



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 02:09 AM UTC

PDB ID : 8OJ0 / pdb_00008oj0
EMDB ID : EMD-16902
Title : 60S ribosomal subunit bound to the E3-UFM1 complex - state 2 (native)
Authors : Penchev, I.; DaRosa, P.A.; Becker, T.; Beckmann, R.; Kopito, R.
Deposited on : 2023-03-23
Resolution : 3.30 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:

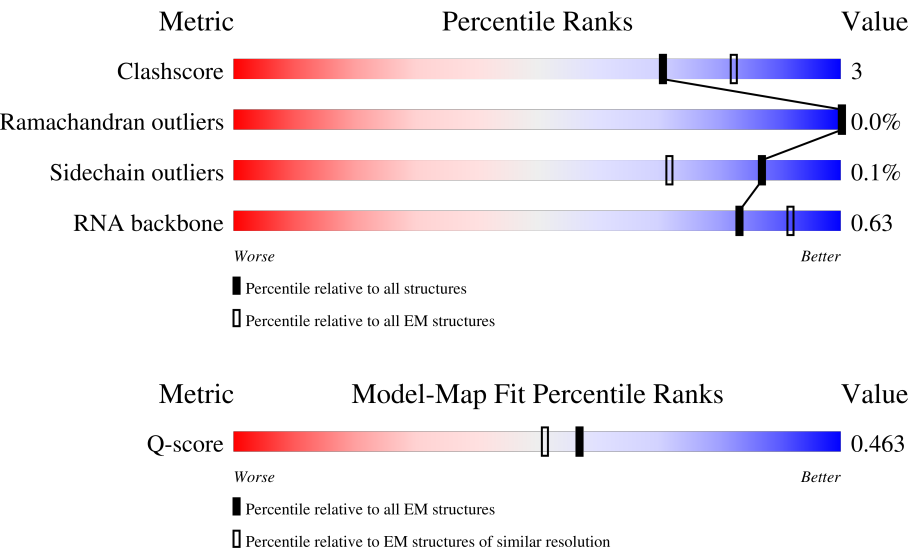
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	1	476	
2	2	68	
3	3	96	

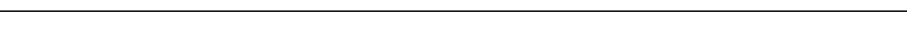
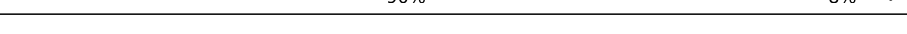
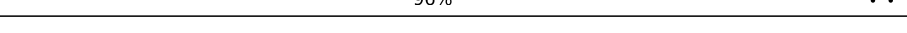
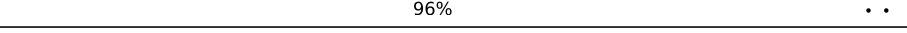
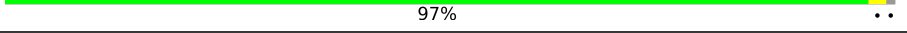
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Mol	Chain	Length	Quality of chain
4	5	5070	
5	7	121	
6	8	157	
7	A	794	
8	B	506	
9	C	314	
10	D	85	
11	K	245	
12	LA	257	
13	LB	403	
14	LC	427	
15	LD	297	
16	LE	288	
17	LF	248	
18	LG	266	
19	LH	192	
20	LI	214	
21	LJ	178	
22	LL	211	
23	LM	215	
24	LN	204	
25	LO	203	
26	LP	184	
27	LQ	188	
28	LR	196	

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Mol	Chain	Length	Quality of chain
29	LS	176	
30	LT	160	
31	LU	128	
32	LV	140	
33	LW	157	
34	LX	156	
35	LY	145	
36	LZ	136	
37	La	148	
38	Lb	159	
39	Lc	115	
40	Ld	125	
41	Le	135	
42	Lf	110	
43	Lg	117	
44	Lh	123	
45	Li	105	
46	Lj	97	
47	Lk	70	
48	Ll	51	
49	Lm	128	
50	Lo	106	
51	Lp	92	
52	Lr	137	
53	Lz	217	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 150098 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 Protein transport protein Sec61 subunit alpha isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	426	Total	C	N	O	S	0	0
			3322	2189	535	577	21		

- Molecule 2 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	62	Total	C	N	O	S	0	0
			494	326	86	79	3		

- Molecule 3 is a protein called Protein transport protein Sec61 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	29	Total	C	N	O	S	0	0
			229	157	36	34	2		

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	3474	Total	C	N	O	P	0	0
			74502	33181	13653	24195	3473		

- Molecule 5 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	120	Total	C	N	O	P	0	0
			2561	1141	456	844	120		

- Molecule 6 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	148	Total	C	N	O	P	0	0
			3152	1407	563	1035	147		

- Molecule 7 is a protein called E3 UFM1-protein ligase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	692	Total	C	N	O	S	0	0
			5479	3453	957	1050	19		

- Molecule 8 is a protein called CDK5 regulatory subunit-associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	403	Total	C	N	O	S	0	0
			3234	2049	545	624	16		

- Molecule 9 is a protein called DDRGK domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	109	Total	C	N	O	S	0	0
			855	539	143	172	1		

- Molecule 10 is a protein called Ubiquitin-fold modifier 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	78	Total	C	N	O	S	0	0
			588	382	96	109	1		

- Molecule 11 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	224	Total	C	N	O	S	0	0
			1704	1061	293	338	12		

- Molecule 12 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LA	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 13 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LB	402	Total	C	N	O	S	0	0
			3239	2060	608	557	14		

- Molecule 14 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LC	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- Molecule 15 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 16 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LE	220	Total	C	N	O	S	0	0
			1765	1136	334	291	4		

- Molecule 17 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 18 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LG	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 19 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 20 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LI	202	Total	C	N	O	S	0	0
			1634	1038	314	269	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LI	87	ILE	MET	conflict	UNP Q96L21

- Molecule 21 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LJ	175	Total	C	N	O	S	0	0
			1401	882	261	252	6		

- Molecule 22 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LL	194	Total	C	N	O	S	0	0
			1573	987	327	255	4		

- Molecule 23 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LM	136	Total	C	N	O	S	0	0
			1120	719	215	179	7		

- Molecule 24 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 25 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 26 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 27 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 28 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LR	155	Total	C	N	O	S	0	0
			1294	808	278	199	9		

- Molecule 29 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 30 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 31 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LU	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 32 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 33 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LW	62	Total	C	N	O	S	0	0
			519	332	101	83	3		

- Molecule 34 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LX	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 35 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LY	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 36 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 37 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 38 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lb	109	Total	C	N	O	S	0	0
			876	546	189	137	4		

- Molecule 39 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 40 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Ld	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 41 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 42 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 43 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 44 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 45 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Li	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 46 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 47 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lk	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 48 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 49 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lm	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 50 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lo	105	Total	C	N	O	S	0	0
			863	542	175	140	6		

- Molecule 51 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Lp	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 52 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 53 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Lz	217	Total	C	N	O	S	0	0
			1744	1114	314	307	9		

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	5	206	Total	Mg	0
			206	206	
54	7	2	Total	Mg	0
			2	2	
54	8	5	Total	Mg	0
			5	5	

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Mol	Chain	Residues	Atoms		AltConf
54	LI	1	Total 1	Mg 1	0
54	LP	1	Total 1	Mg 1	0
54	LV	1	Total 1	Mg 1	0
54	Le	1	Total 1	Mg 1	0
54	Lf	1	Total 1	Mg 1	0
54	Lj	2	Total 2	Mg 2	0

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	Lg	1	Total 1	Zn 1	0
55	Lj	1	Total 1	Zn 1	0
55	Lm	1	Total 1	Zn 1	0
55	Lo	1	Total 1	Zn 1	0
55	Lp	1	Total 1	Zn 1	0

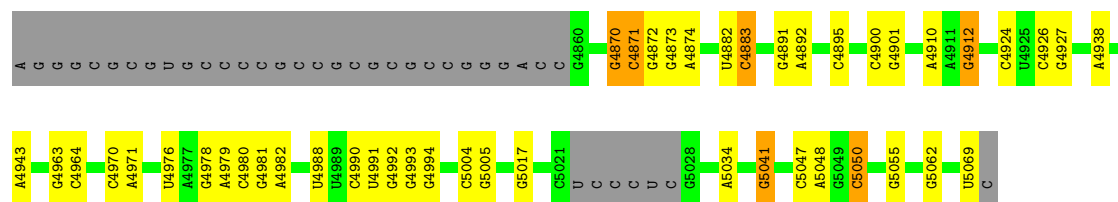


Chain 5: 52% 15% . 31%









- Molecule 5: 5S rRNA

Chain 7: 77% 21% ..



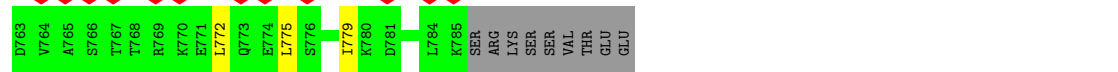
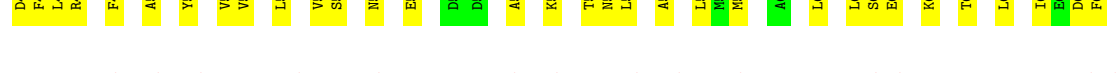
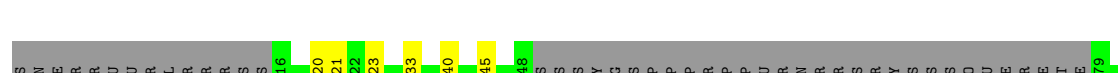
- Molecule 6: 5.8S rRNA

Chain 8: 75% 20% 6%

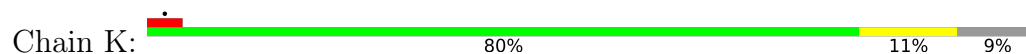


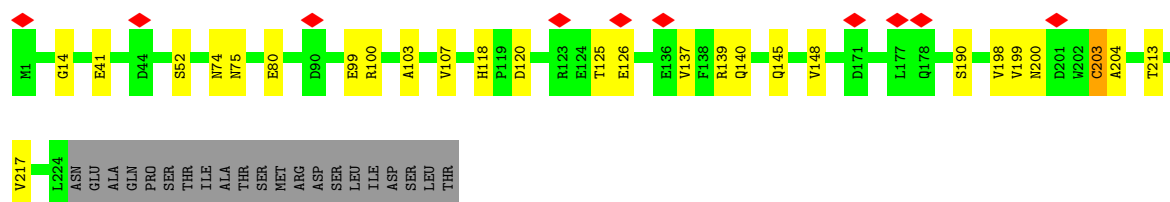
- Molecule 7: E3 UFM1-protein ligase 1

Chain A: 74% 13% 13%



- Molecule 8: CDK5 regulatory subunit-associated protein 3





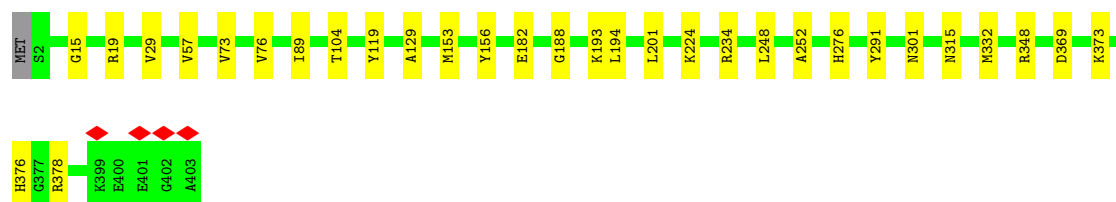
- Molecule 12: 60S ribosomal protein L8

Chain LA: 86% 11%



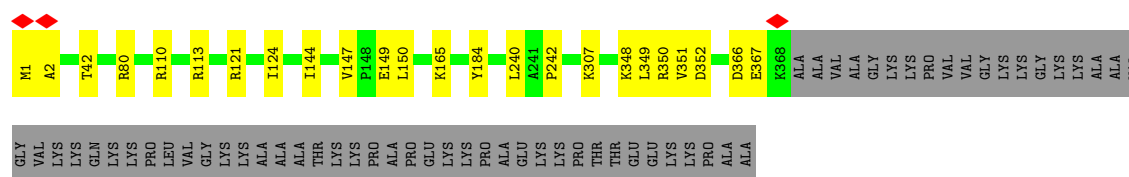
- Molecule 13: 60S ribosomal protein L3

Chain LB: 92% 8%



- Molecule 14: 60S ribosomal protein L4

Chain LC: 81% 6% 14%



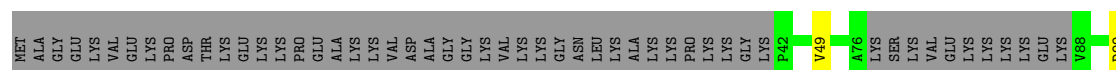
- Molecule 15: 60S ribosomal protein L5

Chain LD: 90% 9%



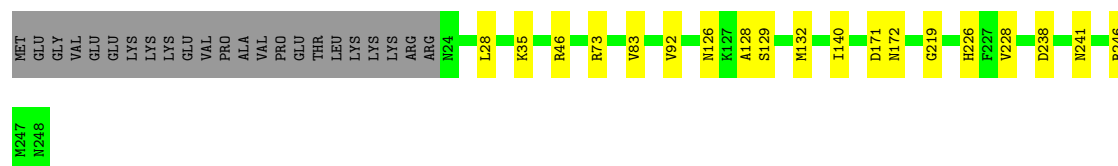
- Molecule 16: 60S ribosomal protein L6

Chain LE: 68% 8% 24%

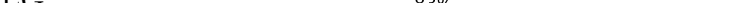


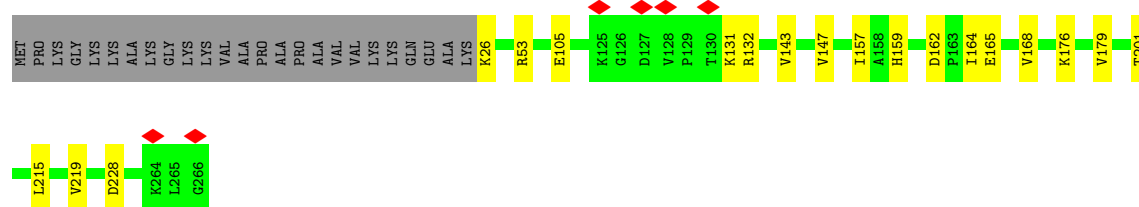
- Molecule 17: 60S ribosomal protein L7

Chain LF: 83% 8% 9%

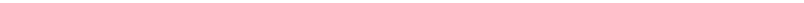


- Molecule 18: 60S ribosomal protein L7a

Chain LG:  83% 7% 9%



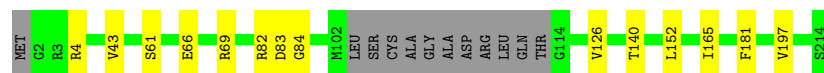
- Molecule 19: 60S ribosomal protein L9

Chain LH:  91% 8%



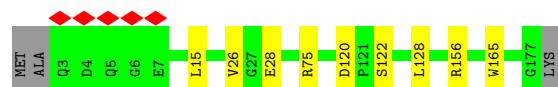
- Molecule 20: Ribosomal protein uL16-like

Chain LI: 88% 7% 6%



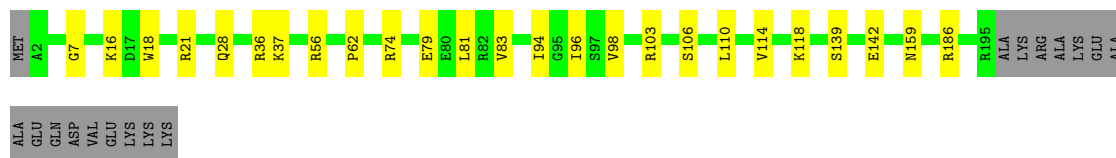
- Molecule 21: 60S ribosomal protein L11

Chain LJ: 93% 5%



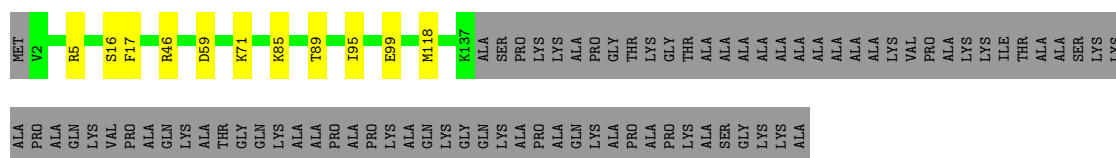
- Molecule 22: 60S ribosomal protein L13

Chain LL:  80% 12% 8%



- Molecule 23: 60S ribosomal protein L14

Chain LM:  58% 5% 37%



- Molecule 24: 60S ribosomal protein L15

Chain LN:  90% 9%



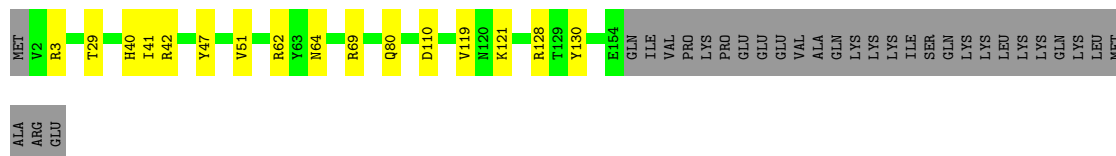
- Molecule 25: 60S ribosomal protein L13a

Chain LO:  90% 9%



- Molecule 26: 60S ribosomal protein L17

Chain LP:  74% 9% 17%



- Molecule 27: 60S ribosomal protein L18

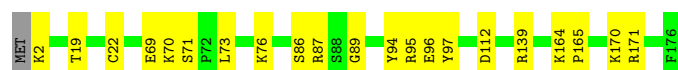
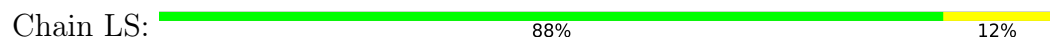
Chain LQ:  89% 10%



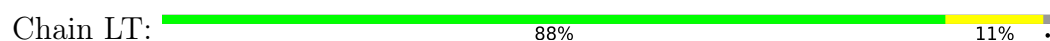
- Molecule 28: 60S ribosomal protein L19



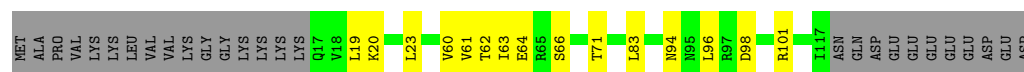
- Molecule 29: 60S ribosomal protein L18a



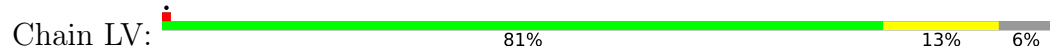
- Molecule 30: 60S ribosomal protein L21



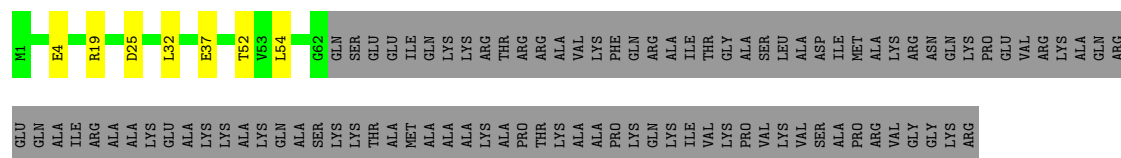
- Molecule 31: 60S ribosomal protein L22



- Molecule 32: 60S ribosomal protein L23

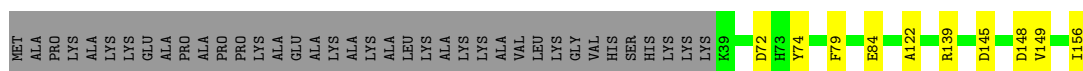


- Molecule 33: 60S ribosomal protein L24



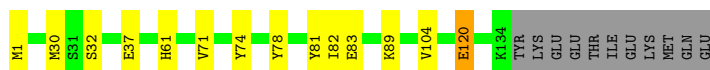
- Molecule 34: 60S ribosomal protein L23a





- Molecule 35: 60S ribosomal protein L26

Chain LY: 83% 9% 8%



- Molecule 36: 60S ribosomal protein L27

Chain LZ: 81% 18% .



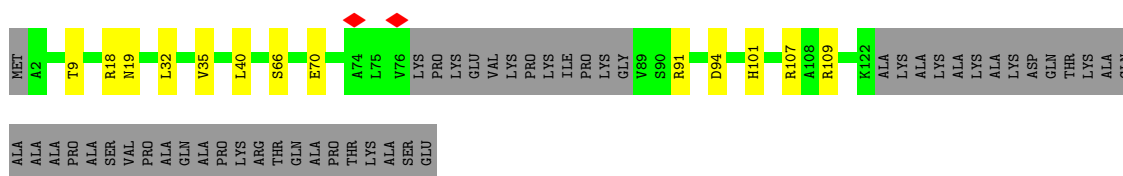
- Molecule 37: 60S ribosomal protein L27a

Chain La: 88% 11% .



- Molecule 38: 60S ribosomal protein L29

Chain Lb: 60% 8% 31%



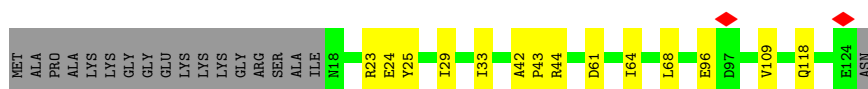
- Molecule 39: 60S ribosomal protein L30

Chain Lc: 77% 8% 15%



- Molecule 40: 60S ribosomal protein L31

Chain Ld: 74% 11% 14%



- Molecule 41: 60S ribosomal protein L32

Chain Le:  88% 7% 5%



- Molecule 42: 60S ribosomal protein L35a

Chain Lf:  92% 7% .

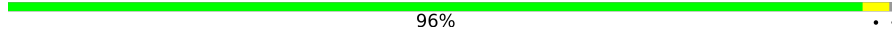


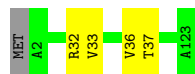
- Molecule 43: 60S ribosomal protein L34

Chain Lg:  90% 8% .



- Molecule 44: 60S ribosomal protein L35

Chain Lh:  96% ..



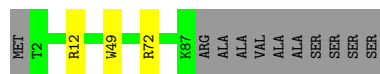
- Molecule 45: 60S ribosomal protein L36

Chain Li:  90% 8% .



- Molecule 46: 60S ribosomal protein L37

Chain Lj:  86% . 11%

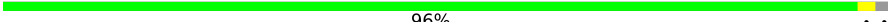


- Molecule 47: 60S ribosomal protein L38

Chain Lk:  84% 14% .



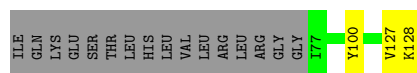
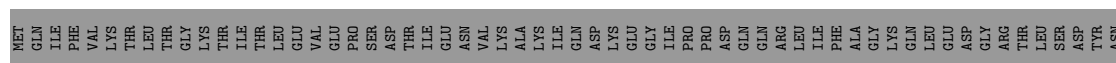
- Molecule 48: 60S ribosomal protein L39

Chain Ll:  96% ..

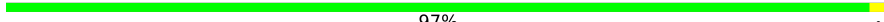


- Molecule 49: Ubiquitin-60S ribosomal protein L40

Chain Lm:  38% . 59%



- Molecule 50: 60S ribosomal protein L36a

Chain Lo:  97% ..



- Molecule 51: 60S ribosomal protein L37a

Chain Lp:  91% 8% .



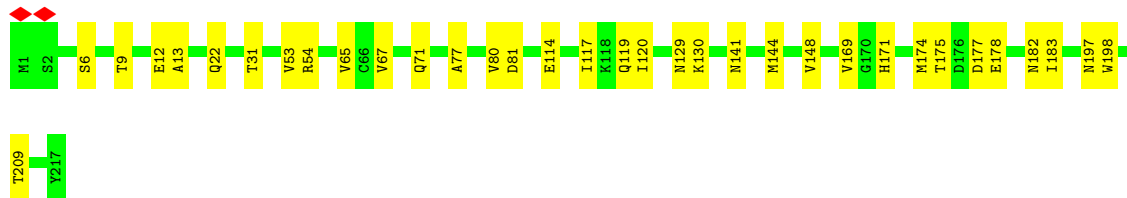
- Molecule 52: 60S ribosomal protein L28

Chain Lr:  80% 11% 9%



- Molecule 53: 60S ribosomal protein L10a

Chain Lz:  84% 16%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20377	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.043	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0055	Depositor
Map size (Å)	392.58, 392.58, 392.58	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	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	1	0.12	0/3393	0.29	0/4597
2	2	0.15	0/504	0.33	0/673
3	3	0.53	0/236	0.92	0/321
4	5	0.07	0/83342	0.20	0/129985
5	7	0.07	0/2861	0.20	0/4459
6	8	0.07	0/3520	0.20	0/5481
7	A	0.10	0/5549	0.23	0/7469
8	B	0.10	0/3280	0.23	0/4426
9	C	0.07	0/864	0.18	0/1169
10	D	0.11	0/601	0.23	0/818
11	K	0.08	0/1728	0.23	0/2351
12	LA	0.10	0/1936	0.23	0/2596
13	LB	0.08	0/3307	0.20	0/4424
14	LC	0.08	0/2981	0.21	0/4002
15	LD	0.09	0/2428	0.20	0/3252
16	LE	0.07	0/1799	0.19	0/2414
17	LF	0.10	0/1905	0.21	0/2539
18	LG	0.09	0/1960	0.21	0/2637
19	LH	0.10	0/1537	0.22	0/2066
20	LI	0.09	0/1673	0.19	0/2234
21	LJ	0.08	0/1424	0.20	0/1904
22	LL	0.09	0/1604	0.21	0/2149
23	LM	0.10	0/1142	0.20	0/1527
24	LN	0.10	0/1746	0.21	0/2338
25	LO	0.10	0/1682	0.22	0/2250
26	LP	0.09	0/1268	0.21	0/1701
27	LQ	0.10	0/1537	0.21	0/2052
28	LR	0.11	0/1310	0.24	0/1734
29	LS	0.09	0/1493	0.22	0/2003
30	LT	0.10	0/1326	0.22	0/1770
31	LU	0.10	0/839	0.22	0/1126
32	LV	0.10	0/993	0.21	0/1332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LW	0.10	0/532	0.19	0/708
34	LX	0.07	0/984	0.19	0/1323
35	LY	0.09	0/1132	0.23	0/1504
36	LZ	0.11	0/1130	0.21	0/1507
37	La	0.07	0/1191	0.19	0/1591
38	Lb	0.11	0/889	0.25	0/1175
39	Lc	0.12	0/774	0.26	0/1038
40	Ld	0.10	0/903	0.23	0/1216
41	Le	0.08	0/1071	0.18	0/1429
42	Lf	0.09	0/895	0.22	0/1198
43	Lg	0.09	0/916	0.21	0/1220
44	Lh	0.09	0/1023	0.21	0/1351
45	Li	0.09	0/843	0.19	0/1115
46	Lj	0.09	0/720	0.19	0/952
47	Lk	0.09	0/575	0.23	0/761
48	Ll	0.10	0/454	0.18	0/599
49	Lm	0.11	0/435	0.22	0/575
50	Lo	0.10	0/877	0.20	0/1156
51	Lp	0.10	0/718	0.21	0/953
52	Lr	0.09	0/1017	0.21	0/1364
53	Lz	0.09	0/1772	0.23	0/2375
All	All	0.09	0/160619	0.21	0/234909

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3322	0	3452	1	0
2	2	494	0	527	0	0
3	3	229	0	245	0	0
4	5	74502	0	37636	390	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	7	2561	0	1295	18	0
6	8	3152	0	1601	13	0
7	A	5479	0	5608	77	0
8	B	3234	0	3287	35	0
9	C	855	0	854	8	0
10	D	588	0	616	0	0
11	K	1704	0	1683	16	0
12	LA	1898	0	1993	23	0
13	LB	3239	0	3376	25	0
14	LC	2927	0	3104	19	0
15	LD	2382	0	2410	23	0
16	LE	1765	0	1917	16	0
17	LF	1870	0	1996	12	0
18	LG	1927	0	2074	14	0
19	LH	1518	0	1601	11	0
20	LI	1634	0	1673	9	0
21	LJ	1401	0	1428	7	0
22	LL	1573	0	1681	19	0
23	LM	1120	0	1187	9	0
24	LN	1701	0	1749	14	0
25	LO	1650	0	1794	16	0
26	LP	1242	0	1269	10	0
27	LQ	1513	0	1628	14	0
28	LR	1294	0	1434	15	0
29	LS	1453	0	1490	15	0
30	LT	1298	0	1366	14	0
31	LU	825	0	850	9	0
32	LV	979	0	1039	13	0
33	LW	519	0	533	5	0
34	LX	967	0	1040	7	0
35	LY	1115	0	1205	11	0
36	LZ	1107	0	1182	15	0
37	La	1162	0	1213	14	0
38	Lb	876	0	948	13	0
39	Lc	764	0	804	7	0
40	Ld	888	0	930	9	0
41	Le	1053	0	1147	7	0
42	Lf	876	0	912	5	0
43	Lg	906	0	998	8	0
44	Lh	1015	0	1148	3	0
45	Li	832	0	917	7	0
46	Lj	705	0	737	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	Lk	569	0	637	8	0
48	Ll	444	0	483	1	0
49	Lm	429	0	465	2	0
50	Lo	863	0	929	2	0
51	Lp	708	0	756	6	0
52	Lr	1002	0	1068	11	0
53	Lz	1744	0	1859	26	0
54	5	206	0	0	0	0
54	7	2	0	0	0	0
54	8	5	0	0	0	0
54	LI	1	0	0	0	0
54	LP	1	0	0	0	0
54	LV	1	0	0	0	0
54	Le	1	0	0	0	0
54	Lf	1	0	0	0	0
54	Lj	2	0	0	0	0
55	Lg	1	0	0	0	0
55	Lj	1	0	0	0	0
55	Lm	1	0	0	0	0
55	Lo	1	0	0	0	0
55	Lp	1	0	0	0	0
All	All	150098	0	113774	856	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 3.

All (856) 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)
7:A:29:GLU:N	7:A:32:CYS:HG	1.66	0.92
4:5:2520:C:O2	4:5:2640:G:N2	2.04	0.90
4:5:3809:G:OP2	4:5:3809:G:N2	2.06	0.88
4:5:2693:G:OP1	47:Lk:35:LYS:NZ	2.06	0.88
4:5:308:G:N2	4:5:308:G:OP2	2.07	0.88
4:5:3962:A:N6	4:5:3965:A:O2'	2.07	0.87
5:7:72:U:O2	5:7:103:A:N6	2.07	0.87
4:5:1293:G:N2	4:5:1293:G:OP2	2.10	0.85
4:5:1818:G:OP2	4:5:1818:G:N2	2.10	0.84
4:5:1326:A:OP2	4:5:4445:U:O2'	1.95	0.84
4:5:3653:A:O2'	12:LA:179:ILE:O	1.94	0.83
4:5:3717:A:OP2	4:5:3735:G:N2	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:4255:A:H62	7:A:652:MET:HE1	1.42	0.83
4:5:2093:A:O2'	4:5:2094:G:O4'	1.96	0.82
4:5:2296:G:O2'	14:LC:242:PRO:O	1.97	0.82
4:5:3748:A:O2'	12:LA:223:SER:OG	1.96	0.81
4:5:3789:C:OP2	4:5:3790:U:O2'	1.98	0.81
4:5:3823:G:OP2	4:5:3823:G:N2	2.14	0.81
12:LA:47:ASP:OD1	12:LA:48:ILE:N	2.14	0.81
4:5:3641:U:OP2	4:5:3646:A:N6	2.14	0.81
4:5:3689:G:O2'	4:5:3818:U:OP2	1.98	0.80
5:7:23:A:N3	5:7:118:C:O2'	2.15	0.80
4:5:1697:G:N2	4:5:2084:C:OP1	2.15	0.80
5:7:119:U:O4	15:LD:258:LYS:NZ	2.15	0.80
7:A:593:LEU:HD22	7:A:595:MET:HE1	1.64	0.79
4:5:62:A:N3	4:5:77:U:O2'	2.16	0.79
8:B:236:SER:OG	8:B:240:GLU:OE1	2.00	0.79
4:5:4620:U:OP2	4:5:4670:C:N4	2.16	0.79
5:7:73:U:OP2	5:7:74:A:O2'	2.01	0.79
29:LS:71:SER:O	29:LS:76:LYS:NZ	2.16	0.78
4:5:2588:C:OP1	4:5:2768:C:O2'	2.01	0.78
1:1:416:TYR:OH	34:LX:156:ILE:OXT	2.02	0.78
4:5:2562:G:N2	4:5:2565:A:OP2	2.15	0.78
4:5:2759:G:O2'	4:5:2760:G:O4'	2.01	0.78
4:5:1562:G:N2	4:5:1565:A:OP2	2.17	0.77
4:5:1269:G:OP2	38:Lb:107:ARG:NH2	2.18	0.77
5:7:7:G:OP1	15:LD:33:ARG:NH1	2.18	0.77
4:5:419:A:N3	4:5:1332:C:O2'	2.18	0.77
4:5:1646:A:O2'	46:Lj:49:TRP:O	2.03	0.76
24:LN:155:VAL:O	24:LN:162:ARG:NH2	2.18	0.76
15:LD:41:LYS:NZ	30:LT:30:TYR:O	2.19	0.76
4:5:483:G:O6	4:5:669:C:N4	2.19	0.75
12:LA:180:LEU:HD21	51:Lp:26:VAL:HG21	1.68	0.75
15:LD:84:PRO:O	15:LD:89:LYS:NZ	2.19	0.75
27:LQ:175:GLU:N	27:LQ:175:GLU:OE1	2.19	0.75
7:A:355:THR:OG1	7:A:364:VAL:O	2.05	0.75
4:5:4115:G:N2	4:5:4115:G:OP2	2.19	0.74
11:K:52:SER:OG	11:K:80:GLU:OE2	2.04	0.74
16:LE:112:MET:O	52:Lr:87:ARG:NH1	2.20	0.74
6:8:75:G:OP2	35:LY:74:TYR:OH	2.06	0.74
4:5:1523:A:N3	4:5:4389:C:O2'	2.21	0.74
9:C:209:GLU:O	9:C:212:SER:OG	2.05	0.74
4:5:3711:A:O2'	4:5:3712:A:O4'	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:2517:A:N3	4:5:2539:C:O2'	2.20	0.74
33:LW:4:GLU:OE2	33:LW:4:GLU:N	2.21	0.74
4:5:3788:C:N4	4:5:3812:C:O4'	2.21	0.73
4:5:2324:C:O2'	41:Le:98:GLU:OE2	2.05	0.73
4:5:3900:G:OP1	4:5:3901:A:O2'	2.02	0.73
4:5:1369:C:OP2	4:5:1370:G:O2'	2.00	0.73
6:8:102:G:OP2	6:8:104:A:O2'	2.07	0.73
4:5:2478:C:O2	4:5:2591:A:O2'	2.07	0.73
4:5:4066:U:O2'	45:Li:59:GLU:OE1	2.06	0.73
30:LT:43:LYS:O	30:LT:58:HIS:ND1	2.22	0.72
34:LX:84:GLU:N	34:LX:84:GLU:OE1	2.23	0.72
4:5:480:C:OP1	52:Lr:67:ARG:NH1	2.22	0.72
4:5:1927:U:OP1	4:5:1949:U:O2'	2.05	0.72
4:5:4045:G:N2	4:5:4048:A:OP2	2.22	0.72
47:Lk:7:GLU:OE1	47:Lk:7:GLU:N	2.22	0.72
4:5:3909:C:O2'	7:A:440:ALA:O	2.08	0.72
4:5:2062:C:OP1	29:LS:2:LYS:N	2.23	0.72
40:Ld:96:GLU:N	40:Ld:96:GLU:OE1	2.23	0.72
44:Lh:32:ARG:O	44:Lh:36:VAL:HG23	1.90	0.72
4:5:5005:G:N2	4:5:5041:G:O2'	2.22	0.71
4:5:4163:U:OP2	18:LG:53:ARG:NH1	2.23	0.71
18:LG:215:LEU:O	18:LG:219:VAL:HG13	1.90	0.71
36:LZ:54:THR:OG1	36:LZ:57:MET:SD	2.45	0.71
7:A:44:GLN:O	9:C:284:ARG:NH2	2.23	0.71
4:5:4147:G:OP1	18:LG:26:LYS:NZ	2.24	0.71
25:LO:186:GLU:N	25:LO:186:GLU:OE1	2.24	0.71
12:LA:142:GLU:OE1	12:LA:142:GLU:N	2.20	0.70
4:5:1890:G:N2	4:5:1890:G:OP2	2.22	0.70
4:5:102:G:HO2'	4:5:1381:U:HO2'	1.40	0.70
4:5:1548:G:O2'	4:5:2812:A:N3	2.22	0.70
18:LG:105:GLU:N	18:LG:105:GLU:OE1	2.23	0.70
4:5:966:A:OP2	4:5:2092:G:N2	2.25	0.70
4:5:2041:A:N7	4:5:4434:C:O2'	2.24	0.70
5:7:117:G:OP1	15:LD:253:TYR:OH	2.09	0.70
4:5:1874:A:O4'	4:5:4213:A:N6	2.25	0.70
4:5:4474:A:OP2	4:5:4476:C:N4	2.24	0.70
37:La:39:HIS:O	37:La:42:ARG:N	2.25	0.70
42:Lf:14:TYR:OH	42:Lf:92:LEU:O	2.06	0.70
4:5:2034:G:OP1	29:LS:86:SER:OG	2.09	0.70
35:LY:37:GLU:N	35:LY:37:GLU:OE2	2.22	0.70
4:5:307:A:N3	4:5:310:G:O2'	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:737:C:OP2	23:LM:71:LYS:NZ	2.21	0.69
4:5:1353:G:O6	27:LQ:85:THR:HG21	1.91	0.69
13:LB:57:VAL:HG22	13:LB:73:VAL:HG22	1.73	0.69
4:5:1865:G:N2	4:5:1868:A:OP2	2.22	0.69
4:5:4255:A:N6	7:A:652:MET:HE1	2.08	0.69
4:5:5055:G:N2	40:Ld:118:GLN:OE1	2.25	0.69
4:5:2394:G:O4'	4:5:2397:G:N2	2.24	0.69
4:5:4694:G:N2	4:5:4694:G:OP1	2.24	0.69
22:LL:139:SER:OG	22:LL:142:GLU:OE1	2.07	0.69
30:LT:149:GLU:OE2	30:LT:149:GLU:N	2.25	0.69
4:5:67:C:OP2	4:5:312:G:N2	2.26	0.69
8:B:483:GLN:NE2	8:B:487:GLU:OE2	2.25	0.69
23:LM:85:LYS:O	23:LM:89:THR:HG23	1.93	0.69
4:5:704:C:N4	4:5:707:C:OP2	2.25	0.69
4:5:4623:G:OP1	13:LB:19:ARG:NH2	2.25	0.69
7:A:590:ALA:HB1	7:A:595:MET:SD	2.33	0.69
4:5:2553:A:OP2	4:5:2574:G:O2'	2.08	0.68
4:5:2407:G:N2	4:5:2407:G:OP2	2.26	0.68
4:5:1872:G:O2'	4:5:4219:A:N3	2.25	0.68
18:LG:164:ILE:O	18:LG:168:VAL:HG13	1.93	0.68
4:5:4927:G:OP2	4:5:4927:G:N2	2.26	0.68
4:5:151:G:OP2	24:LN:4:TYR:OH	2.08	0.68
4:5:276:C:OP2	45:Li:34:THR:HG21	1.94	0.68
4:5:1390:G:N2	4:5:1393:G:OP2	2.27	0.68
4:5:4732:G:N2	4:5:4734:A:N7	2.41	0.68
4:5:4670:C:O2'	4:5:4672:A:OP2	2.11	0.68
40:Ld:24:GLU:OE2	40:Ld:109:VAL:HG11	1.94	0.68
4:5:1378:C:N4	22:LL:159:ASN:O	2.21	0.67
6:8:13:G:O2'	26:LP:121:LYS:O	2.13	0.67
4:5:102:G:O2'	4:5:1381:U:O2'	2.13	0.67
4:5:4522:G:O2'	4:5:4525:C:OP2	2.12	0.67
21:LJ:120:ASP:OD1	21:LJ:122:SER:OG	2.07	0.67
41:Le:86:GLU:OE2	41:Le:114:ARG:NE	2.28	0.67
4:5:1591:U:OP2	4:5:2856:C:O2'	2.13	0.67
4:5:66:A:O2'	4:5:326:C:O2	2.13	0.67
4:5:4626:A:OP2	13:LB:224:LYS:NZ	2.21	0.67
9:C:227:LYS:NZ	9:C:275:GLU:OE2	2.22	0.67
4:5:4322:G:N2	4:5:4325:A:OP2	2.26	0.67
7:A:593:LEU:HD23	7:A:593:LEU:O	1.95	0.67
4:5:2378:G:N2	4:5:2381:A:OP2	2.28	0.66
4:5:2579:G:N2	4:5:2582:A:OP2	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:1741:G:O6	5:7:103:A:O2'	2.09	0.66
25:LO:181:ALA:O	25:LO:185:VAL:HG22	1.95	0.66
4:5:3700:C:O2'	4:5:3774:A:N3	2.27	0.66
4:5:3620:G:OP1	4:5:3622:C:N4	2.29	0.66
4:5:4924:C:O2	4:5:4926:C:N4	2.28	0.66
4:5:4604:G:N2	4:5:4607:A:OP2	2.28	0.66
32:LV:111:GLU:N	32:LV:111:GLU:OE1	2.30	0.65
14:LC:1:MET:SD	14:LC:2:ALA:N	2.69	0.65
4:5:3605:C:OP2	28:LR:71:ARG:NH1	2.29	0.65
4:5:2257:C:O2'	4:5:2259:G:OP2	2.10	0.65
4:5:5047:C:O2'	4:5:5050:C:OP2	2.14	0.65
4:5:2052:G:O2'	4:5:2057:A:N1	2.25	0.65
4:5:3961:G:O2'	4:5:4043:G:N2	2.29	0.65
4:5:3974:G:OP2	4:5:4040:C:N4	2.30	0.64
52:Lr:65:LYS:O	52:Lr:102:TYR:OH	2.13	0.64
4:5:1371:A:N1	6:8:28:C:O2'	2.29	0.64
4:5:222:C:OP2	14:LC:165:LYS:NZ	2.29	0.64
19:LH:103:VAL:HG11	19:LH:144:LEU:HD21	1.80	0.64
4:5:2843:U:O2'	4:5:4632:U:OP1	2.16	0.64
7:A:617:GLU:OE1	7:A:617:GLU:N	2.30	0.64
4:5:2318:G:N2	4:5:2321:G:OP2	2.23	0.63
26:LP:64:ASN:ND2	26:LP:80:GLN:OE1	2.30	0.63
4:5:2844:A:N6	4:5:3839:G:O2'	2.31	0.63
7:A:555:GLU:HG2	7:A:635:ILE:HG21	1.79	0.63
4:5:935:A:O2'	23:LM:46:ARG:NH1	2.32	0.63
7:A:214:GLU:OE2	7:A:239:GLN:NE2	2.32	0.63
4:5:1867:A:N3	4:5:4403:U:O2'	2.29	0.63
7:A:378:GLU:OE1	7:A:378:GLU:N	2.30	0.63
4:5:4272:G:OP2	4:5:4272:G:N2	2.22	0.62
4:5:75:G:O6	22:LL:103:ARG:NH1	2.30	0.62
4:5:2891:U:OP2	28:LR:74:ARG:NE	2.32	0.62
4:5:1279:A:O2'	4:5:1281:G:N7	2.31	0.62
11:K:126:GLU:OE1	11:K:139:ARG:NH1	2.32	0.62
24:LN:120:TRP:NE1	24:LN:122:GLY:O	2.32	0.62
4:5:713:C:O2	16:LE:130:LYS:NZ	2.32	0.62
4:5:1433:A:N6	4:5:1451:G:O2'	2.32	0.62
4:5:4527:G:OP2	4:5:4527:G:N2	2.28	0.62
4:5:46:U:OP2	4:5:47:A:O2'	2.06	0.62
6:8:94:G:OP2	46:Lj:72:ARG:NH1	2.32	0.62
4:5:2809:G:O2'	4:5:4644:G:OP1	2.17	0.61
4:5:88:A:N7	27:LQ:173:LYS:NZ	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:251:ARG:NH1	8:B:217:GLU:OE2	2.33	0.61
16:LE:180:VAL:HG21	16:LE:258:LEU:HD11	1.80	0.61
19:LH:34:LEU:HD12	19:LH:84:VAL:HG13	1.83	0.61
4:5:1554:A:OP1	51:Lp:5:THR:OG1	2.17	0.61
4:5:1952:G:OP1	29:LS:139:ARG:NE	2.33	0.61
44:Lh:33:VAL:O	44:Lh:37:THR:HG23	2.00	0.61
4:5:2091:C:O2	4:5:2094:G:O2'	2.10	0.61
7:A:29:GLU:N	7:A:32:CYS:SG	2.72	0.61
53:Lz:6:SER:OG	53:Lz:9:THR:OG1	2.17	0.61
15:LD:152:ARG:O	15:LD:157:ASN:ND2	2.33	0.61
4:5:4048:A:O2'	4:5:4049:U:OP1	2.18	0.60
15:LD:133:GLU:N	15:LD:133:GLU:OE1	2.34	0.60
4:5:1866:U:OP1	20:LI:4:ARG:NH1	2.34	0.60
8:B:236:SER:OG	8:B:237:THR:N	2.35	0.60
28:LR:43:LYS:NZ	28:LR:47:ASP:OD1	2.32	0.60
7:A:612:LEU:O	7:A:620:LYS:NZ	2.33	0.60
38:Lb:9:THR:HG22	38:Lb:9:THR:O	2.01	0.60
7:A:231:ARG:NH1	8:B:216:CYS:O	2.35	0.60
4:5:1391:A:N3	4:5:4364:G:O2'	2.28	0.60
7:A:545:SER:O	7:A:549:ASN:ND2	2.35	0.60
4:5:1320:U:O2'	4:5:1891:A:N1	2.34	0.60
4:5:2702:C:OP1	31:LU:101:ARG:NH2	2.34	0.60
4:5:4165:C:OP1	18:LG:53:ARG:NH2	2.35	0.59
13:LB:153:MET:CE	13:LB:194:LEU:HD21	2.31	0.59
4:5:1833:G:N2	4:5:1835:G:O4'	2.35	0.59
4:5:4198:G:H21	7:A:445:ILE:HD12	1.67	0.59
4:5:4569:U:OP1	4:5:4982:A:O2'	2.18	0.59
5:7:120:U:O4'	15:LD:262:LYS:NZ	2.35	0.59
7:A:420:GLU:OE2	7:A:423:ARG:NH2	2.35	0.59
4:5:4472:G:O2'	49:Lm:100:TYR:O	2.20	0.59
7:A:57:ILE:HD11	7:A:65:GLU:OE2	2.03	0.59
9:C:241:ARG:N	9:C:244:ASP:OD2	2.34	0.59
30:LT:137:GLU:OE1	30:LT:137:GLU:N	2.34	0.59
4:5:4265:U:N3	15:LD:17:GLN:O	2.36	0.59
4:5:1961:G:N2	4:5:2024:G:O2'	2.33	0.59
7:A:359:SER:HB3	7:A:362:VAL:HG22	1.85	0.59
30:LT:68:THR:HG22	30:LT:69:GLN:H	1.68	0.59
34:LX:122:ALA:N	34:LX:139:ARG:O	2.35	0.59
4:5:53:C:O2'	4:5:2461:G:O2'	2.15	0.58
4:5:4237:C:O3'	4:5:4326:G:N2	2.36	0.58
11:K:99:GLU:OE2	11:K:100:ARG:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LG:165:GLU:OE2	24:LN:26:ARG:NH1	2.36	0.58
8:B:200:SER:OG	8:B:201:LEU:N	2.35	0.58
32:LV:83:ARG:NH2	32:LV:118:THR:O	2.35	0.58
8:B:250:VAL:HG11	8:B:336:ARG:HH21	1.67	0.58
4:5:2045:G:O6	4:5:3870:C:O2'	2.21	0.58
7:A:47:VAL:HG12	7:A:58:THR:HG22	1.85	0.58
30:LT:4:THR:O	30:LT:9:ARG:NE	2.36	0.58
4:5:2758:G:O2'	4:5:2765:A:N3	2.26	0.58
5:7:11:A:N1	5:7:66:G:O2'	2.29	0.58
4:5:4524:G:N3	13:LB:252:ALA:HB1	2.19	0.58
11:K:100:ARG:NH2	33:LW:25:ASP:OD1	2.36	0.58
34:LX:72:ASP:OD1	34:LX:74:TYR:N	2.36	0.58
4:5:1705:G:N2	4:5:1705:G:OP1	2.35	0.58
24:LN:103:GLU:OE2	24:LN:118:SER:OG	2.13	0.58
41:Le:99:ILE:HD12	41:Le:111:ILE:HG21	1.85	0.58
4:5:3687:A:O2'	12:LA:236:GLY:N	2.36	0.57
36:LZ:35:ASP:OD1	36:LZ:35:ASP:N	2.38	0.57
4:5:1669:A:N3	4:5:1852:U:O2'	2.37	0.57
12:LA:117:GLU:O	12:LA:162:ASN:ND2	2.37	0.57
27:LQ:133:GLY:O	27:LQ:136:THR:OG1	2.11	0.57
4:5:4208:U:OP1	4:5:4334:U:O2'	2.19	0.57
4:5:724:C:OP1	14:LC:350:ARG:NE	2.33	0.57
4:5:1886:G:HO2'	4:5:1909:G:HO2'	1.49	0.57
4:5:1315:C:N4	4:5:1316:G:O6	2.38	0.57
4:5:1279:A:OP1	16:LE:131:LYS:NZ	2.32	0.57
4:5:2724:G:O2'	4:5:2726:G:OP2	2.15	0.57
7:A:612:LEU:HD23	7:A:615:LEU:HD12	1.86	0.57
8:B:250:VAL:HG11	8:B:336:ARG:NH2	2.19	0.57
16:LE:99:ASP:N	16:LE:99:ASP:OD1	2.38	0.57
4:5:2658:G:O2'	4:5:2675:G:N2	2.38	0.57
4:5:3662:A:O2'	12:LA:118:GLU:OE1	2.22	0.57
4:5:4768:G:O2'	4:5:4873:G:N1	2.38	0.57
4:5:2404:A:O2'	46:Lj:12:ARG:O	2.20	0.57
8:B:358:MET:C	8:B:358:MET:HE2	2.30	0.57
14:LC:348:LYS:O	14:LC:352:ASP:OD2	2.23	0.57
28:LR:116:ASP:OD1	28:LR:118:HIS:N	2.37	0.56
35:LY:30:MET:HE3	35:LY:78:TYR:HA	1.86	0.56
4:5:2516:G:O2'	43:Lg:62:LYS:NZ	2.38	0.56
4:5:4978:G:O2'	4:5:4980:C:OP2	2.13	0.56
19:LH:43:VAL:HG21	19:LH:73:ILE:HD13	1.86	0.56
4:5:2845:A:H61	4:5:3843:C:H42	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:2869:U:O2'	4:5:2881:A:N7	2.30	0.56
4:5:232:G:O6	35:LY:61:HIS:N	2.35	0.56
4:5:36:U:OP1	4:5:1651:G:N2	2.38	0.56
38:Lb:32:LEU:O	38:Lb:35:VAL:HG22	2.06	0.56
4:5:3696:C:O2'	4:5:3816:A:N1	2.35	0.56
4:5:4156:G:OP2	4:5:4157:A:O2'	2.09	0.56
7:A:723:ASP:OD1	7:A:724:GLN:N	2.39	0.56
7:A:228:GLY:O	7:A:231:ARG:NH1	2.39	0.56
8:B:373:GLU:OE1	8:B:373:GLU:N	2.38	0.56
11:K:103:ALA:O	11:K:107:VAL:HG22	2.06	0.56
11:K:145:GLN:OE1	32:LV:115:SER:OG	2.07	0.56
4:5:4980:C:N3	26:LP:69:ARG:NH2	2.53	0.56
4:5:1704:C:O3'	17:LF:46:ARG:NH1	2.39	0.56
47:Lk:30:ASP:OD1	47:Lk:30:ASP:N	2.39	0.56
53:Lz:65:VAL:HG11	53:Lz:148:VAL:HG13	1.88	0.56
4:5:4541:G:N2	4:5:4544:A:OP2	2.29	0.55
37:La:94:LYS:O	37:La:94:LYS:NZ	2.27	0.55
7:A:362:VAL:HG21	7:A:497:PHE:CD1	2.41	0.55
4:5:2601:A:N6	4:5:2744:A:OP2	2.36	0.55
7:A:616:SER:O	7:A:620:LYS:N	2.36	0.55
8:B:171:THR:N	8:B:178:GLU:OE1	2.39	0.55
4:5:85:G:O2'	4:5:97:G:O6	2.23	0.55
24:LN:43:THR:HG23	24:LN:44:ARG:HG3	1.87	0.55
4:5:76:A:N7	22:LL:74:ARG:NH2	2.54	0.55
17:LF:171:ASP:OD1	17:LF:172:ASN:N	2.40	0.55
4:5:1930:U:OP2	25:LO:49:ARG:NH1	2.37	0.55
13:LB:119:TYR:OH	13:LB:129:ALA:N	2.40	0.55
4:5:4524:G:C2	13:LB:252:ALA:HB1	2.42	0.55
7:A:346:MET:HE3	7:A:346:MET:HA	1.89	0.55
52:Lr:56:ASP:OD1	52:Lr:56:ASP:N	2.36	0.55
5:7:12:U:OP2	5:7:67:C:O2'	2.25	0.55
30:LT:118:GLU:OE1	30:LT:119:ALA:N	2.40	0.55
4:5:1355:G:OP1	27:LQ:108:ARG:NH2	2.39	0.54
4:5:4457:U:O2	13:LB:252:ALA:HB3	2.07	0.54
14:LC:149:GLU:OE2	52:Lr:71:ARG:NE	2.39	0.54
7:A:615:LEU:O	7:A:620:LYS:NZ	2.40	0.54
26:LP:40:HIS:NE2	26:LP:110:ASP:O	2.36	0.54
32:LV:106:VAL:HG12	32:LV:112:MET:HA	1.89	0.54
4:5:1346:C:OP1	27:LQ:148:VAL:HG12	2.07	0.54
4:5:4323:A:OP1	15:LD:179:ARG:NE	2.39	0.54
4:5:4232:U:O4	50:Lo:8:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LD:59:ASP:OD1	15:LD:60:ILE:N	2.40	0.54
36:LZ:120:GLU:HA	36:LZ:120:GLU:OE1	2.07	0.54
11:K:199:VAL:HG23	11:K:204:ALA:HB2	1.90	0.53
12:LA:36:GLU:OE1	12:LA:163:ARG:NH1	2.40	0.53
50:Lo:105:GLN:HA	50:Lo:105:GLN:OE1	2.08	0.53
7:A:320:GLY:O	7:A:321:THR:OG1	2.24	0.53
33:LW:19:ARG:NH2	33:LW:37:GLU:OE2	2.41	0.53
16:LE:281:ILE:HD13	16:LE:286:LEU:HD11	1.91	0.53
4:5:1552:G:O2'	4:5:1553:A:OP2	2.23	0.53
19:LH:100:PRO:O	19:LH:116:ASN:ND2	2.41	0.53
4:5:1573:G:OP1	28:LR:92:LYS:NZ	2.37	0.53
4:5:4580:U:O2'	13:LB:182:GLU:OE2	2.23	0.53
4:5:4912:G:N2	13:LB:156:TYR:OH	2.41	0.53
8:B:198:GLN:OE1	8:B:234:GLY:N	2.42	0.53
37:La:76:ASP:OD1	37:La:77:LYS:N	2.42	0.53
4:5:4323:A:C2	15:LD:146:LEU:HD23	2.44	0.53
4:5:4420:U:O4	4:5:4475:G:N2	2.42	0.53
4:5:4874:A:O2'	29:LS:170:LYS:NZ	2.42	0.53
13:LB:378:ARG:HG2	33:LW:32:LEU:HD21	1.89	0.53
19:LH:106:GLN:C	19:LH:107:GLU:OE1	2.52	0.53
42:Lf:59:THR:OG1	42:Lf:65:ASN:ND2	2.42	0.53
53:Lz:31:THR:N	53:Lz:209:THR:OG1	2.39	0.53
11:K:200:ASN:OD1	11:K:203:CYS:N	2.42	0.52
4:5:1629:G:N1	12:LA:208:GLU:OE1	2.41	0.52
4:5:1807:C:O3'	30:LT:110:LYS:NZ	2.42	0.52
36:LZ:96:VAL:HG22	36:LZ:110:ALA:HB1	1.91	0.52
4:5:1317:U:OP1	37:La:21:ARG:NH1	2.40	0.52
4:5:1879:C:O2'	4:5:1891:A:N3	2.40	0.52
4:5:2094:G:N2	4:5:2095:A:H2'	2.25	0.52
13:LB:369:ASP:OD2	13:LB:373:LYS:NZ	2.41	0.52
6:8:12:G:OP1	26:LP:3:ARG:NH1	2.43	0.52
32:LV:57:VAL:N	32:LV:84:GLN:OE1	2.43	0.52
32:LV:57:VAL:HG13	32:LV:84:GLN:OE1	2.08	0.52
4:5:106:A:O2'	4:5:335:A:N3	2.39	0.52
16:LE:277:LEU:HA	16:LE:281:ILE:HD11	1.90	0.52
4:5:4122:G:N1	43:Lg:98:GLU:OE1	2.43	0.52
12:LA:14:SER:OG	12:LA:15:VAL:N	2.41	0.52
53:Lz:197:ASN:OD1	53:Lz:198:TRP:N	2.42	0.52
4:5:394:G:N2	4:5:397:G:OP2	2.35	0.52
7:A:709:VAL:O	7:A:712:ILE:HG22	2.09	0.52
8:B:241:TRP:HB2	8:B:343:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LF:226:HIS:ND1	17:LF:228:VAL:HG22	2.25	0.52
11:K:190:SER:OG	32:LV:131:ARG:NH1	2.39	0.52
13:LB:376:HIS:O	13:LB:378:ARG:NH1	2.43	0.52
34:LX:145:ASP:O	34:LX:149:VAL:HG23	2.10	0.51
47:Lk:23:VAL:HG22	47:Lk:36:VAL:HG22	1.92	0.51
4:5:1850:A:N3	4:5:2283:G:O2'	2.42	0.51
4:5:1631:A:N7	12:LA:199:VAL:HG21	2.25	0.51
7:A:666:PHE:O	7:A:666:PHE:CD1	2.64	0.51
7:A:709:VAL:HG13	7:A:710:PRO:HD3	1.91	0.51
4:5:1446:C:H2'	4:5:1447:C:C1'	2.41	0.51
4:5:4568:A:O2'	4:5:4981:G:N7	2.44	0.51
8:B:115:SER:O	8:B:119:VAL:HG23	2.10	0.51
8:B:204:ALA:HB1	8:B:360:LEU:HD21	1.91	0.51
8:B:240:GLU:O	8:B:244:GLY:N	2.43	0.51
22:LL:186:ARG:NH1	45:Li:9:VAL:HG11	2.25	0.51
4:5:4446:U:O2'	4:5:4450:U:OP1	2.27	0.51
16:LE:117:PRO:O	52:Lr:112:ARG:NH1	2.41	0.51
31:LU:23:LEU:HG	31:LU:83:LEU:HD21	1.92	0.51
20:LI:61:SER:HA	20:LI:126:VAL:HG12	1.92	0.51
31:LU:60:VAL:HG13	31:LU:61:VAL:HG23	1.93	0.51
40:Ld:23:ARG:NE	40:Ld:25:TYR:OH	2.37	0.51
7:A:359:SER:CB	7:A:362:VAL:HG22	2.40	0.51
4:5:1552:G:O2'	4:5:1574:G:N2	2.42	0.51
16:LE:188:ARG:NH1	16:LE:214:ASP:OD1	2.44	0.51
52:Lr:31:ASN:OD1	52:Lr:34:ALA:N	2.44	0.51
4:5:957:G:N2	4:5:1283:G:OP2	2.44	0.50
4:5:4195:G:OP1	4:5:4221:C:O2'	2.29	0.50
8:B:224:LEU:HD13	8:B:227:LEU:HD12	1.93	0.50
4:5:1577:G:O2'	4:5:1612:G:H4'	2.11	0.50
4:5:2693:G:OP2	4:5:2694:G:O2'	2.21	0.50
7:A:690:SER:OG	7:A:713:ILE:HD11	2.12	0.50
30:LT:94:GLU:OE2	30:LT:94:GLU:HA	2.11	0.50
36:LZ:123:LYS:O	36:LZ:124:THR:OG1	2.22	0.50
4:5:4871:C:N4	29:LS:171:ARG:O	2.44	0.50
5:7:87:G:N2	5:7:90:A:OP2	2.40	0.50
7:A:357:VAL:HG12	7:A:359:SER:O	2.12	0.50
11:K:74:ASN:OD1	11:K:75:ASN:N	2.45	0.50
34:LX:79:PHE:HB2	44:Lh:36:VAL:HG21	1.92	0.50
37:La:92:LYS:C	37:La:92:LYS:HD3	2.36	0.50
4:5:3659:G:OP1	12:LA:241:ARG:NH1	2.44	0.50
4:5:4748:U:OP1	42:Lf:54:LYS:NZ	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LE:164:PHE:HA	16:LE:175:VAL:HG12	1.94	0.50
53:Lz:171:HIS:N	53:Lz:174:MET:SD	2.74	0.50
4:5:1178:G:O2'	15:LD:286:SER:OG	2.23	0.50
4:5:1366:G:N7	22:LL:37:LYS:NZ	2.60	0.50
4:5:1502:G:OP2	27:LQ:65:ARG:NH1	2.43	0.50
4:5:2434:G:O2'	4:5:2527:A:N1	2.40	0.50
4:5:4550:G:OP2	7:A:433:ARG:NH1	2.44	0.50
17:LF:238:ASP:O	17:LF:241:ASN:ND2	2.44	0.50
29:LS:19:THR:HG23	29:LS:22:CYS:H	1.77	0.50
43:Lg:15:THR:HG22	43:Lg:16:ALA:N	2.27	0.50
4:5:1172:C:H3'	4:5:1173:G:H21	1.76	0.50
4:5:4891:G:H21	23:LM:118:MET:CE	2.25	0.50
7:A:37:ASN:OD1	7:A:38:LYS:N	2.45	0.50
11:K:140:GLN:O	11:K:148:VAL:HG11	2.12	0.50
38:Lb:101:HIS:O	38:Lb:109:ARG:NH1	2.44	0.50
53:Lz:31:THR:N	53:Lz:209:THR:HG1	2.10	0.50
4:5:369:G:N2	4:5:372:A:OP2	2.35	0.49
4:5:2406:G:N7	48:Ll:2:SER:N	2.60	0.49
39:Lc:23:LYS:HD2	39:Lc:23:LYS:N	2.26	0.49
4:5:2514:G:OP1	43:Lg:15:THR:HG21	2.12	0.49
7:A:484:ASP:OD1	7:A:485:PHE:N	2.45	0.49
7:A:555:GLU:CG	7:A:635:ILE:HG21	2.42	0.49
4:5:158:A:N1	4:5:276:C:O2'	2.43	0.49
4:5:1682:A:C2	37:La:43:ILE:HD12	2.48	0.49
4:5:2899:C:OP1	28:LR:108:ARG:NH2	2.43	0.49
4:5:4304:A:OP2	4:5:4305:G:N2	2.44	0.49
26:LP:29:THR:HG23	26:LP:119:VAL:HG11	1.93	0.49
28:LR:119:MET:CE	28:LR:145:LEU:HD23	2.43	0.49
30:LT:48:VAL:HG21	30:LT:94:GLU:HG3	1.94	0.49
4:5:1855:G:O6	4:5:1880:G:N2	2.45	0.49
30:LT:93:ILE:HD12	30:LT:94:GLU:N	2.26	0.49
4:5:3677:U:OP2	4:5:3678:G:O2'	2.20	0.49
8:B:395:LYS:O	8:B:399:VAL:HG23	2.12	0.49
4:5:2863:G:O2'	28:LR:82:LYS:O	2.29	0.49
11:K:126:GLU:HG3	11:K:137:VAL:HG11	1.95	0.49
15:LD:64:ILE:HG13	15:LD:105:LEU:HD21	1.93	0.49
32:LV:28:CYS:SG	32:LV:30:ASP:OD2	2.66	0.49
4:5:2737:C:OP1	51:Lp:34:HIS:NE2	2.45	0.49
15:LD:64:ILE:HD13	15:LD:109:LEU:HD22	1.95	0.49
27:LQ:64:SER:OG	27:LQ:89:ASP:OD2	2.25	0.49
4:5:1854:G:N2	4:5:4394:A:O4'	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:14:GLY:HA2	11:K:198:VAL:HG13	1.95	0.49
20:LI:152:LEU:HB3	20:LI:165:ILE:HD12	1.95	0.49
25:LO:39:GLU:OE1	25:LO:39:GLU:N	2.44	0.49
25:LO:84:VAL:HG11	25:LO:102:LEU:HD22	1.94	0.49
40:Ld:29:ILE:O	40:Ld:33:ILE:HG13	2.11	0.49
38:Lb:70:GLU:OE1	38:Lb:70:GLU:N	2.44	0.49
4:5:4190:U:O2'	4:5:4382:G:OP2	2.21	0.49
4:5:4546:A:N7	12:LA:215:ASN:ND2	2.60	0.49
4:5:4648:A:OP1	28:LR:62:ARG:NH1	2.45	0.48
4:5:4873:G:N3	25:LO:175:MET:HE1	2.28	0.48
8:B:205:ILE:CD1	8:B:224:LEU:HD12	2.43	0.48
22:LL:56:ARG:NH1	22:LL:74:ARG:O	2.45	0.48
30:LT:67:VAL:HA	30:LT:72:VAL:HG12	1.95	0.48
4:5:85:G:N2	4:5:98:A:OP2	2.43	0.48
4:5:452:A:N1	4:5:1293:G:N2	2.61	0.48
19:LH:17:ASP:OD1	19:LH:17:ASP:C	2.56	0.48
21:LJ:26:VAL:HG23	21:LJ:28:GLU:H	1.77	0.48
4:5:408:A:O2'	4:5:411:G:OP2	2.15	0.48
4:5:727:C:OP1	17:LF:73:ARG:NH2	2.41	0.48
5:7:17:C:OP1	21:LJ:156:ARG:NH2	2.47	0.48
47:Lk:52:LYS:HA	47:Lk:55:LYS:HG2	1.95	0.48
53:Lz:71:GLN:OE1	53:Lz:71:GLN:N	2.44	0.48
4:5:3771:C:H2'	4:5:3772:U:C6	2.48	0.48
32:LV:40:ILE:HD11	32:LV:76:VAL:HG11	1.95	0.48
35:LY:71:VAL:HG13	35:LY:83:GLU:HG2	1.94	0.48
4:5:1397:A:N1	4:5:1498:G:O2'	2.39	0.48
7:A:32:CYS:O	7:A:36:VAL:HG23	2.13	0.48
7:A:775:LEU:O	7:A:779:ILE:HG13	2.13	0.48
8:B:237:THR:HG23	8:B:240:GLU:H	1.79	0.48
13:LB:76:VAL:HG21	13:LB:332:MET:SD	2.54	0.48
4:5:134:G:OP1	4:5:134:G:N2	2.46	0.48
7:A:309:VAL:O	7:A:313:VAL:HG23	2.12	0.48
36:LZ:94:THR:O	36:LZ:97:ASN:ND2	2.47	0.48
4:5:2695:A:OP1	47:Lk:35:LYS:NZ	2.42	0.48
31:LU:98:ASP:OD1	31:LU:98:ASP:N	2.46	0.48
4:5:3890:A:N6	4:5:4571:A:O4'	2.47	0.48
7:A:486:LEU:HD12	7:A:487:ARG:N	2.29	0.48
22:LL:79:GLU:OE1	22:LL:83:VAL:HG23	2.13	0.48
4:5:1475:G:N2	4:5:1489:G:H22	2.12	0.47
7:A:366:GLU:O	7:A:370:ASN:ND2	2.45	0.47
4:5:90:G:OP2	4:5:92:C:N4	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:156:G:N2	4:5:157:U:O4	2.47	0.47
4:5:1768:C:N4	7:A:659:LYS:O	2.47	0.47
7:A:582:THR:HG21	7:A:630:LEU:HD11	1.97	0.47
29:LS:69:GLU:OE1	29:LS:70:LYS:N	2.48	0.47
53:Lz:178:GLU:OE1	53:Lz:182:ASN:ND2	2.47	0.47
9:C:243:GLN:O	9:C:247:ASN:ND2	2.46	0.47
14:LC:349:LEU:O	14:LC:352:ASP:OD2	2.33	0.47
32:LV:30:ASP:OD2	32:LV:30:ASP:N	2.47	0.47
37:La:103:VAL:HG22	37:La:125:LYS:O	2.14	0.47
4:5:2042:A:O4'	4:5:4462:C:O2'	2.33	0.47
4:5:3878:C:OP1	4:5:4400:G:O2'	2.18	0.47
14:LC:110:ARG:O	14:LC:113:ARG:NH1	2.43	0.47
24:LN:51:LEU:HD12	24:LN:117:ASN:CG	2.40	0.47
4:5:3896:C:O3'	4:5:3897:G:O4'	2.32	0.47
30:LT:111:GLU:OE2	30:LT:111:GLU:C	2.57	0.47
36:LZ:23:ALA:HB1	36:LZ:43:VAL:HG22	1.96	0.47
22:LL:7:GLY:O	37:La:49:HIS:NE2	2.45	0.47
4:5:1637:A:OP1	4:5:1640:C:N4	2.40	0.47
4:5:1687:U:OP2	38:Lb:19:ASN:ND2	2.45	0.47
4:5:1743:A:N1	4:5:1789:C:O2'	2.37	0.47
4:5:3663:A:N6	4:5:4168:G:O2'	2.48	0.47
4:5:4475:G:OP2	19:LH:173:ARG:NH2	2.44	0.47
17:LF:126:ASN:H	17:LF:129:SER:HG	1.62	0.47
18:LG:162:ASP:OD2	18:LG:162:ASP:C	2.57	0.47
27:LQ:42:THR:O	27:LQ:46:VAL:HG23	2.14	0.47
39:Lc:48:LEU:HD12	39:Lc:93:THR:HG23	1.96	0.47
4:5:1648:C:OP2	4:5:1649:U:O2'	2.30	0.47
4:5:2583:C:OP2	43:Lg:76:ARG:NH1	2.48	0.47
4:5:4768:G:O3'	4:5:4873:G:N2	2.47	0.47
11:K:99:GLU:OE1	11:K:125:THR:HG21	2.15	0.47
12:LA:20:VAL:HG12	12:LA:23:ARG:HD2	1.97	0.47
29:LS:95:ARG:NH2	29:LS:112:ASP:OD2	2.47	0.47
4:5:1686:C:O2'	38:Lb:18:ARG:NH2	2.47	0.47
4:5:4589:A:N1	4:5:4621:C:O2'	2.48	0.47
5:7:40:U:O2	21:LJ:75:ARG:NH1	2.47	0.47
4:5:2725:A:H1'	28:LR:93:VAL:HG21	1.96	0.47
4:5:4699:U:H4'	4:5:4700:A:OP1	2.15	0.47
8:B:462:LEU:HD23	8:B:462:LEU:C	2.40	0.47
19:LH:163:GLN:O	19:LH:166:THR:OG1	2.31	0.47
4:5:357:U:O2	4:5:359:A:N6	2.47	0.46
4:5:3690:U:H2'	4:5:3691:G:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:4252:C:OP2	4:5:4253:A:O2'	2.16	0.46
4:5:4586:G:O6	4:5:4717:A:N6	2.48	0.46
4:5:4891:G:H21	23:LM:118:MET:HE1	1.79	0.46
7:A:486:LEU:HD13	7:A:502:ALA:HB1	1.97	0.46
29:LS:86:SER:OG	29:LS:87:ARG:N	2.49	0.46
36:LZ:87:VAL:HG12	36:LZ:89:ILE:HG13	1.96	0.46
52:Lr:27:THR:HG22	52:Lr:27:THR:O	2.15	0.46
53:Lz:169:VAL:HG21	53:Lz:183:ILE:HD13	1.98	0.46
4:5:1644:C:C2	4:5:1645:C:C5	3.03	0.46
13:LB:29:VAL:HG13	13:LB:348:ARG:HD3	1.98	0.46
4:5:1497:A:N6	27:LQ:175:GLU:O	2.49	0.46
31:LU:64:GLU:N	31:LU:64:GLU:OE1	2.49	0.46
4:5:438:G:OP2	41:Le:18:LYS:NZ	2.35	0.46
4:5:1426:G:N1	4:5:1458:C:OP2	2.45	0.46
4:5:4048:A:HO2'	4:5:4049:U:P	2.36	0.46
4:5:4587:G:N2	13:LB:15:GLY:O	2.43	0.46
24:LN:124:ASP:OD1	24:LN:127:TYR:N	2.42	0.46
31:LU:94:ASN:HB3	31:LU:96:LEU:HD13	1.98	0.46
39:Lc:59:GLU:OE1	43:Lg:92:LYS:CE	2.64	0.46
41:Le:78:LEU:O	52:Lr:20:ARG:NH2	2.42	0.46
4:5:2574:G:N7	4:5:2760:G:N2	2.63	0.46
4:5:4266:G:N3	4:5:4266:G:H2'	2.31	0.46
4:5:4537:C:N4	4:5:4538:G:O6	2.48	0.46
4:5:4870:G:OP2	23:LM:5:ARG:NH1	2.45	0.46
4:5:958:G:N2	4:5:1285:U:OP1	2.38	0.46
4:5:3604:A:O3'	4:5:3605:C:O4'	2.34	0.46
7:A:709:VAL:N	7:A:710:PRO:HD2	2.31	0.46
38:Lb:70:GLU:H	38:Lb:70:GLU:CD	2.23	0.46
42:Lf:33:VAL:HG21	42:Lf:42:TYR:CE2	2.51	0.46
15:LD:83:LEU:N	15:LD:84:PRO:CD	2.79	0.46
43:Lg:88:ARG:O	43:Lg:92:LYS:HG3	2.16	0.46
4:5:3813:A:OP1	7:A:421:ARG:NH1	2.46	0.46
13:LB:188:GLY:O	13:LB:193:LYS:NZ	2.49	0.46
14:LC:352:ASP:OD2	14:LC:352:ASP:N	2.44	0.46
25:LO:54:TYR:OH	25:LO:73:PHE:O	2.33	0.46
29:LS:86:SER:N	29:LS:89:GLY:O	2.45	0.46
53:Lz:117:ILE:HA	53:Lz:120:ILE:HD13	1.97	0.46
4:5:2097:U:C2'	17:LF:35:LYS:HZ1	2.28	0.46
27:LQ:83:VAL:HG22	27:LQ:123:PHE:CZ	2.50	0.46
51:Lp:52:VAL:HG13	51:Lp:52:VAL:O	2.16	0.46
53:Lz:141:ASN:N	53:Lz:141:ASN:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LP:128:ARG:NH2	26:LP:130:TYR:OH	2.48	0.45
39:Lc:22:MET:HE2	39:Lc:22:MET:HA	1.97	0.45
4:5:423:G:OP1	26:LP:62:ARG:NH1	2.48	0.45
4:5:911:U:H2'	4:5:912:G:O4'	2.16	0.45
4:5:4883:C:N4	16:LE:181:LEU:O	2.42	0.45
8:B:488:ALA:O	8:B:491:SER:OG	2.33	0.45
53:Lz:12:GLU:OE1	53:Lz:13:ALA:N	2.49	0.45
4:5:1364:U:OP2	22:LL:36:ARG:NH2	2.46	0.45
4:5:1804:A:O2'	4:5:1833:G:O6	2.22	0.45
4:5:3893:C:O2'	4:5:4979:A:N1	2.40	0.45
22:LL:16:LYS:O	22:LL:21:ARG:NH2	2.49	0.45
35:LY:32:SER:OG	35:LY:104:VAL:O	2.34	0.45
4:5:132:G:H2'	4:5:133:C:O4'	2.17	0.45
4:5:1516:G:O2'	22:LL:18:TRP:NE1	2.43	0.45
4:5:2368:A:N6	4:5:2827:G:O2'	2.49	0.45
4:5:2519:U:O2'	4:5:2530:U:O2	2.33	0.45
7:A:486:LEU:HD13	7:A:502:ALA:CB	2.46	0.45
8:B:400:THR:O	8:B:404:VAL:HG23	2.17	0.45
17:LF:83:VAL:HG23	17:LF:83:VAL:O	2.14	0.45
18:LG:143:VAL:O	18:LG:147:VAL:HG23	2.17	0.45
36:LZ:47:ASP:N	36:LZ:69:LYS:O	2.44	0.45
4:5:2089:G:O2'	14:LC:307:LYS:NZ	2.43	0.45
4:5:4566:U:O2'	13:LB:234:ARG:NH1	2.49	0.45
15:LD:23:ARG:O	15:LD:23:ARG:NH1	2.43	0.45
37:La:100:ILE:N	37:La:100:ILE:HD12	2.32	0.45
38:Lb:66:SER:O	38:Lb:70:GLU:OE1	2.34	0.45
53:Lz:114:GLU:OE1	53:Lz:114:GLU:N	2.45	0.45
4:5:3636:C:O2	4:5:3636:C:H2'	2.16	0.45
14:LC:150:LEU:HD12	14:LC:150:LEU:O	2.16	0.45
21:LJ:15:LEU:HD12	21:LJ:165:TRP:HB2	1.98	0.45
4:5:3873:G:H2'	4:5:3874:G:C8	2.52	0.45
17:LF:219:GLY:O	17:LF:246:ARG:NH2	2.50	0.45
27:LQ:63:LEU:HD12	27:LQ:66:MET:HE2	1.98	0.45
36:LZ:100:VAL:HG23	36:LZ:106:LEU:HB3	1.99	0.45
4:5:2838:G:OP1	13:LB:248:LEU:N	2.50	0.45
4:5:4291:G:O2'	4:5:4328:G:N3	2.49	0.45
4:5:4385:A:O2'	4:5:4546:A:OP1	2.28	0.45
4:5:3653:A:C2	4:5:3692:A:H4'	2.52	0.45
9:C:221:ASN:OD1	9:C:222:TYR:N	2.50	0.45
13:LB:89:ILE:HD11	13:LB:201:LEU:HD21	1.99	0.45
17:LF:128:ALA:O	17:LF:132:MET:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LV:107:ASN:OD1	32:LV:111:GLU:N	2.49	0.45
41:Le:82:VAL:O	41:Le:86:GLU:OE1	2.35	0.45
4:5:2288:G:O2'	4:5:2290:C:O5'	2.35	0.45
4:5:4280:A:OP2	15:LD:23:ARG:NH2	2.44	0.45
25:LO:190:ASP:OD2	25:LO:190:ASP:C	2.59	0.45
4:5:1682:A:H2	37:La:43:ILE:HD12	1.82	0.44
4:5:2580:U:O2'	36:LZ:79:HIS:ND1	2.50	0.44
4:5:2779:C:O2'	6:8:112:G:OP1	2.18	0.44
7:A:720:ILE:HD12	7:A:724:GLN:HB3	1.99	0.44
8:B:406:GLU:HA	8:B:409:ILE:HG22	1.98	0.44
28:LR:31:GLU:OE2	28:LR:31:GLU:HA	2.17	0.44
32:LV:42:VAL:O	32:LV:45:ILE:HG22	2.18	0.44
4:5:386:A:OP2	35:LY:89:LYS:NZ	2.46	0.44
4:5:3652:A:H2'	4:5:3653:A:C8	2.53	0.44
4:5:4992:G:H2'	4:5:4993:G:C8	2.53	0.44
30:LT:118:GLU:OE1	30:LT:118:GLU:C	2.59	0.44
45:Li:59:GLU:O	45:Li:63:VAL:HG23	2.17	0.44
45:Li:73:ILE:O	45:Li:77:VAL:HG22	2.16	0.44
4:5:71:C:O2'	22:LL:62:PRO:O	2.34	0.44
4:5:208:A:N3	4:5:232:G:O2'	2.50	0.44
4:5:2378:G:O2'	4:5:2380:G:N7	2.40	0.44
4:5:4254:G:N3	4:5:4254:G:H2'	2.32	0.44
7:A:709:VAL:O	7:A:713:ILE:HG12	2.17	0.44
33:LW:52:THR:HG22	33:LW:54:LEU:H	1.82	0.44
4:5:1424:G:O6	4:5:1462:A:N6	2.50	0.44
7:A:67:ARG:NH2	7:A:103:SER:OG	2.49	0.44
8:B:204:ALA:CB	8:B:360:LEU:HD21	2.47	0.44
9:C:228:VAL:HG12	9:C:267:LYS:HD3	1.99	0.44
29:LS:97:TYR:OH	29:LS:112:ASP:OD2	2.30	0.44
51:Lp:89:LEU:O	51:Lp:92:GLN:NE2	2.51	0.44
53:Lz:67:VAL:HG23	53:Lz:67:VAL:O	2.18	0.44
4:5:1214:C:OP2	38:Lb:91:ARG:NH1	2.46	0.44
4:5:1631:A:C8	12:LA:199:VAL:HG21	2.52	0.44
4:5:1645:C:OP1	14:LC:80:ARG:NH2	2.39	0.44
4:5:2095:A:O2'	17:LF:28:LEU:HD21	2.18	0.44
4:5:4371:G:O2'	4:5:4372:U:OP2	2.28	0.44
16:LE:49:VAL:O	16:LE:49:VAL:HG13	2.18	0.44
16:LE:133:PHE:O	16:LE:138:ARG:NH2	2.49	0.44
22:LL:94:ILE:HD11	22:LL:96:ILE:HD12	2.00	0.44
39:Lc:42:LYS:O	39:Lc:97:ILE:HG23	2.16	0.44
4:5:1327:C:N4	4:5:1328:G:O6	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:3672:G:OP2	4:5:3672:G:N2	2.44	0.44
4:5:3909:C:H2'	4:5:3909:C:O2	2.17	0.44
4:5:4635:A:H3'	4:5:4636:U:H4'	1.99	0.44
6:8:64:U:C2	6:8:65:A:C8	3.06	0.44
7:A:727:LEU:HD11	7:A:775:LEU:HD22	2.00	0.44
20:LI:181:PHE:CZ	20:LI:197:VAL:HG11	2.53	0.44
51:Lp:85:ARG:O	51:Lp:89:LEU:HG	2.18	0.44
52:Lr:26:SER:OG	52:Lr:28:GLU:OE2	2.24	0.44
4:5:2833:A:OP1	40:Ld:44:ARG:NH2	2.51	0.44
4:5:4724:A:O2'	13:LB:104:THR:HG22	2.17	0.44
16:LE:177:GLY:N	16:LE:184:VAL:O	2.49	0.44
4:5:226:G:N7	14:LC:184:TYR:OH	2.39	0.44
4:5:1918:U:O4'	4:5:2065:G:N2	2.51	0.44
7:A:89:ASP:OD1	7:A:90:LEU:N	2.51	0.44
12:LA:13:GLY:O	12:LA:14:SER:OG	2.35	0.44
12:LA:109:GLU:OE1	12:LA:109:GLU:N	2.50	0.44
22:LL:110:LEU:O	22:LL:114:VAL:HG23	2.17	0.44
4:5:4438:U:H2'	4:5:4439:U:O4'	2.18	0.43
4:5:4458:C:H2'	4:5:4459:U:C6	2.53	0.43
4:5:4584:A:C2	4:5:4719:G:C4	3.05	0.43
7:A:355:THR:OG1	7:A:356:VAL:N	2.51	0.43
8:B:341:LEU:HD23	8:B:341:LEU:H	1.82	0.43
26:LP:41:ILE:HG23	26:LP:42:ARG:N	2.33	0.43
29:LS:73:LEU:HD23	29:LS:73:LEU:N	2.33	0.43
45:Li:77:VAL:HG23	45:Li:78:GLY:N	2.33	0.43
47:Lk:50:LYS:O	47:Lk:54:GLU:HG2	2.18	0.43
7:A:80:VAL:HG21	22:LL:118:LYS:HB3	2.01	0.43
7:A:735:VAL:HG12	7:A:772:LEU:HD21	1.99	0.43
14:LC:124:ILE:HD11	14:LC:240:LEU:HD12	1.99	0.43
39:Lc:97:ILE:HG22	39:Lc:98:ASP:OD1	2.17	0.43
4:5:433:A:H2'	4:5:434:A:O4'	2.18	0.43
4:5:711:A:H2'	4:5:712:C:C6	2.53	0.43
4:5:1368:A:C2	35:LY:1:MET:HE3	2.53	0.43
4:5:1914:C:OP2	4:5:1915:C:O2'	2.32	0.43
8:B:203:GLU:O	8:B:207:VAL:HG23	2.18	0.43
13:LB:291:TYR:OH	13:LB:315:ASN:ND2	2.51	0.43
14:LC:144:ILE:O	14:LC:147:VAL:HG22	2.18	0.43
28:LR:7:GLN:NE2	28:LR:35:ALA:O	2.46	0.43
49:Lm:127:VAL:HG23	49:Lm:128:LYS:HD2	2.00	0.43
4:5:2341:A:OP2	37:La:4:ARG:NH2	2.47	0.43
4:5:4237:C:OP1	4:5:4327:C:O2'	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LA:147:ARG:HG3	12:LA:157:VAL:HG22	1.99	0.43
18:LG:157:ILE:HG23	18:LG:201:THR:HG22	2.01	0.43
25:LO:110:PRO:N	25:LO:111:PRO:CD	2.82	0.43
25:LO:175:MET:SD	25:LO:175:MET:C	3.02	0.43
27:LQ:57:ASN:OD1	27:LQ:143:ARG:NH2	2.51	0.43
4:5:1361:G:OP2	22:LL:28:GLN:NE2	2.47	0.43
4:5:3913:G:H4'	4:5:3914:U:OP2	2.18	0.43
8:B:162:TYR:O	8:B:166:LYS:HG3	2.18	0.43
19:LH:106:GLN:O	19:LH:107:GLU:OE1	2.37	0.43
4:5:1786:A:O2'	4:5:1788:A:OP2	2.28	0.43
8:B:348:GLU:OE2	8:B:352:GLN:NE2	2.49	0.43
4:5:73:A:OP1	22:LL:106:SER:OG	2.26	0.43
4:5:3661:G:N7	12:LA:152:SER:OG	2.46	0.43
4:5:4584:A:H2'	4:5:4585:U:O4'	2.19	0.43
4:5:4872:G:C2	25:LO:203:VAL:HG23	2.53	0.43
5:7:42:A:O4'	21:LJ:75:ARG:NE	2.52	0.43
7:A:637:ASP:OD1	7:A:638:PHE:N	2.52	0.43
16:LE:161:ARG:O	16:LE:182:ASN:ND2	2.52	0.43
4:5:1656:U:OP2	37:La:26:ARG:NH2	2.51	0.43
4:5:2877:G:N2	4:5:3824:A:O2'	2.45	0.43
4:5:4323:A:H2	15:LD:146:LEU:HD23	1.80	0.43
5:7:111:C:H2'	5:7:112:U:O4'	2.18	0.43
8:B:205:ILE:HD13	8:B:224:LEU:HD12	2.00	0.43
8:B:241:TRP:CB	8:B:343:LEU:HD21	2.48	0.43
4:5:4873:G:C2	25:LO:175:MET:HE1	2.54	0.43
7:A:366:GLU:OE1	7:A:366:GLU:N	2.50	0.43
9:C:215:PHE:HE2	9:C:240:LEU:HD11	1.83	0.43
7:A:612:LEU:HD22	7:A:624:THR:HG23	2.00	0.42
7:A:732:GLN:O	7:A:736:VAL:HG23	2.19	0.42
8:B:212:VAL:HG21	8:B:223:VAL:HG11	2.00	0.42
11:K:118:HIS:ND1	11:K:120:ASP:OD1	2.50	0.42
22:LL:81:LEU:HD11	22:LL:98:VAL:HG22	2.00	0.42
40:Ld:61:ASP:O	40:Ld:61:ASP:CG	2.61	0.42
7:A:568:ALA:O	7:A:571:LYS:HG2	2.19	0.42
15:LD:64:ILE:CD1	15:LD:109:LEU:HD22	2.48	0.42
16:LE:257:ILE:HG22	16:LE:261:ILE:HD12	2.01	0.42
28:LR:28:GLU:OE2	28:LR:28:GLU:HA	2.19	0.42
38:Lb:94:ASP:OD1	38:Lb:94:ASP:N	2.52	0.42
53:Lz:119:GLN:N	53:Lz:119:GLN:OE1	2.52	0.42
4:5:1643:A:C5	4:5:1644:C:C5	3.08	0.42
4:5:1705:G:H21	4:5:1705:G:P	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:2415:U:H2'	4:5:2416:G:O4'	2.19	0.42
7:A:686:LEU:HG	7:A:709:VAL:HG21	2.00	0.42
27:LQ:88:ASP:OD1	27:LQ:89:ASP:N	2.53	0.42
36:LZ:10:VAL:HG23	36:LZ:86:SER:HA	2.01	0.42
53:Lz:31:THR:H	53:Lz:209:THR:HG1	1.60	0.42
4:5:2046:G:O2'	4:5:2047:A:N7	2.49	0.42
4:5:2525:U:C2	4:5:2527:A:OP2	2.72	0.42
4:5:3648:A:H1'	4:5:3785:A:N6	2.34	0.42
4:5:4454:G:O2'	4:5:4500:U:O2'	2.29	0.42
4:5:4716:C:OP1	13:LB:276:HIS:ND1	2.49	0.42
24:LN:96:ARG:NH2	24:LN:104:GLU:OE1	2.47	0.42
40:Ld:42:ALA:HB3	40:Ld:43:PRO:HD3	2.01	0.42
5:7:110:G:H2'	5:7:111:C:C6	2.55	0.42
23:LM:95:ILE:O	23:LM:99:GLU:HG3	2.19	0.42
29:LS:94:TYR:OH	29:LS:96:GLU:OE1	2.25	0.42
32:LV:27:ASN:ND2	32:LV:100:ASP:OD2	2.51	0.42
4:5:1629:G:N2	12:LA:208:GLU:OE1	2.51	0.42
4:5:4963:G:C6	4:5:4964:C:N4	2.87	0.42
7:A:121:ASP:OD1	7:A:160:ARG:NE	2.52	0.42
7:A:540:LEU:O	7:A:544:VAL:HG23	2.20	0.42
7:A:679:THR:OG1	7:A:684:LEU:HD23	2.20	0.42
15:LD:229:ASN:O	15:LD:230:SER:OG	2.28	0.42
18:LG:179:VAL:HG23	18:LG:179:VAL:O	2.20	0.42
18:LG:228:ASP:N	18:LG:228:ASP:OD1	2.52	0.42
53:Lz:80:VAL:HG23	53:Lz:80:VAL:O	2.19	0.42
4:5:280:G:OP2	24:LN:44:ARG:NH1	2.51	0.42
4:5:1305:C:OP1	6:8:7:U:O2'	2.38	0.42
4:5:1817:U:O2'	4:5:1818:G:H5'	2.19	0.42
4:5:4251:A:H2'	4:5:4252:C:O4'	2.19	0.42
53:Lz:22:GLN:N	53:Lz:22:GLN:OE1	2.53	0.42
4:5:438:G:N2	42:Lf:23:GLU:OE2	2.43	0.42
4:5:1089:G:OP1	4:5:1199:G:N1	2.40	0.42
4:5:1852:U:OP1	37:La:23:GLY:N	2.38	0.42
8:B:355:ASP:O	8:B:358:MET:SD	2.78	0.42
18:LG:176:LYS:HD2	45:Li:43:MET:HE3	2.01	0.42
23:LM:5:ARG:NE	23:LM:59:ASP:OD1	2.46	0.42
38:Lb:9:THR:O	38:Lb:9:THR:CG2	2.67	0.42
53:Lz:53:VAL:HG22	53:Lz:54:ARG:N	2.33	0.42
4:5:3652:A:O2'	12:LA:182:ALA:HB2	2.20	0.42
4:5:3955:G:H2'	4:5:3956:G:C8	2.55	0.42
7:A:513:TYR:O	7:A:517:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:583:ASN:OD1	7:A:584:LEU:N	2.53	0.42
19:LH:41:ILE:HG22	19:LH:43:VAL:HG13	2.01	0.42
31:LU:20:LYS:CD	31:LU:71:THR:HG23	2.50	0.42
34:LX:148:ASP:OD2	34:LX:148:ASP:C	2.63	0.42
37:La:93:ASN:OD1	37:La:95:THR:HG22	2.20	0.42
4:5:1739:G:H2'	4:5:1740:C:C6	2.54	0.42
4:5:4970:C:C2	4:5:4971:A:C8	3.08	0.42
20:LI:181:PHE:CE1	20:LI:197:VAL:HG11	2.55	0.42
4:5:2079:G:H2'	4:5:2080:U:C6	2.55	0.41
4:5:2460:A:O2'	24:LN:96:ARG:NH2	2.52	0.41
4:5:4122:G:O2'	36:LZ:136:PHE:OXT	2.37	0.41
4:5:4678:G:N2	4:5:4713:G:H1'	2.35	0.41
4:5:4749:C:H2'	4:5:4750:G:O4'	2.20	0.41
8:B:183:VAL:HG13	8:B:424:LEU:HD21	2.01	0.41
23:LM:16:SER:HG	23:LM:17:PHE:HD2	1.65	0.41
24:LN:96:ARG:NH1	24:LN:104:GLU:OE1	2.51	0.41
26:LP:47:TYR:O	26:LP:51:VAL:HG23	2.20	0.41
38:Lb:35:VAL:HG21	38:Lb:40:LEU:HD21	2.01	0.41
4:5:3795:A:C6	4:5:3806:G:C6	3.09	0.41
4:5:3909:C:N3	4:5:3910:C:C5	2.88	0.41
28:LR:111:GLU:OE2	28:LR:111:GLU:HA	2.20	0.41
53:Lz:81:ASP:OD1	53:Lz:81:ASP:N	2.53	0.41
53:Lz:129:ASN:OD1	53:Lz:130:LYS:N	2.53	0.41
4:5:67:C:N4	4:5:325:U:O2'	2.50	0.41
4:5:1474:C:H2'	4:5:1475:G:C8	2.55	0.41
4:5:2347:A:C5	41:Le:31:ILE:HD11	2.55	0.41
4:5:2359:U:OP2	4:5:2360:A:O2'	2.31	0.41
4:5:2857:A:H2'	4:5:2858:A:O4'	2.20	0.41
4:5:3910:C:O2'	4:5:4196:G:N2	2.51	0.41
4:5:1418:C:H2'	4:5:1419:G:O4'	2.20	0.41
5:7:6:C:O3'	15:LD:50:ARG:NH2	2.52	0.41
21:LJ:128:LEU:HD23	21:LJ:128:LEU:N	2.36	0.41
53:Lz:77:ALA:O	53:Lz:80:VAL:O	2.38	0.41
4:5:1769:G:C2	4:5:1770:A:C5	3.09	0.41
4:5:2340:C:H4'	14:LC:42:THR:HG23	2.03	0.41
4:5:2599:G:N2	4:5:2747:U:O4	2.53	0.41
4:5:4891:G:C6	4:5:4892:A:C6	3.08	0.41
31:LU:66:SER:O	31:LU:66:SER:OG	2.33	0.41
4:5:4049:U:H3'	4:5:4050:A:H5''	2.03	0.41
4:5:4586:G:OP2	25:LO:74:ARG:NH1	2.53	0.41
7:A:513:TYR:O	7:A:516:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:176:ARG:NH2	8:B:431:ASP:OD1	2.54	0.41
14:LC:121:ARG:O	14:LC:124:ILE:HG22	2.20	0.41
14:LC:348:LYS:O	14:LC:351:VAL:HG12	2.20	0.41
39:Lc:19:GLN:O	39:Lc:23:LYS:HG2	2.21	0.41
4:5:1332:C:H2'	4:5:1333:A:H8	1.85	0.41
4:5:1795:A:N3	5:7:79:U:O2'	2.52	0.41
4:5:4587:G:OP1	25:LO:61:ARG:NH1	2.54	0.41
28:LR:107:ARG:O	28:LR:111:GLU:HG2	2.19	0.41
35:LY:120:GLU:OE1	35:LY:120:GLU:N	2.54	0.41
4:5:177:G:H2'	4:5:178:C:H5''	2.03	0.41
4:5:665:C:O4'	4:5:667:A:N6	2.54	0.41
4:5:1920:C:H3'	4:5:1921:C:H5''	2.02	0.41
6:8:141:C:OP1	24:LN:38:ARG:NH1	2.54	0.41
25:LO:84:VAL:HG11	25:LO:102:LEU:CD2	2.51	0.41
4:5:113:A:OP2	4:5:156:G:N2	2.43	0.41
4:5:731:G:C6	4:5:932:A:C4	3.09	0.41
4:5:2659:A:C2	4:5:2676:A:C8	3.08	0.41
4:5:3634:G:N2	4:5:3636:C:H5''	2.36	0.41
6:8:69:U:H2'	6:8:70:G:O4'	2.20	0.41
7:A:154:THR:O	7:A:158:THR:OG1	2.34	0.41
11:K:213:THR:O	11:K:217:VAL:HG23	2.21	0.41
15:LD:116:ASP:OD1	15:LD:117:LYS:N	2.52	0.41
35:LY:71:VAL:HG22	35:LY:81:TYR:O	2.20	0.41
35:LY:82:ILE:HG22	35:LY:83:GLU:N	2.36	0.41
36:LZ:76:ASN:OD1	36:LZ:77:TYR:N	2.54	0.41
40:Ld:64:ILE:HG23	40:Ld:68:LEU:HD23	2.02	0.41
4:5:492:U:H2'	4:5:493:G:O4'	2.21	0.41
4:5:1882:U:C4	4:5:2279:A:C2	3.09	0.41
4:5:1933:G:H2'	4:5:1934:A:C8	2.56	0.41
4:5:2503:G:O6	12:LA:72:ARG:NH1	2.51	0.41
4:5:3756:A:H2'	4:5:3757:G:C1'	2.50	0.41
7:A:674:GLU:O	7:A:678:VAL:HG23	2.21	0.41
19:LH:107:GLU:OE1	19:LH:111:LEU:CB	2.69	0.41
29:LS:164:LYS:CB	29:LS:165:PRO:CD	2.99	0.41
47:Lk:10:ASP:N	47:Lk:10:ASP:OD2	2.54	0.41
53:Lz:175:THR:OG1	53:Lz:177:ASP:OD1	2.31	0.41
6:8:51:U:O2'	6:8:52:A:C8	2.73	0.40
7:A:78:ASN:OD1	7:A:79:ILE:N	2.54	0.40
20:LI:43:VAL:HG21	20:LI:197:VAL:HG13	2.02	0.40
36:LZ:31:ASP:C	36:LZ:31:ASP:OD2	2.64	0.40
43:Lg:107:LEU:O	43:Lg:110:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:3938:G:H4'	4:5:3939:G:O5'	2.21	0.40
6:8:149:G:O2'	6:8:151:G:OP2	2.39	0.40
7:A:153:LEU:O	7:A:157:LEU:CD2	2.69	0.40
13:LB:153:MET:HE3	13:LB:194:LEU:HD21	2.02	0.40
17:LF:92:VAL:HG13	17:LF:140:ILE:HD12	2.02	0.40
20:LI:82:ARG:NH1	20:LI:83:ASP:OD1	2.54	0.40
20:LI:84:GLY:O	20:LI:140:THR:OG1	2.34	0.40
31:LU:62:THR:C	31:LU:63:ILE:HD12	2.45	0.40
53:Lz:65:VAL:CG1	53:Lz:148:VAL:HG13	2.50	0.40
4:5:2264:C:H2'	4:5:2265:G:O4'	2.21	0.40
4:5:2752:G:H2'	4:5:2753:G:O4'	2.22	0.40
7:A:325:ILE:HG22	7:A:329:LEU:HG	2.03	0.40
24:LN:181:HIS:O	24:LN:195:ARG:NH2	2.47	0.40
52:Lr:97:ILE:HD13	52:Lr:107:ARG:HA	2.02	0.40
53:Lz:144:MET:SD	53:Lz:144:MET:C	3.04	0.40
4:5:2021:G:C2	4:5:2022:C:C5	3.10	0.40
4:5:3950:U:H2'	4:5:3951:G:C1'	2.51	0.40
18:LG:131:LYS:O	18:LG:132:ARG:C	2.65	0.40
25:LO:81:TRP:CZ2	25:LO:99:LEU:HD21	2.56	0.40
4:5:5004:C:H2'	4:5:5005:G:O4'	2.22	0.40
13:LB:301:ASN:O	13:LB:301:ASN:ND2	2.55	0.40
14:LC:366:ASP:OD1	14:LC:367:GLU:N	2.55	0.40
20:LI:66:GLU:OE1	20:LI:69:ARG:NH2	2.55	0.40
53:Lz:174:MET:HE2	53:Lz:178:GLU:OE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	420/476 (88%)	399 (95%)	21 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	60/68 (88%)	58 (97%)	2 (3%)	0	100	100
3	3	27/96 (28%)	25 (93%)	2 (7%)	0	100	100
7	A	684/794 (86%)	671 (98%)	13 (2%)	0	100	100
8	B	397/506 (78%)	390 (98%)	7 (2%)	0	100	100
9	C	107/314 (34%)	107 (100%)	0	0	100	100
10	D	76/85 (89%)	76 (100%)	0	0	100	100
11	K	222/245 (91%)	215 (97%)	7 (3%)	0	100	100
12	LA	246/257 (96%)	239 (97%)	7 (3%)	0	100	100
13	LB	400/403 (99%)	395 (99%)	5 (1%)	0	100	100
14	LC	366/427 (86%)	360 (98%)	6 (2%)	0	100	100
15	LD	291/297 (98%)	285 (98%)	5 (2%)	1 (0%)	36	65
16	LE	214/288 (74%)	207 (97%)	7 (3%)	0	100	100
17	LF	223/248 (90%)	217 (97%)	6 (3%)	0	100	100
18	LG	239/266 (90%)	233 (98%)	6 (2%)	0	100	100
19	LH	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
20	LI	198/214 (92%)	193 (98%)	5 (2%)	0	100	100
21	LJ	173/178 (97%)	170 (98%)	3 (2%)	0	100	100
22	LL	192/211 (91%)	187 (97%)	5 (3%)	0	100	100
23	LM	134/215 (62%)	132 (98%)	2 (2%)	0	100	100
24	LN	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
25	LO	199/203 (98%)	199 (100%)	0	0	100	100
26	LP	151/184 (82%)	148 (98%)	3 (2%)	0	100	100
27	LQ	185/188 (98%)	183 (99%)	2 (1%)	0	100	100
28	LR	153/196 (78%)	149 (97%)	4 (3%)	0	100	100
29	LS	173/176 (98%)	166 (96%)	7 (4%)	0	100	100
30	LT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
31	LU	99/128 (77%)	96 (97%)	2 (2%)	1 (1%)	12	40
32	LV	129/140 (92%)	125 (97%)	4 (3%)	0	100	100
33	LW	60/157 (38%)	59 (98%)	1 (2%)	0	100	100
34	LX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
35	LY	132/145 (91%)	128 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	LZ	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
37	La	145/148 (98%)	139 (96%)	6 (4%)	0	100	100
38	Lb	105/159 (66%)	102 (97%)	3 (3%)	0	100	100
39	Lc	96/115 (84%)	96 (100%)	0	0	100	100
40	Ld	105/125 (84%)	101 (96%)	4 (4%)	0	100	100
41	Le	126/135 (93%)	123 (98%)	3 (2%)	0	100	100
42	Lf	107/110 (97%)	107 (100%)	0	0	100	100
43	Lg	112/117 (96%)	112 (100%)	0	0	100	100
44	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
45	Li	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
46	Lj	84/97 (87%)	84 (100%)	0	0	100	100
47	Lk	67/70 (96%)	67 (100%)	0	0	100	100
48	Ll	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
49	Lm	50/128 (39%)	49 (98%)	1 (2%)	0	100	100
50	Lo	103/106 (97%)	101 (98%)	2 (2%)	0	100	100
51	Lp	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
52	Lr	123/137 (90%)	122 (99%)	1 (1%)	0	100	100
53	Lz	215/217 (99%)	208 (97%)	7 (3%)	0	100	100
All	All	8540/9988 (86%)	8352 (98%)	186 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	LD	4	VAL
31	LU	19	LEU

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	1	361/398 (91%)	360 (100%)	1 (0%)	86	86
2	2	53/59 (90%)	53 (100%)	0	100	100
3	3	26/74 (35%)	25 (96%)	1 (4%)	29	57
7	A	612/704 (87%)	612 (100%)	0	100	100
8	B	360/438 (82%)	360 (100%)	0	100	100
9	C	93/254 (37%)	93 (100%)	0	100	100
10	D	66/72 (92%)	66 (100%)	0	100	100
11	K	194/213 (91%)	192 (99%)	2 (1%)	68	76
12	LA	190/199 (96%)	190 (100%)	0	100	100
13	LB	348/349 (100%)	348 (100%)	0	100	100
14	LC	306/348 (88%)	306 (100%)	0	100	100
15	LD	246/250 (98%)	246 (100%)	0	100	100
16	LE	194/252 (77%)	194 (100%)	0	100	100
17	LF	194/215 (90%)	194 (100%)	0	100	100
18	LG	203/223 (91%)	202 (100%)	1 (0%)	81	83
19	LH	169/171 (99%)	169 (100%)	0	100	100
20	LI	172/181 (95%)	172 (100%)	0	100	100
21	LJ	147/149 (99%)	147 (100%)	0	100	100
22	LL	164/177 (93%)	164 (100%)	0	100	100
23	LM	116/161 (72%)	116 (100%)	0	100	100
24	LN	171/172 (99%)	171 (100%)	0	100	100
25	LO	173/174 (99%)	173 (100%)	0	100	100
26	LP	134/163 (82%)	134 (100%)	0	100	100
27	LQ	164/165 (99%)	164 (100%)	0	100	100
28	LR	138/175 (79%)	138 (100%)	0	100	100
29	LS	156/157 (99%)	156 (100%)	0	100	100
30	LT	139/140 (99%)	139 (100%)	0	100	100
31	LU	91/115 (79%)	91 (100%)	0	100	100
32	LV	101/107 (94%)	101 (100%)	0	100	100
33	LW	54/126 (43%)	54 (100%)	0	100	100
34	LX	106/133 (80%)	106 (100%)	0	100	100
35	LY	124/135 (92%)	123 (99%)	1 (1%)	73	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	LZ	117/118 (99%)	117 (100%)	0	100	100
37	La	120/121 (99%)	120 (100%)	0	100	100
38	Lb	88/126 (70%)	88 (100%)	0	100	100
39	Lc	83/97 (86%)	83 (100%)	0	100	100
40	Ld	98/110 (89%)	98 (100%)	0	100	100
41	Le	114/121 (94%)	114 (100%)	0	100	100
42	Lf	88/89 (99%)	88 (100%)	0	100	100
43	Lg	98/100 (98%)	98 (100%)	0	100	100
44	Lh	109/110 (99%)	109 (100%)	0	100	100
45	Li	86/89 (97%)	86 (100%)	0	100	100
46	Lj	73/80 (91%)	73 (100%)	0	100	100
47	Lk	64/65 (98%)	64 (100%)	0	100	100
48	Ll	47/48 (98%)	47 (100%)	0	100	100
49	Lm	48/116 (41%)	48 (100%)	0	100	100
50	Lo	93/94 (99%)	93 (100%)	0	100	100
51	Lp	74/75 (99%)	74 (100%)	0	100	100
52	Lr	109/121 (90%)	109 (100%)	0	100	100
53	Lz	196/196 (100%)	196 (100%)	0	100	100
All	All	7470/8525 (88%)	7464 (100%)	6 (0%)	87	90

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	452	THR
3	3	77	SER
11	K	41	GLU
11	K	203	CYS
18	LG	159	HIS
35	LY	120	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
7	A	108	GLN
7	A	572	HIS

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Mol	Chain	Res	Type
7	A	627	HIS
7	A	703	HIS
7	A	725	HIS
8	B	140	GLN
8	B	167	GLN
8	B	465	GLN
9	C	299	ASN
11	K	162	HIS
12	LA	22	HIS
12	LA	38	HIS
13	LB	184	GLN
13	LB	322	HIS
14	LC	38	ASN
14	LC	187	GLN
14	LC	310	HIS
14	LC	329	ASN
15	LD	45	ASN
15	LD	198	HIS
15	LD	202	GLN
17	LF	110	GLN
18	LG	82	GLN
18	LG	100	HIS
18	LG	141	ASN
18	LG	227	ASN
19	LH	8	GLN
19	LH	98	HIS
20	LI	73	ASN
20	LI	163	GLN
20	LI	213	HIS
21	LJ	110	GLN
22	LL	67	HIS
24	LN	29	GLN
24	LN	32	GLN
24	LN	158	HIS
26	LP	34	GLN
26	LP	75	GLN
30	LT	54	HIS
30	LT	114	GLN
31	LU	105	ASN
33	LW	50	ASN
33	LW	59	HIS
34	LX	107	HIS

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Mol	Chain	Res	Type
35	LY	96	HIS
37	La	17	HIS
37	La	89	ASN
40	Ld	116	ASN
42	Lf	99	HIS
44	Lh	65	GLN
45	Li	15	HIS
47	Lk	58	GLN
48	Ll	33	ASN
50	Lo	76	ASN
52	Lr	21	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	5	3452/5070 (68%)	382 (11%)	5 (0%)
5	7	119/121 (98%)	5 (4%)	0
6	8	145/157 (92%)	13 (8%)	0
All	All	3716/5348 (69%)	400 (10%)	5 (0%)

All (400) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	5	2	G
4	5	13	U
4	5	39	A
4	5	42	A
4	5	48	G
4	5	59	A
4	5	64	A
4	5	65	A
4	5	73	A
4	5	91	G
4	5	98	A
4	5	110	C
4	5	119	G
4	5	120	A
4	5	134	G
4	5	135	G
4	5	136	C
4	5	141	C

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Mol	Chain	Res	Type
4	5	142	G
4	5	143	C
4	5	159	C
4	5	172	C
4	5	178	C
4	5	179	G
4	5	197	A
4	5	200	U
4	5	209	U
4	5	218	A
4	5	219	G
4	5	233	U
4	5	234	G
4	5	253	G
4	5	266	C
4	5	280	G
4	5	297	U
4	5	316	U
4	5	340	C
4	5	381	U
4	5	387	G
4	5	409	G
4	5	410	A
4	5	412	G
4	5	413	G
4	5	449	C
4	5	450	G
4	5	451	C
4	5	453	G
4	5	454	U
4	5	467	U
4	5	485	C
4	5	662	C
4	5	664	G
4	5	666	G
4	5	669	C
4	5	686	A
4	5	687	U
4	5	697	G
4	5	704	C
4	5	705	G
4	5	731	G

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Mol	Chain	Res	Type
4	5	738	C
4	5	739	G
4	5	740	G
4	5	760	G
4	5	915	A
4	5	917	A
4	5	926	G
4	5	932	A
4	5	933	G
4	5	936	C
4	5	943	A
4	5	944	A
4	5	945	U
4	5	956	A
4	5	960	A
4	5	961	G
4	5	962	C
4	5	965	G
4	5	967	C
4	5	968	C
4	5	969	C
4	5	982	U
4	5	1070	G
4	5	1072	C
4	5	1078	A
4	5	1101	C
4	5	1168	G
4	5	1170	G
4	5	1182	C
4	5	1183	C
4	5	1199	G
4	5	1211	G
4	5	1215	C
4	5	1241	C
4	5	1266	G
4	5	1269	G
4	5	1270	A
4	5	1272	C
4	5	1273	G
4	5	1284	G
4	5	1287	G
4	5	1302	U

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Mol	Chain	Res	Type
4	5	1303	A
4	5	1304	C
4	5	1326	A
4	5	1354	A
4	5	1359	G
4	5	1366	G
4	5	1387	A
4	5	1397	A
4	5	1399	G
4	5	1413	C
4	5	1414	C
4	5	1415	G
4	5	1439	C
4	5	1443	A
4	5	1445	U
4	5	1497	A
4	5	1498	G
4	5	1502	G
4	5	1516	G
4	5	1523	A
4	5	1534	A
4	5	1547	A
4	5	1578	U
4	5	1591	U
4	5	1596	U
4	5	1613	A
4	5	1624	G
4	5	1625	G
4	5	1631	A
4	5	1633	G
4	5	1634	A
4	5	1638	A
4	5	1641	G
4	5	1654	G
4	5	1661	C
4	5	1676	C
4	5	1677	U
4	5	1691	G
4	5	1697	G
4	5	1699	A
4	5	1701	A
4	5	1742	A

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Mol	Chain	Res	Type
4	5	1755	C
4	5	1761	G
4	5	1765	A
4	5	1766	A
4	5	1767	A
4	5	1768	C
4	5	1787	A
4	5	1804	A
4	5	1836	G
4	5	1837	A
4	5	1842	G
4	5	1855	G
4	5	1869	G
4	5	1897	A
4	5	1918	U
4	5	1921	C
4	5	1922	G
4	5	1931	C
4	5	1932	A
4	5	1940	G
4	5	1941	A
4	5	1948	G
4	5	1961	G
4	5	2026	A
4	5	2046	G
4	5	2048	U
4	5	2055	G
4	5	2056	G
4	5	2069	A
4	5	2084	C
4	5	2092	G
4	5	2093	A
4	5	2096	G
4	5	2098	G
4	5	2102	G
4	5	2107	C
4	5	2261	G
4	5	2300	A
4	5	2301	G
4	5	2306	G
4	5	2313	A
4	5	2314	G

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Mol	Chain	Res	Type
4	5	2348	G
4	5	2350	U
4	5	2351	C
4	5	2360	A
4	5	2395	A
4	5	2397	G
4	5	2417	A
4	5	2421	G
4	5	2470	C
4	5	2471	G
4	5	2474	G
4	5	2475	G
4	5	2478	C
4	5	2504	C
4	5	2505	C
4	5	2506	G
4	5	2513	A
4	5	2554	U
4	5	2583	C
4	5	2587	A
4	5	2589	C
4	5	2601	A
4	5	2627	C
4	5	2653	C
4	5	2660	A
4	5	2669	C
4	5	2687	U
4	5	2694	G
4	5	2695	A
4	5	2696	A
4	5	2708	U
4	5	2711	G
4	5	2743	A
4	5	2761	U
4	5	2764	A
4	5	2769	U
4	5	2788	U
4	5	2790	U
4	5	2814	C
4	5	2826	U
4	5	2827	G
4	5	2829	U

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Mol	Chain	Res	Type
4	5	2855	G
4	5	2899	C
4	5	3597	G
4	5	3605	C
4	5	3615	G
4	5	3618	C
4	5	3626	G
4	5	3635	A
4	5	3653	A
4	5	3662	A
4	5	3673	C
4	5	3692	A
4	5	3709	U
4	5	3710	G
4	5	3712	A
4	5	3753	G
4	5	3757	G
4	5	3776	G
4	5	3777	G
4	5	3784	A
4	5	3811	G
4	5	3814	U
4	5	3817	A
4	5	3819	G
4	5	3838	U
4	5	3839	G
4	5	3840	U
4	5	3877	A
4	5	3878	C
4	5	3879	G
4	5	3897	G
4	5	3898	G
4	5	3901	A
4	5	3906	A
4	5	3907	G
4	5	3908	A
4	5	3915	U
4	5	3939	G
4	5	3951	G
4	5	3956	G
4	5	3958	G
4	5	3959	U

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Mol	Chain	Res	Type
4	5	3961	G
4	5	3962	A
4	5	3963	A
4	5	3965	A
4	5	3966	A
4	5	3967	G
4	5	3968	U
4	5	3969	G
4	5	3974	G
4	5	3975	C
4	5	4040	C
4	5	4046	A
4	5	4048	A
4	5	4049	U
4	5	4050	A
4	5	4051	C
4	5	4061	G
4	5	4076	G
4	5	4119	C
4	5	4122	G
4	5	4163	U
4	5	4170	A
4	5	4183	G
4	5	4184	G
4	5	4191	G
4	5	4203	A
4	5	4213	A
4	5	4229	U
4	5	4233	A
4	5	4234	A
4	5	4251	A
4	5	4254	G
4	5	4266	G
4	5	4268	A
4	5	4273	A
4	5	4281	A
4	5	4291	G
4	5	4305	G
4	5	4306	U
4	5	4330	G
4	5	4332	C
4	5	4339	A

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Mol	Chain	Res	Type
4	5	4373	G
4	5	4377	G
4	5	4378	A
4	5	4381	A
4	5	4387	C
4	5	4394	A
4	5	4421	C
4	5	4422	A
4	5	4437	U
4	5	4448	G
4	5	4464	A
4	5	4465	U
4	5	4466	C
4	5	4500	U
4	5	4512	U
4	5	4513	A
4	5	4524	G
4	5	4548	A
4	5	4549	G
4	5	4567	G
4	5	4590	A
4	5	4627	U
4	5	4636	U
4	5	4637	G
4	5	4656	A
4	5	4670	C
4	5	4671	C
4	5	4672	A
4	5	4700	A
4	5	4708	A
4	5	4709	U
4	5	4720	C
4	5	4730	C
4	5	4731	G
4	5	4732	G
4	5	4734	A
4	5	4741	C
4	5	4742	G
4	5	4743	G
4	5	4745	G
4	5	4750	G
4	5	4754	G

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Mol	Chain	Res	Type
4	5	4757	C
4	5	4759	C
4	5	4761	G
4	5	4765	G
4	5	4771	C
4	5	4870	G
4	5	4871	C
4	5	4882	U
4	5	4883	C
4	5	4895	C
4	5	4900	C
4	5	4901	G
4	5	4910	A
4	5	4912	G
4	5	4938	A
4	5	4943	A
4	5	4976	U
4	5	4988	U
4	5	4990	C
4	5	4991	U
4	5	4994	G
4	5	5017	G
4	5	5034	A
4	5	5041	G
4	5	5048	A
4	5	5050	C
4	5	5062	G
4	5	5069	U
5	7	7	G
5	7	53	U
5	7	54	A
5	7	64	G
5	7	110	G
6	8	23	C
6	8	34	U
6	8	35	C
6	8	39	G
6	8	59	A
6	8	62	A
6	8	63	U
6	8	80	A
6	8	87	G

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Mol	Chain	Res	Type
6	8	103	A
6	8	105	C
6	8	110	U
6	8	114	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	5	739	G
4	5	1633	G
4	5	3964	U
4	5	4048	A
4	5	4699	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 225 ligands modelled in this entry, 225 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 ⓘ

There are no chain breaks in this entry.

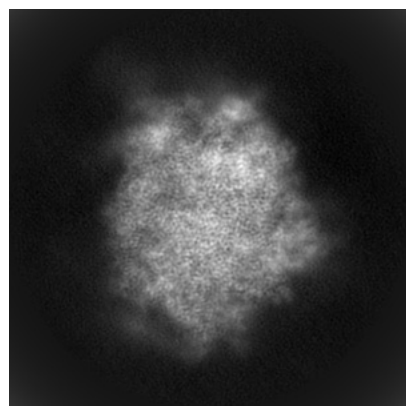
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16902. These allow visual inspection of the internal detail of the map and identification of artifacts.

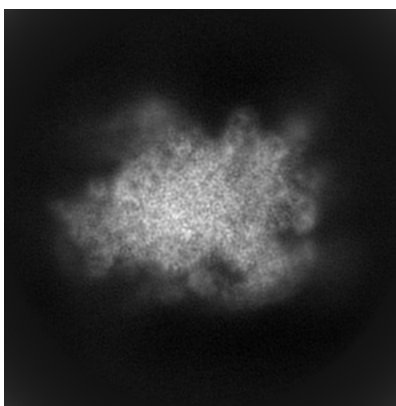
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

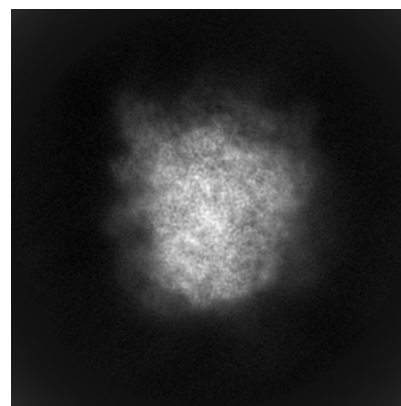
6.1.1 Primary map



X

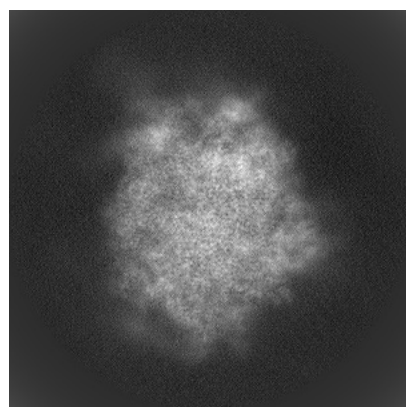


Y

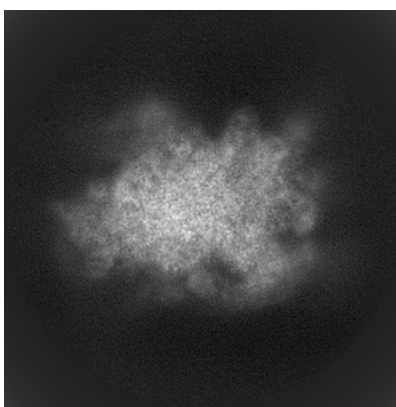


Z

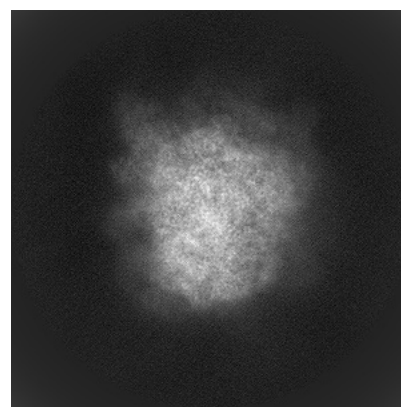
6.1.2 Raw map



X



Y

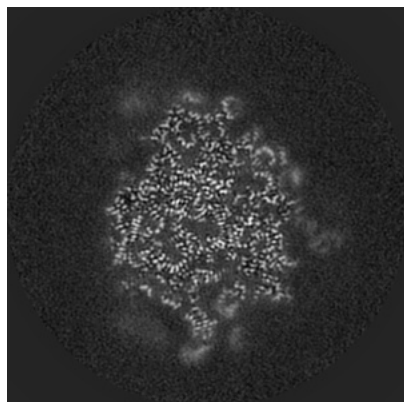


Z

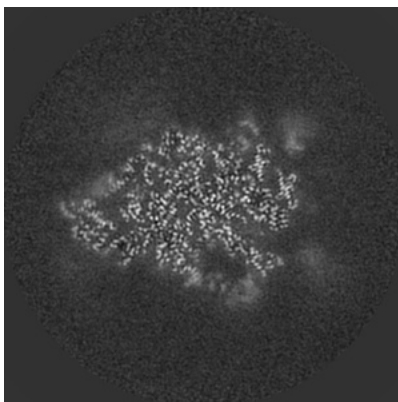
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

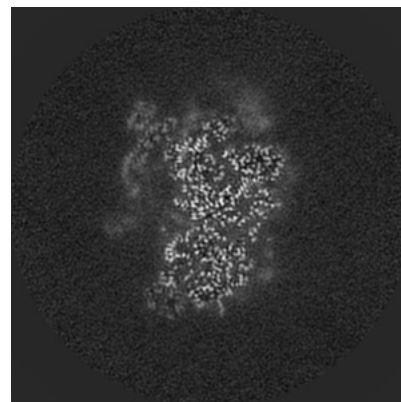
6.2.1 Primary map



X Index: 270

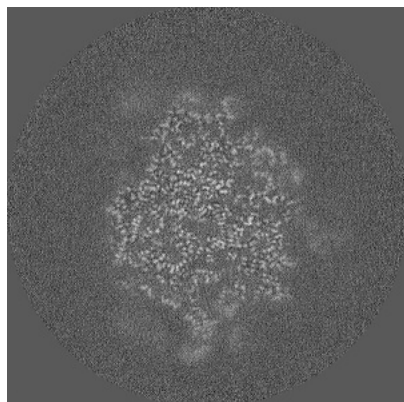


Y Index: 270

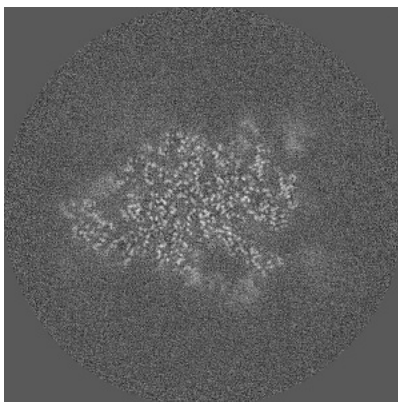


Z Index: 270

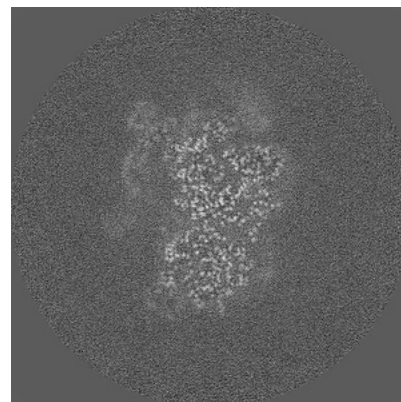
6.2.2 Raw map



X Index: 270



Y Index: 270

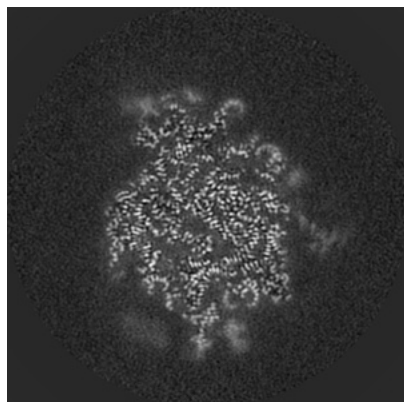


Z Index: 270

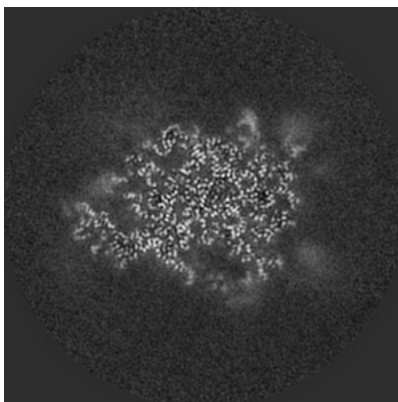
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

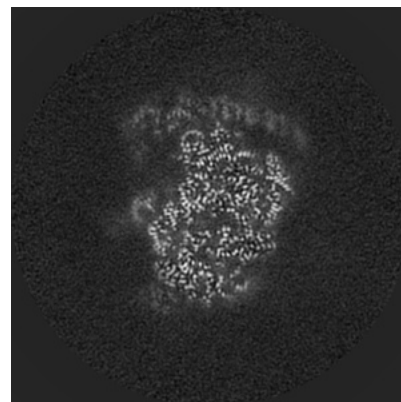
6.3.1 Primary map



X Index: 261

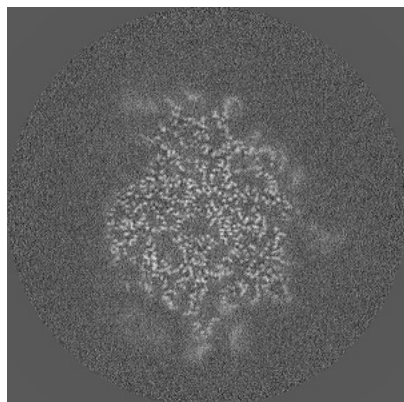


Y Index: 276

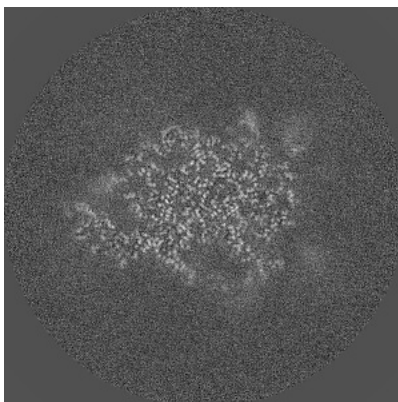


Z Index: 249

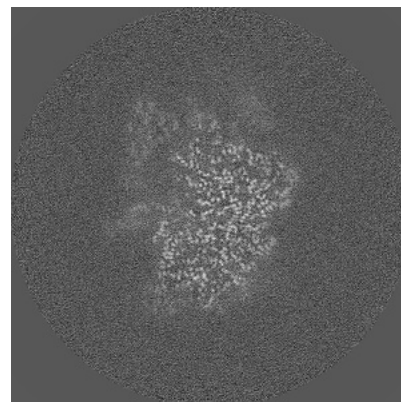
6.3.2 Raw map



X Index: 266



Y Index: 275

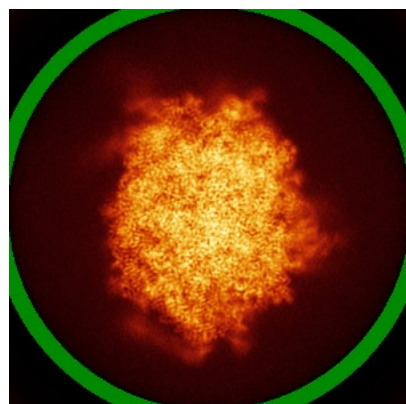


Z Index: 261

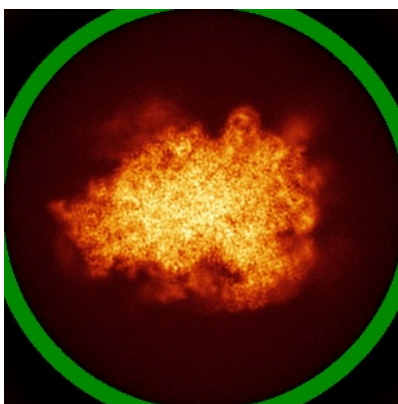
The images above show the largest variance slices of the map in three orthogonal directions.

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

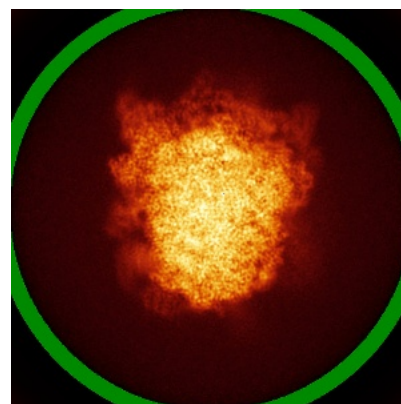
6.4.1 Primary map



X

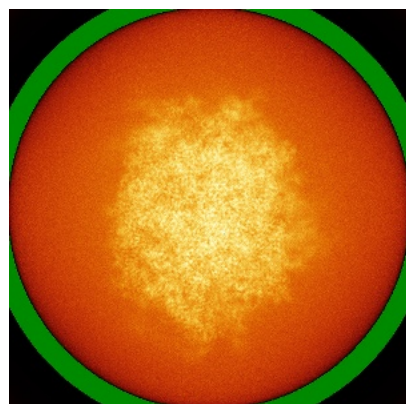


Y

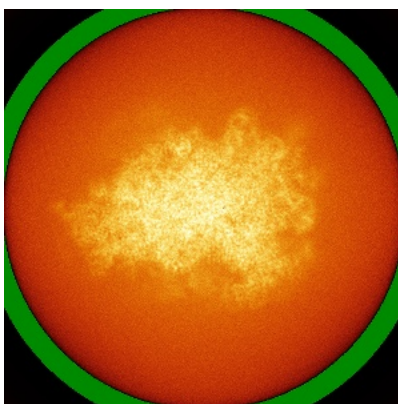


Z

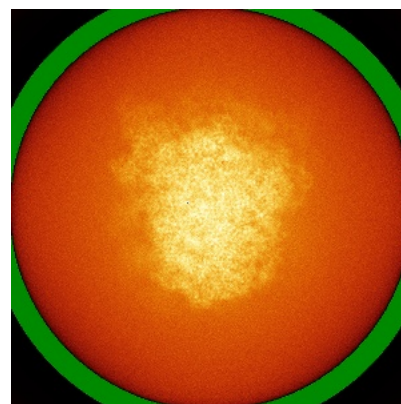
6.4.2 Raw map



X



Y

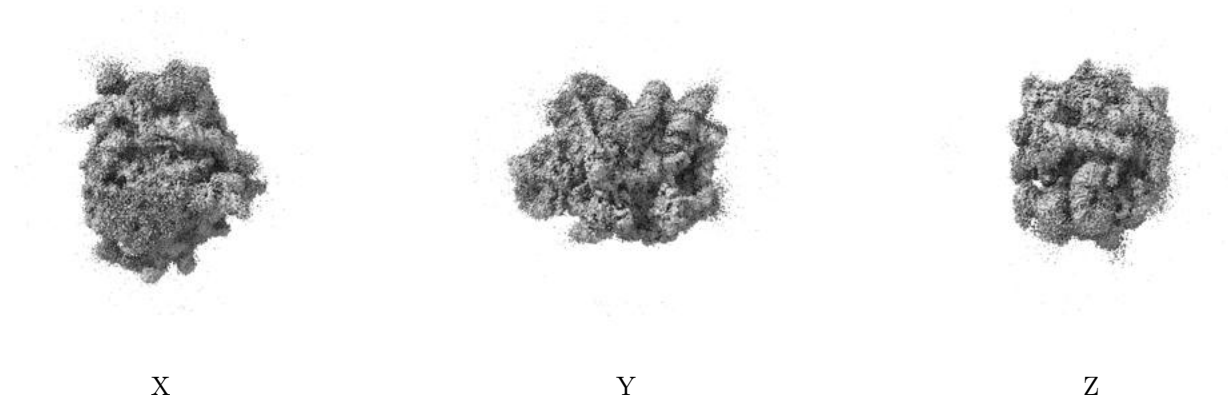


Z

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.

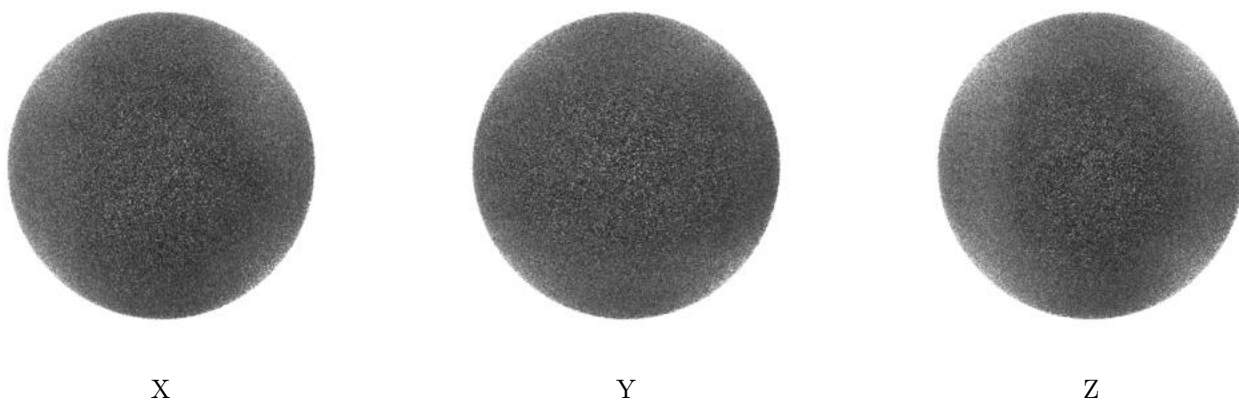
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

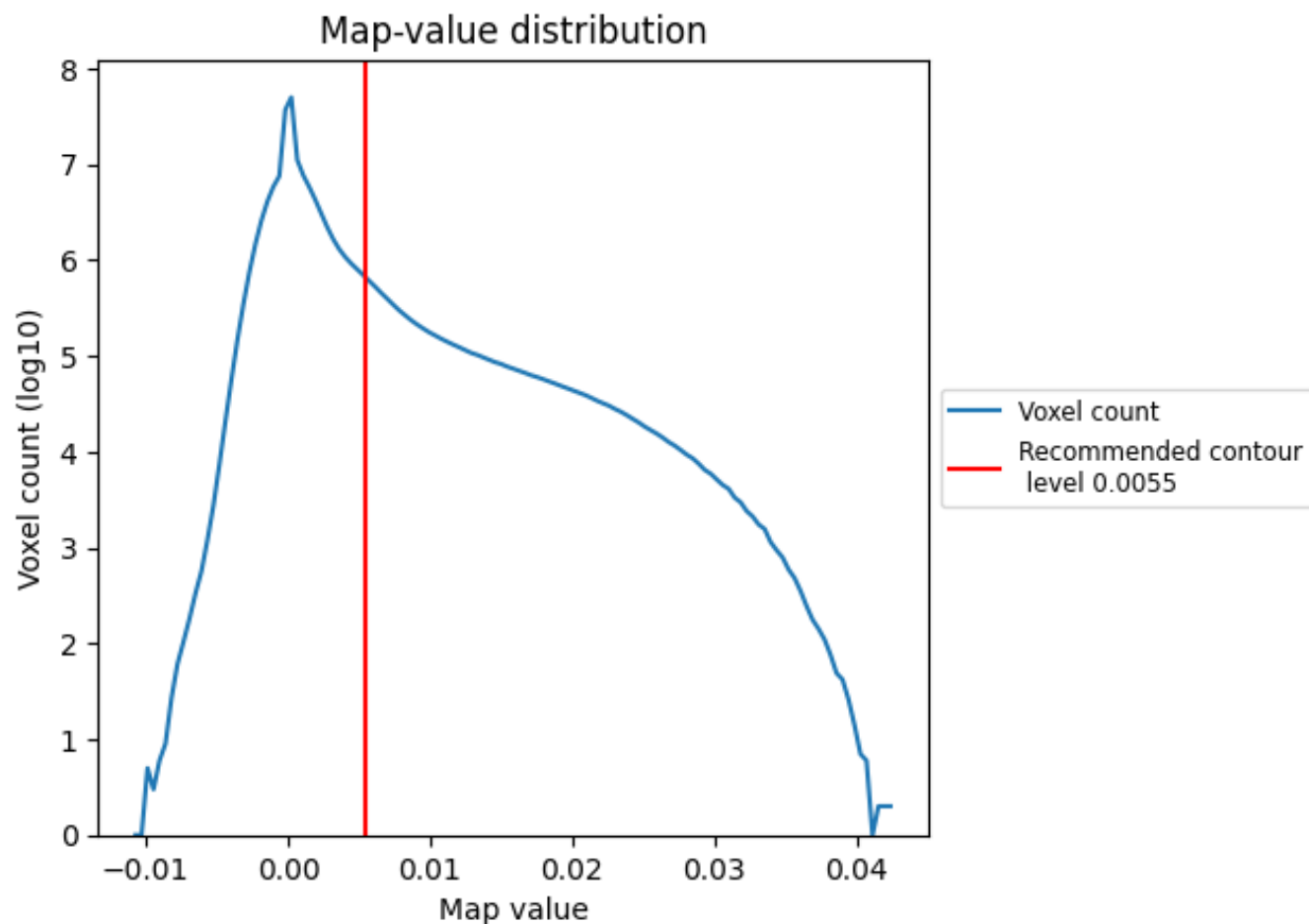
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

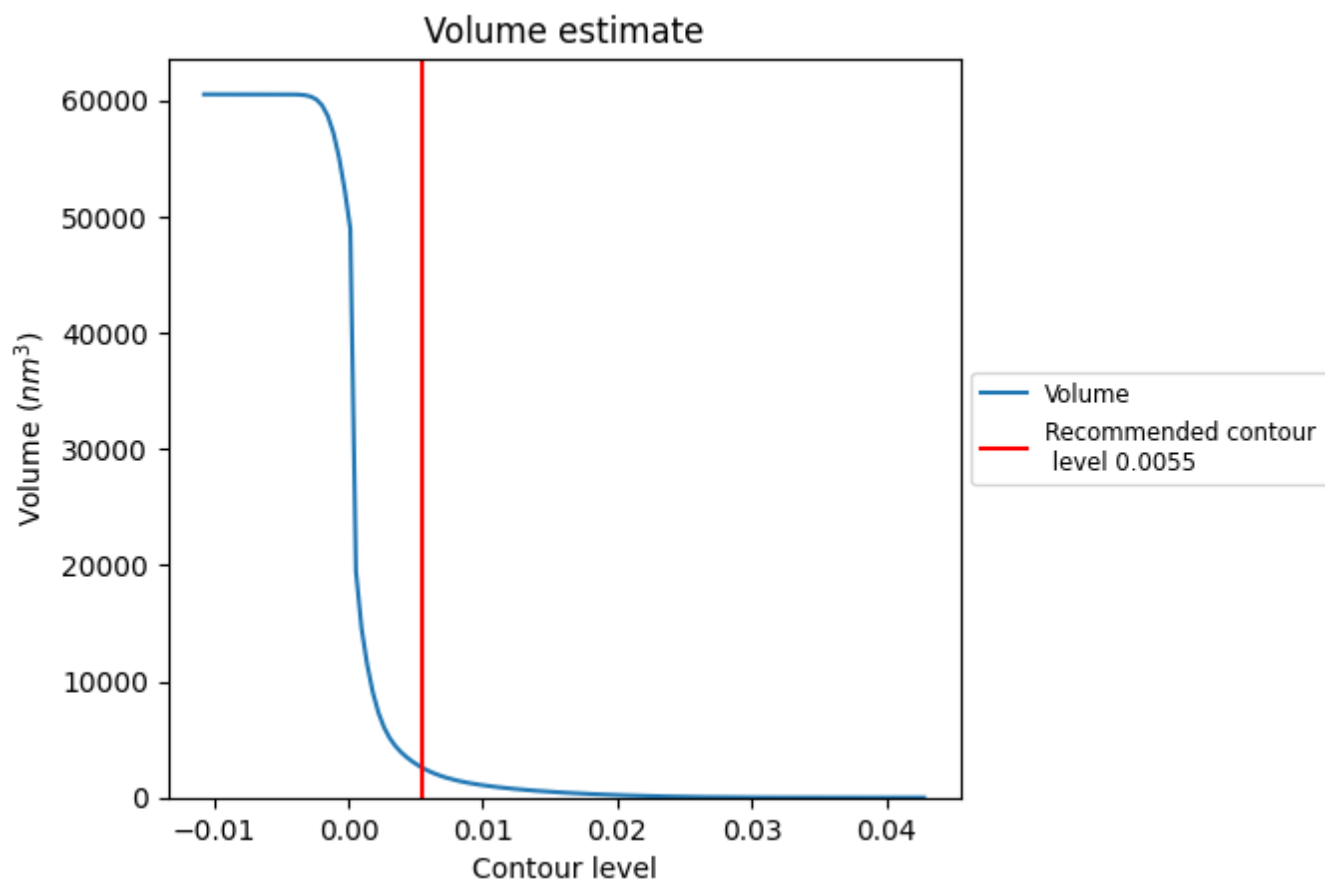
This section contains the results of statistical analysis of the map.

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.

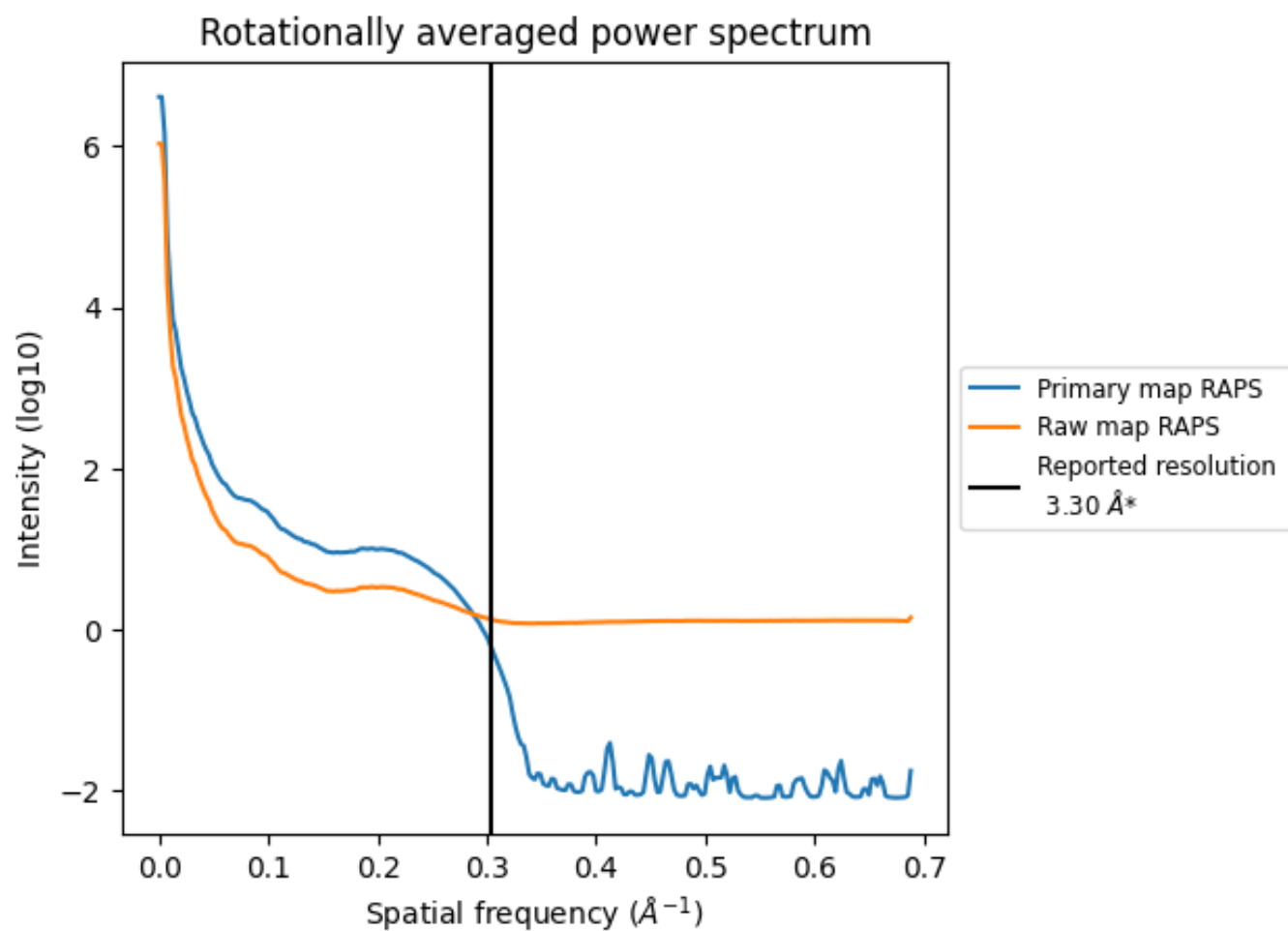
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2573 nm³; this corresponds to an approximate mass of 2324 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](#)

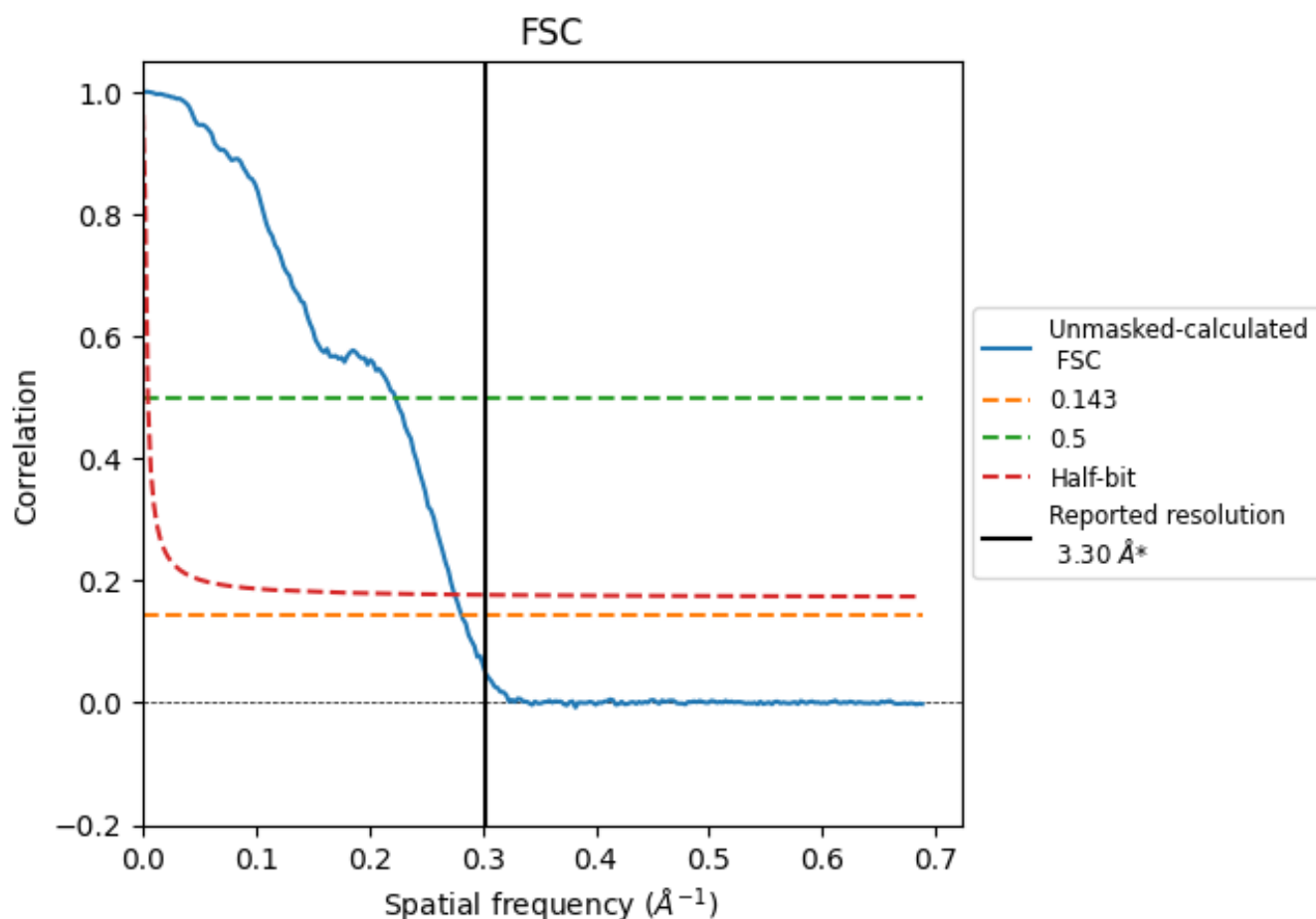


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

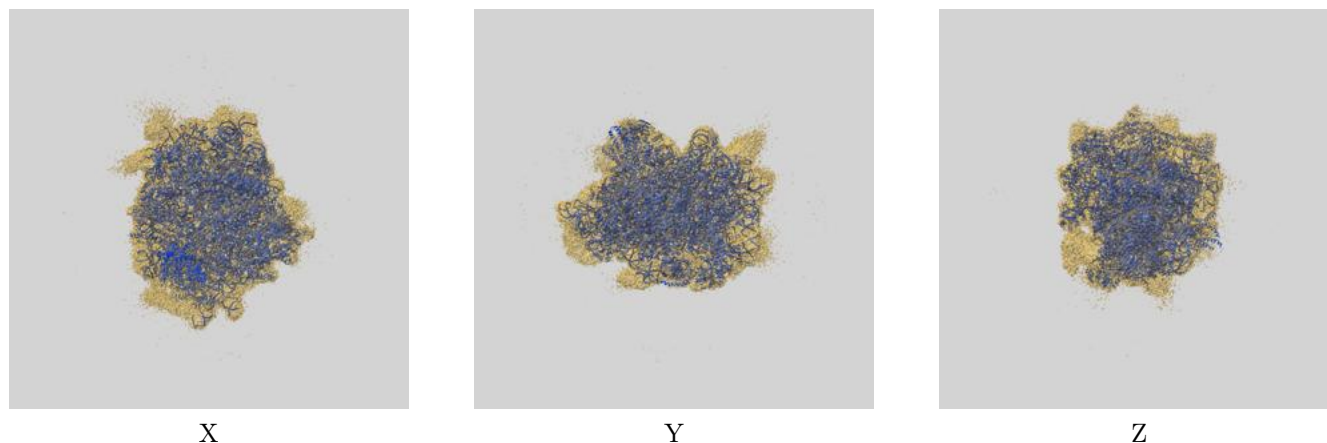
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.55	4.48	3.63

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

9 Map-model fit [i](#)

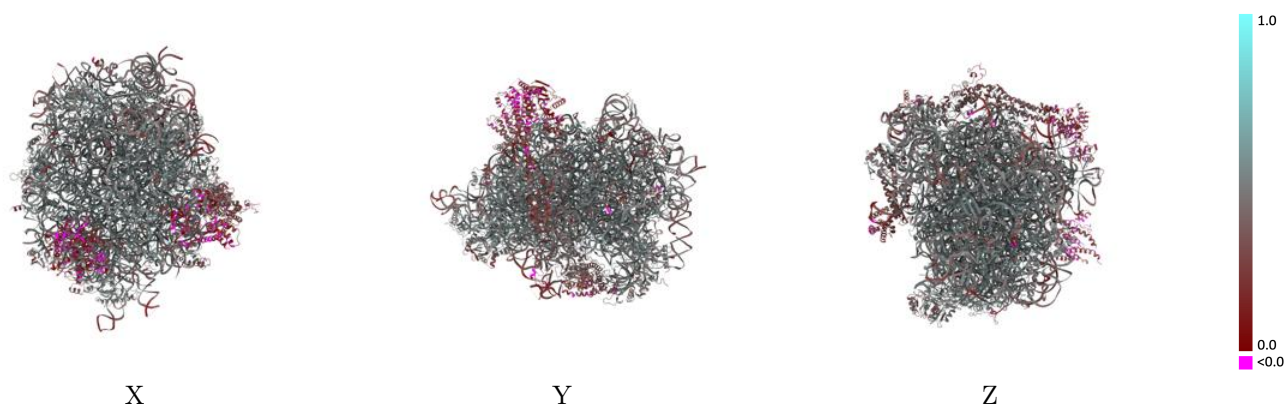
This section contains information regarding the fit between EMDB map EMD-16902 and PDB model 8OJ0. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



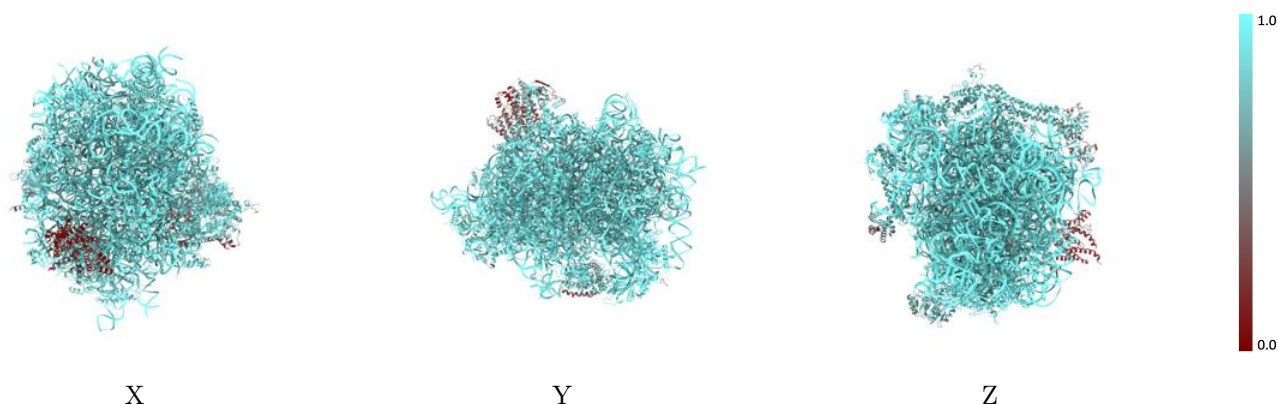
The images above show the 3D surface view of the map at the recommended contour level 0.0055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



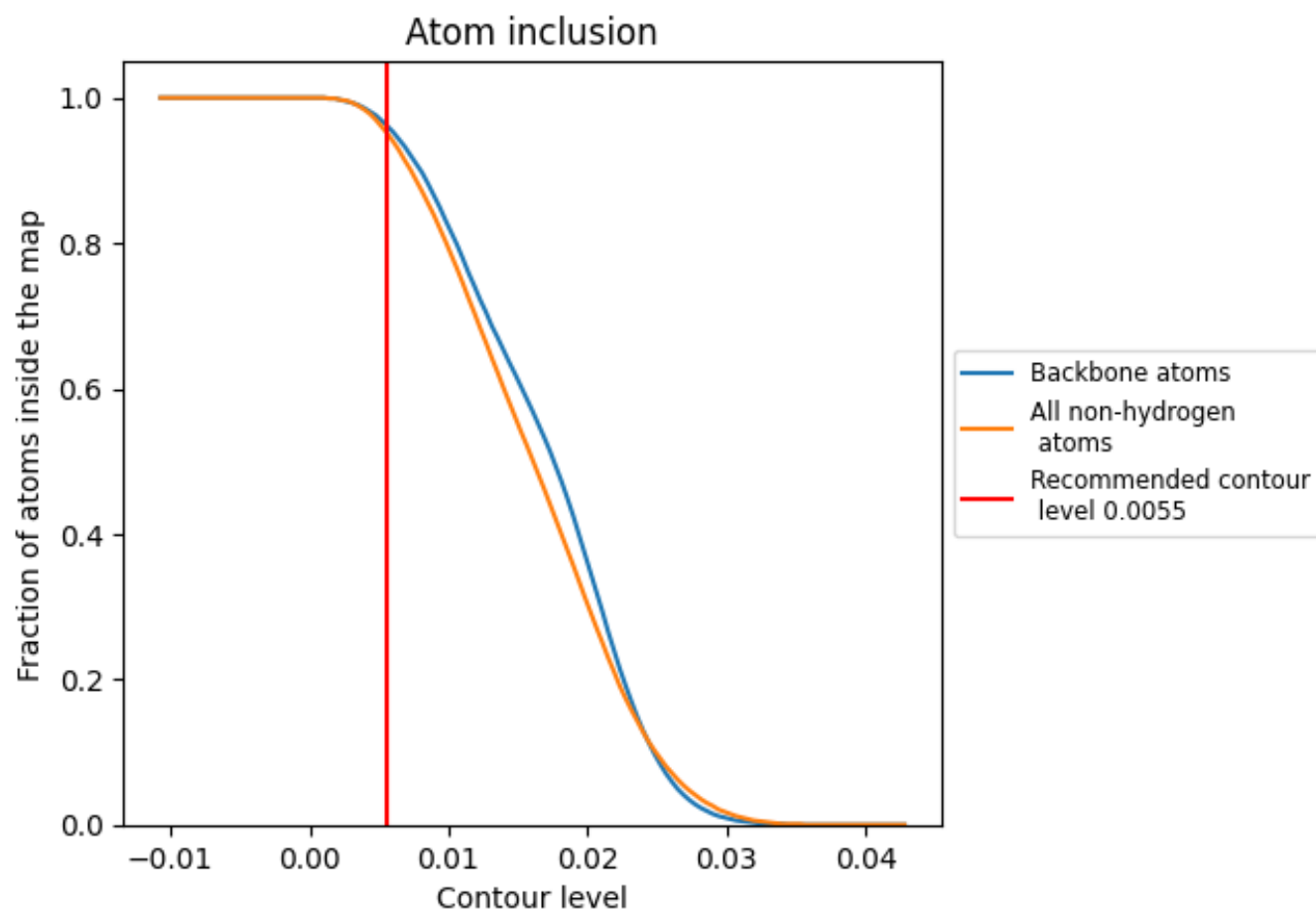
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0055).

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.0055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.4630
1	 0.3380	 0.1740
2	 0.4900	 0.2340
3	 0.0310	 0.0890
5	 0.9960	 0.4760
7	 0.9970	 0.4830
8	 0.9960	 0.4930
A	 0.8250	 0.3310
B	 0.7420	 0.2050
C	 0.7590	 0.1790
D	 0.5320	 0.1230
K	 0.7380	 0.4300
LA	 0.9900	 0.5380
LB	 0.9730	 0.5150
LC	 0.9760	 0.5140
LD	 0.9760	 0.4830
LE	 0.9880	 0.4980
LF	 0.9830	 0.5090
LG	 0.9530	 0.4660
LH	 0.9760	 0.4980
LI	 0.9820	 0.5110
LJ	 0.9430	 0.4590
LL	 0.9740	 0.5010
LM	 0.9820	 0.5000
LN	 0.9960	 0.5420
LO	 0.9810	 0.5110
LP	 0.9860	 0.5250
LQ	 0.9890	 0.5210
LR	 0.9730	 0.5050
LS	 0.9880	 0.5230
LT	 0.9840	 0.5040
LU	 0.9650	 0.4390
LV	 0.9730	 0.5070
LW	 0.9880	 0.5190
LX	 0.9680	 0.5120



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Chain	Atom inclusion	Q-score
LY	 0.9870	 0.5120
LZ	 0.9870	 0.5060
La	 0.9860	 0.5300
Lb	 0.9550	 0.4550
Lc	 0.9600	 0.4890
Ld	 0.9690	 0.5000
Le	 0.9900	 0.5310
Lf	 0.9910	 0.5290
Lg	 0.9790	 0.5120
Lh	 0.9760	 0.5050
Li	 0.9790	 0.5000
Lj	 0.9930	 0.5380
Lk	 0.9250	 0.4620
Ll	 0.9910	 0.5320
Lm	 0.9830	 0.5050
Lo	 0.9790	 0.5180
Lp	 0.9800	 0.5060
Lr	 0.9930	 0.5240
Lz	 0.8800	 0.3660