



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:46 AM UTC

PDB ID : 8OIQ / pdb_00008oiq
EMDB ID : EMD-16896
Title : 39S mammalian mitochondrial large ribosomal subunit with mtRF1 and P-site tRNA
Authors : Saurer, M.; Leibundgut, M.; Scaiola, A.; Schoenhut, T.; Ban, N.
Deposited on : 2023-03-23
Resolution : 3.50 Å (reported)
Based on initial models : ., 7QI4, 7NQH

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:

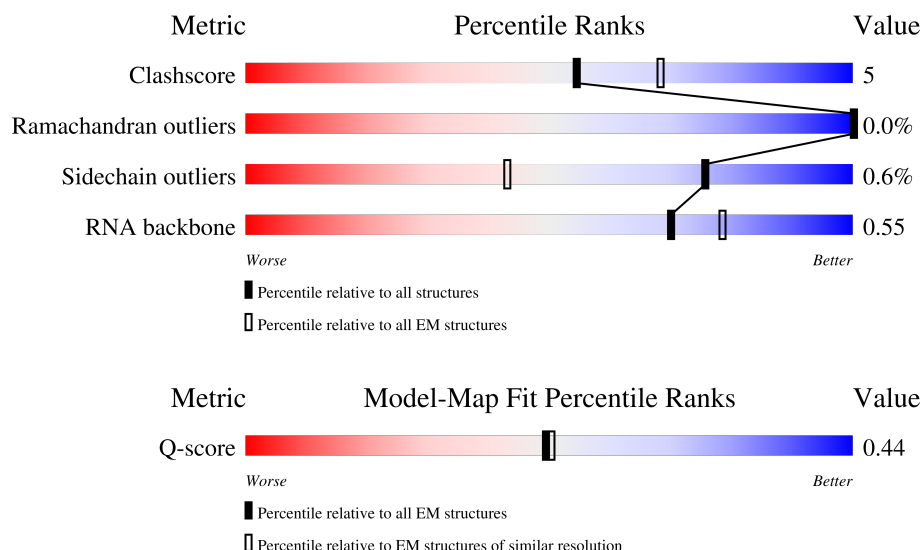
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	B1	198	22% 21% 77%
1	B2	198	14% 12% 86%
1	B3	198	14% 12% 86%

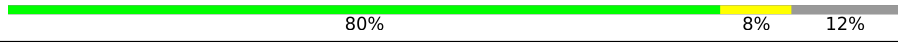
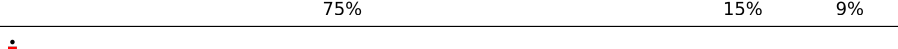
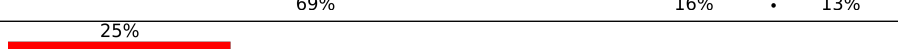
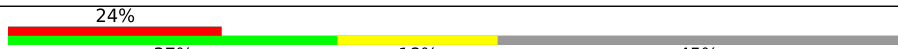
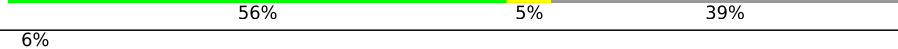
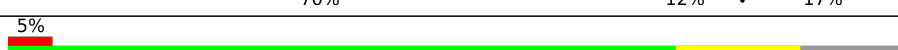
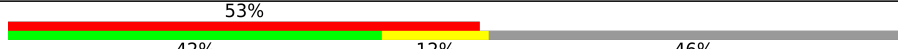
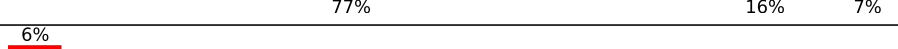
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Mol	Chain	Length	Quality of chain
1	B4	198	
1	B5	198	
1	B6	198	
2	B7	3	
3	B8	1571	
4	B9	73	
5	BA	210	
6	BB	150	
7	BC	216	
8	BD	148	
9	BE	256	
10	BF	250	
11	BG	161	
12	BH	207	
13	BI	65	
14	BJ	95	
15	BK	188	
16	BL	306	
17	BM	399	
18	BN	294	
19	BO	268	
20	BP	257	
21	BQ	192	
22	BR	197	
23	BS	325	

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Mol	Chain	Length	Quality of chain
24	BT	296	
25	BU	251	
26	BV	169	
27	BW	188	
28	BX	303	
29	BY	149	
30	BZ	209	
31	Ba	160	
32	Bb	112	
33	Bc	138	
34	Bd	126	
35	Be	102	
36	Bf	205	
37	Bg	222	
38	Bh	196	
39	Bi	433	
40	Bj	304	
41	Bl	100	
42	Bm	423	
43	Bn	380	
44	Bo	334	
45	Bp	162	
46	Bq	135	
47	Br	142	
48	Bs	159	

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Mol	Chain	Length	Quality of chain
49	Bt	332	
50	Bu	306	
51	Bv	279	
52	Bw	269	
53	Bx	166	
54	By	198	
55	Bz	128	
56	AG	71	
57	Aa	474	

2 Entry composition [i](#)

There are 63 unique types of molecules in this entry. The entry contains 112981 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 Mitochondrial ribosomal protein L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	B1	45	Total	C	N	O	0	0
			317	203	52	62		
1	B2	27	Total	C	N	O	0	0
			213	137	33	43		
1	B3	28	Total	C	N	O	0	0
			222	143	35	44		
1	B4	27	Total	C	N	O	0	0
			213	137	33	43		
1	B5	27	Total	C	N	O	0	0
			213	137	33	43		
1	B6	26	Total	C	N	O	0	0
			205	131	32	42		

- Molecule 2 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B7	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 3 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B8	1571	Total	C	N	O	P	0	0
			33427	15015	6087	10754	1571		

- Molecule 4 is a RNA chain called CP Phe-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	B9	73	Total	C	N	O	P	S	0	0
			1560	703	283	500	73	1		

- Molecule 5 is a protein called Large ribosomal subunit protein uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BA	166	Total	C	N	O	S	0	0
			1374	876	258	234	6		

- Molecule 6 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BB	149	Total	C	N	O	S	0	0
			1184	754	227	201	2		

- Molecule 7 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BC	206	Total	C	N	O	S	0	0
			1678	1056	308	309	5		

- Molecule 8 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BD	112	Total	C	N	O	S	0	0
			867	558	158	148	3		

- Molecule 9 is a protein called Mitochondrial ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BE	244	Total	C	N	O	S	0	0
			2036	1315	363	353	5		

- Molecule 10 is a protein called Mitochondrial ribosomal protein L47.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BF	179	Total	C	N	O	S	0	0
			1548	992	290	260	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BG	118	Total	C	N	O	S	0	0
			968	622	178	165	3		

- Molecule 12 is a protein called Mitochondrial ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BH	110	Total	C	N	O	S	0	0
			902	553	181	162	6		

- Molecule 13 is a protein called Large ribosomal subunit protein bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BI	52	Total	C	N	O	S	0	0
			425	274	78	71	2		

- Molecule 14 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BJ	46	Total	C	N	O	S	0	0
			387	239	89	58	1		

- Molecule 15 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BK	95	Total	C	N	O	S	0	0
			833	539	163	129	2		

- Molecule 16 is a protein called Mitochondrial ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BL	240	Total	C	N	O	S	0	0
			1860	1160	371	319	10		

- Molecule 17 is a protein called ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BM	307	Total	C	N	O	S	0	0
			2420	1554	426	430	10		

- Molecule 18 is a protein called Mitochondrial ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BN	250	Total	C	N	O	S	1	0
			2019	1299	370	344	6		

- Molecule 19 is a protein called Mitochondrial ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BO	202	Total	C	N	O	S	0	0
			1660	1059	311	286	4		

- Molecule 20 is a protein called Mitochondrial ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BP	212	Total	C	N	O	S	0	0
			1705	1100	306	290	9		

- Molecule 21 is a protein called Mitochondrial ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BQ	176	Total	C	N	O	S	0	0
			1339	851	243	243	2		

- Molecule 22 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BR	177	Total	C	N	O	S	0	0
			1447	928	258	254	7		

- Molecule 23 is a protein called Mitochondrial ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BS	115	Total	C	N	O	S	0	0
			896	562	176	154	4		

- Molecule 24 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BT	288	Total	C	N	O	S	0	0
			2312	1473	430	403	6		

- Molecule 25 is a protein called uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BU	222	Total	C	N	O	S	0	0
			1803	1156	331	306	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	237	HIS	TYR	conflict	UNP F1RI89

- Molecule 26 is a protein called bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BV	153	Total	C	N	O	S	0	0
			1240	777	236	222	5		

- Molecule 27 is a protein called Mitochondrial ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BW	143	Total	C	N	O	S	0	0
			1168	733	227	204	4		

- Molecule 28 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BX	225	Total	C	N	O	S	0	0
			1855	1187	321	338	9		

- Molecule 29 is a protein called Mitochondrial ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BY	140	Total	C	N	O	S	0	0
			1159	732	239	185	3		

- Molecule 30 is a protein called Mitochondrial ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BZ	155	Total	C	N	O	S	0	0
			1231	789	219	219	4		

- Molecule 31 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ba	97	Total	C	N	O	S	0	0
			772	481	148	141	2		

- Molecule 32 is a protein called Mitochondrial ribosomal protein L53.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bb	97	Total	C	N	O	S	0	0
			745	461	143	135	6		

- Molecule 33 is a protein called mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bc	84	Total	C	N	O	S	0	0
			716	458	128	127	3		

- Molecule 34 is a protein called Mitochondrial ribosomal protein L55.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bd	69	Total	C	N	O	S	0	0
			571	353	117	98	3		

- Molecule 35 is a protein called Mitochondrial ribosomal protein L57.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Be	94	Total	C	N	O	S	0	0
			780	485	168	126	1		

- Molecule 36 is a protein called mL62 (ICT1).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Bf	151	Total	C	N	O	S	0	0
			1198	738	233	222	5		

- Molecule 37 is a protein called mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bg	135	Total	C	N	O	S	0	0
			1131	692	223	211	5		

- Molecule 38 is a protein called Mitochondrial ribosomal protein S18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bh	162	Total	C	N	O	S	0	0
			1325	845	249	224	7		

- Molecule 39 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bi	387	Total	C	N	O	S	0	0
			3126	2011	548	555	12		

- Molecule 40 is a protein called 39S ribosomal protein L1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bj	164	Total	C	N	O	S	0	0
			1325	853	217	251	4		

- Molecule 41 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bl	38	Total	C	N	O	S	0	0
			335	214	70	47	4		

- Molecule 42 is a protein called Mitochondrial ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bm	393	Total	C	N	O	S	0	0
			3173	2040	556	565	12		

- Molecule 43 is a protein called Mitochondrial ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bn	354	Total	C	N	O	S	0	0
			2952	1876	542	525	9		

- Molecule 44 is a protein called Mitochondrial ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bo	295	Total	C	N	O	S	0	0
			2408	1541	410	441	16		

- Molecule 45 is a protein called Mitochondrial ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Bp	143	Total	C	N	O	S	0	0
			1202	757	217	227	1		

- Molecule 46 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Bq	122	Total	C	N	O	S	0	0
			972	628	168	173	3		

- Molecule 47 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Br	108	Total	C	N	O	S	0	0
			906	570	167	165	4		

- Molecule 48 is a protein called Large ribosomal subunit protein mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Bs	151	Total	C	N	O	S	0	0
			1185	738	227	217	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bs	2	ACE	-	acetylation	UNP F1S8U4

- Molecule 49 is a protein called mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Bt	289	Total	C	N	O	S	0	0
			2319	1486	399	426	8		

- Molecule 50 is a protein called Mitochondrial ribosomal protein L45.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Bu	260	Total	C	N	O	S	0	0
			2138	1370	379	379	10		

- Molecule 51 is a protein called Mitochondrial ribosomal protein L46.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Bv	238	Total	C	N	O	S	0	0
			1948	1240	338	363	7		

- Molecule 52 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Bw	165	Total	C	N	O	S	0	0
			1295	825	224	241	5		

- Molecule 53 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Bx	133	Total	C	N	O	S	0	0
			1097	709	192	194	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bx	59	ARG	LYS	conflict	UNP A0A287A0K2

- Molecule 54 is a protein called Mitochondrial ribosomal protein L50.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	By	109	Total	C	N	O	S	0	0
			893	568	160	162	3		

- Molecule 55 is a protein called Large ribosomal subunit protein mL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Bz	97	Total	C	N	O	S	0	0
			837	539	166	128	4		

- Molecule 56 is a RNA chain called P-site Met-tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AG	71	Total	C	N	O	P	0	0
			1502	673	264	494	71		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AG	69	C	-	insertion	GB 1208989970
AG	70	C	-	insertion	GB 1208989970
AG	71	A	-	insertion	GB 1208989970

- Molecule 57 is a protein called Peptide chain release factor 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Aa	381	Total	C	N	O	S	1	0
			3120	1943	572	592	13		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	446	GLY	-	expression tag	UNP O75570
Aa	447	GLY	-	expression tag	UNP O75570
Aa	448	SER	-	expression tag	UNP O75570
Aa	449	GLY	-	expression tag	UNP O75570
Aa	450	GLY	-	expression tag	UNP O75570
Aa	451	SER	-	expression tag	UNP O75570
Aa	452	GLY	-	expression tag	UNP O75570
Aa	453	ASP	-	expression tag	UNP O75570
Aa	454	TYR	-	expression tag	UNP O75570
Aa	455	LYS	-	expression tag	UNP O75570
Aa	456	ASP	-	expression tag	UNP O75570
Aa	457	HIS	-	expression tag	UNP O75570
Aa	458	ASP	-	expression tag	UNP O75570
Aa	459	GLY	-	expression tag	UNP O75570
Aa	460	ASP	-	expression tag	UNP O75570
Aa	461	TYR	-	expression tag	UNP O75570
Aa	462	LYS	-	expression tag	UNP O75570
Aa	463	ASP	-	expression tag	UNP O75570
Aa	464	HIS	-	expression tag	UNP O75570
Aa	465	ASP	-	expression tag	UNP O75570
Aa	466	ILE	-	expression tag	UNP O75570
Aa	467	ASP	-	expression tag	UNP O75570
Aa	468	TYR	-	expression tag	UNP O75570
Aa	469	LYS	-	expression tag	UNP O75570
Aa	470	ASP	-	expression tag	UNP O75570
Aa	471	ASP	-	expression tag	UNP O75570
Aa	472	ASP	-	expression tag	UNP O75570
Aa	473	ASP	-	expression tag	UNP O75570
Aa	474	LYS	-	expression tag	UNP O75570

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	B8	193	Total	Mg	0
			193	193	
58	B9	1	Total	Mg	0
			1	1	

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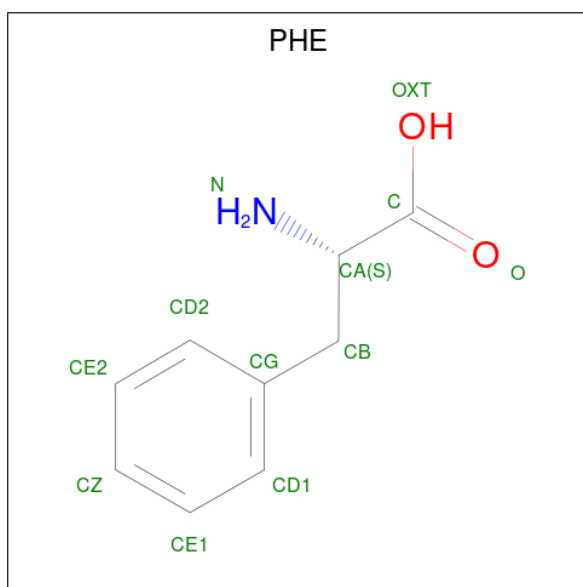
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Mol	Chain	Residues	Atoms		AltConf
58	BL	2	Total 2	Mg 2	0
58	BM	2	Total 2	Mg 2	0
58	BT	1	Total 1	Mg 1	0
58	BV	3	Total 3	Mg 3	0
58	Be	1	Total 1	Mg 1	0
58	Bq	1	Total 1	Mg 1	0
58	Bx	1	Total 1	Mg 1	0

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
59	B8	26	Total 26	K 26	0
59	BL	1	Total 1	K 1	0
59	BU	1	Total 1	K 1	0
59	BW	1	Total 1	K 1	0
59	Be	1	Total 1	K 1	0

- Molecule 60 is PHENYLALANINE (CCD ID: PHE) (formula: C₉H₁₁NO₂).

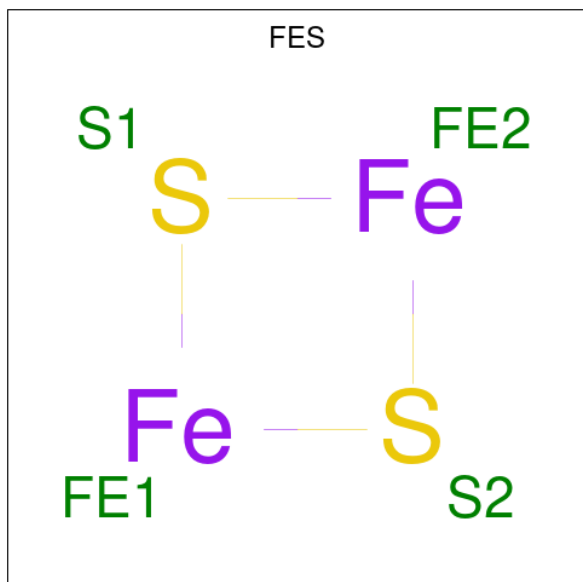


Mol	Chain	Residues	Atoms				AltConf
60	B9	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

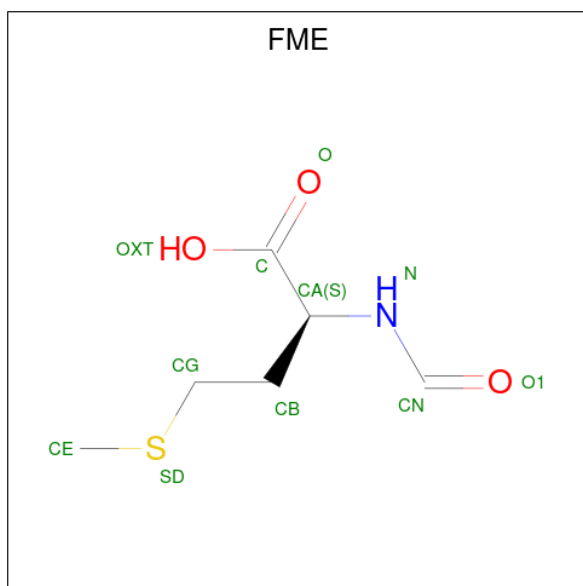
Mol	Chain	Residues	Atoms		AltConf
61	BH	1	Total	Zn	0
			1	1	
61	Bl	1	Total	Zn	0
			1	1	

- Molecule 62 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
62	Bh	1	Total	Fe	S	0
			4	2	2	

- Molecule 63 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).

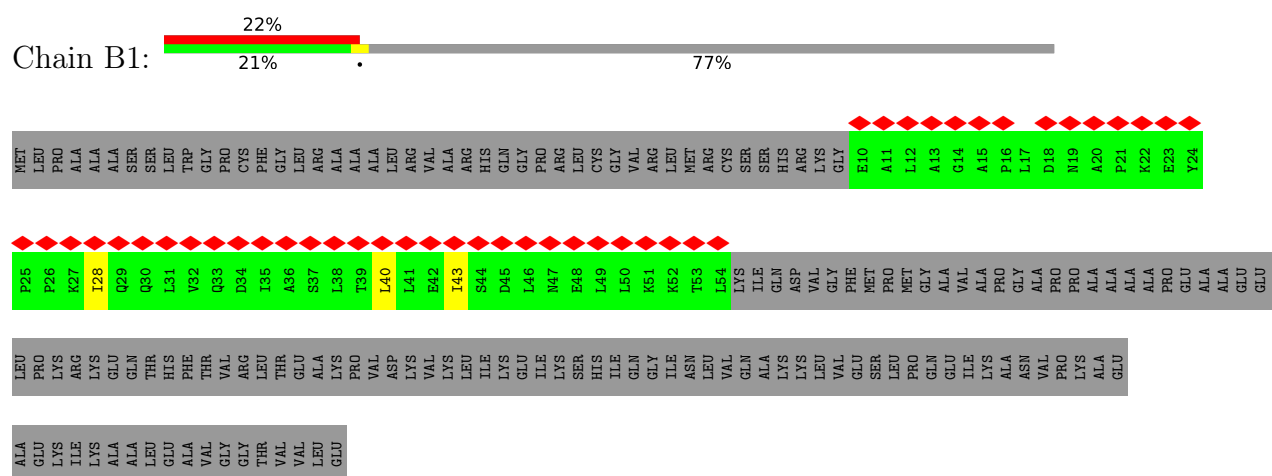


Mol	Chain	Residues	Atoms					AltConf
63	AG	1	Total	C	N	O	S	0
			10	6	1	2	1	

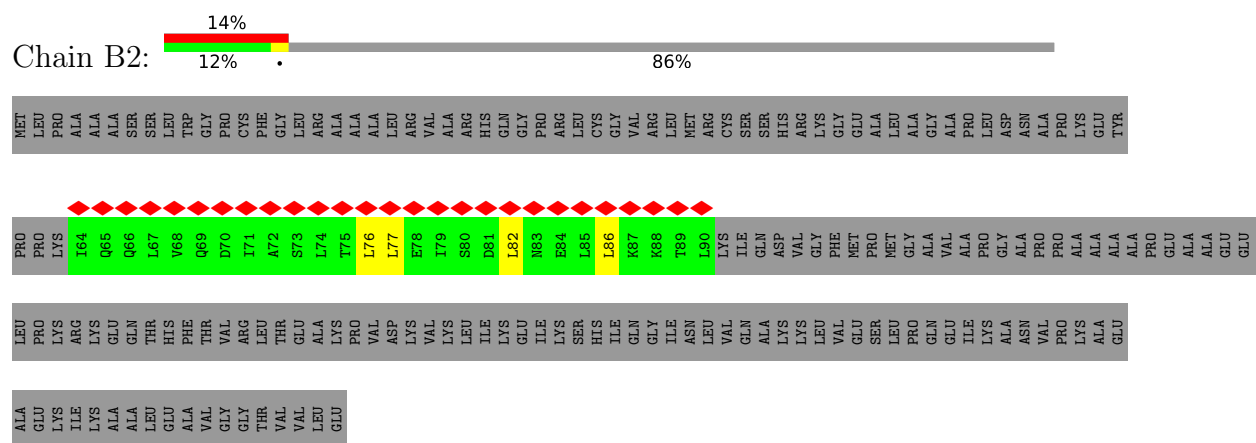
3 Residue-property plots

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

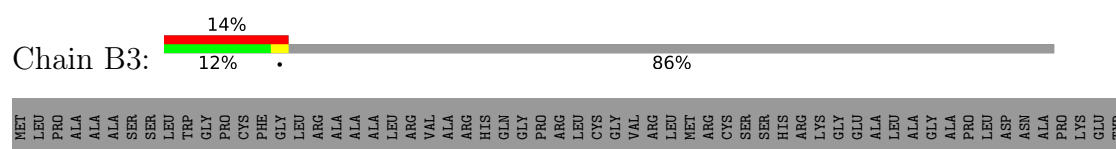
• Molecule 1: Mitochondrial ribosomal protein L12

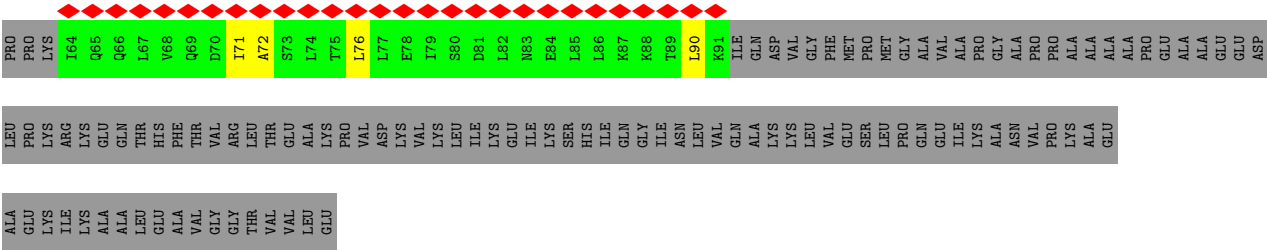


• Molecule 1: Mitochondrial ribosomal protein L12

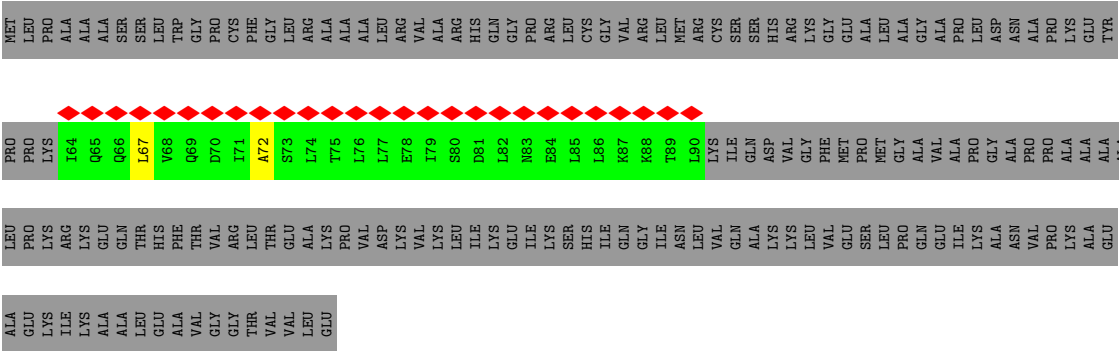


• Molecule 1: Mitochondrial ribosomal protein L12

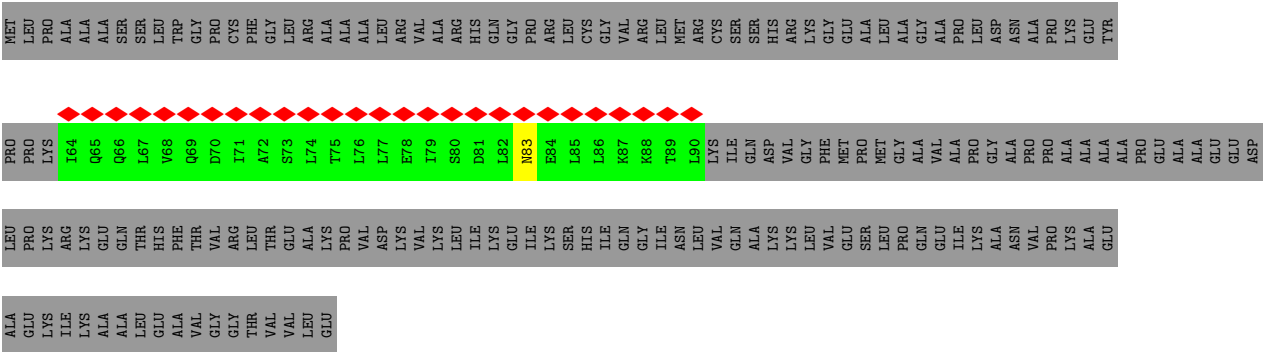




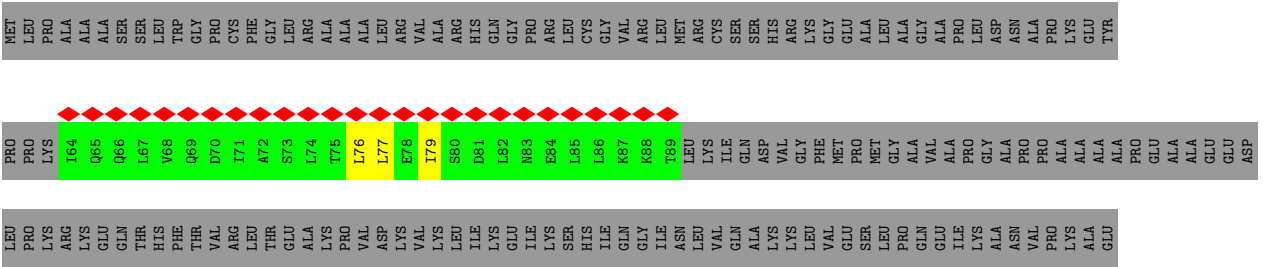
• Molecule 1: Mitochondrial ribosomal protein L12



• Molecule 1: Mitochondrial ribosomal protein L12



• Molecule 1: Mitochondrial ribosomal protein L12

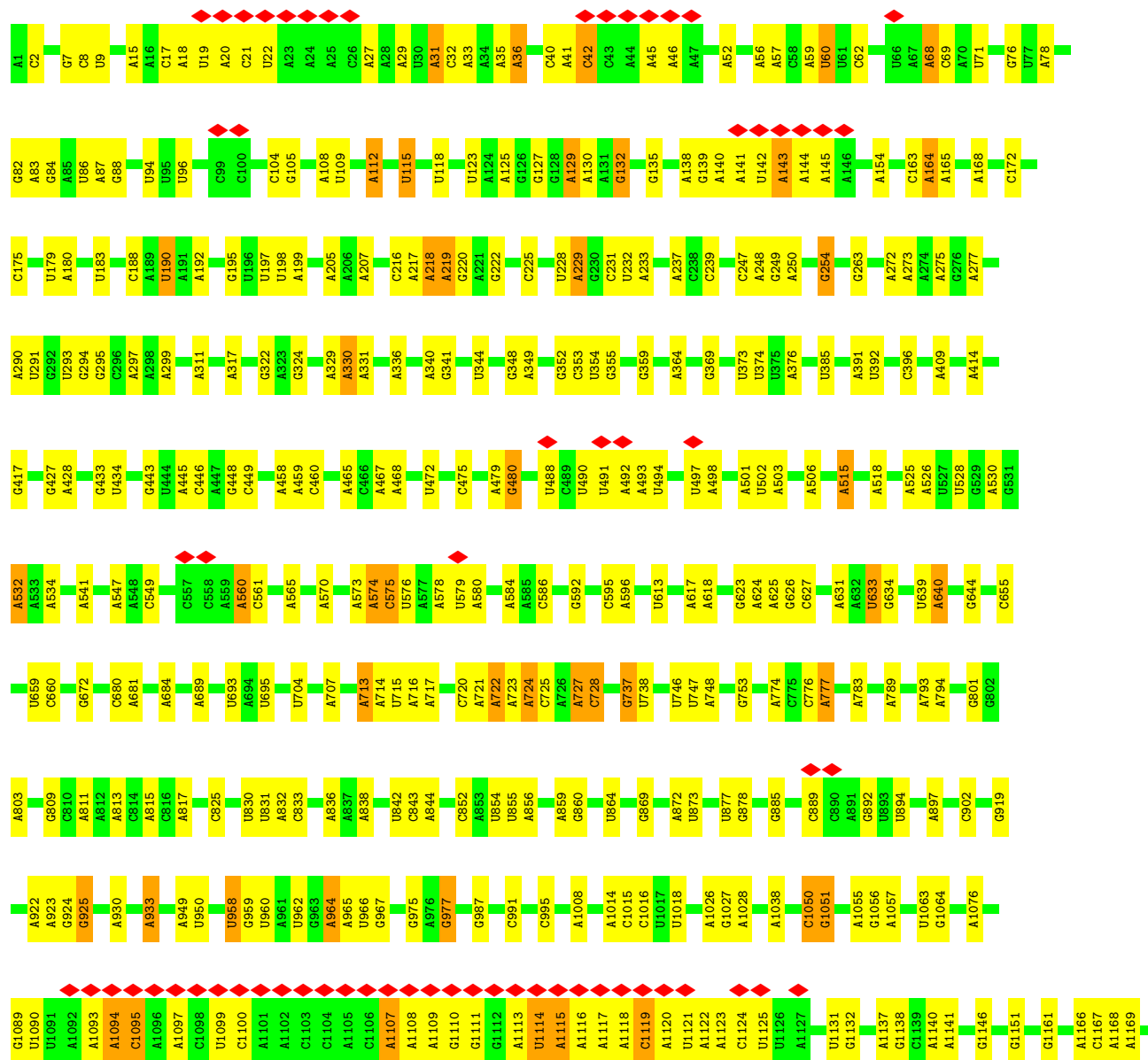


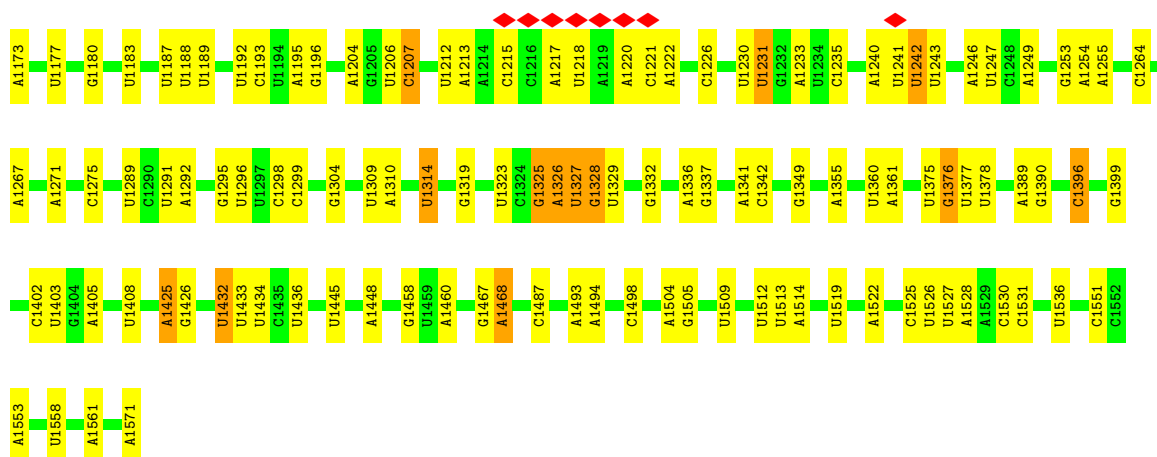
ALA
GLU
LYS
ILE
LYS
LYS
ALA
ALA
LEU
GLU
ALA
VAL
GLY
GLY
THR
VAL
VAL
LEU
GLU

• Molecule 2: E-site tRNA

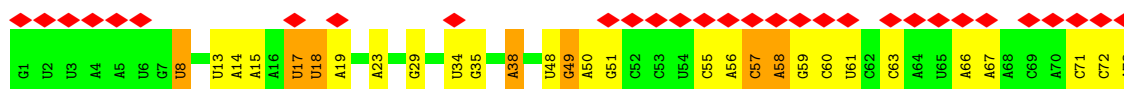
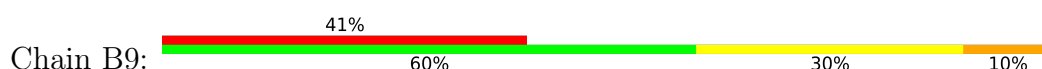


• Molecule 3: 16S rRNA

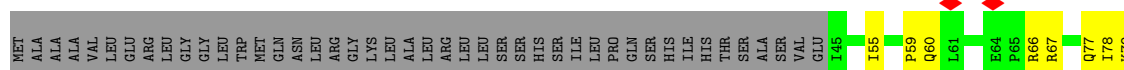




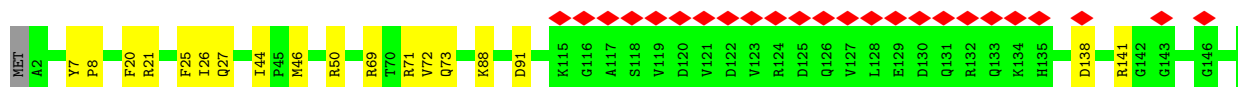
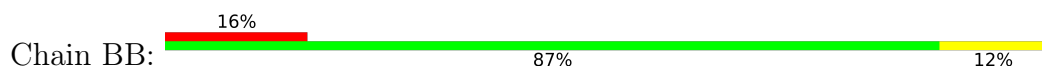
- Molecule 4: CP Phe-tRNA



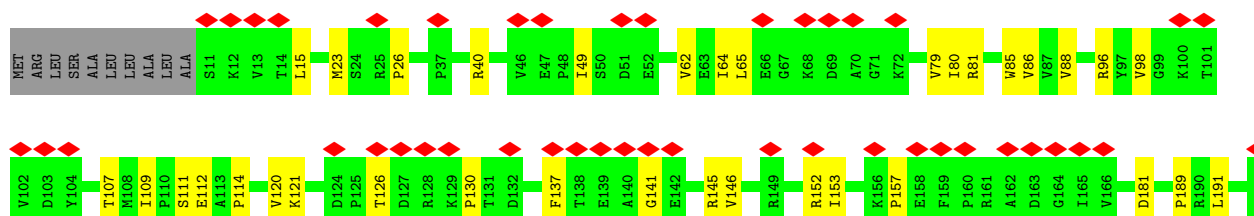
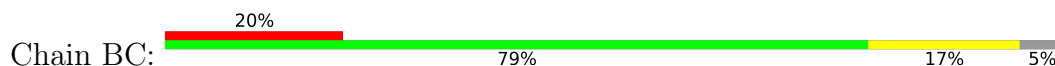
- Molecule 5: Large ribosomal subunit protein uL22m



- Molecule 6: 39S ribosomal protein L23, mitochondrial



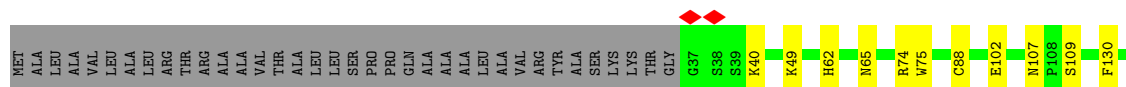
- Molecule 7: uL24m





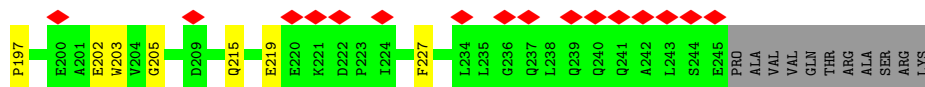
- Molecule 8: 39S ribosomal protein L27, mitochondrial

Chain BD: 68% 8% 24%



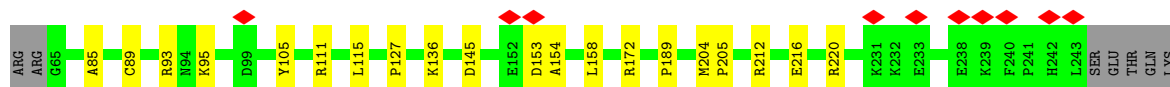
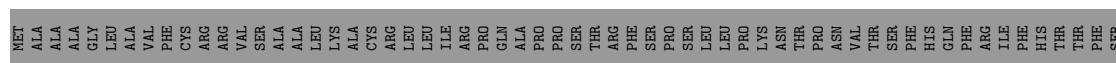
- Molecule 9: Mitochondrial ribosomal protein L28

Chain BE: 11% 84% 11% 5%



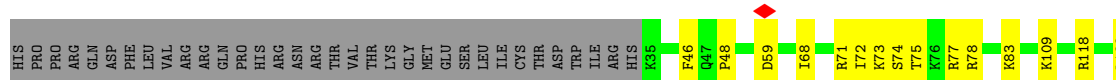
- Molecule 10: Mitochondrial ribosomal protein L47

Chain BF: 64% 8% 28%

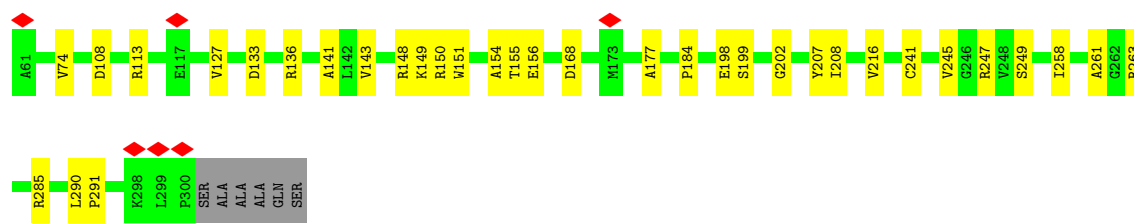


- Molecule 11: Large ribosomal subunit protein uL30m

Chain BG: 62% 11% 27%

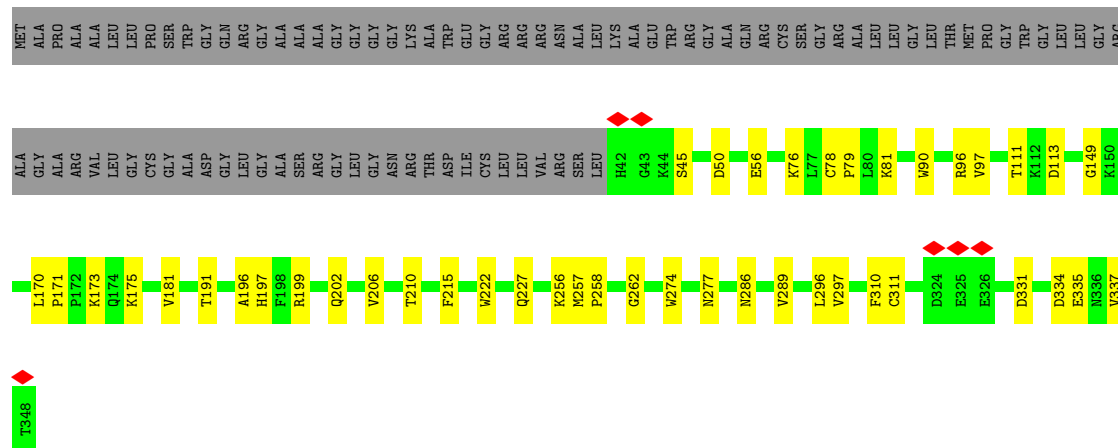


- Molecule 12: Mitochondrial ribosomal protein L32



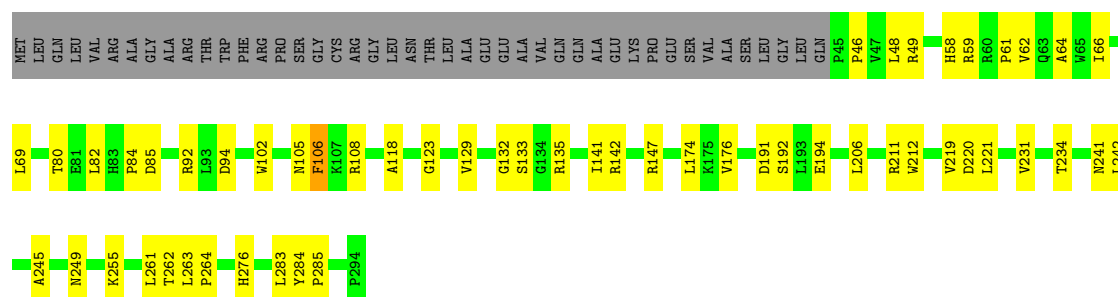
• Molecule 17: ICT1

Chain BM: 66% 11% 23%



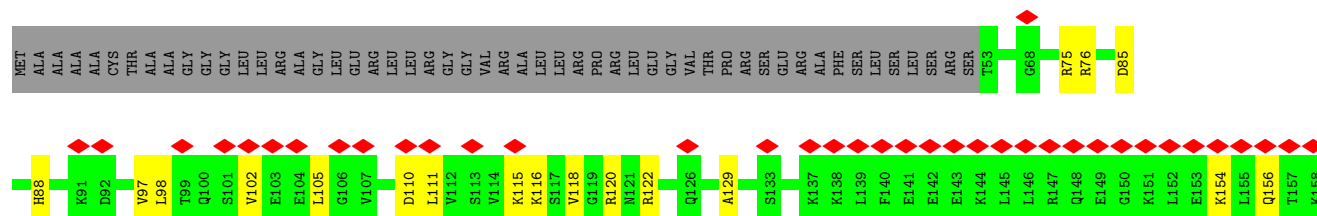
• Molecule 18: Mitochondrial ribosomal protein L4

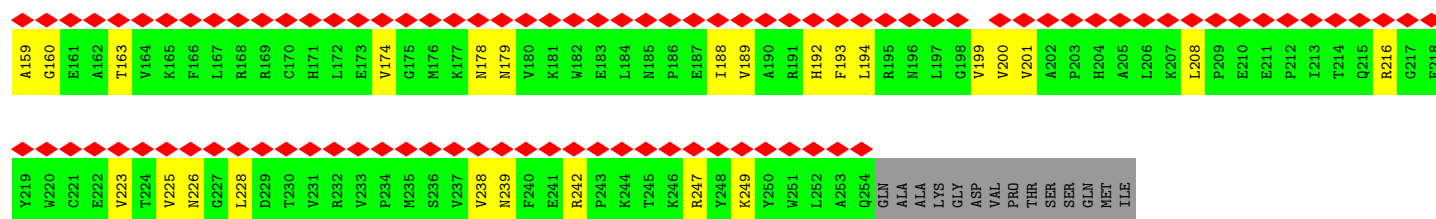
Chain BN: 66% 18% 15%



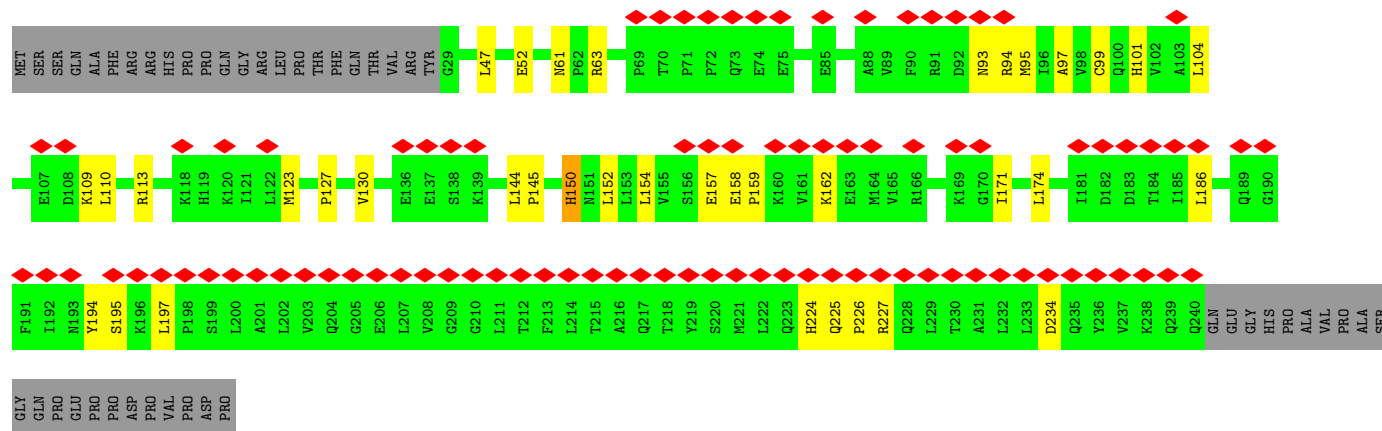
• Molecule 19: Mitochondrial ribosomal protein L9

Chain BO: 59% 16% 25%

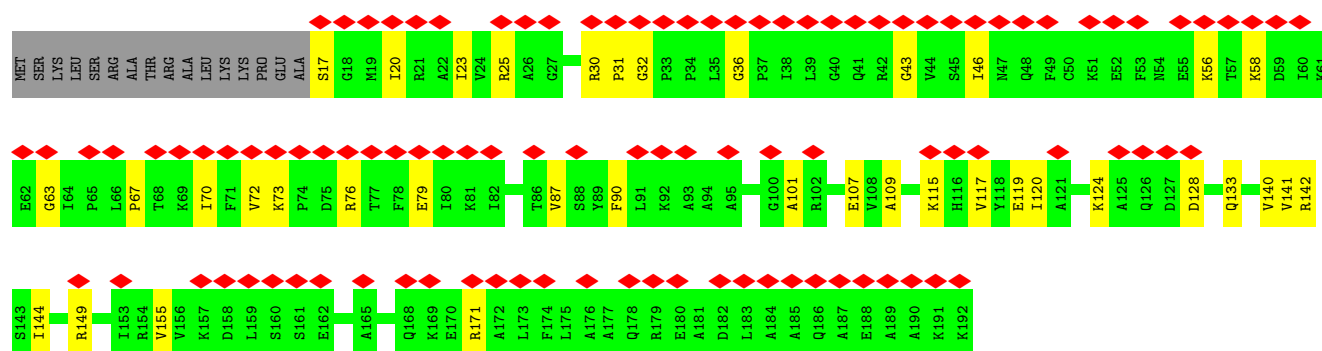
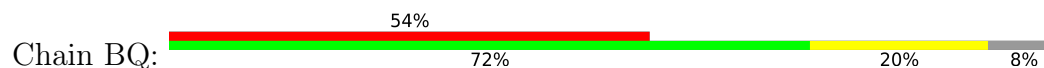




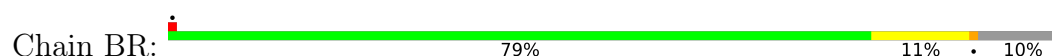
• Molecule 20: Mitochondrial ribosomal protein L10



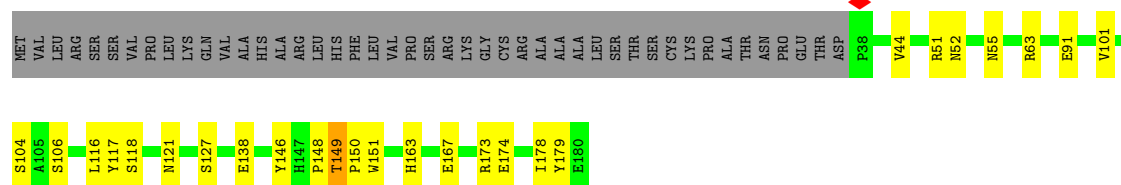
• Molecule 21: Mitochondrial ribosomal protein L11



• Molecule 22: 39S ribosomal protein L13, mitochondrial

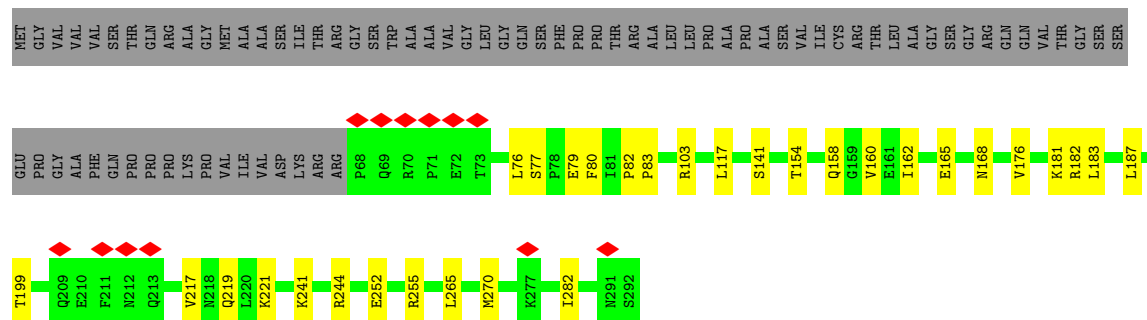


Chain BW: 



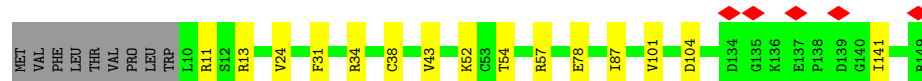
- Molecule 28: 39S ribosomal protein L19, mitochondrial

Chain BX: 



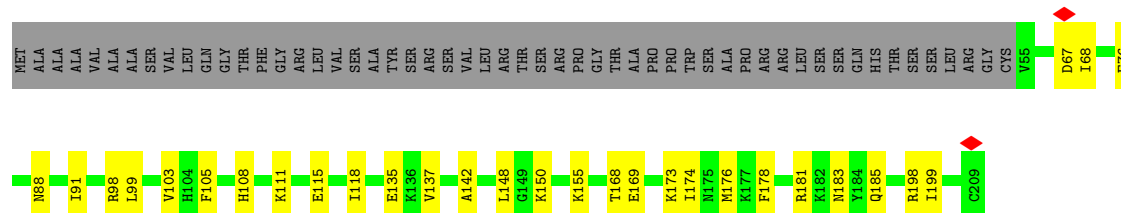
- Molecule 29: Mitochondrial ribosomal protein L20

Chain BY: 



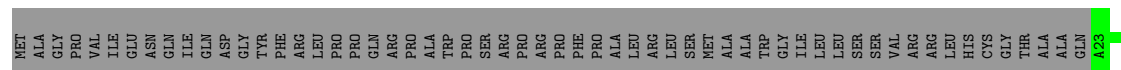
- Molecule 30: Mitochondrial ribosomal protein L21

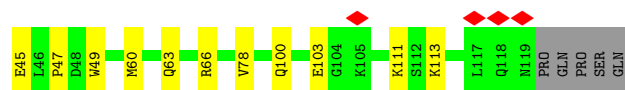
Chain BZ: 



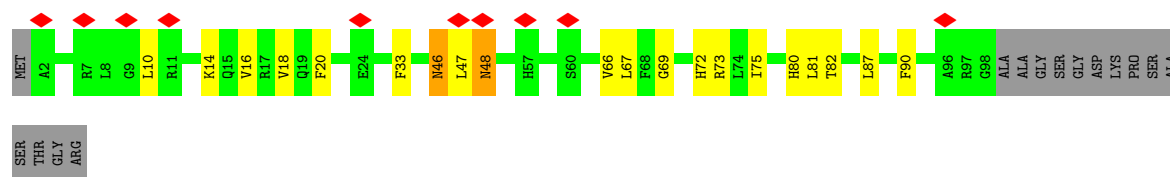
- Molecule 31: 39S ribosomal protein L52, mitochondrial

Chain Ba: 

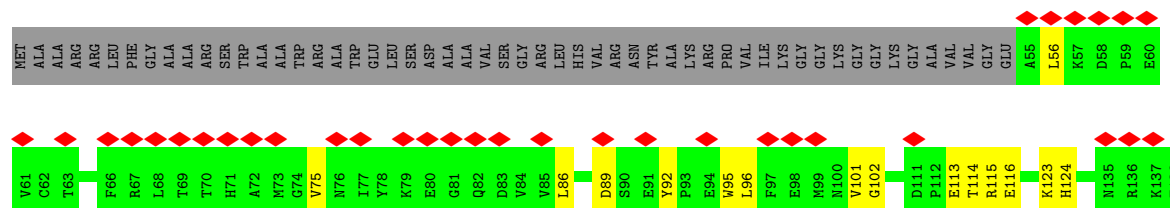




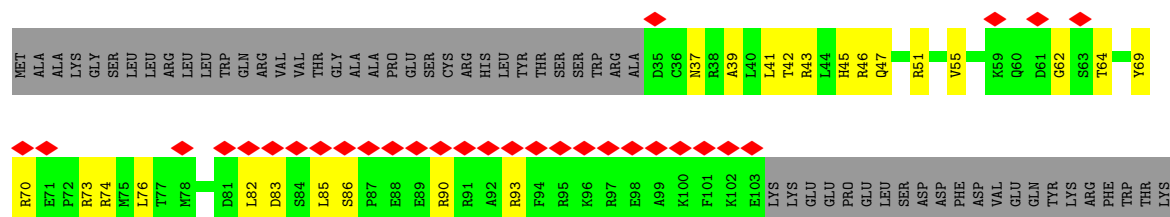
• Molecule 32: Mitochondrial ribosomal protein L53



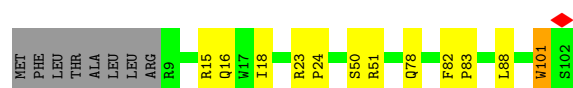
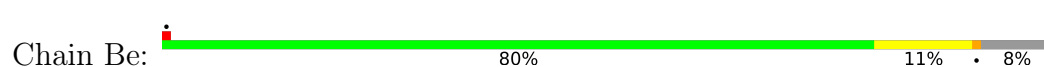
• Molecule 33: mL54



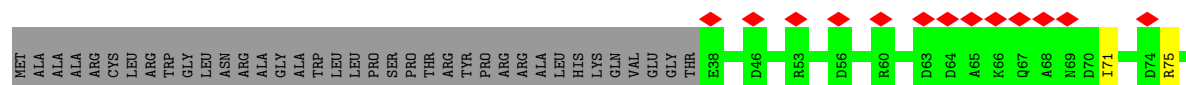
• Molecule 34: Mitochondrial ribosomal protein L55

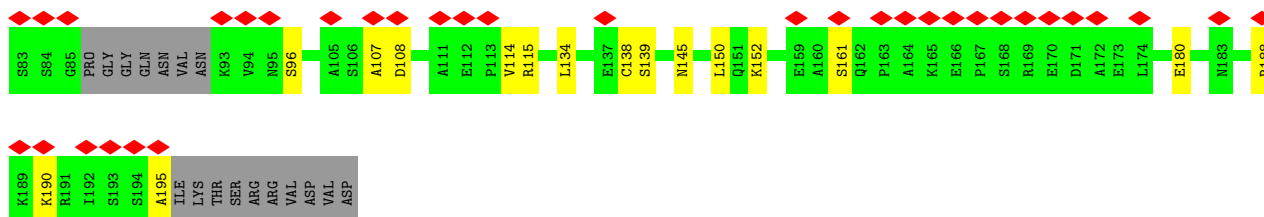


• Molecule 35: Mitochondrial ribosomal protein L57

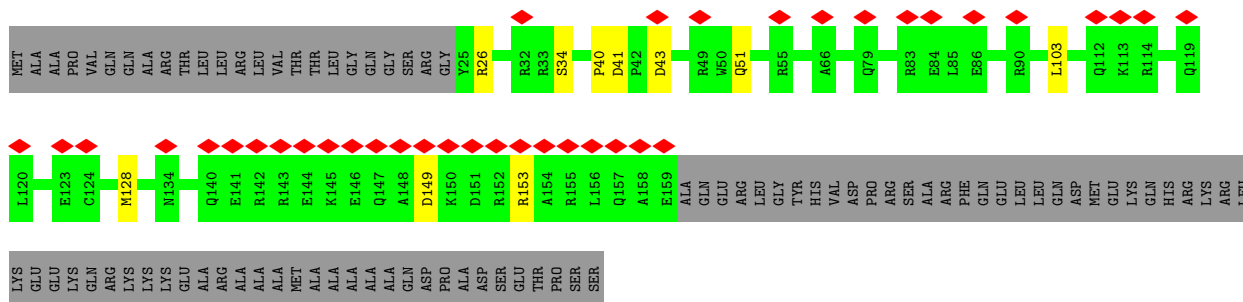


• Molecule 36: mL62 (ICT1)

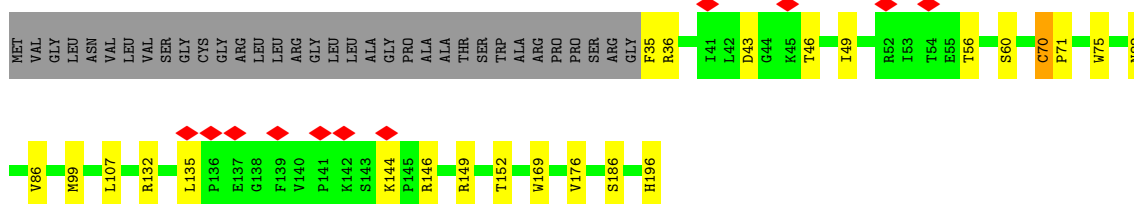
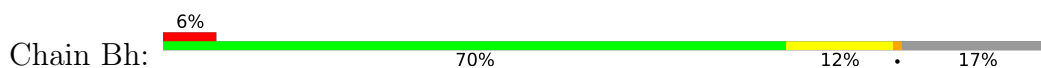




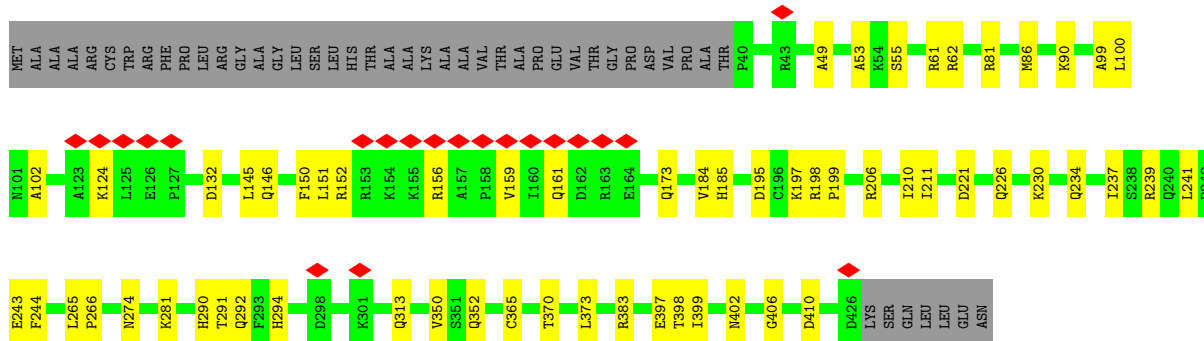
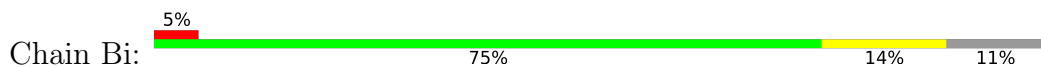
- Molecule 37: mL64



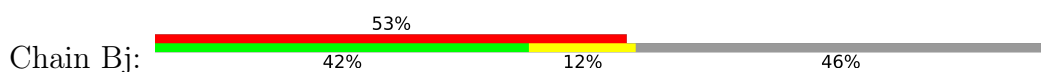
- Molecule 38: Mitochondrial ribosomal protein S18A



- Molecule 39: 39S ribosomal protein S30, mitochondrial

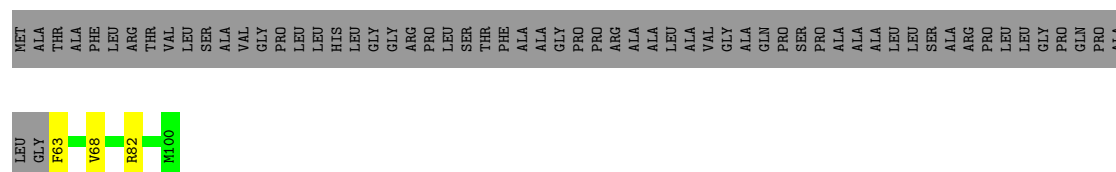


- Molecule 40: 39S ribosomal protein L1, mitochondrial

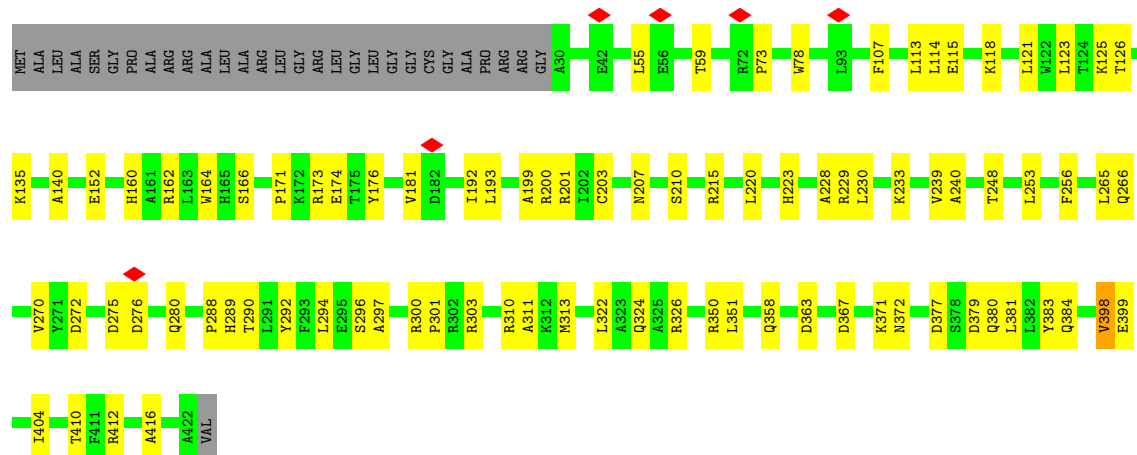




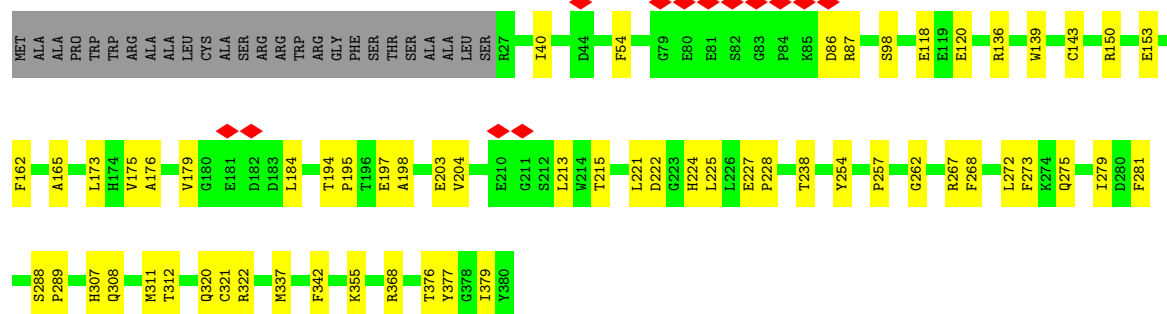
Chain Bl: 35% 1% 62%



Chain Bm:

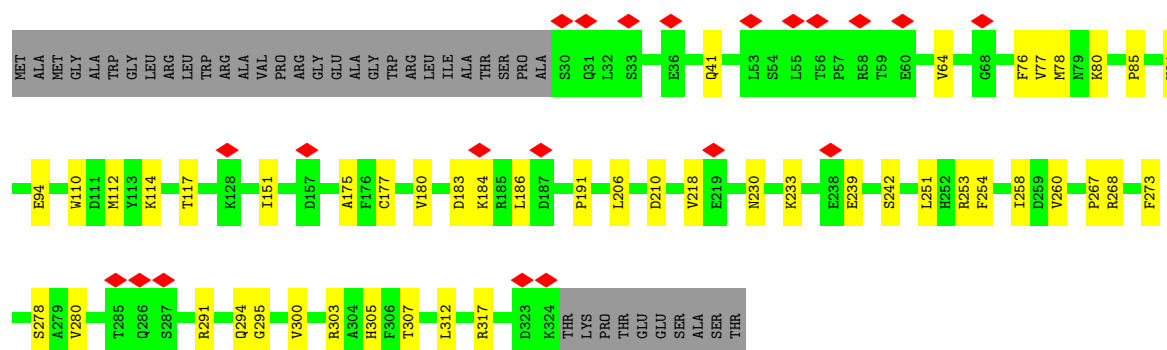


Chain Bn: 



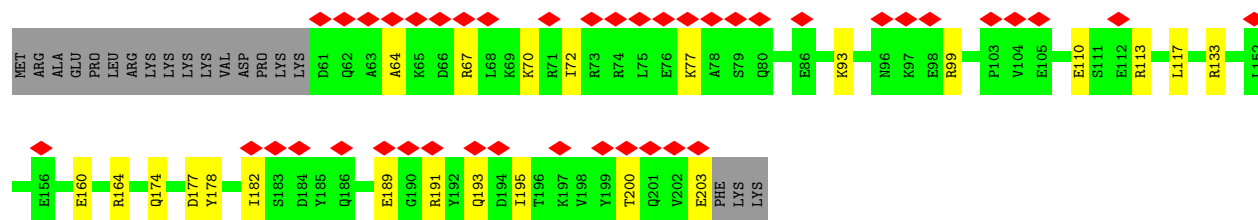
• Molecule 44: Mitochondrial ribosomal protein L39

Chain Bo: 



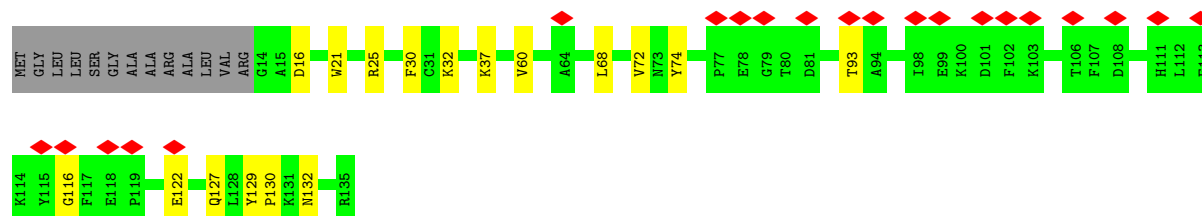
• Molecule 45: Mitochondrial ribosomal protein L40

Chain Bp: 

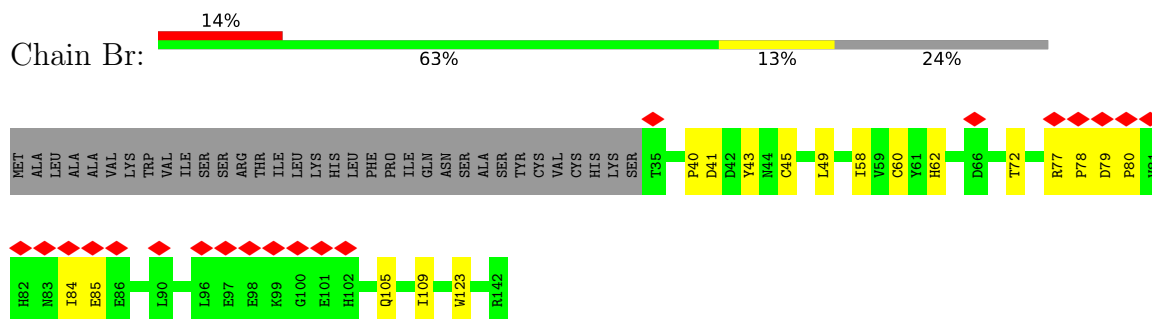


• Molecule 46: 39S ribosomal protein L41, mitochondrial

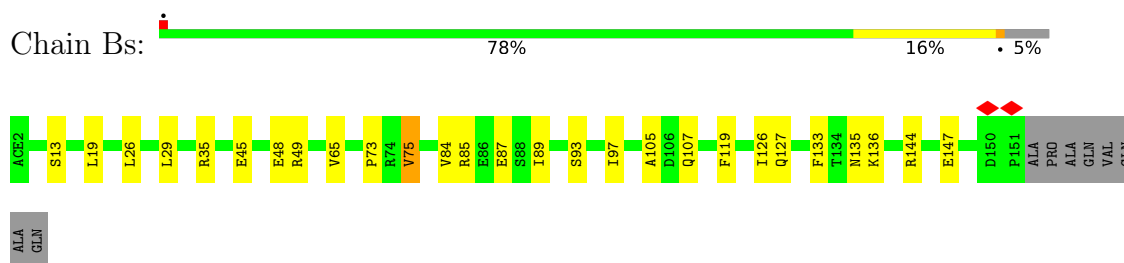
Chain Bq: 



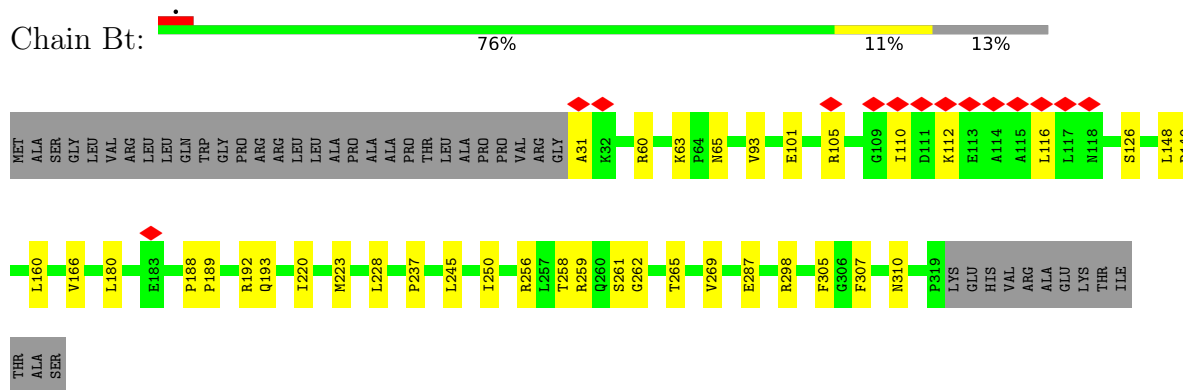
• Molecule 47: mL42



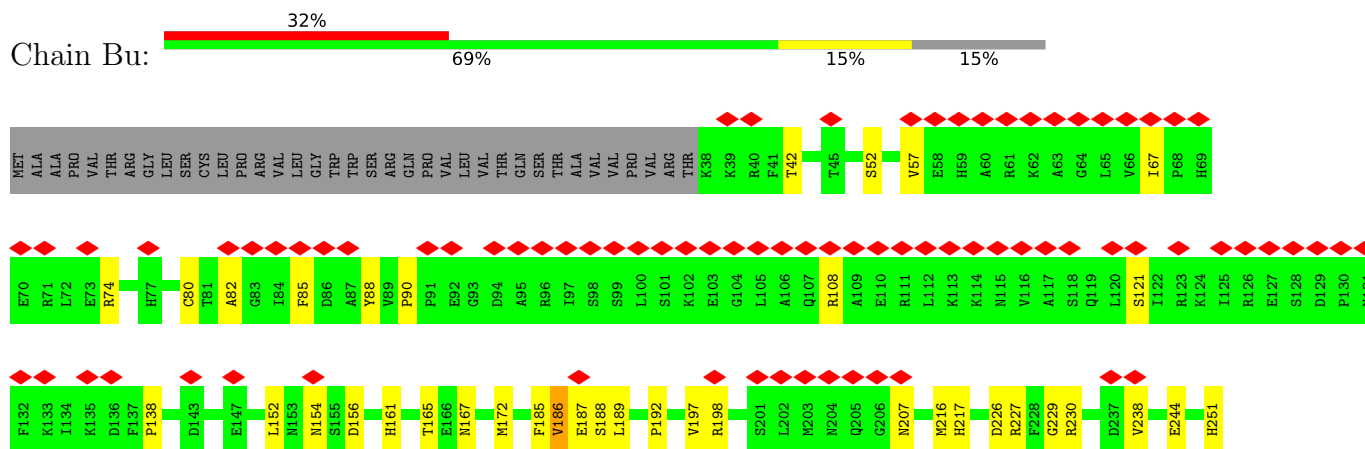
• Molecule 48: Large ribosomal subunit protein mL43

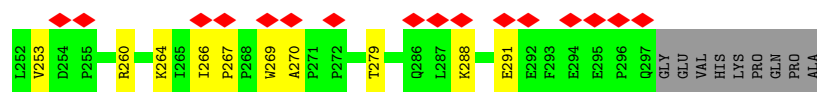


• Molecule 49: mL44

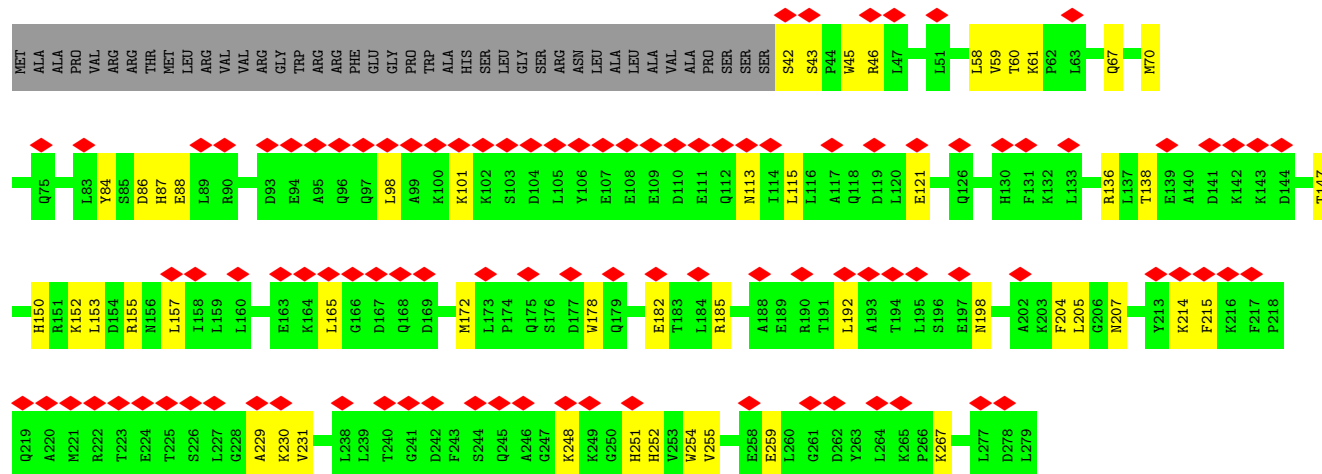


• Molecule 50: Mitochondrial ribosomal protein L45

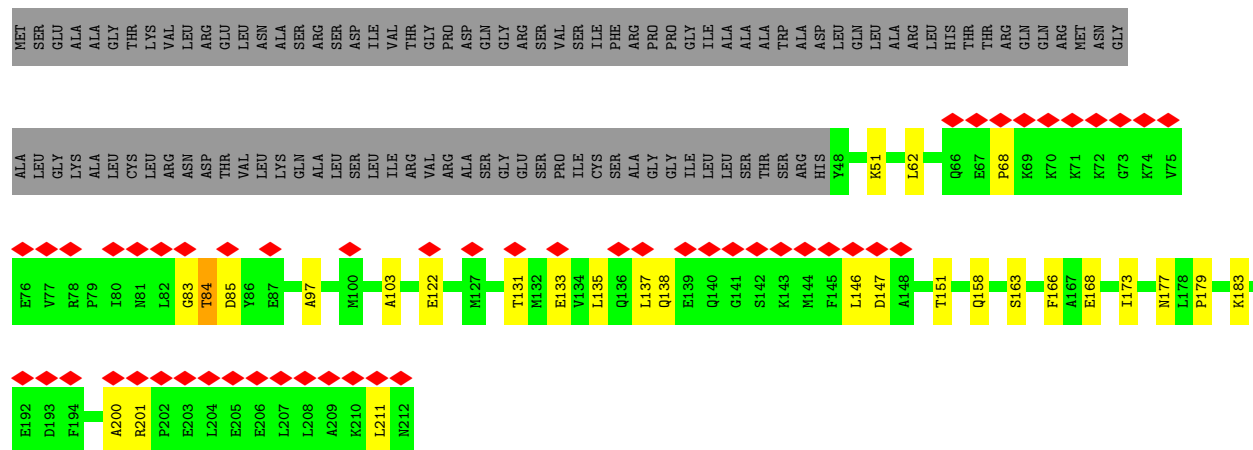




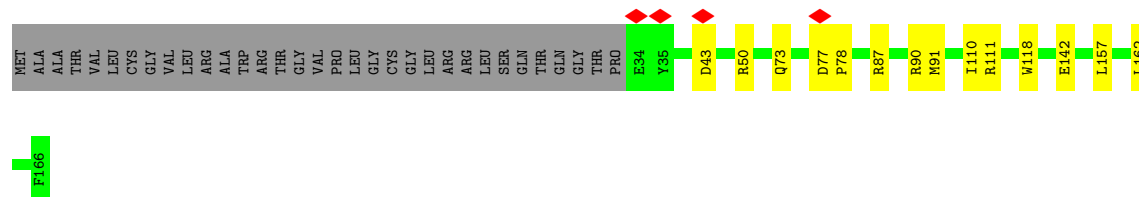
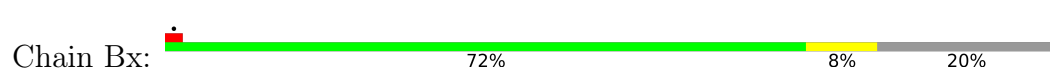
• Molecule 51: Mitochondrial ribosomal protein L46



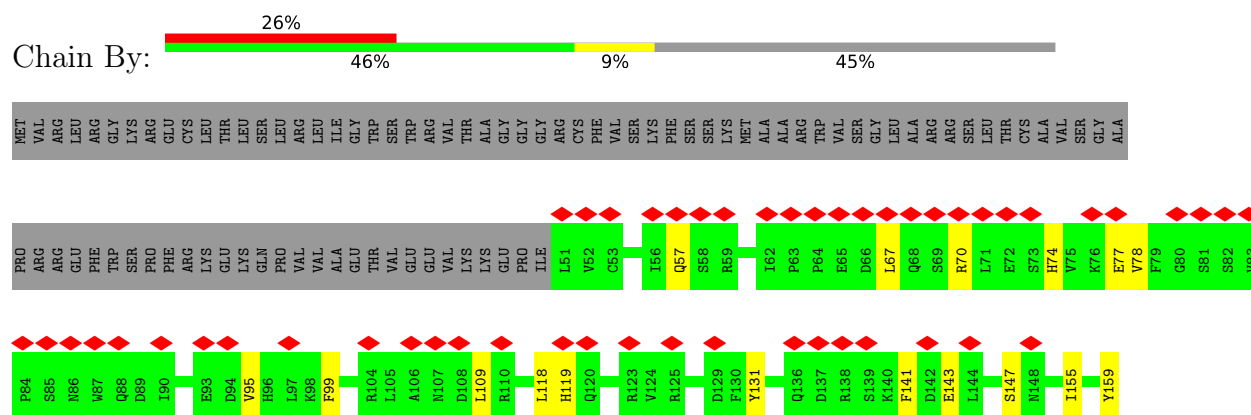
• Molecule 52: 39S ribosomal protein L48, mitochondrial



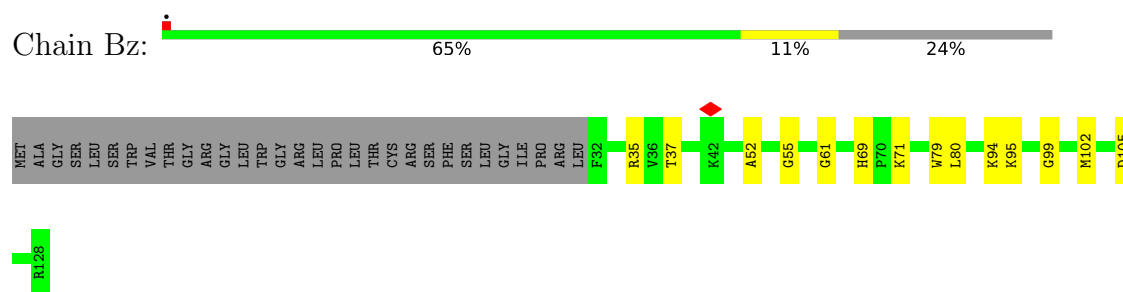
• Molecule 53: 39S ribosomal protein L49, mitochondrial



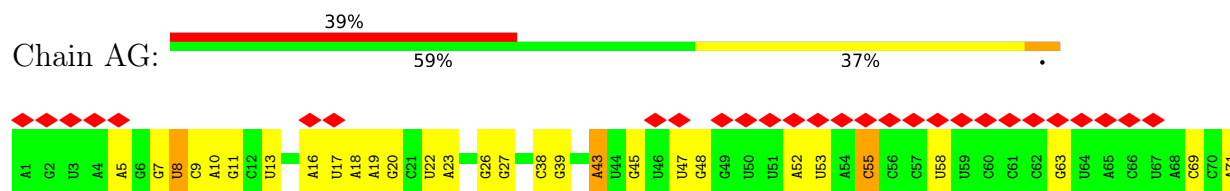
- Molecule 54: Mitochondrial ribosomal protein L50



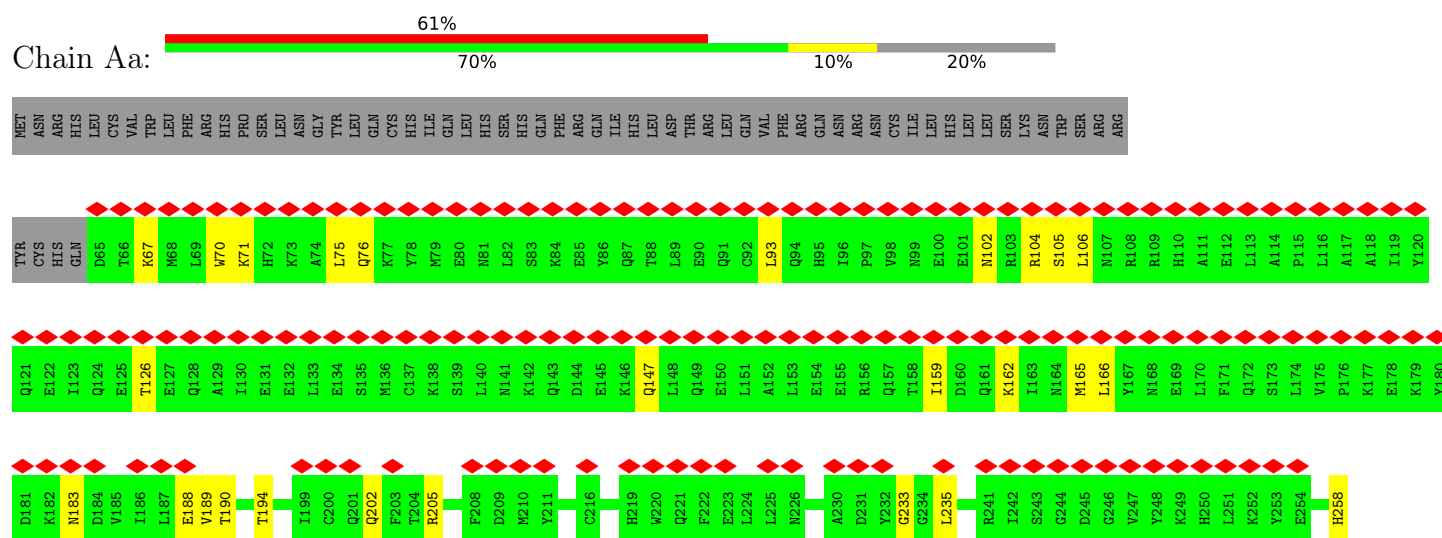
- Molecule 55: Large ribosomal subunit protein mL51



- Molecule 56: P-site Met-tRNA(fMet)



- Molecule 57: Peptide chain release factor 1, mitochondrial





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50622	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.800	Depositor
Minimum map value	-2.487	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.130	Depositor
Recommended contour level	0.5	Depositor
Map size ($\text{\AA}$)	532.5, 532.5, 532.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.065, 1.065, 1.065	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FES, MIA, MG, OMU, AYA, PSU, SAC, ZN, ACE, FME, K, OMG, 1MA

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	B1	0.06	0/319	0.17	0/435
1	B2	0.05	0/212	0.17	0/286
1	B3	0.06	0/221	0.17	0/297
1	B4	0.05	0/212	0.13	0/286
1	B5	0.05	0/212	0.12	0/286
1	B6	0.06	0/204	0.18	0/275
2	B7	0.05	0/68	0.10	0/103
3	B8	0.09	0/37315	0.15	0/58099
4	B9	0.07	0/1712	0.15	0/2659
5	BA	0.10	0/1407	0.21	0/1891
6	BB	0.09	0/1206	0.23	0/1639
7	BC	0.08	0/1719	0.23	0/2329
8	BD	0.10	0/890	0.23	0/1202
9	BE	0.08	0/2093	0.20	0/2835
10	BF	0.08	0/1586	0.19	0/2123
11	BG	0.10	0/993	0.22	0/1341
12	BH	0.09	0/917	0.20	0/1227
13	BI	0.07	0/430	0.22	0/570
14	BJ	0.10	0/395	0.18	0/524
15	BK	0.10	0/853	0.22	0/1136
16	BL	0.10	0/1898	0.24	0/2555
17	BM	0.10	0/2493	0.24	0/3387
18	BN	0.12	0/2080	0.26	0/2830
19	BO	0.08	0/1695	0.22	0/2288
20	BP	0.09	0/1742	0.24	0/2358
21	BQ	0.07	0/1359	0.20	0/1828
22	BR	0.24	1/1481 (0.1%)	0.23	0/2009
23	BS	0.10	0/912	0.24	0/1231
24	BT	0.10	0/2368	0.25	0/3198
25	BU	0.10	0/1850	0.24	0/2491
26	BV	0.10	0/1262	0.23	0/1700
27	BW	0.10	0/1197	0.23	0/1624

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	BX	0.10	0/1898	0.23	0/2562
29	BY	0.10	0/1179	0.20	0/1578
30	BZ	0.11	0/1256	0.24	0/1706
31	Ba	0.09	0/787	0.22	0/1056
32	Bb	0.12	0/747	0.33	0/1006
33	Bc	0.06	0/737	0.21	0/997
34	Bd	0.12	0/580	0.28	0/780
35	Be	0.10	0/798	0.21	0/1073
36	Bf	0.07	0/1214	0.22	0/1630
37	Bg	0.07	0/1157	0.17	0/1560
38	Bh	0.12	0/1364	0.29	0/1849
39	Bi	0.10	0/3206	0.25	0/4354
40	Bj	0.07	0/1350	0.23	0/1823
41	Bl	0.10	0/342	0.19	0/450
42	Bm	0.09	0/3267	0.24	0/4455
43	Bn	0.10	0/3047	0.24	0/4139
44	Bo	0.08	0/2464	0.21	0/3330
45	Bp	0.09	0/1228	0.23	0/1656
46	Bq	0.09	0/1000	0.22	0/1345
47	Br	0.11	0/934	0.29	0/1267
48	Bs	0.11	0/1208	0.26	0/1639
49	Bt	0.09	0/2372	0.23	0/3211
50	Bu	0.09	0/2199	0.23	0/2980
51	Bv	0.07	0/1988	0.19	0/2678
52	Bw	0.10	0/1320	0.29	1/1785 (0.1%)
53	Bx	0.10	0/1135	0.23	0/1549
54	By	0.08	0/917	0.22	0/1248
55	Bz	0.10	0/860	0.21	0/1150
56	AG	0.06	0/1677	0.14	0/2606
57	Aa	0.06	0/3171	0.19	0/4263
All	All	0.10	1/118703 (0.0%)	0.20	1/168767 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BR	4	PHE	C-N	-8.30	1.22	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	Bw	68	PRO	N-CA-CB	7.57	110.37	103.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B1	317	0	309	4	0
1	B2	213	0	234	7	0
1	B3	222	0	247	5	0
1	B4	213	0	234	2	0
1	B5	213	0	234	1	0
1	B6	205	0	223	4	0
2	B7	62	0	34	2	0
3	B8	33427	0	16915	220	0
4	B9	1560	0	798	17	0
5	BA	1374	0	1405	29	0
6	BB	1184	0	1143	12	0
7	BC	1678	0	1683	22	0
8	BD	867	0	886	7	0
9	BE	2036	0	2058	17	0
10	BF	1548	0	1583	17	0
11	BG	968	0	1018	13	0
12	BH	902	0	916	13	0
13	BI	425	0	471	5	0
14	BJ	387	0	413	9	0
15	BK	833	0	883	11	0
16	BL	1860	0	1923	21	0
17	BM	2420	0	2418	29	0
18	BN	2019	0	2062	43	0
19	BO	1660	0	1730	31	0
20	BP	1705	0	1804	27	0
21	BQ	1339	0	1407	27	0
22	BR	1447	0	1441	15	0
23	BS	896	0	946	12	0
24	BT	2312	0	2372	27	0
25	BU	1803	0	1841	17	0
26	BV	1240	0	1260	18	0
27	BW	1168	0	1159	20	0
28	BX	1855	0	1860	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	BY	1159	0	1228	15	0
30	BZ	1231	0	1278	25	0
31	Ba	772	0	773	9	0
32	Bb	745	0	753	13	0
33	Bc	716	0	706	14	0
34	Bd	571	0	579	19	0
35	Be	780	0	792	12	0
36	Bf	1198	0	1192	12	0
37	Bg	1131	0	1093	8	0
38	Bh	1325	0	1354	22	0
39	Bi	3126	0	3153	35	0
40	Bj	1325	0	1351	30	0
41	Bl	335	0	359	3	0
42	Bm	3173	0	3153	55	0
43	Bn	2952	0	2839	47	0
44	Bo	2408	0	2415	27	0
45	Bp	1202	0	1205	29	0
46	Bq	972	0	971	15	0
47	Br	906	0	886	12	0
48	Bs	1185	0	1188	21	0
49	Bt	2319	0	2332	29	0
50	Bu	2138	0	2139	28	0
51	Bv	1948	0	1955	37	0
52	Bw	1295	0	1272	20	0
53	Bx	1097	0	1080	11	0
54	By	893	0	878	14	0
55	Bz	837	0	860	11	0
56	AG	1502	0	764	21	0
57	Aa	3120	0	3124	30	0
58	B8	193	0	0	0	0
58	B9	1	0	0	0	0
58	BL	2	0	0	0	0
58	BM	2	0	0	0	0
58	BT	1	0	0	0	0
58	BV	3	0	0	0	0
58	Be	1	0	0	0	0
58	Bq	1	0	0	0	0
58	Bx	1	0	0	0	0
59	B8	26	0	0	0	0
59	BL	1	0	0	0	0
59	BU	1	0	0	0	0
59	BW	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	Be	1	0	0	0	0
60	B9	11	0	8	1	0
61	BH	1	0	0	0	0
61	Bl	1	0	0	0	0
62	Bh	4	0	0	1	0
63	AG	10	0	10	1	0
All	All	112981	0	95600	1046	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1046) 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)
18:BN:66:ILE:HD11	18:BN:80:THR:HB	1.56	0.86
27:BW:52:ASN:HD22	43:Bn:267:ARG:HD3	1.41	0.84
34:Bd:45:HIS:O	34:Bd:46:ARG:NH1	2.11	0.83
24:BT:47:ARG:HD3	30:BZ:183:ASN:HD22	1.43	0.83
42:Bm:126:THR:HG22	42:Bm:372:ASN:HB2	1.65	0.79
20:BP:95:MET:HB2	20:BP:159:PRO:HB3	1.66	0.78
18:BN:249:ASN:ND2	55:Bz:55:GLY:O	2.16	0.77
3:B8:1396:C:N3	57:Aa:306:ARG:NH2	2.33	0.77
42:Bm:200:ARG:HE	42:Bm:233:LYS:HD2	1.49	0.76
12:BH:144:GLN:HE21	12:BH:173:ARG:HH21	1.32	0.76
9:BE:196:ILE:HG12	9:BE:197:PRO:HD2	1.69	0.75
27:BW:173:ARG:NH1	27:BW:174:GLU:O	2.20	0.74
18:BN:283:LEU:HB2	24:BT:125:ARG:HH12	1.52	0.74
55:Bz:94:LYS:NZ	55:Bz:102:MET:SD	2.61	0.73
3:B8:831:U:OP2	3:B8:836:A:N6	2.22	0.73
42:Bm:140:ALA:HB2	42:Bm:416:ALA:HB2	1.70	0.73
22:BR:2:SAC:H2A3	49:Bt:310:ASN:HD21	1.52	0.73
23:BS:46:LEU:HD12	23:BS:78:ARG:HD3	1.70	0.72
45:Bp:64:ALA:HA	45:Bp:67:ARG:HD2	1.71	0.72
45:Bp:67:ARG:NH2	56:AG:10:A:OP2	2.23	0.72
17:BM:210:THR:OG1	17:BM:262:GLY:O	2.08	0.71
13:BI:59:GLN:HG2	13:BI:60:LYS:HG3	1.72	0.71
38:Bh:149:ARG:HD3	38:Bh:152:THR:HG21	1.72	0.71
39:Bi:237:ILE:HG22	39:Bi:239:ARG:H	1.54	0.71
7:BC:80:ILE:HB	7:BC:85:TRP:HB2	1.72	0.71
39:Bi:397:GLU:HG2	39:Bi:398:THR:HG22	1.72	0.71
20:BP:110:LEU:HD11	21:BQ:133:GLN:HG2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:BM:175:LYS:HD3	17:BM:296:LEU:HB2	1.73	0.70
32:Bb:82:THR:HG23	38:Bh:36:ARG:HH12	1.57	0.70
3:B8:175:C:H5''	22:BR:115:ASN:HB2	1.74	0.70
31:Ba:113:LYS:NZ	43:Bn:311:MET:O	2.24	0.70
3:B8:1207:C:O2'	8:BD:88:CYS:SG	2.49	0.69
51:Bv:67:GLN:HA	51:Bv:70:MET:HE2	1.73	0.69
39:Bi:53:ALA:O	39:Bi:62:ARG:NH2	2.25	0.68
24:BT:119:THR:O	24:BT:123:ASN:ND2	2.27	0.68
39:Bi:152:ARG:HH21	42:Bm:280:GLN:HG2	1.58	0.68
49:Bt:258:THR:HG22	49:Bt:259:ARG:HG3	1.75	0.68
29:BY:54:THR:HG21	30:BZ:176:MET:H	1.57	0.68
49:Bt:105:ARG:HH21	49:Bt:112:LYS:HB2	1.58	0.68
3:B8:129:A:OP1	18:BN:142:ARG:NH2	2.26	0.68
16:BL:74:VAL:HG11	16:BL:149:LYS:HB2	1.76	0.67
55:Bz:35:ARG:NH1	55:Bz:37:THR:O	2.27	0.67
3:B8:565:A:N6	3:B8:1314:U:OP1	2.26	0.67
30:BZ:150:LYS:HE3	47:Br:58:ILE:HD11	1.74	0.67
53:Bx:118:TRP:NE1	53:Bx:142:GLU:OE2	2.28	0.67
17:BM:206:VAL:HG11	17:BM:289:VAL:HB	1.76	0.67
3:B8:1289:U:H5''	41:Bl:68:VAL:HG12	1.76	0.67
3:B8:493:A:O2'	3:B8:494:U:O2	2.11	0.67
1:B1:40:LEU:HB3	1:B4:72:ALA:HA	1.77	0.66
40:Bj:97:TYR:HB3	40:Bj:306:LYS:HB2	1.75	0.66
3:B8:644:G:N2	3:B8:1008:A:OP2	2.28	0.66
44:Bo:85:PRO:HG2	44:Bo:112:MET:HA	1.75	0.66
3:B8:458:A:O2'	3:B8:467:A:O2'	2.14	0.66
3:B8:112:A:N6	3:B8:115:U:OP2	2.27	0.66
25:BU:136:MET:HG3	57:Aa:342:ILE:HD13	1.78	0.66
3:B8:417:G:N3	11:BG:109:LYS:NZ	2.44	0.66
45:Bp:117:LEU:HD21	51:Bv:70:MET:HG2	1.77	0.66
20:BP:104:LEU:H	20:BP:109:LYS:HE3	1.60	0.66
3:B8:183:U:OP1	24:BT:47:ARG:NH1	2.28	0.65
5:BA:105:GLU:OE1	5:BA:116:LYS:NZ	2.29	0.65
18:BN:59:ARG:HH12	24:BT:10:PRO:HD3	1.61	0.65
49:Bt:105:ARG:HH12	49:Bt:110:ILE:HB	1.61	0.65
26:BV:113:ARG:NH2	26:BV:117:ASP:OD2	2.27	0.65
3:B8:125:A:OP1	14:BJ:85:ARG:NH1	2.29	0.65
11:BG:68:ILE:HD11	11:BG:122:LEU:HD13	1.77	0.65
20:BP:224:HIS:HA	20:BP:227:ARG:HE	1.61	0.65
39:Bi:292:GLN:OE1	39:Bi:294:HIS:NE2	2.29	0.65
5:BA:82:LYS:HD3	5:BA:147:ARG:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BX:76:LEU:HD21	28:BX:282:ILE:HD11	1.78	0.65
32:Bb:14:LYS:HE3	32:Bb:69:GLY:HA2	1.77	0.65
50:Bu:90:PRO:HB2	50:Bu:269:TRP:HH2	1.62	0.65
3:B8:1014:A:H5''	29:BY:34:ARG:HH21	1.62	0.64
19:BO:225:VAL:HG22	40:Bj:86:VAL:HB	1.78	0.64
16:BL:113:ARG:O	16:BL:148:ARG:NH2	2.30	0.64
34:Bd:51:ARG:NH1	51:Bv:88:GLU:OE2	2.29	0.64
3:B8:62:C:OP1	19:BO:76:ARG:NH1	2.30	0.64
57:Aa:183:ASN:ND2	57:Aa:289:ASP:OD1	2.31	0.64
5:BA:152:LYS:NZ	5:BA:166:GLU:OE2	2.29	0.64
9:BE:16:LEU:HD12	9:BE:21:TYR:HB3	1.79	0.64
21:BQ:31:PRO:HA	21:BQ:46:ILE:HG21	1.78	0.64
24:BT:114:GLN:OE1	53:Bx:50:ARG:NH1	2.30	0.64
35:Be:24:PRO:HD2	38:Bh:169:TRP:HB2	1.78	0.64
57:Aa:189:VAL:HG12	57:Aa:282:VAL:HG22	1.80	0.64
3:B8:530:A:O2'	3:B8:547:A:N1	2.30	0.64
42:Bm:275:ASP:OD2	42:Bm:326:ARG:NH1	2.31	0.64
27:BW:151:TRP:HH2	43:Bn:54:PHE:HB3	1.63	0.64
40:Bj:290:VAL:HG11	40:Bj:307:ILE:HD13	1.78	0.64
3:B8:639:U:H5'	5:BA:147:ARG:HH12	1.63	0.64
50:Bu:267:PRO:HG2	50:Bu:270:ALA:HB2	1.79	0.63
3:B8:877:U:H5''	3:B8:878:G:H5'	1.80	0.63
51:Bv:113:ASN:ND2	51:Bv:115:LEU:O	2.31	0.63
25:BU:124:VAL:HG12	25:BU:158:ARG:HE	1.63	0.63
56:AG:5:A:H2	56:AG:63:G:H1	1.46	0.63
24:BT:57:ARG:HG2	24:BT:62:ARG:HH21	1.64	0.63
3:B8:127:G:OP2	14:BJ:88:LYS:NZ	2.32	0.63
3:B8:293:U:O2'	3:B8:1434:U:O2'	2.15	0.63
34:Bd:74:ARG:HH22	51:Bv:121:GLU:HB3	1.64	0.63
36:Bf:96:SER:O	36:Bf:145:ASN:ND2	2.33	0.62
57:Aa:394[B]:ARG:NH1	57:Aa:403:GLU:OE1	2.32	0.62
27:BW:51:ARG:NH1	43:Bn:228:PRO:O	2.32	0.62
38:Bh:71:PRO:HD2	38:Bh:107:LEU:HD23	1.81	0.62
44:Bo:210:ASP:OD2	44:Bo:268:ARG:NH1	2.33	0.62
20:BP:93:ASN:ND2	20:BP:157:GLU:OE2	2.32	0.62
31:Ba:63:GLN:OE1	31:Ba:66:ARG:NH1	2.32	0.62
10:BF:204:MET:HE3	10:BF:205:PRO:HD2	1.80	0.62
3:B8:62:C:OP2	19:BO:75:ARG:NH2	2.32	0.61
7:BC:64:ILE:HD11	7:BC:88:VAL:HG21	1.82	0.61
11:BG:78:ARG:O	11:BG:83:LYS:NZ	2.33	0.61
23:BS:43:ASN:HD21	23:BS:117:THR:HB	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:885:G:H1	3:B8:894:U:H3	1.48	0.61
7:BC:126:THR:OG1	7:BC:152:ARG:NH1	2.32	0.61
19:BO:193:PHE:HB3	19:BO:199:VAL:HB	1.81	0.61
32:Bb:66:VAL:HG11	32:Bb:90:PHE:HE1	1.65	0.61
42:Bm:201:ARG:HB3	42:Bm:230:LEU:HD11	1.83	0.61
39:Bi:152:ARG:NH1	42:Bm:276:ASP:OD1	2.34	0.61
47:Br:79:ASP:HB3	47:Br:80:PRO:HD3	1.83	0.61
9:BE:120:ASP:OD2	9:BE:177:HIS:NE2	2.33	0.61
38:Bh:70:CYS:HB3	62:Bh:201:FES:S2	2.40	0.61
51:Bv:46:ARG:H	51:Bv:229:ALA:HA	1.66	0.61
3:B8:1193:C:OP2	15:BK:142:ARG:NH1	2.34	0.60
15:BK:175:ASP:HB3	15:BK:178:GLN:HB2	1.83	0.60
45:Bp:193:GLN:O	52:Bw:133:GLU:N	2.29	0.60
50:Bu:82:ALA:O	50:Bu:167:ASN:ND2	2.34	0.60
53:Bx:73:GLN:HB3	53:Bx:162:LEU:HD11	1.83	0.60
5:BA:92:ILE:HA	5:BA:95:MET:HE2	1.81	0.60
22:BR:26:GLN:NE2	22:BR:147:GLN:OE1	2.34	0.60
18:BN:262:THR:HG22	18:BN:264:PRO:HD2	1.83	0.60
23:BS:34:LYS:HG2	23:BS:35:MET:HG2	1.81	0.60
21:BQ:101:ALA:HB2	21:BQ:109:ALA:HB2	1.84	0.60
3:B8:96:U:N3	37:Bg:34:SER:O	2.35	0.60
5:BA:123:GLN:NE2	5:BA:135:ARG:O	2.35	0.60
3:B8:9:U:O2	3:B8:132:G:N2	2.35	0.60
21:BQ:155:VAL:HG23	33:Bc:101:VAL:HG13	1.84	0.60
34:Bd:70:ARG:NH1	51:Bv:86:ASP:OD2	2.34	0.60
3:B8:216:C:OP2	53:Bx:111:ARG:NH2	2.34	0.59
3:B8:1399:G:O2'	3:B8:1402:C:OP2	2.20	0.59
6:BB:46:MET:HE1	6:BB:72:VAL:HG13	1.84	0.59
32:Bb:73:ARG:HB3	38:Bh:46:THR:HG22	1.84	0.59
3:B8:573:A:H5'	22:BR:29:GLY:HA3	1.84	0.59
7:BC:146:VAL:HG22	7:BC:153:ILE:HG22	1.83	0.59
42:Bm:377:ASP:HB3	42:Bm:380:GLN:HE21	1.68	0.59
51:Bv:185:ARG:HH21	51:Bv:204:PHE:HB2	1.66	0.59
42:Bm:248:THR:HG22	42:Bm:371:LYS:HB2	1.85	0.59
20:BP:47:LEU:HD22	25:BU:226:ILE:HG12	1.84	0.59
27:BW:44:VAL:HG22	43:Bn:225:LEU:HD13	1.84	0.59
48:Bs:85:ARG:NH1	48:Bs:107:GLN:OE1	2.35	0.59
3:B8:869:G:O2'	3:B8:966:U:OP2	2.18	0.59
3:B8:188:C:O2'	3:B8:190:U:OP2	2.19	0.59
42:Bm:115:GLU:HB3	42:Bm:118:LYS:HE2	1.85	0.59
6:BB:71:ARG:NH1	6:BB:73:GLN:OE1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BE:173:ASP:HB3	9:BE:175:GLN:HG2	1.85	0.58
11:BG:71:ARG:NH1	11:BG:73:LYS:O	2.36	0.58
29:BY:57:ARG:NH2	30:BZ:174:ILE:O	2.37	0.58
51:Bv:60:THR:O	51:Bv:136:ARG:NH2	2.29	0.58
3:B8:640:A:OP1	5:BA:147:ARG:NH1	2.36	0.58
55:Bz:69:HIS:HD2	55:Bz:71:LYS:H	1.51	0.58
16:BL:199:SER:HB3	16:BL:207:TYR:HE1	1.69	0.58
30:BZ:198:ARG:NH2	48:Bs:13:SER:OG	2.36	0.58
3:B8:1349:G:HO2'	41:Bl:63:PHE:N	2.02	0.58
26:BV:77:ASP:OD1	26:BV:83:LYS:NZ	2.34	0.58
28:BX:221:LYS:NZ	28:BX:241:LYS:O	2.36	0.58
3:B8:1230:U:H5'	3:B8:1231:U:H5'	1.85	0.58
19:BO:154:LYS:HA	19:BO:228:LEU:HD13	1.85	0.58
19:BO:156:GLN:OE1	19:BO:226:ASN:ND2	2.35	0.58
27:BW:51:ARG:NH2	43:Bn:221:LEU:O	2.37	0.58
38:Bh:35:PHE:N	38:Bh:56:THR:OG1	2.36	0.58
57:Aa:202:GLN:NE2	57:Aa:233:GLY:O	2.37	0.58
3:B8:60:U:O2'	9:BE:96:LYS:O	2.21	0.58
17:BM:90:TRP:NE1	17:BM:311:CYS:SG	2.74	0.58
42:Bm:300:ARG:HE	42:Bm:303:ARG:HH22	1.51	0.58
3:B8:222:G:H1	55:Bz:61:GLY:HA3	1.69	0.58
3:B8:1014:A:OP1	29:BY:34:ARG:NH2	2.37	0.58
3:B8:1275:C:H4'	57:Aa:317:LYS:HG3	1.86	0.58
9:BE:202:GLU:HG3	9:BE:203:TRP:CD1	2.38	0.58
16:BL:133:ASP:OD2	16:BL:136:ARG:NH1	2.37	0.58
50:Bu:244:GLU:HG2	50:Bu:264:LYS:HE2	1.86	0.58
56:AG:9:C:O2'	56:AG:10:A:N7	2.36	0.57
3:B8:195:G:OP1	3:B8:633:U:O2'	2.21	0.57
3:B8:1089:G:N2	3:B8:1124:C:O2	2.35	0.57
22:BR:27:PRO:HG2	22:BR:30:LYS:HB2	1.84	0.57
28:BX:79:GLU:OE2	28:BX:103:ARG:NH2	2.37	0.57
3:B8:987:G:N2	3:B8:991:C:O2'	2.38	0.57
47:Br:72:THR:O	49:Bt:256:ARG:NH2	2.38	0.57
26:BV:33:LEU:HD21	26:BV:59:LEU:HD22	1.85	0.57
36:Bf:71:ILE:HG21	36:Bf:150:LEU:HD22	1.86	0.57
32:Bb:80:HIS:O	38:Bh:36:ARG:NH1	2.32	0.57
34:Bd:62:GLY:HA3	45:Bp:182:ILE:HG12	1.87	0.57
43:Bn:175:VAL:HG22	43:Bn:204:VAL:HG22	1.85	0.57
45:Bp:193:GLN:HB2	52:Bw:133:GLU:HB3	1.86	0.57
21:BQ:149:ARG:NH2	33:Bc:102:GLY:O	2.38	0.57
46:Bq:127:GLN:HB3	46:Bq:130:PRO:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:975:G:O2'	3:B8:977:G:OP2	2.18	0.57
20:BP:97:ALA:HB3	20:BP:154:LEU:HB2	1.87	0.57
27:BW:149:THR:HG22	27:BW:150:PRO:HD2	1.87	0.57
44:Bo:278:SER:O	44:Bo:317:ARG:NH1	2.37	0.57
8:BD:107:ASN:ND2	8:BD:109:SER:OG	2.38	0.57
7:BC:79:VAL:HG12	7:BC:86:VAL:HG12	1.87	0.56
33:Bc:92:TYR:HB3	33:Bc:96:LEU:HD21	1.87	0.56
40:Bj:128:ASP:O	40:Bj:282:ARG:NH2	2.38	0.56
3:B8:472:U:H5''	11:BG:74:SER:HB3	1.86	0.56
40:Bj:118:ASN:OD1	40:Bj:261:ASN:ND2	2.38	0.56
40:Bj:245:VAL:HA	40:Bj:253:LEU:HD22	1.87	0.56
42:Bm:398:VAL:HG22	42:Bm:399:GLU:HG3	1.87	0.56
3:B8:130:A:OP1	18:BN:147:ARG:NH2	2.38	0.56
3:B8:164:A:OP1	29:BY:52:LYS:NZ	2.34	0.56
3:B8:217:A:HO2'	3:B8:219:A:HO2'	1.53	0.56
10:BF:89:CYS:SG	10:BF:93:ARG:NH1	2.79	0.56
10:BF:127:PRO:HB3	50:Bu:67:ILE:HD11	1.87	0.56
16:BL:290:LEU:HD12	16:BL:291:PRO:HD2	1.87	0.56
24:BT:140:LEU:HG	24:BT:156:VAL:HG11	1.86	0.56
24:BT:247:ILE:HD11	24:BT:256:LEU:HD13	1.87	0.56
45:Bp:203:GLU:OE1	52:Bw:201:ARG:NH1	2.37	0.56
46:Bq:16:ASP:OD1	46:Bq:25:ARG:NH1	2.36	0.56
52:Bw:97:ALA:HB3	52:Bw:103:ALA:HB2	1.87	0.56
3:B8:528:U:O3'	33:Bc:115:ARG:NH2	2.38	0.56
15:BK:172:TYR:HB2	15:BK:175:ASP:HB2	1.88	0.56
42:Bm:140:ALA:HB1	42:Bm:412:ARG:HG2	1.87	0.56
42:Bm:160:HIS:HA	42:Bm:164:TRP:HB2	1.88	0.56
51:Bv:192:LEU:O	51:Bv:198:ASN:ND2	2.39	0.56
52:Bw:122:GLU:OE1	52:Bw:158:GLN:NE2	2.38	0.56
28:BX:252:GLU:OE1	28:BX:255:ARG:NH2	2.38	0.56
39:Bi:86:MET:O	39:Bi:274:ASN:ND2	2.39	0.56
42:Bm:59:THR:HB	42:Bm:73:PRO:HG3	1.87	0.56
50:Bu:154:ASN:ND2	50:Bu:156:ASP:OD2	2.39	0.56
3:B8:1355:A:O2'	3:B8:1460:A:N1	2.39	0.56
53:Bx:110:ILE:HD11	53:Bx:157:LEU:HD13	1.88	0.56
3:B8:1131:U:H2'	3:B8:1132:G:H8	1.70	0.56
19:BO:98:LEU:HD23	19:BO:129:ALA:HB2	1.88	0.56
24:BT:44:ARG:HG3	24:BT:45:ARG:HG3	1.87	0.56
40:Bj:128:ASP:N	40:Bj:289:PHE:O	2.38	0.56
18:BN:69:LEU:HD22	18:BN:206:LEU:HD21	1.88	0.56
33:Bc:89:ASP:HA	33:Bc:92:TYR:HD2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Bs:73:PRO:HB2	48:Bs:89:ILE:HG13	1.88	0.56
3:B8:672:G:H4'	14:BJ:58:PRO:HB2	1.86	0.56
21:BQ:87:VAL:HG22	21:BQ:124:LYS:HE3	1.88	0.56
23:BS:145:VAL:HG11	28:BX:160:VAL:HG11	1.88	0.56
17:BM:111:THR:OG1	17:BM:113:ASP:OD1	2.23	0.55
51:Bv:178:TRP:NE1	51:Bv:182:GLU:O	2.39	0.55
3:B8:526:A:H5''	21:BQ:142:ARG:HH21	1.71	0.55
7:BC:121:LYS:HE3	7:BC:130:PRO:HB2	1.88	0.55
50:Bu:80:CYS:SG	50:Bu:165:THR:OG1	2.58	0.55
57:Aa:70:TRP:HA	57:Aa:75:LEU:HD23	1.87	0.55
3:B8:71:U:H3	3:B8:94:U:H3	1.55	0.55
36:Bf:107:ALA:O	36:Bf:115:ARG:NH2	2.26	0.55
7:BC:49:ILE:O	7:BC:81:ARG:NH2	2.38	0.55
10:BF:220:ARG:NH2	55:Bz:105:ASP:OD2	2.40	0.55
17:BM:50:ASP:OD1	26:BV:139:ARG:NH2	2.39	0.55
27:BW:163:HIS:NE2	27:BW:167:GLU:OE2	2.39	0.55
51:Bv:255:VAL:HB	51:Bv:259:GLU:HG3	1.89	0.55
28:BX:183:LEU:HD21	28:BX:219:GLN:HG3	1.89	0.55
45:Bp:67:ARG:CZ	56:AG:43:A:H4'	2.37	0.55
50:Bu:192:PRO:HB3	50:Bu:216:MET:HG2	1.89	0.55
13:BI:16:ILE:HD12	13:BI:64:SER:HA	1.88	0.55
57:Aa:162:LYS:HE2	57:Aa:166:LEU:HD11	1.88	0.55
25:BU:96:TYR:OH	25:BU:129:LYS:NZ	2.38	0.55
39:Bi:243:GLU:HA	39:Bi:350:VAL:HG21	1.88	0.55
42:Bm:228:ALA:HB3	42:Bm:292:TYR:HB2	1.89	0.55
49:Bt:60:ARG:NH1	49:Bt:65:ASN:O	2.38	0.55
2:B7:76:A:OP2	3:B8:1255:A:O2'	2.25	0.55
39:Bi:370:THR:HG22	39:Bi:383:ARG:HG3	1.89	0.55
57:Aa:306:ARG:NH1	57:Aa:319:ASP:OD1	2.40	0.55
19:BO:201:VAL:HG22	40:Bj:86:VAL:HG13	1.89	0.55
26:BV:30:GLN:NE2	26:BV:78:PHE:O	2.35	0.55
30:BZ:105:PHE:HE1	31:Ba:49:TRP:HB3	1.72	0.55
36:Bf:188:ARG:HH12	43:Bn:179:VAL:HG11	1.71	0.55
38:Bh:43:ASP:O	38:Bh:46:THR:OG1	2.23	0.55
44:Bo:80:LYS:NZ	44:Bo:117:THR:O	2.38	0.55
3:B8:995:C:H5''	26:BV:13:ARG:HH12	1.70	0.55
43:Bn:87:ARG:NH2	43:Bn:153:GLU:OE2	2.40	0.55
47:Br:80:PRO:HB2	47:Br:84:ILE:HG12	1.89	0.55
50:Bu:189:LEU:HB2	50:Bu:217:HIS:HD2	1.72	0.55
11:BG:75:THR:HB	11:BG:83:LYS:HG2	1.88	0.54
44:Bo:273:PHE:HB2	44:Bo:300:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BA:155:ARG:HH11	5:BA:165:MET:HE2	1.71	0.54
45:Bp:160:GLU:O	51:Bv:207:ASN:ND2	2.39	0.54
3:B8:1095:C:H4'	19:BO:247:ARG:HD2	1.90	0.54
16:BL:168:ASP:HA	16:BL:184:PRO:HD3	1.89	0.54
19:BO:201:VAL:HG13	40:Bj:86:VAL:HG22	1.87	0.54
21:BQ:115:LYS:HD2	33:Bc:86:LEU:HD13	1.88	0.54
42:Bm:135:LYS:HD3	42:Bm:239:VAL:HG23	1.88	0.54
47:Br:62:HIS:ND1	47:Br:62:HIS:O	2.39	0.54
50:Bu:186:VAL:HG22	50:Bu:187:GLU:HG3	1.89	0.54
3:B8:1487:C:OP1	28:BX:141:SER:OG	2.22	0.54
6:BB:26:ILE:HD12	6:BB:44:ILE:HG22	1.88	0.54
26:BV:16:ARG:NH2	26:BV:50:ASP:OD2	2.40	0.54
34:Bd:37:ASN:HD21	51:Bv:61:LYS:HB2	1.72	0.54
43:Bn:307:HIS:HB2	43:Bn:311:MET:HE2	1.90	0.54
6:BB:88:LYS:NZ	6:BB:91:ASP:OD1	2.41	0.54
39:Bi:49:ALA:O	39:Bi:61:ARG:NH1	2.40	0.54
21:BQ:128:ASP:OD1	21:BQ:128:ASP:N	2.41	0.54
28:BX:182:ARG:HD3	28:BX:187:LEU:HD11	1.90	0.54
54:By:77:GLU:HG3	54:By:78:VAL:HG13	1.90	0.54
3:B8:7:G:OP2	3:B8:7:G:N2	2.40	0.54
25:BU:134:LYS:HB3	25:BU:138:GLN:HE21	1.73	0.54
42:Bm:215:ARG:NH1	42:Bm:367:ASP:OD1	2.33	0.54
3:B8:1329:U:O2	57:Aa:313:GLN:NE2	2.40	0.53
24:BT:141:VAL:HG21	43:Bn:377:TYR:CE1	2.43	0.53
42:Bm:125:LYS:HG2	42:Bm:371:LYS:HG3	1.90	0.53
3:B8:1131:U:H2'	3:B8:1132:G:C8	2.44	0.53
3:B8:1177:U:H4'	25:BU:144:LYS:HD3	1.90	0.53
7:BC:98:VAL:HG21	7:BC:109:ILE:HD12	1.91	0.53
57:Aa:194:THR:HG21	57:Aa:381:GLN:HG3	1.89	0.53
34:Bd:55:VAL:HG21	34:Bd:69:TYR:HB3	1.90	0.53
48:Bs:26:LEU:HD21	48:Bs:29:LEU:HD11	1.89	0.53
3:B8:123:U:O2	3:B8:254:G:N2	2.40	0.53
38:Bh:144:LYS:H	38:Bh:144:LYS:HD2	1.74	0.53
48:Bs:144:ARG:HB2	48:Bs:147:GLU:HB2	1.90	0.53
3:B8:1396:C:H5	57:Aa:317:LYS:HD2	1.74	0.53
4:B9:18:U:H5'	4:B9:57:C:C5	2.44	0.53
4:B9:66:A:H2'	4:B9:67:A:C8	2.44	0.53
30:BZ:148:LEU:HB2	47:Br:58:ILE:HB	1.90	0.53
3:B8:29:A:N3	3:B8:35:A:O2'	2.38	0.53
40:Bj:117:PRO:HB2	40:Bj:261:ASN:HD21	1.73	0.53
48:Bs:133:PHE:HZ	49:Bt:261:SER:HB2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BZ:135:GLU:N	30:BZ:135:GLU:OE1	2.42	0.53
40:Bj:143:VAL:HG22	40:Bj:242:GLU:HA	1.90	0.53
3:B8:218:A:N6	3:B8:229:A:O4'	2.42	0.53
44:Bo:206:LEU:HD21	44:Bo:254:PHE:HE2	1.74	0.53
55:Bz:99:GLY:HA2	55:Bz:102:MET:HE2	1.90	0.53
3:B8:1192:U:OP2	15:BK:142:ARG:NH2	2.41	0.52
5:BA:96:SER:H	5:BA:99:GLN:HE21	1.57	0.52
16:BL:258:ILE:HG23	16:BL:263:ARG:HB3	1.90	0.52
57:Aa:395:VAL:HG23	57:Aa:407:ILE:HG12	1.92	0.52
3:B8:1110:G:OP2	19:BO:242:ARG:NE	2.43	0.52
31:Ba:111:LYS:N	43:Bn:308:GLN:OE1	2.41	0.52
50:Bu:161:HIS:O	50:Bu:260:ARG:NH2	2.43	0.52
24:BT:153:ASN:HB2	24:BT:256:LEU:HD23	1.92	0.52
32:Bb:67:LEU:HD12	32:Bb:72:HIS:O	2.09	0.52
3:B8:353:C:O2	3:B8:1267:A:O2'	2.26	0.52
13:BI:34:ARG:NH1	13:BI:38:ARG:O	2.43	0.52
17:BM:227:GLN:OE1	17:BM:227:GLN:N	2.42	0.52
3:B8:78:A:OP2	15:BK:108:LYS:NZ	2.36	0.52
15:BK:168:ARG:NH1	15:BK:170:ASN:OD1	2.42	0.52
18:BN:92:ARG:HB2	18:BN:176:VAL:HG11	1.91	0.52
52:Bw:173:ILE:O	52:Bw:177:ASN:ND2	2.33	0.52
19:BO:189:VAL:HG21	19:BO:208:LEU:HD21	1.90	0.52
22:BR:15:ALA:HB1	49:Bt:269:VAL:HG21	1.91	0.52
51:Bv:157:LEU:HB3	51:Bv:254:TRP:HB3	1.92	0.52
32:Bb:46:ASN:OD1	32:Bb:46:ASN:N	2.40	0.52
33:Bc:114:THR:HG22	33:Bc:116:GLU:H	1.75	0.52
51:Bv:147:THR:HG21	51:Bv:248:LYS:HB3	1.90	0.52
3:B8:41:A:H2'	3:B8:42:C:H4'	1.91	0.52
3:B8:1292:A:N6	3:B8:1304:G:O2'	2.42	0.52
10:BF:85:ALA:N	46:Bq:72:VAL:O	2.42	0.52
54:By:143:GLU:O	54:By:147:SER:OG	2.27	0.52
1:B6:76:LEU:HA	1:B6:79:ILE:HG12	1.91	0.51
3:B8:31:A:H1'	14:BJ:73:LEU:HD12	1.92	0.51
17:BM:196:ALA:O	17:BM:199:ARG:NH1	2.43	0.51
42:Bm:201:ARG:HD3	42:Bm:230:LEU:HD21	1.91	0.51
21:BQ:17:SER:N	21:BQ:72:VAL:O	2.43	0.51
3:B8:1108:A:O2'	19:BO:239:ASN:ND2	2.43	0.51
6:BB:21:ARG:NH1	10:BF:145:ASP:OD1	2.42	0.51
42:Bm:123:LEU:HD22	42:Bm:220:LEU:HD21	1.92	0.51
44:Bo:41:GLN:HB3	44:Bo:258:ILE:HD12	1.92	0.51
3:B8:8:C:H5	49:Bt:31:ALA:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Bd:39:ALA:HB3	52:Bw:179:PRO:HG3	1.93	0.51
42:Bm:240:ALA:H	42:Bm:358:GLN:HE22	1.59	0.51
44:Bo:183:ASP:OD1	44:Bo:184:LYS:N	2.44	0.51
21:BQ:25:ARG:NH1	21:BQ:63:GLY:O	2.43	0.51
26:BV:55:TYR:HE1	28:BX:270:MET:HB2	1.75	0.51
51:Bv:205:LEU:HB3	52:Bw:168:GLU:HG3	1.93	0.51
3:B8:776:C:O2'	3:B8:777:A:H2'	2.11	0.51
3:B8:1231:U:H5''	15:BK:135:LYS:HD3	1.92	0.51
39:Bi:195:ASP:HB2	39:Bi:234:GLN:HB2	1.92	0.51
40:Bj:105:LEU:HD12	40:Bj:108:LYS:HD3	1.93	0.51
3:B8:624:A:O2'	18:BN:108:ARG:NH1	2.41	0.51
9:BE:227:PHE:HD1	10:BF:158:LEU:HD12	1.75	0.51
40:Bj:133:LYS:HG2	40:Bj:134:LYS:H	1.76	0.51
20:BP:113:ARG:HH11	20:BP:123:MET:HG3	1.75	0.51
3:B8:317:A:OP1	14:BJ:59:SER:OG	2.25	0.51
9:BE:174:PRO:O	9:BE:184:ARG:NH2	2.41	0.51
27:BW:91:GLU:HG3	27:BW:106:SER:HB3	1.93	0.51
3:B8:216:C:O3'	53:Bx:90:ARG:NH1	2.44	0.51
7:BC:112:GLU:OE2	50:Bu:74:ARG:NH1	2.44	0.51
3:B8:84:G:OP2	15:BK:113:ARG:NH2	2.43	0.50
9:BE:167:LEU:HD21	9:BE:202:GLU:HB3	1.93	0.50
39:Bi:184:VAL:HG12	42:Bm:193:LEU:HA	1.93	0.50
51:Bv:98:LEU:HD23	51:Bv:101:LYS:HD2	1.92	0.50
55:Bz:69:HIS:CD2	55:Bz:71:LYS:H	2.29	0.50
3:B8:528:U:O2'	33:Bc:115:ARG:NH2	2.45	0.50
3:B8:843:C:O2'	16:BL:258:ILE:O	2.23	0.50
11:BG:148:ARG:HD2	11:BG:151:LEU:HD11	1.93	0.50
42:Bm:310:ARG:HA	42:Bm:313:MET:HE2	1.93	0.50
1:B3:71:ILE:HG12	1:B4:67:LEU:HD13	1.92	0.50
36:Bf:114:VAL:HG22	36:Bf:161:SER:HA	1.94	0.50
3:B8:1161:G:OP1	8:BD:49:LYS:NZ	2.37	0.50
3:B8:1187:U:O2'	3:B8:1189:U:OP2	2.29	0.50
39:Bi:100:LEU:O	39:Bi:313:GLN:NE2	2.38	0.50
56:AG:26:G:H2'	56:AG:27:G:H8	1.76	0.50
16:BL:198:GLU:OE2	16:BL:202:GLY:N	2.41	0.50
39:Bi:146:GLN:HA	39:Bi:150:PHE:HB2	1.92	0.50
3:B8:575:C:H5	38:Bh:186:SER:HA	1.77	0.50
48:Bs:133:PHE:HB3	49:Bt:259:ARG:HD3	1.94	0.50
49:Bt:112:LYS:HE3	49:Bt:116:LEU:HB2	1.92	0.50
1:B2:77:LEU:HD23	20:BP:197:LEU:HD22	1.92	0.50
5:BA:98:ASP:OD2	44:Bo:94:GLU:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Bv:138:THR:OG1	51:Bv:150:HIS:O	2.28	0.50
3:B8:659:U:H5''	39:Bi:55:SER:HB2	1.94	0.49
5:BA:210:LEU:HB3	48:Bs:119:PHE:CE1	2.47	0.49
18:BN:62:VAL:HG23	54:By:119:HIS:HB3	1.93	0.49
24:BT:12:ALA:HB2	35:Be:88:LEU:HD13	1.94	0.49
3:B8:1512:U:OP2	41:Bl:82:ARG:NH1	2.46	0.49
51:Bv:42:SER:OG	51:Bv:43:SER:N	2.45	0.49
53:Bx:77:ASP:HB2	53:Bx:78:PRO:HD3	1.93	0.49
19:BO:223:VAL:HG13	40:Bj:86:VAL:HG21	1.94	0.49
3:B8:52:A:O2'	3:B8:349:A:N3	2.44	0.49
12:BH:152:PRO:HG3	12:BH:173:ARG:HH11	1.77	0.49
25:BU:36:VAL:HG21	33:Bc:124:HIS:HB3	1.95	0.49
9:BE:41:VAL:HG11	9:BE:83:GLU:HB3	1.94	0.49
19:BO:156:GLN:HE22	19:BO:226:ASN:HB2	1.75	0.49
20:BP:99:CYS:O	20:BP:152:LEU:N	2.41	0.49
21:BQ:20:ILE:HB	21:BQ:70:ILE:HB	1.94	0.49
45:Bp:77:LYS:NZ	56:AG:48:G:OP2	2.36	0.49
3:B8:1458:G:O2'	3:B8:1467:G:O6	2.28	0.49
18:BN:102:TRP:O	18:BN:106:PHE:HB3	2.13	0.49
21:BQ:117:VAL:HG12	21:BQ:141:VAL:HG23	1.95	0.49
24:BT:112:PRO:HB3	24:BT:152:VAL:HG12	1.95	0.49
45:Bp:191:ARG:HE	45:Bp:193:GLN:HE22	1.61	0.49
7:BC:65:LEU:HD11	7:BC:121:LYS:HE2	1.93	0.49
35:Be:15:ARG:HB3	35:Be:18:ILE:HG12	1.94	0.49
12:BH:132:LYS:NZ	12:BH:136:GLU:OE2	2.43	0.49
45:Bp:67:ARG:HH22	56:AG:10:A:P	2.35	0.49
3:B8:299:A:OP2	3:B8:833:C:N4	2.46	0.49
17:BM:96:ARG:NH2	17:BM:197:HIS:O	2.45	0.49
19:BO:102:VAL:HB	19:BO:105:LEU:HB2	1.94	0.49
23:BS:75:LEU:HD21	23:BS:105:VAL:HG21	1.95	0.49
42:Bm:107:PHE:HB2	42:Bm:265:LEU:HD22	1.95	0.49
45:Bp:77:LYS:HZ3	56:AG:48:G:P	2.35	0.49
3:B8:644:G:OP1	12:BH:93:ARG:NH1	2.45	0.49
3:B8:1124:C:H2'	3:B8:1125:U:C6	2.48	0.49
17:BM:334:ASP:HB3	17:BM:337:VAL:HG23	1.95	0.49
21:BQ:43:GLY:HA3	21:BQ:76:ARG:HH11	1.78	0.49
24:BT:109:ARG:HH21	24:BT:125:ARG:HB2	1.77	0.49
31:Ba:47:PRO:HA	31:Ba:60:MET:HE3	1.95	0.49
3:B8:480:G:OP2	30:BZ:108:HIS:ND1	2.44	0.48
3:B8:644:G:P	12:BH:93:ARG:HH12	2.35	0.48
4:B9:49:G:N2	4:B9:63:C:O2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BT:203:ARG:HH21	24:BT:262:PRO:HA	1.78	0.48
48:Bs:75:VAL:HG13	48:Bs:87:GLU:HB2	1.95	0.48
56:AG:47:U:H3	56:AG:58:U:H3	1.61	0.48
25:BU:72:ILE:HD11	25:BU:96:TYR:CZ	2.48	0.48
40:Bj:108:LYS:HE2	40:Bj:112:LEU:HD11	1.93	0.48
56:AG:22:U:H2'	56:AG:23:A:H8	1.78	0.48
57:Aa:188:GLU:HB2	57:Aa:283:ILE:HB	1.95	0.48
20:BP:61:ASN:HD22	20:BP:63:ARG:H	1.59	0.48
3:B8:1336:A:H2'	3:B8:1337:G:H8	1.78	0.48
7:BC:191:LEU:HD12	46:Bq:116:GLY:HA3	1.94	0.48
17:BM:206:VAL:HG13	17:BM:297:VAL:HG13	1.94	0.48
39:Bi:173:GLN:HE22	42:Bm:203:CYS:HB3	1.77	0.48
43:Bn:86:ASP:OD1	43:Bn:86:ASP:N	2.44	0.48
48:Bs:45:GLU:OE1	48:Bs:49:ARG:NH1	2.46	0.48
50:Bu:138:PRO:HB2	50:Bu:192:PRO:HG2	1.96	0.48
57:Aa:389:ASN:HB3	57:Aa:394[A]:ARG:HG3	1.94	0.48
43:Bn:173:LEU:HD12	43:Bn:272:LEU:HD22	1.94	0.48
1:B3:76:LEU:HD11	1:B6:79:ILE:HG21	1.95	0.48
26:BV:32:LEU:HB3	26:BV:52:LEU:HD22	1.96	0.48
3:B8:844:A:O2'	3:B8:873:U:OP1	2.29	0.48
4:B9:29:G:OP1	45:Bp:133:ARG:NH2	2.46	0.48
20:BP:123:MET:HE3	20:BP:152:LEU:HD11	1.95	0.48
39:Bi:281:LYS:NZ	42:Bm:166:SER:O	2.46	0.48
3:B8:515:A:H2'	3:B8:541:A:H5'	1.96	0.48
3:B8:525:A:N6	3:B8:532:A:OP2	2.46	0.48
3:B8:1196:G:OP2	43:Bn:368:ARG:NH1	2.47	0.48
19:BO:118:VAL:HG13	19:BO:122:ARG:HE	1.79	0.48
25:BU:211:ASN:ND2	25:BU:213:TRP:O	2.45	0.48
27:BW:138:GLU:OE1	43:Bn:136:ARG:NH1	2.47	0.48
40:Bj:96:ILE:HG21	40:Bj:303:LEU:HD13	1.96	0.48
49:Bt:237:PRO:HG3	49:Bt:298:ARG:HE	1.79	0.48
3:B8:1425:A:O2'	56:AG:69:C:OP2	2.29	0.48
9:BE:117:GLU:OE1	9:BE:190:ARG:NH2	2.46	0.48
30:BZ:115:GLU:HG2	48:Bs:19:LEU:HD11	1.95	0.48
42:Bm:322:LEU:HG	42:Bm:326:ARG:HH12	1.79	0.48
50:Bu:185:PHE:HZ	50:Bu:188:SER:HB2	1.79	0.48
51:Bv:45:TRP:CG	51:Bv:230:LYS:HE3	2.49	0.48
3:B8:76:G:H3'	15:BK:163:THR:HG21	1.96	0.48
3:B8:560:A:H3'	3:B8:561:C:O2	2.14	0.48
18:BN:220:ASP:O	18:BN:245:ALA:N	2.46	0.48
43:Bn:139:TRP:CD1	43:Bn:143:CYS:HG	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Bt:101:GLU:O	49:Bt:105:ARG:HG2	2.13	0.48
3:B8:1323:U:O2'	3:B8:1327:U:OP1	2.32	0.47
3:B8:1360:U:H2'	3:B8:1361:A:H8	1.78	0.47
32:Bb:16:VAL:HG22	32:Bb:66:VAL:HG13	1.96	0.47
42:Bm:288:PRO:HD2	42:Bm:324:GLN:CD	2.39	0.47
47:Br:40:PRO:HG2	47:Br:43:TYR:HE1	1.79	0.47
57:Aa:190:THR:OG1	57:Aa:281:SER:OG	2.31	0.47
3:B8:143:A:H2'	3:B8:144:A:C8	2.48	0.47
3:B8:154:A:OP1	12:BH:95:ARG:NH2	2.47	0.47
44:Bo:305:HIS:CD2	44:Bo:307:THR:H	2.32	0.47
60:B9:101:PHE:HB2	51:Bv:165:LEU:HG	1.95	0.47
17:BM:196:ALA:HB1	17:BM:199:ARG:HH12	1.78	0.47
18:BN:133:SER:HB2	18:BN:135[B]:ARG:HH21	1.79	0.47
20:BP:94:ARG:HH21	20:BP:158:GLU:H	1.60	0.47
23:BS:32:ILE:HD11	23:BS:103:ASN:HB3	1.96	0.47
3:B8:76:G:O2'	3:B8:88:G:O6	2.32	0.47
6:BB:20:PHE:O	10:BF:105:TYR:OH	2.28	0.47
18:BN:123:GLY:HA3	18:BN:142:ARG:HG2	1.97	0.47
1:B2:76:LEU:HB3	20:BP:197:LEU:HD23	1.96	0.47
1:B2:77:LEU:HD11	20:BP:186:LEU:HD21	1.97	0.47
3:B8:623:G:O2'	18:BN:105:ASN:ND2	2.47	0.47
4:B9:73:A:H61	51:Bv:231:VAL:HG21	1.79	0.47
6:BB:138:ASP:HB3	6:BB:141:ARG:HG2	1.96	0.47
9:BE:40:PRO:HB3	9:BE:43:TYR:CZ	2.50	0.47
24:BT:111:ASP:OD1	24:BT:111:ASP:N	2.48	0.47
39:Bi:145:LEU:HD22	39:Bi:402:ASN:HA	1.96	0.47
3:B8:723:A:H3'	3:B8:724:A:H5''	1.96	0.47
3:B8:1458:G:N2	3:B8:1468:A:OP2	2.39	0.47
11:BG:59:ASP:O	35:Be:51:ARG:NH2	2.47	0.47
44:Bo:191:PRO:HD2	44:Bo:280:VAL:HG21	1.96	0.47
3:B8:1242:U:H3	13:BI:27:GLY:C	2.23	0.47
7:BC:23:MET:SD	7:BC:114:PRO:HG3	2.54	0.47
15:BK:126:LYS:HE2	15:BK:148:VAL:HG11	1.96	0.47
20:BP:225:GLN:HB2	20:BP:226:PRO:HD3	1.95	0.47
27:BW:178:ILE:HG22	27:BW:179:TYR:HD2	1.80	0.47
29:BY:24:VAL:HG11	29:BY:43:VAL:HG22	1.96	0.47
31:Ba:100:GLN:NE2	31:Ba:103:GLU:OE2	2.48	0.47
32:Bb:33:PHE:HD1	32:Bb:87:LEU:HD12	1.79	0.47
35:Be:82:PHE:CG	35:Be:83:PRO:HD2	2.50	0.47
38:Bh:176:VAL:HG21	38:Bh:196:HIS:CE1	2.49	0.47
40:Bj:61:ALA:N	40:Bj:134:LYS:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:Bn:222:ASP:OD1	43:Bn:222:ASP:N	2.48	0.47
43:Bn:257:PRO:HB3	43:Bn:268:PHE:CZ	2.50	0.47
45:Bp:93:LYS:NZ	45:Bp:99:ARG:HH12	2.13	0.47
49:Bt:148:LEU:HD13	49:Bt:149:PRO:HD2	1.96	0.47
51:Bv:58:LEU:N	51:Bv:153:LEU:O	2.44	0.47
3:B8:33:A:C6	46:Bq:30:PHE:HB2	2.50	0.47
18:BN:220:ASP:OD1	18:BN:221:LEU:N	2.46	0.47
21:BQ:141:VAL:HG11	33:Bc:95:TRP:HZ3	1.80	0.47
24:BT:72:THR:OG1	24:BT:77:ARG:NH2	2.48	0.47
45:Bp:70:LYS:NZ	56:AG:47:U:OP1	2.39	0.47
47:Br:49:LEU:HD23	47:Br:60:CYS:HB3	1.97	0.47
50:Bu:152:LEU:HD11	50:Bu:172:MET:HB2	1.97	0.47
57:Aa:93:LEU:HD21	57:Aa:106:LEU:HB2	1.96	0.47
11:BG:46:PHE:O	35:Be:50:SER:OG	2.24	0.47
17:BM:97:VAL:O	17:BM:197:HIS:NE2	2.48	0.47
20:BP:162:LYS:HE3	20:BP:195:SER:HB2	1.97	0.47
28:BX:77:SER:HB2	28:BX:80:PHE:HD2	1.79	0.47
39:Bi:244:PHE:HE2	39:Bi:365:CYS:HB3	1.80	0.47
1:B1:28:ILE:HG23	1:B2:82:LEU:HD12	1.97	0.47
44:Bo:78:MET:HE1	44:Bo:91:HIS:CE1	2.50	0.47
50:Bu:85:PHE:HB2	50:Bu:198:ARG:HH21	1.80	0.47
3:B8:294:G:H5'	5:BA:159:ARG:HD2	1.96	0.46
5:BA:55:ILE:O	50:Bu:227:ARG:NH2	2.45	0.46
17:BM:277:ASN:ND2	17:BM:331:ASP:OD1	2.49	0.46
19:BO:116:LYS:HE2	19:BO:120:ARG:NH2	2.29	0.46
36:Bf:138:CYS:SG	36:Bf:139:SER:N	2.88	0.46
37:Bg:40:PRO:HG3	37:Bg:51:GLN:HB3	1.95	0.46
3:B8:197:U:O2'	29:BY:38:CYS:SG	2.61	0.46
3:B8:1295:G:H2'	3:B8:1298:C:H42	1.79	0.46
17:BM:274:TRP:HE1	17:BM:286:ASN:HB2	1.81	0.46
18:BN:58:HIS:CD2	18:BN:59:ARG:HG3	2.51	0.46
35:Be:101:TRP:NE1	48:Bs:48:GLU:OE2	2.37	0.46
37:Bg:43:ASP:OD1	37:Bg:43:ASP:N	2.48	0.46
3:B8:396:C:O2'	3:B8:414:A:N6	2.33	0.46
3:B8:644:G:O6	5:BA:81:SER:OG	2.27	0.46
3:B8:801:G:O2'	23:BS:36:THR:HG22	2.15	0.46
24:BT:208:GLU:HB3	37:Bg:103:LEU:HD11	1.97	0.46
28:BX:117:LEU:HG	28:BX:176:VAL:HG22	1.97	0.46
34:Bd:86:SER:O	34:Bd:90:ARG:N	2.34	0.46
40:Bj:115:THR:OG1	40:Bj:116:ASN:N	2.48	0.46
43:Bn:197:GLU:OE1	43:Bn:197:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B8:86:U:H2'	3:B8:87:A:H8	1.80	0.46
11:BG:72:ILE:HD11	11:BG:118:ARG:HB2	1.97	0.46
18:BN:94:ASP:OD1	18:BN:94:ASP:N	2.44	0.46
22:BR:37:VAL:HG13	22:BR:42:LEU:HB2	1.97	0.46
29:BY:101:VAL:HG23	30:BZ:111:LYS:HB2	1.97	0.46
30:BZ:142:ALA:O	48:Bs:127:GLN:NE2	2.49	0.46
42:Bm:125:LYS:HG3	42:Bm:253:LEU:HD11	1.96	0.46
44:Bo:112:MET:HB2	44:Bo:267:PRO:HB3	1.97	0.46
3:B8:1111:G:H5'	40:Bj:116:ASN:HB2	1.97	0.46
5:BA:66:ARG:HH21	50:Bu:230:ARG:HD2	1.81	0.46
25:BU:124:VAL:HA	25:BU:158:ARG:HH21	1.81	0.46
39:Bi:132:ASP:OD1	39:Bi:132:ASP:N	2.45	0.46
39:Bi:410:ASP:OD1	39:Bi:410:ASP:N	2.48	0.46
2:B7:76:A:O2'	3:B8:1235:C:N3	2.39	0.46
3:B8:1326:A:O2'	3:B8:1328:G:OP2	2.33	0.46
16:BL:141:ALA:HB2	16:BL:154:ALA:HB2	1.96	0.46
30:BZ:168:THR:OG1	30:BZ:169:GLU:N	2.47	0.46
42:Bm:210:SER:OG	42:Bm:223:HIS:ND1	2.45	0.46
3:B8:188:C:H3'	30:BZ:181:ARG:NH2	2.29	0.46
3:B8:1360:U:H2'	3:B8:1361:A:C8	2.50	0.46
4:B9:50:A:H2'	4:B9:51:G:C8	2.51	0.46
17:BM:78:CYS:HB3	17:BM:81:LYS:HB2	1.98	0.46
27:BW:104:SER:HG	43:Bn:150:ARG:HH22	1.59	0.46
57:Aa:67:LYS:HG2	57:Aa:71:LYS:HE3	1.98	0.46
3:B8:1116:A:H2'	3:B8:1117:A:O4'	2.16	0.46
27:BW:118:SER:HB3	27:BW:121:ASN:OD1	2.15	0.46
28:BX:165:GLU:HB2	28:BX:168:ASN:HB2	1.97	0.46
43:Bn:238:THR:HG21	43:Bn:281:PHE:HB2	1.98	0.46
45:Bp:200:THR:HG22	52:Bw:200:ALA:HB3	1.98	0.46
4:B9:18:U:H2'	4:B9:19:A:C8	2.51	0.46
43:Bn:40:ILE:HD11	52:Bw:62:LEU:HD22	1.98	0.46
1:B5:83:ASN:ND2	20:BP:234:ASP:OD1	2.49	0.46
3:B8:17:C:H2'	3:B8:18:A:O4'	2.16	0.46
3:B8:443:G:H5''	25:BU:134:LYS:HD3	1.98	0.46
4:B9:51:G:H1	4:B9:60:C:H42	1.64	0.46
4:B9:59:G:H2'	4:B9:60:C:C6	2.50	0.46
3:B8:250:A:N6	3:B8:341:G:O6	2.48	0.45
27:BW:52:ASN:OD1	27:BW:55:ASN:N	2.49	0.45
32:Bb:81:LEU:HD21	38:Bh:49:ILE:HG22	1.98	0.45
8:BD:62:HIS:H	8:BD:65:ASN:ND2	2.14	0.45
22:BR:112:LEU:HD13	22:BR:121:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BV:38:ARG:NH2	26:BV:82:GLU:OE1	2.49	0.45
31:Ba:113:LYS:NZ	43:Bn:312:THR:OG1	2.35	0.45
49:Bt:166:VAL:HG11	49:Bt:192:ARG:HG3	1.98	0.45
50:Bu:226:ASP:OD1	50:Bu:227:ARG:N	2.49	0.45
50:Bu:251:HIS:HE1	50:Bu:253:VAL:HB	1.81	0.45
57:Aa:126:THR:HG22	57:Aa:159:ILE:HG23	1.98	0.45
3:B8:220:G:N3	3:B8:231:C:O2'	2.49	0.45
3:B8:860:G:O5'	16:BL:136:ARG:NH2	2.48	0.45
11:BG:48:PRO:HD3	35:Be:50:SER:OG	2.16	0.45
18:BN:231:VAL:HG13	37:Bg:26:ARG:HD2	1.99	0.45
21:BQ:119:GLU:HG2	33:Bc:75:VAL:HG11	1.97	0.45
22:BR:155:LEU:HB2	38:Bh:86:VAL:HG11	1.98	0.45
3:B8:1051:G:N2	12:BH:79:ALA:HA	2.32	0.45
4:B9:38:MIA:H131	4:B9:38:MIA:N1	2.32	0.45
4:B9:72:C:O4'	51:Bv:267:LYS:NZ	2.37	0.45
47:Br:109:ILE:HG23	47:Br:123:TRP:HB2	1.97	0.45
3:B8:1377:U:H2'	3:B8:1378:U:C6	2.52	0.45
19:BO:85:ASP:HB3	19:BO:88:HIS:HD2	1.81	0.45
30:BZ:67:ASP:OD1	30:BZ:68:ILE:N	2.49	0.45
44:Bo:175:ALA:HB1	44:Bo:295:GLY:O	2.16	0.45
52:Bw:135:LEU:HD22	52:Bw:146:LEU:HA	1.98	0.45
42:Bm:272:ASP:OD1	42:Bm:272:ASP:N	2.48	0.45
49:Bt:60:ARG:HD2	49:Bt:63:LYS:HD2	1.99	0.45
57:Aa:102:ASN:O	57:Aa:105:SER:OG	2.30	0.45
17:BM:45:SER:O	44:Bo:303:ARG:NH2	2.49	0.45
18:BN:66:ILE:HD13	18:BN:263:LEU:HD11	1.98	0.45
27:BW:104:SER:OG	43:Bn:150:ARG:NH2	2.34	0.45
38:Bh:60:SER:HB2	38:Bh:75:TRP:CH2	2.52	0.45
45:Bp:99:ARG:HB2	51:Bv:84:TYR:H	1.81	0.45
47:Br:105:GLN:O	47:Br:109:ILE:HG12	2.16	0.45
51:Bv:172:MET:HE2	51:Bv:172:MET:HB3	1.87	0.45
3:B8:217:A:O2'	3:B8:219:A:O2'	2.28	0.45
3:B8:295:G:N3	3:B8:297:A:N6	2.64	0.45
3:B8:721:A:H5''	42:Bm:301:PRO:HB3	1.97	0.45
16:BL:149:LYS:HE2	42:Bm:114:LEU:HD11	1.99	0.45
36:Bf:190:LYS:NZ	43:Bn:184:LEU:O	2.45	0.45
56:AG:26:G:H2'	56:AG:27:G:C8	2.52	0.45
3:B8:165:A:H5''	29:BY:31:PHE:CE1	2.52	0.45
3:B8:1137:A:H2'	3:B8:1138:G:H8	1.81	0.45
16:BL:155:THR:O	16:BL:249:SER:HB3	2.17	0.45
17:BM:222:TRP:CD1	17:BM:256:LYS:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:BN:61:PRO:HA	18:BN:84:PRO:HD3	1.99	0.45
34:Bd:64:THR:O	45:Bp:178:TYR:N	2.49	0.45
43:Bn:198:ALA:O	43:Bn:254:TYR:OH	2.35	0.45
45:Bp:110:GLU:OE2	45:Bp:113:ARG:NH1	2.50	0.45
3:B8:22:U:O4	10:BF:172:ARG:NH1	2.47	0.45
20:BP:52:GLU:HG2	25:BU:250:ARG:HH12	1.81	0.45
45:Bp:174:GLN:HG2	52:Bw:183:LYS:HG2	1.99	0.45
1:B3:72:ALA:HB1	1:B6:77:LEU:HG	1.99	0.44
5:BA:77:GLN:H	5:BA:171:HIS:CD2	2.35	0.44
17:BM:202:GLN:HA	17:BM:310:PHE:HE2	1.82	0.44
19:BO:194:LEU:HD13	19:BO:200:VAL:HG22	1.98	0.44
21:BQ:23:ILE:HG13	21:BQ:67:PRO:HA	1.99	0.44
30:BZ:118:ILE:HD13	30:BZ:199:ILE:HD11	1.99	0.44
42:Bm:289:HIS:ND1	42:Bm:290:THR:OG1	2.45	0.44
51:Bv:215:PHE:CE1	51:Bv:229:ALA:HB3	2.52	0.44
57:Aa:162:LYS:HA	57:Aa:165:MET:HE2	1.98	0.44
10:BF:136:LYS:NZ	46:Bq:74:TYR:OH	2.44	0.44
19:BO:216:ARG:NH2	19:BO:239:ASN:OD1	2.50	0.44
22:BR:156:ASP:OD1	22:BR:156:ASP:N	2.50	0.44
26:BV:150:LEU:HD23	44:Bo:312:LEU:HD21	1.99	0.44
32:Bb:46:ASN:HB2	32:Bb:48:ASN:OD1	2.16	0.44
40:Bj:130:THR:HG22	40:Bj:131:LEU:H	1.82	0.44
45:Bp:67:ARG:HD3	56:AG:43:A:C5'	2.47	0.44
48:Bs:93:SER:O	48:Bs:97:ILE:HG12	2.18	0.44
49:Bt:148:LEU:HD22	49:Bt:305:PHE:HB3	1.99	0.44
52:Bw:84:THR:HG22	52:Bw:85:ASP:H	1.82	0.44
56:AG:38:C:H2'	56:AG:39:G:C8	2.52	0.44
5:BA:132:VAL:HG11	5:BA:138:LEU:HD21	2.00	0.44
42:Bm:297:ALA:HB3	42:Bm:303:ARG:HG3	1.98	0.44
48:Bs:126:ILE:O	48:Bs:127:GLN:HG2	2.18	0.44
50:Bu:88:TYR:OH	50:Bu:108:ARG:NH1	2.50	0.44
1:B2:77:LEU:HG	20:BP:194:TYR:HD2	1.82	0.44
28:BX:221:LYS:HB3	28:BX:244:ARG:HG2	1.99	0.44
29:BY:11:ARG:NH1	29:BY:13:ARG:HD2	2.32	0.44
34:Bd:62:GLY:HA3	45:Bp:182:ILE:H	1.81	0.44
43:Bn:176:ALA:HB1	43:Bn:184:LEU:HG	2.00	0.44
48:Bs:35:ARG:HG2	54:By:159:TYR:CZ	2.53	0.44
49:Bt:93:VAL:HG12	49:Bt:180:LEU:HD22	1.99	0.44
3:B8:290:A:O2'	3:B8:794:A:OP1	2.35	0.44
3:B8:1140:A:H2'	3:B8:1141:A:H8	1.82	0.44
5:BA:202:ARG:NH1	49:Bt:287:GLU:OE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BC:181:ASP:O	10:BF:95:LYS:NZ	2.50	0.44
20:BP:99:CYS:N	20:BP:152:LEU:O	2.49	0.44
21:BQ:107:GLU:OE1	21:BQ:171:ARG:NH1	2.46	0.44
39:Bi:156:ARG:HH11	39:Bi:161:GLN:HA	1.83	0.44
39:Bi:198:ARG:HD3	39:Bi:199:PRO:HD2	2.00	0.44
42:Bm:380:GLN:HB3	42:Bm:410:THR:HG22	1.99	0.44
44:Bo:218:VAL:HG21	44:Bo:251:LEU:HD12	2.00	0.44
3:B8:132:G:O2'	7:BC:40:ARG:O	2.36	0.44
3:B8:135:G:N1	3:B8:138:A:OP2	2.51	0.44
3:B8:813:A:N6	3:B8:815:A:N1	2.66	0.44
3:B8:1531:C:OP2	38:Bh:146:ARG:NH2	2.50	0.44
10:BF:189:PRO:HD3	42:Bm:78:TRP:CZ2	2.53	0.44
12:BH:130:VAL:HG13	26:BV:132:PRO:HB2	2.00	0.44
13:BI:54:VAL:HB	37:Bg:128:MET:HE3	1.98	0.44
18:BN:284:TYR:HB2	18:BN:285:PRO:HD2	2.00	0.44
19:BO:188:ILE:HG12	40:Bj:112:LEU:HA	1.99	0.44
27:BW:117:TYR:CZ	43:Bn:120:GLU:HG2	2.53	0.44
32:Bb:48:ASN:OD1	32:Bb:48:ASN:N	2.50	0.44
52:Bw:163:SER:HG	52:Bw:166:PHE:HB2	1.83	0.44
3:B8:364:A:O2'	3:B8:385:U:H5''	2.17	0.44
3:B8:467:A:OP1	35:Be:15:ARG:NH2	2.44	0.44
3:B8:1050:C:H2'	3:B8:1327:U:H4'	1.98	0.44
17:BM:149:GLY:O	17:BM:173:LYS:HD2	2.18	0.44
17:BM:257:MET:HG3	17:BM:258:PRO:HD2	1.98	0.44
25:BU:65:GLU:OE1	25:BU:65:GLU:N	2.45	0.44
34:Bd:82:LEU:HD12	34:Bd:85:LEU:HD12	1.99	0.44
49:Bt:105:ARG:HA	49:Bt:105:ARG:HH11	1.82	0.44
5:BA:101:LEU:HD22	5:BA:116:LYS:HG3	2.00	0.44
5:BA:210:LEU:HD12	29:BY:104:ASP:HB3	1.99	0.44
6:BB:8:PRO:HG3	46:Bq:132:ASN:O	2.18	0.44
23:BS:104:ASN:ND2	28:BX:158:GLN:OE1	2.41	0.44
30:BZ:178:PHE:HD1	30:BZ:185:GLN:HG2	1.83	0.44
43:Bn:221:LEU:HB2	43:Bn:267:ARG:HG3	1.99	0.44
4:B9:58:A:H2'	4:B9:59:G:C8	2.53	0.44
9:BE:215:GLN:NE2	9:BE:219:GLU:OE2	2.45	0.44
42:Bm:162:ARG:HD2	42:Bm:383:TYR:OH	2.18	0.44
3:B8:249:G:N2	3:B8:344:U:O2	2.51	0.43
3:B8:680:C:H2'	3:B8:681:A:H8	1.83	0.43
3:B8:1166:A:N6	3:B8:1173:A:OP2	2.50	0.43
4:B9:17:U:H1'	43:Bn:98:SER:HA	1.99	0.43
17:BM:56:GLU:HG2	26:BV:154:ARG:HH12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:BN:132:GLY:HA3	50:Bu:42:THR:HG21	2.00	0.43
19:BO:178:ASN:H	19:BO:178:ASN:HD22	1.65	0.43
22:BR:132:ASP:OD1	22:BR:132:ASP:N	2.51	0.43
27:BW:52:ASN:HD21	43:Bn:320:GLN:HE22	1.66	0.43
1:B1:40:LEU:HA	1:B1:43:ILE:HD12	2.00	0.43
3:B8:774:A:OP1	39:Bi:81:ARG:NH2	2.36	0.43
3:B8:1118:A:H5''	3:B8:1119:C:H2'	2.01	0.43
3:B8:1325:G:H5'	3:B8:1326:A:H5''	1.99	0.43
4:B9:17:U:OP2	4:B9:58:A:N6	2.51	0.43
7:BC:15:LEU:HD21	7:BC:26:PRO:HB3	2.00	0.43
7:BC:145:ARG:HH22	7:BC:157:PRO:HD3	1.83	0.43
16:BL:127:VAL:HG22	16:BL:143:VAL:HG22	2.01	0.43
57:Aa:393:ASP:OD1	57:Aa:407:ILE:HG13	2.19	0.43
3:B8:613:U:H5'	18:BN:255:LYS:HE3	2.01	0.43
17:BM:97:VAL:HG22	17:BM:181:VAL:HG21	1.99	0.43
17:BM:151:THR:HG23	17:BM:171:PRO:HB2	2.00	0.43
19:BO:97:VAL:HG22	19:BO:111:LEU:HD23	2.00	0.43
39:Bi:197:LYS:HB3	39:Bi:230:LYS:HE3	2.00	0.43
51:Bv:87:HIS:NE2	51:Bv:121:GLU:OE2	2.51	0.43
56:AG:18:A:H2'	56:AG:43:A:N6	2.34	0.43
3:B8:930:A:N6	3:B8:958:U:OP2	2.38	0.43
43:Bn:194:THR:HB	43:Bn:197:GLU:OE1	2.19	0.43
3:B8:1376:OMG:H1'	3:B8:1405:A:N3	2.34	0.43
12:BH:138:ARG:HA	12:BH:141:MET:HE2	2.01	0.43
17:BM:79:PRO:HB3	17:BM:191:THR:HG23	2.01	0.43
18:BN:69:LEU:HD21	18:BN:212:TRP:HH2	1.84	0.43
42:Bm:174:GLU:HA	42:Bm:296:SER:HB2	2.00	0.43
51:Bv:251:HIS:HD2	51:Bv:252:HIS:HD2	1.66	0.43
3:B8:144:A:H2'	3:B8:145:A:C8	2.54	0.43
3:B8:330:A:H8	3:B8:830:U:O2'	2.02	0.43
3:B8:1117:A:H4'	40:Bj:75:TYR:CE2	2.54	0.43
3:B8:1531:C:H1'	38:Bh:135:LEU:HD12	2.01	0.43
6:BB:25:PHE:CE1	10:BF:111:ARG:HD3	2.53	0.43
16:BL:156:GLU:N	16:BL:247:ARG:O	2.51	0.43
19:BO:115:LYS:HE3	19:BO:118:VAL:HG21	2.00	0.43
21:BQ:115:LYS:NZ	33:Bc:86:LEU:HB2	2.34	0.43
27:BW:116:LEU:HD21	27:BW:127:SER:OG	2.18	0.43
27:BW:146:TYR:CE2	27:BW:148:PRO:HB3	2.54	0.43
34:Bd:83:ASP:HA	34:Bd:90:ARG:HH21	1.84	0.43
52:Bw:131:THR:HG23	52:Bw:151:THR:HG22	2.01	0.43
54:By:67:LEU:HD11	54:By:131:TYR:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B2:76:LEU:HD12	20:BP:194:TYR:CZ	2.54	0.43
3:B8:715:U:H2'	3:B8:716:A:H8	1.83	0.43
3:B8:722:A:H5'	42:Bm:300:ARG:HB3	1.99	0.43
3:B8:842:U:O2'	16:BL:261:ALA:HB2	2.19	0.43
5:BA:151:LEU:HB2	5:BA:167:LYS:HB2	2.01	0.43
21:BQ:32:GLY:O	21:BQ:36:GLY:N	2.37	0.43
46:Bq:21:TRP:HE3	46:Bq:25:ARG:HH21	1.66	0.43
3:B8:1336:A:H2'	3:B8:1337:G:C8	2.54	0.43
7:BC:62:VAL:HB	7:BC:120:VAL:HG13	2.01	0.43
18:BN:234:THR:HG21	18:BN:242:LEU:HB2	2.01	0.43
21:BQ:140:VAL:O	21:BQ:144:ILE:HG12	2.19	0.43
34:Bd:55:VAL:HG22	34:Bd:73:ARG:O	2.19	0.43
44:Bo:151:ILE:HG21	44:Bo:180:VAL:HG21	2.01	0.43
49:Bt:105:ARG:NH2	49:Bt:112:LYS:HB2	2.31	0.43
57:Aa:284:VAL:HG13	57:Aa:375:GLN:HE22	1.82	0.43
3:B8:118:U:OP1	14:BJ:91:LYS:N	2.51	0.43
3:B8:207:A:H61	3:B8:237:A:H5'	1.84	0.43
3:B8:291:U:H4'	3:B8:793:A:H4'	2.01	0.43
3:B8:467:A:H62	3:B8:468:A:H62	1.66	0.43
3:B8:894:U:O2'	16:BL:285:ARG:O	2.31	0.43
3:B8:1089:G:H2'	3:B8:1090:U:C6	2.53	0.43
3:B8:1309:U:H2'	3:B8:1310:A:C8	2.54	0.43
5:BA:60:GLN:NE2	5:BA:67:ARG:HB2	2.34	0.43
8:BD:74:ARG:HD3	8:BD:75:TRP:CZ2	2.54	0.43
16:BL:177:ALA:HB1	16:BL:245:VAL:HG11	2.00	0.43
18:BN:241:ASN:HD21	55:Bz:52:ALA:HB1	1.84	0.43
18:BN:276:HIS:O	53:Bx:90:ARG:NH2	2.52	0.43
24:BT:142:GLU:N	24:BT:142:GLU:OE1	2.52	0.43
34:Bd:76:LEU:HD11	52:Bw:147:ASP:OD2	2.17	0.43
36:Bf:75:ARG:NH1	36:Bf:108:ASP:OD1	2.52	0.43
49:Bt:220:ILE:O	49:Bt:223:MET:HG2	2.19	0.43
17:BM:274:TRP:NE1	17:BM:286:ASN:HB2	2.34	0.42
19:BO:159:ALA:O	19:BO:163:THR:HG23	2.18	0.42
40:Bj:123:LEU:HD21	40:Bj:125:LEU:HD21	2.01	0.42
42:Bm:113:LEU:HD12	42:Bm:311:ALA:HB1	1.99	0.42
43:Bn:224:HIS:CE1	43:Bn:227:GLU:H	2.37	0.42
46:Bq:129:TYR:HB3	46:Bq:130:PRO:HD3	2.00	0.42
51:Bv:152:LYS:HB3	51:Bv:155:ARG:HB2	2.01	0.42
1:B2:76:LEU:HB2	20:BP:194:TYR:CE2	2.55	0.42
9:BE:163:ARG:NH1	42:Bm:55:LEU:HD11	2.34	0.42
23:BS:62:ASN:OD1	23:BS:63:LYS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BX:154:THR:HB	28:BX:199:THR:HG22	2.01	0.42
43:Bn:288:SER:HB3	43:Bn:289:PRO:HD3	2.00	0.42
44:Bo:177:CYS:HB3	44:Bo:294:GLN:HG2	2.01	0.42
3:B8:660:C:O3'	26:BV:81:THR:OG1	2.32	0.42
3:B8:727:A:OP2	42:Bm:300:ARG:NH2	2.52	0.42
3:B8:1109:A:H8	19:BO:179:ASN:HD21	1.68	0.42
4:B9:8:U:H3	4:B9:13:U:H3	1.67	0.42
9:BE:20:ILE:HD12	9:BE:20:ILE:H	1.84	0.42
10:BF:153:ASP:OD1	10:BF:154:ALA:N	2.52	0.42
18:BN:174:LEU:HD21	18:BN:249:ASN:HA	2.01	0.42
42:Bm:181:VAL:HG21	42:Bm:294:LEU:HD22	2.02	0.42
43:Bn:279:ILE:HG12	43:Bn:307:HIS:HD2	1.83	0.42
50:Bu:121:SER:OG	50:Bu:197:VAL:O	2.37	0.42
3:B8:232:U:H2'	3:B8:233:A:H8	1.84	0.42
3:B8:832:A:N1	14:BJ:52:ARG:NH1	2.68	0.42
4:B9:51:G:N2	4:B9:61:U:O2	2.53	0.42
3:B8:198:U:H2'	3:B8:199:A:C8	2.54	0.42
3:B8:1115:A:H2'	3:B8:1116:A:O4'	2.20	0.42
9:BE:6:VAL:HG13	9:BE:11:TRP:HE1	1.84	0.42
12:BH:156:THR:HG23	12:BH:173:ARG:HG3	2.01	0.42
24:BT:97:SER:OG	24:BT:143:GLU:HB3	2.20	0.42
42:Bm:166:SER:HB3	42:Bm:171:PRO:HG3	2.01	0.42
43:Bn:162:PHE:HB3	43:Bn:165:ALA:HB3	2.02	0.42
51:Bv:58:LEU:HB3	51:Bv:153:LEU:HB3	2.01	0.42
56:AG:38:C:H2'	56:AG:39:G:H8	1.83	0.42
3:B8:532:A:OP1	33:Bc:123:LYS:NZ	2.40	0.42
3:B8:789:A:O2'	17:BM:215:PHE:O	2.26	0.42
3:B8:1108:A:H5'	19:BO:249:LYS:HE3	2.01	0.42
6:BB:27:GLN:HG2	10:BF:115:LEU:HB3	2.00	0.42
11:BG:134:MET:HE1	31:Ba:78:VAL:HG21	2.00	0.42
16:BL:108:ASP:OD2	16:BL:150:ARG:NE	2.52	0.42
17:BM:76:LYS:HG3	17:BM:170:LEU:HD21	2.00	0.42
18:BN:191:ASP:O	18:BN:192:SER:OG	2.37	0.42
23:BS:46:LEU:CD1	23:BS:78:ARG:HD3	2.44	0.42
42:Bm:192:ILE:HD11	42:Bm:199:ALA:HB2	2.01	0.42
44:Bo:76:PHE:HB3	44:Bo:78:MET:HE2	2.00	0.42
46:Bq:68:LEU:HD12	46:Bq:68:LEU:HA	1.88	0.42
54:By:141:PHE:HE1	54:By:155:ILE:HG21	1.85	0.42
56:AG:19:A:H2'	56:AG:20:G:H8	1.85	0.42
3:B8:803:A:H61	3:B8:811:A:H61	1.66	0.42
3:B8:1530:C:H4'	38:Bh:132:ARG:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BO:110:ASP:OD1	19:BO:111:LEU:N	2.52	0.42
26:BV:46:TRP:CD1	26:BV:122:ALA:HB2	2.54	0.42
26:BV:110:ILE:HD13	26:BV:110:ILE:HA	1.85	0.42
39:Bi:291:THR:HG22	39:Bi:352:GLN:HB2	2.01	0.42
43:Bn:262:GLY:HA3	43:Bn:342:PHE:HB2	2.01	0.42
49:Bt:245:LEU:HD22	49:Bt:250:ILE:HD12	2.02	0.42
3:B8:1296:U:O4	57:Aa:104:ARG:HD2	2.19	0.42
7:BC:107:THR:O	7:BC:109:ILE:HG13	2.19	0.42
8:BD:139:GLU:HG3	27:BW:63:ARG:HG3	2.02	0.42
11:BG:77:ARG:O	25:BU:228:LYS:NZ	2.51	0.42
20:BP:127:PRO:HG2	20:BP:130:VAL:HG22	2.01	0.42
29:BY:78:GLU:CD	48:Bs:135:ASN:HD22	2.27	0.42
34:Bd:41:LEU:HD11	51:Bv:67:GLN:HB3	2.02	0.42
42:Bm:207:ASN:HD21	42:Bm:229:ARG:HD2	1.84	0.42
44:Bo:110:TRP:CE2	44:Bo:114:LYS:HE3	2.54	0.42
44:Bo:239:GLU:O	44:Bo:242:SER:OG	2.37	0.42
51:Bv:84:TYR:HD1	51:Bv:88:GLU:HB3	1.85	0.42
3:B8:1408:U:O4'	63:AG:101:FME:HE2	2.20	0.42
15:BK:183:ARG:NH2	43:Bn:355:LYS:O	2.53	0.42
18:BN:46:PRO:HB3	54:By:99:PHE:CE2	2.54	0.42
18:BN:85:ASP:OD1	53:Bx:87:ARG:NH2	2.53	0.42
23:BS:58:ILE:HD11	23:BS:76:ALA:HB2	2.02	0.42
29:BY:57:ARG:HH12	30:BZ:173:LYS:HB3	1.85	0.42
39:Bi:397:GLU:HB3	39:Bi:406:GLY:HA3	2.01	0.42
42:Bm:173:ARG:HA	42:Bm:176:TYR:CE2	2.54	0.42
45:Bp:93:LYS:HZ3	45:Bp:99:ARG:HH12	1.65	0.42
49:Bt:188:PRO:N	49:Bt:189:PRO:HD2	2.35	0.42
3:B8:68:A:H61	55:Bz:95:LYS:NZ	2.18	0.42
14:BJ:85:ARG:HE	14:BJ:90:ARG:HG3	1.84	0.42
19:BO:174:VAL:HG13	19:BO:192:HIS:CD2	2.54	0.42
21:BQ:43:GLY:HA3	21:BQ:76:ARG:NH1	2.35	0.42
23:BS:98:PRO:HA	28:BX:162:ILE:HG12	2.01	0.42
26:BV:34:THR:OG1	26:BV:81:THR:HG22	2.20	0.42
30:BZ:98:ARG:HB3	48:Bs:126:ILE:HD13	2.01	0.42
45:Bp:164:ARG:HD3	52:Bw:83:GLY:HA2	2.02	0.42
3:B8:838:A:H1'	3:B8:933:A:H61	1.85	0.41
3:B8:1177:U:O2'	25:BU:64:ARG:O	2.38	0.41
5:BA:154:ILE:HG13	50:Bu:52:SER:HB3	2.02	0.41
12:BH:182:PRO:HG2	12:BH:185:PHE:HB2	2.02	0.41
21:BQ:30:ARG:HE	33:Bc:56:LEU:HD21	1.85	0.41
31:Ba:45:GLU:HG3	31:Ba:63:GLN:HE22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Bf:195:ALA:HB2	43:Bn:203:GLU:HB3	2.02	0.41
42:Bm:363:ASP:OD1	42:Bm:363:ASP:N	2.48	0.41
44:Bo:186:LEU:O	44:Bo:291:ARG:NH2	2.53	0.41
44:Bo:253:ARG:HG3	44:Bo:258:ILE:HG12	2.02	0.41
3:B8:36:A:C4	46:Bq:32:LYS:HG3	2.55	0.41
3:B8:465:A:N6	35:Be:16:GLN:OE1	2.53	0.41
3:B8:680:C:H2'	3:B8:681:A:C8	2.55	0.41
3:B8:1116:A:H4'	40:Bj:294:PHE:CE1	2.54	0.41
9:BE:159:MET:HB3	9:BE:205:GLY:HA2	2.02	0.41
16:BL:198:GLU:HB3	16:BL:241:CYS:HB3	2.01	0.41
54:By:70:ARG:HH11	54:By:109:LEU:HD23	1.85	0.41
3:B8:1212:U:H2'	3:B8:1213:A:C8	2.55	0.41
3:B8:1513:U:H2'	3:B8:1514:A:H8	1.85	0.41
34:Bd:42:THR:OG1	34:Bd:43:ARG:N	2.53	0.41
50:Bu:207:ASN:HA	50:Bu:253:VAL:HG21	2.02	0.41
3:B8:2:C:O2'	5:BA:147:ARG:O	2.32	0.41
21:BQ:73:LYS:HE2	21:BQ:79:GLU:HG3	2.02	0.41
24:BT:26:ASN:OD1	24:BT:26:ASN:N	2.54	0.41
26:BV:129:ASN:OD1	26:BV:129:ASN:N	2.54	0.41
29:BY:141:ILE:HG21	30:BZ:76:GLU:HG2	2.03	0.41
35:Be:23:ARG:HA	35:Be:24:PRO:HD3	1.87	0.41
38:Bh:35:PHE:N	38:Bh:56:THR:HG1	2.16	0.41
39:Bi:151:LEU:HD11	42:Bm:207:ASN:HB3	2.01	0.41
43:Bn:118:GLU:CD	43:Bn:118:GLU:H	2.29	0.41
3:B8:727:A:O2'	3:B8:728:C:O4'	2.33	0.41
3:B8:1230:U:H5'	3:B8:1231:U:C5'	2.50	0.41
30:BZ:103:VAL:HG12	30:BZ:137:VAL:HG22	2.02	0.41
45:Bp:177:ASP:O	51:Bv:59:VAL:HA	2.20	0.41
3:B8:449:C:H4'	3:B8:1319:G:O2'	2.20	0.41
3:B8:925:G:N2	3:B8:964:A:OP2	2.32	0.41
16:BL:74:VAL:O	16:BL:151:TRP:NE1	2.50	0.41
17:BM:334:ASP:OD1	17:BM:335:GLU:N	2.54	0.41
18:BN:283:LEU:HB2	24:BT:125:ARG:NH1	2.29	0.41
36:Bf:180:GLU:OE2	43:Bn:322:ARG:NH1	2.53	0.41
49:Bt:160:LEU:HD11	49:Bt:223:MET:HE3	2.02	0.41
3:B8:655:C:C6	12:BH:138:ARG:HB3	2.55	0.41
3:B8:1122:A:H2'	3:B8:1123:A:C8	2.55	0.41
7:BC:202:MET:HE3	7:BC:202:MET:HB2	1.84	0.41
18:BN:64:ALA:HA	54:By:118:LEU:HD12	2.03	0.41
18:BN:141:ILE:O	18:BN:142:ARG:HD3	2.21	0.41
22:BR:17:VAL:HG11	48:Bs:136:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BR:177:ARG:HB2	38:Bh:36:ARG:HH21	1.86	0.41
30:BZ:135:GLU:HB2	30:BZ:155:LYS:HG2	2.02	0.41
36:Bf:134:LEU:HD21	36:Bf:152:LYS:HD2	2.03	0.41
52:Bw:137:LEU:HD12	52:Bw:138:GLN:H	1.84	0.41
57:Aa:307:ALA:HB2	57:Aa:321:ALA:HB2	2.03	0.41
3:B8:247:C:H2'	3:B8:248:A:C8	2.56	0.41
3:B8:838:A:H1'	3:B8:933:A:N6	2.36	0.41
5:BA:79:LYS:HA	5:BA:79:LYS:HD2	1.90	0.41
37:Bg:149:ASP:OD2	37:Bg:153:ARG:NH2	2.54	0.41
47:Br:84:ILE:HG22	47:Br:85:GLU:HG3	2.02	0.41
57:Aa:70:TRP:CE2	57:Aa:76:GLN:HG2	2.55	0.41
57:Aa:205:ARG:HB2	57:Aa:235:LEU:HD13	2.02	0.41
57:Aa:393:ASP:O	57:Aa:405:ARG:NE	2.45	0.41
3:B8:219:A:H5'	53:Bx:91:MET:HG3	2.03	0.41
3:B8:299:A:H61	3:B8:1432:U:H3	1.69	0.41
3:B8:627:C:N4	24:BT:39:ARG:HD2	2.36	0.41
3:B8:1107:A:H2'	3:B8:1108:A:O4'	2.21	0.41
3:B8:1115:A:H1'	40:Bj:296:ARG:NH1	2.36	0.41
4:B9:14:A:H2'	4:B9:15:A:O4'	2.21	0.41
5:BA:78:ILE:HG22	5:BA:80:TYR:H	1.86	0.41
6:BB:50:ARG:NH1	6:BB:69:ARG:HA	2.35	0.41
7:BC:137:PHE:CZ	7:BC:141:GLY:HA2	2.56	0.41
10:BF:105:TYR:CE2	46:Bq:60:VAL:HG12	2.56	0.41
10:BF:212:ARG:O	10:BF:216:GLU:HG2	2.21	0.41
18:BN:49:ARG:HB3	18:BN:80:THR:OG1	2.21	0.41
18:BN:62:VAL:HG13	18:BN:82:LEU:HB2	2.03	0.41
18:BN:211:ARG:HH12	54:By:57:GLN:HG3	1.86	0.41
20:BP:94:ARG:HH21	20:BP:158:GLU:N	2.19	0.41
25:BU:54:GLU:H	25:BU:54:GLU:CD	2.28	0.41
25:BU:154:VAL:HG11	25:BU:160:ILE:HD11	2.03	0.41
28:BX:181:LYS:HD2	28:BX:217:VAL:HG22	2.02	0.41
29:BY:87:ILE:HD13	29:BY:87:ILE:HA	1.92	0.41
32:Bb:18:VAL:HG12	32:Bb:20:PHE:HD1	1.86	0.41
34:Bd:46:ARG:HG3	34:Bd:47:GLN:H	1.85	0.41
39:Bi:184:VAL:HG23	39:Bi:185:HIS:CD2	2.56	0.41
39:Bi:265:LEU:N	39:Bi:266:PRO:HA	2.36	0.41
40:Bj:72:ILE:HA	40:Bj:75:TYR:CD2	2.56	0.41
40:Bj:95:GLN:HG3	40:Bj:96:ILE:HG13	2.03	0.41
40:Bj:119:GLN:HB2	40:Bj:260:LEU:HB2	2.02	0.41
43:Bn:215:THR:HB	43:Bn:273:PHE:HB2	2.02	0.41
48:Bs:65:VAL:HB	54:By:155:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Bu:288:LYS:NZ	50:Bu:291:GLU:HB2	2.36	0.41
54:By:74:HIS:O	54:By:78:VAL:HG22	2.21	0.41
56:AG:8:U:H5'	56:AG:45:G:H5'	2.02	0.41
57:Aa:258:HIS:HB3	57:Aa:388:TYR:HE1	1.86	0.41
3:B8:354:U:H2'	3:B8:355:G:H8	1.84	0.41
3:B8:574:A:H61	38:Bh:82:ASN:ND2	2.19	0.41
3:B8:737:G:H2'	3:B8:738:U:C6	2.56	0.41
3:B8:1114:U:O4	40:Bj:299:THR:HG22	2.21	0.41
8:BD:102:GLU:HB2	8:BD:130:PHE:CD1	2.56	0.41
12:BH:181:ARG:NH1	12:BH:187:GLN:HB2	2.36	0.41
24:BT:115:PRO:HD3	24:BT:255:MET:HG2	2.03	0.41
34:Bd:93:ARG:HD2	45:Bp:189:GLU:OE2	2.21	0.41
44:Bo:230:ASN:HB3	44:Bo:233:LYS:HB2	2.03	0.41
45:Bp:72:ILE:HD11	52:Bw:211:LEU:HD11	2.03	0.41
52:Bw:51:LYS:HD3	52:Bw:51:LYS:HA	1.90	0.41
39:Bi:241:LEU:HD11	39:Bi:290:HIS:HA	2.03	0.40
43:Bn:195:PRO:HG3	43:Bn:321:CYS:SG	2.62	0.40
48:Bs:26:LEU:HD22	48:Bs:105:ALA:HA	2.02	0.40
54:By:118:LEU:HD23	54:By:118:LEU:HA	1.92	0.40
55:Bz:79:TRP:CD1	55:Bz:80:LEU:HG	2.56	0.40
56:AG:16:A:H5'	56:AG:55:C:N3	2.36	0.40
3:B8:8:C:N4	3:B8:108:A:OP2	2.54	0.40
3:B8:391:A:N6	35:Be:78:GLN:OE1	2.54	0.40
3:B8:1094:A:H2'	3:B8:1118:A:N1	2.36	0.40
5:BA:210:LEU:HD11	30:BZ:111:LYS:HD2	2.02	0.40
6:BB:7:TYR:CE1	46:Bq:37:LYS:HG3	2.56	0.40
7:BC:189:PRO:O	46:Bq:93:THR:OG1	2.25	0.40
14:BJ:66:LYS:HA	14:BJ:71:ARG:HH11	1.86	0.40
18:BN:219:VAL:HG21	18:BN:261:LEU:HD23	2.03	0.40
22:BR:63:ARG:NH1	22:BR:130:ASP:OD2	2.54	0.40
37:Bg:41:ASP:OD1	37:Bg:41:ASP:N	2.54	0.40
40:Bj:119:GLN:O	40:Bj:260:LEU:N	2.55	0.40
42:Bm:351:LEU:HD21	42:Bm:379:ASP:HA	2.03	0.40
46:Bq:122:GLU:HA	46:Bq:127:GLN:HE21	1.86	0.40
1:B3:76:LEU:HD21	1:B6:79:ILE:HD13	2.04	0.40
3:B8:713:A:H2'	3:B8:714:A:C8	2.56	0.40
5:BA:59:PRO:HA	50:Bu:229:GLY:HA2	2.04	0.40
18:BN:48:LEU:HD22	54:By:95:VAL:HG12	2.03	0.40
20:BP:144:LEU:N	20:BP:145:PRO:HD2	2.36	0.40
21:BQ:25:ARG:HB3	21:BQ:63:GLY:H	1.85	0.40
21:BQ:115:LYS:HE3	21:BQ:115:LYS:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BT:287:ASP:HB3	24:BT:290:LEU:HD13	2.03	0.40
30:BZ:99:LEU:HD23	30:BZ:142:ALA:HB2	2.04	0.40
39:Bi:90:LYS:HD2	39:Bi:226:GLN:HB2	2.04	0.40
39:Bi:211:ILE:HD11	39:Bi:221:ASP:HB3	2.03	0.40
42:Bm:350:ARG:NH1	42:Bm:381:LEU:HD11	2.36	0.40
43:Bn:213:LEU:HB2	43:Bn:275:GLN:HG3	2.02	0.40
44:Bo:77:VAL:O	50:Bu:279:THR:HG23	2.21	0.40
45:Bp:93:LYS:NZ	51:Bv:86:ASP:OD1	2.46	0.40
49:Bt:228:LEU:HB2	49:Bt:307:PHE:CD1	2.56	0.40
1:B1:40:LEU:HD21	1:B3:90:LEU:HD11	2.03	0.40
3:B8:218:A:C5	43:Bn:379:ILE:HG21	2.56	0.40
3:B8:348:G:C8	18:BN:118:ALA:HB2	2.57	0.40
3:B8:717:A:O2'	42:Bm:266:GLN:HG3	2.22	0.40
3:B8:919:G:H4'	56:AG:13:U:H4'	2.02	0.40
5:BA:189:THR:HG23	5:BA:192:ALA:H	1.87	0.40
7:BC:96:ARG:NH1	7:BC:111:SER:OG	2.55	0.40
21:BQ:90:PHE:CD2	21:BQ:120:ILE:HD12	2.57	0.40
22:BR:140:ASN:HA	49:Bt:262:GLY:HA2	2.03	0.40
28:BX:82:PRO:HA	28:BX:83:PRO:HD3	1.95	0.40
30:BZ:88:ASN:HA	30:BZ:91:ILE:HG22	2.04	0.40
39:Bi:99:ALA:HB3	39:Bi:102:ALA:HB2	2.03	0.40
39:Bi:206:ARG:HD3	39:Bi:373:LEU:HB3	2.02	0.40
47:Br:77:ARG:HB2	47:Br:78:PRO:HD3	2.01	0.40
49:Bt:105:ARG:NH1	49:Bt:110:ILE:HB	2.34	0.40
51:Bv:214:LYS:HG2	51:Bv:230:LYS:HG2	2.02	0.40
53:Bx:43:ASP:OD1	53:Bx:43:ASP:N	2.51	0.40
3:B8:1519:U:H5'	38:Bh:99:MET:O	2.21	0.40
18:BN:192:SER:OG	18:BN:194:GLU:OE1	2.24	0.40
19:BO:160:GLY:O	19:BO:163:THR:OG1	2.30	0.40
20:BP:101:HIS:HB3	20:BP:150:HIS:ND1	2.36	0.40
24:BT:127:VAL:HG21	24:BT:138:VAL:HG21	2.04	0.40
36:Bf:190:LYS:HE2	43:Bn:184:LEU:HD23	2.02	0.40
42:Bm:384:GLN:HB3	42:Bm:404:ILE:O	2.22	0.40
44:Bo:64:VAL:HB	44:Bo:76:PHE:HB2	2.04	0.40
49:Bt:126:SER:OG	49:Bt:193:GLN:NE2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B1	43/198 (22%)	40 (93%)	3 (7%)	0	100	100
1	B2	25/198 (13%)	25 (100%)	0	0	100	100
1	B3	26/198 (13%)	26 (100%)	0	0	100	100
1	B4	25/198 (13%)	25 (100%)	0	0	100	100
1	B5	25/198 (13%)	25 (100%)	0	0	100	100
1	B6	24/198 (12%)	24 (100%)	0	0	100	100
5	BA	164/210 (78%)	158 (96%)	6 (4%)	0	100	100
6	BB	147/150 (98%)	145 (99%)	2 (1%)	0	100	100
7	BC	204/216 (94%)	196 (96%)	8 (4%)	0	100	100
8	BD	110/148 (74%)	109 (99%)	1 (1%)	0	100	100
9	BE	242/256 (94%)	240 (99%)	2 (1%)	0	100	100
10	BF	177/250 (71%)	175 (99%)	2 (1%)	0	100	100
11	BG	116/161 (72%)	114 (98%)	2 (2%)	0	100	100
12	BH	108/207 (52%)	108 (100%)	0	0	100	100
13	BI	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
14	BJ	44/95 (46%)	44 (100%)	0	0	100	100
15	BK	93/188 (50%)	92 (99%)	1 (1%)	0	100	100
16	BL	238/306 (78%)	230 (97%)	7 (3%)	1 (0%)	30	62
17	BM	305/399 (76%)	295 (97%)	10 (3%)	0	100	100
18	BN	249/294 (85%)	246 (99%)	3 (1%)	0	100	100
19	BO	200/268 (75%)	192 (96%)	8 (4%)	0	100	100
20	BP	210/257 (82%)	208 (99%)	2 (1%)	0	100	100
21	BQ	174/192 (91%)	170 (98%)	4 (2%)	0	100	100
22	BR	175/197 (89%)	170 (97%)	5 (3%)	0	100	100
23	BS	113/325 (35%)	111 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	BT	286/296 (97%)	274 (96%)	12 (4%)	0	100	100
25	BU	220/251 (88%)	216 (98%)	4 (2%)	0	100	100
26	BV	151/169 (89%)	147 (97%)	4 (3%)	0	100	100
27	BW	141/188 (75%)	134 (95%)	7 (5%)	0	100	100
28	BX	223/303 (74%)	221 (99%)	2 (1%)	0	100	100
29	BY	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
30	BZ	153/209 (73%)	149 (97%)	4 (3%)	0	100	100
31	Ba	95/160 (59%)	94 (99%)	1 (1%)	0	100	100
32	Bb	95/112 (85%)	90 (95%)	5 (5%)	0	100	100
33	Bc	82/138 (59%)	82 (100%)	0	0	100	100
34	Bd	67/126 (53%)	64 (96%)	3 (4%)	0	100	100
35	Be	92/102 (90%)	88 (96%)	4 (4%)	0	100	100
36	Bf	147/205 (72%)	143 (97%)	4 (3%)	0	100	100
37	Bg	133/222 (60%)	132 (99%)	1 (1%)	0	100	100
38	Bh	160/196 (82%)	154 (96%)	6 (4%)	0	100	100
39	Bi	385/433 (89%)	370 (96%)	14 (4%)	1 (0%)	36	67
40	Bj	160/304 (53%)	155 (97%)	5 (3%)	0	100	100
41	Bl	36/100 (36%)	36 (100%)	0	0	100	100
42	Bm	391/423 (92%)	380 (97%)	11 (3%)	0	100	100
43	Bn	352/380 (93%)	336 (96%)	16 (4%)	0	100	100
44	Bo	293/334 (88%)	282 (96%)	11 (4%)	0	100	100
45	Bp	141/162 (87%)	135 (96%)	6 (4%)	0	100	100
46	Bq	120/135 (89%)	114 (95%)	6 (5%)	0	100	100
47	Br	106/142 (75%)	101 (95%)	5 (5%)	0	100	100
48	Bs	149/159 (94%)	145 (97%)	4 (3%)	0	100	100
49	Bt	287/332 (86%)	282 (98%)	5 (2%)	0	100	100
50	Bu	258/306 (84%)	251 (97%)	7 (3%)	0	100	100
51	Bv	236/279 (85%)	232 (98%)	4 (2%)	0	100	100
52	Bw	163/269 (61%)	151 (93%)	12 (7%)	0	100	100
53	Bx	131/166 (79%)	128 (98%)	3 (2%)	0	100	100
54	By	107/198 (54%)	105 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	Bz	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
57	Aa	380/474 (80%)	372 (98%)	8 (2%)	0	100	100
All	All	9260/12922 (72%)	9010 (97%)	248 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	Bi	159	VAL
16	BL	208	ILE

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	B1	30/157 (19%)	30 (100%)	0	100	100
1	B2	26/157 (17%)	25 (96%)	1 (4%)	29	55
1	B3	27/157 (17%)	27 (100%)	0	100	100
1	B4	26/157 (17%)	26 (100%)	0	100	100
1	B5	26/157 (17%)	26 (100%)	0	100	100
1	B6	25/157 (16%)	25 (100%)	0	100	100
5	BA	144/180 (80%)	144 (100%)	0	100	100
6	BB	116/134 (87%)	116 (100%)	0	100	100
7	BC	185/192 (96%)	185 (100%)	0	100	100
8	BD	91/115 (79%)	90 (99%)	1 (1%)	65	74
9	BE	219/229 (96%)	218 (100%)	1 (0%)	81	80
10	BF	164/226 (73%)	164 (100%)	0	100	100
11	BG	110/150 (73%)	110 (100%)	0	100	100
12	BH	99/177 (56%)	99 (100%)	0	100	100
13	BI	49/60 (82%)	48 (98%)	1 (2%)	48	67
14	BJ	41/78 (53%)	41 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	BK	87/162 (54%)	87 (100%)	0	100	100
16	BL	193/248 (78%)	192 (100%)	1 (0%)	81	80
17	BM	263/320 (82%)	263 (100%)	0	100	100
18	BN	218/251 (87%)	216 (99%)	2 (1%)	70	76
19	BO	181/228 (79%)	180 (99%)	1 (1%)	78	79
20	BP	192/231 (83%)	189 (98%)	3 (2%)	55	70
21	BQ	138/151 (91%)	136 (99%)	2 (1%)	59	71
22	BR	155/173 (90%)	154 (99%)	1 (1%)	78	79
23	BS	99/243 (41%)	98 (99%)	1 (1%)	68	75
24	BT	245/249 (98%)	245 (100%)	0	100	100
25	BU	190/210 (90%)	189 (100%)	1 (0%)	81	80
26	BV	132/143 (92%)	132 (100%)	0	100	100
27	BW	123/161 (76%)	121 (98%)	2 (2%)	55	70
28	BX	204/266 (77%)	203 (100%)	1 (0%)	81	80
29	BY	118/127 (93%)	118 (100%)	0	100	100
30	BZ	136/178 (76%)	136 (100%)	0	100	100
31	Ba	77/129 (60%)	77 (100%)	0	100	100
32	Bb	79/88 (90%)	74 (94%)	5 (6%)	16	42
33	Bc	79/114 (69%)	78 (99%)	1 (1%)	61	72
34	Bd	60/114 (53%)	60 (100%)	0	100	100
35	Be	75/82 (92%)	74 (99%)	1 (1%)	61	72
36	Bf	126/177 (71%)	126 (100%)	0	100	100
37	Bg	115/183 (63%)	115 (100%)	0	100	100
38	Bh	149/173 (86%)	148 (99%)	1 (1%)	76	78
39	Bi	340/373 (91%)	337 (99%)	3 (1%)	70	76
40	Bj	150/267 (56%)	149 (99%)	1 (1%)	76	78
41	Bl	36/77 (47%)	36 (100%)	0	100	100
42	Bm	348/365 (95%)	343 (99%)	5 (1%)	59	71
43	Bn	310/328 (94%)	308 (99%)	2 (1%)	78	79
44	Bo	271/299 (91%)	270 (100%)	1 (0%)	84	81
45	Bp	132/150 (88%)	131 (99%)	1 (1%)	73	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	Bq	100/108 (93%)	100 (100%)	0	100	100
47	Br	103/133 (77%)	101 (98%)	2 (2%)	50	68
48	Bs	130/135 (96%)	128 (98%)	2 (2%)	57	71
49	Bt	251/284 (88%)	250 (100%)	1 (0%)	84	81
50	Bu	236/275 (86%)	232 (98%)	4 (2%)	53	70
51	Bv	210/242 (87%)	210 (100%)	0	100	100
52	Bw	135/226 (60%)	134 (99%)	1 (1%)	76	78
53	Bx	122/147 (83%)	122 (100%)	0	100	100
54	By	103/178 (58%)	103 (100%)	0	100	100
55	Bz	88/113 (78%)	88 (100%)	0	100	100
57	Aa	339/424 (80%)	337 (99%)	2 (1%)	78	79
All	All	8216/11008 (75%)	8164 (99%)	52 (1%)	76	79

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B2	86	LEU
8	BD	40	LYS
9	BE	196	ILE
13	BI	50	VAL
16	BL	216	VAL
18	BN	106	PHE
18	BN	129	VAL
19	BO	238	VAL
20	BP	150	HIS
20	BP	171	ILE
20	BP	174	LEU
21	BQ	56	LYS
21	BQ	58	LYS
22	BR	67	PHE
23	BS	89	HIS
25	BU	59	VAL
27	BW	101	VAL
27	BW	149	THR
28	BX	265	LEU
32	Bb	10	LEU
32	Bb	46	ASN
32	Bb	47	LEU

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Mol	Chain	Res	Type
32	Bb	48	ASN
32	Bb	75	ILE
33	Bc	113	GLU
35	Be	101	TRP
38	Bh	70	CYS
39	Bi	124	LYS
39	Bi	210	ILE
39	Bi	399	ILE
40	Bj	130	THR
42	Bm	121	LEU
42	Bm	152	GLU
42	Bm	256	PHE
42	Bm	270	VAL
42	Bm	398	VAL
43	Bn	337	MET
43	Bn	376	THR
44	Bo	260	VAL
45	Bp	195	ILE
47	Br	41	ASP
47	Br	45	CYS
48	Bs	75	VAL
48	Bs	84	VAL
49	Bt	265	THR
50	Bu	57	VAL
50	Bu	186	VAL
50	Bu	238	VAL
50	Bu	266	ILE
52	Bw	84	THR
57	Aa	147	GLN
57	Aa	284	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

Mol	Chain	Res	Type
5	BA	60	GLN
5	BA	99	GLN
5	BA	113	GLN
5	BA	171	HIS
5	BA	193	HIS
5	BA	199	GLN
5	BA	208	HIS
6	BB	82	HIS

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Mol	Chain	Res	Type
8	BD	107	ASN
9	BE	89	HIS
10	BF	197	ASN
12	BH	83	ASN
12	BH	96	ASN
12	BH	144	GLN
13	BI	45	HIS
14	BJ	57	GLN
15	BK	118	HIS
15	BK	154	GLN
16	BL	183	HIS
16	BL	228	GLN
16	BL	236	GLN
17	BM	52	HIS
17	BM	117	HIS
17	BM	125	GLN
17	BM	139	ASN
17	BM	156	HIS
17	BM	277	ASN
18	BN	58	HIS
18	BN	97	HIS
18	BN	223	HIS
18	BN	241	ASN
18	BN	277	ASN
19	BO	88	HIS
19	BO	148	GLN
19	BO	178	ASN
19	BO	239	ASN
20	BP	61	ASN
20	BP	73	GLN
20	BP	115	GLN
20	BP	142	ASN
20	BP	151	ASN
20	BP	224	HIS
21	BQ	84	GLN
21	BQ	103	HIS
21	BQ	133	GLN
22	BR	40	GLN
22	BR	89	GLN
22	BR	160	GLN
23	BS	33	GLN
23	BS	52	HIS

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Mol	Chain	Res	Type
23	BS	59	HIS
23	BS	142	GLN
24	BT	87	HIS
24	BT	94	GLN
24	BT	264	GLN
25	BU	101	HIS
25	BU	138	GLN
25	BU	209	ASN
26	BV	98	GLN
26	BV	116	GLN
27	BW	52	ASN
27	BW	96	HIS
27	BW	147	HIS
28	BX	175	GLN
28	BX	209	GLN
28	BX	253	GLN
29	BY	70	ASN
29	BY	147	GLN
30	BZ	79	HIS
30	BZ	183	ASN
33	Bc	82	GLN
33	Bc	124	HIS
34	Bd	60	GLN
35	Be	30	GLN
35	Be	33	GLN
35	Be	85	HIS
36	Bf	103	HIS
36	Bf	142	GLN
36	Bf	162	GLN
37	Bg	106	GLN
37	Bg	119	GLN
37	Bg	130	GLN
38	Bh	112	HIS
38	Bh	196	HIS
39	Bi	104	ASN
39	Bi	107	GLN
39	Bi	148	HIS
39	Bi	173	GLN
39	Bi	201	HIS
39	Bi	228	ASN
39	Bi	240	GLN
39	Bi	379	GLN

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Mol	Chain	Res	Type
39	Bi	414	GLN
40	Bj	276	ASN
41	Bl	99	GLN
42	Bm	119	GLN
42	Bm	149	ASN
42	Bm	160	HIS
42	Bm	186	GLN
42	Bm	266	GLN
42	Bm	280	GLN
42	Bm	343	GLN
42	Bm	358	GLN
42	Bm	380	GLN
43	Bn	307	HIS
44	Bo	91	HIS
44	Bo	197	HIS
44	Bo	274	GLN
44	Bo	305	HIS
45	Bp	158	HIS
45	Bp	186	GLN
45	Bp	193	GLN
48	Bs	24	GLN
48	Bs	81	ASN
48	Bs	127	GLN
48	Bs	129	GLN
49	Bt	42	GLN
49	Bt	69	HIS
49	Bt	123	GLN
49	Bt	193	GLN
50	Bu	69	HIS
50	Bu	115	ASN
50	Bu	207	ASN
51	Bv	67	GLN
51	Bv	251	HIS
52	Bw	54	HIS
52	Bw	92	ASN
52	Bw	136	GLN
53	Bx	93	ASN
53	Bx	155	GLN
54	By	88	GLN
54	By	96	HIS
55	Bz	65	ASN
55	Bz	69	HIS

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Mol	Chain	Res	Type
57	Aa	124	GLN
57	Aa	164	ASN
57	Aa	183	ASN
57	Aa	202	GLN
57	Aa	258	HIS
57	Aa	336	GLN
57	Aa	381	GLN
57	Aa	392	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B7	2/3 (66%)	1 (50%)	0
3	B8	1570/1571 (99%)	262 (16%)	0
4	B9	72/73 (98%)	13 (18%)	0
56	AG	70/71 (98%)	9 (12%)	0
All	All	1714/1718 (99%)	285 (16%)	0

All (285) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B7	76	A
3	B8	15	A
3	B8	19	U
3	B8	20	A
3	B8	21	C
3	B8	27	A
3	B8	31	A
3	B8	32	C
3	B8	36	A
3	B8	40	C
3	B8	42	C
3	B8	45	A
3	B8	46	A
3	B8	56	A
3	B8	57	A
3	B8	59	A
3	B8	60	U
3	B8	68	A
3	B8	69	C
3	B8	82	G

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Mol	Chain	Res	Type
3	B8	83	A
3	B8	104	C
3	B8	105	G
3	B8	109	U
3	B8	112	A
3	B8	115	U
3	B8	129	A
3	B8	132	G
3	B8	139	G
3	B8	140	A
3	B8	141	A
3	B8	142	U
3	B8	143	A
3	B8	163	C
3	B8	164	A
3	B8	168	A
3	B8	172	C
3	B8	179	U
3	B8	180	A
3	B8	190	U
3	B8	192	A
3	B8	205	A
3	B8	218	A
3	B8	219	A
3	B8	225	C
3	B8	228	U
3	B8	229	A
3	B8	239	C
3	B8	254	G
3	B8	263	G
3	B8	272	A
3	B8	273	A
3	B8	275	A
3	B8	277	A
3	B8	311	A
3	B8	322	G
3	B8	324	G
3	B8	329	A
3	B8	330	A
3	B8	331	A
3	B8	336	A
3	B8	340	A

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Mol	Chain	Res	Type
3	B8	352	G
3	B8	359	G
3	B8	369	G
3	B8	373	U
3	B8	374	U
3	B8	376	A
3	B8	392	U
3	B8	409	A
3	B8	427	G
3	B8	428	A
3	B8	433	G
3	B8	434	U
3	B8	445	A
3	B8	446	C
3	B8	448	G
3	B8	459	A
3	B8	460	C
3	B8	475	C
3	B8	479	A
3	B8	480	G
3	B8	488	U
3	B8	490	U
3	B8	491	U
3	B8	492	A
3	B8	497	U
3	B8	498	A
3	B8	501	A
3	B8	502	U
3	B8	503	A
3	B8	506	A
3	B8	515	A
3	B8	518	A
3	B8	532	A
3	B8	534	A
3	B8	549	C
3	B8	560	A
3	B8	570	A
3	B8	574	A
3	B8	575	C
3	B8	576	U
3	B8	578	A
3	B8	579	U

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Mol	Chain	Res	Type
3	B8	580	A
3	B8	584	A
3	B8	586	C
3	B8	592	G
3	B8	595	C
3	B8	596	A
3	B8	617	A
3	B8	618	A
3	B8	625	A
3	B8	626	G
3	B8	631	A
3	B8	633	U
3	B8	634	G
3	B8	640	A
3	B8	684	A
3	B8	689	A
3	B8	693	U
3	B8	695	U
3	B8	704	U
3	B8	707	A
3	B8	713	A
3	B8	720	C
3	B8	722	A
3	B8	724	A
3	B8	725	C
3	B8	727	A
3	B8	728	C
3	B8	737	G
3	B8	746	U
3	B8	747	U
3	B8	748	A
3	B8	753	G
3	B8	777	A
3	B8	783	A
3	B8	809	G
3	B8	817	A
3	B8	825	C
3	B8	852	C
3	B8	854	U
3	B8	855	U
3	B8	856	A
3	B8	859	A

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Mol	Chain	Res	Type
3	B8	864	U
3	B8	872	A
3	B8	889	C
3	B8	892	G
3	B8	897	A
3	B8	902	C
3	B8	922	A
3	B8	923	A
3	B8	924	G
3	B8	925	G
3	B8	933	A
3	B8	950	U
3	B8	958	U
3	B8	959	G
3	B8	960	U
3	B8	962	U
3	B8	964	A
3	B8	965	A
3	B8	967	G
3	B8	977	G
3	B8	1015	C
3	B8	1016	C
3	B8	1018	U
3	B8	1026	A
3	B8	1027	G
3	B8	1028	A
3	B8	1038	A
3	B8	1050	C
3	B8	1051	G
3	B8	1055	A
3	B8	1056	G
3	B8	1057	A
3	B8	1063	U
3	B8	1064	G
3	B8	1076	A
3	B8	1093	A
3	B8	1094	A
3	B8	1095	C
3	B8	1097	A
3	B8	1099	U
3	B8	1100	C
3	B8	1107	A

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Mol	Chain	Res	Type
3	B8	1113	A
3	B8	1114	U
3	B8	1115	A
3	B8	1119	C
3	B8	1120	A
3	B8	1121	U
3	B8	1146	G
3	B8	1167	C
3	B8	1168	A
3	B8	1169	A
3	B8	1180	G
3	B8	1183	U
3	B8	1188	U
3	B8	1195	A
3	B8	1204	A
3	B8	1206	U
3	B8	1207	C
3	B8	1215	C
3	B8	1217	A
3	B8	1218	U
3	B8	1220	A
3	B8	1221	C
3	B8	1222	A
3	B8	1226	C
3	B8	1231	U
3	B8	1233	A
3	B8	1240	A
3	B8	1241	U
3	B8	1242	U
3	B8	1243	U
3	B8	1246	A
3	B8	1247	U
3	B8	1249	A
3	B8	1253	G
3	B8	1254	A
3	B8	1264	C
3	B8	1271	A
3	B8	1291	U
3	B8	1299	C
3	B8	1314	U
3	B8	1325	G
3	B8	1326	A

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Mol	Chain	Res	Type
3	B8	1327	U
3	B8	1328	G
3	B8	1332	G
3	B8	1341	A
3	B8	1342	C
3	B8	1389	A
3	B8	1390	G
3	B8	1396	C
3	B8	1425	A
3	B8	1426	G
3	B8	1432	U
3	B8	1433	U
3	B8	1436	U
3	B8	1445	U
3	B8	1448	A
3	B8	1468	A
3	B8	1493	A
3	B8	1494	A
3	B8	1498	C
3	B8	1504	A
3	B8	1505	G
3	B8	1509	U
3	B8	1522	A
3	B8	1525	C
3	B8	1526	U
3	B8	1527	U
3	B8	1528	A
3	B8	1536	U
3	B8	1551	C
3	B8	1553	A
3	B8	1558	U
3	B8	1561	A
3	B8	1571	A
4	B9	8	U
4	B9	17	U
4	B9	18	U
4	B9	23	A
4	B9	34	U
4	B9	35	G
4	B9	48	U
4	B9	49	G
4	B9	55	C

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Mol	Chain	Res	Type
4	B9	56	A
4	B9	57	C
4	B9	58	A
4	B9	71	C
56	AG	7	G
56	AG	8	U
56	AG	11	G
56	AG	17	U
56	AG	43	A
56	AG	52	A
56	AG	53	U
56	AG	55	C
56	AG	71	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

9 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	OMG	B8	1376	3	23,26,27	1.17	3 (13%)	32,38,41	1.83	5 (15%)
3	PSU	B8	1403	3	18,21,22	1.39	2 (11%)	21,30,33	1.99	4 (19%)
22	SAC	BR	2	22	7,8,9	0.56	0	7,9,11	1.02	1 (14%)
3	OMU	B8	1375	3,59	19,22,23	1.20	3 (15%)	25,31,34	1.77	5 (20%)
3	1MA	B8	949	3	21,25,26	0.43	0	30,37,40	0.75	1 (3%)
4	MIA	B9	38	4	28,31,32	0.62	1 (3%)	38,44,47	3.99	1 (2%)
6	AYA	BB	2	6	6,7,8	0.78	0	6,8,10	0.56	0
32	AYA	Bb	2	32	6,7,8	0.72	0	6,8,10	0.68	0
3	OMG	B8	1151	3,59,56	23,26,27	1.17	3 (13%)	32,38,41	1.84	6 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	B8	1376	3	-	0/9/27/28	0/3/3/3
3	PSU	B8	1403	3	-	0/7/25/26	0/2/2/2
22	SAC	BR	2	22	-	4/7/8/10	-
3	OMU	B8	1375	3,59	-	0/9/27/28	0/2/2/2
3	1MA	B8	949	3	-	0/7/25/26	0/3/3/3
4	MIA	B9	38	4	-	0/15/33/34	0/3/3/3
6	AYA	BB	2	6	-	1/5/6/8	-
32	AYA	Bb	2	32	-	4/5/6/8	-
3	OMG	B8	1151	3,59,56	-	0/9/27/28	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B8	1403	PSU	C6-C5	3.33	1.39	1.35
3	B8	1376	OMG	C5-C4	3.05	1.47	1.38
3	B8	1151	OMG	C5-C4	3.00	1.47	1.38
3	B8	1403	PSU	C4-N3	-2.70	1.33	1.38
3	B8	1376	OMG	C6-N1	-2.60	1.34	1.38
3	B8	1151	OMG	C6-N1	-2.57	1.34	1.38
3	B8	1375	OMU	C4-N3	-2.55	1.34	1.38
4	B9	38	MIA	C2-S10	2.37	1.77	1.75
3	B8	1375	OMU	C2-N3	-2.17	1.34	1.38
3	B8	1151	OMG	C5-N7	-2.08	1.34	1.39
3	B8	1376	OMG	C5-N7	-2.08	1.34	1.39
3	B8	1375	OMU	C5-C4	-2.04	1.39	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B9	38	MIA	C11-S10-C2	24.38	120.54	102.25
3	B8	1403	PSU	N1-C2-N3	6.18	121.69	115.17
3	B8	1376	OMG	C5-C4-N3	-5.69	119.33	128.39
3	B8	1151	OMG	C5-C4-N3	-5.60	119.47	128.39
3	B8	1375	OMU	C4-N3-C2	-4.74	120.73	126.61
3	B8	1151	OMG	C2-N3-C4	4.59	120.20	112.30
3	B8	1376	OMG	C2-N3-C4	4.56	120.15	112.30
3	B8	1376	OMG	N9-C4-N3	4.35	134.65	125.95
3	B8	1151	OMG	N9-C4-N3	4.32	134.58	125.95
3	B8	1375	OMU	N3-C2-N1	4.15	120.29	114.89

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B8	1403	PSU	C4-N3-C2	-3.97	120.90	126.37
3	B8	1375	OMU	C5-C4-N3	3.77	120.07	114.80
3	B8	1403	PSU	O2-C2-N1	-3.51	119.17	122.79
3	B8	1375	OMU	O4-C4-C5	-3.09	119.84	125.16
3	B8	1151	OMG	C6-C5-N7	2.97	135.70	130.29
3	B8	1376	OMG	C6-C5-N7	2.94	135.64	130.29
22	BR	2	SAC	O-C-CA	-2.58	118.13	124.77
3	B8	1375	OMU	O2-C2-N1	-2.36	119.72	122.80
3	B8	1376	OMG	C4-C5-N7	-2.26	107.08	110.67
3	B8	1151	OMG	C4-C5-N7	-2.21	107.17	110.67
3	B8	949	1MA	N1-C6-N6	2.11	125.02	119.71
3	B8	1151	OMG	O6-C6-C5	-2.10	120.98	126.53
3	B8	1403	PSU	C5-C6-N1	-2.01	119.35	122.14

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	BB	2	AYA	O-C-CA-CB
22	BR	2	SAC	C2A-C1A-N-CA
22	BR	2	SAC	OAC-C1A-N-CA
22	BR	2	SAC	C-CA-CB-OG
32	Bb	2	AYA	O-C-CA-CB
32	Bb	2	AYA	CM-CT-N-CA
32	Bb	2	AYA	OT-CT-N-CA
22	BR	2	SAC	N-CA-CB-OG
32	Bb	2	AYA	C-CA-N-CT

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B8	1376	OMG	1	0
22	BR	2	SAC	1	0
4	B9	38	MIA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 240 ligands modelled in this entry, 237 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
63	FME	AG	101	56	8,9,10	0.57	0	8,9,11	0.92	1 (12%)
60	PHE	B9	101	4	10,11,12	0.39	0	8,13,15	0.20	0
62	FES	Bh	201	38,20	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	PHE	B9	101	4	-	1/5/6/8	0/1/1/1
63	FME	AG	101	56	-	2/7/9/11	-
62	FES	Bh	201	38,20	-	-	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	AG	101	FME	O-C-CA	-2.55	118.21	124.77

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	B9	101	PHE	O-C-CA-CB
63	AG	101	FME	O1-CN-N-CA
63	AG	101	FME	CB-CA-N-CN

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	AG	101	FME	1	0
60	B9	101	PHE	1	0
62	Bh	201	FES	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

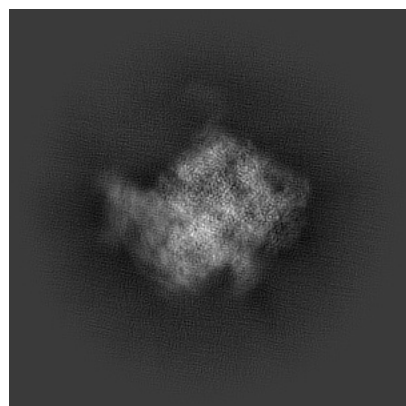
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16896. These allow visual inspection of the internal detail of the map and identification of artifacts.

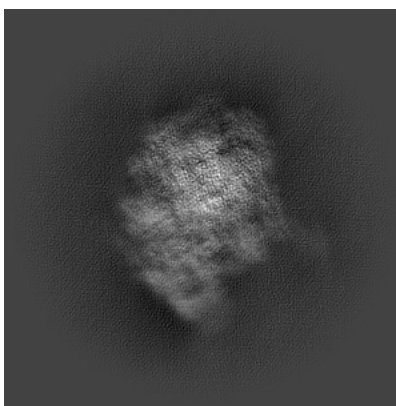
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

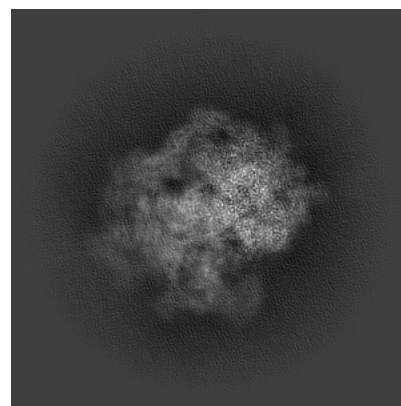
6.1.1 Primary map



X

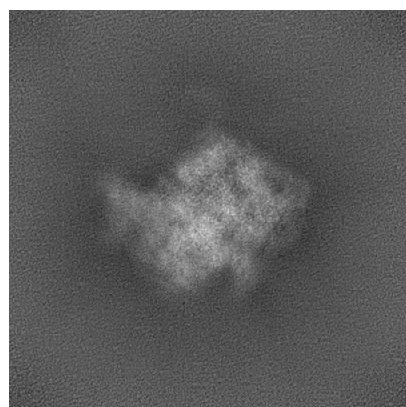


Y

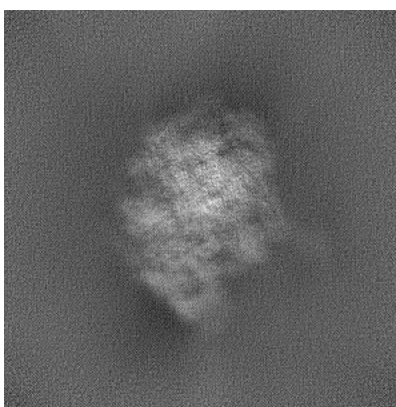


Z

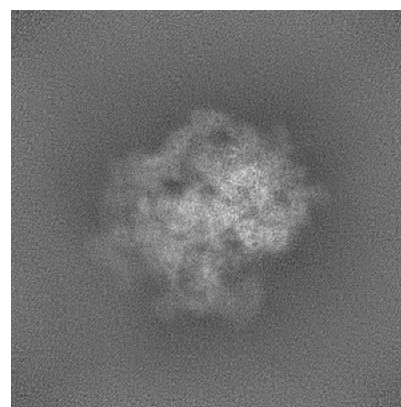
6.1.2 Raw map



X



Y

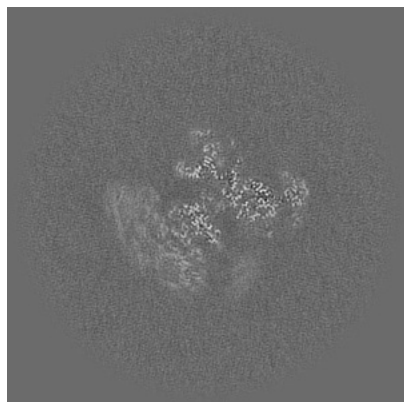


Z

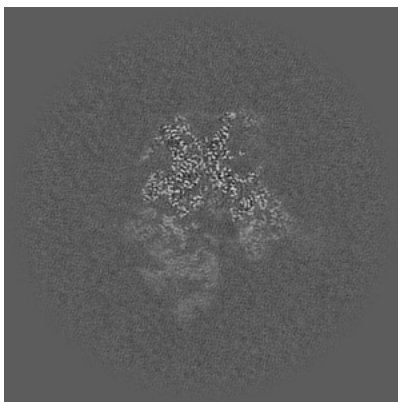
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

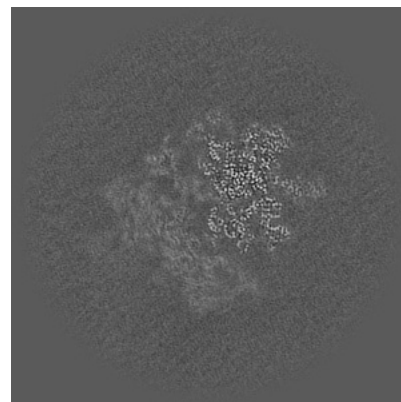
6.2.1 Primary map



X Index: 250

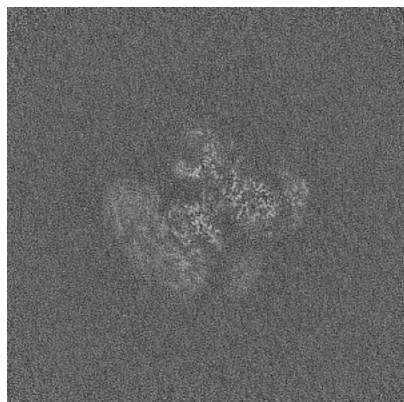


Y Index: 250

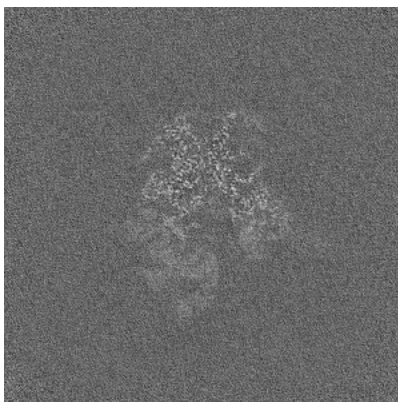


Z Index: 250

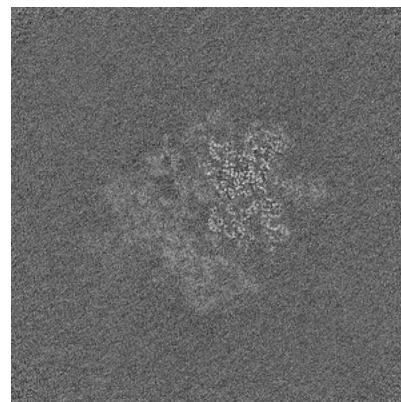
6.2.2 Raw map



X Index: 250



Y Index: 250

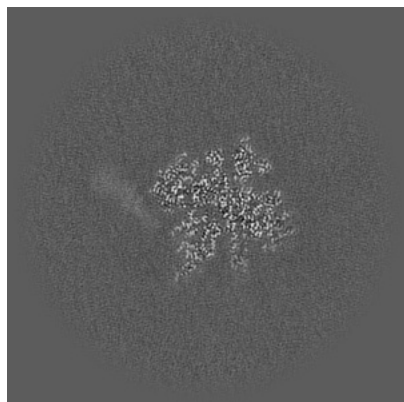


Z Index: 250

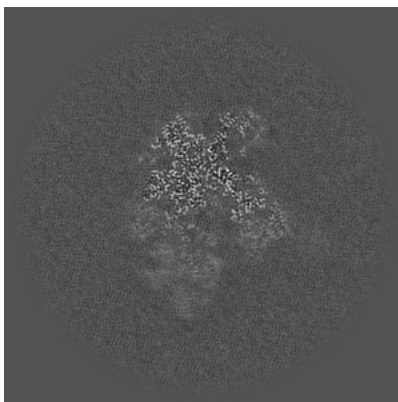
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

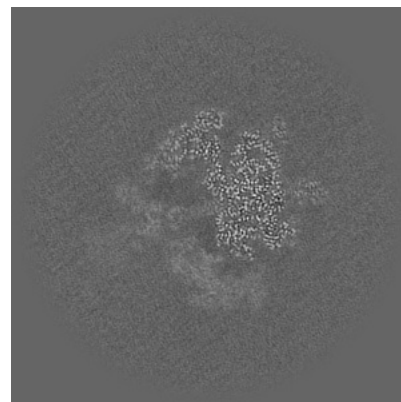
6.3.1 Primary map



X Index: 291

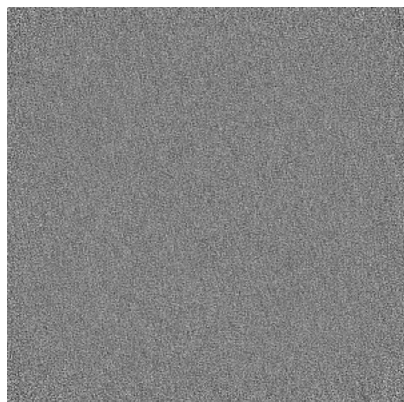


Y Index: 247

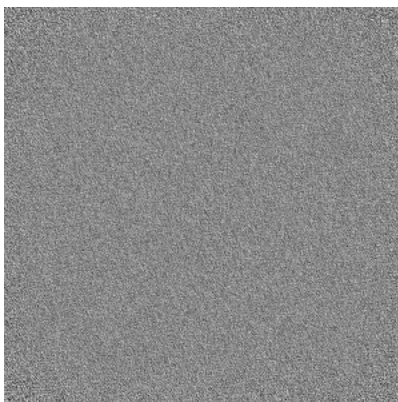


Z Index: 263

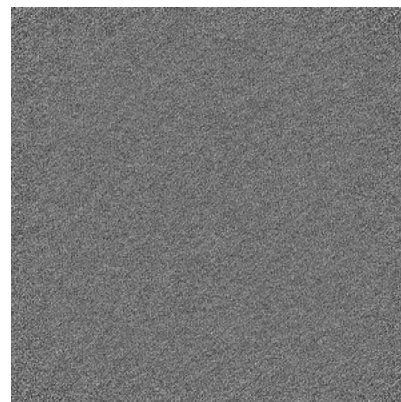
6.3.2 Raw map



X Index: 0



Y Index: 0

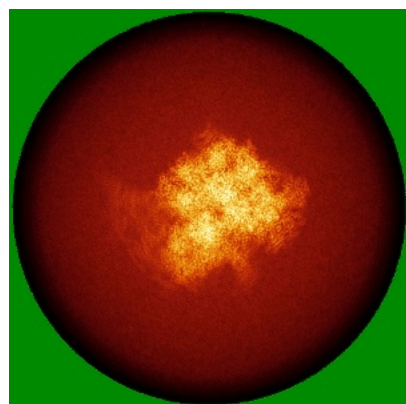


Z Index: 0

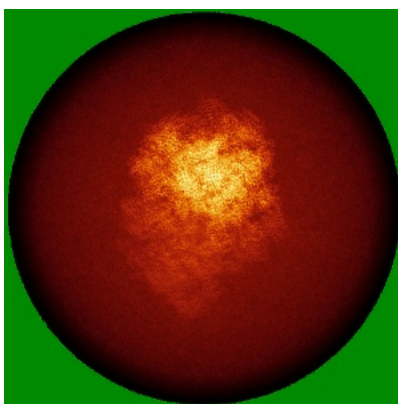
The images above show the largest variance slices of the map in three orthogonal directions.

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

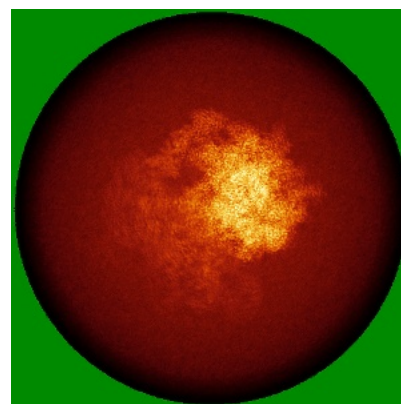
6.4.1 Primary map



X

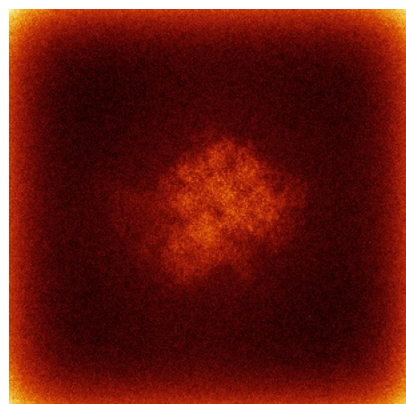


Y

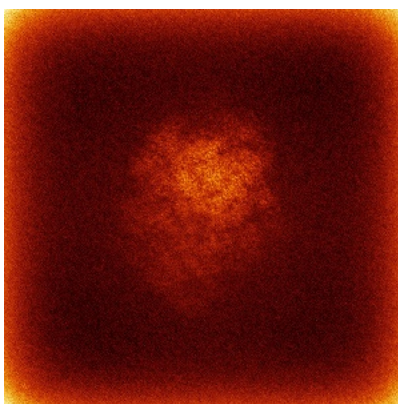


Z

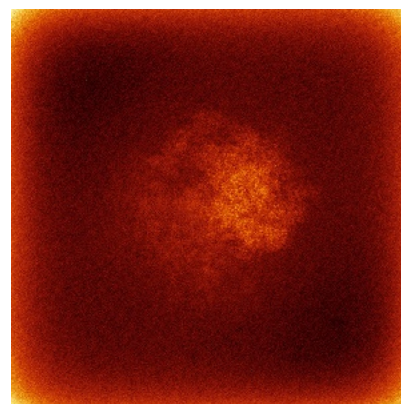
6.4.2 Raw map



X



Y

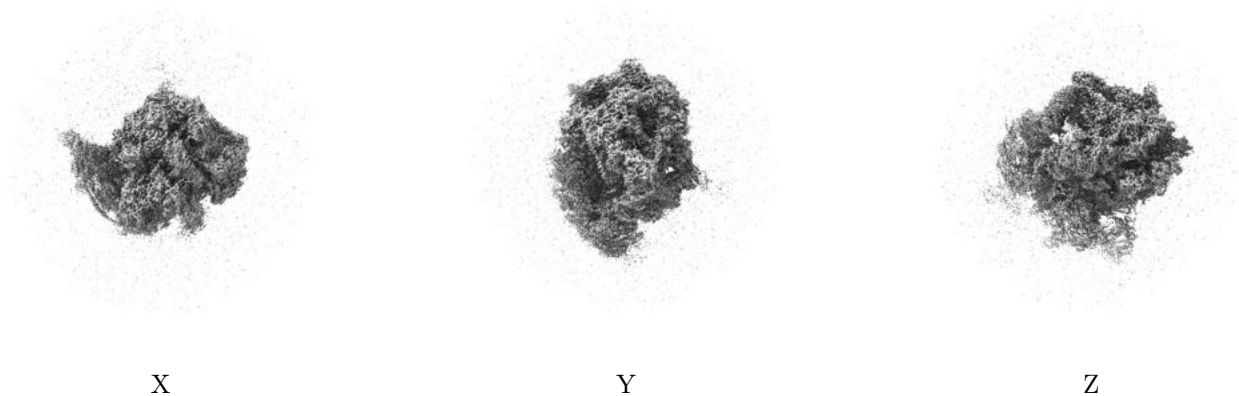


Z

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.

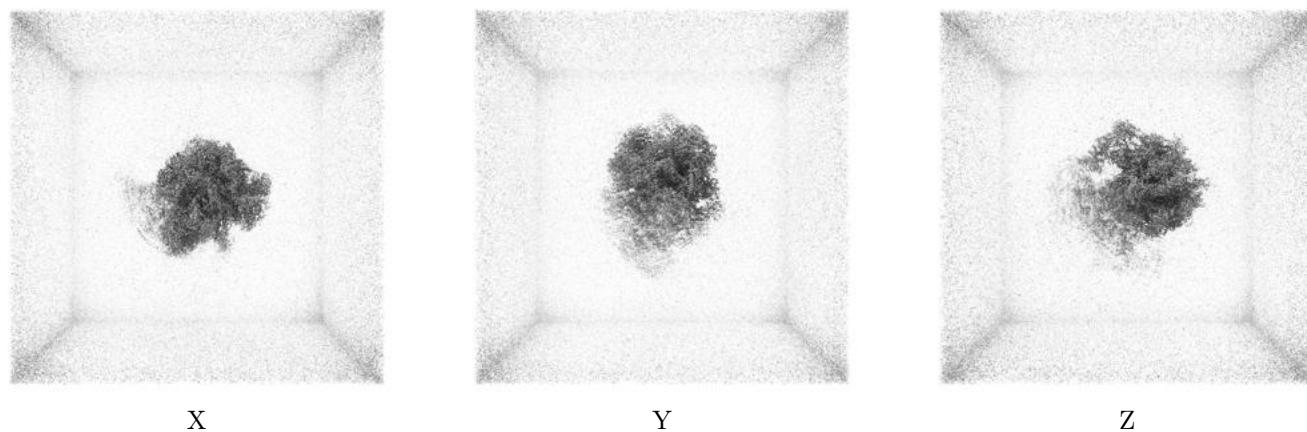
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

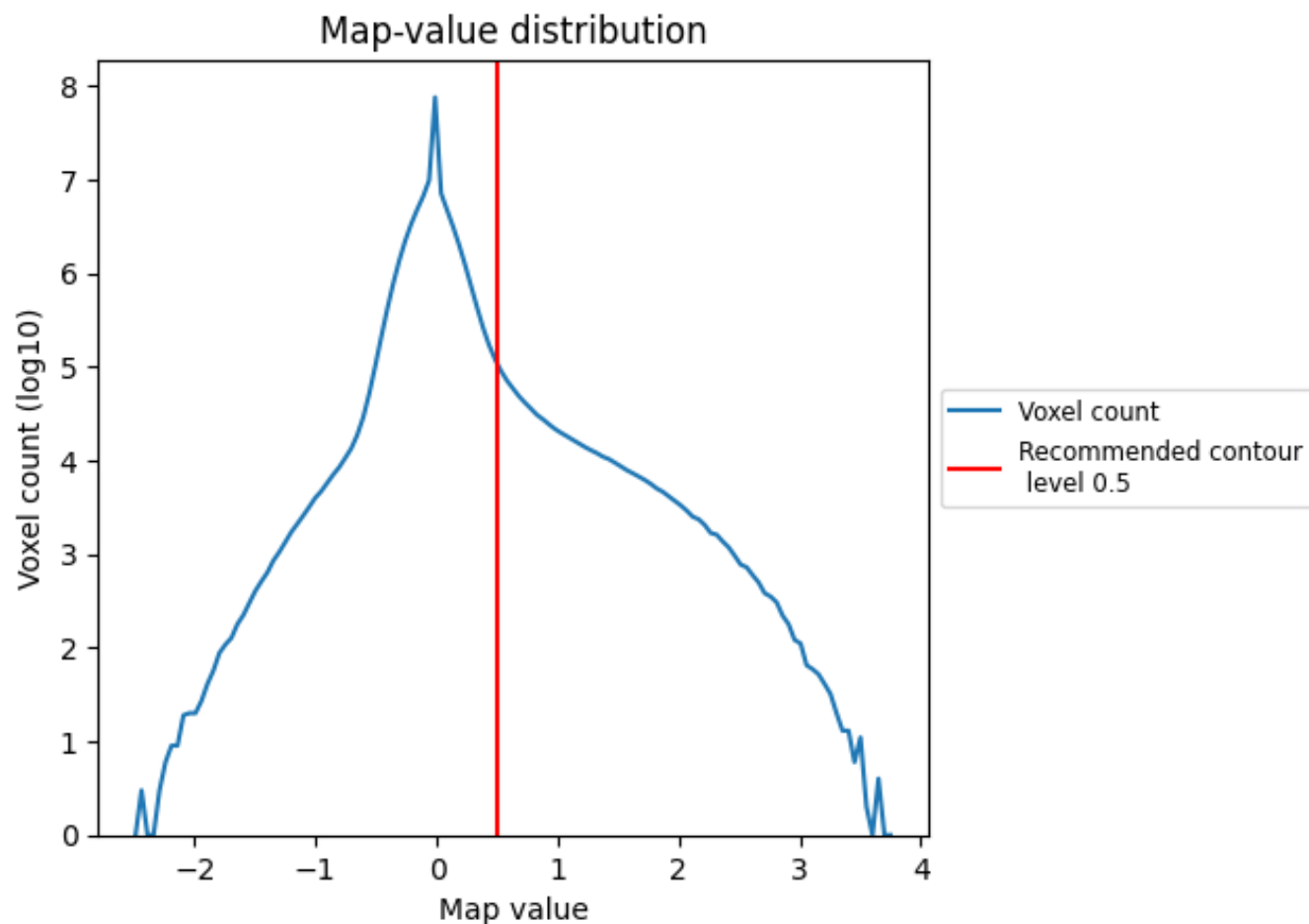
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

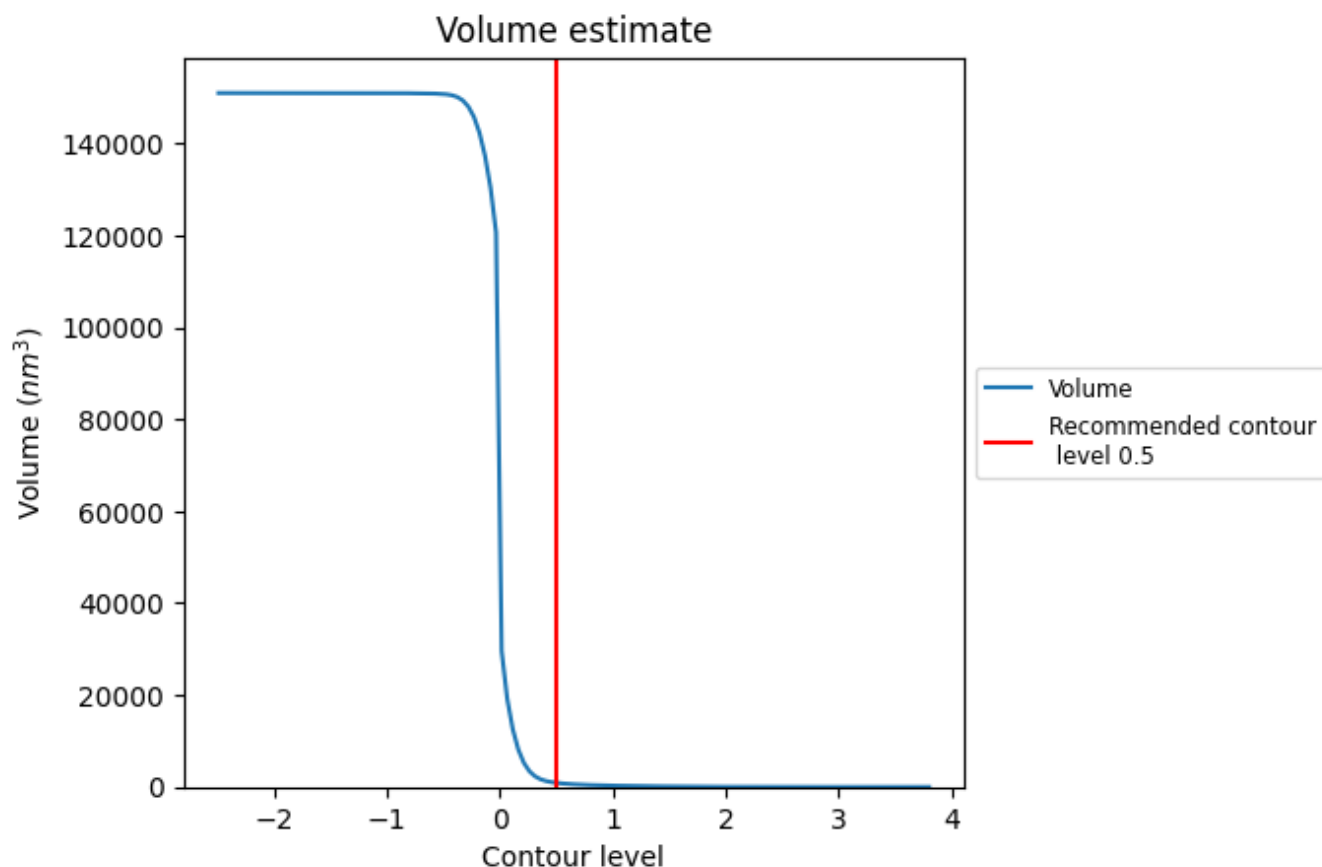
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

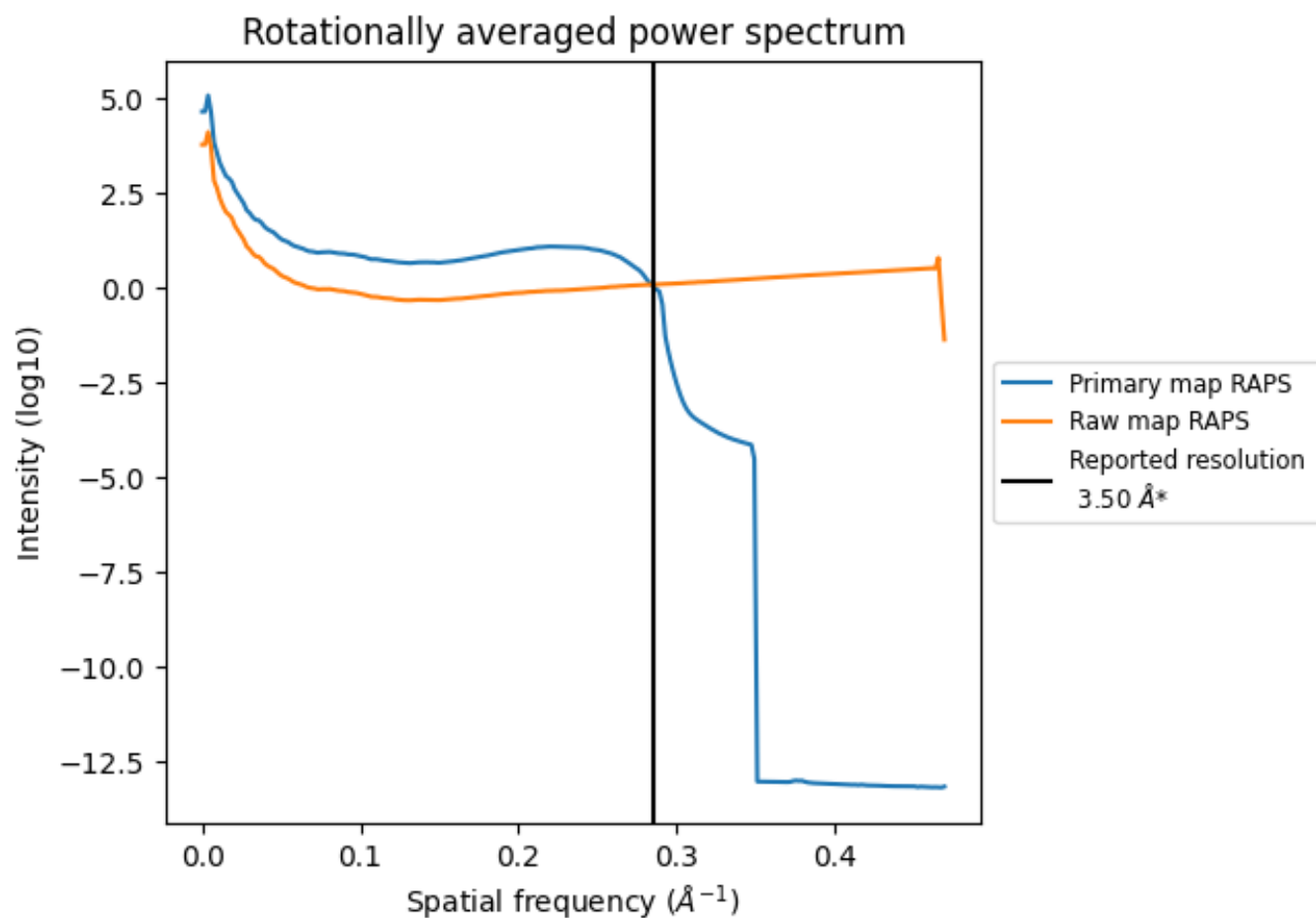
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 905 nm^3 ; this corresponds to an approximate mass of 817 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 ⓘ

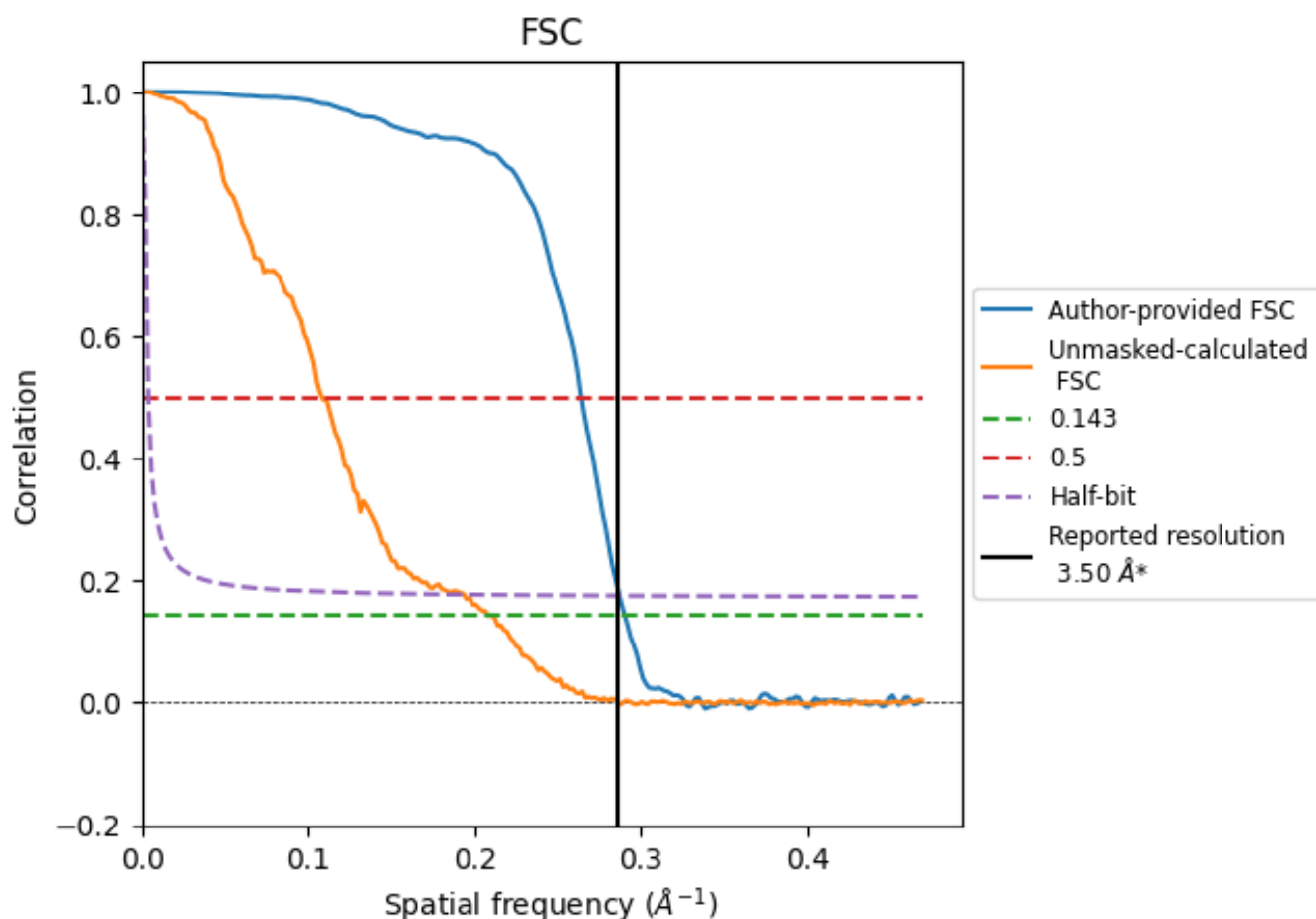


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

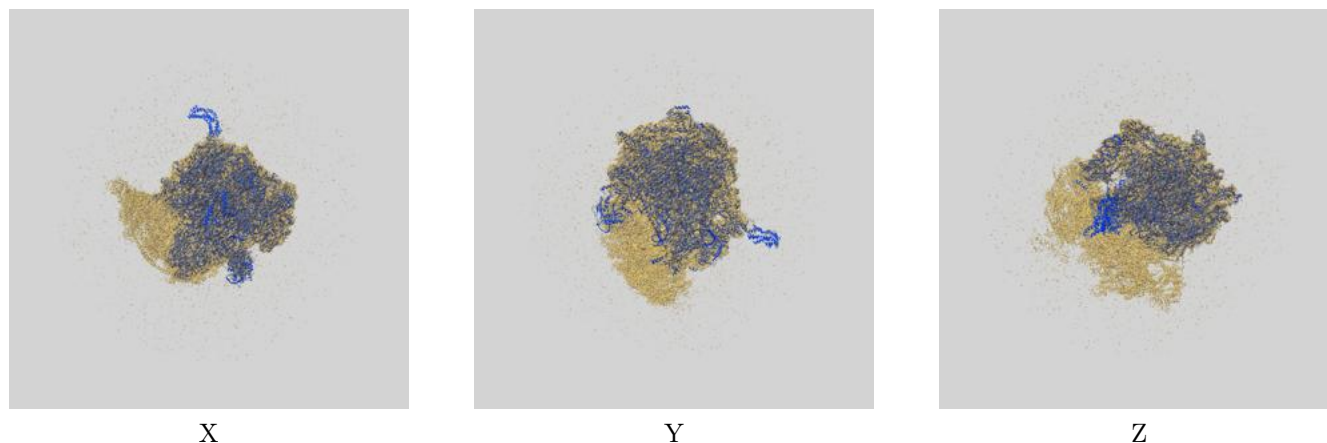
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.44	3.78	3.48
Unmasked-calculated*	4.80	9.23	5.16

*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 4.80 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

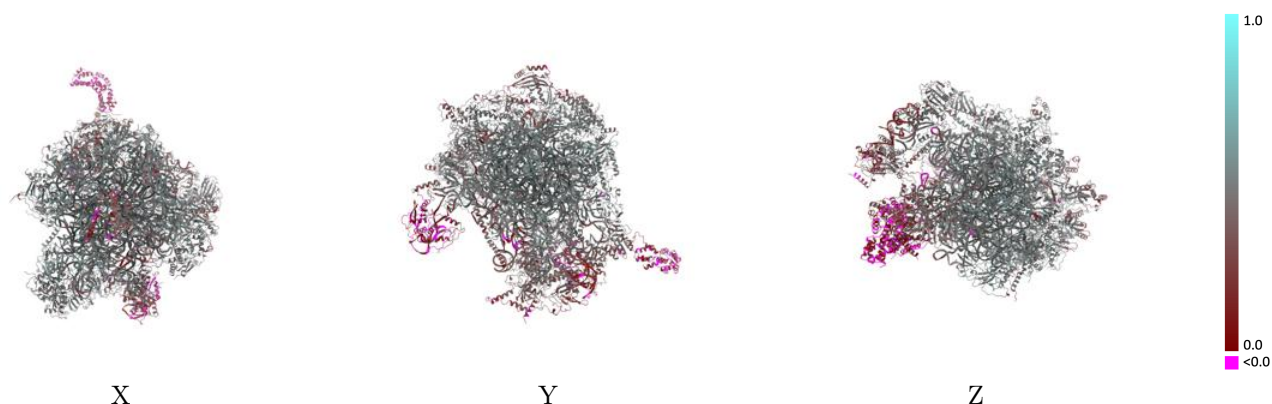
This section contains information regarding the fit between EMDB map EMD-16896 and PDB model 8OIQ. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay [i](#)



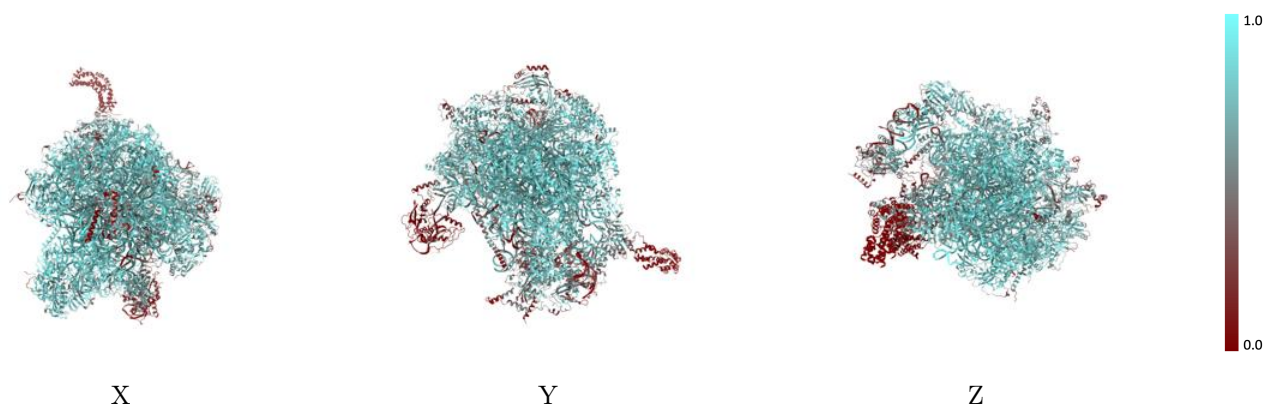
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



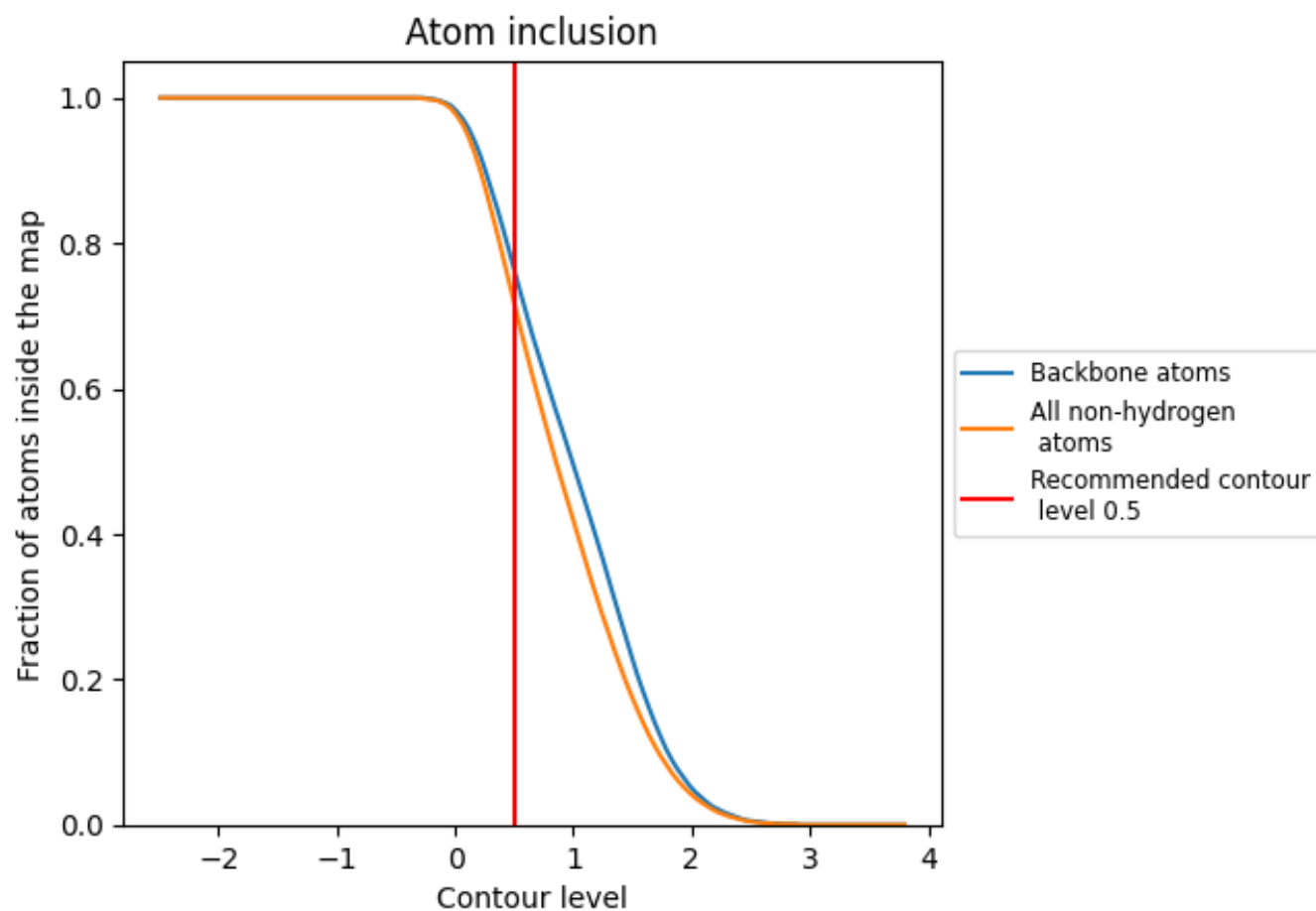
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7180	 0.4400
AG	 0.4970	 0.2890
Aa	 0.2050	 0.2120
B1	 0.0350	 0.1140
B2	 0.0190	 0.0840
B3	 0.0040	 0.0300
B4	 0.0000	 0.0580
B5	 0.0000	 0.0230
B6	 0.0000	 0.1040
B7	 0.0650	 0.1160
B8	 0.8600	 0.4750
B9	 0.5470	 0.3000
BA	 0.7980	 0.5140
BB	 0.7380	 0.4670
BC	 0.5800	 0.4200
BD	 0.8270	 0.5200
BE	 0.6880	 0.4490
BF	 0.7760	 0.4820
BG	 0.8290	 0.5030
BH	 0.7880	 0.5010
BI	 0.5940	 0.4180
BJ	 0.8700	 0.5320
BK	 0.8490	 0.5340
BL	 0.8170	 0.5020
BM	 0.8200	 0.5020
BN	 0.8170	 0.5120
BO	 0.2900	 0.2460
BP	 0.4590	 0.3120
BQ	 0.3480	 0.2810
BR	 0.8470	 0.5160
BS	 0.7840	 0.5100
BT	 0.7930	 0.4960
BU	 0.8260	 0.5090
BV	 0.8190	 0.5210
BW	 0.7730	 0.4910



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Chain	Atom inclusion	Q-score
BX	 0.7600	 0.4910
BY	 0.8330	 0.5210
BZ	 0.8220	 0.5090
Ba	 0.7680	 0.4810
Bb	 0.6300	 0.4050
Bc	 0.4880	 0.3300
Bd	 0.4560	 0.3370
Be	 0.8630	 0.5220
Bf	 0.5440	 0.4040
Bg	 0.5520	 0.3990
Bh	 0.7960	 0.4820
Bi	 0.7890	 0.4830
Bj	 0.0580	 0.0750
Bl	 0.8660	 0.5290
Bm	 0.7800	 0.4760
Bn	 0.7690	 0.4650
Bo	 0.7190	 0.4560
Bp	 0.5200	 0.3680
Bq	 0.6630	 0.4440
Br	 0.6750	 0.4630
Bs	 0.8190	 0.5130
Bt	 0.7760	 0.4760
Bu	 0.5020	 0.3710
Bv	 0.4480	 0.2810
Bw	 0.5440	 0.4000
Bx	 0.7990	 0.4980
By	 0.4460	 0.4140
Bz	 0.8420	 0.5210