



Full wwPDB EM Validation Report ⓘ

May 16, 2026 – 01:37 PM EDT

PDB ID : 9PHC / pdb_00009phc
EMDB ID : EMD-71645
Title : In vitro reconstituted complex of purified *S. pombe* large ribosomal subunit and SNOR
Authors : Gluc, M.; Jomaa, A.
Deposited on : 2025-07-09
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

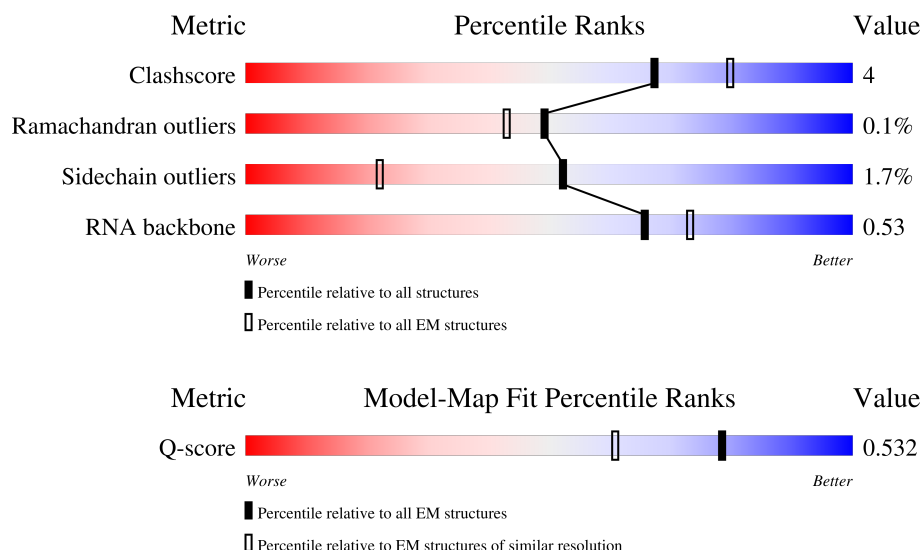
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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.













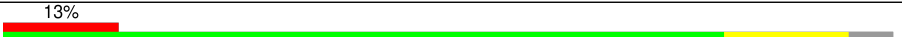


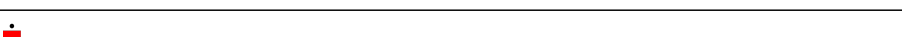
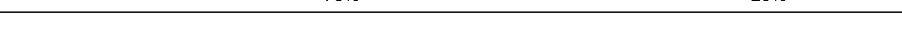
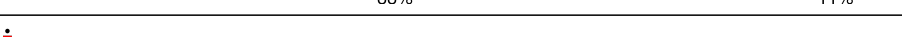



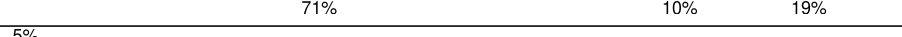





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	B0	106	
2	B1	94	
3	B2	3498	














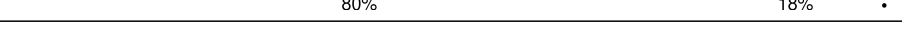


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Mol	Chain	Length	Quality of chain
4	B3	246	
5	B4	165	
6	BN	253	
7	BO	388	
8	BP	363	
9	BQ	294	
10	BR	195	
11	BS	251	
12	BT	259	
13	BU	189	
14	BV	221	
15	BW	174	
16	BX	208	
17	BY	134	
18	BZ	201	
19	Ba	197	
20	Bb	187	
21	Bc	187	
22	Bd	193	
23	Be	176	
24	Bf	160	
25	Bg	117	
26	Bh	139	
27	Bi	149	
28	Bj	141	

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Mol	Chain	Length	Quality of chain
29	Bk	126	 79%20%..
30	Bl	136	 74%25%.
31	Bm	148	 87%12%.
32	Bn	61	 89%8%.
33	Bo	109	 6%70%17%14%
34	Bp	113	 84%7%9%
35	Bq	127	 91%7%
36	Br	108	 85%11%.
37	Bs	111	 79%16%5%
38	Bt	122	 89%11%.
39	Bu	99	 84%12%.
40	Bv	91	 84%7%10%
41	Bw	74	 80%14%7%
42	Bx	51	 14%80%18%.
43	By	134	 83%16%..
44	HS	106	 21%73%19%6%

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 122816 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 Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B0	93	Total	C	N	O	S	0	0
			758	479	152	122	5		

- Molecule 2 is a protein called Large ribosomal subunit protein eL43A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	93	Total	C	N	O	S	0	0
			718	442	147	123	6		

- Molecule 3 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B2	3139	Total	C	N	O	P	0	0
			67111	29989	12096	21887	3139		

- Molecule 4 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B3	119	Total	C	N	O	P	0	0
			2539	1133	454	833	119		

- Molecule 5 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B4	157	Total	C	N	O	P	0	0
			3332	1491	583	1101	157		

- Molecule 6 is a protein called Large ribosomal subunit protein uL2C.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BN	248	Total	C	N	O	S	0	0
			1872	1166	377	324	5		

- Molecule 7 is a protein called Large ribosomal subunit protein uL3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BO	384	Total	C	N	O	S	0	0
			3050	1929	576	535	10		

- Molecule 8 is a protein called Large ribosomal subunit protein uL4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BP	362	Total	C	N	O	S	0	0
			2799	1768	538	490	3		

- Molecule 9 is a protein called Large ribosomal subunit protein uL18B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BQ	287	Total	C	N	O	S	0	0
			2312	1461	410	437	4		

- Molecule 10 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BR	162	Total	C	N	O	S	0	0
			1251	802	231	215	3		

- Molecule 11 is a protein called Large ribosomal subunit protein uL30C.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BS	233	Total	C	N	O	S	0	0
			1897	1211	349	334	3		

- Molecule 12 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BT	229	Total	C	N	O	S	0	0
			1772	1135	325	309	3		

- Molecule 13 is a protein called Large ribosomal subunit protein uL6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BU	168	Total	C	N	O	S	0	0
			1319	828	244	242	5		

- Molecule 14 is a protein called Large ribosomal subunit protein uL16A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BV	209	Total	C	N	O	S	0	0
			1679	1060	318	293	8		

- Molecule 15 is a protein called Large ribosomal subunit protein uL5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BW	167	Total	C	N	O	S	0	0
			1346	854	252	235	5		

- Molecule 16 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BX	207	Total	C	N	O	S	0	0
			1654	1034	329	290	1		

- Molecule 17 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BY	130	Total	C	N	O	S	0	0
			1038	662	198	174	4		

- Molecule 18 is a protein called Large ribosomal subunit protein eL15B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BZ	200	Total	C	N	O	S	0	0
			1676	1050	348	275	3		

- Molecule 19 is a protein called Large ribosomal subunit protein uL13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Ba	196	Total	C	N	O	S	0	0
			1545	991	294	256	4		

- Molecule 20 is a protein called Large ribosomal subunit protein uL22A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Bb	152	Total	C	N	O	S	0	0
			1212	770	229	210	3		

- Molecule 21 is a protein called Large ribosomal subunit protein eL18B.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Bc	186	Total	C	N	O	0	0
			1487	937	300	250		

- Molecule 22 is a protein called Large ribosomal subunit protein eL19B.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Bd	157	Total	C	N	O	S	0	0
			1301	809	275	212	5		

- Molecule 23 is a protein called Large ribosomal subunit protein eL20A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Be	173	Total	C	N	O	S	0	0
			1423	916	268	234	5		

- Molecule 24 is a protein called Large ribosomal subunit protein eL21B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Bf	159	Total	C	N	O	S	0	0
			1286	810	247	226	3		

- Molecule 25 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Bg	99	Total	C	N	O	0	0
			798	518	138	142		

- Molecule 26 is a protein called Large ribosomal subunit protein uL14B.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Bh	134	Total	C	N	O	S	0	0
			999	630	184	177	8		

- Molecule 27 is a protein called Large ribosomal subunit protein eL24B.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Bi	63	Total	C	N	O	S	0	0
			523	336	102	82	3		

- Molecule 28 is a protein called Large ribosomal subunit protein uL23A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Bj	118	Total	C	N	O	S	0	0
			947	605	175	166	1		

- Molecule 29 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Bk	125	Total	C	N	O	S	0	0
			998	622	201	173	2		

- Molecule 30 is a protein called Large ribosomal subunit protein eL27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Bl	135	Total	C	N	O	S	0	0
			1078	698	200	178	2		

- Molecule 31 is a protein called Large ribosomal subunit protein uL15B.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bm	147	Total	C	N	O	S	0	0
			1171	740	235	194	2		

- Molecule 32 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Bn	59	Total	C	N	O	0	0
			495	299	112	84		

- Molecule 33 is a protein called Large ribosomal subunit protein eL30A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bo	94	Total	C	N	O	S	0	0
			705	450	121	130	4		

- Molecule 34 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bp	103	Total	C	N	O	S	0	0
			857	538	167	149	3		

- Molecule 35 is a protein called Large ribosomal subunit protein eL32A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Bq	118	Total	C	N	O	S	0	0
			944	591	191	157	5		

- Molecule 36 is a protein called Large ribosomal subunit protein eL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Br	104	Total	C	N	O	S	0	0
			831	531	160	137	3		

- Molecule 37 is a protein called Large ribosomal subunit protein eL34B.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bs	106	Total	C	N	O	S	0	0
			858	538	176	142	2		

- Molecule 38 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bt	121	Total	C	N	O		0	0
			999	629	194	176			

- Molecule 39 is a protein called Large ribosomal subunit protein eL36B.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bu	95	Total	C	N	O	S	0	0
			759	472	159	127	1		

- Molecule 40 is a protein called Large ribosomal subunit protein eL37B.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bv	82	Total	C	N	O	S	0	0
			652	399	140	106	7		

- Molecule 41 is a protein called Large ribosomal subunit protein eL38A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bw	69	Total	C	N	O	S	0	0
			560	355	103	101	1		

- Molecule 42 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bx	50	Total	C	N	O	S	0	0
			436	273	98	64	1		

- Molecule 43 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	By	133	Total	C	N	O	S	0	0
			1031	641	203	186	1		

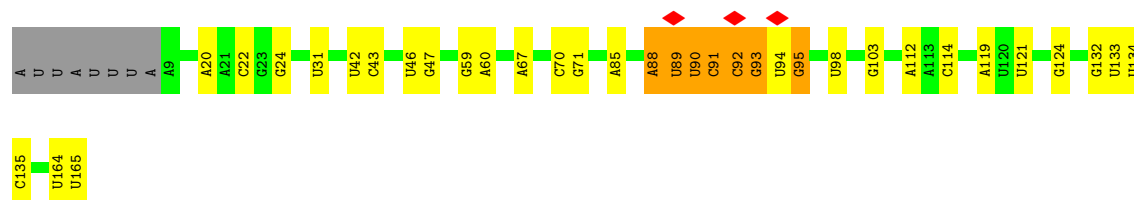
- Molecule 44 is a protein called SDO1-like protein C21C3.19.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	HS	100	Total	C	N	O	S	0	0
			795	494	140	159	2		

- Molecule 45 is ZINC ION (CCD ID: ZN) (formula: Zn).

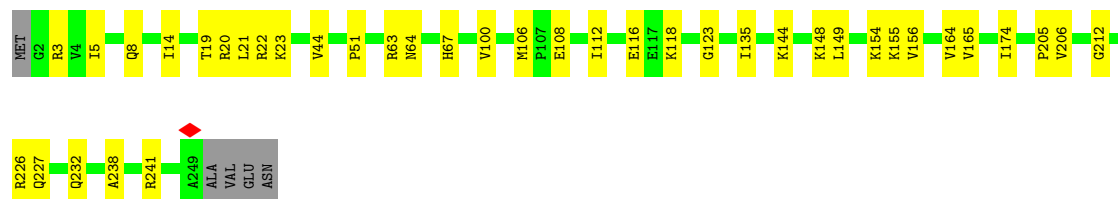
Mol	Chain	Residues	Atoms		AltConf
45	B0	1	Total	Zn	0
			1	1	
45	B1	1	Total	Zn	0
			1	1	
45	Bv	1	Total	Zn	0
			1	1	





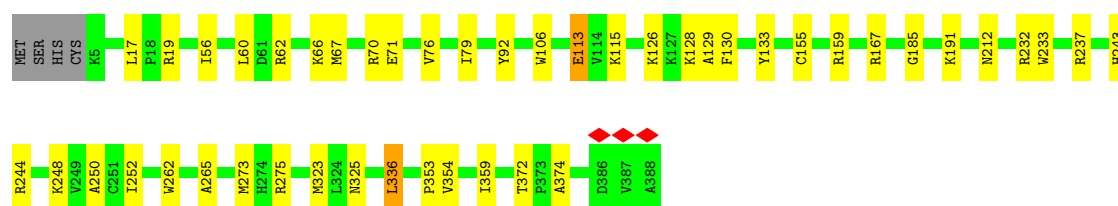
- Molecule 6: Large ribosomal subunit protein uL2C

Chain BN: 83% 15%



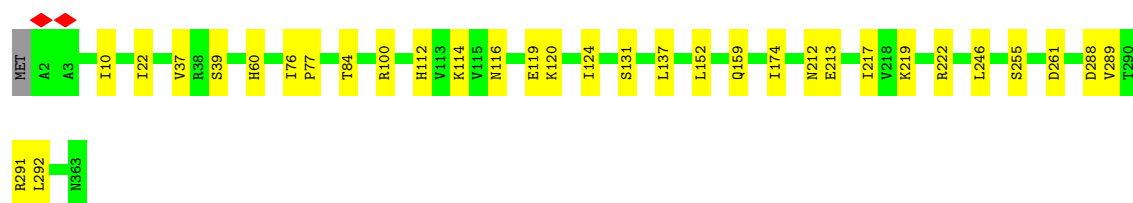
- Molecule 7: Large ribosomal subunit protein uL3A

Chain BO: 87% 11%



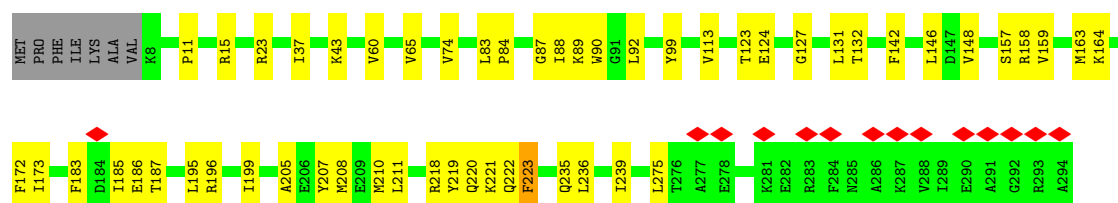
- Molecule 8: Large ribosomal subunit protein uL4A

Chain BP: 91% 9%

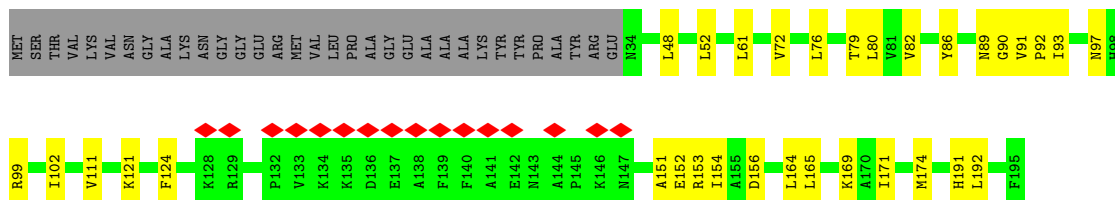


- Molecule 9: Large ribosomal subunit protein uL18B

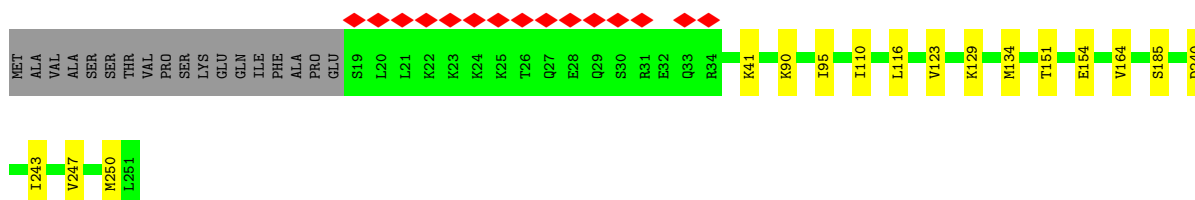
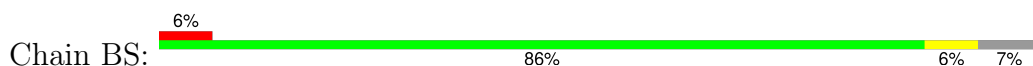
Chain BQ: 5% 79% 18%



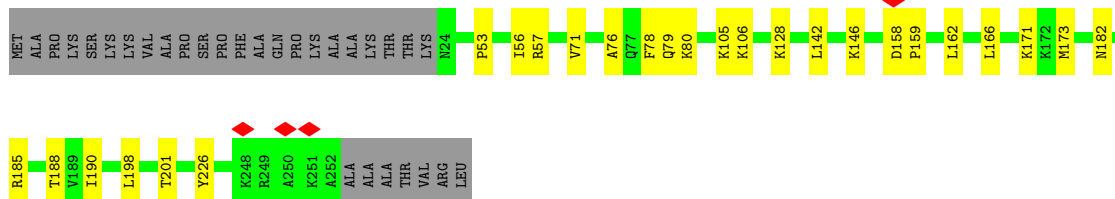
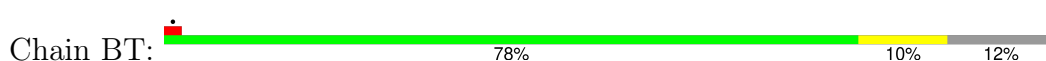
- Molecule 10: Large ribosomal subunit protein eL6



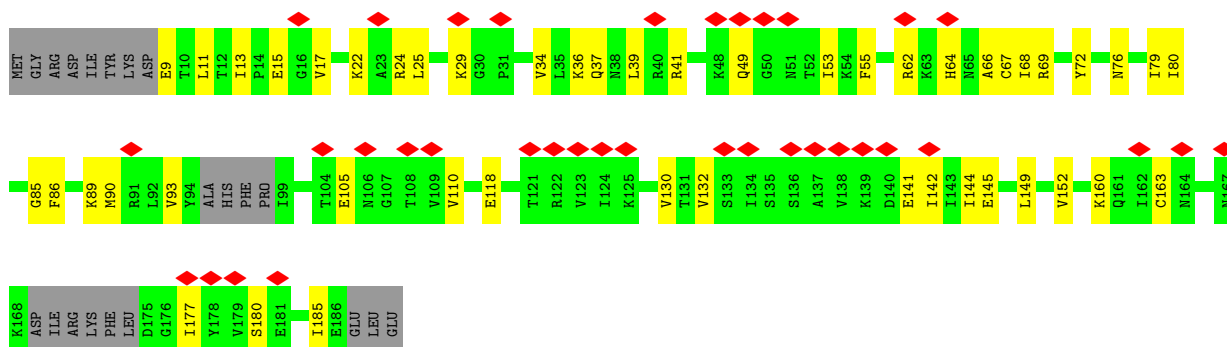
- Molecule 11: Large ribosomal subunit protein uL30C



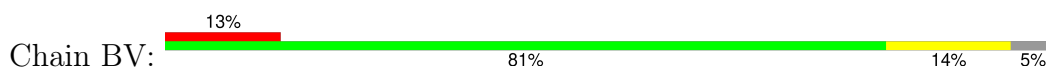
- Molecule 12: Large ribosomal subunit protein eL8

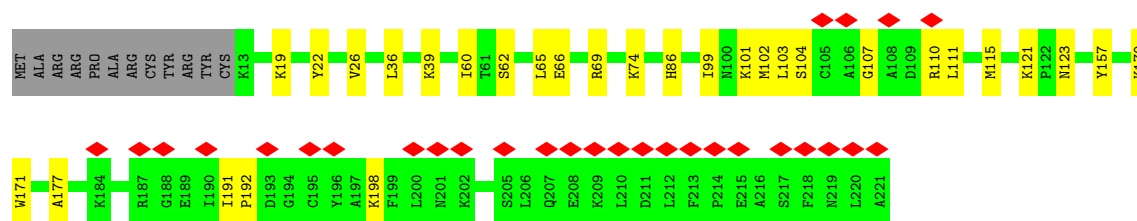


- Molecule 13: Large ribosomal subunit protein uL6B

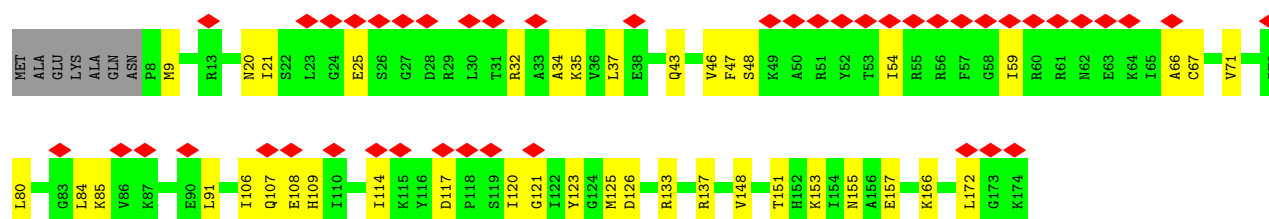
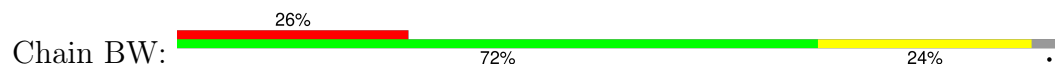


- Molecule 14: Large ribosomal subunit protein uL16A

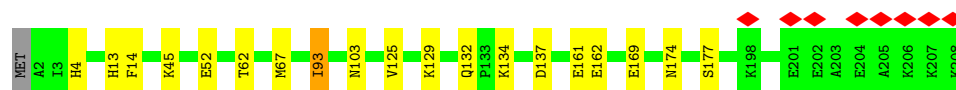




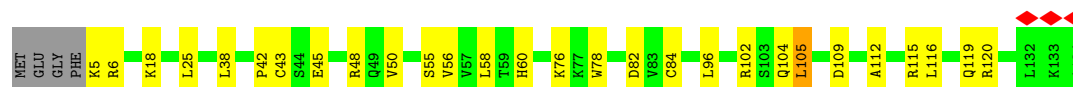
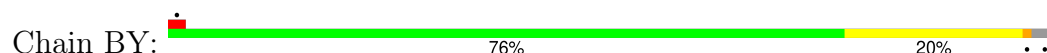
- Molecule 15: Large ribosomal subunit protein uL5A



- Molecule 16: Large ribosomal subunit protein eL13



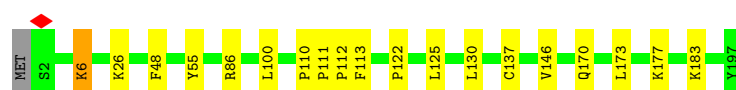
- Molecule 17: Large ribosomal subunit protein eL14



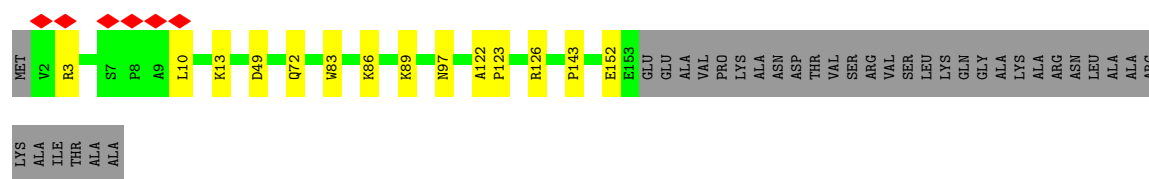
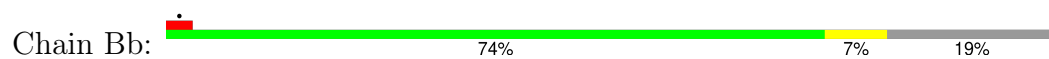
- Molecule 18: Large ribosomal subunit protein eL15B



- Molecule 19: Large ribosomal subunit protein uL13A



- Molecule 20: Large ribosomal subunit protein uL22A



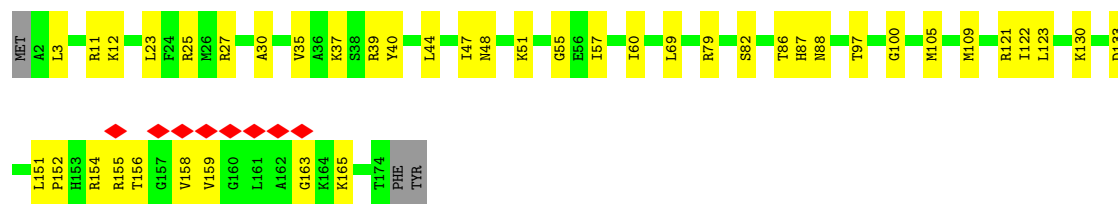
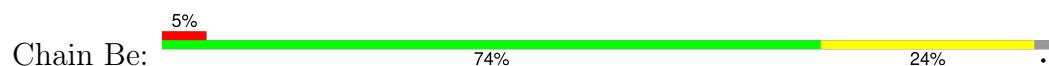
- Molecule 21: Large ribosomal subunit protein eL18B



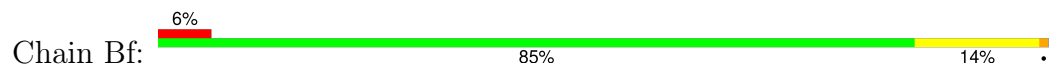
- Molecule 22: Large ribosomal subunit protein eL19B



- Molecule 23: Large ribosomal subunit protein eL20A



- Molecule 24: Large ribosomal subunit protein eL21B



- Molecule 25: Large ribosomal subunit protein eL22







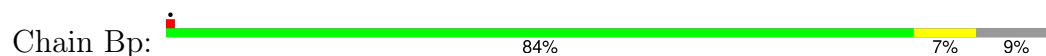
- Molecule 32: Large ribosomal subunit protein eL29



- Molecule 33: Large ribosomal subunit protein eL30A



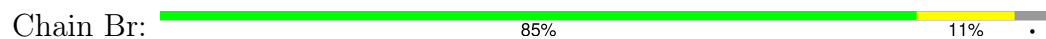
- Molecule 34: Large ribosomal subunit protein eL31



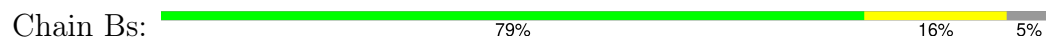
- Molecule 35: Large ribosomal subunit protein eL32A



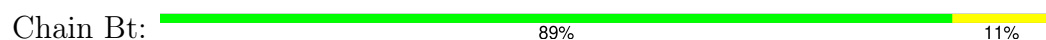
- Molecule 36: Large ribosomal subunit protein eL33A



- Molecule 37: Large ribosomal subunit protein eL34B

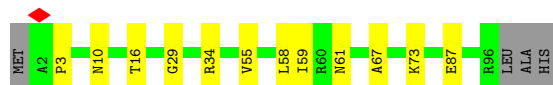
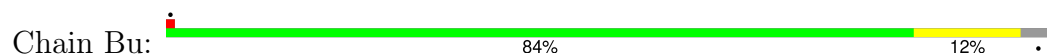


- Molecule 38: Large ribosomal subunit protein uL29

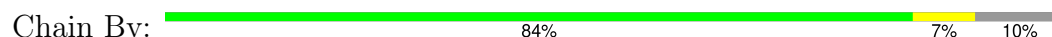




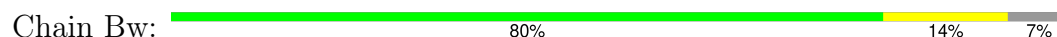
- Molecule 39: Large ribosomal subunit protein eL36B



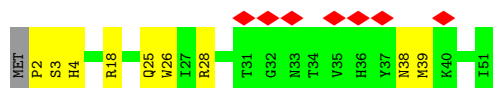
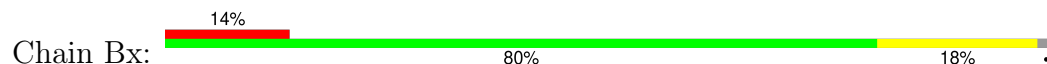
- Molecule 40: Large ribosomal subunit protein eL37B



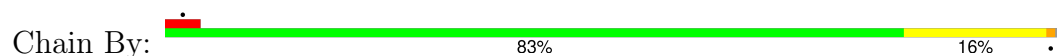
- Molecule 41: Large ribosomal subunit protein eL38A



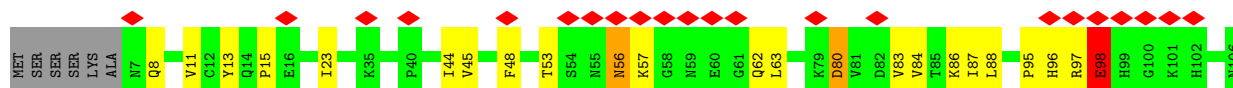
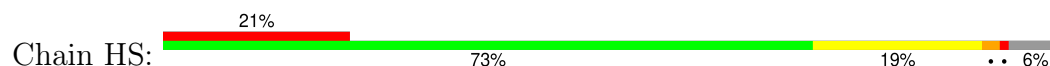
- Molecule 42: Large ribosomal subunit protein eL39



- Molecule 43: Large ribosomal subunit protein eL28



- Molecule 44: SDO1-like protein C21C3.19



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110548	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.002	Depositor
Map size (Å)	430.08, 430.08, 430.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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	B0	0.10	0/772	0.28	0/1025
2	B1	0.11	0/727	0.37	0/973
3	B2	0.08	0/75119	0.18	0/117094
4	B3	0.07	0/2838	0.15	0/4422
5	B4	0.08	0/3723	0.16	0/5796
6	BN	0.13	0/1910	0.31	0/2575
7	BO	0.11	0/3116	0.29	0/4190
8	BP	0.11	0/2852	0.29	0/3850
9	BQ	0.14	0/2361	0.40	0/3173
10	BR	0.12	0/1275	0.33	0/1719
11	BS	0.11	0/1929	0.33	1/2583 (0.0%)
12	BT	0.13	0/1801	0.36	0/2430
13	BU	0.23	0/1330	0.53	0/1789
14	BV	0.11	0/1712	0.31	0/2294
15	BW	0.15	0/1369	0.41	0/1830
16	BX	0.12	0/1686	0.28	0/2267
17	BY	0.11	0/1054	0.29	0/1413
18	BZ	0.11	0/1717	0.31	1/2306 (0.0%)
19	Ba	0.11	0/1575	0.28	0/2109
20	Bb	0.10	0/1237	0.31	0/1661
21	Bc	0.11	0/1511	0.28	0/2021
22	Bd	0.11	0/1320	0.31	0/1757
23	Be	0.12	0/1458	0.31	0/1961
24	Bf	0.11	0/1314	0.29	0/1771
25	Bg	0.14	0/812	0.40	0/1090
26	Bh	0.13	0/1015	0.36	0/1369
27	Bi	0.13	0/534	0.39	0/709
28	Bj	0.12	0/963	0.33	0/1296
29	Bk	0.12	0/1008	0.32	0/1341
30	Bl	0.17	0/1101	0.40	0/1477
31	Bm	0.13	0/1200	0.33	0/1611
32	Bn	0.11	0/503	0.28	0/664

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Bo	0.13	0/714	0.33	0/961
34	Bp	0.11	0/872	0.31	0/1172
35	Bq	0.11	0/958	0.30	0/1278
36	Br	0.11	0/853	0.31	0/1146
37	Bs	0.13	0/870	0.31	0/1165
38	Bt	0.11	0/1008	0.31	0/1340
39	Bu	0.09	0/766	0.23	0/1017
40	Bv	0.09	0/666	0.26	0/881
41	Bw	0.20	0/566	0.56	0/757
42	Bx	0.13	0/447	0.44	0/597
43	By	0.11	0/1045	0.31	0/1404
44	HS	0.13	0/808	0.36	0/1092
All	All	0.10	0/132415	0.24	2/195376 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	BZ	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	BS	240	ASP	CB-CA-C	-5.62	110.08	116.54
18	BZ	148	ILE	N-CA-C	-5.10	107.74	112.43

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	BZ	183	SER	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B0	758	0	815	3	0
2	B1	718	0	751	8	0
3	B2	67111	0	33740	265	0
4	B3	2539	0	1283	16	0
5	B4	3332	0	1684	14	0
6	BN	1872	0	1917	25	0
7	BO	3050	0	3125	33	0
8	BP	2799	0	2925	16	0
9	BQ	2312	0	2272	41	0
10	BR	1251	0	1337	18	0
11	BS	1897	0	1984	9	0
12	BT	1772	0	1866	17	0
13	BU	1319	0	1389	44	0
14	BV	1679	0	1718	26	0
15	BW	1346	0	1397	27	0
16	BX	1654	0	1705	12	0
17	BY	1038	0	1115	18	0
18	BZ	1676	0	1712	16	0
19	Ba	1545	0	1641	16	0
20	Bb	1212	0	1239	10	0
21	Bc	1487	0	1597	10	0
22	Bd	1301	0	1393	14	0
23	Be	1423	0	1488	28	0
24	Bf	1286	0	1310	15	0
25	Bg	798	0	834	10	0
26	Bh	999	0	1047	15	0
27	Bi	523	0	555	9	0
28	Bj	947	0	1012	11	0
29	Bk	998	0	1090	16	0
30	Bl	1078	0	1154	22	0
31	Bm	1171	0	1215	11	0
32	Bn	495	0	504	4	0
33	Bo	705	0	746	12	0
34	Bp	857	0	891	4	0
35	Bq	944	0	1005	3	0
36	Br	831	0	858	5	0
37	Bs	858	0	925	13	0
38	Bt	999	0	1092	8	0
39	Bu	759	0	840	6	0
40	Bv	652	0	663	3	0
41	Bw	560	0	608	9	0
42	Bx	436	0	463	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	By	1031	0	1080	16	0
44	HS	795	0	788	15	0
45	B0	1	0	0	0	0
45	B1	1	0	0	0	0
45	Bv	1	0	0	0	0
All	All	122816	0	88773	809	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 4.

All (809) 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)
3:B2:2356:U:H3	3:B2:2360:G:H22	1.25	0.82
7:BO:76:VAL:HG21	7:BO:323:MET:HE3	1.60	0.82
11:BS:41:LYS:HE3	11:BS:41:LYS:HA	1.62	0.81
15:BW:48:SER:HB2	15:BW:66:ALA:HB3	1.65	0.78
23:Be:97:THR:HG23	23:Be:100:GLY:H	1.47	0.78
23:Be:88:ASN:HD21	24:Bf:156:TYR:H	1.33	0.76
23:Be:47:ILE:HD12	23:Be:48:ASN:HD22	1.51	0.74
30:Bl:84:ARG:HB3	33:Bo:68:LEU:HD11	1.70	0.73
26:Bh:15:MET:HE1	26:Bh:56:CYS:HB2	1.69	0.73
3:B2:1380:A:H2'	43:By:44:ARG:HH22	1.52	0.72
21:Bc:72:ARG:HB2	21:Bc:75:ALA:HB2	1.72	0.72
3:B2:167:G:H1	3:B2:268:U:H3	1.38	0.71
13:BU:130:VAL:HG12	13:BU:144:ILE:HD11	1.72	0.71
15:BW:21:ILE:HD11	15:BW:67:CYS:HB2	1.72	0.70
7:BO:19:ARG:HB2	7:BO:232:ARG:HH21	1.57	0.69
3:B2:2526:A:H61	3:B2:2605:U:H3	1.41	0.69
7:BO:273:MET:HE3	7:BO:275:ARG:HH12	1.57	0.69
3:B2:1742:G:H22	3:B2:1781:G:H22	1.40	0.69
23:Be:79:ARG:HG2	23:Be:123:LEU:HD21	1.75	0.69
3:B2:856:C:H5''	6:BN:20:ARG:HD3	1.74	0.69
3:B2:551:C:H42	3:B2:575:G:H21	1.41	0.68
8:BP:37:VAL:HG21	8:BP:246:LEU:HD21	1.75	0.68
15:BW:125:MET:HE2	15:BW:125:MET:HA	1.76	0.67
3:B2:2852:U:H4'	24:Bf:7:ILE:HG22	1.75	0.67
15:BW:155:ASN:HD21	15:BW:157:GLU:HG3	1.58	0.67
35:Bq:84:MET:HE3	35:Bq:84:MET:HA	1.75	0.67
11:BS:90:LYS:HG2	24:Bf:135:PRO:HG2	1.77	0.67
3:B2:1875:U:H5'	3:B2:1877:C:H41	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Be:154:ARG:HG2	23:Be:155:ARG:H	1.61	0.66
3:B2:2300:C:H2'	3:B2:2318:C:H42	1.61	0.66
3:B2:2329:U:H2'	3:B2:2330:A:C8	2.31	0.66
4:B3:46:C:H5''	9:BQ:158:ARG:HH11	1.61	0.66
37:Bs:41:ILE:HG13	37:Bs:56:ALA:HB2	1.77	0.65
29:Bk:54:GLN:HB3	29:Bk:107:LYS:HB3	1.79	0.65
43:By:64:VAL:H	43:By:87:ILE:HD11	1.60	0.65
2:B1:5:THR:HG21	2:B1:9:GLY:H	1.62	0.64
3:B2:1080:A:H2'	14:BV:22:TYR:HE2	1.62	0.64
7:BO:115:LYS:HD2	7:BO:129:ALA:HB3	1.79	0.64
9:BQ:83:LEU:HB3	9:BQ:88:ILE:HB	1.80	0.64
27:Bi:50:SER:HA	27:Bi:55:TYR:HD2	1.62	0.64
6:BN:106:MET:HE1	6:BN:112:ILE:HG21	1.81	0.63
12:BT:190:ILE:HD11	12:BT:198:LEU:HD21	1.79	0.63
3:B2:1588:A:H4'	3:B2:1589:U:H5'	1.79	0.63
3:B2:590:U:H2'	3:B2:591:G:H4'	1.81	0.63
3:B2:2373:C:H4'	44:HS:95:PRO:HD2	1.80	0.63
4:B3:51:G:H21	15:BW:9:MET:HE1	1.64	0.63
13:BU:105:GLU:HG3	13:BU:110:VAL:HA	1.81	0.63
2:B1:86:ARG:HG2	2:B1:86:ARG:HH11	1.62	0.63
3:B2:253:U:H3'	3:B2:254:G:H8	1.64	0.63
3:B2:1995:G:H21	3:B2:3463:A:H8	1.45	0.62
3:B2:1380:A:H2'	43:By:44:ARG:NH2	2.14	0.62
3:B2:1386:G:H4'	43:By:44:ARG:HH21	1.63	0.62
3:B2:1599:A:H1'	3:B2:1600:C:H5	1.64	0.62
6:BN:23:LYS:HE3	6:BN:23:LYS:HA	1.80	0.62
43:By:21:LYS:HD3	43:By:29:GLN:HG2	1.80	0.62
3:B2:3369:A:H4'	3:B2:3370:U:H3'	1.81	0.62
3:B2:1575:A:H62	3:B2:1586:G:H21	1.45	0.62
3:B2:1386:G:H4'	43:By:44:ARG:NH2	2.13	0.62
9:BQ:218:ARG:HA	9:BQ:221:LYS:HG2	1.81	0.62
6:BN:116:GLU:HG2	6:BN:123:GLY:H	1.65	0.61
3:B2:690:A:H1'	16:BX:14:PHE:HE2	1.65	0.61
3:B2:3490:A:H5''	3:B2:3491:A:H5''	1.82	0.61
9:BQ:183:PHE:HD2	9:BQ:185:ILE:HG22	1.64	0.61
9:BQ:37:ILE:HD12	9:BQ:37:ILE:O	2.00	0.61
23:Be:37:LYS:HG2	23:Be:57:ILE:HG13	1.81	0.61
9:BQ:146:LEU:HD22	9:BQ:163:MET:HG3	1.82	0.61
3:B2:1868:C:H4'	3:B2:1869:C:OP1	2.01	0.60
9:BQ:132:THR:HB	9:BQ:172:PHE:HB2	1.84	0.60
41:Bw:53:LYS:HA	41:Bw:56:LYS:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B2:2452:G:H22	3:B2:2484:G:H1'	1.67	0.60
3:B2:182:G:H22	3:B2:248:G:H1	1.48	0.60
3:B2:2605:U:HO2'	3:B2:2606:U:H6	1.49	0.59
13:BU:13:ILE:HD11	13:BU:53:ILE:HG23	1.85	0.59
42:Bx:18:ARG:HG3	42:Bx:18:ARG:HH11	1.67	0.59
42:Bx:39:MET:HE3	42:Bx:39:MET:HA	1.84	0.59
3:B2:2186:C:H2'	3:B2:2187:A:C8	2.37	0.59
13:BU:93:VAL:H	13:BU:177:ILE:HG23	1.66	0.59
3:B2:250:A:H2'	3:B2:252:A:H5''	1.82	0.59
8:BP:288:ASP:HB2	43:By:4:SER:HB2	1.83	0.59
12:BT:158:ASP:HB3	12:BT:159:PRO:HD3	1.84	0.59
9:BQ:163:MET:HG2	9:BQ:173:ILE:HD11	1.84	0.59
13:BU:85:GLY:HA3	13:BU:185:ILE:HG13	1.84	0.59
3:B2:3389:G:H21	3:B2:3390:G:H5'	1.67	0.59
3:B2:543:G:H1	3:B2:583:C:H41	1.49	0.59
4:B3:33:U:H1'	9:BQ:210:MET:HE1	1.84	0.59
3:B2:1127:U:H1'	24:Bf:129:ARG:HE	1.67	0.58
3:B2:3264:U:H3	3:B2:3382:C:H42	1.50	0.58
12:BT:182:ASN:HB3	12:BT:185:ARG:HB3	1.84	0.58
15:BW:32:ARG:HH21	15:BW:35:LYS:HB3	1.68	0.58
3:B2:2343:A:H2'	3:B2:2344:A:H2'	1.84	0.58
3:B2:2304:G:H1	3:B2:2316:A:H61	1.50	0.58
30:Bl:42:VAL:HB	30:Bl:74:VAL:HG22	1.86	0.58
3:B2:1742:G:H22	3:B2:1781:G:N2	2.00	0.58
3:B2:1850:A:H5''	3:B2:2668:C:H42	1.68	0.58
3:B2:2528:G:H1	3:B2:2603:C:H42	1.50	0.58
8:BP:112:HIS:HB3	18:BZ:201:ARG:HB2	1.85	0.58
27:Bi:50:SER:HA	27:Bi:55:TYR:CD2	2.38	0.58
29:Bk:58:ILE:HG22	29:Bk:59:ARG:HG2	1.86	0.58
3:B2:2428:U:H5''	7:BO:237:ARG:HD3	1.86	0.57
8:BP:152:LEU:HD21	8:BP:174:ILE:HD12	1.85	0.57
3:B2:2667:G:H2'	3:B2:2669:G:H8	1.69	0.57
10:BR:154:ILE:H	10:BR:154:ILE:HD12	1.67	0.57
3:B2:1095:G:OP1	3:B2:1129:G:H5'	2.05	0.57
9:BQ:89:LYS:HG3	9:BQ:90:TRP:CE3	2.40	0.57
12:BT:78:PHE:O	12:BT:79:GLN:HG3	2.04	0.57
3:B2:3289:G:N2	3:B2:3299:U:H1'	2.20	0.57
18:BZ:80:THR:HG21	18:BZ:87:GLN:HA	1.86	0.57
33:Bo:28:LYS:HB2	33:Bo:100:ASP:HB2	1.87	0.57
7:BO:56:ILE:HG22	7:BO:359:ILE:HA	1.87	0.56
13:BU:11:LEU:HB3	13:BU:53:ILE:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Bx:25:GLN:CD	42:Bx:25:GLN:H	2.13	0.56
3:B2:3261:U:H3	3:B2:3385:G:H1	1.53	0.56
19:Ba:110:PRO:HB2	19:Ba:112:PRO:HD2	1.87	0.56
29:Bk:56:THR:HB	29:Bk:66:GLU:HG2	1.88	0.56
23:Be:158:VAL:HG13	23:Be:163:GLY:HA3	1.88	0.56
2:B1:16:VAL:HG12	3:B2:1982:G:C8	2.40	0.56
8:BP:289:VAL:HA	8:BP:292:LEU:HB2	1.87	0.56
9:BQ:88:ILE:HG22	9:BQ:88:ILE:O	2.05	0.56
17:BY:105:LEU:HB3	17:BY:109:ASP:HB2	1.87	0.56
3:B2:2289:G:H1	3:B2:2328:G:H22	1.53	0.56
6:BN:112:ILE:HG22	6:BN:165:VAL:HA	1.86	0.56
3:B2:192:C:H2'	3:B2:193:U:H4'	1.87	0.56
3:B2:3267:A:H5''	3:B2:3268:U:H5'	1.88	0.56
38:Bt:20:LEU:HB2	38:Bt:56:ILE:HG21	1.87	0.56
3:B2:3014:A:H61	3:B2:3022:C:H42	1.54	0.56
22:Bd:15:LEU:HD23	22:Bd:52:ARG:HB2	1.87	0.56
3:B2:3435:U:H4'	3:B2:3436:A:H5'	1.88	0.55
17:BY:48:ARG:HD2	23:Be:69:LEU:HD13	1.88	0.55
3:B2:1525:A:N7	42:Bx:2:PRO:HB3	2.20	0.55
11:BS:151:THR:HG23	11:BS:247:VAL:HG11	1.89	0.55
3:B2:3278:A:H2'	3:B2:3279:A:C8	2.42	0.55
22:Bd:26:PRO:HA	22:Bd:29:ILE:HD11	1.89	0.55
5:B4:90:U:O2'	5:B4:91:C:H5''	2.07	0.55
18:BZ:118:SER:HB3	18:BZ:132:VAL:HG12	1.89	0.55
3:B2:414:G:H1'	5:B4:24:G:N2	2.22	0.55
3:B2:3450:C:H42	3:B2:3458:U:H3	1.55	0.55
27:Bi:56:ARG:HB2	27:Bi:57:ARG:HH12	1.71	0.55
26:Bh:81:VAL:HG12	26:Bh:82:ARG:HG3	1.88	0.55
29:Bk:43:LYS:HG3	29:Bk:124:LYS:HE2	1.87	0.55
3:B2:1916:G:H4'	22:Bd:63:ILE:HG21	1.89	0.54
18:BZ:113:LEU:HB2	18:BZ:134:LEU:HD23	1.88	0.54
4:B3:75:G:H1'	4:B3:76:U:H5	1.72	0.54
24:Bf:126:VAL:HG13	24:Bf:127:GLN:H	1.71	0.54
29:Bk:56:THR:HG23	29:Bk:104:VAL:HG13	1.89	0.54
29:Bk:59:ARG:HB2	29:Bk:102:LYS:HG3	1.90	0.54
38:Bt:14:GLU:CD	38:Bt:14:GLU:H	2.14	0.54
3:B2:1271:A:H61	3:B2:1275:A:H3'	1.73	0.54
3:B2:2322:G:H2'	3:B2:2323:C:O4'	2.08	0.54
3:B2:253:U:H3'	3:B2:254:G:C8	2.42	0.54
4:B3:61:U:H5''	9:BQ:275:LEU:HD22	1.90	0.54
27:Bi:60:LYS:HD2	27:Bi:60:LYS:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Bo:83:LEU:HD12	33:Bo:93:VAL:HB	1.90	0.54
10:BR:61:LEU:HD11	10:BR:102:ILE:HG13	1.90	0.54
12:BT:71:VAL:HG23	12:BT:76:ALA:HB2	1.90	0.54
6:BN:21:LEU:HB3	6:BN:51:PRO:HG3	1.90	0.54
18:BZ:39:ALA:HB3	18:BZ:61:ILE:HG22	1.90	0.54
6:BN:19:THR:HG22	6:BN:22:ARG:HG3	1.90	0.53
41:Bw:16:ARG:HH21	41:Bw:62:PRO:HG3	1.72	0.53
14:BV:170:LYS:HA	14:BV:177:ALA:HA	1.90	0.53
34:Bp:82:ARG:HD2	34:Bp:92:LEU:HD13	1.90	0.53
43:By:57:GLN:HG3	43:By:65:VAL:HG13	1.90	0.53
3:B2:396:G:H1'	20:Bb:97:ASN:HD21	1.73	0.53
6:BN:148:LYS:HG3	6:BN:154:LYS:HE3	1.90	0.53
15:BW:34:ALA:HB2	15:BW:47:PHE:HZ	1.72	0.53
19:Ba:6:LYS:HD3	19:Ba:6:LYS:H	1.73	0.53
3:B2:1951:A:H61	3:B2:2427:C:H42	1.57	0.53
3:B2:1662:U:H4'	3:B2:1664:A:O2'	2.09	0.53
3:B2:787:G:H1	3:B2:804:A:H61	1.55	0.53
10:BR:165:LEU:HD12	10:BR:169:LYS:HE3	1.89	0.53
29:Bk:118:ILE:HD12	29:Bk:118:ILE:H	1.73	0.53
43:By:42:ALA:HB3	43:By:45:PHE:HD2	1.74	0.53
22:Bd:105:LEU:HD22	22:Bd:135:LYS:HG3	1.89	0.53
13:BU:130:VAL:HG13	13:BU:152:VAL:HG12	1.91	0.52
11:BS:129:LYS:HB2	24:Bf:133:ALA:HB3	1.90	0.52
13:BU:17:VAL:HG21	13:BU:79:ILE:HD11	1.92	0.52
13:BU:69:ARG:HH22	13:BU:72:TYR:HD2	1.57	0.52
24:Bf:84:TYR:HB2	32:Bn:24:PRO:HD3	1.91	0.52
31:Bm:71:PRO:HG2	31:Bm:108:TYR:HA	1.90	0.52
13:BU:11:LEU:HD22	13:BU:72:TYR:HE1	1.75	0.52
24:Bf:126:VAL:HG22	24:Bf:128:LEU:HG	1.91	0.52
15:BW:71:VAL:HG12	15:BW:71:VAL:O	2.09	0.52
2:B1:86:ARG:HG2	2:B1:86:ARG:NH1	2.25	0.52
5:B4:91:C:H42	29:Bk:51:ARG:HH21	1.58	0.52
9:BQ:113:VAL:HG11	9:BQ:142:PHE:HE2	1.74	0.52
36:Br:49:ARG:HH11	36:Br:49:ARG:HB2	1.74	0.52
41:Bw:55:GLU:CD	41:Bw:55:GLU:H	2.18	0.52
3:B2:3289:G:H22	3:B2:3299:U:H1'	1.74	0.52
7:BO:372:THR:HG22	7:BO:374:ALA:H	1.75	0.52
36:Br:14:HIS:HB2	36:Br:99:LEU:HD11	1.91	0.52
3:B2:1332:A:H4'	3:B2:1333:A:H5'	1.92	0.52
13:BU:24:ARG:HB3	13:BU:39:LEU:HB2	1.91	0.52
23:Be:154:ARG:HG2	23:Be:155:ARG:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Bk:111:ASP:H	29:Bk:114:ARG:HB3	1.75	0.52
3:B2:2186:C:H2'	3:B2:2187:A:H8	1.74	0.52
10:BR:111:VAL:HG12	10:BR:164:LEU:HD11	1.91	0.52
30:Bl:4:ILE:HG22	30:Bl:5:LEU:HG	1.92	0.51
30:Bl:15:ARG:HD2	30:Bl:79:HIS:CD2	2.45	0.51
3:B2:3336:G:H2'	3:B2:3337:A:C8	2.45	0.51
23:Be:11:ARG:HB3	23:Be:23:LEU:HD23	1.93	0.51
3:B2:3291:C:H2'	3:B2:3292:U:H2'	1.91	0.51
8:BP:116:ASN:HB2	8:BP:119:GLU:HG3	1.93	0.51
15:BW:109:HIS:CE1	15:BW:123:TYR:H	2.28	0.51
21:Bc:69:LEU:HD12	21:Bc:141:LEU:HD13	1.92	0.51
3:B2:447:C:H1'	3:B2:505:G:N3	2.25	0.51
3:B2:1665:A:H5'	30:Bl:67:ARG:NH1	2.25	0.51
7:BO:79:ILE:HD13	7:BO:336:LEU:HD11	1.92	0.51
3:B2:3130:C:C2	13:BU:118:GLU:HG2	2.45	0.51
34:Bp:21:MET:HE1	34:Bp:40:GLU:HB2	1.93	0.51
10:BR:52:LEU:HD13	10:BR:80:LEU:HD11	1.92	0.51
6:BN:5:ILE:HG12	6:BN:8:GLN:HB2	1.92	0.51
16:BX:174:ASN:HB3	16:BX:177:SER:HB2	1.93	0.51
33:Bo:39:THR:HG22	33:Bo:45:ALA:HB2	1.91	0.51
42:Bx:25:GLN:HA	42:Bx:28:ARG:HD3	1.92	0.51
3:B2:305:A:H8	39:Bu:29:GLY:HA2	1.75	0.51
9:BQ:207:TYR:HD1	9:BQ:210:MET:HE3	1.76	0.51
20:Bb:13:LYS:HD3	20:Bb:152:GLU:HB2	1.93	0.51
3:B2:3333:G:H1	3:B2:3354:U:H3	1.59	0.50
3:B2:263:A:H2'	3:B2:264:G:H8	1.75	0.50
3:B2:1290:A:H1'	3:B2:1312:U:H1'	1.91	0.50
3:B2:2281:U:H5''	3:B2:2282:G:H5'	1.93	0.50
8:BP:159:GLN:HA	8:BP:217:ILE:HB	1.93	0.50
3:B2:505:G:H3'	3:B2:506:G:H21	1.77	0.50
3:B2:1379:U:H5'	3:B2:1389:A:H61	1.76	0.50
23:Be:79:ARG:HG3	23:Be:121:ARG:HB3	1.94	0.50
39:Bu:61:ASN:N	39:Bu:61:ASN:HD22	2.09	0.50
41:Bw:52:LYS:HE2	41:Bw:52:LYS:H	1.77	0.50
3:B2:263:A:H2'	3:B2:264:G:C8	2.47	0.50
44:HS:53:THR:HG21	44:HS:56:ASN:O	2.12	0.50
3:B2:3093:G:H1'	3:B2:3498:U:H5'	1.93	0.50
15:BW:37:LEU:HD12	15:BW:67:CYS:HB3	1.94	0.50
26:Bh:83:GLN:HA	26:Bh:100:ASN:HB3	1.94	0.50
27:Bi:56:ARG:HB2	27:Bi:57:ARG:NH1	2.26	0.50
32:Bn:18:ARG:HG2	32:Bn:18:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BP:291:ARG:NH1	8:BP:291:ARG:HB2	2.27	0.50
15:BW:120:ILE:HD12	15:BW:121:GLY:H	1.77	0.50
19:Ba:122:PRO:HA	19:Ba:125:LEU:HD12	1.92	0.50
2:B1:17:ARG:HG3	2:B1:18:TYR:CE1	2.47	0.50
3:B2:3335:U:H3'	3:B2:3336:G:H21	1.77	0.50
26:Bh:24:ILE:HD13	26:Bh:37:TYR:HB2	1.94	0.50
3:B2:97:U:OP2	16:BX:13:HIS:HD2	1.95	0.49
16:BX:125:VAL:HB	16:BX:137:ASP:HA	1.93	0.49
3:B2:1095:G:H8	3:B2:1098:G:H1'	1.77	0.49
9:BQ:87:GLY:HA2	9:BQ:89:LYS:NZ	2.28	0.49
3:B2:932:G:H1'	3:B2:1624:A:N6	2.28	0.49
7:BO:60:LEU:HD11	7:BO:62:ARG:HH21	1.77	0.49
9:BQ:65:VAL:HG12	9:BQ:74:VAL:HG22	1.94	0.49
31:Bm:85:GLU:CD	31:Bm:85:GLU:H	2.20	0.49
4:B3:2:U:H3	4:B3:117:G:H1	1.59	0.49
8:BP:219:LYS:HA	8:BP:222:ARG:HD3	1.93	0.49
19:Ba:111:PRO:N	19:Ba:112:PRO:HD2	2.27	0.49
44:HS:84:VAL:O	44:HS:88:LEU:HD22	2.12	0.49
3:B2:1679:A:H62	37:Bs:68:ASN:HD21	1.60	0.49
11:BS:95:ILE:HD12	11:BS:243:ILE:HD11	1.94	0.49
3:B2:2329:U:H5'	6:BN:241:ARG:NH2	2.28	0.49
3:B2:3328:U:H4'	3:B2:3329:G:O5'	2.12	0.49
7:BO:212:ASN:HD21	7:BO:354:VAL:H	1.61	0.49
3:B2:445:G:H1	3:B2:647:A:H61	1.61	0.49
3:B2:2770:C:H5''	3:B2:2771:A:C8	2.48	0.49
7:BO:76:VAL:HG12	7:BO:325:ASN:HA	1.95	0.49
7:BO:167:ARG:HG2	7:BO:167:ARG:HH11	1.78	0.49
23:Be:12:LYS:HA	23:Be:55:GLY:HA2	1.94	0.49
5:B4:92:C:H4'	5:B4:93:G:C8	2.47	0.49
9:BQ:183:PHE:CD2	9:BQ:185:ILE:HG22	2.47	0.49
14:BV:62:SER:HA	14:BV:65:LEU:HD12	1.94	0.49
15:BW:155:ASN:HD22	15:BW:157:GLU:H	1.60	0.49
26:Bh:105:VAL:HA	26:Bh:111:MET:HA	1.94	0.49
9:BQ:148:VAL:HG12	9:BQ:159:VAL:HG21	1.95	0.49
3:B2:1696:G:H2'	3:B2:1697:G:C8	2.48	0.48
3:B2:3002:G:H5'	3:B2:3003:G:OP2	2.13	0.48
3:B2:3144:C:H5	3:B2:3187:A:H62	1.61	0.48
3:B2:3389:G:H5''	3:B2:3390:G:C8	2.48	0.48
14:BV:103:LEU:HD11	44:HS:23:ILE:HG21	1.95	0.48
3:B2:588:G:C6	3:B2:589:U:H1'	2.49	0.48
3:B2:1589:U:H5	3:B2:1593:A:H61	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Bk:88:LYS:HD3	29:Bk:92:ALA:HB3	1.95	0.48
3:B2:2770:C:H2'	3:B2:2773:A:H62	1.77	0.48
7:BO:262:TRP:H	7:BO:262:TRP:CD1	2.31	0.48
40:Bv:69:LYS:HE3	40:Bv:69:LYS:HB2	1.50	0.48
3:B2:1073:U:H4'	14:BV:198:LYS:NZ	2.28	0.48
3:B2:1423:G:H5''	35:Bq:98:SER:HB3	1.93	0.48
9:BQ:99:TYR:HE1	9:BQ:164:LYS:HG3	1.79	0.48
21:Bc:7:ARG:HB3	21:Bc:10:VAL:HG21	1.93	0.48
31:Bm:89:LYS:HG2	31:Bm:90:TYR:CD2	2.48	0.48
1:B0:65:THR:HG22	1:B0:89:LYS:HD2	1.95	0.48
13:BU:89:LYS:O	13:BU:180:SER:HB3	2.13	0.48
7:BO:67:MET:HE3	7:BO:70:ARG:HB2	1.94	0.48
13:BU:76:ASN:O	13:BU:80:ILE:HG22	2.14	0.48
44:HS:56:ASN:HB3	44:HS:57:LYS:H	1.53	0.48
3:B2:164:G:H2'	3:B2:165:A:C8	2.48	0.48
25:Bg:43:LYS:H	25:Bg:43:LYS:HD2	1.79	0.48
38:Bt:84:GLN:HG2	38:Bt:86:LYS:HZ3	1.79	0.48
3:B2:1639:U:H4'	3:B2:1890:A:H4'	1.95	0.48
3:B2:2867:C:H4'	3:B2:2868:C:OP2	2.14	0.48
3:B2:3329:G:OP2	3:B2:3329:G:H8	1.97	0.48
20:Bb:89:LYS:HE2	20:Bb:89:LYS:HB3	1.63	0.48
3:B2:2667:G:H2'	3:B2:2669:G:C8	2.48	0.48
9:BQ:84:PRO:HB3	9:BQ:89:LYS:HB3	1.96	0.48
3:B2:443:C:H2'	3:B2:444:A:C8	2.49	0.48
3:B2:1096:A:H4'	3:B2:1097:C:H3'	1.94	0.48
5:B4:88:A:H4'	5:B4:89:U:O5'	2.13	0.48
23:Be:25:ARG:HH22	23:Be:27:ARG:HD2	1.78	0.48
41:Bw:56:LYS:N	41:Bw:56:LYS:HE2	2.29	0.48
5:B4:22:C:H5''	20:Bb:123:PRO:HG3	1.96	0.47
13:BU:93:VAL:O	13:BU:177:ILE:HG12	2.14	0.47
17:BY:38:LEU:HD13	17:BY:50:VAL:HG22	1.95	0.47
8:BP:10:ILE:HD11	8:BP:22:ILE:HG13	1.95	0.47
3:B2:3217:U:H1'	3:B2:3218:A:H5''	1.96	0.47
9:BQ:84:PRO:HD3	9:BQ:92:LEU:HD21	1.95	0.47
10:BR:72:VAL:HA	10:BR:82:VAL:HG23	1.96	0.47
15:BW:80:LEU:O	15:BW:84:LEU:HG	2.15	0.47
28:Bj:132:LEU:HD23	28:Bj:132:LEU:HA	1.73	0.47
37:Bs:43:ARG:HG3	37:Bs:43:ARG:HH11	1.78	0.47
3:B2:1086:A:H5''	3:B2:2732:A:H61	1.79	0.47
5:B4:90:U:H1'	5:B4:91:C:C6	2.50	0.47
14:BV:99:ILE:HG22	14:BV:123:ASN:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B2:2330:A:H4'	3:B2:2332:A:H5'	1.96	0.47
4:B3:33:U:C2	9:BQ:210:MET:HE1	2.50	0.47
8:BP:60:HIS:CE1	8:BP:100:ARG:HD3	2.49	0.47
13:BU:9:GLU:O	13:BU:9:GLU:HG2	2.14	0.47
13:BU:86:PHE:CE2	13:BU:149:LEU:HB2	2.50	0.47
25:Bg:33:TYR:HD2	25:Bg:81:PHE:CD2	2.32	0.47
3:B2:445:G:C4	3:B2:446:U:H5	2.32	0.47
3:B2:2687:G:H4'	3:B2:2689:C:C2	2.49	0.47
3:B2:2995:A:H3'	3:B2:2996:G:H8	1.79	0.47
3:B2:3359:U:H5''	3:B2:3361:U:H5	1.79	0.47
7:BO:92:TYR:HE2	7:BO:159:ARG:HD2	1.79	0.47
12:BT:106:LYS:HB2	12:BT:106:LYS:HE2	1.68	0.47
17:BY:18:LYS:HB2	17:BY:55:SER:HB2	1.96	0.47
33:Bo:64:TYR:HE2	37:Bs:97:GLU:HG2	1.79	0.47
3:B2:1319:U:H3'	3:B2:1320:G:H8	1.80	0.47
3:B2:3115:U:H3'	3:B2:3116:U:H5''	1.96	0.47
3:B2:3267:A:H61	3:B2:3378:A:H61	1.61	0.47
3:B2:3284:G:H2'	3:B2:3284:G:N3	2.30	0.47
6:BN:3:ARG:HB2	6:BN:206:VAL:HG22	1.96	0.47
22:Bd:57:MET:HA	22:Bd:57:MET:HE2	1.95	0.47
7:BO:19:ARG:HD3	7:BO:273:MET:HE1	1.97	0.47
22:Bd:144:ARG:HB2	22:Bd:144:ARG:NH1	2.30	0.47
3:B2:1080:A:H2'	14:BV:22:TYR:CE2	2.46	0.47
3:B2:3338:A:H2'	3:B2:3339:A:C8	2.50	0.47
14:BV:19:LYS:HD2	14:BV:26:VAL:HB	1.97	0.47
27:Bi:6:CYS:HB2	27:Bi:32:VAL:HG23	1.97	0.47
29:Bk:49:VAL:HG12	29:Bk:105:ILE:HD11	1.97	0.47
3:B2:2328:G:O2'	6:BN:241:ARG:HB2	2.14	0.47
3:B2:3249:U:H3	3:B2:3392:A:H2'	1.80	0.47
3:B2:3295:U:C4	13:BU:22:LYS:HE2	2.50	0.47
5:B4:20:A:H5''	20:Bb:3:ARG:HB3	1.96	0.47
13:BU:29:LYS:HD2	13:BU:29:LYS:C	2.40	0.47
15:BW:172:LEU:HD23	15:BW:172:LEU:H	1.78	0.47
25:Bg:52:VAL:HA	25:Bg:64:ILE:O	2.15	0.47
18:BZ:106:VAL:HG11	18:BZ:132:VAL:HG21	1.96	0.46
3:B2:3379:A:H2'	3:B2:3380:A:C8	2.50	0.46
13:BU:68:ILE:HD12	13:BU:69:ARG:N	2.30	0.46
14:BV:121:LYS:HE3	44:HS:48:PHE:CD2	2.49	0.46
19:Ba:170:GLN:OE1	19:Ba:170:GLN:HA	2.15	0.46
37:Bs:70:LYS:HE2	37:Bs:70:LYS:HB2	1.68	0.46
42:Bx:26:TRP:H	42:Bx:26:TRP:CD1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B2:1011:G:H1	3:B2:1135:G:H21	1.63	0.46
3:B2:1073:U:H4'	14:BV:198:LYS:HZ3	1.81	0.46
3:B2:1659:G:O6	3:B2:1874:U:H1'	2.16	0.46
43:By:63:GLY:H	43:By:127:GLN:HE22	1.61	0.46
3:B2:997:A:H5''	16:BX:4:HIS:HB3	1.98	0.46
3:B2:1103:U:H3	3:B2:1119:G:H1	1.63	0.46
3:B2:2724:U:H3	3:B2:2744:G:H1	1.62	0.46
8:BP:76:ILE:HD12	8:BP:77:PRO:HD2	1.97	0.46
9:BQ:127:GLY:HA2	9:BQ:195:LEU:HD12	1.97	0.46
13:BU:142:ILE:O	13:BU:142:ILE:HD12	2.15	0.46
30:Bl:83:THR:HG22	37:Bs:93:PHE:CZ	2.51	0.46
36:Br:60:VAL:HG12	36:Br:61:ARG:HG3	1.97	0.46
38:Bt:4:LYS:HB2	38:Bt:7:GLU:HB2	1.97	0.46
3:B2:2187:A:H2'	3:B2:2188:A:H5''	1.96	0.46
3:B2:3315:A:H61	17:BY:115:ARG:HH21	1.63	0.46
5:B4:91:C:H4'	5:B4:92:C:H5''	1.98	0.46
6:BN:205:PRO:HG3	6:BN:212:GLY:HA3	1.97	0.46
7:BO:60:LEU:HD22	7:BO:67:MET:HB3	1.96	0.46
9:BQ:87:GLY:HA2	9:BQ:89:LYS:HZ2	1.81	0.46
17:BY:120:ARG:HD3	19:Ba:183:LYS:HG3	1.96	0.46
24:Bf:17:ARG:HB2	24:Bf:22:HIS:CE1	2.51	0.46
30:Bl:46:VAL:HA	30:Bl:70:PRO:HA	1.98	0.46
30:Bl:59:ALA:O	30:Bl:62:ILE:HG13	2.15	0.46
33:Bo:24:MET:HE1	33:Bo:87:CYS:HA	1.97	0.46
5:B4:89:U:OP2	5:B4:90:U:H5'	2.16	0.46
8:BP:131:SER:HA	8:BP:137:LEU:HD21	1.98	0.46
20:Bb:72:GLN:HE22	20:Bb:83:TRP:HE1	1.64	0.46
29:Bk:49:VAL:HG21	29:Bk:79:LEU:HD21	1.98	0.46
4:B3:75:G:N2	23:Be:51:LYS:HG2	2.31	0.46
10:BR:191:HIS:CD2	10:BR:192:LEU:HG	2.51	0.46
23:Be:30:ALA:HB1	23:Be:35:VAL:HB	1.98	0.46
27:Bi:59:HIS:O	27:Bi:60:LYS:HG3	2.15	0.46
3:B2:680:C:H2'	3:B2:681:A:C8	2.51	0.46
3:B2:1012:A:H2'	3:B2:1013:U:O4'	2.16	0.46
3:B2:2329:U:H5'	6:BN:241:ARG:HH22	1.80	0.46
3:B2:2342:U:N3	3:B2:2343:A:H1'	2.31	0.46
3:B2:2605:U:O2'	3:B2:2606:U:H6	1.99	0.46
3:B2:2993:G:H2'	3:B2:2993:G:N3	2.30	0.46
14:BV:66:GLU:HA	14:BV:66:GLU:OE1	2.15	0.46
28:Bj:68:SER:O	28:Bj:72:MET:HG2	2.16	0.46
28:Bj:72:MET:HE1	28:Bj:141:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Bl:87:LEU:HD13	30:Bl:89:LEU:H	1.80	0.46
3:B2:763:G:C4	3:B2:765:G:H1'	2.51	0.46
12:BT:53:PRO:HG2	12:BT:56:ILE:HG13	1.98	0.46
7:BO:248:LYS:HB3	7:BO:248:LYS:HE2	1.63	0.46
13:BU:53:ILE:HD12	13:BU:53:ILE:C	2.41	0.46
18:BZ:73:ARG:NH1	18:BZ:92:LEU:HD11	2.31	0.46
30:Bl:42:VAL:HA	30:Bl:74:VAL:HA	1.98	0.46
44:HS:62:GLN:HG2	44:HS:63:LEU:H	1.81	0.46
3:B2:3246:A:H4'	7:BO:128:LYS:O	2.16	0.45
3:B2:3288:G:H2'	3:B2:3289:G:C8	2.51	0.45
10:BR:93:ILE:HG22	10:BR:124:PHE:HE1	1.80	0.45
14:BV:110:ARG:HG3	14:BV:111:LEU:H	1.81	0.45
3:B2:2441:G:H5''	20:Bb:86:LYS:HB2	1.98	0.45
3:B2:2659:G:N2	3:B2:2673:U:H1'	2.31	0.45
3:B2:2716:G:H22	14:BV:111:LEU:HD12	1.81	0.45
3:B2:3055:C:H2'	3:B2:3056:G:C8	2.51	0.45
12:BT:166:LEU:HD23	12:BT:166:LEU:HA	1.79	0.45
3:B2:31:C:H4'	18:BZ:96:ARG:HD3	1.99	0.45
3:B2:178:U:H2'	3:B2:179:G:C8	2.51	0.45
3:B2:713:G:H5'	3:B2:714:A:N7	2.32	0.45
3:B2:2300:C:H2'	3:B2:2318:C:N4	2.29	0.45
3:B2:3289:G:N3	3:B2:3289:G:H2'	2.31	0.45
3:B2:788:G:H4'	3:B2:789:A:O4'	2.16	0.45
15:BW:106:ILE:HG12	15:BW:125:MET:O	2.15	0.45
30:Bl:136:PHE:HB2	37:Bs:88:ARG:HG2	1.98	0.45
3:B2:164:G:H2'	3:B2:165:A:H8	1.81	0.45
3:B2:574:U:H2'	3:B2:575:G:C4	2.52	0.45
3:B2:1095:G:O2'	3:B2:1096:A:H5'	2.16	0.45
3:B2:1875:U:H5'	3:B2:1877:C:N4	2.28	0.45
3:B2:3336:G:H2'	3:B2:3337:A:H8	1.81	0.45
3:B2:3362:C:H3'	3:B2:3363:C:H5''	1.98	0.45
13:BU:11:LEU:HD22	13:BU:72:TYR:CE1	2.51	0.45
31:Bm:75:LEU:HD23	31:Bm:75:LEU:HA	1.86	0.45
41:Bw:52:LYS:HE2	41:Bw:52:LYS:N	2.31	0.45
3:B2:2527:A:H61	3:B2:2604:U:H3	1.65	0.45
7:BO:56:ILE:HG21	7:BO:323:MET:HE1	1.98	0.45
23:Be:37:LYS:HE2	23:Be:57:ILE:HG21	1.99	0.45
40:Bv:64:MET:O	40:Bv:68:LYS:HG3	2.17	0.45
43:By:97:LYS:NZ	43:By:97:LYS:HB3	2.32	0.45
3:B2:2702:G:H5'	6:BN:232:GLN:HB3	1.97	0.45
9:BQ:222:GLN:O	9:BQ:223:PHE:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BU:86:PHE:CZ	13:BU:149:LEU:HB2	2.52	0.45
2:B1:49:ARG:HB2	2:B1:55:TRP:CZ3	2.51	0.45
3:B2:123:A:OP1	12:BT:105:LYS:HE3	2.16	0.45
3:B2:3283:A:O2'	3:B2:3284:G:H8	2.00	0.45
15:BW:107:GLN:HG2	15:BW:108:GLU:HG3	1.98	0.45
25:Bg:27:VAL:HG13	25:Bg:61:ILE:HD11	1.98	0.45
3:B2:1064:C:H2'	3:B2:1065:U:C6	2.52	0.45
3:B2:1319:U:H3'	3:B2:1320:G:C8	2.52	0.45
13:BU:15:GLU:H	13:BU:15:GLU:CD	2.24	0.45
13:BU:55:PHE:HB3	13:BU:68:ILE:HG22	1.98	0.45
18:BZ:57:GLN:HE21	18:BZ:57:GLN:HB2	1.62	0.45
19:Ba:173:LEU:HD12	19:Ba:173:LEU:HA	1.84	0.45
21:Bc:21:GLU:HA	21:Bc:21:GLU:OE1	2.17	0.45
21:Bc:160:LYS:HD2	21:Bc:160:LYS:HA	1.74	0.45
33:Bo:47:LEU:HD12	33:Bo:48:ILE:N	2.32	0.45
3:B2:3470:G:H2'	3:B2:3470:G:N3	2.30	0.45
3:B2:3117:A:H61	3:B2:3128:A:H5''	1.81	0.44
6:BN:226:ARG:HB2	6:BN:238:ALA:HB2	1.97	0.44
9:BQ:196:ARG:O	9:BQ:199:ILE:HG22	2.18	0.44
17:BY:76:LYS:HE3	17:BY:76:LYS:HB3	1.87	0.44
22:Bd:105:LEU:HD23	22:Bd:138:LEU:HD23	1.99	0.44
33:Bo:16:ILE:HG12	33:Bo:76:TYR:CE2	2.52	0.44
3:B2:183:A:O2'	3:B2:184:C:H5'	2.17	0.44
34:Bp:11:GLN:HB3	34:Bp:92:LEU:HD11	2.00	0.44
3:B2:2923:G:H22	14:BV:104:SER:HB3	1.81	0.44
8:BP:212:ASN:HD22	8:BP:255:SER:HB3	1.82	0.44
10:BR:89:ASN:HB3	10:BR:91:VAL:HG22	1.99	0.44
11:BS:116:LEU:HD21	11:BS:123:VAL:HG12	1.99	0.44
12:BT:162:LEU:HA	18:BZ:7:LEU:HD21	1.99	0.44
37:Bs:100:ILE:HD12	37:Bs:101:VAL:N	2.31	0.44
44:HS:83:VAL:O	44:HS:87:ILE:HG12	2.18	0.44
3:B2:546:G:H2'	3:B2:548:U:C5	2.52	0.44
3:B2:1844:C:H2'	3:B2:1845:A:C8	2.53	0.44
9:BQ:131:LEU:HD23	9:BQ:172:PHE:HE1	1.82	0.44
10:BR:86:TYR:CD1	10:BR:90:GLY:HA2	2.52	0.44
43:By:104:GLY:HA3	43:By:113:VAL:HG22	1.99	0.44
16:BX:129:LYS:HB2	16:BX:129:LYS:HE2	1.72	0.44
17:BY:112:ALA:O	17:BY:116:LEU:HD12	2.18	0.44
31:Bm:96:GLU:H	31:Bm:96:GLU:CD	2.24	0.44
3:B2:116:A:H5''	3:B2:273:A:N3	2.33	0.44
3:B2:1071:U:H2'	3:B2:1072:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B2:1127:U:H1'	24:Bf:129:ARG:NE	2.32	0.44
3:B2:3209:A:H3'	3:B2:3210:A:C8	2.53	0.44
3:B2:3247:U:H5'	3:B2:3394:C:H1'	1.99	0.44
12:BT:78:PHE:C	12:BT:80:LYS:H	2.26	0.44
15:BW:80:LEU:HD12	15:BW:80:LEU:HA	1.74	0.44
21:Bc:179:ARG:HG3	31:Bm:51:GLY:HA3	1.99	0.44
26:Bh:35:ASN:HB2	26:Bh:66:LYS:HB3	2.00	0.44
28:Bj:88:LYS:HE2	28:Bj:88:LYS:HB3	1.70	0.44
33:Bo:40:LEU:HD23	33:Bo:40:LEU:HA	1.85	0.44
3:B2:1759:G:H4'	3:B2:1772:U:H4'	1.99	0.44
3:B2:1941:A:H2'	3:B2:1942:A:H8	1.82	0.44
6:BN:14:ILE:HD13	6:BN:14:ILE:HA	1.89	0.44
12:BT:171:LYS:HG2	12:BT:226:TYR:CD2	2.53	0.44
14:BV:101:LYS:HA	14:BV:101:LYS:HD3	1.68	0.44
29:Bk:22:PRO:HG2	29:Bk:25:VAL:HG23	1.99	0.44
30:Bl:92:LEU:HD13	30:Bl:114:VAL:HG22	1.99	0.44
7:BO:185:GLY:H	7:BO:191:LYS:HZ2	1.65	0.44
13:BU:25:LEU:HB3	13:BU:36:LYS:HZ1	1.83	0.44
14:BV:102:MET:HE2	14:BV:102:MET:HB2	1.84	0.44
26:Bh:61:LEU:HB3	26:Bh:75:ILE:HD11	1.99	0.44
44:HS:44:ILE:HG22	44:HS:45:VAL:HG13	1.99	0.44
3:B2:1520:G:H21	37:Bs:6:THR:HG22	1.82	0.44
3:B2:1800:G:H22	3:B2:1804:C:H41	1.64	0.44
3:B2:2669:G:N3	3:B2:2669:G:H2'	2.32	0.44
7:BO:113:GLU:H	7:BO:113:GLU:HG3	1.60	0.44
12:BT:142:LEU:HD13	12:BT:201:THR:HG21	2.00	0.44
13:BU:69:ARG:HA	13:BU:69:ARG:CZ	2.48	0.44
17:BY:6:ARG:HD2	17:BY:60:HIS:CE1	2.53	0.44
22:Bd:114:LYS:HG3	22:Bd:146:LYS:HZ1	1.83	0.44
22:Bd:114:LYS:HG3	22:Bd:146:LYS:NZ	2.33	0.44
29:Bk:97:GLY:C	29:Bk:98:ILE:HD13	2.43	0.44
3:B2:2525:G:H1	3:B2:2606:U:H3	1.65	0.43
6:BN:144:LYS:HB3	6:BN:156:VAL:HG13	2.00	0.43
7:BO:212:ASN:ND2	7:BO:353:PRO:HA	2.33	0.43
9:BQ:83:LEU:N	9:BQ:84:PRO:HD2	2.33	0.43
12:BT:146:LYS:HE3	12:BT:146:LYS:HB2	1.75	0.43
12:BT:185:ARG:O	12:BT:188:THR:HG22	2.17	0.43
13:BU:90:MET:HE3	13:BU:160:LYS:HE2	2.00	0.43
26:Bh:59:MET:HE3	26:Bh:59:MET:HB2	1.96	0.43
33:Bo:49:LEU:HB2	33:Bo:96:LEU:HG	2.00	0.43
3:B2:613:A:N6	3:B2:635:G:H1'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B2:2345:C:H42	3:B2:2394:C:N4	2.16	0.43
3:B2:3329:G:H1	3:B2:3358:U:H3	1.66	0.43
3:B2:3374:A:H5'	3:B2:3375:U:H5'	2.00	0.43
6:BN:100:VAL:HG22	6:BN:164:VAL:HG22	1.98	0.43
14:BV:115:MET:HE3	14:BV:115:MET:HB3	1.78	0.43
23:Be:151:LEU:HD22	23:Be:152:PRO:HD2	1.99	0.43
42:Bx:25:GLN:H	42:Bx:25:GLN:NE2	2.14	0.43
3:B2:1234:A:H2'	3:B2:1235:A:C8	2.53	0.43
3:B2:2319:C:O2'	3:B2:2517:G:H5'	2.19	0.43
3:B2:2342:U:C4	3:B2:2343:A:H1'	2.53	0.43
3:B2:2607:A:H2'	3:B2:2608:C:C6	2.54	0.43
12:BT:71:VAL:HG12	18:BZ:21:PHE:CZ	2.53	0.43
17:BY:42:PRO:HG3	17:BY:78:TRP:CG	2.53	0.43
37:Bs:23:ILE:HD13	37:Bs:33:LEU:HD13	2.00	0.43
41:Bw:19:ASP:HB2	41:Bw:40:SER:HB2	1.99	0.43
3:B2:641:G:H2'	3:B2:642:A:C8	2.54	0.43
3:B2:1891:C:H41	42:Bx:3:SER:HB2	1.83	0.43
3:B2:2000:A:H2'	3:B2:2001:A:C8	2.54	0.43
6:BN:227:GLN:HA	6:BN:227:GLN:OE1	2.18	0.43
7:BO:106:TRP:HB2	7:BO:133:TYR:CE2	2.54	0.43
14:BV:36:LEU:HD21	14:BV:69:ARG:HD2	2.01	0.43
32:Bn:18:ARG:HG2	32:Bn:18:ARG:NH1	2.33	0.43
3:B2:2188:A:H4'	3:B2:2188:A:OP1	2.19	0.43
13:BU:64:HIS:O	13:BU:67:CYS:HB2	2.18	0.43
17:BY:104:GLN:HA	17:BY:104:GLN:OE1	2.18	0.43
34:Bp:56:VAL:HG13	34:Bp:60:LEU:HD23	1.99	0.43
37:Bs:91:ARG:O	37:Bs:95:ILE:HG13	2.18	0.43
44:HS:13:TYR:CE2	44:HS:15:PRO:HD3	2.53	0.43
3:B2:1844:C:H2'	3:B2:1845:A:H8	1.84	0.43
3:B2:2662:U:H3	3:B2:2669:G:H1	1.67	0.43
3:B2:3418:U:H1'	3:B2:3419:G:OP2	2.18	0.43
15:BW:20:ASN:HB3	15:BW:126:ASP:OD2	2.18	0.43
20:Bb:122:ALA:HB3	20:Bb:143:PRO:HG2	2.00	0.43
23:Be:165:LYS:HB2	23:Be:165:LYS:HE2	1.55	0.43
1:B0:61:LYS:HB2	1:B0:61:LYS:HE3	1.86	0.43
2:B1:36:ARG:HG3	2:B1:48:LYS:HE2	1.99	0.43
3:B2:1790:A:H4'	3:B2:1791:G:H5'	2.01	0.43
3:B2:2923:G:N2	14:BV:104:SER:HB3	2.33	0.43
13:BU:29:LYS:HB3	13:BU:34:VAL:HG23	2.00	0.43
14:BV:191:ILE:HD12	14:BV:192:PRO:HD2	2.00	0.43
16:BX:134:LYS:HD2	16:BX:134:LYS:HA	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:BY:43:CYS:HB3	17:BY:45:GLU:OE1	2.19	0.43
24:Bf:126:VAL:HG13	24:Bf:127:GLN:N	2.32	0.43
3:B2:1242:U:OP1	13:BU:62:ARG:HB3	2.19	0.43
3:B2:2330:A:H2'	3:B2:2334:G:O6	2.18	0.43
3:B2:3116:U:H2'	3:B2:3117:A:C8	2.54	0.43
6:BN:63:ARG:HE	6:BN:63:ARG:HB3	1.61	0.43
7:BO:130:PHE:HD1	7:BO:130:PHE:H	1.67	0.43
13:BU:62:ARG:HH12	13:BU:66:ALA:HB2	1.83	0.43
17:BY:25:LEU:HD12	17:BY:25:LEU:HA	1.85	0.43
19:Ba:177:LYS:HE3	19:Ba:177:LYS:HB3	1.92	0.43
28:Bj:114:ARG:HD3	28:Bj:120:LYS:HE3	2.01	0.43
44:HS:97:ARG:C	44:HS:98:GLU:HG3	2.44	0.43
2:B1:30:GLU:HG2	2:B1:34:HIS:CE1	2.54	0.43
3:B2:1221:A:H2'	3:B2:1221:A:N3	2.34	0.43
16:BX:132:GLN:N	16:BX:132:GLN:OE1	2.52	0.43
21:Bc:125:LEU:HD23	21:Bc:125:LEU:HA	1.89	0.43
22:Bd:132:PHE:CE2	22:Bd:138:LEU:HD13	2.53	0.43
23:Be:44:LEU:HA	23:Be:44:LEU:HD12	1.77	0.43
30:Bl:26:LEU:HD23	30:Bl:96:ILE:HB	2.00	0.43
30:Bl:54:THR:HG22	30:Bl:57:MET:HE2	2.00	0.43
30:Bl:55:LYS:HB2	30:Bl:55:LYS:HE2	1.68	0.43
3:B2:277:G:H5''	18:BZ:14:LYS:NZ	2.34	0.43
3:B2:715:U:H2'	3:B2:716:G:N2	2.33	0.43
3:B2:1234:A:H61	3:B2:1331:G:H2'	1.84	0.43
9:BQ:221:LYS:HE3	9:BQ:221:LYS:HB2	1.79	0.43
12:BT:173:MET:HE2	12:BT:173:MET:HB3	1.96	0.43
22:Bd:143:GLN:OE1	22:Bd:143:GLN:HA	2.17	0.43
23:Be:109:MET:HE3	23:Be:109:MET:HB3	1.77	0.43
26:Bh:90:LYS:HD2	26:Bh:90:LYS:HA	1.64	0.43
38:Bt:65:ARG:O	38:Bt:69:ARG:HG3	2.19	0.43
43:By:52:LYS:HB3	43:By:108:TYR:CE1	2.54	0.43
3:B2:948:G:H5'	3:B2:949:A:OP1	2.19	0.42
4:B3:44:C:P	15:BW:137:ARG:HH12	2.42	0.42
10:BR:171:ILE:HG21	10:BR:174:MET:HE3	2.01	0.42
13:BU:36:LYS:HE3	13:BU:37:GLN:H	1.84	0.42
13:BU:86:PHE:CD1	13:BU:149:LEU:HD23	2.54	0.42
16:BX:169:GLU:CD	16:BX:169:GLU:H	2.26	0.42
20:Bb:126:ARG:HB2	20:Bb:126:ARG:CZ	2.48	0.42
21:Bc:14:GLN:H	21:Bc:14:GLN:HG2	1.56	0.42
3:B2:185:G:H2'	3:B2:186:A:H8	1.84	0.42
3:B2:1877:C:H2'	3:B2:1878:A:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B2:1888:G:P	28:Bj:113:ILE:HD12	2.59	0.42
4:B3:54:A:O2'	4:B3:55:A:H8	2.02	0.42
11:BS:250:MET:HE2	11:BS:250:MET:HB3	1.86	0.42
13:BU:145:GLU:HA	13:BU:145:GLU:OE2	2.18	0.42
39:Bu:58:LEU:HB3	39:Bu:67:ALA:HB2	2.01	0.42
3:B2:1295:G:H21	3:B2:1308:C:H42	1.67	0.42
3:B2:2330:A:H2'	3:B2:2334:G:C6	2.54	0.42
3:B2:3130:C:O2	13:BU:118:GLU:HG2	2.19	0.42
6:BN:118:LYS:HB3	6:BN:118:LYS:HE2	1.84	0.42
11:BS:110:ILE:HG23	11:BS:134:MET:HG2	2.01	0.42
24:Bf:51:GLY:HA3	24:Bf:92:ARG:HG3	2.02	0.42
27:Bi:47:ARG:HG3	27:Bi:54:LEU:HB3	2.01	0.42
9:BQ:186:GLU:CD	9:BQ:187:THR:HG23	2.44	0.42
3:B2:277:G:H5''	18:BZ:14:LYS:HZ1	1.85	0.42
4:B3:12:U:H4'	4:B3:13:A:OP2	2.20	0.42
9:BQ:23:ARG:HD2	9:BQ:23:ARG:O	2.20	0.42
13:BU:49:GLN:OE1	13:BU:49:GLN:N	2.52	0.42
14:BV:39:LYS:HA	14:BV:86:HIS:CD2	2.55	0.42
23:Be:47:ILE:CD1	23:Be:48:ASN:HD22	2.28	0.42
29:Bk:124:LYS:HD3	29:Bk:124:LYS:N	2.34	0.42
31:Bm:78:LEU:HD23	31:Bm:78:LEU:HA	1.84	0.42
35:Bq:7:ILE:HD13	35:Bq:7:ILE:HA	1.90	0.42
3:B2:3042:G:C2	7:BO:250:ALA:HB1	2.55	0.42
4:B3:12:U:H1'	4:B3:108:G:H21	1.84	0.42
9:BQ:157:SER:C	9:BQ:159:VAL:H	2.28	0.42
26:Bh:36:LEU:HD23	26:Bh:36:LEU:HA	1.92	0.42
41:Bw:55:GLU:HG2	41:Bw:56:LYS:HE3	2.01	0.42
43:By:28:ILE:HD12	43:By:28:ILE:O	2.20	0.42
3:B2:70:A:H2	3:B2:72:C:H42	1.67	0.42
3:B2:2662:U:H1'	3:B2:2670:A:C2	2.55	0.42
3:B2:3284:G:H3'	3:B2:3285:G:H4'	2.00	0.42
28:Bj:133:ASP:HA	28:Bj:136:ASN:HD22	1.84	0.42
3:B2:446:U:H1'	3:B2:447:C:C5	2.54	0.42
3:B2:1287:G:H2'	3:B2:1288:C:C6	2.54	0.42
3:B2:2933:A:H4'	14:BV:74:LYS:HE3	2.02	0.42
3:B2:3003:G:H2'	3:B2:3004:U:C6	2.55	0.42
7:BO:126:LYS:HB2	7:BO:128:LYS:HG3	2.02	0.42
14:BV:107:GLY:HA2	44:HS:8:GLN:CD	2.45	0.42
25:Bg:16:ALA:O	25:Bg:20:VAL:HG12	2.19	0.42
26:Bh:79:ILE:HD11	26:Bh:131:ILE:HD12	2.02	0.42
28:Bj:65:PRO:HG2	28:Bj:138:ILE:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Bl:76:ASN:HB3	30:Bl:79:HIS:ND1	2.34	0.42
38:Bt:22:GLU:OE1	38:Bt:22:GLU:HA	2.20	0.42
3:B2:2622:C:H2'	3:B2:2623:G:C8	2.55	0.42
9:BQ:124:GLU:OE1	9:BQ:124:GLU:HA	2.20	0.42
19:Ba:130:LEU:HD12	19:Ba:130:LEU:HA	1.91	0.42
31:Bm:38:LEU:HG	31:Bm:53:PHE:CE2	2.55	0.42
33:Bo:40:LEU:HD13	33:Bo:65:TYR:HB3	2.00	0.42
3:B2:3002:G:H2'	3:B2:3002:G:N3	2.35	0.42
3:B2:3342:G:H5'	3:B2:3345:G:H8	1.85	0.42
9:BQ:235:GLN:O	9:BQ:239:ILE:HD12	2.18	0.42
13:BU:149:LEU:HA	13:BU:152:VAL:HG22	2.02	0.42
17:BY:115:ARG:O	17:BY:119:GLN:HG3	2.20	0.42
19:Ba:48:PHE:HA	19:Ba:137:CYS:SG	2.60	0.42
19:Ba:55:TYR:CE2	19:Ba:146:VAL:HG11	2.55	0.42
25:Bg:12:TYR:HE2	25:Bg:69:PHE:HB3	1.85	0.42
28:Bj:39:LEU:HD23	28:Bj:39:LEU:H	1.85	0.42
29:Bk:65:ARG:HD2	29:Bk:65:ARG:HA	1.81	0.42
6:BN:108:GLU:HA	6:BN:135:ILE:HG22	2.01	0.41
7:BO:66:LYS:HB3	7:BO:66:LYS:HE3	1.94	0.41
10:BR:121:LYS:HE2	10:BR:121:LYS:HB3	1.61	0.41
15:BW:54:ILE:H	15:BW:59:ILE:HG12	1.83	0.41
16:BX:67:MET:HE3	16:BX:67:MET:HB3	1.86	0.41
23:Be:40:TYR:CZ	23:Be:44:LEU:HD22	2.55	0.41
30:Bl:4:ILE:HD13	30:Bl:4:ILE:HA	1.93	0.41
3:B2:186:A:H2'	3:B2:187:U:H4'	2.02	0.41
3:B2:588:G:H2'	3:B2:589:U:H4'	2.02	0.41
3:B2:3335:U:H3'	3:B2:3336:G:N2	2.34	0.41
5:B4:90:U:H1'	5:B4:91:C:C5	2.55	0.41
13:BU:160:LYS:HD2	13:BU:163:CYS:SG	2.60	0.41
15:BW:148:VAL:HG23	15:BW:153:LYS:NZ	2.35	0.41
17:BY:102:ARG:HH11	17:BY:102:ARG:HB2	1.86	0.41
24:Bf:7:ILE:HG13	24:Bf:54:HIS:HD2	1.85	0.41
30:Bl:103:GLU:OE2	30:Bl:103:GLU:N	2.53	0.41
39:Bu:55:VAL:O	39:Bu:59:ILE:HG13	2.20	0.41
3:B2:1025:G:N3	3:B2:2732:A:H2'	2.35	0.41
3:B2:1094:A:H4'	3:B2:1095:G:OP2	2.20	0.41
13:BU:90:MET:O	13:BU:141:GLU:HG2	2.21	0.41
19:Ba:86:ARG:HG3	19:Ba:100:LEU:HD22	2.03	0.41
23:Be:57:ILE:HD13	23:Be:57:ILE:HA	1.88	0.41
25:Bg:39:LYS:HB2	25:Bg:39:LYS:HE3	1.61	0.41
3:B2:414:G:H1'	5:B4:24:G:H22	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B2:2966:G:H5''	3:B2:2967:A:H5'	2.02	0.41
3:B2:2975:U:O2	7:BO:250:ALA:HB3	2.19	0.41
7:BO:233:TRP:CD1	7:BO:265:ALA:HB1	2.55	0.41
10:BR:99:ARG:HA	10:BR:99:ARG:HD3	1.72	0.41
15:BW:117:ASP:HB2	15:BW:120:ILE:HG23	2.02	0.41
16:BX:93:ILE:HD12	16:BX:93:ILE:HA	1.85	0.41
26:Bh:47:ARG:HG2	26:Bh:50:ARG:NH1	2.36	0.41
44:HS:8:GLN:HB2	44:HS:96:HIS:HB3	2.02	0.41
3:B2:1255:C:H2'	3:B2:1256:A:H8	1.84	0.41
3:B2:1559:G:H5'	3:B2:1885:G:OP2	2.21	0.41
3:B2:2344:A:H4'	3:B2:2345:C:OP1	2.19	0.41
3:B2:2995:A:H3'	3:B2:2996:G:C8	2.56	0.41
3:B2:3218:A:H2	13:BU:41:ARG:HH21	1.68	0.41
9:BQ:223:PHE:CD1	9:BQ:223:PHE:C	2.99	0.41
10:BR:79:THR:HG22	10:BR:97:ASN:HA	2.02	0.41
10:BR:151:ALA:O	10:BR:152:GLU:HB3	2.19	0.41
31:Bm:70:ARG:HD2	31:Bm:128:TYR:CD2	2.55	0.41
41:Bw:7:ASP:OD1	41:Bw:9:LYS:HG2	2.21	0.41
43:By:90:ALA:HB3	43:By:94:LYS:CE	2.50	0.41
44:HS:80:ASP:O	44:HS:84:VAL:HG23	2.21	0.41
3:B2:3327:A:H5'	3:B2:3328:U:OP2	2.21	0.41
5:B4:46:U:H5	38:Bt:84:GLN:O	2.03	0.41
9:BQ:43:LYS:HE2	9:BQ:43:LYS:HB2	1.65	0.41
21:Bc:144:LYS:HB2	21:Bc:147:ALA:HB2	2.03	0.41
26:Bh:47:ARG:HD2	26:Bh:48:LEU:H	1.85	0.41
27:Bi:55:TYR:HE1	27:Bi:59:HIS:ND1	2.18	0.41
37:Bs:106:LYS:HE3	37:Bs:106:LYS:HB3	1.86	0.41
3:B2:1884:G:H5''	3:B2:1885:G:H5'	2.03	0.41
3:B2:3338:A:H2'	3:B2:3339:A:H8	1.84	0.41
5:B4:94:U:H4'	5:B4:95:G:N7	2.36	0.41
6:BN:64:ASN:HD22	6:BN:67:HIS:H	1.69	0.41
6:BN:149:LEU:HD11	6:BN:155:LYS:HD2	2.02	0.41
15:BW:155:ASN:ND2	15:BW:157:GLU:HG3	2.31	0.41
18:BZ:174:ILE:HD13	18:BZ:174:ILE:HA	1.90	0.41
19:Ba:110:PRO:HG2	19:Ba:113:PHE:CD2	2.55	0.41
23:Be:105:MET:HE1	23:Be:122:ILE:HD11	2.03	0.41
23:Be:130:LYS:HB3	23:Be:133:ASP:OD1	2.21	0.41
23:Be:154:ARG:HH11	23:Be:156:THR:HA	1.85	0.41
26:Bh:56:CYS:SG	26:Bh:83:GLN:HG2	2.60	0.41
38:Bt:73:LYS:HB3	38:Bt:73:LYS:HE3	1.76	0.41
40:Bv:10:MET:HE2	40:Bv:10:MET:HB3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B2:176:A:H2'	3:B2:177:G:H8	1.85	0.41
3:B2:551:C:N4	3:B2:575:G:H21	2.13	0.41
3:B2:2343:A:H2'	3:B2:2344:A:C2'	2.50	0.41
3:B2:2931:C:H4'	14:BV:157:TYR:HD2	1.85	0.41
3:B2:3272:U:C2	19:Ba:6:LYS:HD2	2.56	0.41
4:B3:39:C:O2'	15:BW:43:GLN:HB3	2.21	0.41
24:Bf:50:LYS:HB3	24:Bf:50:LYS:HE3	1.73	0.41
25:Bg:30:PHE:O	25:Bg:34:LEU:HD23	2.20	0.41
36:Br:48:LYS:HD3	36:Br:105:PRO:HD2	2.02	0.41
43:By:19:LEU:HD11	43:By:29:GLN:HB3	2.02	0.41
3:B2:588:G:N1	3:B2:589:U:H1'	2.36	0.41
3:B2:822:U:H4'	8:BP:114:LYS:O	2.21	0.41
3:B2:2994:C:N4	3:B2:3125:A:H61	2.18	0.41
3:B2:3283:A:OP2	13:BU:22:LYS:HA	2.21	0.41
3:B2:3368:A:H1'	10:BR:92:PRO:HG3	2.01	0.41
9:BQ:205:ALA:O	9:BQ:208:MET:HB2	2.21	0.41
9:BQ:236:LEU:HD23	9:BQ:236:LEU:HA	1.83	0.41
10:BR:76:LEU:HD23	10:BR:76:LEU:HA	1.90	0.41
14:BV:60:ILE:H	14:BV:60:ILE:HG13	1.51	0.41
15:BW:85:LYS:HA	15:BW:85:LYS:HD3	1.73	0.41
15:BW:166:LYS:HE3	15:BW:166:LYS:HB2	1.83	0.41
19:Ba:26:LYS:HD2	19:Ba:26:LYS:HA	1.87	0.41
22:Bd:135:LYS:O	22:Bd:139:ILE:HG13	2.20	0.41
23:Be:35:VAL:O	23:Be:39:ARG:HG2	2.21	0.41
24:Bf:104:ASP:O	24:Bf:108:ARG:HG3	2.21	0.41
25:Bg:8:VAL:O	25:Bg:8:VAL:HG13	2.21	0.41
28:Bj:73:LYS:O	28:Bj:77:ASP:HB2	2.21	0.41
30:Bl:15:ARG:HH22	37:Bs:83:ASN:ND2	2.19	0.41
39:Bu:3:PRO:HD3	39:Bu:10:ASN:HB2	2.02	0.41
3:B2:185:G:H2'	3:B2:186:A:C8	2.56	0.41
3:B2:1103:U:H4'	3:B2:1104:G:OP1	2.21	0.41
3:B2:1941:A:H2'	3:B2:1942:A:C8	2.54	0.41
3:B2:2203:G:O2'	22:Bd:82:LYS:HD3	2.21	0.41
11:BS:129:LYS:HA	11:BS:129:LYS:HD2	1.84	0.41
8:BP:120:LYS:O	8:BP:124:ILE:HG13	2.21	0.40
9:BQ:11:PRO:O	9:BQ:15:ARG:HG3	2.21	0.40
9:BQ:211:LEU:HD21	9:BQ:219:TYR:HA	2.03	0.40
16:BX:62:THR:HG21	31:Bm:66:ASN:HD22	1.85	0.40
18:BZ:183:SER:O	18:BZ:184:PRO:C	2.64	0.40
25:Bg:30:PHE:HA	25:Bg:81:PHE:HE2	1.85	0.40
3:B2:906:U:OP1	3:B2:907:G:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B2:2764:C:H2'	3:B2:2765:G:H8	1.86	0.40
4:B3:28:C:H1'	4:B3:54:A:H61	1.85	0.40
7:BO:244:ARG:HE	7:BO:244:ARG:HB2	1.63	0.40
9:BQ:220:GLN:HA	9:BQ:220:GLN:OE1	2.22	0.40
10:BR:151:ALA:C	10:BR:153:ARG:H	2.29	0.40
13:BU:29:LYS:HA	13:BU:34:VAL:HA	2.03	0.40
14:BV:171:TRP:CD1	14:BV:171:TRP:C	2.99	0.40
30:Bl:91:ASN:HD22	30:Bl:91:ASN:C	2.30	0.40
31:Bm:123:ILE:HA	31:Bm:143:VAL:O	2.21	0.40
36:Br:51:CYS:HB3	36:Br:69:TRP:CZ3	2.56	0.40
44:HS:11:VAL:HG12	44:HS:87:ILE:HG22	2.04	0.40
1:B0:66:LYS:NZ	1:B0:66:LYS:HB2	2.36	0.40
3:B2:2380:U:H3	3:B2:2388:G:H1	1.69	0.40
3:B2:3001:C:H1'	3:B2:3002:G:OP2	2.22	0.40
3:B2:3267:A:H61	3:B2:3378:A:N6	2.19	0.40
7:BO:17:LEU:HD21	7:BO:233:TRP:HH2	1.86	0.40
19:Ba:55:TYR:HE2	19:Ba:146:VAL:HG11	1.85	0.40
30:Bl:22:LYS:HD3	30:Bl:129:TRP:CZ3	2.57	0.40
3:B2:2656:A:O2'	3:B2:2657:A:H8	2.05	0.40
3:B2:3043:C:H4'	7:BO:243:HIS:H	1.86	0.40
3:B2:3332:U:H3	3:B2:3355:G:H1	1.69	0.40
4:B3:53:U:H1'	4:B3:54:A:C8	2.56	0.40
15:BW:25:GLU:H	15:BW:25:GLU:CD	2.30	0.40
17:BY:6:ARG:HB3	17:BY:58:LEU:HD23	2.03	0.40
17:BY:102:ARG:HB2	17:BY:102:ARG:NH1	2.37	0.40
28:Bj:62:ILE:HD13	28:Bj:85:VAL:HG12	2.03	0.40
30:Bl:128:ALA:O	30:Bl:132:THR:HG23	2.22	0.40
32:Bn:47:ASN:HA	32:Bn:50:THR:HG22	2.03	0.40
33:Bo:40:LEU:HD23	33:Bo:45:ALA:HB3	2.02	0.40
39:Bu:34:ARG:HH11	39:Bu:34:ARG:HG2	1.87	0.40
42:Bx:2:PRO:C	42:Bx:4:HIS:H	2.29	0.40
3:B2:57:A:H5'	18:BZ:157:LYS:HE2	2.02	0.40
3:B2:316:A:H1'	3:B2:2310:A:N3	2.37	0.40
3:B2:587:U:H6	3:B2:587:U:H2'	1.72	0.40
3:B2:948:G:H4'	3:B2:949:A:O5'	2.22	0.40
3:B2:2344:A:C8	3:B2:2349:G:C6	3.10	0.40
3:B2:2764:C:H2'	3:B2:2765:G:C8	2.56	0.40
4:B3:75:G:H22	23:Be:51:LYS:HG2	1.86	0.40
17:BY:5:LYS:HE3	17:BY:5:LYS:HB3	1.92	0.40
20:Bb:10:LEU:HA	20:Bb:10:LEU:HD12	1.86	0.40
21:Bc:72:ARG:HA	21:Bc:72:ARG:HD2	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Bd:115:ILE:HG22	22:Bd:146:LYS:HZ2	1.86	0.40
26:Bh:87:TRP:HH2	26:Bh:97:PHE:HE1	1.68	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	B0	91/106 (86%)	86 (94%)	5 (6%)	0	100	100
2	B1	91/94 (97%)	87 (96%)	4 (4%)	0	100	100
6	BN	246/253 (97%)	238 (97%)	8 (3%)	0	100	100
7	BO	382/388 (98%)	367 (96%)	14 (4%)	1 (0%)	36	66
8	BP	360/363 (99%)	350 (97%)	10 (3%)	0	100	100
9	BQ	285/294 (97%)	259 (91%)	25 (9%)	1 (0%)	30	60
10	BR	160/195 (82%)	145 (91%)	15 (9%)	0	100	100
11	BS	231/251 (92%)	223 (96%)	8 (4%)	0	100	100
12	BT	227/259 (88%)	218 (96%)	9 (4%)	0	100	100
13	BU	162/189 (86%)	153 (94%)	9 (6%)	0	100	100
14	BV	207/221 (94%)	201 (97%)	6 (3%)	0	100	100
15	BW	165/174 (95%)	150 (91%)	13 (8%)	2 (1%)	10	34
16	BX	205/208 (99%)	201 (98%)	4 (2%)	0	100	100
17	BY	128/134 (96%)	127 (99%)	1 (1%)	0	100	100
18	BZ	198/201 (98%)	187 (94%)	11 (6%)	0	100	100
19	Ba	194/197 (98%)	191 (98%)	3 (2%)	0	100	100
20	Bb	150/187 (80%)	144 (96%)	6 (4%)	0	100	100
21	Bc	184/187 (98%)	181 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	Bd	155/193 (80%)	151 (97%)	3 (2%)	1 (1%)	21	51
23	Be	171/176 (97%)	166 (97%)	4 (2%)	1 (1%)	21	51
24	Bf	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
25	Bg	97/117 (83%)	89 (92%)	8 (8%)	0	100	100
26	Bh	132/139 (95%)	127 (96%)	5 (4%)	0	100	100
27	Bi	61/149 (41%)	59 (97%)	2 (3%)	0	100	100
28	Bj	116/141 (82%)	111 (96%)	5 (4%)	0	100	100
29	Bk	123/126 (98%)	122 (99%)	1 (1%)	0	100	100
30	Bl	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
31	Bm	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
32	Bn	57/61 (93%)	54 (95%)	3 (5%)	0	100	100
33	Bo	92/109 (84%)	90 (98%)	2 (2%)	0	100	100
34	Bp	101/113 (89%)	99 (98%)	2 (2%)	0	100	100
35	Bq	116/127 (91%)	113 (97%)	3 (3%)	0	100	100
36	Br	102/108 (94%)	100 (98%)	2 (2%)	0	100	100
37	Bs	104/111 (94%)	102 (98%)	2 (2%)	0	100	100
38	Bt	119/122 (98%)	114 (96%)	5 (4%)	0	100	100
39	Bu	93/99 (94%)	91 (98%)	2 (2%)	0	100	100
40	Bv	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
41	Bw	67/74 (90%)	66 (98%)	1 (2%)	0	100	100
42	Bx	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
43	By	131/134 (98%)	126 (96%)	5 (4%)	0	100	100
44	HS	98/106 (92%)	83 (85%)	12 (12%)	3 (3%)	3	12
All	All	6164/6692 (92%)	5908 (96%)	247 (4%)	9 (0%)	49	77

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	BW	46	VAL
15	BW	133	ARG
22	Bd	35	ALA
44	HS	56	ASN
44	HS	80	ASP
44	HS	98	GLU

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Mol	Chain	Res	Type
7	BO	155	CYS
9	BQ	223	PHE
23	Be	159	VAL

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	B0	84/93 (90%)	83 (99%)	1 (1%)	63	87
2	B1	74/75 (99%)	72 (97%)	2 (3%)	39	74
6	BN	188/192 (98%)	186 (99%)	2 (1%)	65	87
7	BO	318/326 (98%)	314 (99%)	4 (1%)	61	86
8	BP	293/294 (100%)	289 (99%)	4 (1%)	59	85
9	BQ	235/241 (98%)	233 (99%)	2 (1%)	70	89
10	BR	132/155 (85%)	130 (98%)	2 (2%)	57	84
11	BS	198/213 (93%)	195 (98%)	3 (2%)	57	84
12	BT	182/212 (86%)	180 (99%)	2 (1%)	65	87
13	BU	149/168 (89%)	148 (99%)	1 (1%)	76	91
14	BV	177/187 (95%)	177 (100%)	0	100	100
15	BW	141/146 (97%)	138 (98%)	3 (2%)	47	79
16	BX	166/167 (99%)	160 (96%)	6 (4%)	31	66
17	BY	110/113 (97%)	105 (96%)	5 (4%)	24	58
18	BZ	175/176 (99%)	173 (99%)	2 (1%)	65	87
19	Ba	159/160 (99%)	158 (99%)	1 (1%)	78	92
20	Bb	124/149 (83%)	123 (99%)	1 (1%)	73	90
21	Bc	157/158 (99%)	156 (99%)	1 (1%)	78	92
22	Bd	136/163 (83%)	134 (98%)	2 (2%)	57	84
23	Be	151/154 (98%)	146 (97%)	5 (3%)	33	69
24	Bf	138/139 (99%)	131 (95%)	7 (5%)	21	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	Bg	86/103 (84%)	86 (100%)	0	100	100
26	Bh	103/107 (96%)	100 (97%)	3 (3%)	37	73
27	Bi	57/121 (47%)	55 (96%)	2 (4%)	32	67
28	Bj	105/122 (86%)	102 (97%)	3 (3%)	37	73
29	Bk	110/111 (99%)	107 (97%)	3 (3%)	39	74
30	Bl	114/115 (99%)	110 (96%)	4 (4%)	32	67
31	Bm	122/123 (99%)	120 (98%)	2 (2%)	55	83
32	Bn	50/51 (98%)	49 (98%)	1 (2%)	48	80
33	Bo	75/87 (86%)	75 (100%)	0	100	100
34	Bp	94/102 (92%)	93 (99%)	1 (1%)	65	87
35	Bq	100/107 (94%)	100 (100%)	0	100	100
36	Br	91/94 (97%)	88 (97%)	3 (3%)	33	69
37	Bs	91/96 (95%)	90 (99%)	1 (1%)	65	87
38	Bt	106/107 (99%)	104 (98%)	2 (2%)	50	81
39	Bu	81/84 (96%)	78 (96%)	3 (4%)	30	65
40	Bv	68/71 (96%)	66 (97%)	2 (3%)	37	73
41	Bw	63/66 (96%)	63 (100%)	0	100	100
42	Bx	46/47 (98%)	45 (98%)	1 (2%)	45	78
43	By	112/113 (99%)	110 (98%)	2 (2%)	51	82
44	HS	92/97 (95%)	90 (98%)	2 (2%)	45	78
All	All	5253/5605 (94%)	5162 (98%)	91 (2%)	52	83

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B0	59	HIS
2	B1	5	THR
2	B1	71	TRP
6	BN	44	VAL
6	BN	174	ILE
7	BO	71	GLU
7	BO	113	GLU
7	BO	252	ILE
7	BO	336	LEU
8	BP	39	SER

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Mol	Chain	Res	Type
8	BP	84	THR
8	BP	213	GLU
8	BP	261	ASP
9	BQ	60	VAL
9	BQ	123	THR
10	BR	48	LEU
10	BR	156	ASP
11	BS	154	GLU
11	BS	164	VAL
11	BS	185	SER
12	BT	57	ARG
12	BT	128	LYS
13	BU	132	VAL
15	BW	91	LEU
15	BW	114	ILE
15	BW	151	THR
16	BX	45	LYS
16	BX	52	GLU
16	BX	93	ILE
16	BX	103	ASN
16	BX	161	GLU
16	BX	162	GLU
17	BY	56	VAL
17	BY	82	ASP
17	BY	84	CYS
17	BY	96	LEU
17	BY	105	LEU
18	BZ	10	LEU
18	BZ	117	ASN
19	Ba	6	LYS
20	Bb	49	ASP
21	Bc	84	ILE
22	Bd	37	SER
22	Bd	50	VAL
23	Be	3	LEU
23	Be	60	ILE
23	Be	82	SER
23	Be	86	THR
23	Be	87	HIS
24	Bf	3	HIS
24	Bf	21	GLU
24	Bf	71	SER

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Mol	Chain	Res	Type
24	Bf	96	VAL
24	Bf	103	GLN
24	Bf	104	ASP
24	Bf	141	VAL
26	Bh	40	SER
26	Bh	79	ILE
26	Bh	108	LYS
27	Bi	1	MET
27	Bi	59	HIS
28	Bj	68	SER
28	Bj	123	VAL
28	Bj	132	LEU
29	Bk	41	GLN
29	Bk	56	THR
29	Bk	117	LEU
30	Bl	29	ILE
30	Bl	33	SER
30	Bl	95	LEU
30	Bl	100	THR
31	Bm	86	THR
31	Bm	144	VAL
32	Bn	56	GLN
34	Bp	85	SER
36	Br	28	THR
36	Br	64	LYS
36	Br	103	LEU
37	Bs	105	LEU
38	Bt	35	ILE
38	Bt	115	LEU
39	Bu	16	THR
39	Bu	73	LYS
39	Bu	87	GLU
40	Bv	46	SER
40	Bv	65	SER
42	Bx	38	ASN
43	By	35	VAL
43	By	65	VAL
44	HS	86	LYS
44	HS	98	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	B0	27	GLN
6	BN	64	ASN
6	BN	193	ASN
6	BN	216	GLN
7	BO	226	ASN
7	BO	277	GLN
7	BO	319	ASN
8	BP	60	HIS
8	BP	112	HIS
8	BP	118	ASN
8	BP	245	HIS
8	BP	316	GLN
8	BP	344	ASN
9	BQ	63	GLN
10	BR	75	GLN
10	BR	186	ASN
11	BS	29	GLN
11	BS	120	ASN
11	BS	208	ASN
11	BS	242	HIS
12	BT	41	GLN
12	BT	191	HIS
12	BT	192	GLN
13	BU	100	ASN
14	BV	14	ASN
14	BV	162	GLN
15	BW	43	GLN
15	BW	109	HIS
15	BW	152	HIS
15	BW	155	ASN
16	BX	8	GLN
16	BX	19	GLN
16	BX	37	GLN
16	BX	174	ASN
17	BY	123	GLN
18	BZ	32	GLN
18	BZ	57	GLN
18	BZ	87	GLN
19	Ba	47	HIS
19	Ba	97	GLN
19	Ba	116	GLN
20	Bb	54	HIS
20	Bb	72	GLN

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Mol	Chain	Res	Type
20	Bb	97	ASN
20	Bb	120	ASN
20	Bb	125	GLN
22	Bd	39	GLN
23	Be	48	ASN
23	Be	87	HIS
24	Bf	3	HIS
24	Bf	54	HIS
26	Bh	134	ASN
28	Bj	136	ASN
31	Bm	44	HIS
31	Bm	125	GLN
32	Bn	11	ASN
32	Bn	12	GLN
32	Bn	19	ASN
32	Bn	43	GLN
34	Bp	50	GLN
35	Bq	17	HIS
35	Bq	75	ASN
37	Bs	29	ASN
37	Bs	67	HIS
37	Bs	83	ASN
38	Bt	15	ASN
38	Bt	25	GLN
38	Bt	61	ASN
38	Bt	84	GLN
39	Bu	61	ASN
40	Bv	13	ASN
40	Bv	76	ASN
42	Bx	36	HIS
43	By	127	GLN
44	HS	69	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	B2	3132/3498 (89%)	618 (19%)	20 (0%)
4	B3	118/246 (47%)	16 (13%)	1 (0%)
5	B4	156/165 (94%)	30 (19%)	1 (0%)
All	All	3406/3909 (87%)	664 (19%)	22 (0%)

All (664) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	B2	40	A
3	B2	43	A
3	B2	49	A
3	B2	59	G
3	B2	60	A
3	B2	65	A
3	B2	66	A
3	B2	92	G
3	B2	105	G
3	B2	109	A
3	B2	110	G
3	B2	116	A
3	B2	118	U
3	B2	121	A
3	B2	122	A
3	B2	162	A
3	B2	163	A
3	B2	167	G
3	B2	170	G
3	B2	172	U
3	B2	174	U
3	B2	175	G
3	B2	180	U
3	B2	183	A
3	B2	184	C
3	B2	185	G
3	B2	187	U
3	B2	188	C
3	B2	189	G
3	B2	190	G
3	B2	191	U
3	B2	192	C
3	B2	193	U
3	B2	194	A
3	B2	197	U
3	B2	198	U
3	B2	207	C
3	B2	217	G
3	B2	220	A
3	B2	225	G
3	B2	226	A
3	B2	239	U
3	B2	241	G

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Mol	Chain	Res	Type
3	B2	246	U
3	B2	247	U
3	B2	248	G
3	B2	249	G
3	B2	250	A
3	B2	251	U
3	B2	252	A
3	B2	254	G
3	B2	256	C
3	B2	257	A
3	B2	258	U
3	B2	259	A
3	B2	260	U
3	B2	263	A
3	B2	277	G
3	B2	291	G
3	B2	292	A
3	B2	303	A
3	B2	313	U
3	B2	331	A
3	B2	337	U
3	B2	347	C
3	B2	359	A
3	B2	360	A
3	B2	383	A
3	B2	384	G
3	B2	399	A
3	B2	406	U
3	B2	407	A
3	B2	411	C
3	B2	412	G
3	B2	429	G
3	B2	430	A
3	B2	437	G
3	B2	444	A
3	B2	446	U
3	B2	447	C
3	B2	448	U
3	B2	506	G
3	B2	507	U
3	B2	509	A
3	B2	510	G

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Mol	Chain	Res	Type
3	B2	532	A
3	B2	533	A
3	B2	540	A
3	B2	541	G
3	B2	545	A
3	B2	546	G
3	B2	547	G
3	B2	548	U
3	B2	549	G
3	B2	575	G
3	B2	577	U
3	B2	578	U
3	B2	579	A
3	B2	581	A
3	B2	582	G
3	B2	587	U
3	B2	588	G
3	B2	589	U
3	B2	590	U
3	B2	591	G
3	B2	592	U
3	B2	594	A
3	B2	602	A
3	B2	603	C
3	B2	613	A
3	B2	616	A
3	B2	624	U
3	B2	627	G
3	B2	628	U
3	B2	634	G
3	B2	636	A
3	B2	645	U
3	B2	646	A
3	B2	674	A
3	B2	702	A
3	B2	706	U
3	B2	708	U
3	B2	714	A
3	B2	715	U
3	B2	717	A
3	B2	732	A
3	B2	742	A

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Mol	Chain	Res	Type
3	B2	761	U
3	B2	762	U
3	B2	763	G
3	B2	764	U
3	B2	765	G
3	B2	766	G
3	B2	770	G
3	B2	786	C
3	B2	788	G
3	B2	804	A
3	B2	806	G
3	B2	809	U
3	B2	812	A
3	B2	813	G
3	B2	817	G
3	B2	838	A
3	B2	849	A
3	B2	862	A
3	B2	875	A
3	B2	889	G
3	B2	893	C
3	B2	906	U
3	B2	911	U
3	B2	928	A
3	B2	939	G
3	B2	940	G
3	B2	946	A
3	B2	948	G
3	B2	949	A
3	B2	956	G
3	B2	969	G
3	B2	976	C
3	B2	991	C
3	B2	992	U
3	B2	993	C
3	B2	1009	C
3	B2	1011	G
3	B2	1012	A
3	B2	1033	G
3	B2	1034	A
3	B2	1047	C
3	B2	1049	U

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Mol	Chain	Res	Type
3	B2	1050	G
3	B2	1051	G
3	B2	1052	G
3	B2	1056	G
3	B2	1057	G
3	B2	1058	A
3	B2	1059	A
3	B2	1060	U
3	B2	1061	U
3	B2	1064	C
3	B2	1065	U
3	B2	1066	C
3	B2	1067	A
3	B2	1073	U
3	B2	1079	A
3	B2	1081	C
3	B2	1095	G
3	B2	1096	A
3	B2	1098	G
3	B2	1104	G
3	B2	1113	U
3	B2	1123	G
3	B2	1125	C
3	B2	1126	A
3	B2	1127	U
3	B2	1128	C
3	B2	1129	G
3	B2	1130	A
3	B2	1135	G
3	B2	1148	G
3	B2	1155	U
3	B2	1159	U
3	B2	1162	G
3	B2	1175	U
3	B2	1176	G
3	B2	1186	C
3	B2	1209	G
3	B2	1211	A
3	B2	1212	U
3	B2	1227	C
3	B2	1239	U
3	B2	1240	G

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Mol	Chain	Res	Type
3	B2	1245	U
3	B2	1252	A
3	B2	1253	G
3	B2	1266	U
3	B2	1267	G
3	B2	1268	G
3	B2	1270	C
3	B2	1272	U
3	B2	1273	G
3	B2	1275	A
3	B2	1276	A
3	B2	1277	G
3	B2	1279	C
3	B2	1287	G
3	B2	1293	G
3	B2	1294	A
3	B2	1295	G
3	B2	1296	U
3	B2	1297	G
3	B2	1300	U
3	B2	1305	A
3	B2	1310	C
3	B2	1311	C
3	B2	1313	G
3	B2	1314	C
3	B2	1316	G
3	B2	1317	A
3	B2	1318	A
3	B2	1319	U
3	B2	1333	A
3	B2	1334	A
3	B2	1338	G
3	B2	1340	U
3	B2	1344	G
3	B2	1361	A
3	B2	1379	U
3	B2	1380	A
3	B2	1388	G
3	B2	1390	A
3	B2	1420	U
3	B2	1433	U
3	B2	1434	G

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Mol	Chain	Res	Type
3	B2	1451	G
3	B2	1453	A
3	B2	1468	G
3	B2	1471	C
3	B2	1484	G
3	B2	1530	C
3	B2	1542	C
3	B2	1557	U
3	B2	1570	G
3	B2	1588	A
3	B2	1589	U
3	B2	1590	G
3	B2	1593	A
3	B2	1594	G
3	B2	1595	U
3	B2	1596	U
3	B2	1598	C
3	B2	1600	C
3	B2	1606	U
3	B2	1607	U
3	B2	1608	C
3	B2	1611	G
3	B2	1613	C
3	B2	1614	U
3	B2	1615	C
3	B2	1616	C
3	B2	1617	U
3	B2	1618	A
3	B2	1622	A
3	B2	1624	A
3	B2	1628	A
3	B2	1640	A
3	B2	1657	U
3	B2	1664	A
3	B2	1665	A
3	B2	1674	C
3	B2	1677	A
3	B2	1678	A
3	B2	1679	A
3	B2	1680	U
3	B2	1682	A
3	B2	1692	C

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Mol	Chain	Res	Type
3	B2	1718	C
3	B2	1741	U
3	B2	1742	G
3	B2	1745	C
3	B2	1746	U
3	B2	1755	A
3	B2	1764	U
3	B2	1765	C
3	B2	1781	G
3	B2	1790	A
3	B2	1791	G
3	B2	1800	G
3	B2	1802	C
3	B2	1806	U
3	B2	1807	G
3	B2	1811	A
3	B2	1816	G
3	B2	1819	G
3	B2	1821	G
3	B2	1837	G
3	B2	1838	A
3	B2	1849	G
3	B2	1869	C
3	B2	1870	U
3	B2	1871	U
3	B2	1872	G
3	B2	1873	U
3	B2	1875	U
3	B2	1876	U
3	B2	1877	C
3	B2	1894	A
3	B2	1897	A
3	B2	1901	C
3	B2	1904	C
3	B2	1905	A
3	B2	1933	G
3	B2	1934	A
3	B2	1935	U
3	B2	1941	A
3	B2	1961	G
3	B2	1962	C
3	B2	2005	U

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Mol	Chain	Res	Type
3	B2	2187	A
3	B2	2188	A
3	B2	2190	U
3	B2	2200	U
3	B2	2201	A
3	B2	2209	G
3	B2	2210	G
3	B2	2219	A
3	B2	2230	A
3	B2	2232	A
3	B2	2246	A
3	B2	2257	G
3	B2	2294	G
3	B2	2295	A
3	B2	2297	U
3	B2	2298	G
3	B2	2300	C
3	B2	2301	A
3	B2	2306	G
3	B2	2308	A
3	B2	2311	A
3	B2	2316	A
3	B2	2321	A
3	B2	2322	G
3	B2	2323	C
3	B2	2324	G
3	B2	2325	C
3	B2	2328	G
3	B2	2329	U
3	B2	2331	A
3	B2	2332	A
3	B2	2337	G
3	B2	2341	G
3	B2	2343	A
3	B2	2344	A
3	B2	2346	U
3	B2	2347	A
3	B2	2348	U
3	B2	2349	G
3	B2	2350	A
3	B2	2353	C
3	B2	2355	C

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Mol	Chain	Res	Type
3	B2	2360	G
3	B2	2361	G
3	B2	2362	U
3	B2	2367	A
3	B2	2369	A
3	B2	2372	C
3	B2	2376	G
3	B2	2386	U
3	B2	2395	G
3	B2	2398	U
3	B2	2401	A
3	B2	2403	G
3	B2	2422	U
3	B2	2423	G
3	B2	2424	U
3	B2	2461	A
3	B2	2462	C
3	B2	2463	G
3	B2	2481	G
3	B2	2482	G
3	B2	2485	A
3	B2	2489	A
3	B2	2490	A
3	B2	2491	G
3	B2	2492	A
3	B2	2499	U
3	B2	2507	A
3	B2	2521	U
3	B2	2522	U
3	B2	2523	G
3	B2	2524	U
3	B2	2525	G
3	B2	2606	U
3	B2	2607	A
3	B2	2608	C
3	B2	2610	U
3	B2	2611	A
3	B2	2619	A
3	B2	2620	A
3	B2	2622	C
3	B2	2627	U
3	B2	2632	A

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Mol	Chain	Res	Type
3	B2	2634	U
3	B2	2635	U
3	B2	2636	A
3	B2	2638	U
3	B2	2644	U
3	B2	2645	A
3	B2	2648	C
3	B2	2649	U
3	B2	2656	A
3	B2	2660	U
3	B2	2661	U
3	B2	2662	U
3	B2	2663	C
3	B2	2664	U
3	B2	2665	U
3	B2	2666	C
3	B2	2667	G
3	B2	2668	C
3	B2	2669	G
3	B2	2670	A
3	B2	2680	C
3	B2	2688	A
3	B2	2701	G
3	B2	2702	G
3	B2	2709	G
3	B2	2721	A
3	B2	2730	A
3	B2	2743	G
3	B2	2747	U
3	B2	2751	A
3	B2	2752	A
3	B2	2768	A
3	B2	2769	A
3	B2	2771	A
3	B2	2772	G
3	B2	2773	A
3	B2	2774	A
3	B2	2775	A
3	B2	2776	U
3	B2	2784	A
3	B2	2786	A
3	B2	2789	A

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Mol	Chain	Res	Type
3	B2	2799	A
3	B2	2809	G
3	B2	2823	G
3	B2	2824	U
3	B2	2848	G
3	B2	2850	C
3	B2	2868	C
3	B2	2872	G
3	B2	2873	A
3	B2	2889	G
3	B2	2891	G
3	B2	2895	G
3	B2	2896	A
3	B2	2898	A
3	B2	2899	A
3	B2	2903	A
3	B2	2905	C
3	B2	2912	A
3	B2	2913	U
3	B2	2918	G
3	B2	2925	G
3	B2	2933	A
3	B2	2934	G
3	B2	2937	U
3	B2	2938	U
3	B2	2940	A
3	B2	2955	U
3	B2	2957	U
3	B2	2962	C
3	B2	2966	G
3	B2	2971	C
3	B2	2982	A
3	B2	2984	C
3	B2	2992	A
3	B2	2993	G
3	B2	2994	C
3	B2	2996	G
3	B2	2997	A
3	B2	3001	C
3	B2	3002	G
3	B2	3003	G
3	B2	3018	U

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Mol	Chain	Res	Type
3	B2	3030	U
3	B2	3031	A
3	B2	3036	A
3	B2	3050	U
3	B2	3051	A
3	B2	3066	A
3	B2	3067	G
3	B2	3078	C
3	B2	3091	G
3	B2	3093	G
3	B2	3108	A
3	B2	3117	A
3	B2	3155	G
3	B2	3174	A
3	B2	3176	G
3	B2	3182	G
3	B2	3189	C
3	B2	3195	C
3	B2	3197	G
3	B2	3200	U
3	B2	3216	C
3	B2	3218	A
3	B2	3226	A
3	B2	3227	U
3	B2	3238	A
3	B2	3239	A
3	B2	3248	U
3	B2	3249	U
3	B2	3250	U
3	B2	3254	G
3	B2	3260	A
3	B2	3261	U
3	B2	3265	U
3	B2	3266	U
3	B2	3268	U
3	B2	3269	A
3	B2	3275	A
3	B2	3276	A
3	B2	3281	A
3	B2	3282	G
3	B2	3283	A
3	B2	3284	G

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Mol	Chain	Res	Type
3	B2	3285	G
3	B2	3286	U
3	B2	3287	A
3	B2	3288	G
3	B2	3289	G
3	B2	3290	A
3	B2	3291	C
3	B2	3294	G
3	B2	3295	U
3	B2	3296	U
3	B2	3297	C
3	B2	3298	C
3	B2	3299	U
3	B2	3300	A
3	B2	3301	C
3	B2	3302	U
3	B2	3305	C
3	B2	3306	C
3	B2	3307	U
3	B2	3308	G
3	B2	3317	A
3	B2	3318	A
3	B2	3319	G
3	B2	3322	G
3	B2	3326	G
3	B2	3327	A
3	B2	3329	G
3	B2	3338	A
3	B2	3345	G
3	B2	3347	G
3	B2	3352	A
3	B2	3355	G
3	B2	3359	U
3	B2	3360	G
3	B2	3363	C
3	B2	3365	U
3	B2	3371	U
3	B2	3372	C
3	B2	3373	C
3	B2	3374	A
3	B2	3375	U
3	B2	3376	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B2	3385	G
3	B2	3386	U
3	B2	3387	G
3	B2	3388	C
3	B2	3390	G
3	B2	3391	A
3	B2	3392	A
3	B2	3394	C
3	B2	3395	G
3	B2	3404	G
3	B2	3405	C
3	B2	3418	U
3	B2	3419	G
3	B2	3420	U
3	B2	3442	U
3	B2	3443	A
3	B2	3446	G
3	B2	3450	C
3	B2	3453	U
3	B2	3455	U
3	B2	3456	U
3	B2	3457	G
3	B2	3468	C
3	B2	3476	A
3	B2	3479	C
3	B2	3483	U
3	B2	3484	G
3	B2	3491	A
3	B2	3498	U
4	B3	7	G
4	B3	12	U
4	B3	13	A
4	B3	22	A
4	B3	33	U
4	B3	35	C
4	B3	53	U
4	B3	54	A
4	B3	55	A
4	B3	63	A
4	B3	64	G
4	B3	75	G
4	B3	100	A

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Mol	Chain	Res	Type
4	B3	110	G
4	B3	116	G
4	B3	119	U
5	B4	31	U
5	B4	42	U
5	B4	43	C
5	B4	47	G
5	B4	59	G
5	B4	60	A
5	B4	67	A
5	B4	70	C
5	B4	71	G
5	B4	85	A
5	B4	88	A
5	B4	89	U
5	B4	90	U
5	B4	91	C
5	B4	92	C
5	B4	93	G
5	B4	95	G
5	B4	98	U
5	B4	103	G
5	B4	112	A
5	B4	114	C
5	B4	119	A
5	B4	121	U
5	B4	124	G
5	B4	132	G
5	B4	133	U
5	B4	134	U
5	B4	135	C
5	B4	164	U
5	B4	165	U

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	B2	290	G
3	B2	382	A
3	B2	948	G
3	B2	1094	A
3	B2	1103	U

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Mol	Chain	Res	Type
3	B2	1269	C
3	B2	1272	U
3	B2	1868	C
3	B2	1876	U
3	B2	2347	A
3	B2	2867	C
3	B2	2993	G
3	B2	3001	C
3	B2	3217	U
3	B2	3260	A
3	B2	3286	U
3	B2	3298	C
3	B2	3328	U
3	B2	3373	C
3	B2	3418	U
4	B3	12	U
5	B4	88	A

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 3 ligands modelled in this entry, 3 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

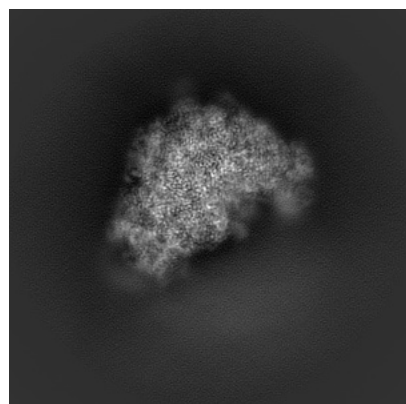
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71645. These allow visual inspection of the internal detail of the map and identification of artifacts.

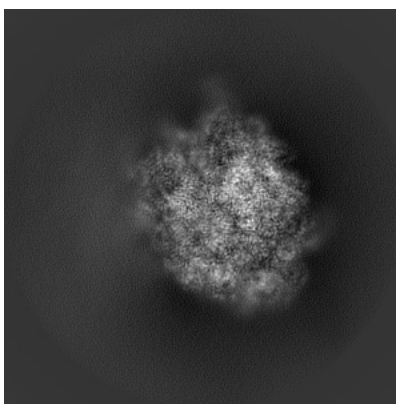
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

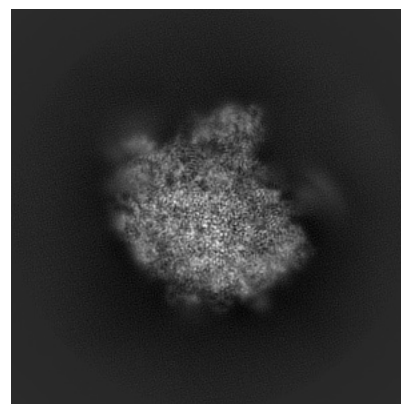
6.1.1 Primary map



X

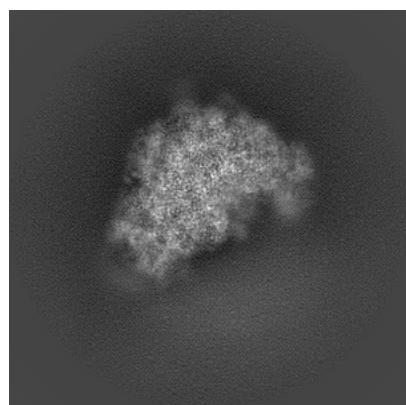


Y

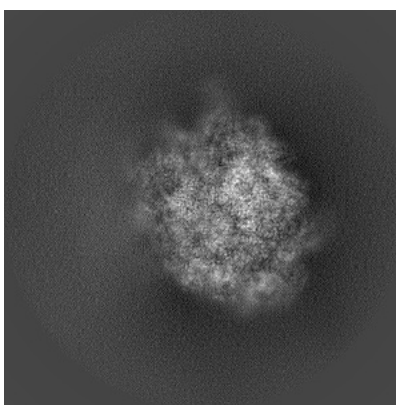


Z

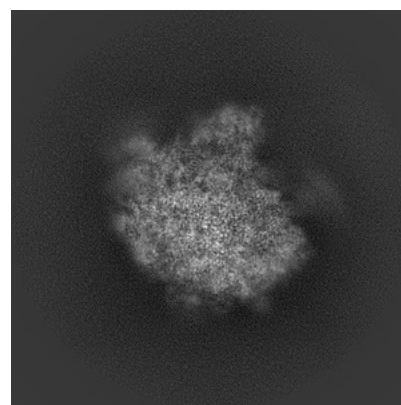
6.1.2 Raw map



X



Y

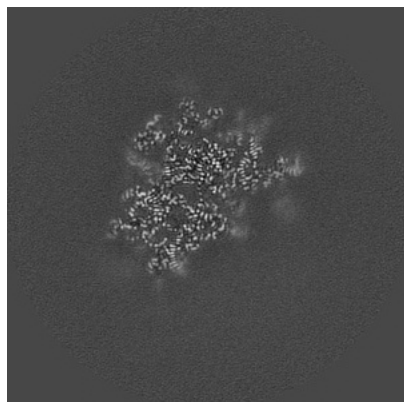


Z

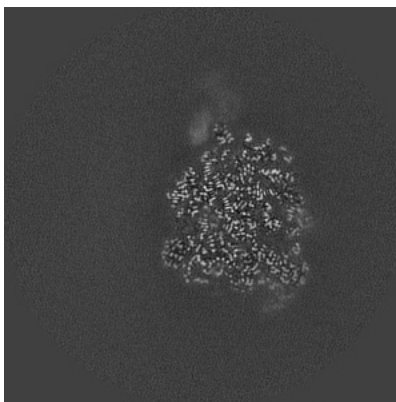
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

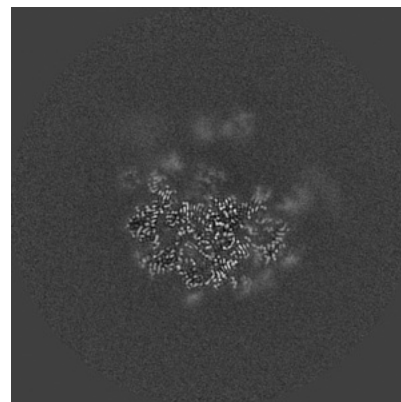
6.2.1 Primary map



X Index: 256

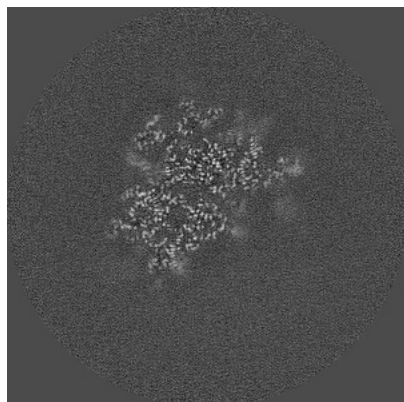


Y Index: 256

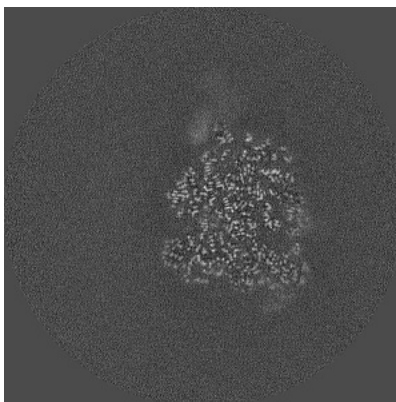


Z Index: 256

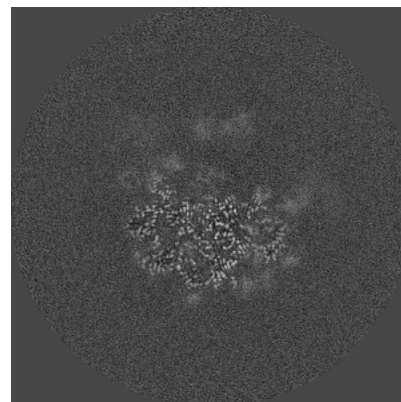
6.2.2 Raw map



X Index: 256



Y Index: 256

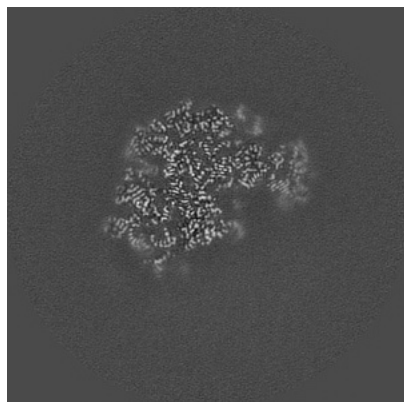


Z Index: 256

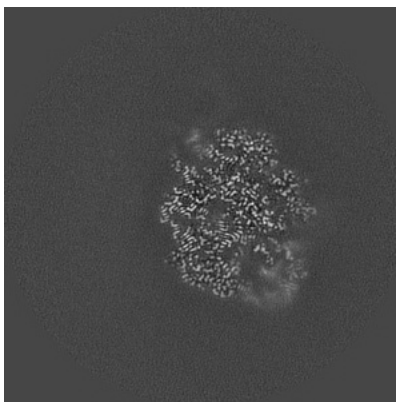
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

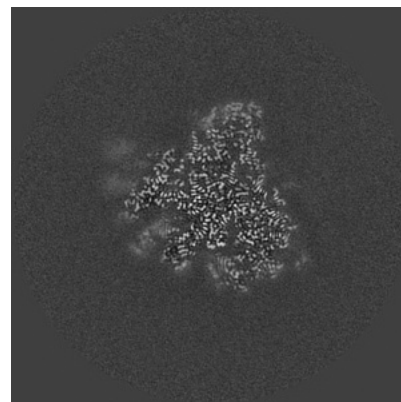
6.3.1 Primary map



X Index: 271

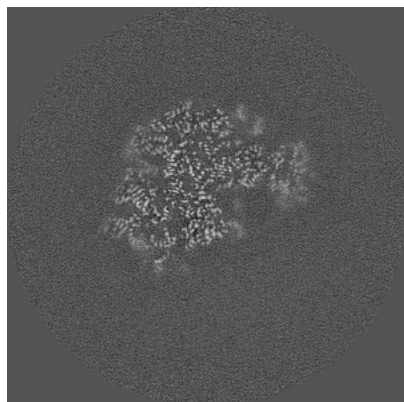


Y Index: 241

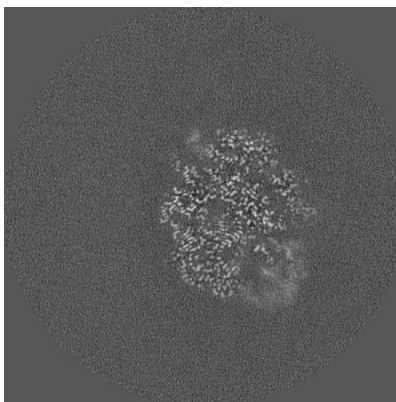


Z Index: 306

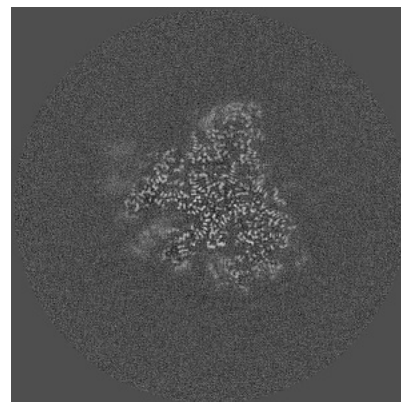
6.3.2 Raw map



X Index: 271



Y Index: 241

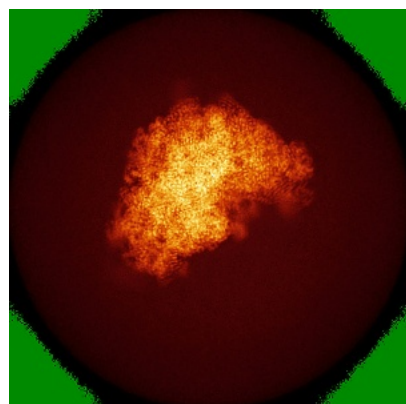


Z Index: 306

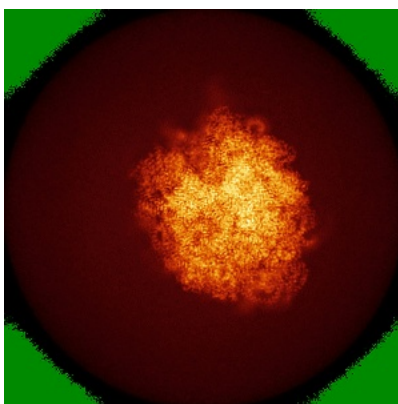
The images above show the largest variance slices of the map in three orthogonal directions.

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

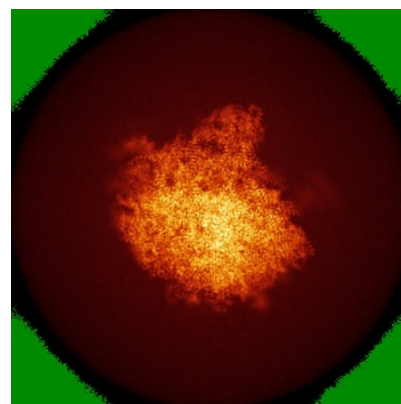
6.4.1 Primary map



X

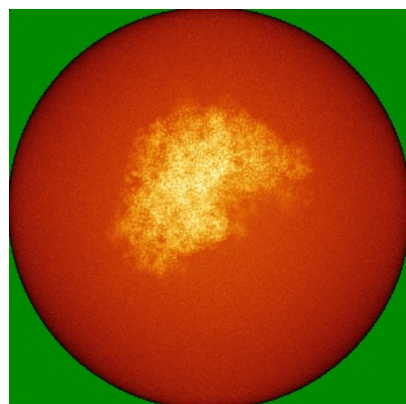


Y

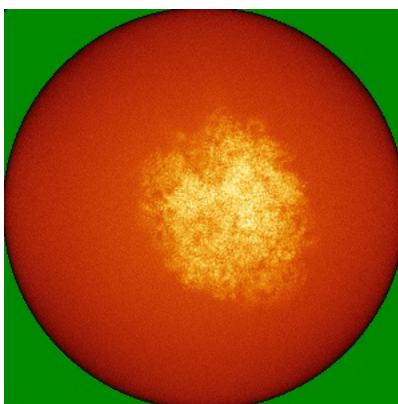


Z

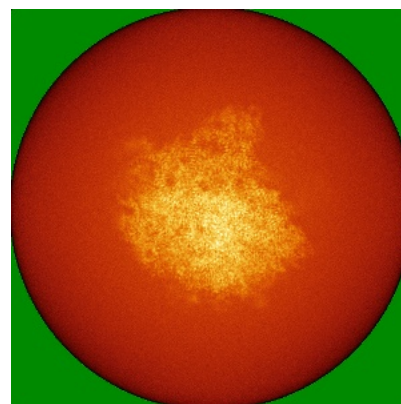
6.4.2 Raw map



X



Y

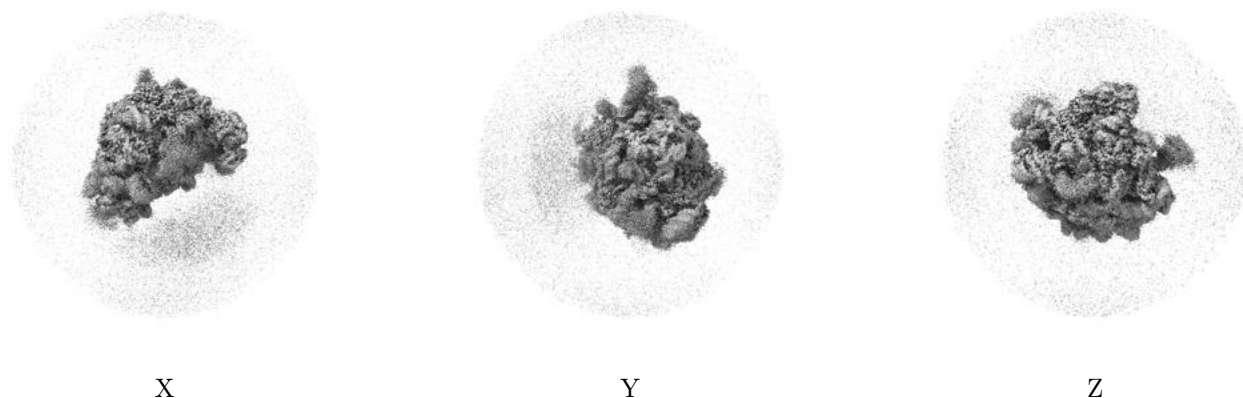


Z

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.

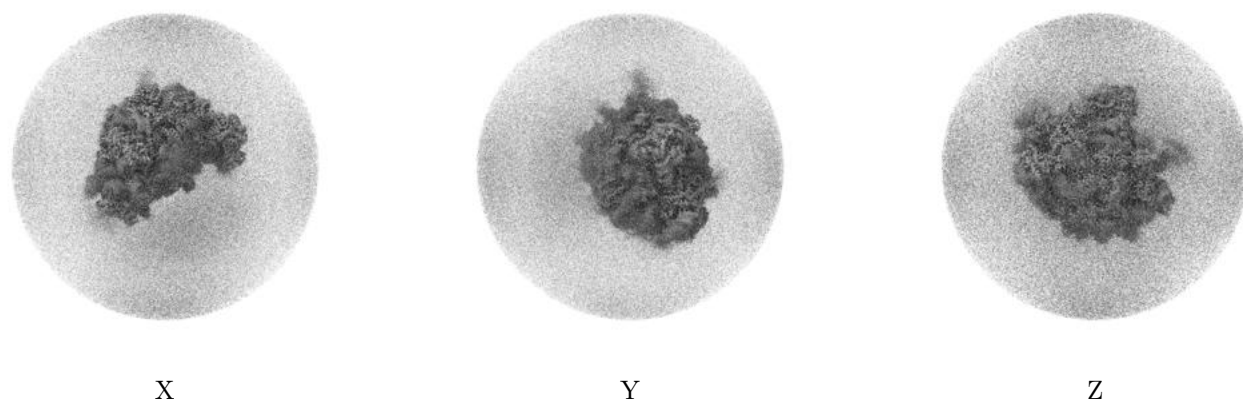
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.002. 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.

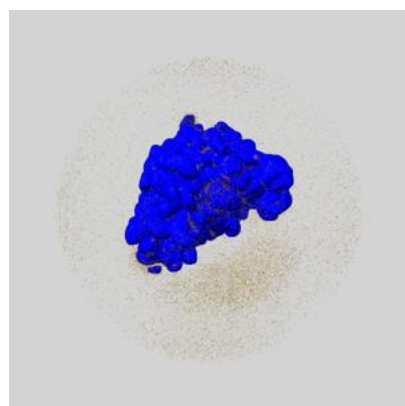
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

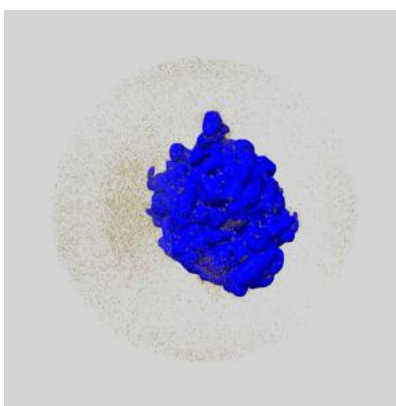
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

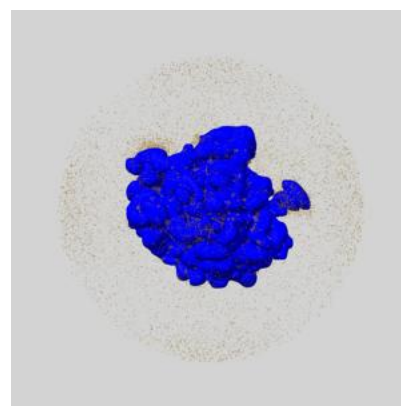
6.6.1 emd_71645_msk_1.map [i](#)



X



Y

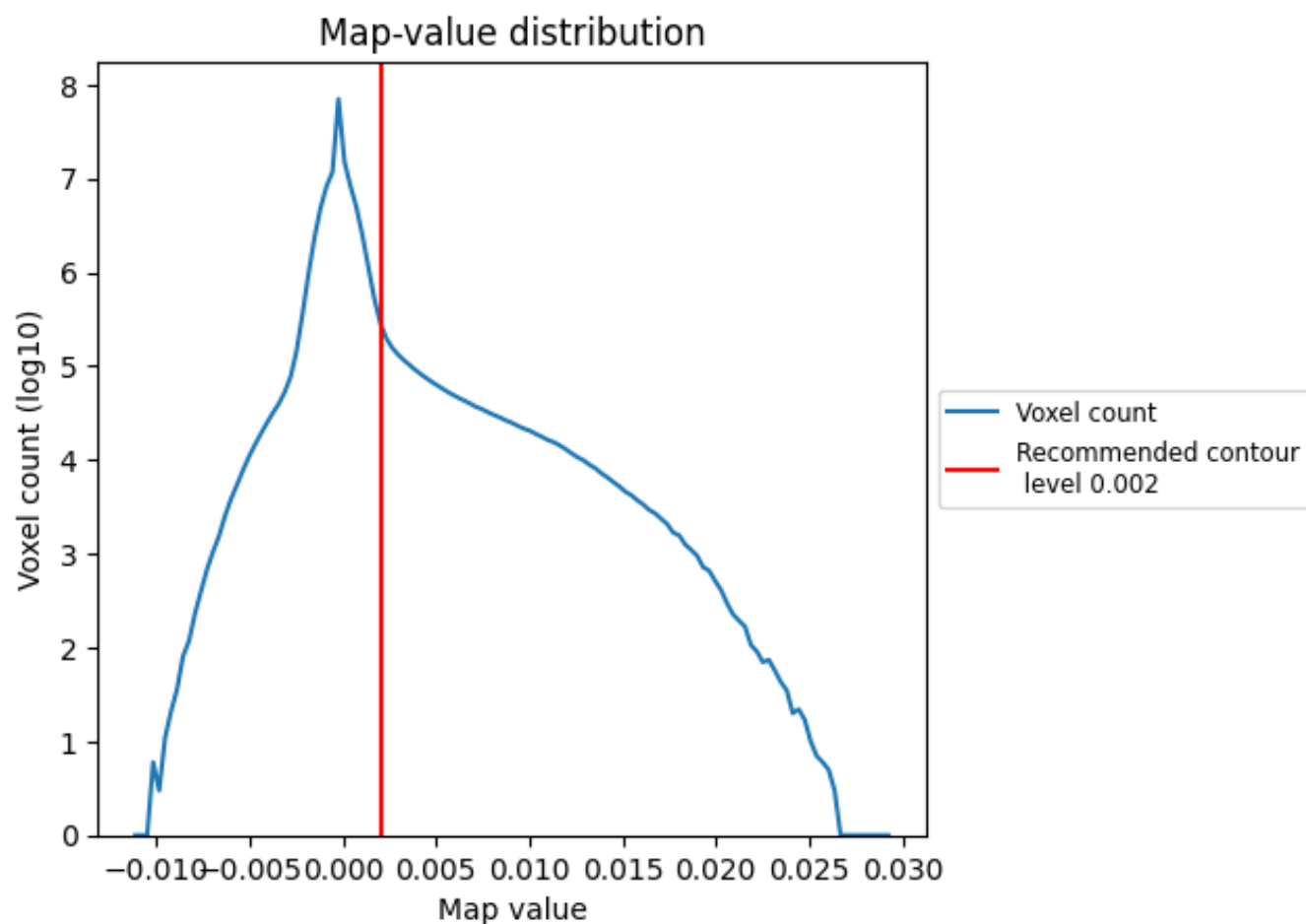


Z

7 Map analysis [i](#)

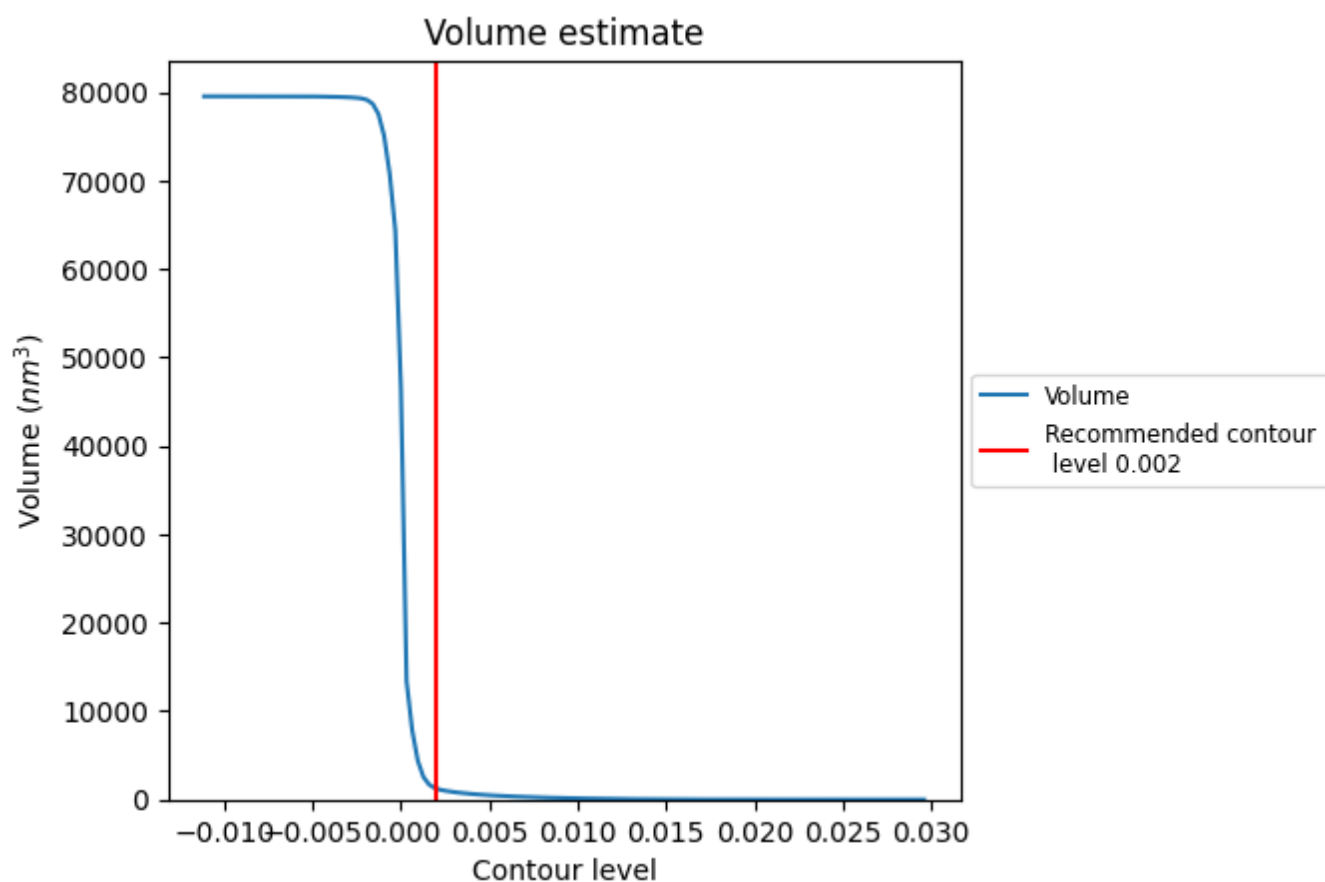
This section contains the results of statistical analysis of the map.

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.

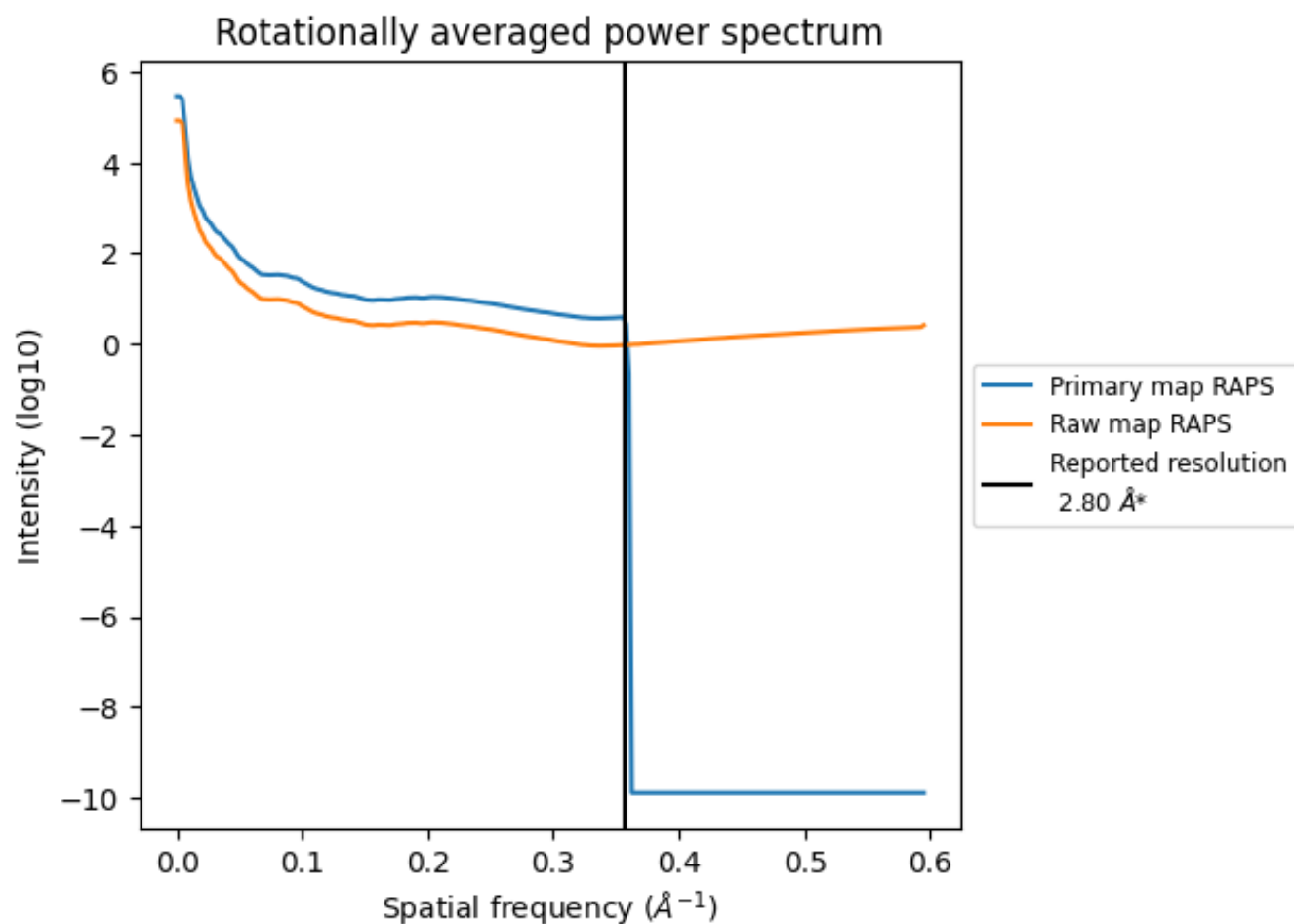
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1250 nm^3 ; this corresponds to an approximate mass of 1129 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

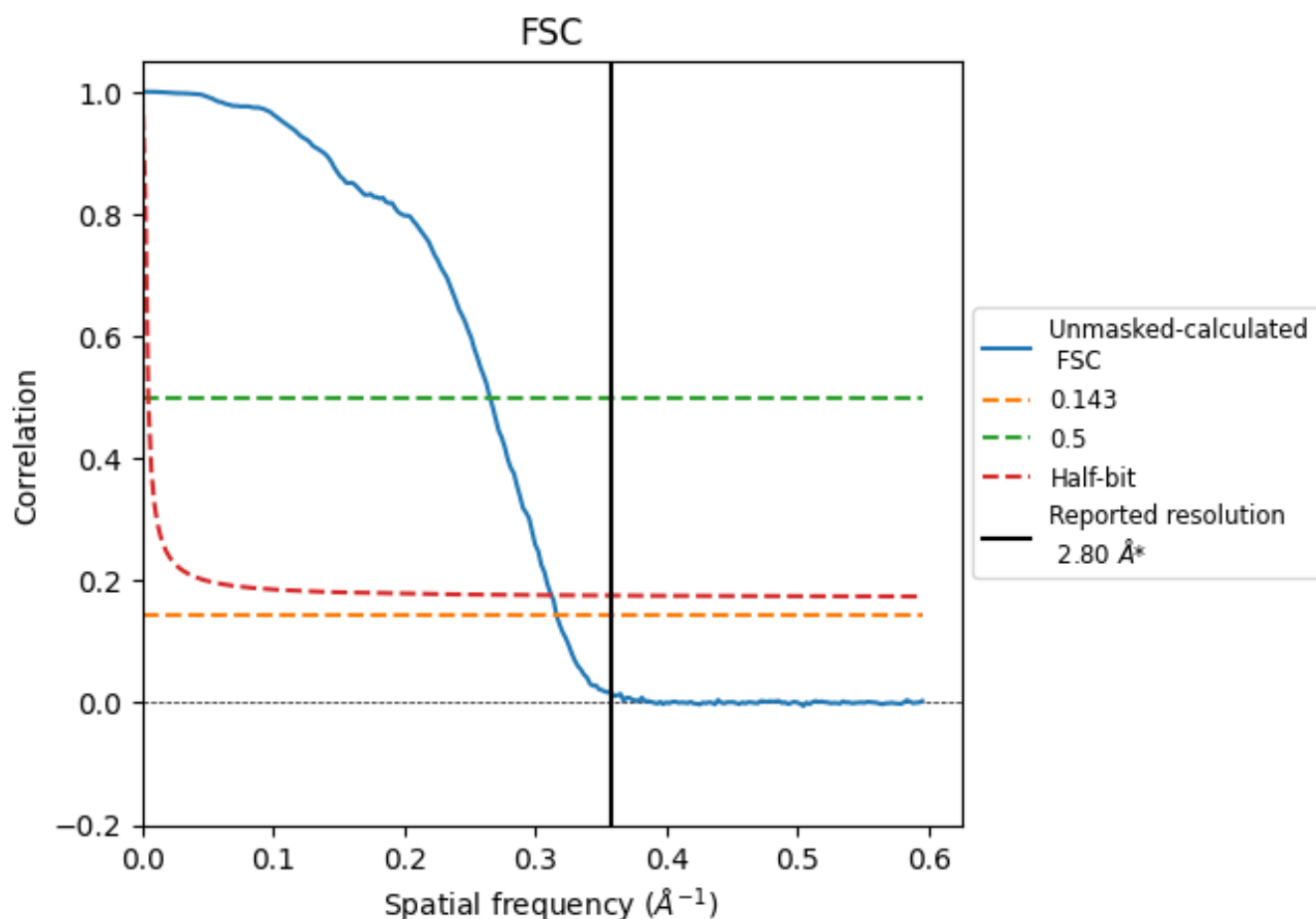


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

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 0.357 \AA^{-1}

8.2 Resolution estimates [i](#)

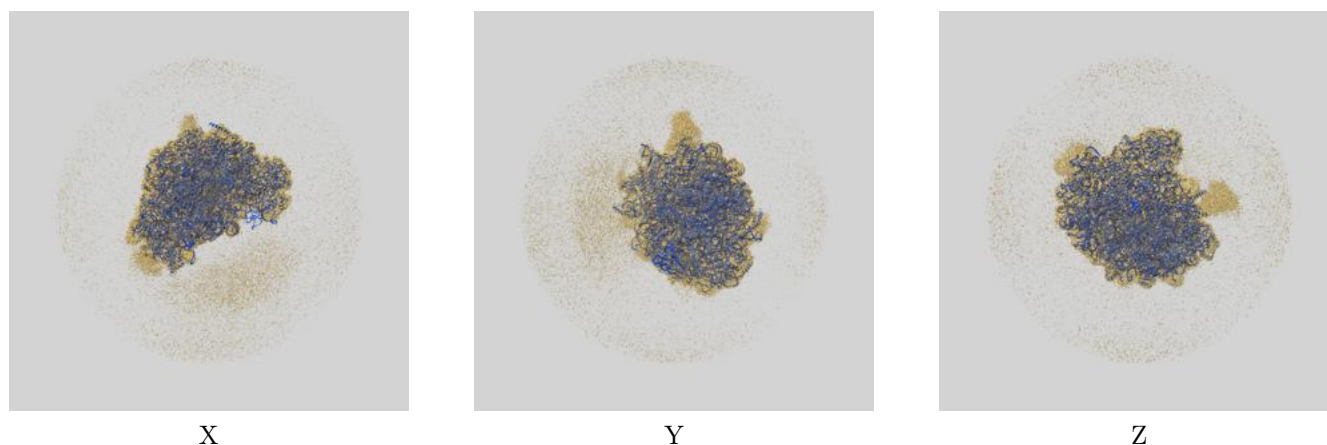
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.16	3.77	3.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.16 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

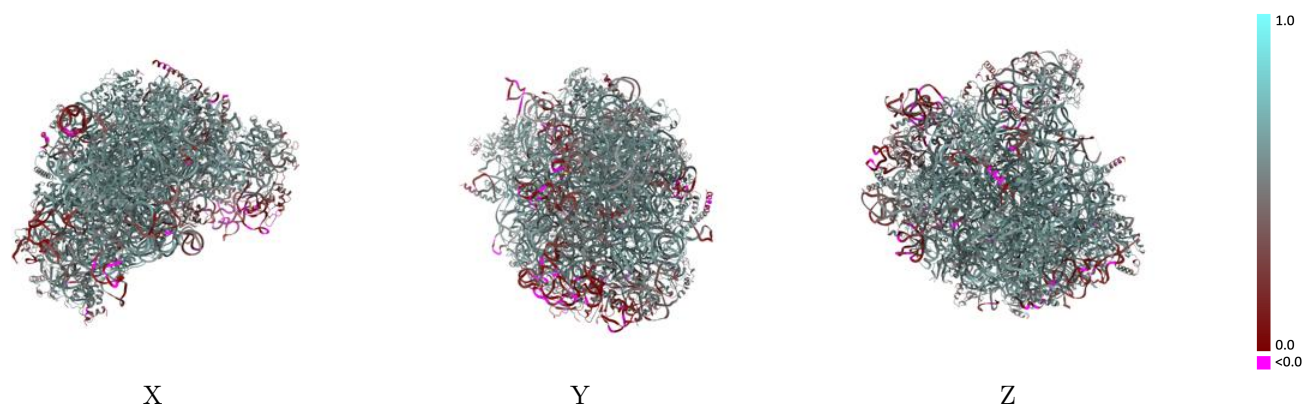
This section contains information regarding the fit between EMDB map EMD-71645 and PDB model 9PHC. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.002 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](#)



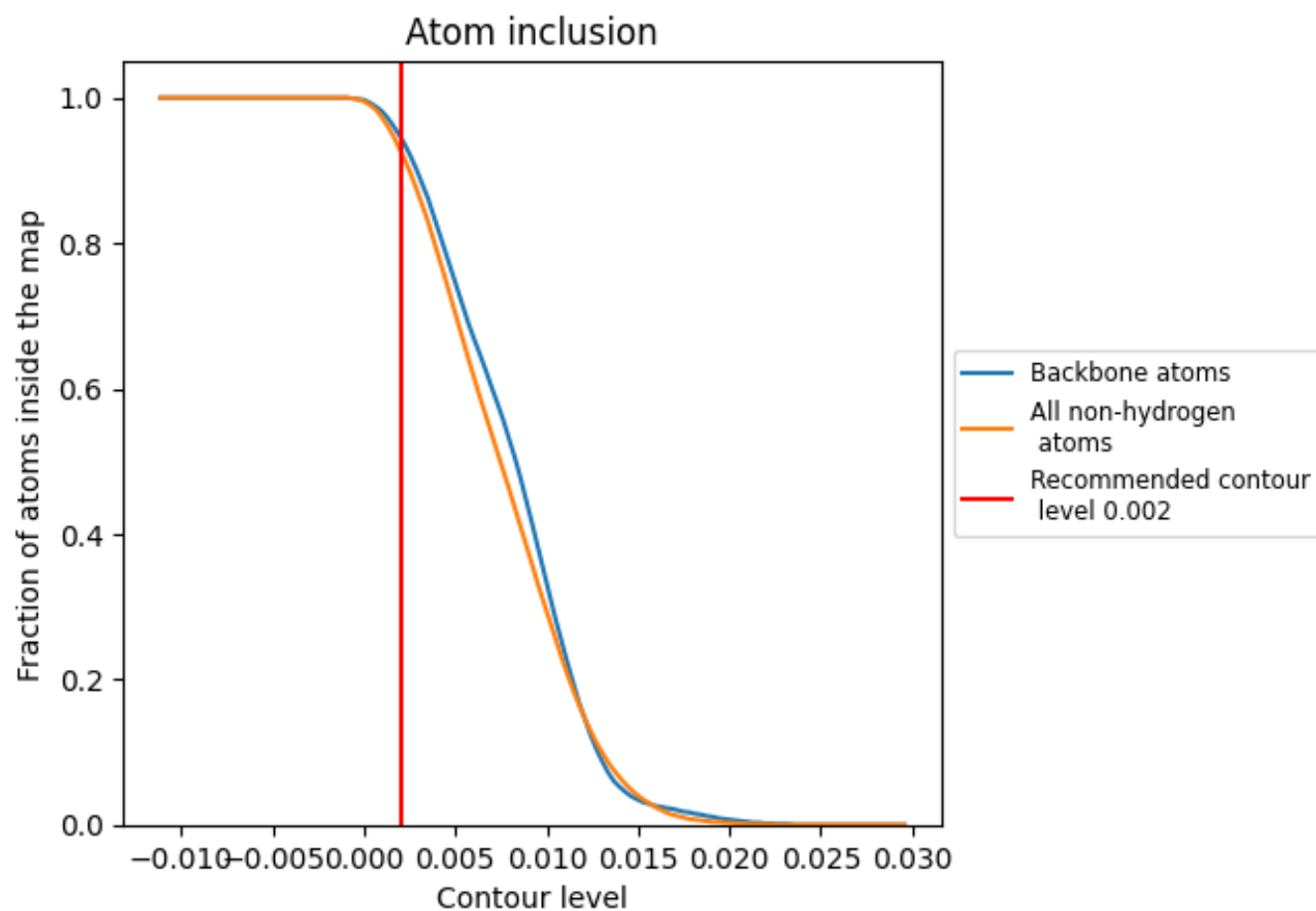
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.002).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.002) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9270	 0.5320
B0	 0.8650	 0.5290
B1	 0.9460	 0.5710
B2	 0.9380	 0.5230
B3	 0.9840	 0.5530
B4	 0.9660	 0.5520
BN	 0.9720	 0.6110
BO	 0.9710	 0.5980
BP	 0.9730	 0.6020
BQ	 0.8890	 0.4920
BR	 0.8570	 0.4950
BS	 0.8920	 0.5600
BT	 0.9250	 0.5450
BU	 0.6160	 0.2690
BV	 0.7830	 0.4690
BW	 0.6460	 0.2700
BX	 0.9280	 0.5720
BY	 0.9360	 0.5280
BZ	 0.9880	 0.6230
Ba	 0.9710	 0.5890
Bb	 0.9290	 0.5800
Bc	 0.9620	 0.6010
Bd	 0.9060	 0.5470
Be	 0.9320	 0.5720
Bf	 0.8920	 0.5360
Bg	 0.7650	 0.3960
Bh	 0.9590	 0.5820
Bi	 0.9190	 0.5460
Bj	 0.9630	 0.5770
Bk	 0.9640	 0.5760
Bl	 0.9240	 0.5140
Bm	 0.9740	 0.6120
Bn	 0.9310	 0.5720
Bo	 0.8570	 0.4890
Bp	 0.9440	 0.5700



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Chain	Atom inclusion	Q-score
Bq	 0.9700	 0.6060
Br	 0.9730	 0.6040
Bs	 0.9660	 0.5990
Bt	 0.9530	 0.5720
Bu	 0.9450	 0.5670
Bv	 0.9840	 0.6180
Bw	 0.9010	 0.4840
Bx	 0.8100	 0.4910
By	 0.9060	 0.5460
HS	 0.5540	 0.3290