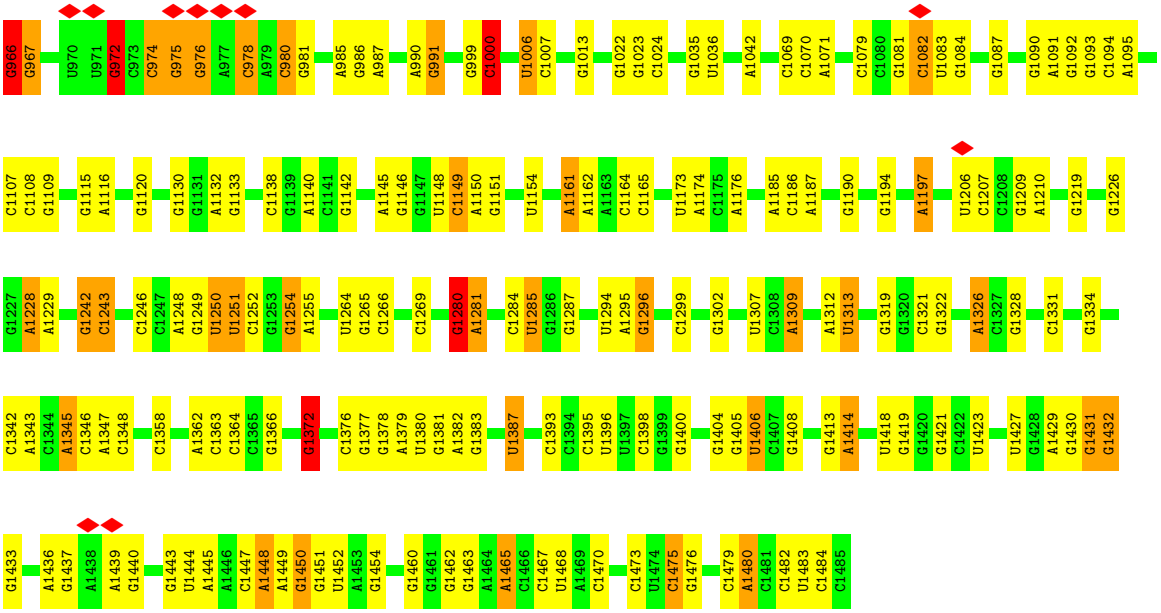
3 Residue-property plots (i)

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

- Molecule 1: 16S ribosomal RNA

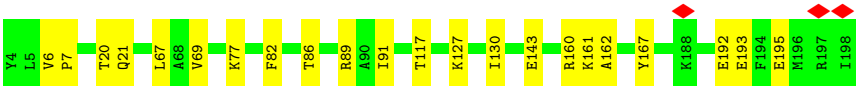
Chain A:





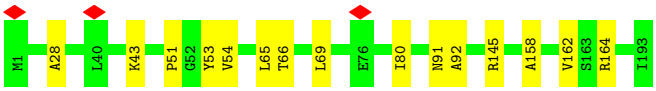
- Molecule 2: 30S ribosomal protein S2

Chain B:



- Molecule 3: 30S ribosomal protein S3

Chain C:

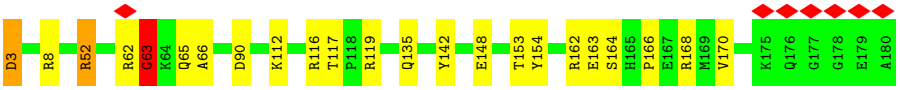


- Molecule 4: 30S ribosomal protein S3Ae

Chain D:

- Molecule 5: 30S ribosomal protein S4

Chain E:

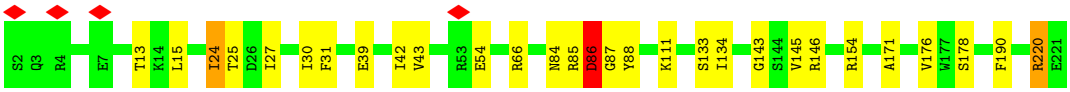


- Molecule 6: 30S ribosomal protein S4e

Chain F: 83% 17%

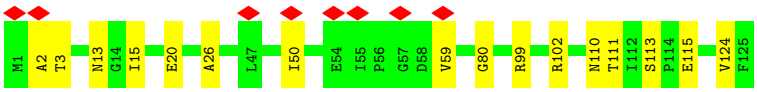
• Molecule 7: 30S ribosomal protein S5

Chain G: 87% 12%



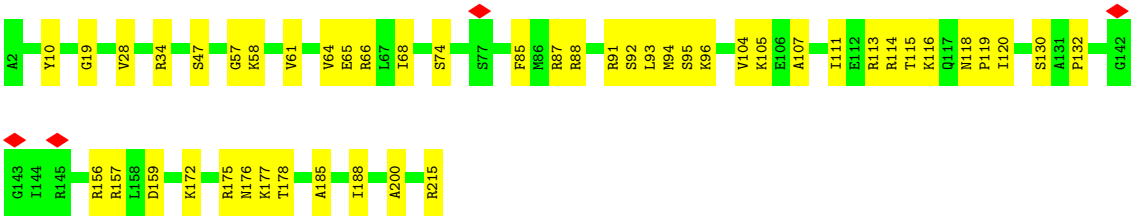
• Molecule 8: 30S ribosomal protein S6e

Chain H: 6% 87% 13%



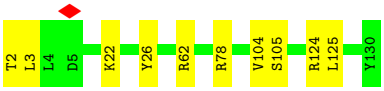
• Molecule 9: 30S ribosomal protein S7

Chain I: 78% 22%



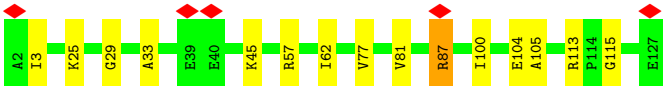
• Molecule 10: 30S ribosomal protein S8

Chain J: 92% 8%



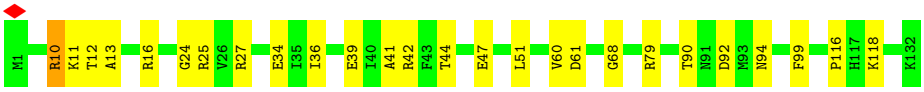
• Molecule 11: 30S ribosomal protein S8e

Chain K: 88% 11%



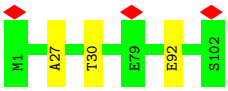
• Molecule 12: 30S ribosomal protein S9

Chain L: 80% 19%



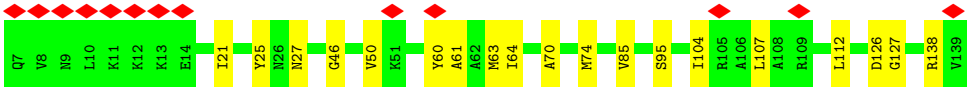
• Molecule 13: 30S ribosomal protein S10

Chain M: 97%



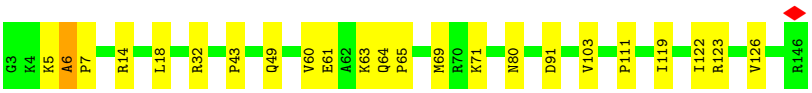
• Molecule 14: 30S ribosomal protein S11

Chain N: 10% 86% 14%



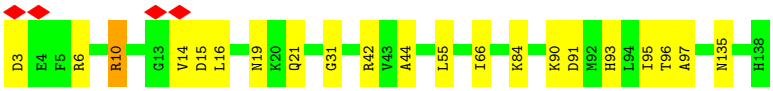
• Molecule 15: 30S ribosomal protein S12

Chain O: 84% 15%



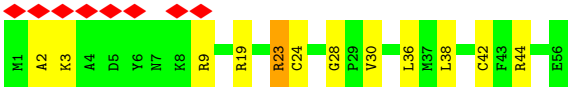
• Molecule 16: 30S ribosomal protein S13

Chain P: 85% 15%



• Molecule 17: 30S ribosomal protein S14 type Z

Chain Q: 14% 79% 20%

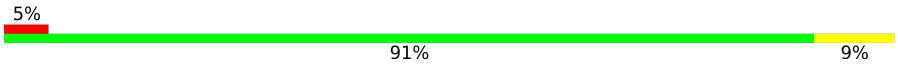


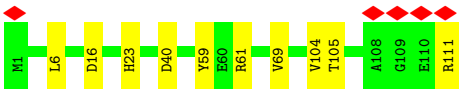
• Molecule 18: 30S ribosomal protein S15

Chain R: 91% 7%

• Molecule 19: 30S ribosomal protein S17

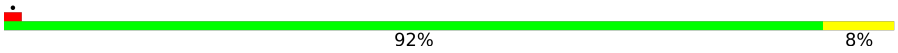
Chain S:

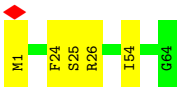




• Molecule 20: 30S ribosomal protein S17e

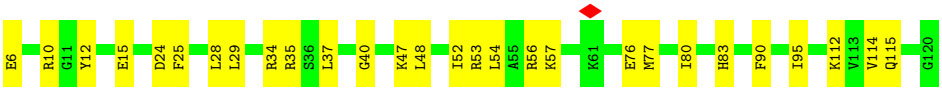
Chain T:





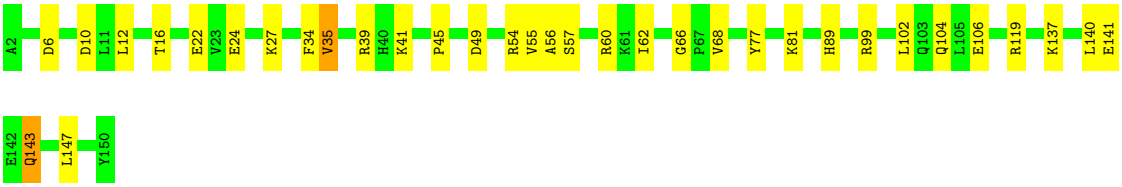
• Molecule 21: 30S ribosomal protein S19P

Chain U:



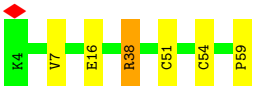
• Molecule 22: 30S ribosomal protein S19e

Chain V:



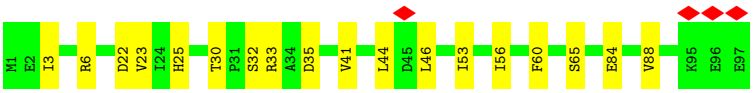
• Molecule 23: RNA-binding protein

Chain W:



• Molecule 24: 30S ribosomal protein S24e

Chain X:

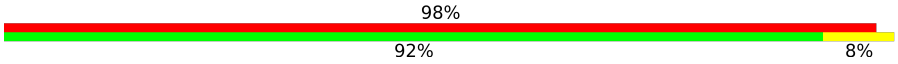


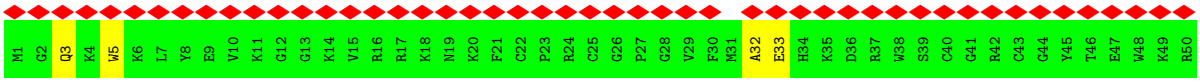
• Molecule 25: 30S ribosomal protein S27e

Chain Y:

• Molecule 26: 30S ribosomal protein S27ae

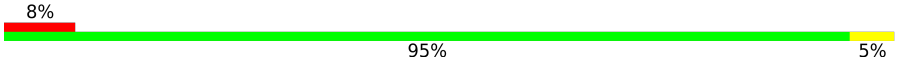
Chain Z:

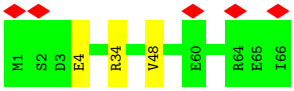




• Molecule 27: 30S ribosomal protein S28e

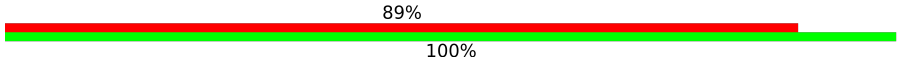
Chain a:

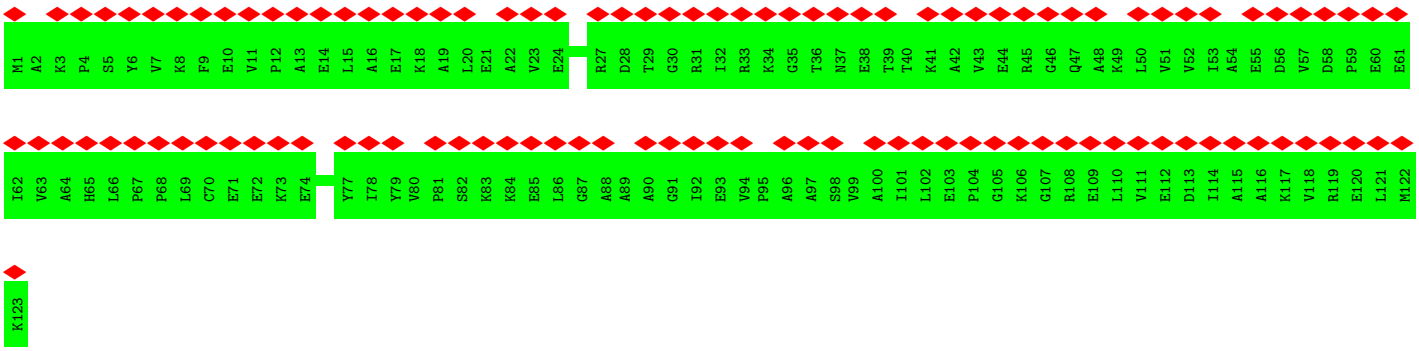




• Molecule 28: 50S ribosomal protein L7Ae

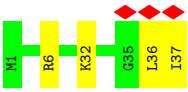
Chain b:





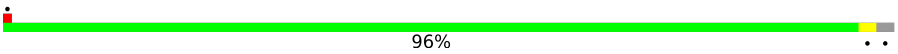
• Molecule 29: LSU ribosomal protein L41E

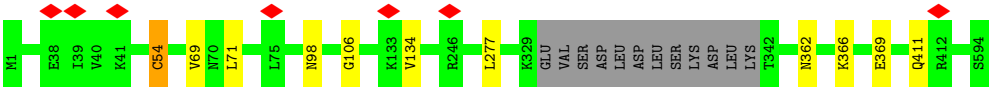
Chain c:



• Molecule 30: ATPase

Chain d:


96%


M1
E38
T39
V40
K41
C54
V69
N70
L71
L75
N98
G106
K133
V134
R246
L277
K329
GLU
VAL
SER
ASP
LEU
ASP
LEU
SER
LYS
ASP
LEU
LYS
T342
N362
K366
E369
Q411
R412
S594

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	293010	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	49.493	Depositor
Minimum map value	-24.478	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.121	Depositor
Recommended contour level	5.0	Depositor
Map size (Å)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, SF4, ANP

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	1.61	104/35726 (0.3%)	1.32	233/55763 (0.4%)
2	B	0.74	0/1602	0.66	0/2167
3	C	0.76	0/1548	0.68	0/2076
4	D	0.65	0/1547	0.69	1/2076 (0.0%)
5	E	0.80	0/1499	0.75	2/2011 (0.1%)
6	F	0.90	0/2007	0.71	0/2708
7	G	0.91	0/1747	0.74	2/2351 (0.1%)
8	H	0.61	0/974	0.72	0/1306
9	I	0.90	2/1734 (0.1%)	0.69	1/2326 (0.0%)
10	J	0.94	0/1042	0.71	0/1399
11	K	0.79	0/1007	0.73	0/1342
12	L	0.91	0/1053	0.73	1/1408 (0.1%)
13	M	0.71	0/826	0.69	0/1107
14	N	0.61	0/1024	0.66	0/1377
15	O	0.89	0/1148	0.74	0/1529
16	P	0.88	1/1131 (0.1%)	0.74	0/1524
17	Q	0.82	0/469	0.64	0/618
18	R	0.74	0/1248	0.71	2/1672 (0.1%)
19	S	0.90	0/936	0.64	0/1260
20	T	0.72	0/547	0.57	0/726
21	U	0.91	0/968	0.67	0/1292
22	V	1.01	1/1250 (0.1%)	0.78	2/1688 (0.1%)
23	W	0.86	0/449	0.66	0/610
24	X	0.80	0/811	0.65	0/1085
25	Y	0.73	0/481	0.72	0/648
26	Z	0.32	0/429	0.62	0/568
27	a	0.74	0/516	0.72	0/692
28	b	0.34	0/949	0.60	0/1282
29	c	1.05	0/357	0.84	0/462
30	d	0.77	1/4701 (0.0%)	0.64	0/6338
All	All	1.28	109/69726 (0.2%)	1.09	244/101411 (0.2%)

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	A	0	3
2	B	0	1
All	All	0	4

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	19	ASN	CA-CB	-10.17	1.26	1.53
1	A	830	C	C2-O2	-8.92	1.16	1.24
9	I	96	LYS	CA-CB	-8.45	1.35	1.53
1	A	352	C	C2-O2	-7.93	1.17	1.24
1	A	379	G	N3-C4	-7.63	1.30	1.35
1	A	379	G	C2-N3	-6.95	1.27	1.32
1	A	1294	U	C2-N3	-6.92	1.32	1.37
1	A	512	C	C4-C5	-6.56	1.37	1.43
1	A	1326	A	N9-C4	-6.52	1.33	1.37
1	A	830	C	N3-C4	-6.48	1.29	1.33
1	A	294	C	C4-C5	-6.46	1.37	1.43
1	A	829	C	C4-C5	-6.39	1.37	1.43
1	A	956	C	N3-C4	-6.32	1.29	1.33
1	A	510	G	C2-N3	-6.32	1.27	1.32
1	A	341	A	C6-N6	-6.23	1.28	1.33
1	A	510	G	C2-N2	-6.21	1.28	1.34
1	A	510	G	N3-C4	-6.14	1.31	1.35
1	A	352	C	N3-C4	-6.03	1.29	1.33
1	A	379	G	C2-N2	-6.00	1.28	1.34
1	A	103	C	C5-C6	-6.00	1.29	1.34
1	A	1138	C	N1-C6	-5.93	1.33	1.37
1	A	564	A	N9-C4	-5.89	1.34	1.37
1	A	17	C	C4-C5	-5.85	1.38	1.43
1	A	103	C	C4-C5	-5.85	1.38	1.43
1	A	512	C	C5-C6	-5.85	1.29	1.34
1	A	866	A	C6-N6	-5.83	1.29	1.33
1	A	274	C	C5-C6	-5.77	1.29	1.34
1	A	829	C	C5-C6	-5.73	1.29	1.34
1	A	18	C	C5-C6	-5.72	1.29	1.34
1	A	1348	C	N1-C6	-5.71	1.33	1.37
1	A	274	C	C4-C5	-5.69	1.38	1.43
1	A	350	A	N9-C4	-5.69	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	672	A	N9-C4	-5.69	1.34	1.37
1	A	22	G	C6-N1	-5.66	1.35	1.39
30	d	54	CYS	CB-SG	-5.66	1.72	1.81
1	A	526	G	C6-N1	-5.66	1.35	1.39
1	A	813	G	C8-N7	-5.64	1.27	1.30
1	A	765	C	C5-C6	-5.62	1.29	1.34
1	A	812	A	N9-C4	-5.61	1.34	1.37
1	A	349	A	N9-C4	-5.61	1.34	1.37
1	A	1342	C	C5-C6	-5.58	1.29	1.34
1	A	274	C	C4-N4	-5.57	1.28	1.33
1	A	90	C	C4-C5	-5.56	1.38	1.43
1	A	1022	G	C6-N1	-5.54	1.35	1.39
1	A	372	C	C4-N4	-5.53	1.28	1.33
1	A	1451	G	N9-C4	-5.51	1.33	1.38
1	A	372	C	C4-C5	-5.50	1.38	1.43
1	A	826	C	C5-C6	-5.50	1.29	1.34
1	A	764	G	C6-N1	-5.48	1.35	1.39
1	A	687	A	N9-C4	-5.47	1.34	1.37
1	A	101	G	C6-N1	-5.45	1.35	1.39
1	A	448	G	C8-N7	-5.45	1.27	1.30
1	A	90	C	C5-C6	-5.44	1.29	1.34
1	A	386	C	C4-C5	-5.44	1.38	1.43
1	A	379	G	N9-C4	-5.41	1.33	1.38
1	A	1024	C	C5-C6	-5.39	1.30	1.34
1	A	112	A	N9-C4	-5.37	1.34	1.37
1	A	1454	G	C6-N1	-5.36	1.35	1.39
1	A	813	G	N7-C5	-5.36	1.36	1.39
1	A	510	G	N1-C2	-5.32	1.33	1.37
1	A	277	G	C8-N7	-5.32	1.27	1.30
1	A	489	A	N9-C4	-5.31	1.34	1.37
1	A	765	C	C4-C5	-5.29	1.38	1.43
1	A	869	G	N7-C5	-5.28	1.36	1.39
9	I	64	VAL	CB-CG2	-5.27	1.41	1.52
1	A	803	C	C5-C6	-5.27	1.30	1.34
1	A	820	A	N7-C5	-5.27	1.36	1.39
1	A	1467	C	N3-C4	-5.27	1.30	1.33
1	A	769	C	C5-C6	-5.25	1.30	1.34
1	A	449	C	C4-C5	-5.24	1.38	1.43
1	A	764	G	C8-N7	-5.23	1.27	1.30
1	A	16	G	C8-N7	-5.23	1.27	1.30
1	A	757	A	N9-C4	-5.22	1.34	1.37
1	A	823	C	N1-C6	-5.22	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	562	C	N1-C6	-5.21	1.34	1.37
1	A	450	A	C6-N6	-5.21	1.29	1.33
1	A	298	A	N9-C4	-5.21	1.34	1.37
1	A	767	G	N9-C4	-5.20	1.33	1.38
1	A	1345	A	C6-N6	-5.18	1.29	1.33
1	A	865	A	C6-N6	-5.17	1.29	1.33
1	A	13	C	C4-C5	-5.16	1.38	1.43
22	V	55	VAL	CB-CG2	-5.16	1.42	1.52
1	A	27	C	C4-C5	-5.15	1.38	1.43
1	A	280	A	C6-N6	-5.15	1.29	1.33
1	A	509	G	C6-N1	-5.15	1.35	1.39
1	A	515	A	N9-C4	-5.15	1.34	1.37
1	A	27	C	C5-C6	-5.13	1.30	1.34
1	A	294	C	C5-C6	-5.13	1.30	1.34
1	A	357	C	C5-C6	-5.13	1.30	1.34
1	A	448	G	N7-C5	-5.12	1.36	1.39
1	A	26	A	C6-N6	-5.12	1.29	1.33
1	A	684	G	C6-N1	-5.11	1.35	1.39
1	A	295	C	N1-C6	-5.09	1.34	1.37
1	A	293	C	C5-C6	-5.08	1.30	1.34
1	A	510	G	N9-C4	-5.07	1.33	1.38
1	A	337	C	C4-C5	-5.06	1.39	1.43
1	A	1451	G	C2-N3	-5.06	1.28	1.32
1	A	82	G	C6-N1	-5.06	1.36	1.39
1	A	384	C	C4-C5	-5.06	1.39	1.43
1	A	379	G	N1-C2	-5.04	1.33	1.37
1	A	93	A	N7-C5	-5.04	1.36	1.39
1	A	83	C	N1-C6	-5.04	1.34	1.37
1	A	1448	A	N9-C4	-5.03	1.34	1.37
1	A	500	C	C4-C5	-5.02	1.39	1.43
1	A	93	A	C6-N6	-5.02	1.29	1.33
1	A	13	C	C4-N4	-5.01	1.29	1.33
1	A	18	C	C4-C5	-5.01	1.39	1.43
1	A	348	A	N9-C4	-5.01	1.34	1.37
1	A	823	C	C4-C5	-5.01	1.39	1.43

All (244) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	966	G	N1-C6-O6	-21.94	106.73	119.90
1	A	966	G	C5-C6-O6	20.78	141.07	128.60
1	A	956	C	N3-C4-N4	-19.90	104.07	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	956	C	C5-C4-N4	18.06	132.84	120.20
1	A	466	G	C4-N9-C1'	12.11	142.24	126.50
1	A	466	G	C6-C5-N7	-11.89	123.26	130.40
1	A	466	G	C8-N9-C1'	-11.52	112.03	127.00
1	A	379	G	N3-C2-N2	-11.10	112.13	119.90
1	A	466	G	N3-C4-N9	10.60	132.36	126.00
1	A	448	G	N3-C2-N2	10.46	127.22	119.90
1	A	379	G	N9-C4-C5	10.34	109.54	105.40
1	A	957	C	N3-C2-O2	-10.25	114.72	121.90
1	A	466	G	C4-C5-N7	10.19	114.88	110.80
1	A	448	G	C6-C5-N7	-9.95	124.43	130.40
1	A	379	G	N3-C4-N9	-9.93	120.04	126.00
1	A	466	G	N3-C2-N2	9.74	126.72	119.90
1	A	352	C	C6-N1-C2	-9.64	116.44	120.30
1	A	448	G	N1-C2-N2	-9.52	107.63	116.20
1	A	449	C	C5-C4-N4	-9.21	113.76	120.20
1	A	957	C	N1-C2-O2	9.18	124.41	118.90
1	A	466	G	N9-C4-C5	-9.17	101.73	105.40
1	A	313	C	C2-N1-C1'	8.79	128.47	118.80
1	A	466	G	N1-C2-N2	-8.11	108.90	116.20
1	A	379	G	C5-C6-O6	7.69	133.21	128.60
1	A	1448	A	C5-N7-C8	-7.63	100.09	103.90
1	A	294	C	C5-C4-N4	-7.59	114.89	120.20
1	A	830	C	C6-N1-C2	-7.51	117.30	120.30
1	A	294	C	N1-C2-O2	7.50	123.40	118.90
1	A	972	G	C5-C6-O6	7.50	133.10	128.60
1	A	379	G	N1-C6-O6	-7.39	115.47	119.90
1	A	313	C	C6-N1-C1'	-7.28	112.07	120.80
1	A	352	C	N1-C2-O2	-7.24	114.55	118.90
1	A	313	C	N1-C2-O2	7.20	123.22	118.90
1	A	379	G	C8-N9-C4	-7.13	103.55	106.40
1	A	347	G	N3-C4-N9	-7.12	121.73	126.00
1	A	448	G	C4-C5-N7	7.10	113.64	110.80
1	A	1450	G	O5'-P-OP1	-7.02	99.38	105.70
1	A	1000	C	N3-C2-O2	-7.01	116.99	121.90
1	A	830	C	N3-C2-O2	-7.00	117.00	121.90
1	A	972	G	N1-C6-O6	-6.97	115.72	119.90
1	A	352	C	N3-C2-O2	-6.96	117.03	121.90
1	A	829	C	N1-C2-O2	6.95	123.07	118.90
1	A	337	C	C5-C4-N4	-6.89	115.37	120.20
1	A	466	G	N7-C8-N9	6.87	116.53	113.10
1	A	813	G	C4-C5-N7	6.84	113.54	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	957	C	C6-N1-C2	-6.83	117.57	120.30
1	A	510	G	N3-C4-N9	-6.82	121.91	126.00
1	A	697	C	C2-N1-C1'	6.78	126.26	118.80
5	E	63	GLY	N-CA-C	6.78	130.04	113.10
1	A	1326	A	C6-N1-C2	6.65	122.59	118.60
1	A	437	A	N1-C6-N6	-6.63	114.62	118.60
1	A	579	G	C2-N3-C4	-6.59	108.61	111.90
1	A	372	C	N3-C4-C5	6.56	124.52	121.90
1	A	103	C	N1-C2-O2	6.50	122.80	118.90
1	A	512	C	N1-C2-O2	6.50	122.80	118.90
1	A	697	C	C6-N1-C1'	-6.49	113.01	120.80
1	A	881	C	C6-N1-C2	-6.48	117.71	120.30
1	A	604	G	C2-N3-C4	-6.47	108.66	111.90
1	A	1107	C	C2-N1-C1'	6.47	125.92	118.80
1	A	701	G	C2-N3-C4	-6.46	108.67	111.90
1	A	448	G	N3-C4-N9	6.45	129.87	126.00
1	A	90	C	N1-C2-O2	6.39	122.73	118.90
1	A	466	G	C5-N7-C8	-6.35	101.12	104.30
1	A	341	A	C5-C6-N1	6.34	120.87	117.70
1	A	357	C	C5-C4-N4	-6.33	115.77	120.20
1	A	1475	C	N1-C2-O2	6.31	122.69	118.90
1	A	735	A	O4'-C1'-N9	6.28	113.23	108.20
1	A	437	A	C8-N9-C4	-6.24	103.30	105.80
1	A	375	C	N1-C2-O2	6.22	122.63	118.90
1	A	845	G	C2-N3-C4	-6.21	108.80	111.90
1	A	1467	C	N1-C2-O2	6.18	122.61	118.90
1	A	313	C	N3-C2-O2	-6.17	117.58	121.90
1	A	499	G	C2-N3-C4	-6.16	108.82	111.90
1	A	352	C	C6-N1-C1'	6.11	128.13	120.80
1	A	576	G	C4-C5-N7	6.11	113.24	110.80
1	A	1070	C	N3-C2-O2	-6.10	117.63	121.90
1	A	1448	A	C4-C5-N7	6.10	113.75	110.70
1	A	282	G	C2-N3-C4	-6.05	108.88	111.90
1	A	510	G	C2-N3-C4	-6.04	108.88	111.90
1	A	1451	G	N3-C2-N2	-6.03	115.68	119.90
1	A	526	G	C2-N3-C4	-5.99	108.90	111.90
1	A	812	A	C5-N7-C8	-5.99	100.90	103.90
1	A	64	G	C2-N3-C4	-5.99	108.90	111.90
1	A	517	G	C8-N9-C1'	5.98	134.78	127.00
1	A	449	C	N3-C4-C5	5.98	124.29	121.90
1	A	101	G	C2-N3-C4	-5.97	108.91	111.90
1	A	294	C	N3-C4-N4	5.97	122.18	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	701	G	N7-C8-N9	5.97	116.08	113.10
1	A	376	G	C2-N3-C4	-5.96	108.92	111.90
1	A	17	C	C5-C4-N4	-5.96	116.03	120.20
1	A	870	G	N7-C8-N9	5.93	116.06	113.10
1	A	708	G	C2-N3-C4	-5.89	108.95	111.90
1	A	84	G	C2-N3-C4	-5.84	108.98	111.90
1	A	352	C	N1-C2-N3	5.84	123.29	119.20
1	A	1326	A	N1-C2-N3	-5.83	126.39	129.30
1	A	372	C	C5-C4-N4	-5.82	116.13	120.20
1	A	1475	C	C2-N1-C1'	5.80	125.18	118.80
1	A	1248	A	N1-C2-N3	-5.80	126.40	129.30
1	A	1448	A	N7-C8-N9	5.79	116.69	113.80
1	A	1450	G	N3-C4-C5	5.78	131.49	128.60
18	R	131	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	A	814	C	N1-C2-O2	5.71	122.33	118.90
1	A	448	G	C4-N9-C1'	5.71	133.92	126.50
1	A	342	G	C2-N3-C4	-5.70	109.05	111.90
1	A	1451	G	N3-C4-N9	-5.69	122.59	126.00
1	A	545	G	C2-N3-C4	-5.67	109.06	111.90
1	A	547	C	N3-C4-C5	5.67	124.17	121.90
1	A	448	G	N9-C4-C5	-5.66	103.14	105.40
1	A	767	G	N3-C4-N9	-5.66	122.60	126.00
1	A	1450	G	N3-C2-N2	-5.66	115.94	119.90
1	A	449	C	N3-C4-N4	5.65	121.95	118.00
1	A	414	C	C5-C4-N4	-5.64	116.25	120.20
1	A	512	C	C5-C4-N4	-5.64	116.25	120.20
1	A	956	C	C6-N1-C1'	5.61	127.53	120.80
1	A	1475	C	C5-C4-N4	-5.61	116.28	120.20
1	A	870	G	C5-N7-C8	-5.60	101.50	104.30
1	A	826	C	N3-C4-C5	5.58	124.13	121.90
1	A	999	G	C4-C5-N7	5.57	113.03	110.80
1	A	21	A	N1-C6-N6	5.57	121.94	118.60
1	A	866	A	C5-N7-C8	-5.57	101.12	103.90
1	A	767	G	C2-N3-C4	-5.55	109.13	111.90
1	A	999	G	N1-C6-O6	5.54	123.23	119.90
4	D	142	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	A	966	G	C6-C5-N7	5.52	133.71	130.40
1	A	340	C	N1-C2-O2	5.51	122.21	118.90
1	A	1322	G	C2-N3-C4	-5.51	109.14	111.90
1	A	446	G	C2-N3-C4	-5.50	109.15	111.90
1	A	386	C	C5-C4-N4	-5.50	116.35	120.20
1	A	347	G	N3-C4-C5	5.49	131.35	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1107	C	C6-N1-C1'	-5.48	114.22	120.80
1	A	1437	G	N3-C4-N9	-5.48	122.71	126.00
1	A	103	C	C2-N1-C1'	5.48	124.83	118.80
1	A	1450	G	N3-C4-N9	-5.47	122.72	126.00
1	A	860	A	P-O3'-C3'	5.46	126.26	119.70
1	A	864	G	C2-N3-C4	-5.46	109.17	111.90
1	A	634	G	C2-N3-C4	-5.46	109.17	111.90
12	L	10	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	813	G	C5-N7-C8	-5.46	101.57	104.30
1	A	1024	C	N3-C4-C5	5.45	124.08	121.90
1	A	999	G	C2-N3-C4	-5.45	109.18	111.90
1	A	1460	G	C4-C5-N7	5.45	112.98	110.80
1	A	466	G	N3-C4-C5	-5.44	125.88	128.60
1	A	84	G	N3-C4-N9	-5.44	122.73	126.00
1	A	1326	A	N1-C6-N6	5.44	121.86	118.60
7	G	86	ASP	N-CA-C	-5.44	96.32	111.00
1	A	1451	G	N3-C4-C5	5.42	131.31	128.60
1	A	840	C	C5-C4-N4	-5.42	116.41	120.20
1	A	93	A	N7-C8-N9	5.41	116.50	113.80
1	A	19	G	C2-N3-C4	-5.40	109.20	111.90
1	A	379	G	C8-N9-C1'	5.39	134.01	127.00
1	A	670	G	N3-C4-N9	-5.39	122.76	126.00
1	A	676	G	C2-N3-C4	-5.39	109.20	111.90
1	A	765	C	N3-C4-C5	5.39	124.06	121.90
5	E	52	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	A	1447	C	C5-C4-N4	-5.39	116.43	120.20
1	A	1280	G	P-O3'-C3'	5.38	126.16	119.70
1	A	870	G	C4-C5-N7	5.38	112.95	110.80
1	A	1070	C	N1-C2-O2	5.38	122.13	118.90
22	V	54	ARG	NE-CZ-NH1	5.37	122.98	120.30
7	G	66	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	510	G	C5-C6-O6	5.35	131.81	128.60
1	A	829	C	C5-C4-N4	-5.34	116.46	120.20
1	A	1470	C	C5-C4-N4	-5.33	116.47	120.20
1	A	1362	A	O4'-C1'-N9	5.32	112.45	108.20
1	A	812	A	N7-C8-N9	5.31	116.46	113.80
1	A	765	C	C5-C4-N4	-5.30	116.49	120.20
1	A	1023	G	C2-N3-C4	-5.30	109.25	111.90
1	A	1473	C	N3-C4-C5	5.30	124.02	121.90
1	A	813	G	C2-N3-C4	-5.29	109.26	111.90
1	A	821	G	C2-N3-C4	-5.28	109.26	111.90
1	A	999	G	C5-C6-O6	-5.28	125.43	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1307	U	O4'-C1'-N1	5.28	112.42	108.20
1	A	90	C	C5-C4-N4	-5.28	116.51	120.20
1	A	375	C	C2-N1-C1'	5.27	124.59	118.80
1	A	669	C	N3-C4-C5	5.27	124.01	121.90
1	A	510	G	N1-C6-O6	-5.26	116.74	119.90
1	A	313	C	P-O3'-C3'	5.26	126.02	119.70
1	A	723	G	C2-N3-C4	-5.26	109.27	111.90
1	A	137	G	C2-N3-C4	-5.25	109.27	111.90
1	A	810	G	C2-N3-C4	-5.25	109.27	111.90
1	A	411	U	O4'-C1'-N1	5.25	112.40	108.20
1	A	386	C	N1-C2-O2	5.24	122.05	118.90
1	A	972	G	N3-C4-N9	-5.24	122.86	126.00
1	A	711	G	C2-N3-C4	-5.24	109.28	111.90
1	A	387	C	C5-C4-N4	-5.23	116.54	120.20
1	A	1475	C	C6-N1-C1'	-5.23	114.52	120.80
1	A	282	G	N3-C4-N9	-5.22	122.86	126.00
1	A	1006	U	P-O3'-C3'	5.22	125.97	119.70
22	V	99	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	21	A	C5-C6-N6	-5.21	119.54	123.70
1	A	450	A	C5-C6-N6	-5.21	119.53	123.70
1	A	1342	C	C5-C4-N4	-5.21	116.56	120.20
1	A	1468	U	N3-C4-O4	5.20	123.04	119.40
1	A	448	G	C4-C5-C6	5.20	121.92	118.80
1	A	340	C	C2-N1-C1'	5.20	124.52	118.80
1	A	340	C	C5-C4-N4	-5.20	116.56	120.20
1	A	386	C	C2-N1-C1'	5.19	124.51	118.80
1	A	813	G	C6-C5-N7	-5.19	127.29	130.40
1	A	840	C	N3-C4-C5	5.19	123.98	121.90
1	A	1013	G	N7-C8-N9	5.18	115.69	113.10
1	A	90	C	C2-N1-C1'	5.18	124.50	118.80
1	A	523	G	N7-C8-N9	5.18	115.69	113.10
1	A	152	C	N1-C2-O2	5.18	122.01	118.90
1	A	608	A	C5-C6-N1	5.18	120.29	117.70
18	R	124	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	594	C	C5-C4-N4	-5.17	116.58	120.20
1	A	505	A	C4-N9-C1'	5.17	135.60	126.30
1	A	93	A	C5-N7-C8	-5.16	101.32	103.90
1	A	1280	G	C8-N9-C4	-5.16	104.34	106.40
1	A	870	G	C6-C5-N7	-5.16	127.31	130.40
1	A	1343	A	N1-C6-N6	5.16	121.69	118.60
1	A	560	C	C5-C4-N4	-5.16	116.59	120.20
1	A	551	A	C5-C6-N1	5.15	120.28	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	14	C	C6-N1-C2	-5.15	118.24	120.30
1	A	27	C	N1-C2-O2	5.14	121.99	118.90
1	A	1372	G	C5-C6-O6	5.14	131.68	128.60
1	A	16	G	N7-C8-N9	5.13	115.67	113.10
1	A	1345	A	C4-C5-N7	5.13	113.27	110.70
1	A	684	G	C2-N3-C4	-5.13	109.34	111.90
1	A	103	C	C5-C4-N4	-5.12	116.61	120.20
1	A	286	G	N3-C2-N2	-5.12	116.31	119.90
1	A	512	C	C2-N1-C1'	5.12	124.43	118.80
1	A	999	G	N9-C4-C5	-5.10	103.36	105.40
1	A	466	G	C4-C5-C6	5.10	121.86	118.80
9	I	156	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	379	G	C6-C5-N7	5.10	133.46	130.40
1	A	1468	U	C5-C4-O4	-5.09	122.84	125.90
1	A	575	U	C5-C6-N1	5.07	125.24	122.70
1	A	956	C	C2-N1-C1'	-5.07	113.22	118.80
1	A	1364	C	C2-N1-C1'	5.07	124.38	118.80
1	A	523	G	C5-N7-C8	-5.07	101.76	104.30
1	A	551	A	C4-C5-N7	5.07	113.23	110.70
1	A	845	G	N3-C4-C5	5.07	131.13	128.60
1	A	1294	U	O4'-C1'-N1	5.06	112.25	108.20
1	A	999	G	C6-C5-N7	-5.05	127.37	130.40
1	A	336	G	O4'-C1'-N9	5.05	112.24	108.20
1	A	517	G	C4-N9-C1'	-5.05	119.94	126.50
1	A	437	A	N7-C8-N9	5.04	116.32	113.80
1	A	295	C	C5-C4-N4	-5.02	116.69	120.20
1	A	1364	C	N1-C2-O2	5.02	121.91	118.90
1	A	999	G	N1-C2-N2	-5.01	111.69	116.20
1	A	519	G	C2-N3-C4	-5.01	109.39	111.90
1	A	83	C	N3-C4-C5	5.01	123.90	121.90
1	A	286	G	C2-N3-C4	-5.00	109.40	111.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1000	C	Sidechain
1	A	352	C	Sidechain
1	A	830	C	Sidechain
2	B	6	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	31920	0	16102	146	0
2	B	1571	0	1624	12	0
3	C	1526	0	1611	7	0
4	D	1520	0	1583	19	0
5	E	1476	0	1545	16	0
6	F	1963	0	2043	25	0
7	G	1721	0	1780	20	0
8	H	961	0	1010	11	0
9	I	1704	0	1754	34	0
10	J	1022	0	1053	6	0
11	K	997	0	1078	10	0
12	L	1040	0	1101	17	0
13	M	819	0	871	2	0
14	N	1005	0	1029	11	0
15	O	1131	0	1225	22	0
16	P	1109	0	1137	14	0
17	Q	459	0	483	8	0
18	R	1225	0	1314	8	0
19	S	913	0	933	6	0
20	T	540	0	559	4	0
21	U	949	0	1000	19	0
22	V	1218	0	1231	22	0
23	W	435	0	414	4	0
24	X	799	0	823	13	0
25	Y	475	0	512	5	0
26	Z	417	0	421	5	0
27	a	514	0	547	0	0
28	b	936	0	978	0	0
29	c	351	0	418	0	0
30	d	4622	0	4729	0	0
31	A	27	0	0	0	0
31	d	2	0	0	0	0
32	Q	1	0	0	0	0
32	W	2	0	0	0	0
32	Y	1	0	0	0	0
33	d	16	0	0	0	0
34	d	62	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	65449	0	50932	397	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 5.

All (397) 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)
15:O:6:ALA:CB	15:O:7:PRO:HD3	1.39	1.41
15:O:6:ALA:CB	15:O:7:PRO:CD	2.17	1.21
15:O:6:ALA:HB3	15:O:7:PRO:HD3	1.37	1.04
15:O:6:ALA:HB1	15:O:7:PRO:CD	1.83	1.02
15:O:6:ALA:HB3	15:O:7:PRO:CD	1.90	1.00
1:A:448:G:N7	1:A:466:G:N2	2.12	0.97
15:O:61:GLU:HG2	15:O:69:MET:SD	2.04	0.96
15:O:6:ALA:HB1	15:O:7:PRO:HD3	0.94	0.94
4:D:173:GLU:O	4:D:176:LYS:O	1.89	0.89
1:A:699:G:OP2	18:R:124:ARG:NH2	2.10	0.84
1:A:1326:A:OP2	9:I:58:LYS:NZ	2.10	0.84
12:L:27:ARG:NH1	22:V:6:ASP:OD1	2.13	0.82
9:I:111:ILE:O	9:I:114:ARG:O	1.99	0.81
9:I:113:ARG:O	9:I:116:LYS:NZ	2.13	0.80
12:L:36:ILE:O	12:L:42:ARG:NH1	2.15	0.80
1:A:952:A:C6	1:A:975:G:C6	2.70	0.80
7:G:86:ASP:O	7:G:171:ALA:O	2.00	0.79
1:A:1309:A:OP1	17:Q:19:ARG:NH2	2.16	0.78
1:A:858:U:OP2	15:O:123:ARG:NH2	2.19	0.76
9:I:111:ILE:O	9:I:114:ARG:C	2.25	0.75
14:N:126:ASP:OD1	14:N:127:GLY:N	2.19	0.75
1:A:1285:U:O2'	9:I:85:PHE:O	2.05	0.75
1:A:856:A:OP1	15:O:32:ARG:NH1	2.19	0.75
1:A:949:A:N6	1:A:978:C:O2'	2.20	0.75
1:A:940:G:O2'	1:A:942:C:N4	2.20	0.74
24:X:33:ARG:NH1	24:X:53:ILE:O	2.21	0.74
5:E:52:ARG:NH1	7:G:154:ARG:O	2.19	0.74
1:A:950:U:O2'	26:Z:3:GLN:NE2	2.21	0.74
1:A:1372:G:O6	1:A:1423:U:O4	2.05	0.74
1:A:585:A:N3	10:J:105:SER:OG	2.20	0.74
12:L:90:THR:OG1	12:L:92:ASP:OD1	2.04	0.74
1:A:1387:U:OP1	11:K:45:LYS:NZ	2.18	0.74
1:A:281:U:OP1	5:E:8:ARG:NH2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1264:U:OP2	21:U:35:ARG:NH2	2.21	0.73
1:A:754:U:O2'	1:A:848:A:N1	2.22	0.73
1:A:700:U:OP1	1:A:765:C:O2'	2.07	0.73
1:A:1149:C:O2'	1:A:1154:U:O4	2.07	0.73
1:A:1284:C:O2'	9:I:175:ARG:NH1	2.22	0.72
2:B:67:LEU:HD12	2:B:89:ARG:O	1.89	0.72
1:A:951:G:O2'	1:A:952:A:O4'	2.02	0.72
1:A:190:A:N3	1:A:207:C:O2'	2.20	0.72
1:A:420:U:O2'	24:X:56:ILE:O	2.08	0.72
1:A:537:A:O2'	1:A:584:U:O4	2.07	0.71
9:I:10:TYR:OH	9:I:19:GLY:O	2.04	0.71
9:I:92:SER:OG	9:I:93:LEU:N	2.24	0.70
1:A:1194:G:OP2	22:V:41:LYS:NZ	2.21	0.70
1:A:1254:G:N2	1:A:1281:A:OP2	2.24	0.70
22:V:57:SER:OG	22:V:77:TYR:OH	2.05	0.70
1:A:308:U:O2'	8:H:99:ARG:NH1	2.25	0.70
25:Y:20:CYS:SG	25:Y:24:GLY:N	2.65	0.70
1:A:1251:U:O4	16:P:21:GLN:NE2	2.24	0.69
2:B:127:LYS:HA	2:B:130:ILE:HD12	1.73	0.69
21:U:6:GLU:N	21:U:6:GLU:OE1	2.25	0.69
1:A:837:G:O2'	1:A:853:G:O6	2.11	0.69
8:H:59:VAL:HG13	8:H:124:VAL:O	1.93	0.69
1:A:1405:G:O2'	1:A:1406:U:O4'	2.11	0.69
1:A:939:C:O2	1:A:1162:A:N6	2.25	0.68
1:A:950:U:OP1	1:A:951:G:N2	2.22	0.68
1:A:278:C:O2'	5:E:3:ASP:O	2.05	0.68
2:B:160:ARG:NH1	2:B:195:GLU:OE1	2.27	0.68
22:V:39:ARG:O	22:V:81:LYS:NZ	2.23	0.68
6:F:131:ARG:NH1	6:F:141:ASN:OD1	2.27	0.68
1:A:940:G:O6	1:A:980:C:O2'	2.13	0.67
8:H:3:THR:OG1	8:H:20:GLU:OE2	2.11	0.67
21:U:29:LEU:O	21:U:34:ARG:NH1	2.27	0.67
1:A:708:G:H1	1:A:755:G:HO2'	1.41	0.67
22:V:143:GLN:N	22:V:143:GLN:OE1	2.28	0.67
16:P:42:ARG:NH2	22:V:45:PRO:O	2.28	0.67
3:C:28:ALA:HB2	3:C:53:TYR:HD2	1.60	0.67
26:Z:33:GLU:N	26:Z:33:GLU:OE1	2.28	0.67
6:F:217:ASP:OD1	6:F:221:GLU:N	2.28	0.66
11:K:3:ILE:O	11:K:29:GLY:N	2.27	0.66
1:A:925:A:N6	1:A:1173:U:O5'	2.29	0.66
4:D:22:TRP:O	4:D:39:THR:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:6:ARG:NH2	16:P:55:LEU:O	2.28	0.66
7:G:15:LEU:HD11	7:G:30:ILE:HD13	1.77	0.66
5:E:90:ASP:OD1	7:G:154:ARG:NH2	2.29	0.66
14:N:25:TYR:HH	14:N:95:SER:HG	1.44	0.65
18:R:131:ARG:O	19:S:111:ARG:NH1	2.29	0.65
2:B:77:LYS:NZ	2:B:193:GLU:O	2.28	0.65
1:A:463:G:OP2	15:O:71:LYS:NZ	2.30	0.65
4:D:146:ARG:NH1	4:D:147:ASP:OD1	2.29	0.65
16:P:95:ILE:HG22	16:P:96:THR:H	1.60	0.65
24:X:41:VAL:O	24:X:44:LEU:O	2.15	0.65
8:H:113:SER:OG	8:H:115:GLU:OE1	2.04	0.64
9:I:105:LYS:NZ	12:L:39:GLU:OE2	2.29	0.64
21:U:54:LEU:O	21:U:57:LYS:C	2.36	0.64
1:A:1092:G:OP2	1:A:1092:G:N2	2.23	0.64
1:A:306:A:N6	1:A:314:A:OP2	2.29	0.64
1:A:393:C:OP1	5:E:117:THR:HG21	1.97	0.64
19:S:16:ASP:OD2	19:S:23:HIS:ND1	2.29	0.63
21:U:53:ARG:NH1	21:U:76:GLU:OE2	2.31	0.62
7:G:143:GLY:O	7:G:146:ARG:NH1	2.33	0.62
2:B:117:THR:HG1	2:B:167:TYR:HH	1.48	0.62
15:O:43:PRO:O	15:O:80:ASN:ND2	2.32	0.61
5:E:163:GLU:OE1	5:E:168:ARG:NH2	2.33	0.61
7:G:13:THR:OG1	7:G:39:GLU:OE2	2.18	0.61
21:U:54:LEU:O	21:U:57:LYS:O	2.19	0.60
1:A:940:G:C2	1:A:1161:A:N7	2.69	0.60
8:H:110:ASN:OD1	8:H:111:THR:N	2.34	0.60
6:F:126:ARG:NH2	6:F:230:ALA:O	2.34	0.60
9:I:68:ILE:HG22	9:I:104:VAL:HG21	1.84	0.60
20:T:25:SER:OG	20:T:26:ARG:N	2.34	0.60
1:A:27:C:O2	15:O:49:GLN:NE2	2.35	0.60
16:P:15:ASP:OD1	16:P:15:ASP:N	2.34	0.60
1:A:610:G:OP1	1:A:675:C:O2'	2.13	0.59
1:A:931:A:O2'	1:A:991:G:OP1	2.10	0.59
1:A:666:U:O2'	1:A:667:G:OP1	2.15	0.59
1:A:952:A:N6	1:A:975:G:C6	2.70	0.59
22:V:12:LEU:O	22:V:16:THR:HG22	2.02	0.59
6:F:33:ARG:NH1	6:F:80:ASP:OD2	2.36	0.59
18:R:2:ALA:HB1	18:R:6:ALA:HB3	1.83	0.59
22:V:27:LYS:O	22:V:104:GLN:NE2	2.33	0.59
1:A:686:A:O3'	18:R:2:ALA:HB2	2.01	0.59
1:A:632:G:OP1	14:N:27:ASN:ND2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:24:ILE:O	7:G:24:ILE:HG22	2.00	0.59
1:A:1254:G:O2'	1:A:1255:A:OP2	2.17	0.59
7:G:15:LEU:HD11	7:G:30:ILE:CD1	2.33	0.59
1:A:974:C:OP2	26:Z:5:TRP:NE1	2.35	0.59
1:A:69:C:N4	1:A:72:G:OP2	2.36	0.58
10:J:2:THR:OG1	10:J:3:LEU:N	2.28	0.58
1:A:645:U:O2'	1:A:646:A:OP1	2.21	0.58
22:V:137:LYS:NZ	22:V:141:GLU:OE2	2.31	0.58
8:H:50:ILE:HD12	8:H:50:ILE:H	1.69	0.58
1:A:460:G:N2	15:O:65:PRO:O	2.37	0.58
1:A:1254:G:H22	1:A:1280:G:HO2'	1.51	0.57
11:K:57:ARG:NH1	11:K:115:GLY:O	2.37	0.57
15:O:14:ARG:O	15:O:18:LEU:HD23	2.04	0.57
1:A:463:G:HO2'	1:A:478:C:HO2'	1.49	0.57
9:I:57:GLY:O	9:I:61:VAL:HG23	2.05	0.57
12:L:47:GLU:OE1	12:L:79:ARG:NH2	2.38	0.57
1:A:892:G:N1	1:A:1287:G:OP2	2.33	0.57
22:V:24:GLU:N	22:V:24:GLU:OE2	2.38	0.57
1:A:341:A:N3	1:A:353:U:O2'	2.31	0.57
6:F:165:LEU:HD12	6:F:175:GLU:HB3	1.86	0.57
1:A:966:G:N2	17:Q:2:ALA:O	2.38	0.57
1:A:1265:G:O6	21:U:35:ARG:NH1	2.37	0.57
16:P:96:THR:OG1	16:P:97:ALA:N	2.36	0.57
6:F:15:ALA:O	6:F:23:ARG:NH1	2.37	0.57
7:G:39:GLU:HB2	7:G:42:ILE:HD12	1.85	0.56
9:I:111:ILE:HD11	9:I:119:PRO:CB	2.36	0.56
21:U:77:MET:O	21:U:95:ILE:HG21	2.04	0.56
24:X:25:HIS:NE2	24:X:65:SER:OG	2.34	0.56
9:I:111:ILE:HG21	9:I:188:ILE:HD11	1.86	0.56
9:I:172:LYS:O	9:I:176:ASN:ND2	2.36	0.56
14:N:46:GLY:O	14:N:50:VAL:HG22	2.06	0.56
1:A:361:G:OP1	6:F:12:ARG:NH2	2.38	0.55
1:A:1132:A:OP1	20:T:1:MET:N	2.34	0.55
7:G:43:VAL:HG21	7:G:111:LYS:O	2.05	0.55
6:F:192:ASN:OD1	6:F:195:ARG:NH1	2.37	0.55
17:Q:36:LEU:HD22	17:Q:38:LEU:HD12	1.87	0.55
12:L:13:ALA:HA	12:L:68:GLY:HA3	1.88	0.55
1:A:1462:G:N1	1:A:1465:A:OP2	2.35	0.55
4:D:106:ARG:NE	4:D:108:ASP:OD1	2.40	0.55
1:A:1226:G:O2'	1:A:1228:A:N7	2.36	0.55
9:I:107:ALA:O	9:I:111:ILE:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:78:ARG:O	10:J:124:ARG:NH1	2.39	0.54
2:B:192:GLU:N	2:B:192:GLU:OE1	2.38	0.54
3:C:51:PRO:HA	3:C:54:VAL:HG22	1.89	0.54
18:R:87:ASP:OD1	18:R:88:LEU:N	2.39	0.54
1:A:664:A:OP2	4:D:132:ARG:NH2	2.39	0.54
19:S:59:TYR:O	19:S:61:ARG:NH1	2.35	0.54
1:A:462:A:O2'	15:O:91:ASP:OD1	2.12	0.54
1:A:956:C:C4	1:A:966:G:C6	2.96	0.54
1:A:1479:C:O2'	1:A:1480:A:O5'	2.26	0.54
25:Y:16:LEU:HD11	25:Y:56:LEU:HD21	1.90	0.54
1:A:966:G:O2'	1:A:967:G:OP1	2.23	0.53
15:O:119:ILE:CG2	15:O:122:ILE:HD12	2.39	0.53
1:A:1165:C:O2'	17:Q:9:ARG:NH1	2.39	0.53
1:A:1250:U:OP2	1:A:1252:C:N4	2.42	0.53
3:C:158:ALA:O	3:C:162:VAL:HG22	2.08	0.53
2:B:69:VAL:HG12	2:B:91:ILE:HB	1.90	0.53
6:F:88:MET:N	6:F:102:VAL:O	2.41	0.53
1:A:1299:C:N3	9:I:95:SER:OG	2.41	0.53
15:O:60:VAL:HG21	15:O:122:ILE:HD11	1.90	0.53
12:L:11:LYS:O	12:L:12:THR:OG1	2.25	0.52
9:I:111:ILE:HD11	9:I:119:PRO:HB3	1.90	0.52
1:A:1296:G:O6	12:L:10:ARG:NH2	2.42	0.52
1:A:176:A:O2'	1:A:178:G:N7	2.38	0.52
15:O:6:ALA:HB3	15:O:7:PRO:HD2	1.87	0.52
16:P:14:VAL:HG12	16:P:14:VAL:O	2.08	0.52
1:A:419:G:H21	24:X:30:THR:HG22	1.74	0.52
1:A:892:G:O6	9:I:87:ARG:NH1	2.41	0.52
4:D:60:THR:O	4:D:60:THR:OG1	2.26	0.51
6:F:58:THR:HG22	6:F:60:ARG:H	1.75	0.51
15:O:61:GLU:CG	15:O:69:MET:SD	2.90	0.51
1:A:1081:G:C6	1:A:1083:U:C4	2.98	0.51
1:A:1313:U:OP2	22:V:89:HIS:NE2	2.44	0.51
14:N:21:ILE:HB	14:N:85:VAL:HG12	1.93	0.51
2:B:67:LEU:HD11	2:B:91:ILE:HG13	1.92	0.51
3:C:65:LEU:O	3:C:69:LEU:HD23	2.11	0.51
12:L:25:ARG:N	12:L:61:ASP:OD1	2.43	0.51
9:I:132:PRO:O	9:I:157:ARG:NE	2.40	0.51
4:D:106:ARG:NE	4:D:126:MET:SD	2.84	0.51
1:A:88:G:O6	1:A:315:C:N4	2.44	0.51
4:D:31:PHE:O	4:D:34:LYS:NZ	2.44	0.51
12:L:34:GLU:OE2	12:L:34:GLU:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:92:GLU:OE2	13:M:92:GLU:N	2.38	0.51
1:A:245:G:N7	11:K:113:ARG:NH2	2.53	0.50
1:A:596:U:HO2'	1:A:597:G:H8	1.59	0.50
21:U:114:VAL:O	21:U:115:GLN:NE2	2.44	0.50
4:D:105:THR:OG1	4:D:131:ARG:O	2.17	0.50
6:F:167:LYS:O	6:F:171:ARG:N	2.40	0.50
9:I:130:SER:OG	9:I:200:ALA:HB1	2.12	0.50
22:V:22:GLU:N	22:V:22:GLU:OE1	2.44	0.50
1:A:607:G:H22	1:A:684:G:H1	1.58	0.50
14:N:25:TYR:OH	14:N:95:SER:OG	2.19	0.50
5:E:135:GLN:NE2	24:X:60:PHE:O	2.45	0.50
22:V:49:ASP:OD1	22:V:49:ASP:N	2.39	0.50
1:A:472:G:OP2	1:A:472:G:N2	2.44	0.49
5:E:166:PRO:O	5:E:170:VAL:HG23	2.12	0.49
9:I:47:SER:N	9:I:65:GLU:OE2	2.37	0.49
3:C:91:ASN:OD1	3:C:92:ALA:N	2.45	0.49
5:E:142:TYR:OH	5:E:148:GLU:OE1	2.29	0.49
22:V:62:ILE:HD11	22:V:102:LEU:HD21	1.93	0.49
19:S:40:ASP:N	19:S:40:ASP:OD2	2.45	0.49
1:A:199:C:HO2'	1:A:200:U:P	2.33	0.49
1:A:394:G:O5'	5:E:116:ARG:NH2	2.40	0.49
1:A:660:C:O2'	1:A:677:C:O4'	2.31	0.49
6:F:158:TYR:CZ	6:F:176:ILE:HD11	2.47	0.49
17:Q:23:ARG:NH1	17:Q:42:CYS:SG	2.85	0.49
14:N:74:MET:HB3	14:N:112:LEU:HD21	1.95	0.49
1:A:700:U:H2'	1:A:701:G:O4'	2.13	0.49
3:C:66:THR:HB	3:C:80:ILE:HD12	1.94	0.49
6:F:85:VAL:HG12	6:F:102:VAL:HG21	1.95	0.49
4:D:167:SER:OG	4:D:168:GLY:N	2.45	0.48
4:D:22:TRP:C	4:D:39:THR:O	2.51	0.48
6:F:68:GLU:OE1	6:F:70:ARG:NH2	2.46	0.48
16:P:10:ARG:HG2	16:P:14:VAL:HG13	1.94	0.48
6:F:37:HIS:HB2	6:F:42:SER:OG	2.12	0.48
21:U:15:GLU:OE1	21:U:15:GLU:N	2.40	0.48
14:N:63:MET:HG3	14:N:64:ILE:HD12	1.95	0.48
8:H:13:ASN:HB2	8:H:15:ILE:HG22	1.96	0.48
23:W:51:CYS:O	23:W:54:CYS:O	2.30	0.48
1:A:469:G:O2'	1:A:477:A:N1	2.35	0.48
1:A:771:A:OP2	10:J:22:LYS:NZ	2.45	0.48
5:E:3:ASP:OD1	5:E:3:ASP:N	2.46	0.48
6:F:183:ALA:HB3	6:F:199:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:G:O2'	1:A:1082:C:H2'	2.13	0.48
5:E:63:GLY:C	5:E:65:GLN:H	2.16	0.47
7:G:84:ASN:C	7:G:86:ASP:H	2.18	0.47
1:A:170:A:O3'	6:F:155:LYS:NZ	2.43	0.47
4:D:138:GLU:OE1	4:D:142:ARG:NH2	4.33	0.47
18:R:34:GLU:O	18:R:38:VAL:HG23	2.14	0.47
6:F:164:VAL:HG13	6:F:173:VAL:HG13	1.95	0.47
1:A:419:G:H21	24:X:30:THR:CG2	2.28	0.47
1:A:690:G:O2'	18:R:55:ARG:NH1	2.48	0.47
6:F:125:LEU:HD13	6:F:142:LEU:HD13	1.97	0.47
21:U:56:ARG:HG3	21:U:80:ILE:HD11	1.95	0.47
24:X:32:SER:OG	24:X:35:ASP:OD2	2.28	0.47
2:B:161:LYS:O	2:B:162:ALA:HB3	2.14	0.47
4:D:32:GLY:O	4:D:34:LYS:N	2.44	0.47
15:O:119:ILE:HG22	15:O:122:ILE:HD12	1.97	0.47
4:D:42:ASP:OD1	4:D:42:ASP:N	2.44	0.47
25:Y:47:VAL:HG12	25:Y:56:LEU:HG	1.96	0.47
1:A:975:G:N2	1:A:976:G:N3	2.62	0.46
8:H:80:GLY:C	8:H:111:THR:HG22	2.36	0.46
1:A:965:A:OP1	21:U:47:LYS:NZ	2.48	0.46
1:A:550:A:O2'	6:F:23:ARG:NE	2.47	0.46
1:A:68:C:O2'	1:A:69:C:OP1	2.29	0.46
9:I:66:ARG:NH2	9:I:159:ASP:OD1	2.44	0.46
19:S:6:LEU:HD23	19:S:6:LEU:H	1.81	0.46
22:V:66:GLY:O	22:V:68:VAL:N	2.49	0.46
1:A:952:A:C6	1:A:975:G:O6	2.69	0.46
1:A:1372:G:H1	1:A:1423:U:H3	1.64	0.46
7:G:133:SER:OG	7:G:134:ILE:N	2.49	0.46
22:V:102:LEU:HD22	22:V:119:ARG:HD2	1.98	0.46
1:A:86:A:C6	1:A:311:G:C6	3.04	0.45
9:I:111:ILE:HD13	9:I:188:ILE:HD11	1.98	0.45
12:L:24:GLY:N	12:L:60:VAL:O	2.49	0.45
1:A:956:C:N4	1:A:966:G:N1	2.64	0.45
1:A:1197:A:OP1	22:V:60:ARG:NH2	2.36	0.45
14:N:70:ALA:HB2	14:N:107:LEU:HD23	1.97	0.45
14:N:104:ILE:HA	14:N:107:LEU:HD12	1.97	0.45
22:V:16:THR:HG23	22:V:56:ALA:HB1	1.98	0.45
26:Z:5:TRP:CG	26:Z:5:TRP:O	2.69	0.45
10:J:26:TYR:OH	10:J:62:ARG:NH1	2.49	0.45
21:U:37:LEU:O	21:U:40:GLY:N	2.49	0.45
25:Y:37:VAL:HB	25:Y:47:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:A:C5	1:A:975:G:O6	2.70	0.45
6:F:221:GLU:N	6:F:221:GLU:OE1	2.50	0.45
1:A:662:C:O2	4:D:100:VAL:HG11	2.17	0.45
1:A:1246:C:O2'	9:I:177:LYS:NZ	2.29	0.45
21:U:48:LEU:HD23	21:U:52:ILE:HD12	1.99	0.45
3:C:162:VAL:HG23	3:C:164:ARG:NE	2.32	0.45
10:J:104:VAL:HG22	10:J:125:LEU:HD23	1.98	0.45
2:B:20:THR:HG22	2:B:21:GLN:H	1.82	0.45
7:G:86:ASP:OD2	7:G:220:ARG:HG3	2.16	0.45
16:P:84:LYS:N	16:P:91:ASP:OD2	2.49	0.45
9:I:114:ARG:O	9:I:116:LYS:N	2.49	0.45
22:V:106:GLU:OE1	22:V:119:ARG:NH1	2.49	0.45
1:A:1209:G:HO2'	1:A:1210:A:H8	1.63	0.45
14:N:60:TYR:O	14:N:61:ALA:HB3	2.17	0.45
6:F:144:ASP:OD2	6:F:146:SER:OG	2.18	0.45
12:L:116:PRO:O	12:L:118:LYS:NZ	2.49	0.45
1:A:956:C:C4	1:A:966:G:N1	2.85	0.44
6:F:127:ILE:O	6:F:141:ASN:O	2.35	0.44
16:P:84:LYS:O	21:U:10:ARG:NH1	2.50	0.44
1:A:360:U:O3'	6:F:12:ARG:NH2	2.50	0.44
21:U:24:ASP:OD1	21:U:25:PHE:N	2.49	0.44
11:K:104:GLU:O	11:K:105:ALA:HB3	2.18	0.44
24:X:6:ARG:NH1	24:X:22:ASP:OD2	2.50	0.44
9:I:28:VAL:HG11	9:I:34:ARG:HA	2.00	0.44
1:A:952:A:C5	1:A:975:G:C6	3.06	0.44
4:D:117:ASP:OD1	4:D:117:ASP:N	2.47	0.44
8:H:2:ALA:O	8:H:26:ALA:HB1	2.18	0.44
1:A:2:U:O2'	7:G:178:SER:O	2.36	0.44
1:A:116:U:H2'	1:A:117:C:O4'	2.18	0.44
1:A:618:U:OP2	4:D:193:LYS:NZ	2.46	0.44
1:A:906:A:OP1	21:U:112:LYS:NZ	2.48	0.44
1:A:949:A:OP2	1:A:950:U:N3	2.50	0.44
8:H:59:VAL:HG13	8:H:124:VAL:C	2.38	0.44
1:A:266:G:O2'	1:A:267:A:OP2	2.28	0.43
17:Q:28:GLY:O	17:Q:30:VAL:N	2.51	0.43
1:A:694:C:H2'	1:A:695:G:O4'	2.18	0.43
11:K:62:ILE:O	11:K:77:VAL:N	2.51	0.43
1:A:437:A:N3	1:A:437:A:H2'	2.33	0.43
1:A:940:G:C4	1:A:1161:A:N6	2.86	0.43
9:I:111:ILE:HG22	9:I:185:ALA:HB1	1.99	0.43
1:A:941:A:N6	1:A:985:A:O2'	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:43:GLU:O	4:D:45:GLU:N	2.52	0.43
1:A:1081:G:N1	1:A:1083:U:N3	2.66	0.43
7:G:145:VAL:HG11	7:G:190:PHE:HA	2.01	0.43
18:R:99:ARG:NH2	18:R:119:GLU:OE2	2.49	0.43
4:D:173:GLU:O	4:D:176:LYS:C	2.55	0.43
5:E:65:GLN:O	5:E:66:ALA:HB3	2.17	0.43
23:W:51:CYS:HB3	23:W:54:CYS:SG	2.59	0.43
1:A:543:C:H2'	1:A:544:U:O4'	2.18	0.43
1:A:972:G:H21	26:Z:32:ALA:HB3	1.83	0.43
5:E:162:ARG:NE	5:E:164:SER:OG	2.48	0.43
23:W:7:VAL:HG11	23:W:16:GLU:HG2	2.01	0.43
1:A:251:G:N2	1:A:254:C:OP2	2.49	0.43
1:A:645:U:HO2'	1:A:646:A:P	2.39	0.43
1:A:1069:C:O2'	12:L:16:ARG:NH1	2.51	0.43
2:B:143:GLU:OE1	2:B:143:GLU:N	2.51	0.43
11:K:81:VAL:HG23	11:K:100:ILE:HB	2.00	0.43
1:A:1381:G:O2'	1:A:1414:A:N6	2.39	0.42
16:P:31:GLY:O	16:P:93:HIS:NE2	2.47	0.42
1:A:1431:G:O2'	1:A:1432:G:OP1	2.30	0.42
24:X:3:ILE:HD13	24:X:23:VAL:HG22	2.02	0.42
1:A:575:U:H2'	1:A:576:G:H4'	2.00	0.42
16:P:16:LEU:H	16:P:16:LEU:HD23	1.84	0.42
1:A:513:U:O2'	1:A:865:A:OP1	2.33	0.42
1:A:1285:U:O4	9:I:91:ARG:NH2	2.41	0.42
7:G:84:ASN:OD1	7:G:88:TYR:N	2.52	0.42
22:V:10:ASP:N	22:V:10:ASP:OD1	2.51	0.42
1:A:255:A:O3'	11:K:87:ARG:NH1	2.52	0.42
1:A:1186:C:OP1	1:A:1252:C:O2'	2.31	0.42
2:B:82:PHE:O	2:B:86:THR:OG1	2.34	0.42
13:M:27:ALA:O	13:M:30:THR:C	2.57	0.42
16:P:44:ALA:HB2	16:P:66:ILE:CD1	2.49	0.42
12:L:51:LEU:HD23	12:L:99:PHE:CD1	2.55	0.42
6:F:185:VAL:HG21	6:F:230:ALA:HB1	2.02	0.42
21:U:12:TYR:CD2	21:U:28:LEU:HD21	2.55	0.42
1:A:92:C:O2'	1:A:93:A:OP2	2.24	0.42
11:K:33:ALA:HB2	11:K:57:ARG:CG	2.50	0.42
1:A:309:G:O6	11:K:25:LYS:NZ	2.38	0.41
1:A:1000:C:O2'	17:Q:44:ARG:NH1	2.48	0.41
5:E:117:THR:HG22	5:E:119:ARG:H	1.84	0.41
9:I:176:ASN:ND2	9:I:178:THR:HG22	2.35	0.41
1:A:897:G:N7	16:P:135:ASN:ND2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1321:C:O2	9:I:95:SER:HB3	2.20	0.41
9:I:118:ASN:OD1	9:I:120:ILE:N	2.51	0.41
15:O:103:VAL:CG2	15:O:126:VAL:HG13	2.49	0.41
23:W:38:ARG:NH2	23:W:59:PRO:O	2.53	0.41
15:O:103:VAL:HG22	15:O:126:VAL:HG13	2.02	0.41
20:T:1:MET:N	20:T:1:MET:SD	2.94	0.41
1:A:911:G:O2'	1:A:1148:U:OP1	2.35	0.41
5:E:153:THR:HG22	5:E:154:TYR:N	2.35	0.41
7:G:27:ILE:HG12	7:G:31:PHE:HE2	1.85	0.41
9:I:65:GLU:HA	9:I:68:ILE:HG12	2.02	0.41
12:L:41:ALA:O	12:L:44:THR:OG1	2.36	0.41
24:X:41:VAL:O	24:X:44:LEU:C	2.59	0.41
7:G:54:GLU:OE1	7:G:54:GLU:N	2.46	0.41
7:G:86:ASP:HB3	7:G:87:GLY:H	1.56	0.41
19:S:104:VAL:HG12	19:S:105:THR:N	2.35	0.41
24:X:44:LEU:O	24:X:46:LEU:N	2.54	0.41
1:A:318:G:O2'	8:H:102:ARG:O	2.37	0.41
22:V:35:VAL:O	22:V:35:VAL:HG23	2.21	0.41
1:A:313:C:O2'	1:A:314:A:OP2	2.27	0.41
1:A:656:G:H2'	1:A:657:G:C8	2.56	0.41
1:A:1242:G:HO2'	1:A:1243:C:P	2.44	0.41
1:A:1299:C:O2	9:I:94:MET:HG3	2.21	0.41
7:G:27:ILE:HG12	7:G:31:PHE:CE2	2.56	0.41
12:L:94:ASN:OD1	12:L:94:ASN:N	2.54	0.41
17:Q:23:ARG:HB3	17:Q:24:CYS:H	1.72	0.41
25:Y:63:VAL:HG12	25:Y:64:LEU:N	2.35	0.41
1:A:157:A:O2'	1:A:158:U:O2	2.23	0.40
1:A:10:G:H8	1:A:1345:A:HO2'	1.67	0.40
1:A:912:A:N3	1:A:917:A:O2'	2.49	0.40
22:V:140:LEU:CD1	22:V:147:LEU:HD23	2.51	0.40
24:X:84:GLU:O	24:X:88:VAL:HG23	2.21	0.40
9:I:74:SER:OG	9:I:88:ARG:O	2.39	0.40
1:A:940:G:N2	1:A:1161:A:OP2	2.36	0.40
12:L:92:ASP:OD1	12:L:92:ASP:N	2.43	0.40
20:T:24:PHE:CD1	20:T:54:ILE:HD12	2.57	0.40
21:U:83:HIS:HB3	21:U:90:PHE:HB3	2.03	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	193/195 (99%)	174 (90%)	18 (9%)	1 (0%)	29	61
3	C	191/193 (99%)	182 (95%)	9 (5%)	0	100	100
4	D	182/184 (99%)	161 (88%)	20 (11%)	1 (0%)	29	61
5	E	176/178 (99%)	157 (89%)	17 (10%)	2 (1%)	14	41
6	F	239/241 (99%)	211 (88%)	26 (11%)	2 (1%)	19	49
7	G	218/220 (99%)	201 (92%)	16 (7%)	1 (0%)	29	61
8	H	123/125 (98%)	109 (89%)	14 (11%)	0	100	100
9	I	212/214 (99%)	199 (94%)	12 (6%)	1 (0%)	29	61
10	J	127/129 (98%)	113 (89%)	14 (11%)	0	100	100
11	K	124/126 (98%)	110 (89%)	14 (11%)	0	100	100
12	L	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
13	M	100/102 (98%)	91 (91%)	9 (9%)	0	100	100
14	N	131/133 (98%)	117 (89%)	14 (11%)	0	100	100
15	O	142/144 (99%)	128 (90%)	10 (7%)	4 (3%)	5	17
16	P	134/136 (98%)	122 (91%)	12 (9%)	0	100	100
17	Q	54/56 (96%)	44 (82%)	10 (18%)	0	100	100
18	R	149/151 (99%)	139 (93%)	9 (6%)	1 (1%)	22	53
19	S	109/111 (98%)	101 (93%)	8 (7%)	0	100	100
20	T	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
21	U	113/115 (98%)	103 (91%)	10 (9%)	0	100	100
22	V	147/149 (99%)	138 (94%)	6 (4%)	3 (2%)	7	24
23	W	54/56 (96%)	44 (82%)	10 (18%)	0	100	100
24	X	95/97 (98%)	87 (92%)	8 (8%)	0	100	100
25	Y	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
26	Z	48/50 (96%)	38 (79%)	10 (21%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	a	64/66 (97%)	51 (80%)	12 (19%)	1 (2%)	9	31
28	b	121/123 (98%)	110 (91%)	11 (9%)	0	100	100
29	c	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
30	d	578/594 (97%)	501 (87%)	73 (13%)	4 (1%)	22	53
All	All	4112/4184 (98%)	3700 (90%)	391 (10%)	21 (0%)	32	61

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	O	6	ALA
15	O	63	LYS
22	V	35	VAL
5	E	63	GLY
7	G	85	ARG
30	d	362	ASN
5	E	112	LYS
22	V	143	GLN
27	a	4	GLU
2	B	7	PRO
4	D	177	GLU
15	O	64	GLN
22	V	34	PHE
9	I	115	THR
30	d	98	ASN
30	d	277	LEU
6	F	205	PHE
6	F	206	PRO
18	R	63	VAL
15	O	111	PRO
30	d	106	GLY

5.3.2 Protein sidechains (i)

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	169/169 (100%)	169 (100%)	0	100	100
3	C	155/155 (100%)	153 (99%)	2 (1%)	69	91
4	D	159/159 (100%)	159 (100%)	0	100	100
5	E	157/157 (100%)	155 (99%)	2 (1%)	69	91
6	F	212/212 (100%)	212 (100%)	0	100	100
7	G	182/182 (100%)	177 (97%)	5 (3%)	44	78
8	H	103/105 (98%)	103 (100%)	0	100	100
9	I	178/178 (100%)	177 (99%)	1 (1%)	86	96
10	J	105/105 (100%)	105 (100%)	0	100	100
11	K	102/102 (100%)	101 (99%)	1 (1%)	76	93
12	L	108/108 (100%)	108 (100%)	0	100	100
13	M	91/91 (100%)	91 (100%)	0	100	100
14	N	100/100 (100%)	99 (99%)	1 (1%)	76	93
15	O	118/118 (100%)	117 (99%)	1 (1%)	81	94
16	P	114/114 (100%)	111 (97%)	3 (3%)	46	79
17	Q	46/46 (100%)	44 (96%)	2 (4%)	29	62
18	R	130/130 (100%)	129 (99%)	1 (1%)	81	94
19	S	98/98 (100%)	97 (99%)	1 (1%)	76	93
20	T	59/59 (100%)	59 (100%)	0	100	100
21	U	103/103 (100%)	103 (100%)	0	100	100
22	V	124/124 (100%)	124 (100%)	0	100	100
23	W	50/50 (100%)	49 (98%)	1 (2%)	55	84
24	X	86/86 (100%)	86 (100%)	0	100	100
25	Y	56/56 (100%)	56 (100%)	0	100	100
26	Z	42/42 (100%)	42 (100%)	0	100	100
27	a	55/55 (100%)	53 (96%)	2 (4%)	35	69
28	b	98/98 (100%)	98 (100%)	0	100	100
29	c	35/35 (100%)	31 (89%)	4 (11%)	5	18
30	d	504/519 (97%)	497 (99%)	7 (1%)	67	90
All	All	3539/3556 (100%)	3505 (99%)	34 (1%)	77	93

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	43	LYS
3	C	145	ARG
5	E	3	ASP
5	E	62	ARG
7	G	24	ILE
7	G	25	THR
7	G	86	ASP
7	G	176	VAL
7	G	220	ARG
9	I	215	ARG
11	K	87	ARG
14	N	138	ARG
15	O	5	LYS
16	P	3	ASP
16	P	10	ARG
16	P	90	LYS
17	Q	3	LYS
17	Q	23	ARG
18	R	138	LYS
19	S	69	VAL
23	W	38	ARG
27	a	34	ARG
27	a	48	VAL
29	c	6	ARG
29	c	32	LYS
29	c	36	LEU
29	c	37	ILE
30	d	54	CYS
30	d	69	VAL
30	d	71	LEU
30	d	134	VAL
30	d	366	LYS
30	d	369	GLU
30	d	411	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	21	GLN
2	B	177	ASN
6	F	121	ASN
8	H	13	ASN
11	K	5	GLN

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Mol	Chain	Res	Type
12	L	5	GLN
19	S	29	HIS
26	Z	3	GLN
30	d	70	ASN
30	d	126	ASN
30	d	158	ASN
30	d	164	HIS
30	d	448	ASN
30	d	450	HIS
30	d	456	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1484/1485 (99%)	303 (20%)	34 (2%)

All (303) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	C
1	A	14	C
1	A	33	U
1	A	39	U
1	A	40	C
1	A	42	G
1	A	45	U
1	A	47	A
1	A	65	G
1	A	69	C
1	A	71	U
1	A	78	A
1	A	82	G
1	A	92	C
1	A	93	A
1	A	96	A
1	A	98	C
1	A	107	A
1	A	109	C
1	A	119	G
1	A	135	G
1	A	141	C

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Mol	Chain	Res	Type
1	A	158	U
1	A	168	G
1	A	174	G
1	A	177	G
1	A	186	G
1	A	190	A
1	A	192	A
1	A	193	G
1	A	198	U
1	A	199	C
1	A	200	U
1	A	201	G
1	A	205	G
1	A	216	G
1	A	225	C
1	A	229	U
1	A	230	U
1	A	232	G
1	A	235	A
1	A	236	G
1	A	243	G
1	A	251	G
1	A	252	C
1	A	258	A
1	A	264	A
1	A	265	A
1	A	266	G
1	A	267	A
1	A	274	C
1	A	286	G
1	A	291	A
1	A	306	A
1	A	309	G
1	A	313	C
1	A	314	A
1	A	315	C
1	A	317	G
1	A	329	A
1	A	332	G
1	A	337	C
1	A	338	A
1	A	339	G

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Mol	Chain	Res	Type
1	A	341	A
1	A	343	G
1	A	347	G
1	A	348	A
1	A	352	C
1	A	357	C
1	A	358	A
1	A	378	G
1	A	382	A
1	A	391	G
1	A	393	C
1	A	394	G
1	A	395	U
1	A	399	A
1	A	400	A
1	A	401	C
1	A	402	G
1	A	412	U
1	A	419	G
1	A	424	A
1	A	425	A
1	A	427	A
1	A	436	A
1	A	437	A
1	A	438	U
1	A	439	A
1	A	448	G
1	A	450	A
1	A	453	G
1	A	454	C
1	A	460	G
1	A	461	C
1	A	469	G
1	A	474	A
1	A	475	A
1	A	489	A
1	A	503	U
1	A	505	A
1	A	506	U
1	A	509	G
1	A	514	A
1	A	515	A

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Mol	Chain	Res	Type
1	A	518	C
1	A	519	G
1	A	521	C
1	A	529	G
1	A	538	A
1	A	547	C
1	A	560	C
1	A	575	U
1	A	576	G
1	A	580	G
1	A	596	U
1	A	599	G
1	A	608	A
1	A	629	U
1	A	630	A
1	A	631	G
1	A	645	U
1	A	646	A
1	A	662	C
1	A	665	G
1	A	666	U
1	A	667	G
1	A	674	G
1	A	677	C
1	A	691	G
1	A	698	G
1	A	703	G
1	A	724	A
1	A	736	U
1	A	737	A
1	A	742	G
1	A	758	A
1	A	760	G
1	A	771	A
1	A	789	G
1	A	790	A
1	A	817	U
1	A	819	A
1	A	832	G
1	A	834	G
1	A	837	G
1	A	849	G

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Mol	Chain	Res	Type
1	A	861	A
1	A	866	A
1	A	869	G
1	A	873	G
1	A	881	C
1	A	882	U
1	A	883	A
1	A	890	G
1	A	893	G
1	A	908	U
1	A	916	A
1	A	917	A
1	A	919	G
1	A	920	C
1	A	922	G
1	A	923	G
1	A	924	G
1	A	925	A
1	A	930	C
1	A	941	A
1	A	942	C
1	A	943	G
1	A	947	G
1	A	949	A
1	A	950	U
1	A	951	G
1	A	952	A
1	A	954	G
1	A	957	C
1	A	958	A
1	A	960	G
1	A	961	C
1	A	965	A
1	A	966	G
1	A	967	G
1	A	972	G
1	A	974	C
1	A	975	G
1	A	976	G
1	A	978	C
1	A	980	C
1	A	981	G

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Mol	Chain	Res	Type
1	A	986	G
1	A	987	A
1	A	991	G
1	A	1006	U
1	A	1007	C
1	A	1035	G
1	A	1036	U
1	A	1042	A
1	A	1071	A
1	A	1079	C
1	A	1082	C
1	A	1084	G
1	A	1087	G
1	A	1090	G
1	A	1091	A
1	A	1093	G
1	A	1094	C
1	A	1095	A
1	A	1108	C
1	A	1109	G
1	A	1115	G
1	A	1116	A
1	A	1120	G
1	A	1130	G
1	A	1133	G
1	A	1140	A
1	A	1142	G
1	A	1145	A
1	A	1146	G
1	A	1149	C
1	A	1150	A
1	A	1151	G
1	A	1161	A
1	A	1164	C
1	A	1174	A
1	A	1176	A
1	A	1185	A
1	A	1187	A
1	A	1190	G
1	A	1197	A
1	A	1206	U
1	A	1207	C

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Mol	Chain	Res	Type
1	A	1219	G
1	A	1228	A
1	A	1229	A
1	A	1243	C
1	A	1249	G
1	A	1250	U
1	A	1251	U
1	A	1254	G
1	A	1266	C
1	A	1269	C
1	A	1281	A
1	A	1285	U
1	A	1295	A
1	A	1296	G
1	A	1302	G
1	A	1309	A
1	A	1312	A
1	A	1313	U
1	A	1319	G
1	A	1328	G
1	A	1331	C
1	A	1334	G
1	A	1346	C
1	A	1347	A
1	A	1358	C
1	A	1363	C
1	A	1366	G
1	A	1372	G
1	A	1376	C
1	A	1377	G
1	A	1378	G
1	A	1379	A
1	A	1380	U
1	A	1382	A
1	A	1383	G
1	A	1387	U
1	A	1393	C
1	A	1395	C
1	A	1396	U
1	A	1398	C
1	A	1400	G
1	A	1404	G

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Mol	Chain	Res	Type
1	A	1406	U
1	A	1408	G
1	A	1413	G
1	A	1414	A
1	A	1418	U
1	A	1419	G
1	A	1421	G
1	A	1427	U
1	A	1429	A
1	A	1430	G
1	A	1432	G
1	A	1433	G
1	A	1436	A
1	A	1439	A
1	A	1440	G
1	A	1443	G
1	A	1445	A
1	A	1448	A
1	A	1449	A
1	A	1450	G
1	A	1452	U
1	A	1463	G
1	A	1465	A
1	A	1475	C
1	A	1476	G
1	A	1480	A
1	A	1482	C
1	A	1483	U
1	A	1484	C

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	38	G
1	A	68	C
1	A	92	C
1	A	199	C
1	A	228	A
1	A	235	A
1	A	266	G
1	A	290	G
1	A	313	C

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Mol	Chain	Res	Type
1	A	401	C
1	A	411	U
1	A	437	A
1	A	438	U
1	A	453	G
1	A	460	G
1	A	574	U
1	A	575	U
1	A	630	A
1	A	661	G
1	A	831	U
1	A	860	A
1	A	882	U
1	A	966	G
1	A	974	C
1	A	990	A
1	A	1006	U
1	A	1150	A
1	A	1206	U
1	A	1242	G
1	A	1249	G
1	A	1280	G
1	A	1295	A
1	A	1431	G
1	A	1444	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 33 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
34	ANP	d	603	31	29,33,33	4.61	15 (51%)	31,52,52	2.25	5 (16%)
33	SF4	d	601	30	0,12,12	-	-	-		
33	SF4	d	602	30	0,12,12	-	-	-		
34	ANP	d	605	31	29,33,33	4.61	15 (51%)	31,52,52	2.12	3 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	ANP	d	603	31	-	7/14/38/38	0/3/3/3
33	SF4	d	601	30	-	-	0/6/5/5
33	SF4	d	602	30	-	-	0/6/5/5
34	ANP	d	605	31	-	4/14/38/38	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	d	603	ANP	C2'-C1'	-15.95	1.29	1.53
34	d	605	ANP	C2'-C1'	-15.66	1.30	1.53
34	d	605	ANP	O4'-C1'	14.69	1.61	1.41
34	d	603	ANP	O4'-C1'	14.50	1.61	1.41
34	d	603	ANP	O4'-C4'	-6.68	1.30	1.45
34	d	605	ANP	O4'-C4'	-6.48	1.30	1.45
34	d	605	ANP	PB-O3A	4.35	1.64	1.59
34	d	603	ANP	PB-O3A	3.75	1.63	1.59
34	d	603	ANP	O3'-C3'	-3.26	1.35	1.43
34	d	605	ANP	C6-N6	3.11	1.45	1.34
34	d	605	ANP	O3'-C3'	-3.07	1.35	1.43
34	d	603	ANP	C6-N6	3.03	1.45	1.34
34	d	603	ANP	C5-C4	-2.97	1.33	1.40
34	d	605	ANP	PB-O1B	2.95	1.50	1.46
34	d	605	ANP	PG-O1G	2.87	1.50	1.46
34	d	605	ANP	C5-C4	-2.77	1.33	1.40
34	d	603	ANP	O2'-C2'	2.68	1.49	1.43
34	d	605	ANP	O2'-C2'	2.67	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	d	603	ANP	PB-O2B	-2.63	1.49	1.56
34	d	603	ANP	PG-O2G	-2.62	1.49	1.56
34	d	605	ANP	PB-O2B	-2.53	1.49	1.56
34	d	603	ANP	PG-O3G	-2.43	1.50	1.56
34	d	605	ANP	PB-N3B	2.35	1.69	1.63
34	d	603	ANP	PB-N3B	2.33	1.69	1.63
34	d	603	ANP	PG-N3B	2.31	1.69	1.63
34	d	603	ANP	PG-O1G	2.26	1.49	1.46
34	d	603	ANP	PB-O1B	2.25	1.49	1.46
34	d	605	ANP	PG-O3G	-2.21	1.50	1.56
34	d	605	ANP	PG-O2G	-2.17	1.50	1.56
34	d	605	ANP	PG-N3B	2.09	1.68	1.63

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	d	605	ANP	C5-C6-N6	7.37	131.55	120.35
34	d	603	ANP	C5-C6-N6	7.10	131.14	120.35
34	d	603	ANP	N3-C2-N1	-5.71	119.75	128.68
34	d	605	ANP	N3-C2-N1	-5.23	120.51	128.68
34	d	605	ANP	N6-C6-N1	-4.78	108.66	118.57
34	d	603	ANP	N6-C6-N1	-4.77	108.68	118.57
34	d	603	ANP	C3'-C2'-C1'	3.87	106.81	100.98
34	d	603	ANP	PB-O3A-PA	-2.70	123.09	132.62

There are no chirality outliers.

All (11) torsion outliers are listed below:

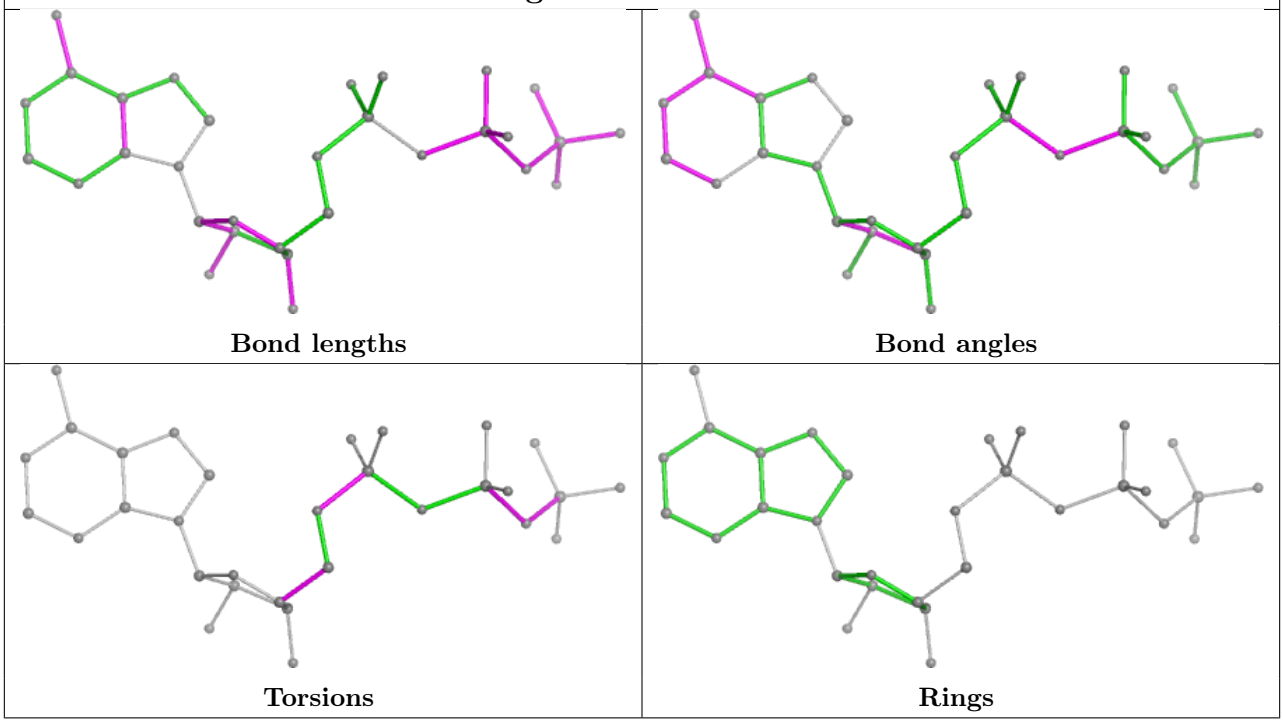
Mol	Chain	Res	Type	Atoms
34	d	603	ANP	PB-N3B-PG-O1G
34	d	603	ANP	PG-N3B-PB-O1B
34	d	603	ANP	C5'-O5'-PA-O1A
34	d	603	ANP	C5'-O5'-PA-O2A
34	d	603	ANP	C5'-O5'-PA-O3A
34	d	605	ANP	PB-N3B-PG-O1G
34	d	603	ANP	O4'-C4'-C5'-O5'
34	d	605	ANP	O4'-C4'-C5'-O5'
34	d	603	ANP	C3'-C4'-C5'-O5'
34	d	605	ANP	PB-O3A-PA-O2A
34	d	605	ANP	PB-O3A-PA-O1A

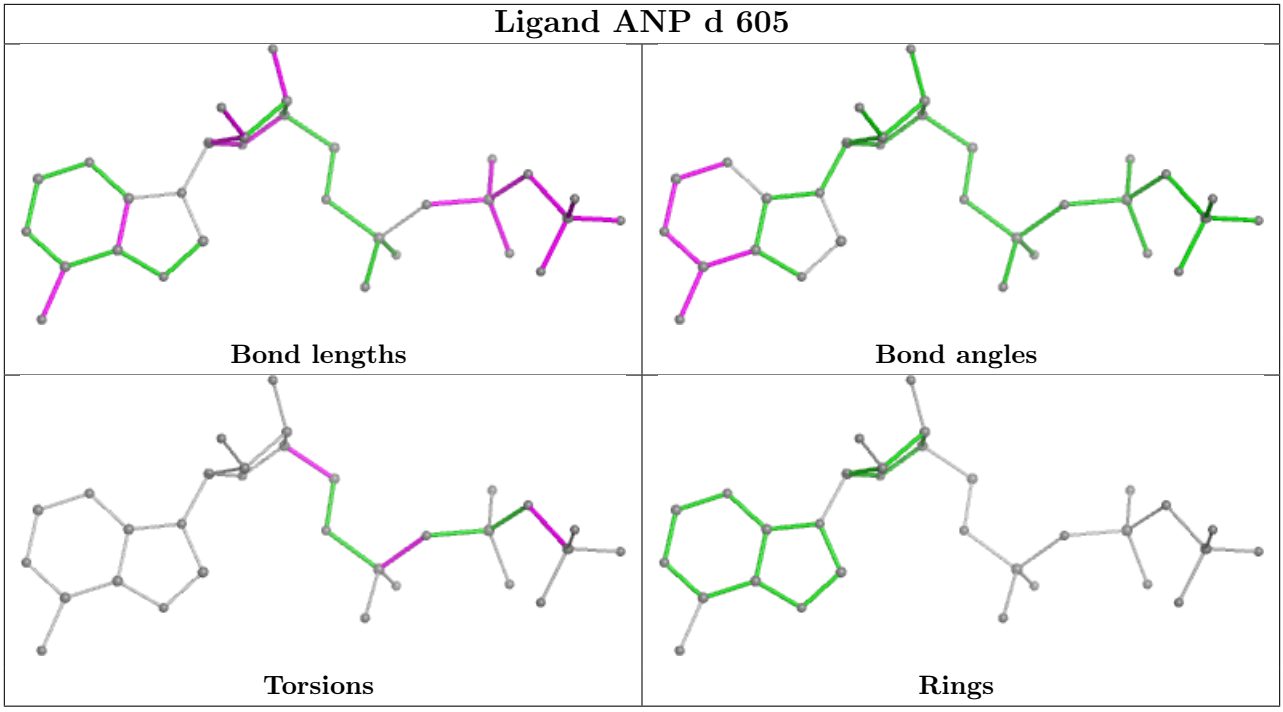
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ANP d 603





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.

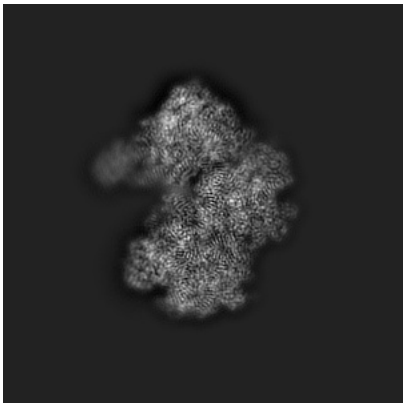
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10519. These allow visual inspection of the internal detail of the map and identification of artifacts.

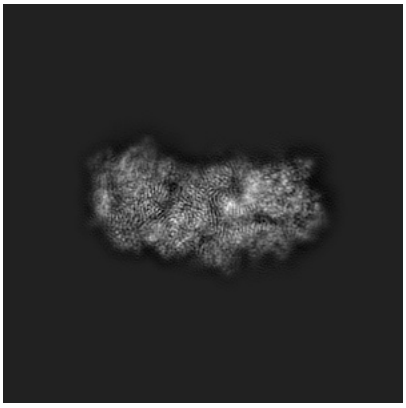
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

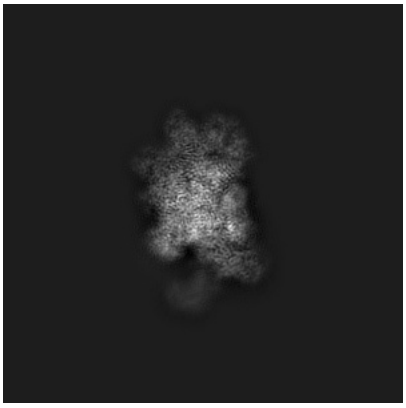
6.1.1 Primary map



X



Y

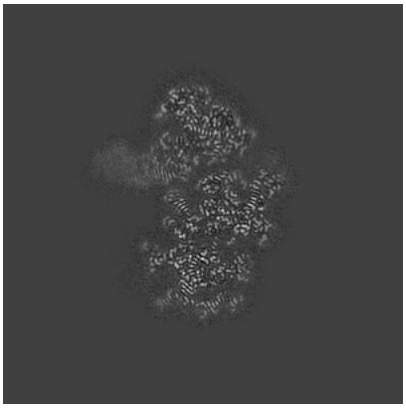


Z

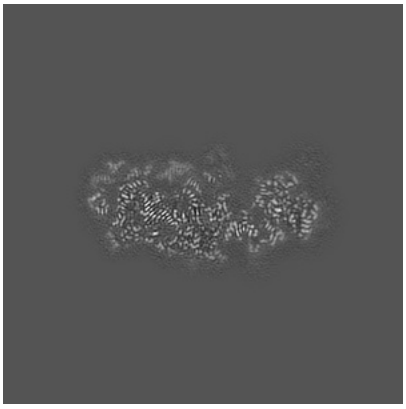
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

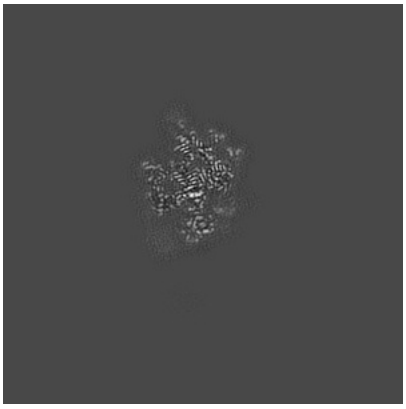
6.2.1 Primary map



X Index: 180



Y Index: 180

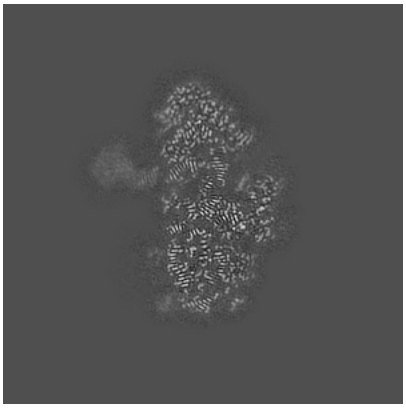


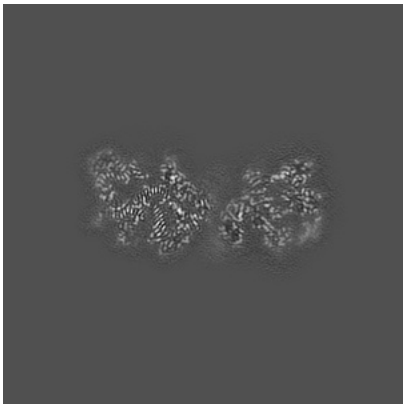
Z Index: 180

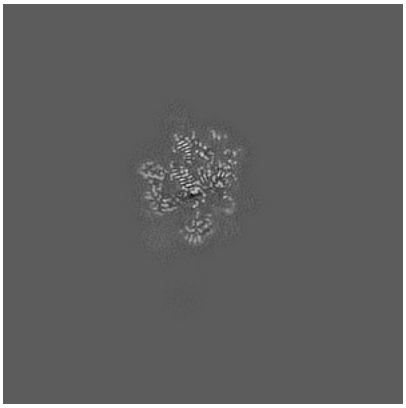
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 173

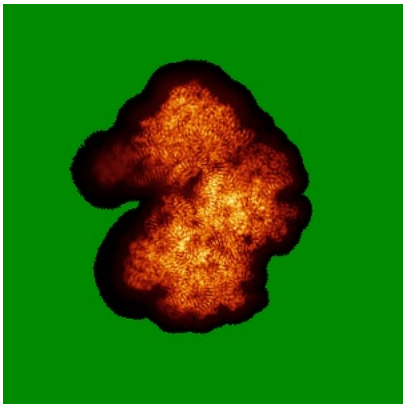

Y Index: 159

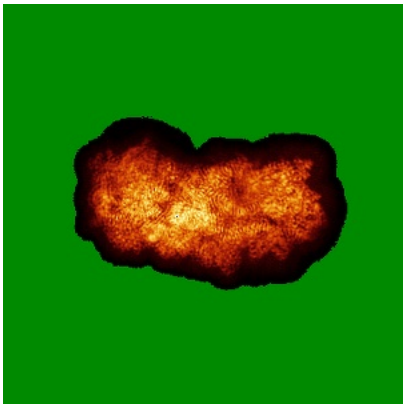

Z Index: 182

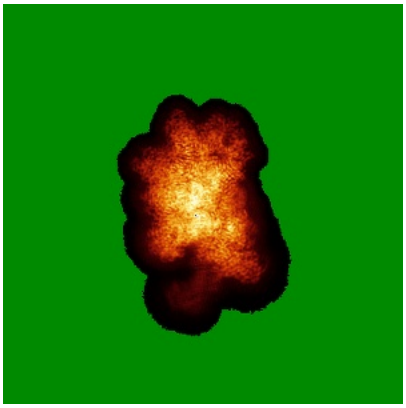
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

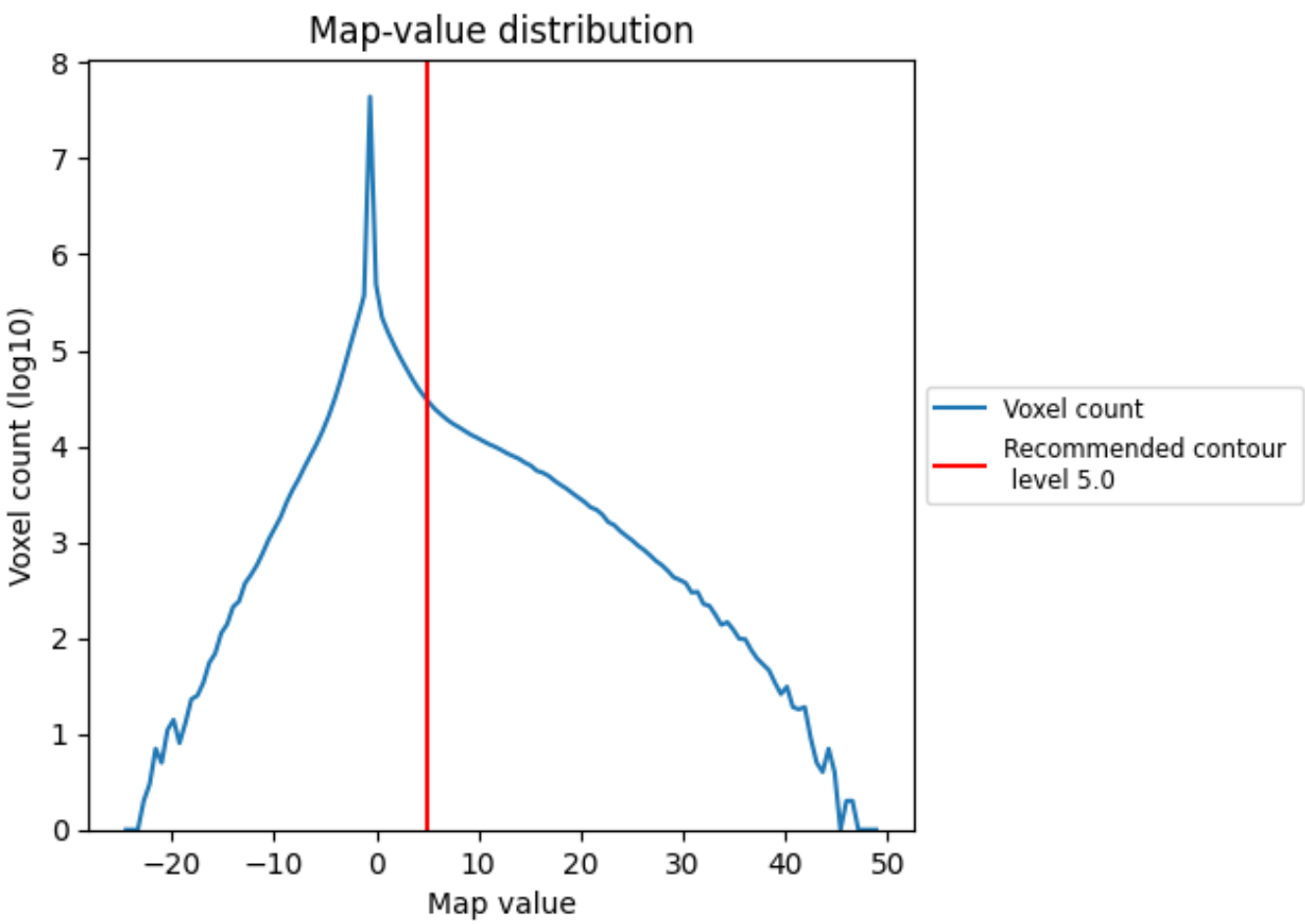
6.6 Mask visualisation (i)

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

7 Map analysis (i)

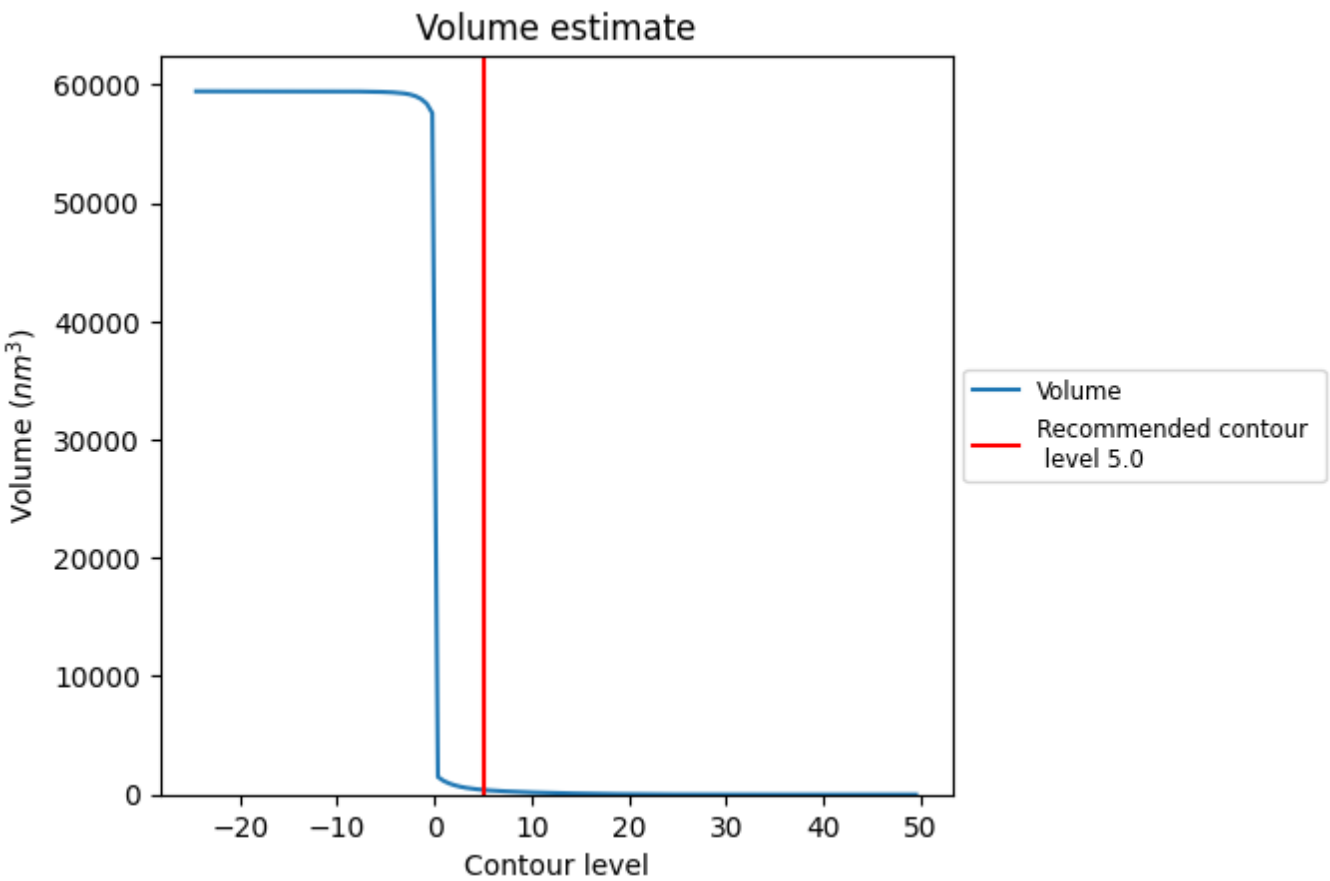
This section contains the results of statistical analysis of the map.

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.

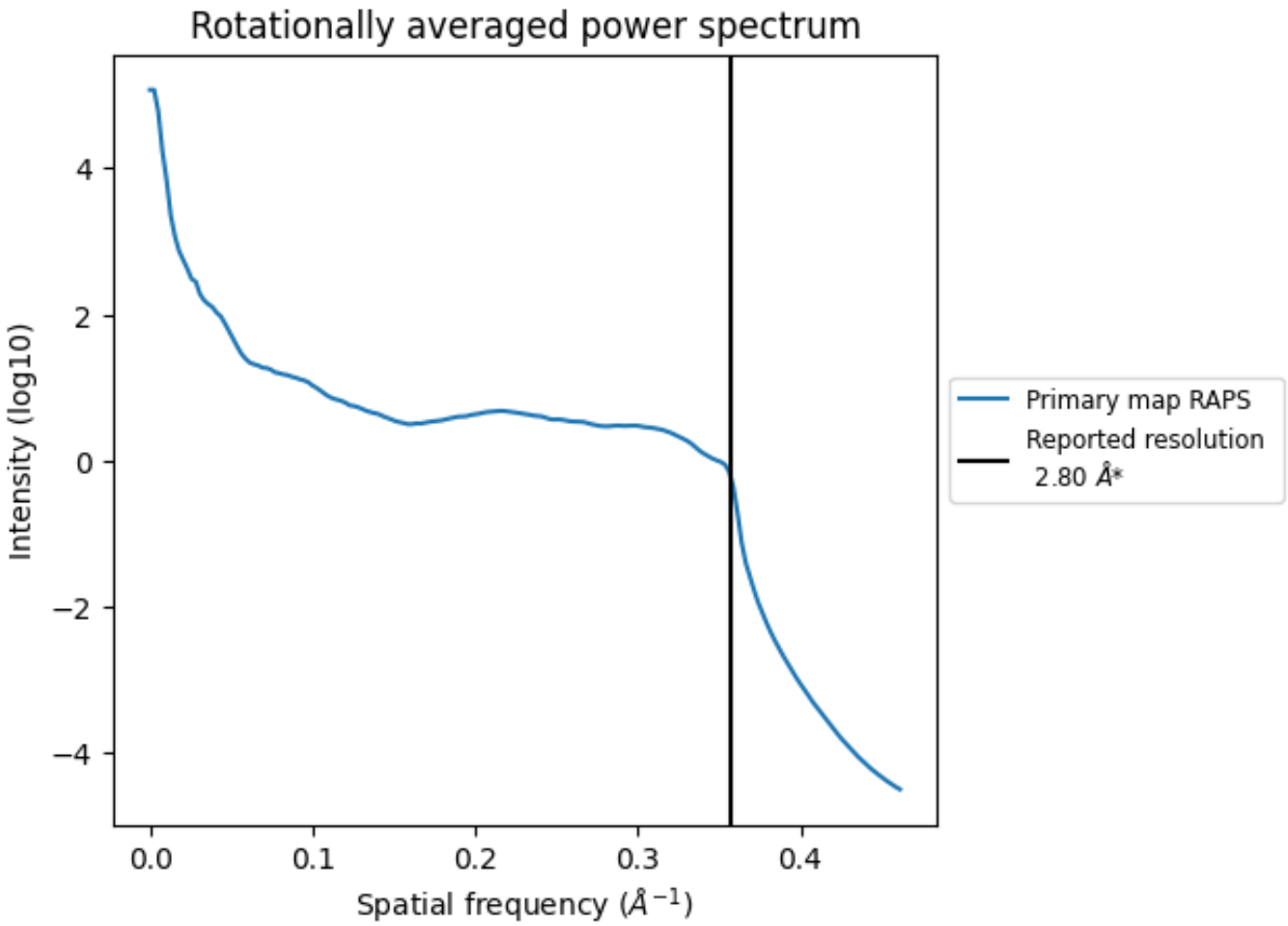
7.2 Volume estimate (i)



The volume at the recommended contour level is 397 nm^3; this corresponds to an approximate mass of 358 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 (i)

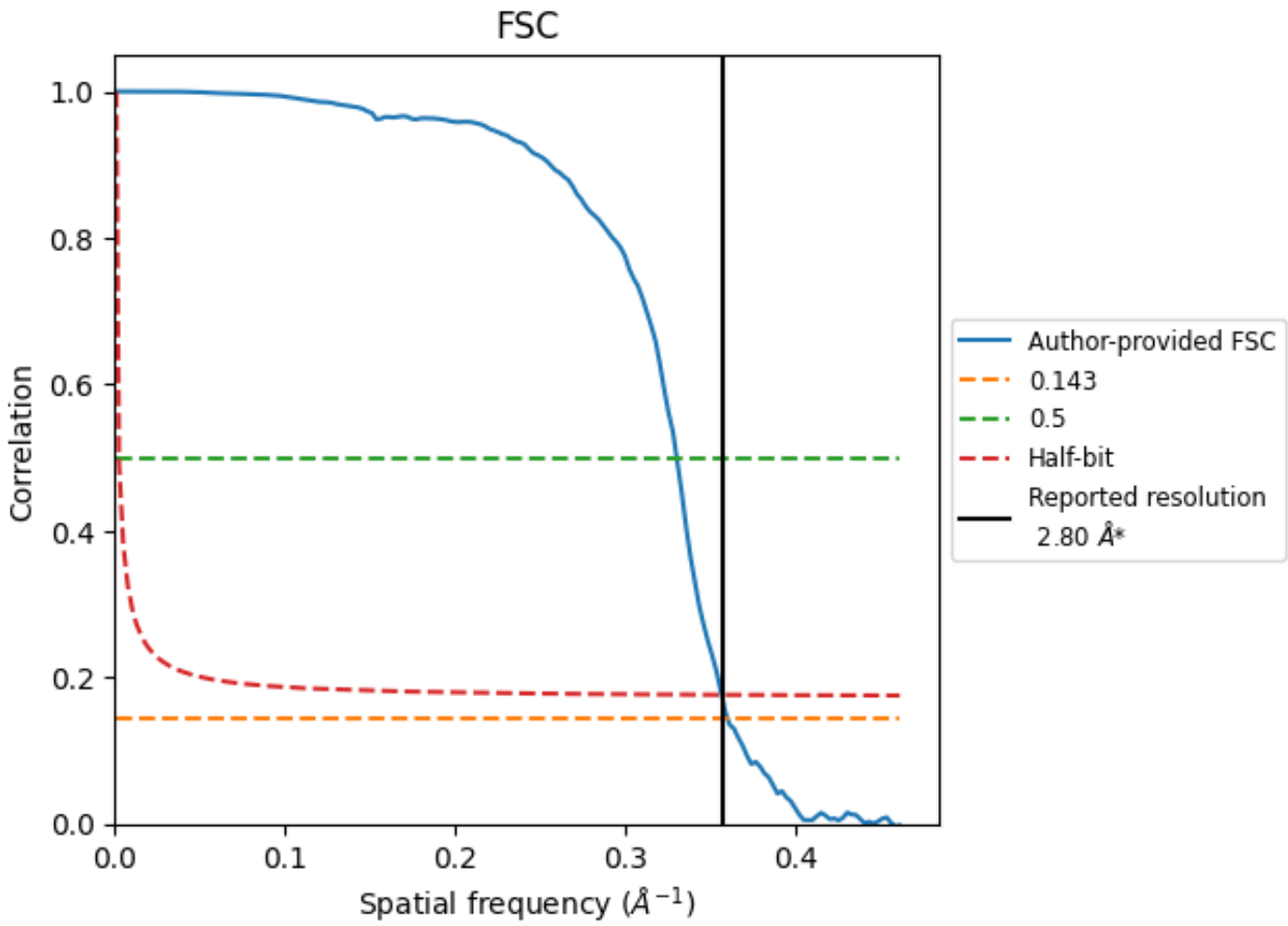


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

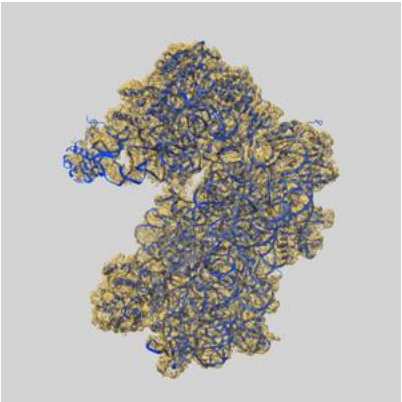
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.78	3.03	2.80
Unmasked-calculated*	-	-	-

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

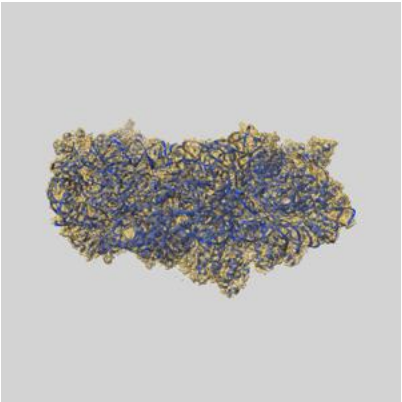
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10519 and PDB model 6TMF. Per-residue inclusion information can be found in section 3 on page 11.

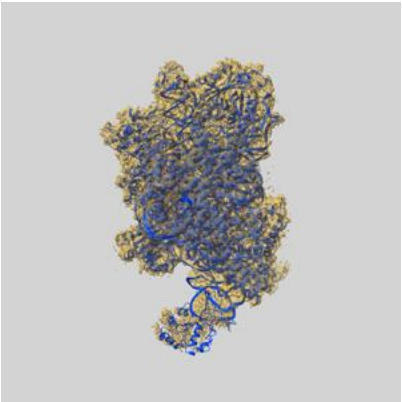
9.1 Map-model overlay (i)



X



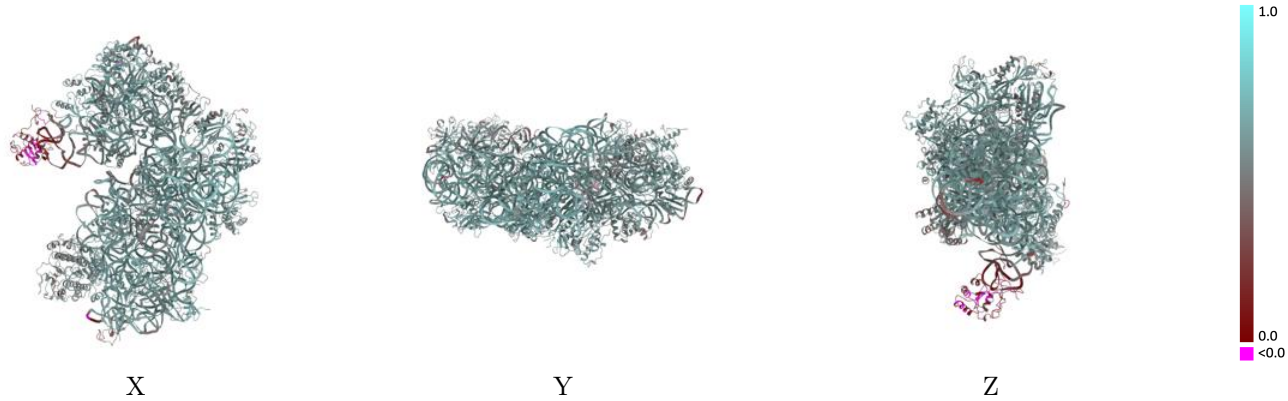
Y



Z

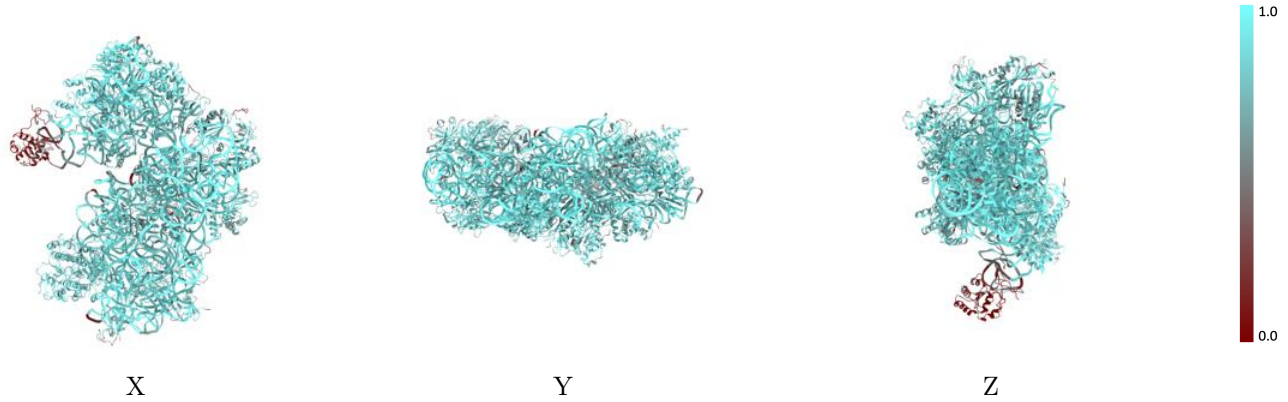
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



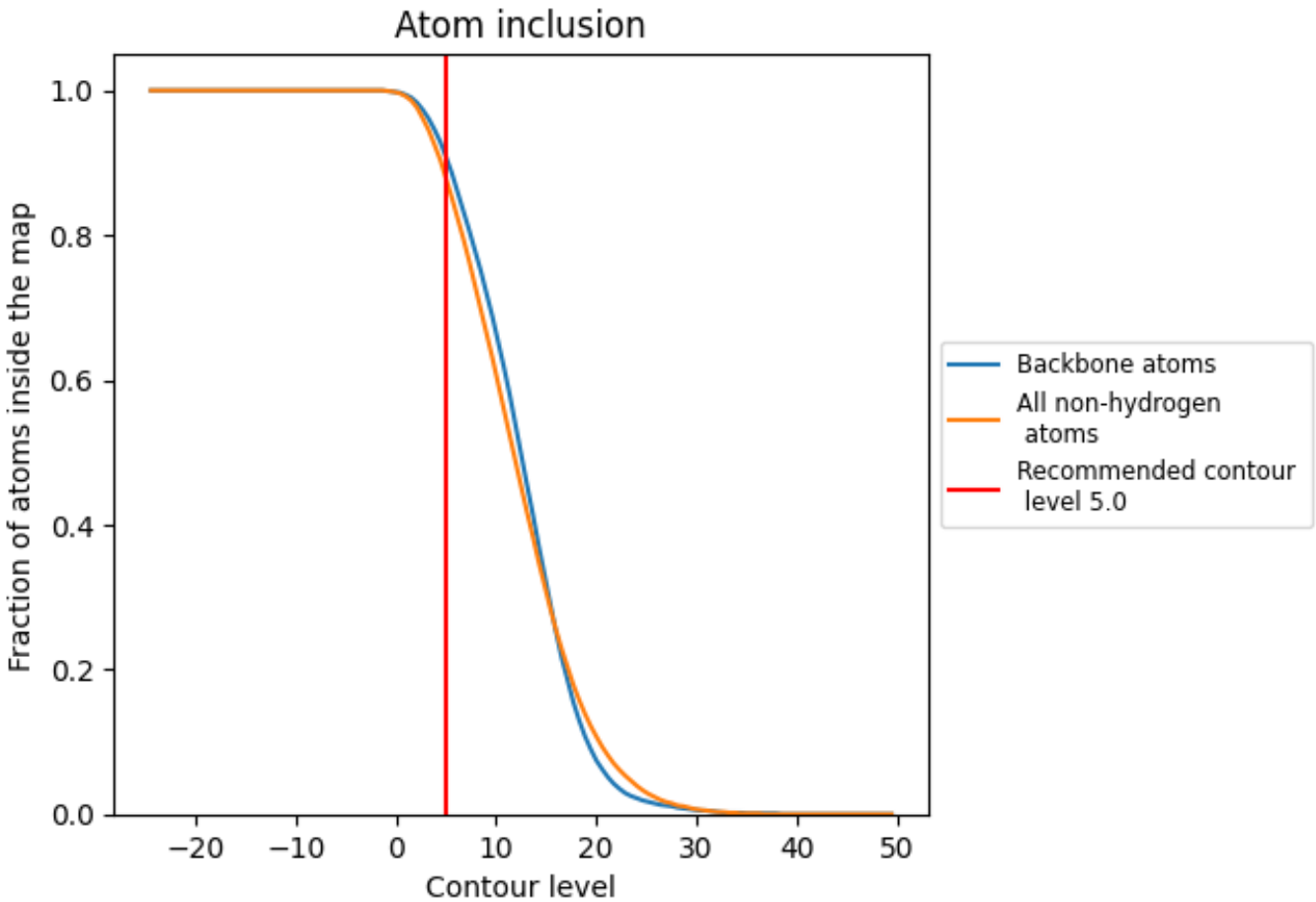
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.0).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (5.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8780	0.5830
A	0.9430	0.6100
B	0.8350	0.5900
C	0.8270	0.5380
D	0.7900	0.5580
E	0.8350	0.5960
F	0.8870	0.6140
G	0.8670	0.6190
H	0.7700	0.5410
I	0.8770	0.5710
J	0.8890	0.6280
K	0.8500	0.5990
L	0.9030	0.5970
M	0.8020	0.5180
N	0.7290	0.5510
O	0.8480	0.6160
P	0.8970	0.5660
Q	0.7730	0.5410
R	0.8450	0.5930
S	0.8530	0.6000
T	0.8380	0.5450
U	0.8910	0.5730
V	0.9100	0.5880
W	0.8780	0.6120
X	0.8020	0.5870
Y	0.7700	0.5530
Z	0.0680	0.1720
a	0.8010	0.5280
b	0.1220	0.1360
c	0.8370	0.6170
d	0.8380	0.5340