



Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 05:57 pm BST

PDB ID : 6GB2 / pdb_00006gb2
EMDB ID : EMD-4370
Title : Unique features of mammalian mitochondrial translation initiation revealed by cryo-EM. This file contains the 39S ribosomal subunit.
Authors : Kummer, E.; Leibundgut, M.; Boehringer, D.; Ban, N.
Deposited on : 2018-04-13
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

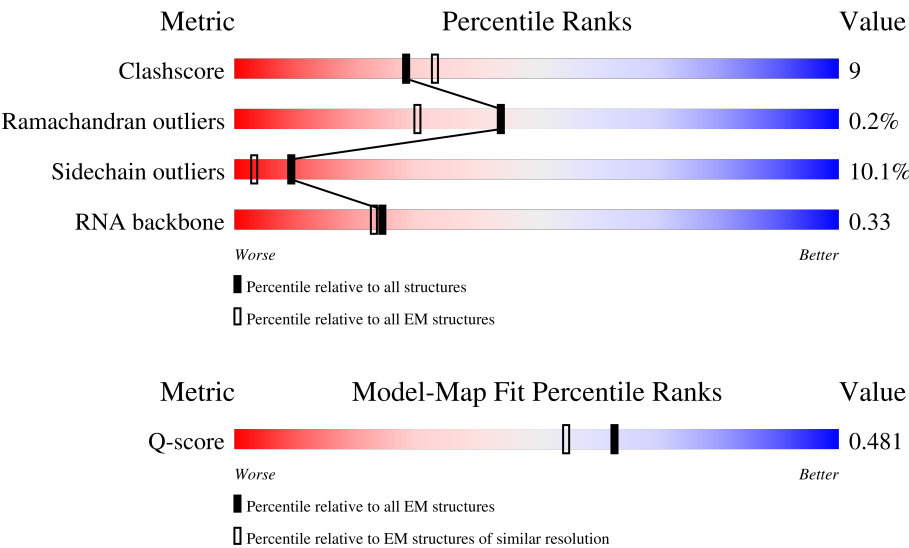
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	BL	198	
1	CL	198	
1	DL	198	

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Mol	Chain	Length	Quality of chain
1	EL	198	
1	FL	198	
1	GL	198	
1	HL	198	
2	B0	148	
3	B1	256	
4	B2	252	
5	B3	161	
6	B4	126	
7	B5	188	
8	B6	65	
9	B7	95	
10	B8	188	
11	B9	100	
12	BA	1571	
13	BB	73	
14	BC	657	
15	BD	306	
16	BE	348	
17	BF	294	
18	BI	268	
19	BJ	262	
20	BK	192	
21	BN	178	
22	BO	145	

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Mol	Chain	Length	Quality of chain
23	BP	296	
24	BQ	251	
25	BR	169	
26	BS	180	
27	BT	292	
28	BU	149	
29	BV	209	
30	BW	210	
31	BX	150	
32	BY	216	
33	Ba	423	
34	Bb	380	
35	Bc	334	
36	Bd	206	
37	Be	135	
38	Bf	142	
39	Bg	159	
40	Bh	332	
41	Bi	306	
42	Bj	279	
43	Bk	212	
44	Bl	166	
45	Bm	159	
46	Bn	128	
47	Bo	124	

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Mol	Chain	Length	Quality of chain
48	Bp	112	
49	Bq	138	
50	Bt	102	
51	Bu	205	
52	Bv	222	
53	Bw	433	
54	Bx	196	
55	Bz	82	
56	AV	71	

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 111109 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	CL	45	Total	C	N	O	0	0
			317	203	52	62		
1	DL	27	Total	C	N	O	0	0
			213	137	33	43		
1	EL	28	Total	C	N	O	0	0
			222	143	35	44		
1	FL	27	Total	C	N	O	0	0
			213	137	33	43		
1	GL	27	Total	C	N	O	0	0
			213	137	33	43		
1	HL	26	Total	C	N	O	0	0
			205	131	32	42		
1	BL	70	Total	C	N	O	0	0
			537	346	93	98		

- Molecule 2 is a protein called Mitochondrial ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B0	110	Total	C	N	O	S	0	0
			857	553	156	145	3		

- Molecule 3 is a protein called Mitochondrial ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B1	244	Total	C	N	O	S	0	0
			2036	1315	363	353	5		

- Molecule 4 is a protein called Mitochondrial ribosomal protein L47.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B2	179	Total	C	N	O	S	0	0
			1548	992	290	260	6		

- Molecule 5 is a protein called 'Mitochondrial ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B3	118	Total	C	N	O	S	0	0
			968	622	178	165	3		

- Molecule 6 is a protein called 'Mitochondrial ribosomal protein L55.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B4	45	Total	C	N	O	S	0	0
			381	239	77	62	3		

- Molecule 7 is a protein called Mitochondrial ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B5	110	Total	C	N	O	S	0	0
			902	553	181	162	6		

- Molecule 8 is a protein called Mitochondrial ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B6	52	Total	C	N	O	S	0	0
			425	274	78	71	2		

- Molecule 9 is a protein called Mitochondrial ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B7	46	Total	C	N	O	S	0	0
			387	239	89	58	1		

- Molecule 10 is a protein called Mitochondrial ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B8	95	Total	C	N	O	S	0	0
			833	539	163	129	2		

- Molecule 11 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B9	38	Total	C	N	O	S	0	0
			335	214	70	47	4		

- Molecule 12 is a RNA chain called 16S ribosomal RNA, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BA	1549	Total	C	N	O	P	0	0
			32950	14798	5993	10610	1549		

- Molecule 13 is a RNA chain called CP tRNAPhe, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BB	67	Total	C	N	O	P	0	0
			1427	640	261	459	67		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	72	C	-	insertion	GB 76262549
BB	73	A	-	insertion	GB 76262549

- Molecule 14 is a protein called Translation initiation factor IF-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BC	571	Total	C	N	O	S	0	0
			4364	2743	765	839	17		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	71	SER	-	expression tag	UNP P46199
BC	72	GLY	-	expression tag	UNP P46199
BC	73	GLY	-	expression tag	UNP P46199
BC	74	SER	-	expression tag	UNP P46199
BC	75	GLY	-	expression tag	UNP P46199
BC	76	SER	-	expression tag	UNP P46199
BC	77	GLY	-	expression tag	UNP P46199

- Molecule 15 is a protein called Mitochondrial ribosomal protein L2.

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

- Molecule 16 is a protein called ICT1.

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

- Molecule 17 is a protein called Mitochondrial ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BF	250	Total	C	N	O	S	0	0
			2011	1294	367	344	6		

- Molecule 18 is a protein called Mitochondrial ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BI	98	Total	C	N	O		0	0
			805	509	155	141			

- Molecule 19 is a protein called Mitochondrial ribosomal protein L10.

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

- Molecule 20 is a protein called Mitochondrial ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BK	176	Total	C	N	O	S	0	0
			1303	830	236	235	2		

- Molecule 21 is a protein called Mitochondrial ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BN	177	Total	C	N	O	S	0	0
			1444	926	258	253	7		

- Molecule 22 is a protein called Mitochondrial ribosomal protein L14.

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

- Molecule 23 is a protein called Mitochondrial ribosomal protein L15.

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

- Molecule 24 is a protein called Mitochondrial ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BQ	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
BQ	237	HIS	TYR	conflict	UNP F1RI89

- Molecule 25 is a protein called Mitochondrial ribosomal protein L17.

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

- Molecule 26 is a protein called Mitochondrial ribosomal protein L18.

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

- Molecule 27 is a protein called Mitochondrial ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BT	223	Total	C	N	O	S	0	0
			1845	1181	319	336	9		

- Molecule 28 is a protein called Mitochondrial ribosomal protein L20.

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

- Molecule 29 is a protein called Mitochondrial ribosomal protein L21.

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

- Molecule 30 is a protein called Mitochondrial ribosomal protein L22.

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

- Molecule 31 is a protein called Mitochondrial ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BX	149	Total	C	N	O	S	0	0
			1181	752	227	200	2		

- Molecule 32 is a protein called Mitochondrial ribosomal protein L24.

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

- Molecule 33 is a protein called Mitochondrial ribosomal protein L37.

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

- Molecule 34 is a protein called Mitochondrial ribosomal protein L38.

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

- Molecule 35 is a protein called Mitochondrial ribosomal protein L39.

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

- Molecule 36 is a protein called Mitochondrial ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Bd	99	Total	C	N	O	S	0	0
			832	528	148	155	1		

- Molecule 37 is a protein called Mitochondrial ribosomal protein L41.

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

- Molecule 38 is a protein called Mitochondrial ribosomal protein L42.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bf	108	Total	C	N	O	S	0	0
			827	519	154	150	4		

- Molecule 39 is a protein called Mitochondrial ribosomal protein L43.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bg	148	Total	C	N	O	S	0	0
			1167	727	225	212	3		

- Molecule 40 is a protein called Mitochondrial ribosomal protein L44.

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

- Molecule 41 is a protein called Mitochondrial ribosomal protein L45.

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

- Molecule 42 is a protein called Mitochondrial ribosomal protein L46.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bj	217	Total	C	N	O	S	0	0
			1775	1137	311	321	6		

- Molecule 43 is a protein called Mitochondrial ribosomal protein L48.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bk	136	Total	C	N	O	S	0	0
			1087	692	185	205	5		

- Molecule 44 is a protein called Mrpl34.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bl	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
Bl	59	ARG	LYS	conflict	UNP A0A0R4J8D6

- Molecule 45 is a protein called Mitochondrial ribosomal protein L50.

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

- Molecule 46 is a protein called Mitochondrial ribosomal protein L51.

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

- Molecule 47 is a protein called Mitochondrial ribosomal protein L52.

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

- Molecule 48 is a protein called mL53, MRPL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Bp	97	Total	C	N	O	S	0	0
			742	459	143	134	6		

- Molecule 49 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Bq	68	Total	C	N	O	S	0	0
			542	344	102	95	1		

- Molecule 50 is a protein called Mitochondrial ribosomal protein L57.

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

- Molecule 51 is a protein called Mitochondrial ribosomal protein L58.

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

- Molecule 52 is a protein called 'Mitochondrial ribosomal protein L59.

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

- Molecule 53 is a protein called mL65, MRPS30.

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

- Molecule 54 is a protein called Mitochondrial ribosomal protein S18A.

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

- Molecule 55 is a protein called unassigned secondary structure elements.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	Bz	82	Total	C	N	O	0	0
			410	246	82	82		

- Molecule 56 is a RNA chain called P-site fMet-tRNA^{Met}, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AV	71	Total	C	N	O	P	0	0
			1498	673	264	491	70		

There are 3 discrepancies between the modelled and reference sequences:

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

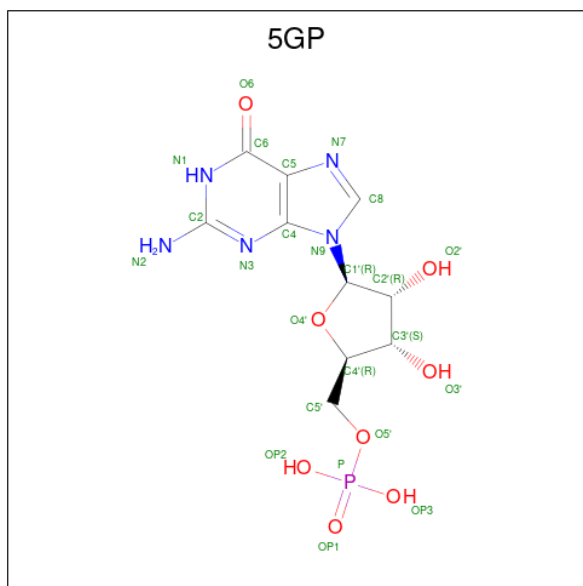
- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	B3	1	Total	Mg	0
			1	1	
57	BA	203	Total	Mg	0
			203	203	
57	BB	1	Total	Mg	0
			1	1	
57	BC	1	Total	Mg	0
			1	1	
57	BD	3	Total	Mg	0
			3	3	
57	BP	2	Total	Mg	0
			2	2	
57	BQ	1	Total	Mg	0
			1	1	
57	Be	2	Total	Mg	0
			2	2	
57	Bl	1	Total	Mg	0
			1	1	
57	Bt	1	Total	Mg	0
			1	1	

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

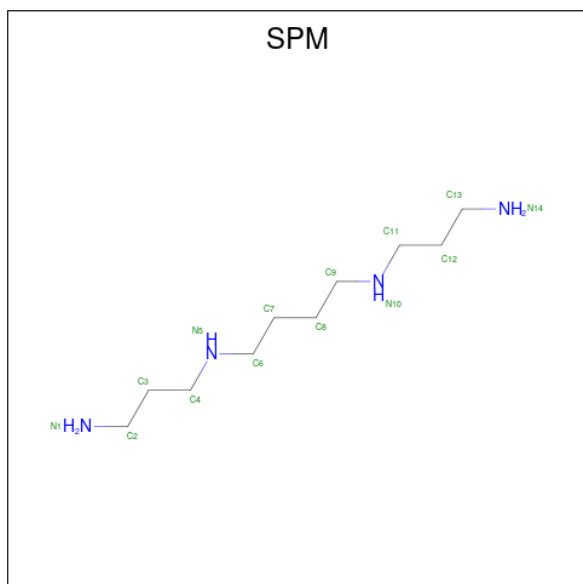
Mol	Chain	Residues	Atoms		AltConf
58	B5	1	Total	Zn	0
			1	1	
58	B9	1	Total	Zn	0
			1	1	
58	BJ	1	Total	Zn	0
			1	1	

- Molecule 59 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					AltConf
59	BA	1	Total	C	N	O	P	0
			24	10	5	8	1	
59	BA	1	Total	C	N	O	P	0
			24	10	5	8	1	

- Molecule 60 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



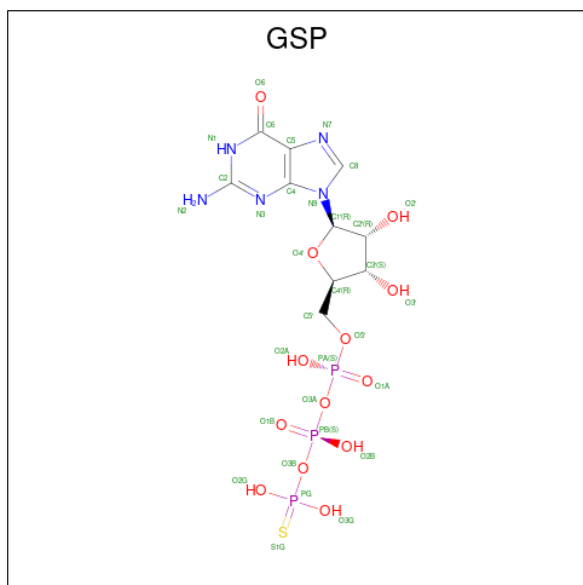
Mol	Chain	Residues	Atoms				AltConf
60	BA	1	Total	C	N		0
			14	10	4		

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Mol	Chain	Residues	Atoms			AltConf
60	BR	1	Total	C	N	0
			14	10	4	

- Molecule 61 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$) (labeled as "Ligand of Interest" by depositor).

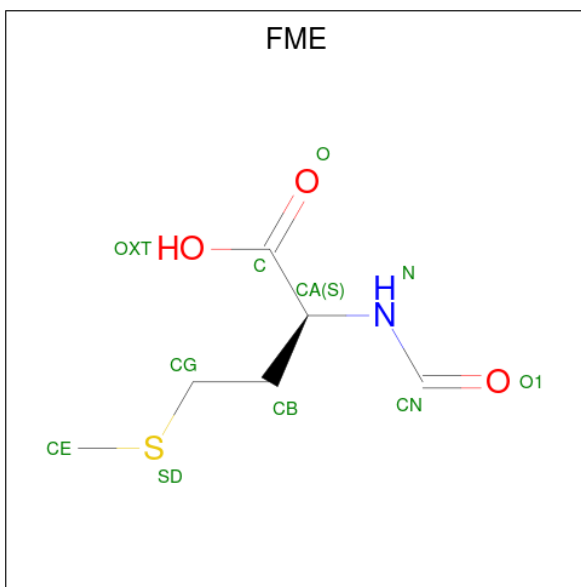


Mol	Chain	Residues	Atoms						AltConf
61	BC	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	

- Molecule 62 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
62	BC	1	Total	Na	0
			1	1	

- Molecule 63 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$) (labeled as "Ligand of Interest" by depositor).



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

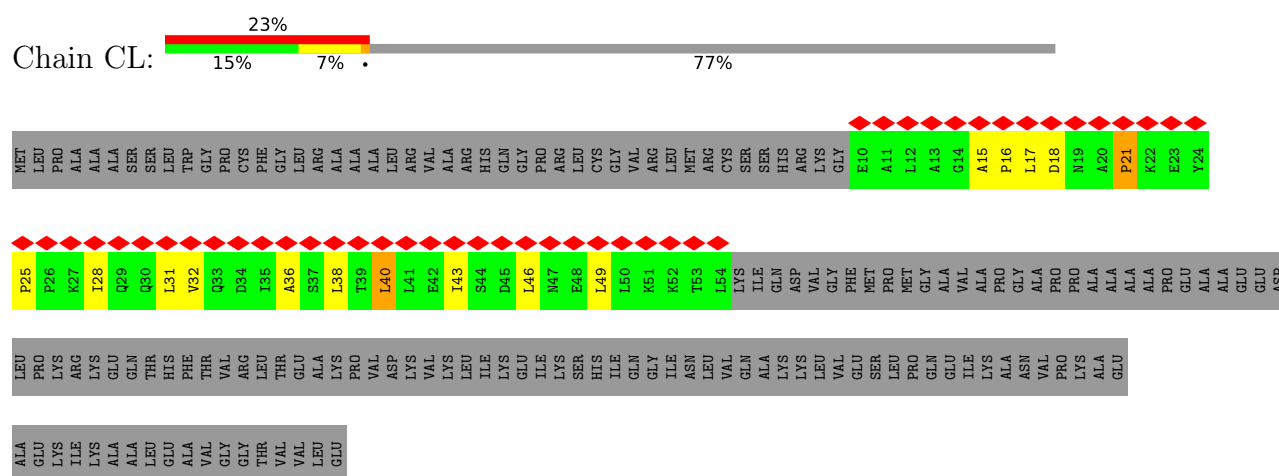
- Molecule 64 is water.

Mol	Chain	Residues	Atoms		AltConf
64	BC	2	Total	O	0
			2	2	

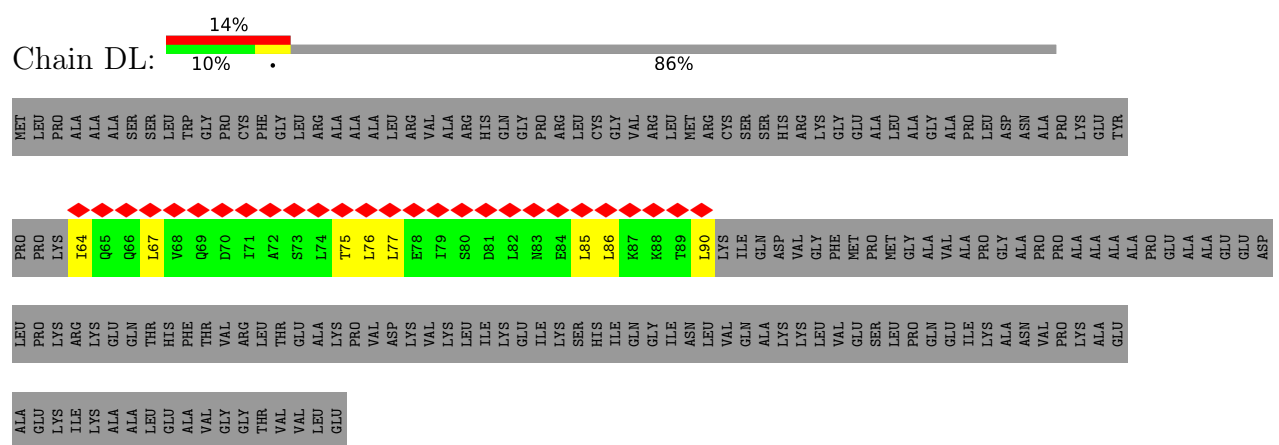
3 Residue-property plots

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.

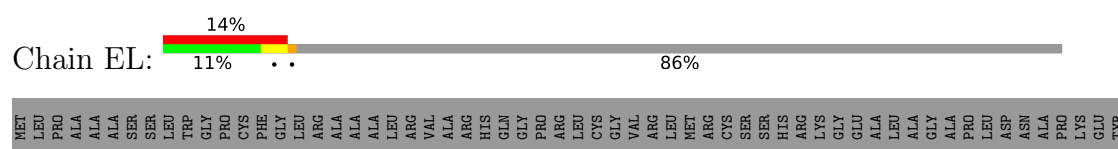
• Molecule 1: Mitochondrial ribosomal protein L12

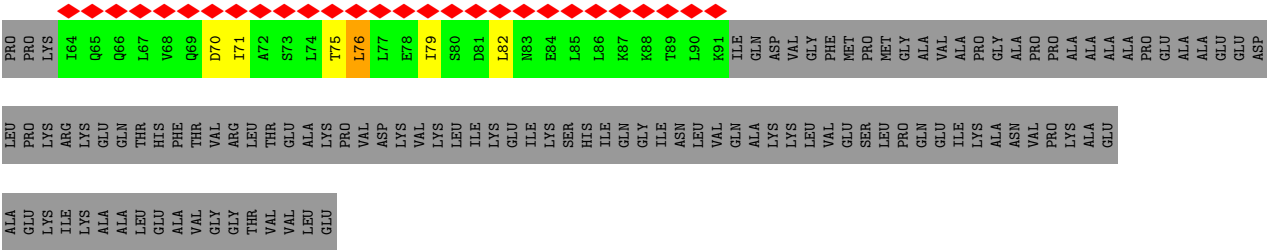


• Molecule 1: Mitochondrial ribosomal protein L12

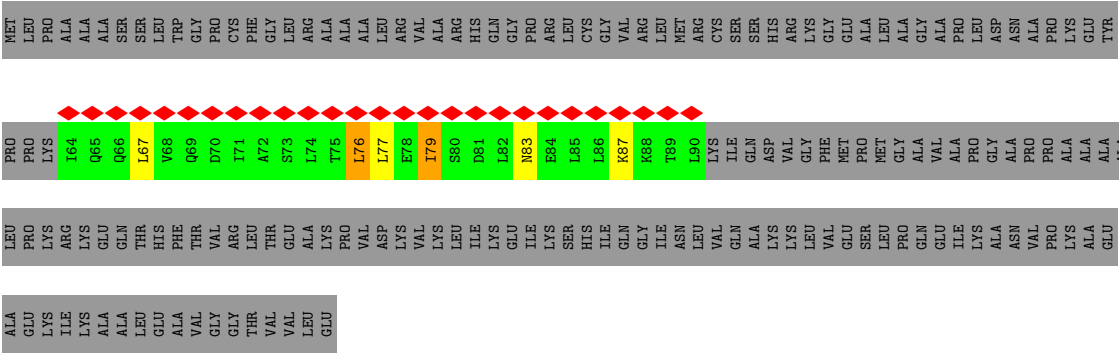


• Molecule 1: Mitochondrial ribosomal protein L12

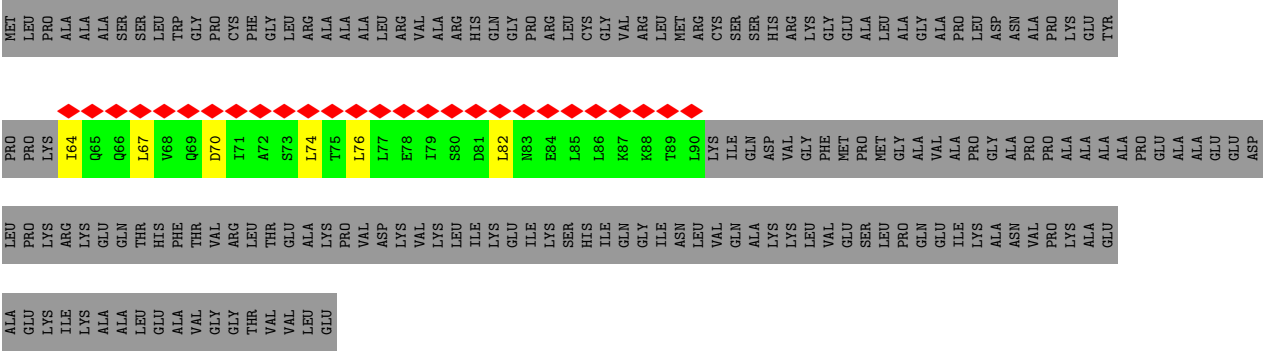




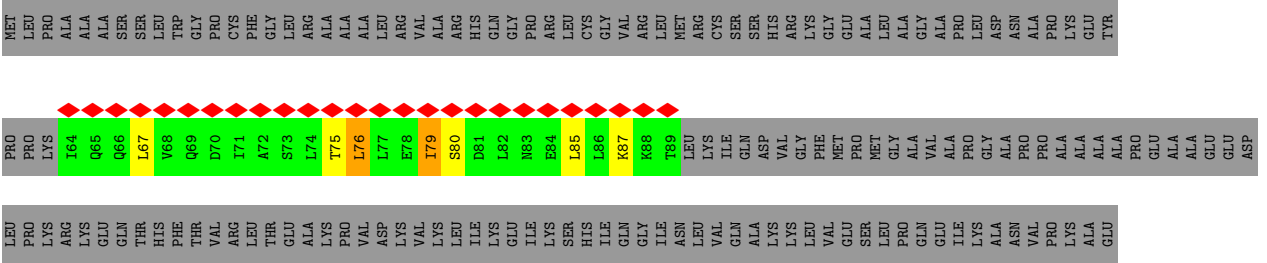
• Molecule 1: Mitochondrial ribosomal protein L12



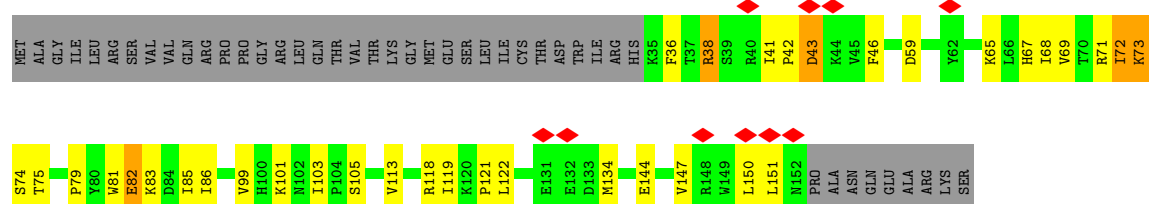
• Molecule 1: Mitochondrial ribosomal protein L12



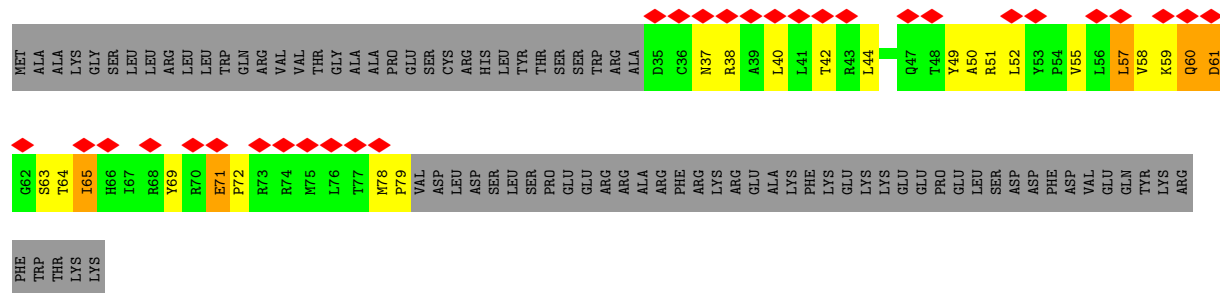
• Molecule 1: Mitochondrial ribosomal protein L12



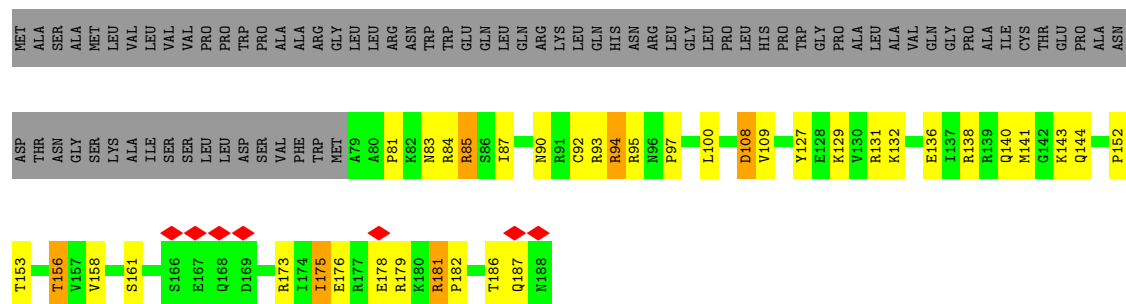
- Molecule 5: 'Mitochondrial ribosomal protein L30



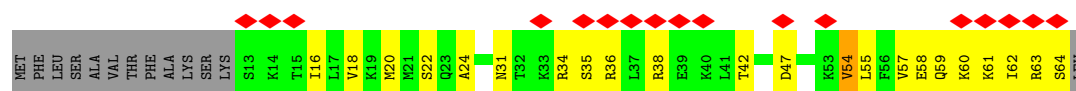
- Molecule 6: 'Mitochondrial ribosomal protein L55



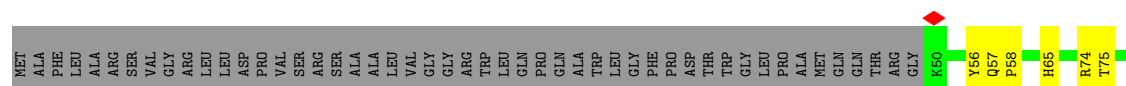
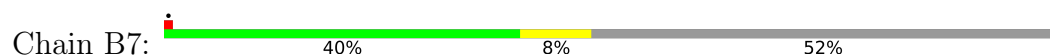
- Molecule 7: Mitochondrial ribosomal protein L32



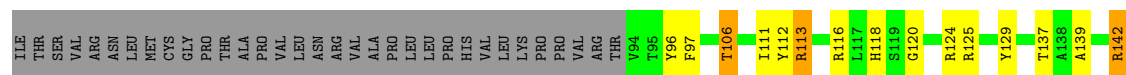
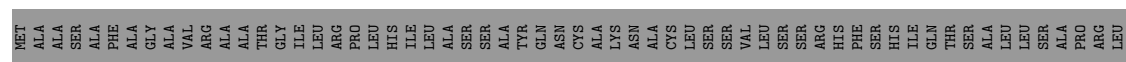
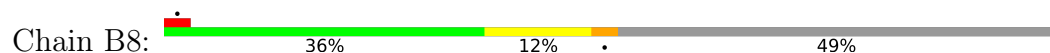
- Molecule 8: Mitochondrial ribosomal protein L33



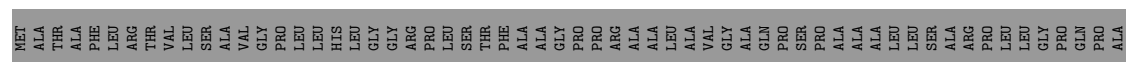
• Molecule 9: Mitochondrial ribosomal protein L34



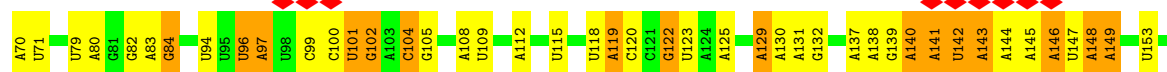
• Molecule 10: Mitochondrial ribosomal protein L35

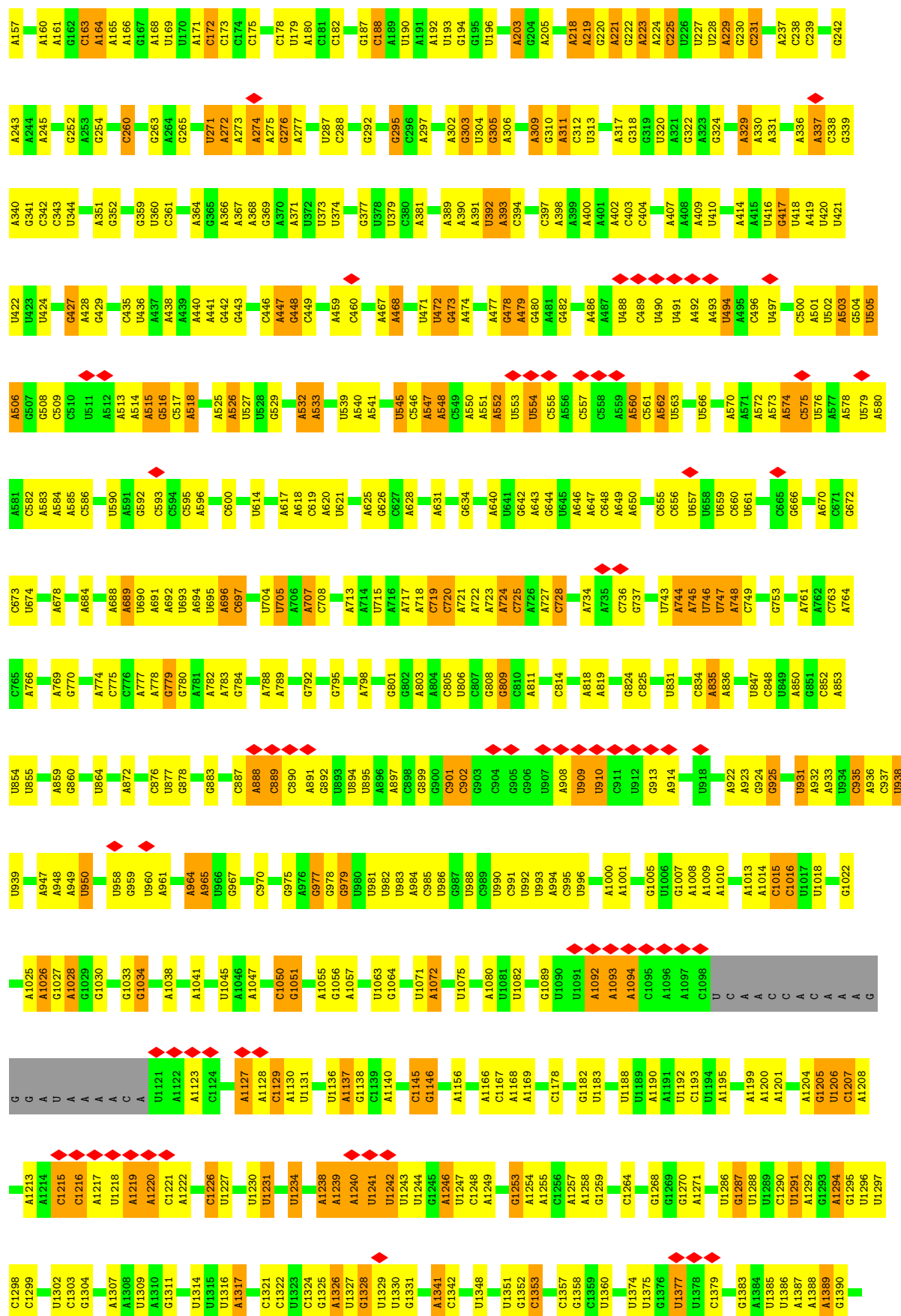


• Molecule 11: Ribosomal protein



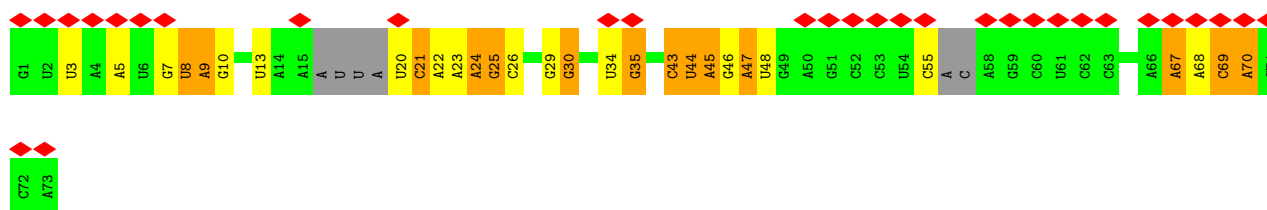
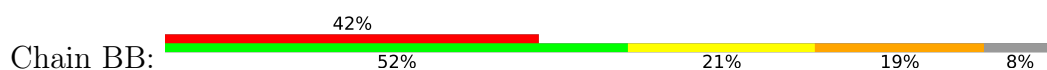
• Molecule 12: 16S ribosomal RNA, mitochondrial



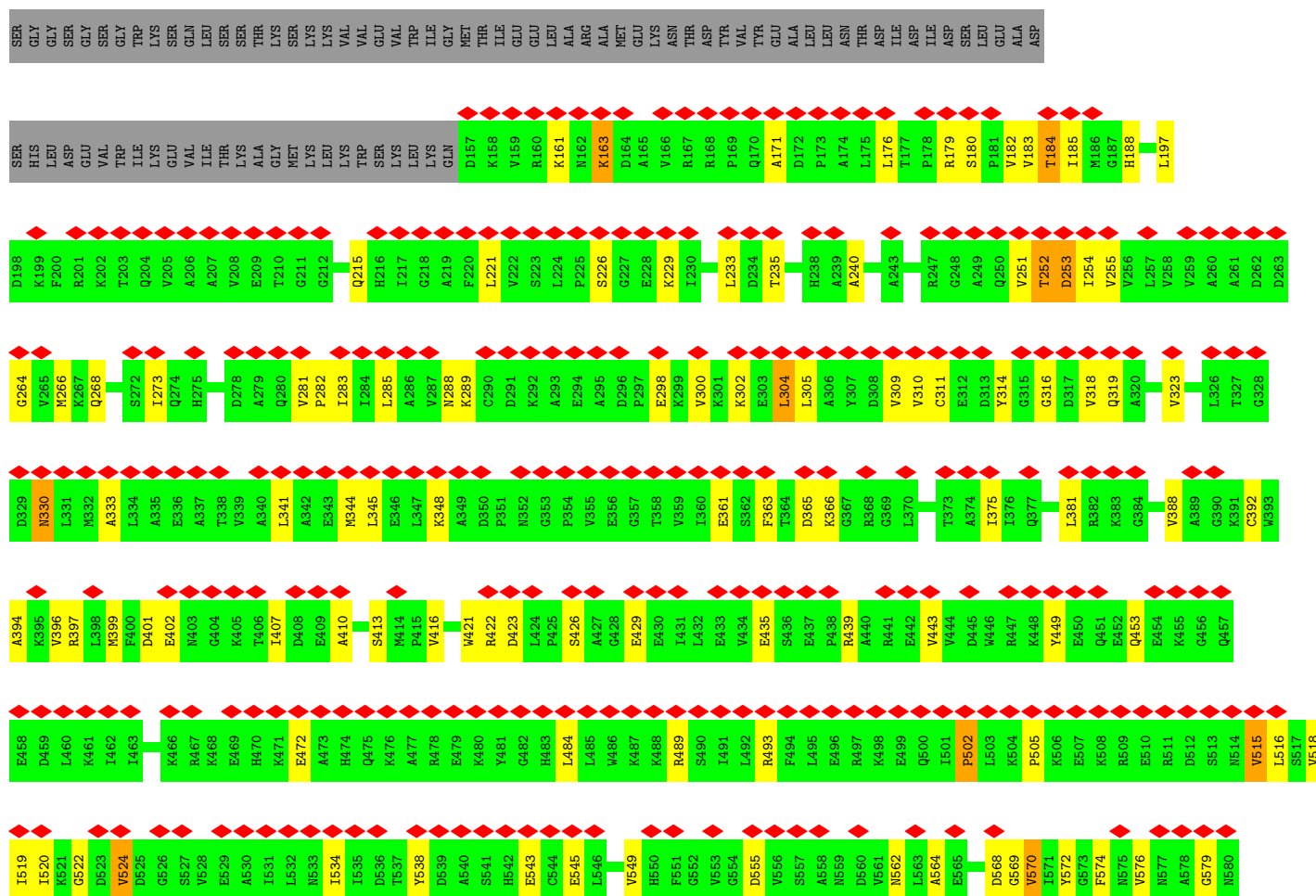


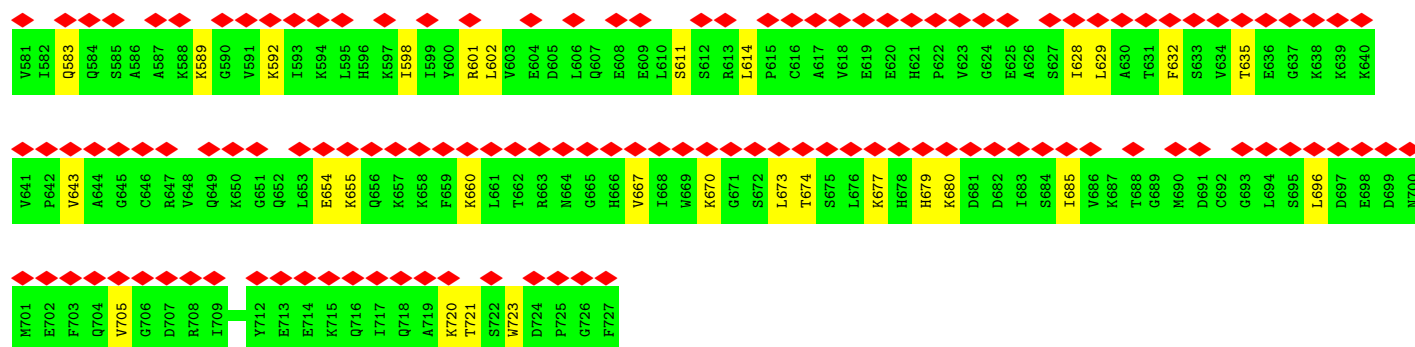


• Molecule 13: CP tRNAPhe, mitochondrial

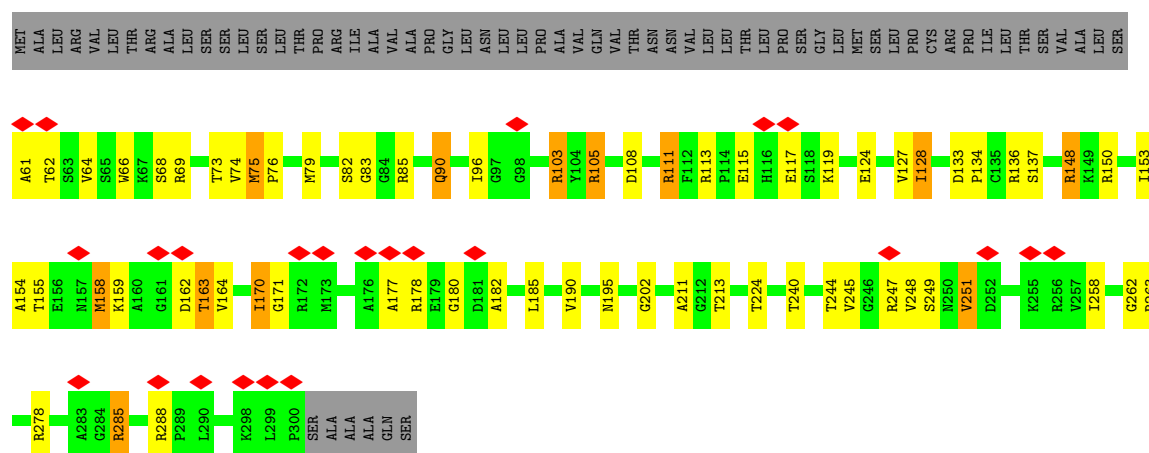


• Molecule 14: Translation initiation factor IF-2, mitochondrial

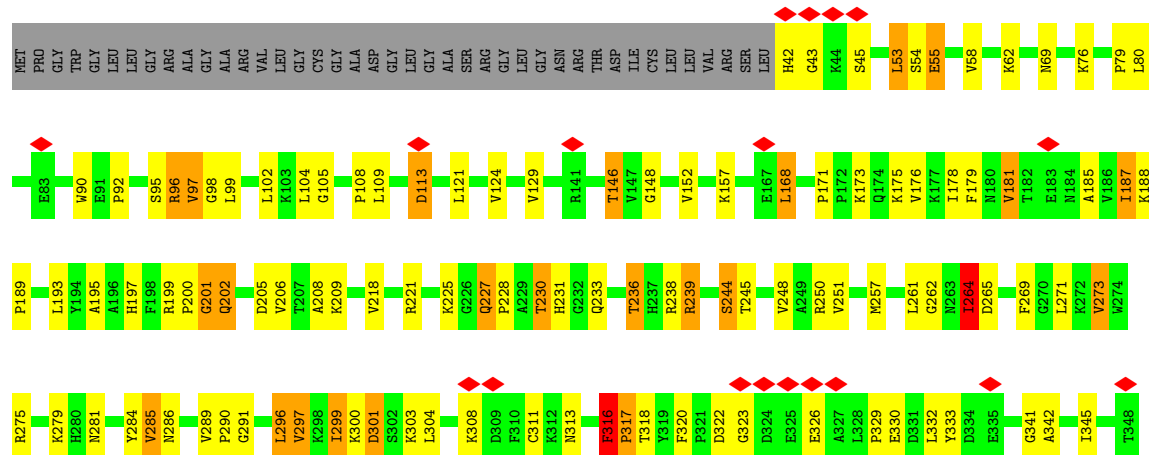




• Molecule 15: Mitochondrial ribosomal protein L2



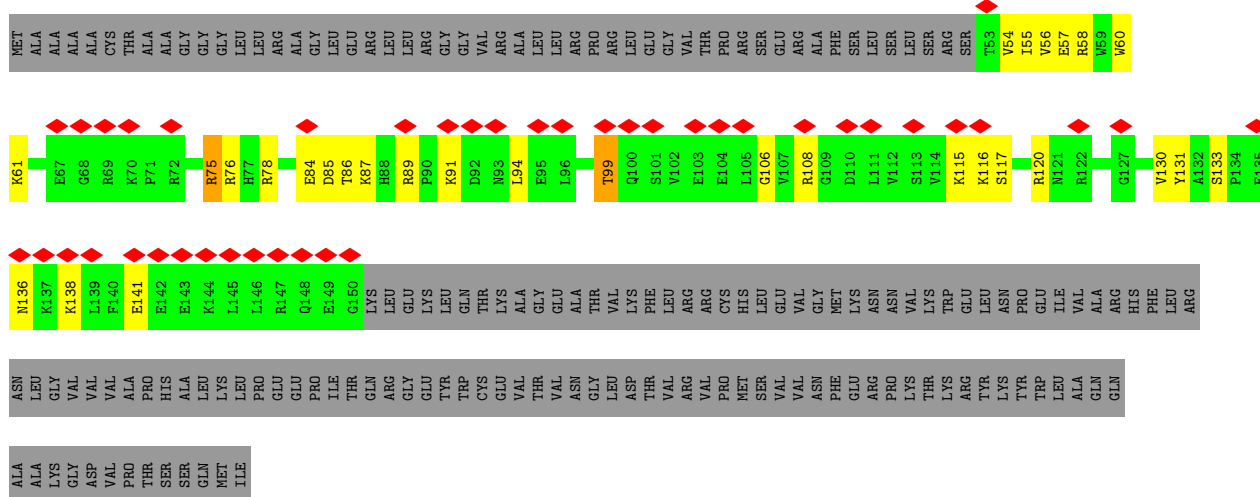
• Molecule 16: ICT1



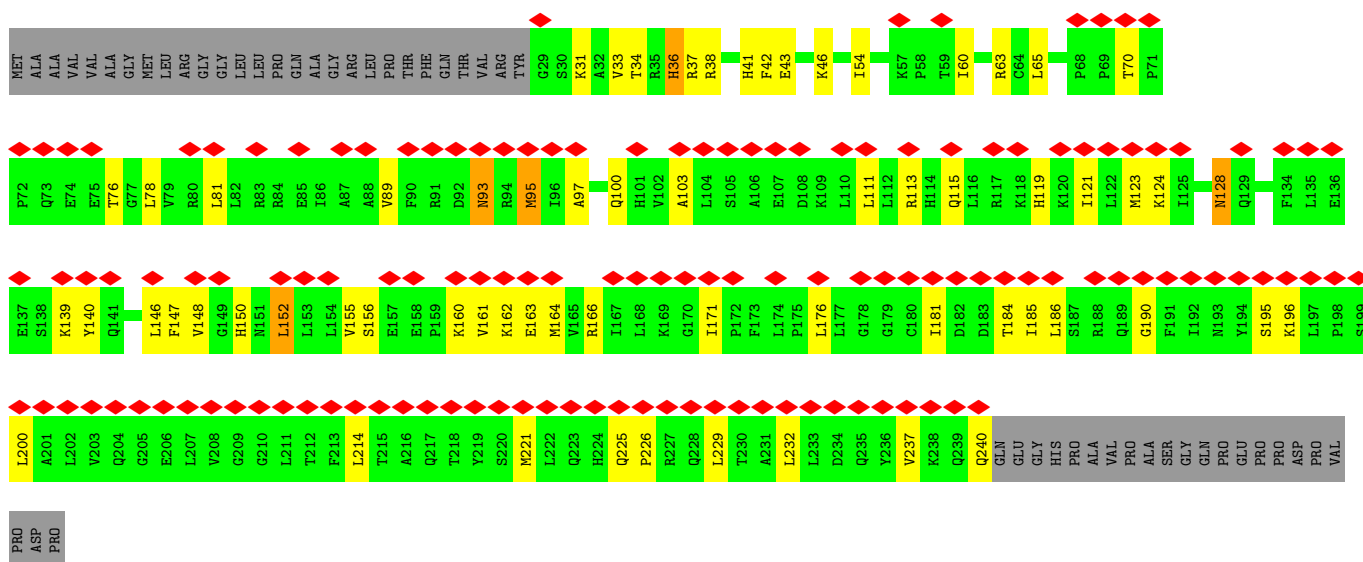
• Molecule 17: Mitochondrial ribosomal protein L4



- Molecule 18: Mitochondrial ribosomal protein L9

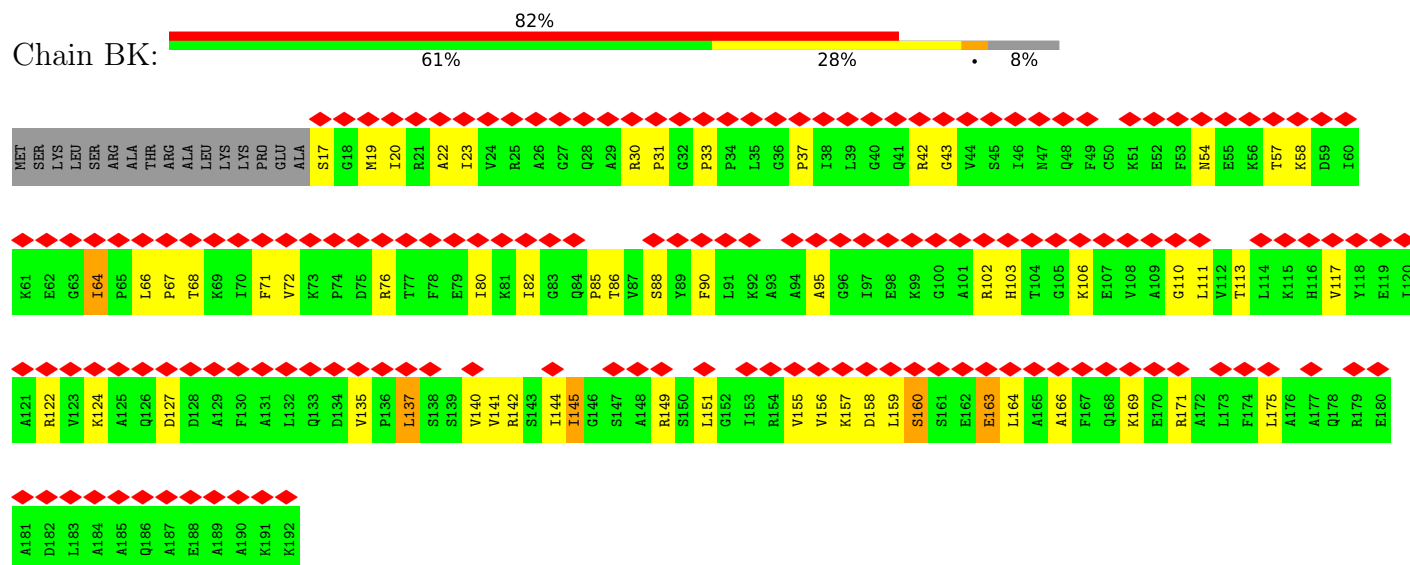


- Molecule 19: Mitochondrial ribosomal protein L10



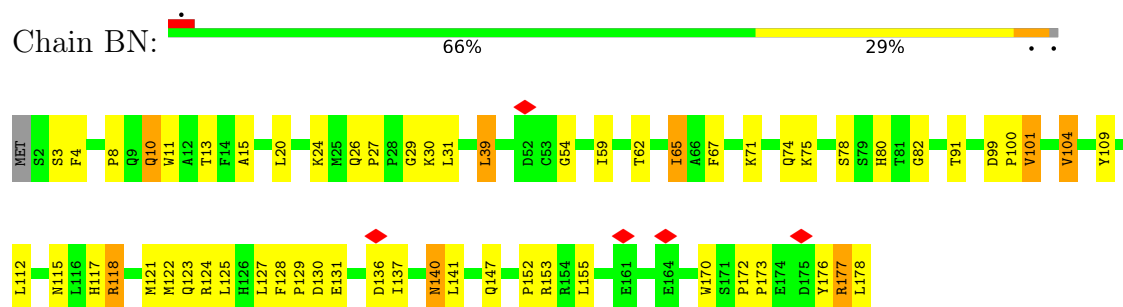
- Molecule 20: Mitochondrial ribosomal protein L11

Chain BK:



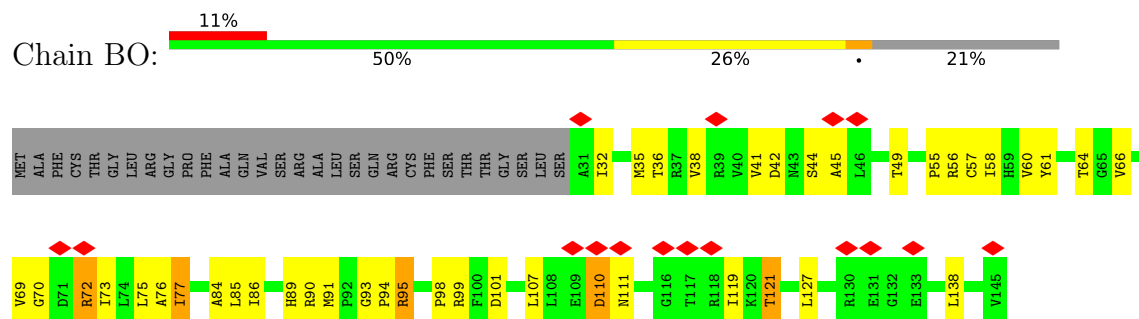
- Molecule 21: Mitochondrial ribosomal protein L13

Chain BN:



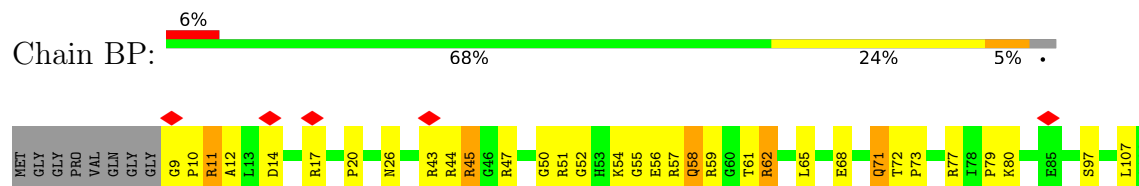
- Molecule 22: Mitochondrial ribosomal protein L14

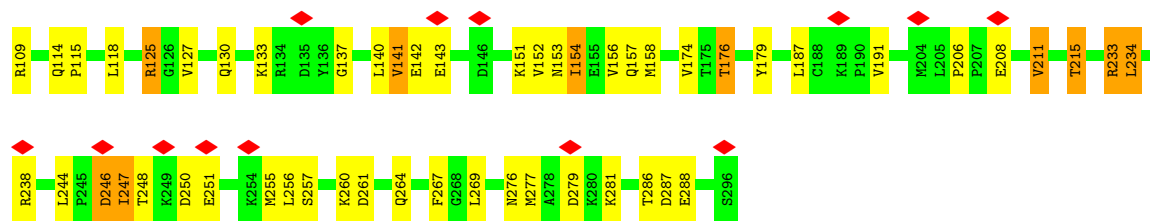
Chain BO:



- Molecule 23: Mitochondrial ribosomal protein L15

Chain BP:

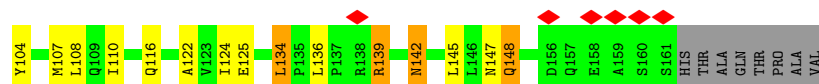




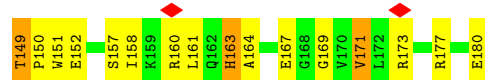
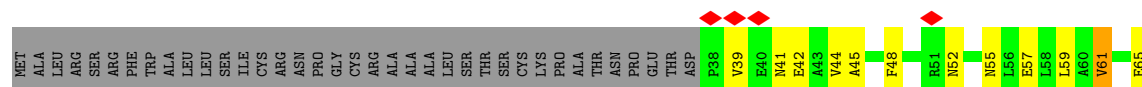
• Molecule 24: Mitochondrial ribosomal protein L16



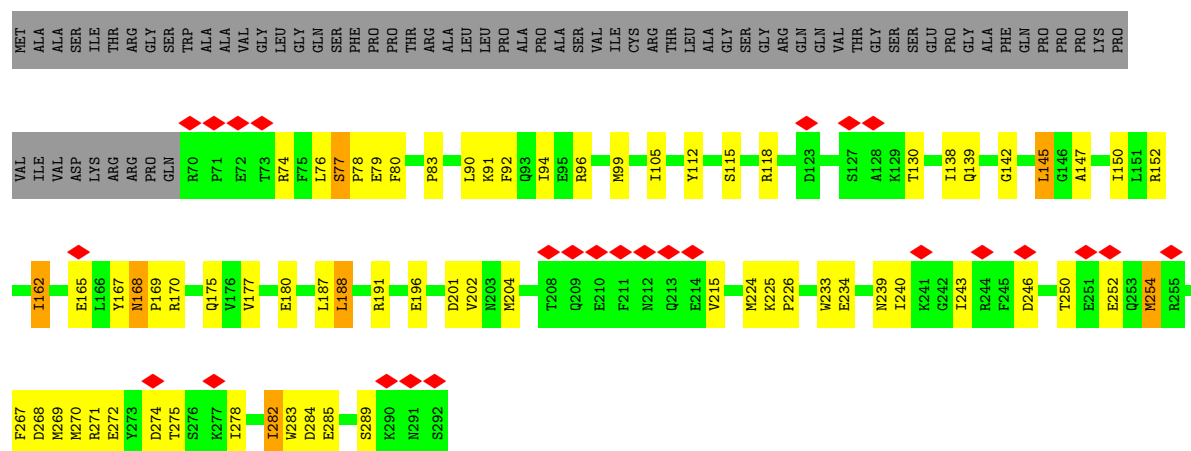
• Molecule 25: Mitochondrial ribosomal protein L17



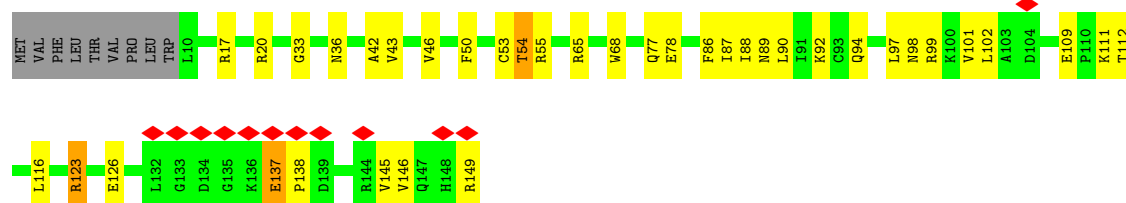
• Molecule 26: Mitochondrial ribosomal protein L18



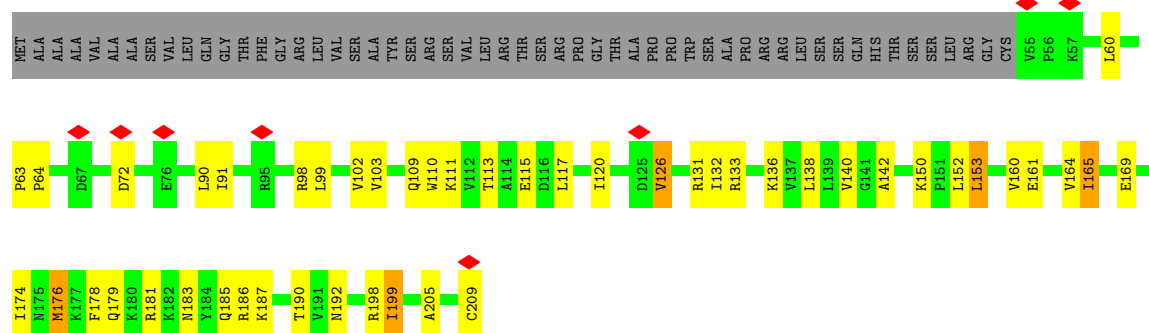
• Molecule 27: Mitochondrial ribosomal protein L19



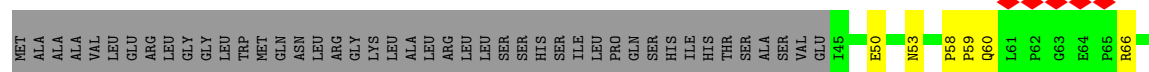
• Molecule 28: Mitochondrial ribosomal protein L20

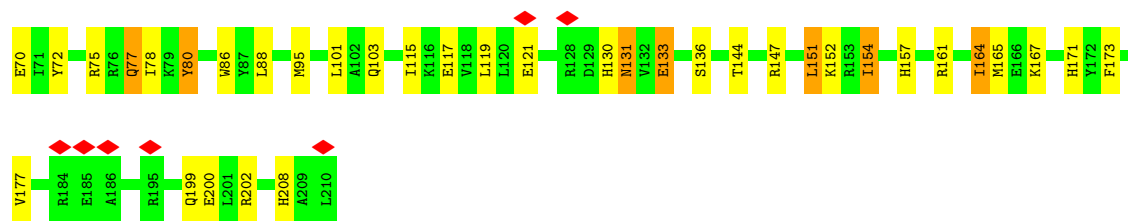


• Molecule 29: Mitochondrial ribosomal protein L21

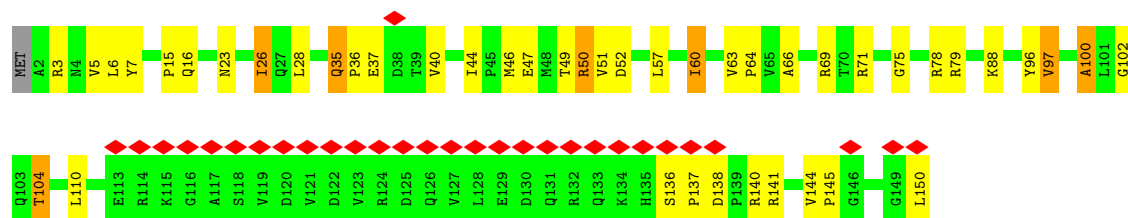


• Molecule 30: Mitochondrial ribosomal protein L22

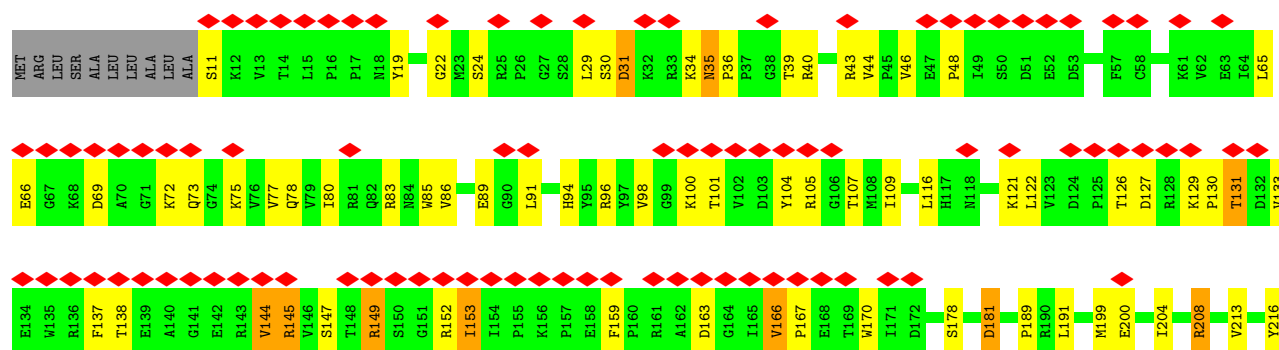
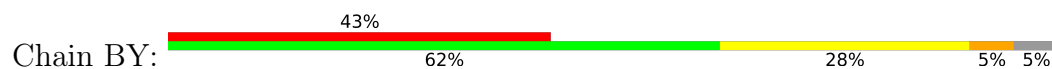




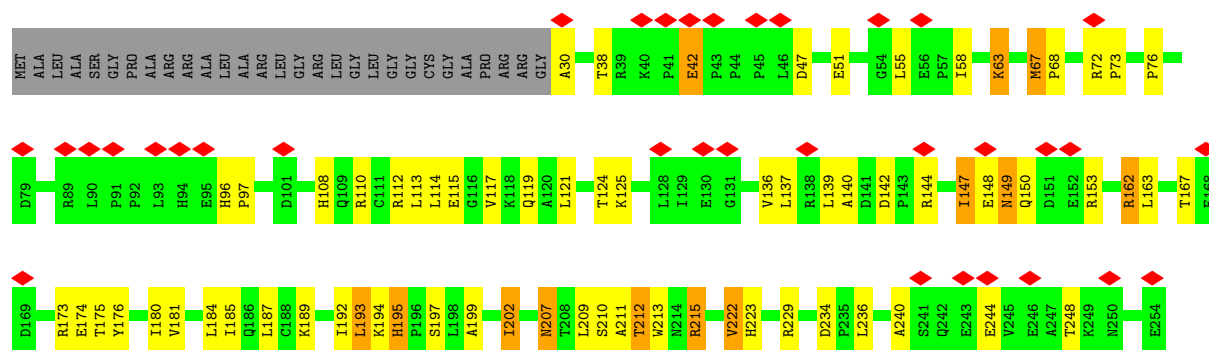
• Molecule 31: Mitochondrial ribosomal protein L23

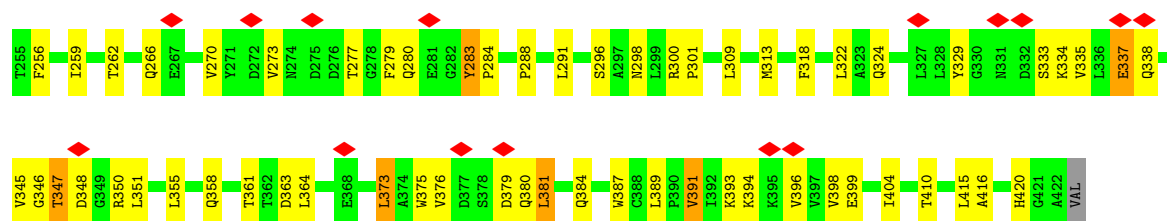


• Molecule 32: Mitochondrial ribosomal protein L24

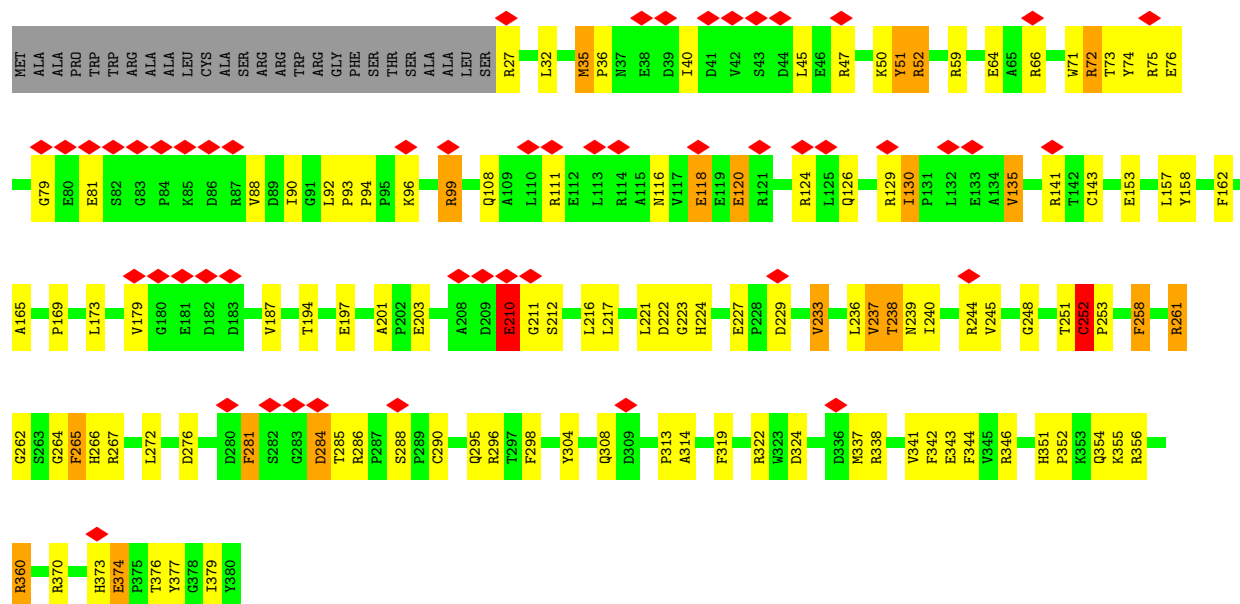


• Molecule 33: Mitochondrial ribosomal protein L37

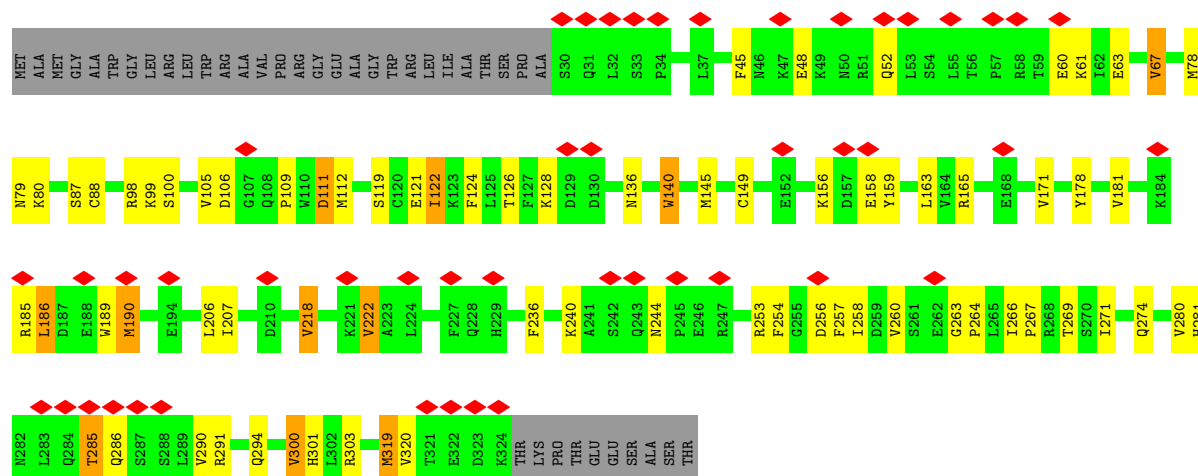




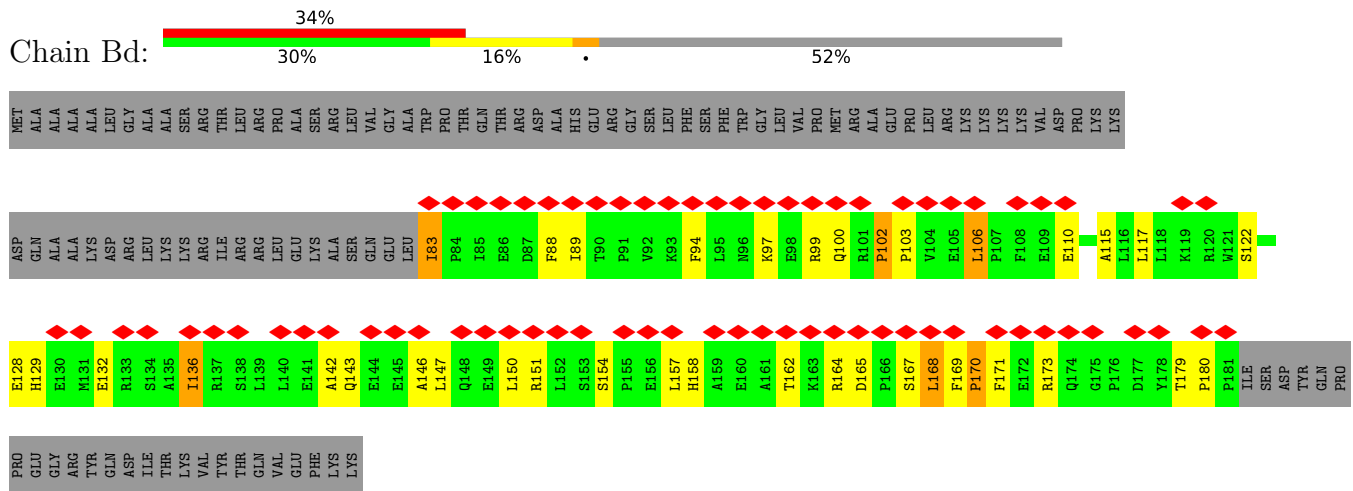
• Molecule 34: Mitochondrial ribosomal protein L38



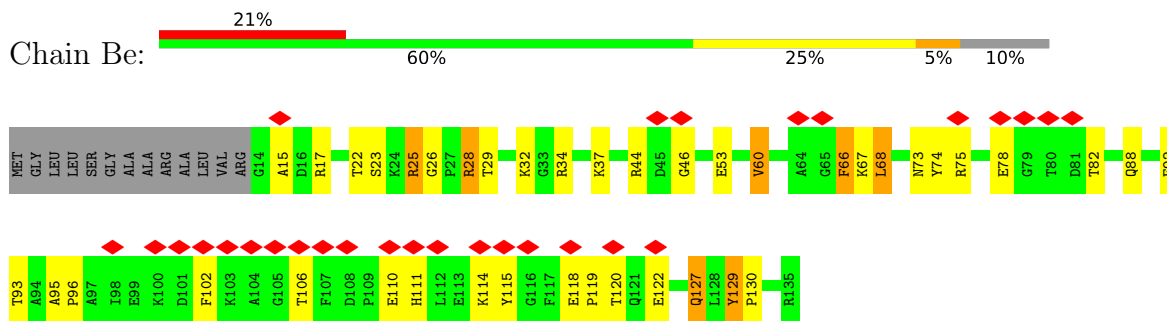
• Molecule 35: Mitochondrial ribosomal protein L39



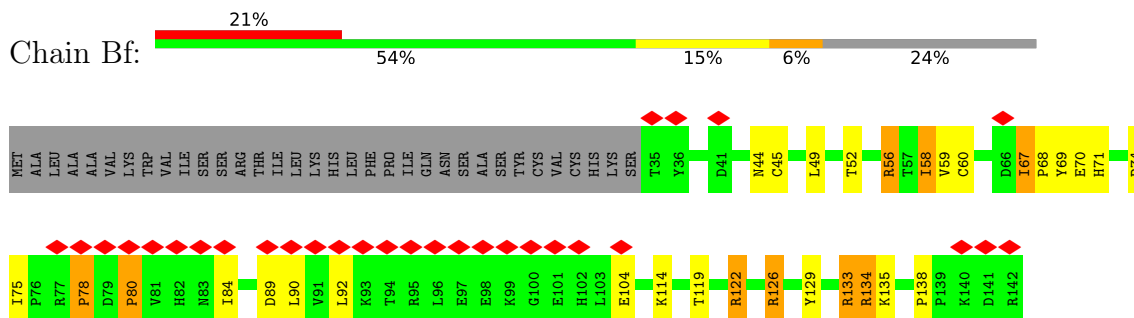
• Molecule 36: Mitochondrial ribosomal protein L40



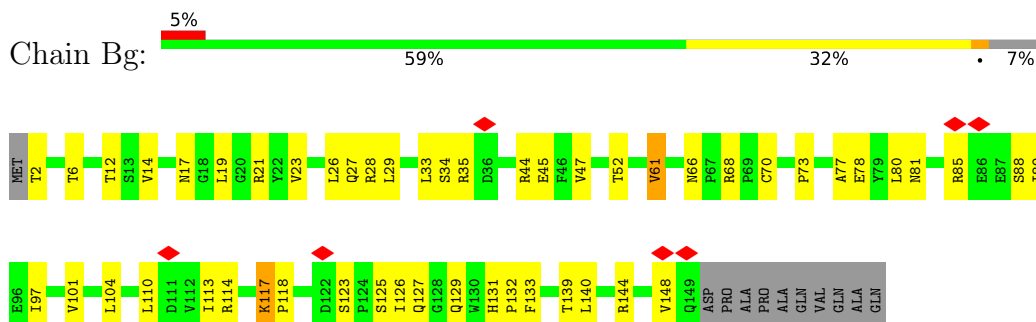
- Molecule 37: Mitochondrial ribosomal protein L41



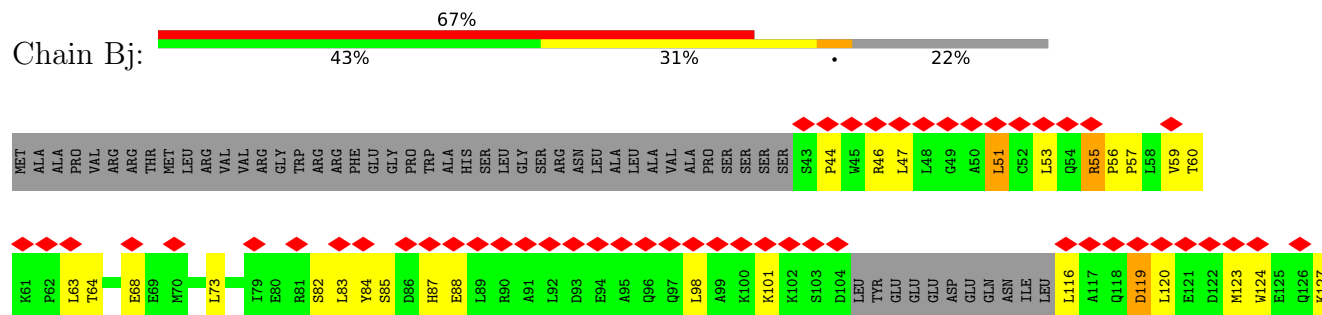
- Molecule 38: Mitochondrial ribosomal protein L42

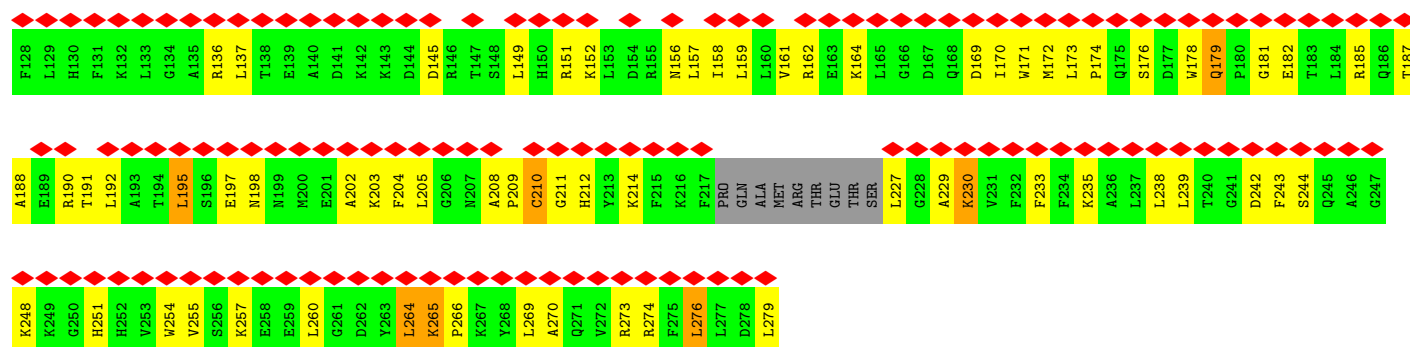


- Molecule 39: Mitochondrial ribosomal protein L43

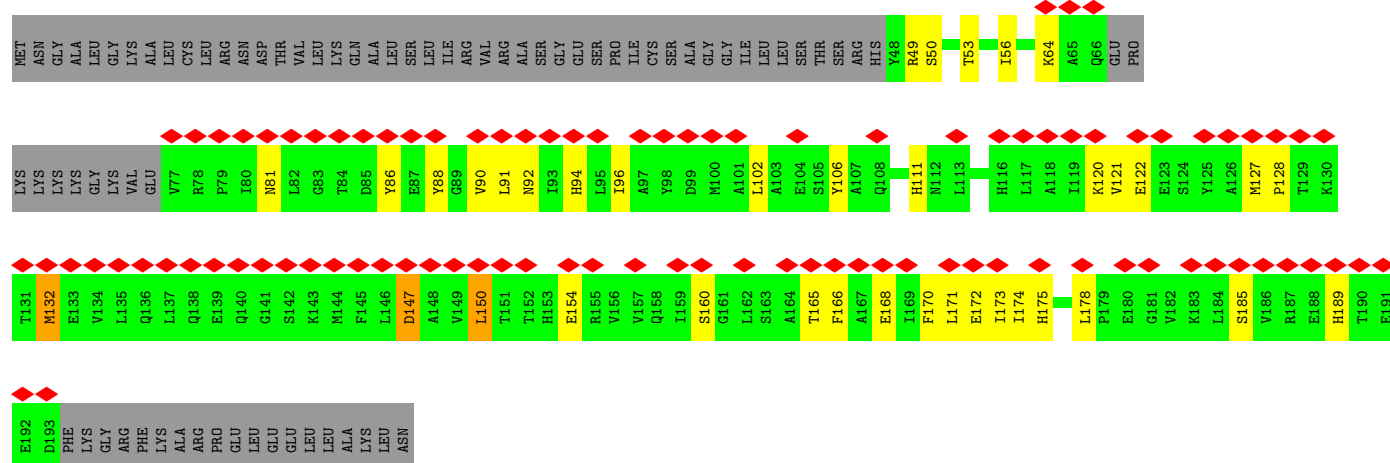


- Molecule 40: Mitochondrial ribosomal protein L44

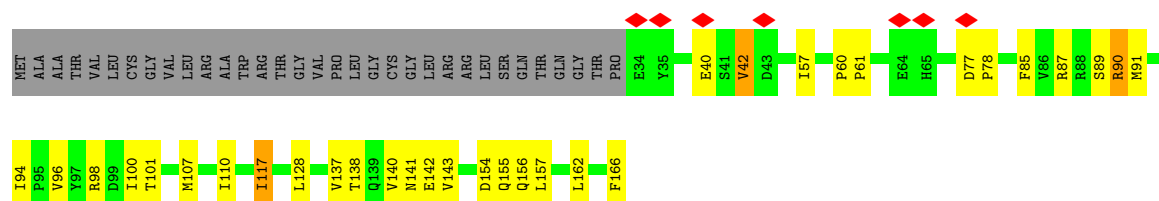




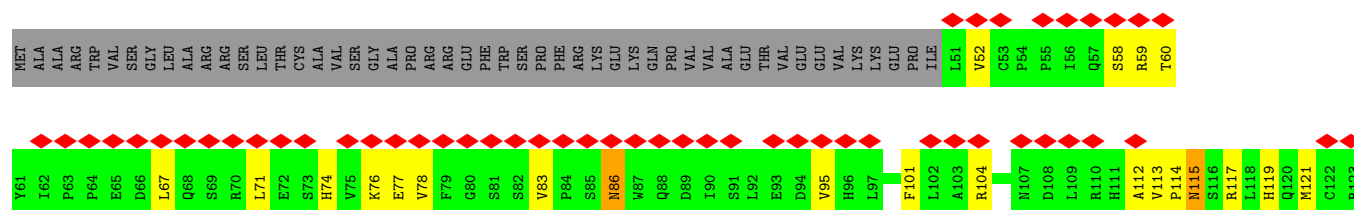
• Molecule 43: Mitochondrial ribosomal protein L48



• Molecule 44: Mrpl34

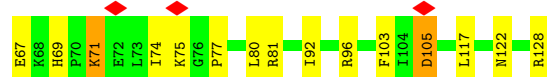


• Molecule 45: Mitochondrial ribosomal protein L50

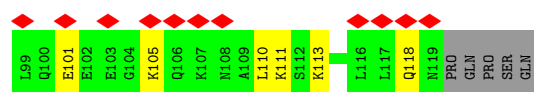




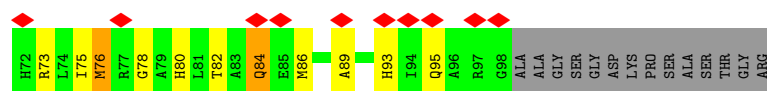
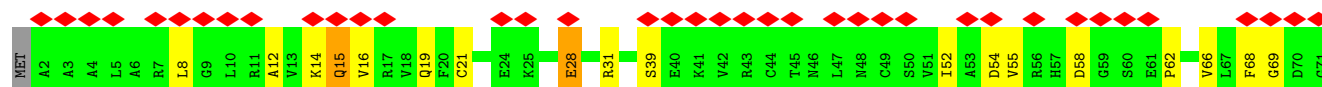
• Molecule 46: Mitochondrial ribosomal protein L51



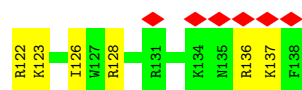
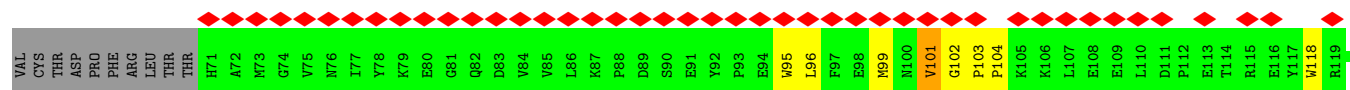
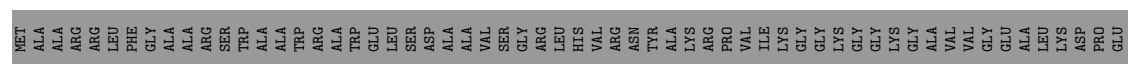
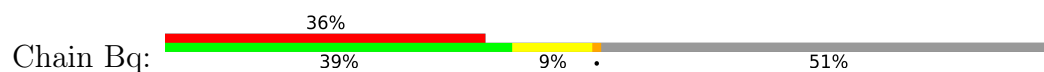
• Molecule 47: Mitochondrial ribosomal protein L52



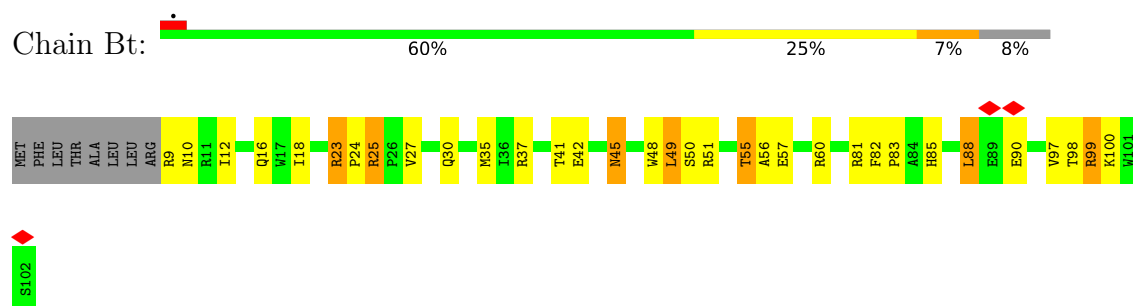
• Molecule 48: mL53, MRPL53



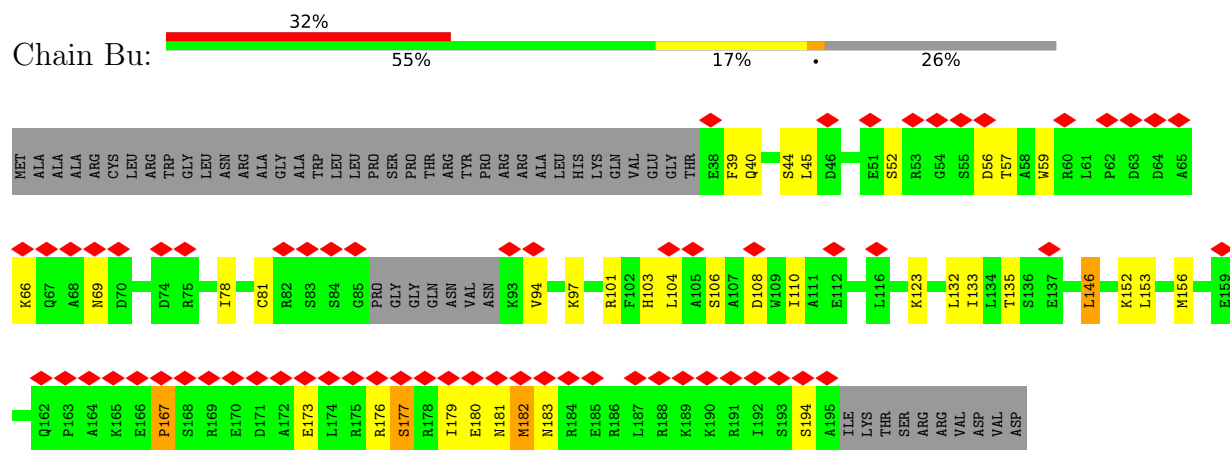
• Molecule 49: Uncharacterized protein



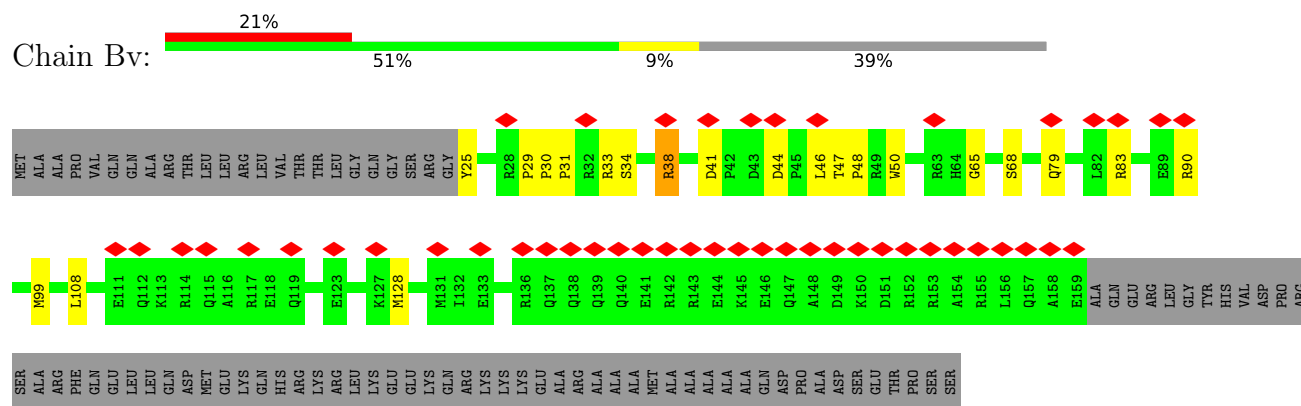
- Molecule 50: Mitochondrial ribosomal protein L57



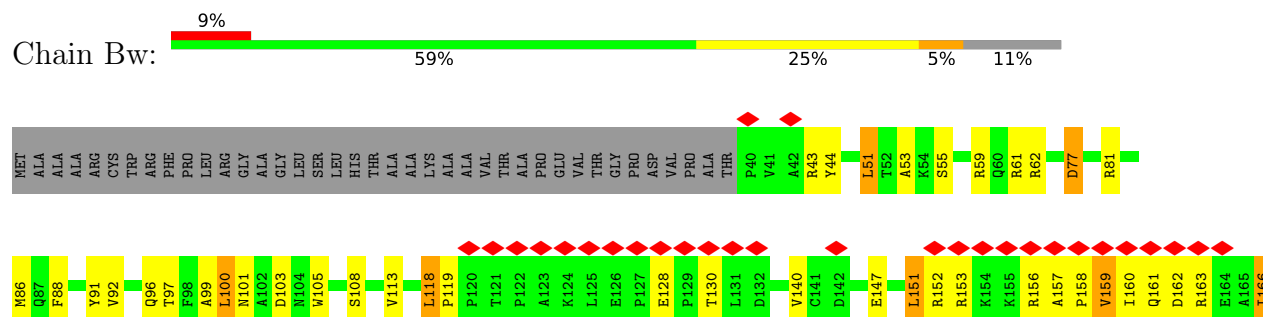
- Molecule 51: Mitochondrial ribosomal protein L58

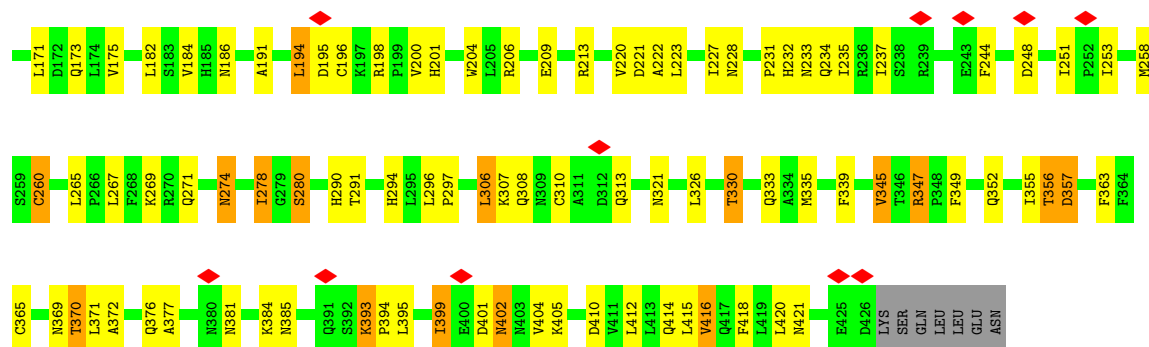


- Molecule 52: 'Mitochondrial ribosomal protein L59

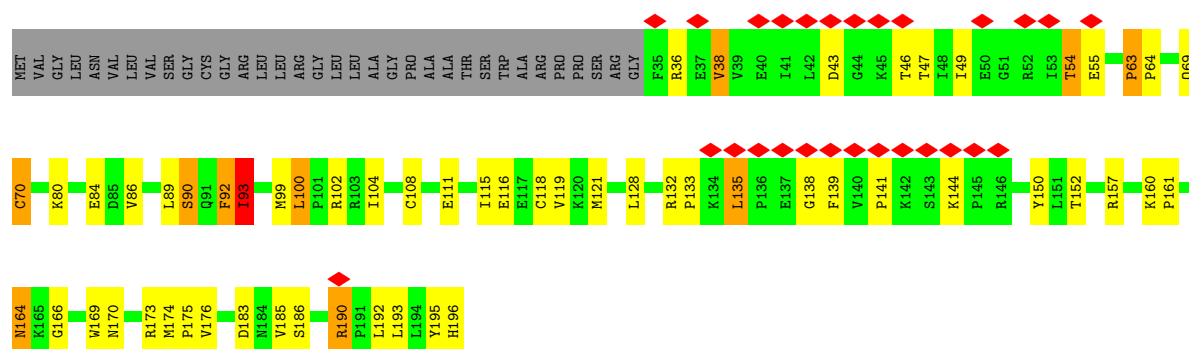


- Molecule 53: mL65, MRPS30





• Molecule 54: Mitochondrial ribosomal protein S18A



• Molecule 55: unassigned secondary structure elements



• Molecule 56: P-site fMet-tRNA^{Met}, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75666	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.658	Depositor
Minimum map value	-0.328	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	390.59, 390.59, 390.59	wwPDB
Map dimensions	281, 281, 281	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GSP, MG, 5GP, FME, ZN, SPM

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	BL	0.53	0/542	0.83	0/729
1	CL	0.70	0/319	1.17	4/435 (0.9%)
1	DL	0.54	0/212	0.70	0/286
1	EL	0.63	0/221	0.83	0/297
1	FL	0.59	0/212	0.74	0/286
1	GL	0.63	0/212	0.67	0/286
1	HL	0.68	0/204	0.72	0/275
2	B0	0.56	0/880	0.87	1/1189 (0.1%)
3	B1	0.42	0/2093	0.82	0/2835
4	B2	0.45	0/1586	0.84	1/2123 (0.0%)
5	B3	0.49	0/993	0.99	3/1341 (0.2%)
6	B4	0.35	0/388	0.97	2/523 (0.4%)
7	B5	0.43	0/917	0.88	2/1227 (0.2%)
8	B6	0.42	0/430	0.91	2/570 (0.4%)
9	B7	0.60	0/395	0.82	0/524
10	B8	0.51	0/853	0.89	0/1136
11	B9	0.50	0/342	0.78	0/450
12	BA	0.31	0/36903	0.46	0/57455
13	BB	0.23	0/1595	0.35	0/2475
14	BC	0.43	0/4432	0.83	4/5989 (0.1%)
15	BD	0.45	0/1898	0.93	3/2555 (0.1%)
16	BE	0.50	0/2493	1.02	14/3387 (0.4%)
17	BF	0.53	0/2069	0.95	5/2816 (0.2%)
18	BI	0.43	0/819	0.87	1/1101 (0.1%)
19	BJ	0.47	0/1742	0.87	5/2358 (0.2%)
20	BK	0.46	0/1323	0.87	1/1785 (0.1%)
21	BN	0.52	0/1487	0.89	3/2017 (0.1%)
22	BO	0.45	0/912	0.87	0/1231
23	BP	0.50	0/2368	0.89	5/3198 (0.2%)
24	BQ	0.46	0/1850	0.85	1/2491 (0.0%)
25	BR	0.47	0/1262	0.84	0/1700
26	BS	0.46	0/1197	0.90	2/1624 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	BT	0.42	0/1888	0.86	3/2548 (0.1%)
28	BU	0.57	0/1179	0.89	2/1578 (0.1%)
29	BV	0.55	0/1256	0.97	5/1706 (0.3%)
30	BW	0.51	0/1407	0.88	2/1891 (0.1%)
31	BX	0.48	0/1211	0.94	2/1646 (0.1%)
32	BY	0.40	0/1719	0.89	2/2329 (0.1%)
33	Ba	0.43	0/3267	0.88	4/4455 (0.1%)
34	Bb	0.44	0/3047	0.93	8/4139 (0.2%)
35	Bc	0.39	0/2464	0.87	4/3330 (0.1%)
36	Bd	0.44	0/853	0.92	3/1153 (0.3%)
37	Be	0.44	0/1000	0.98	8/1345 (0.6%)
38	Bf	0.45	0/851	0.94	5/1159 (0.4%)
39	Bg	0.48	0/1191	0.98	6/1614 (0.4%)
40	Bh	0.47	0/2372	0.95	9/3211 (0.3%)
41	Bi	0.44	0/2199	0.95	9/2980 (0.3%)
42	Bj	0.40	0/1811	0.83	0/2436
43	Bk	0.39	0/1108	0.82	0/1499
44	Bl	0.48	0/1135	0.84	0/1549
45	Bm	0.40	0/917	0.80	0/1248
46	Bn	0.50	0/860	0.93	0/1150
47	Bo	0.43	0/787	0.81	3/1056 (0.3%)
48	Bp	0.43	0/752	0.90	3/1013 (0.3%)
49	Bq	0.46	0/558	0.85	2/756 (0.3%)
50	Bt	0.50	0/798	1.03	4/1073 (0.4%)
51	Bu	0.37	0/1214	0.79	1/1630 (0.1%)
52	Bv	0.37	0/1157	0.71	0/1560
53	Bw	0.47	0/3206	0.92	9/4354 (0.2%)
54	Bx	0.51	0/1364	0.97	5/1849 (0.3%)
55	Bz	0.51	0/404	0.67	0/556
56	AV	0.24	0/1673	0.37	0/2602
All	All	0.42	0/116797	0.76	158/166109 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	B4	0	1
16	BE	0	1
26	BS	0	1
34	Bb	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
46	Bn	0	1
All	All	0	5

There are no bond length outliers.

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Bh	284	GLY	CA-C-N	12.91	132.96	120.31
40	Bh	284	GLY	C-N-CA	12.91	132.96	120.31
41	Bi	89	VAL	CA-C-N	9.45	130.11	120.38
41	Bi	89	VAL	C-N-CA	9.45	130.11	120.38
6	B4	71	GLU	CA-C-N	8.92	128.56	119.82
6	B4	71	GLU	C-N-CA	8.92	128.56	119.82
50	Bt	23	ARG	CA-C-N	8.57	130.55	119.84
50	Bt	23	ARG	C-N-CA	8.57	130.55	119.84
15	BD	119	LYS	CA-C-N	8.46	128.10	119.56
15	BD	119	LYS	C-N-CA	8.46	128.10	119.56
37	Be	129	TYR	CA-C-N	-8.43	111.11	119.87
37	Be	129	TYR	C-N-CA	-8.43	111.11	119.87
8	B6	47	ASP	CA-C-N	8.14	127.82	119.19
8	B6	47	ASP	C-N-CA	8.14	127.82	119.19
14	BC	505	PRO	N-CA-CB	8.07	110.03	101.88
54	Bx	63	PRO	CA-C-N	8.05	127.72	119.19
54	Bx	63	PRO	C-N-CA	8.05	127.72	119.19
16	BE	239	ARG	CA-C-N	8.04	127.69	119.82
16	BE	239	ARG	C-N-CA	8.04	127.69	119.82
50	Bt	25	ARG	CA-C-N	7.87	128.03	120.31
50	Bt	25	ARG	C-N-CA	7.87	128.03	120.31
39	Bg	117	LYS	CA-C-N	7.75	127.41	119.82
39	Bg	117	LYS	C-N-CA	7.75	127.41	119.82
53	Bw	381	ASN	CA-C-N	7.72	127.37	119.19
53	Bw	381	ASN	C-N-CA	7.72	127.37	119.19
35	Bc	263	GLY	CA-C-N	7.60	127.51	120.21
35	Bc	263	GLY	C-N-CA	7.60	127.51	120.21
16	BE	345	ILE	N-CA-C	7.46	119.07	109.30
1	CL	21	PRO	N-CA-CB	7.42	111.04	103.25
24	BQ	69	LEU	N-CA-C	-7.39	104.26	113.28
48	Bp	21	CYS	CA-C-N	7.30	127.94	119.47
48	Bp	21	CYS	C-N-CA	7.30	127.94	119.47
32	BY	35	ASN	CA-C-N	7.24	127.84	120.38
32	BY	35	ASN	C-N-CA	7.24	127.84	120.38
1	CL	16	PRO	N-CA-CB	7.11	110.85	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	BC	502	PRO	N-CA-CB	7.07	110.67	103.25
16	BE	316	PHE	N-CA-C	6.74	121.70	108.21
38	Bf	80	PRO	N-CA-CB	6.70	110.28	103.25
16	BE	201	GLY	N-CA-C	-6.67	97.38	113.18
51	Bu	167	PRO	N-CA-CB	6.66	110.24	103.25
17	BF	121	ARG	N-CA-C	6.64	119.52	111.82
40	Bh	184	PHE	CA-C-N	-6.57	113.39	119.82
40	Bh	184	PHE	C-N-CA	-6.57	113.39	119.82
19	BJ	70	THR	CA-C-N	6.56	127.14	120.38
19	BJ	70	THR	C-N-CA	6.56	127.14	120.38
1	CL	17	LEU	N-CA-C	6.49	116.63	108.45
53	Bw	186	ASN	CA-C-N	6.45	126.14	119.56
53	Bw	186	ASN	C-N-CA	6.45	126.14	119.56
36	Bd	102	PRO	N-CA-C	6.43	118.55	110.70
34	Bb	265	PHE	N-CA-C	6.41	119.03	111.02
54	Bx	164	ASN	N-CA-C	6.40	121.24	113.17
38	Bf	78	PRO	N-CA-CB	6.38	109.95	103.25
49	Bq	102	GLY	N-CA-C	6.38	125.35	112.34
1	CL	18	ASP	N-CA-C	6.38	118.76	111.11
31	BX	102	GLY	N-CA-C	-6.37	106.34	115.64
33	Ba	347	THR	N-CA-C	6.32	119.56	108.75
23	BP	9	GLY	CA-C-N	6.32	127.74	119.84
23	BP	9	GLY	C-N-CA	6.32	127.74	119.84
17	BF	195	LEU	CA-C-N	6.31	127.73	119.84
17	BF	195	LEU	C-N-CA	6.31	127.73	119.84
16	BE	304	LEU	CA-C-N	6.21	125.43	118.97
16	BE	304	LEU	C-N-CA	6.21	125.43	118.97
20	BK	160	SER	N-CA-C	6.21	118.59	111.02
37	Be	46	GLY	N-CA-C	-6.20	107.71	115.08
49	Bq	103	PRO	N-CA-C	6.17	118.23	110.70
53	Bw	198	ARG	CA-C-N	6.11	126.13	119.90
53	Bw	198	ARG	C-N-CA	6.11	126.13	119.90
26	BS	52	ASN	CA-C-N	6.11	125.73	119.56
26	BS	52	ASN	C-N-CA	6.11	125.73	119.56
34	Bb	374	GLU	CA-C-N	-6.09	113.70	119.85
34	Bb	374	GLU	C-N-CA	-6.09	113.70	119.85
53	Bw	100	LEU	CA-C-N	-6.08	114.14	123.14
53	Bw	100	LEU	C-N-CA	-6.08	114.14	123.14
17	BF	126	LYS	CA-C-N	6.05	125.67	119.56
17	BF	126	LYS	C-N-CA	6.05	125.67	119.56
18	BI	106	GLY	N-CA-C	6.01	118.69	110.69
54	Bx	135	LEU	CA-C-N	6.00	126.43	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	Bx	135	LEU	C-N-CA	6.00	126.43	119.47
41	Bi	67	ILE	CA-C-N	-5.99	113.51	119.56
41	Bi	67	ILE	C-N-CA	-5.99	113.51	119.56
39	Bg	123	SER	CA-C-N	5.97	125.59	119.56
39	Bg	123	SER	C-N-CA	5.97	125.59	119.56
19	BJ	171	ILE	CA-C-N	5.97	125.52	119.19
19	BJ	171	ILE	C-N-CA	5.97	125.52	119.19
41	Bi	266	ILE	CA-C-N	5.95	123.95	119.66
41	Bi	266	ILE	C-N-CA	5.95	123.95	119.66
16	BE	230	THR	N-CA-C	5.92	120.78	113.50
29	BV	205	ALA	CA-C-N	5.92	125.62	119.82
29	BV	205	ALA	C-N-CA	5.92	125.62	119.82
5	B3	103	ILE	CA-C-N	5.88	125.58	119.05
5	B3	103	ILE	C-N-CA	5.88	125.58	119.05
5	B3	113	VAL	N-CA-C	5.83	117.77	112.29
16	BE	262	GLY	N-CA-C	5.82	121.71	114.37
15	BD	128	ILE	N-CA-C	5.81	116.45	110.82
40	Bh	63	LYS	CA-C-N	5.78	125.25	119.24
40	Bh	63	LYS	C-N-CA	5.78	125.25	119.24
33	Ba	283	TYR	CA-C-N	5.74	125.60	119.28
33	Ba	283	TYR	C-N-CA	5.74	125.60	119.28
7	B5	181	ARG	CA-C-N	5.72	125.68	119.78
7	B5	181	ARG	C-N-CA	5.72	125.68	119.78
38	Bf	90	LEU	N-CA-C	-5.72	105.80	112.89
30	BW	130	HIS	CA-C-N	-5.71	115.00	123.11
30	BW	130	HIS	C-N-CA	-5.71	115.00	123.11
2	B0	74	ARG	N-CA-C	-5.67	104.53	112.12
48	Bp	58	ASP	N-CA-C	5.64	119.34	112.23
37	Be	26	GLY	CA-C-N	5.63	126.88	119.84
37	Be	26	GLY	C-N-CA	5.63	126.88	119.84
23	BP	72	THR	CA-C-N	5.60	125.61	119.89
23	BP	72	THR	C-N-CA	5.60	125.61	119.89
40	Bh	188	PRO	N-CA-C	5.57	117.50	110.70
37	Be	15	ALA	CB-CA-C	-5.57	109.17	115.79
16	BE	323	GLY	N-CA-C	5.56	119.41	112.73
34	Bb	211	GLY	N-CA-C	-5.56	100.00	113.18
34	Bb	201	ALA	CA-C-N	5.53	125.73	120.31
34	Bb	201	ALA	C-N-CA	5.53	125.73	120.31
35	Bc	244	ASN	CA-C-N	5.53	125.62	119.32
35	Bc	244	ASN	C-N-CA	5.53	125.62	119.32
31	BX	100	ALA	N-CA-C	5.51	118.12	111.40
53	Bw	357	ASP	N-CA-C	-5.50	101.51	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	BE	244	SER	N-CA-C	5.49	115.09	107.73
16	BE	291	GLY	N-CA-C	-5.49	104.43	110.96
40	Bh	187	PRO	CA-C-N	5.49	126.03	120.38
40	Bh	187	PRO	C-N-CA	5.49	126.03	120.38
41	Bi	185	PHE	CA-C-N	-5.34	117.74	122.97
41	Bi	185	PHE	C-N-CA	-5.34	117.74	122.97
36	Bd	165	ASP	CA-C-N	5.31	125.02	119.82
36	Bd	165	ASP	C-N-CA	5.31	125.02	119.82
29	BV	72	ASP	CA-C-N	5.26	125.57	119.47
29	BV	72	ASP	C-N-CA	5.26	125.57	119.47
21	BN	130	ASP	CA-C-N	-5.22	115.05	122.77
21	BN	130	ASP	C-N-CA	-5.22	115.05	122.77
28	BU	137	GLU	CA-C-N	-5.22	114.42	119.90
28	BU	137	GLU	C-N-CA	-5.22	114.42	119.90
29	BV	165	ILE	CB-CA-C	-5.22	105.14	111.87
34	Bb	252	CYS	CA-C-N	5.21	125.15	119.78
34	Bb	252	CYS	C-N-CA	5.21	125.15	119.78
16	BE	97	VAL	CB-CA-C	-5.21	105.62	111.45
14	BC	235	THR	CA-C-N	5.21	125.20	119.89
14	BC	235	THR	C-N-CA	5.21	125.20	119.89
33	Ba	76	PRO	O-C-N	5.17	123.58	121.15
27	BT	188	LEU	N-CA-C	-5.17	106.66	113.17
47	Bo	46	LEU	CA-C-N	5.14	126.27	119.84
47	Bo	46	LEU	C-N-CA	5.14	126.27	119.84
4	B2	190	TRP	N-CA-C	5.13	117.61	111.71
38	Bf	138	PRO	CA-C-N	5.13	125.12	119.89
38	Bf	138	PRO	C-N-CA	5.13	125.12	119.89
39	Bg	66	ASN	CA-C-N	-5.12	114.52	119.90
39	Bg	66	ASN	C-N-CA	-5.12	114.52	119.90
23	BP	206	PRO	O-C-N	5.12	123.56	121.15
47	Bo	40	TYR	CA-CB-CG	5.11	123.09	113.90
27	BT	168	ASN	CA-C-N	5.10	124.82	119.82
27	BT	168	ASN	C-N-CA	5.10	124.82	119.82
19	BJ	36	HIS	N-CA-C	5.09	119.18	112.92
41	Bi	173	VAL	N-CA-C	5.09	116.55	111.00
37	Be	60	VAL	CA-C-N	5.08	125.29	120.31
37	Be	60	VAL	C-N-CA	5.08	125.29	120.31
21	BN	54	GLY	N-CA-C	-5.01	101.30	113.18
16	BE	308	LYS	N-CA-C	5.00	117.11	111.11

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	B4	61	ASP	Peptide
16	BE	316	PHE	Peptide
26	BS	69	GLY	Peptide
34	Bb	210	GLU	Peptide
46	Bn	65	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BL	537	0	591	12	0
1	CL	317	0	309	12	0
1	DL	213	0	234	7	0
1	EL	222	0	247	6	0
1	FL	213	0	234	7	0
1	GL	213	0	234	5	0
1	HL	205	0	223	9	0
2	B0	857	0	878	20	0
3	B1	2036	0	2058	45	0
4	B2	1548	0	1583	27	0
5	B3	968	0	1018	26	0
6	B4	381	0	400	19	0
7	B5	902	0	916	33	0
8	B6	425	0	471	16	0
9	B7	387	0	413	7	0
10	B8	833	0	883	21	0
11	B9	335	0	359	11	0
12	BA	32950	0	16673	363	0
13	BB	1427	0	726	14	0
14	BC	4364	0	4371	82	0
15	BD	1860	0	1923	40	0
16	BE	2420	0	2418	75	0
17	BF	2011	0	2049	62	0
18	BI	805	0	845	26	0
19	BJ	1705	0	1804	46	0
20	BK	1303	0	1343	39	0
21	BN	1444	0	1437	49	0
22	BO	896	0	946	34	0
23	BP	2312	0	2373	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	BQ	1803	0	1841	32	0
25	BR	1240	0	1260	27	0
26	BS	1168	0	1159	49	0
27	BT	1845	0	1856	42	0
28	BU	1159	0	1228	23	0
29	BV	1231	0	1278	28	0
30	BW	1374	0	1405	28	0
31	BX	1181	0	1139	31	0
32	BY	1678	0	1683	44	0
33	Ba	3173	0	3153	88	0
34	Bb	2952	0	2840	91	0
35	Bc	2408	0	2415	53	0
36	Bd	832	0	828	41	0
37	Be	972	0	971	33	0
38	Bf	827	0	736	30	0
39	Bg	1167	0	1173	37	0
40	Bh	2319	0	2332	64	0
41	Bi	2138	0	2139	61	0
42	Bj	1775	0	1797	74	0
43	Bk	1087	0	1080	34	0
44	Bl	1097	0	1080	13	0
45	Bm	893	0	878	26	0
46	Bn	837	0	860	31	0
47	Bo	772	0	773	19	0
48	Bp	742	0	749	20	0
49	Bq	542	0	485	14	0
50	Bt	780	0	792	22	0
51	Bu	1198	0	1192	23	0
52	Bv	1131	0	1093	15	0
53	Bw	3126	0	3153	91	0
54	Bx	1325	0	1354	53	0
55	Bz	410	0	404	5	0
56	AV	1498	0	765	9	0
57	B3	1	0	0	0	0
57	BA	203	0	0	0	0
57	BB	1	0	0	0	0
57	BC	1	0	0	0	0
57	BD	3	0	0	0	0
57	BP	2	0	0	0	0
57	BQ	1	0	0	0	0
57	Be	2	0	0	0	0
57	Bl	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	Bt	1	0	0	0	0
58	B5	1	0	0	0	0
58	B9	1	0	0	0	0
58	BJ	1	0	0	0	0
59	BA	48	0	24	0	0
60	BA	14	0	26	2	0
60	BR	14	0	26	0	0
61	BC	32	0	12	1	0
62	BC	1	0	0	0	0
63	AV	10	0	10	0	0
64	BC	2	0	0	0	0
All	All	111109	0	93948	1934	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 9.

All (1934) 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)
26:BS:85:ARG:HB3	26:BS:120:ARG:HH12	1.20	1.04
37:Be:44:ARG:HH12	53:Bw:157:ALA:HB3	1.20	1.02
37:Be:25:ARG:HG2	37:Be:25:ARG:HH11	1.26	0.99
35:Bc:186:LEU:HG	35:Bc:189:TRP:HE1	1.29	0.98
35:Bc:294:GLN:HE22	35:Bc:320:VAL:H	1.13	0.94
17:BF:287:ARG:HD2	52:Bv:33:ARG:HH12	1.31	0.94
42:Bj:235:LYS:HZ2	43:Bk:172:GLU:HG2	1.32	0.91
10:B8:183:ARG:HH12	34:Bb:354:GLN:HE21	1.19	0.90
14:BC:397:ARG:HH21	14:BC:422:ARG:HH12	1.21	0.89
12:BA:49:A:OP1	18:BI:78:ARG:NH1	2.06	0.88
28:BU:54:THR:HG21	29:BV:176:MET:H	1.39	0.88
36:Bd:167:SER:O	42:Bj:203:LYS:NZ	2.06	0.87
26:BS:130:ARG:NH1	34:Bb:129:ARG:HH11	1.71	0.87
26:BS:160:ARG:HH12	34:Bb:126:GLN:HB3	1.39	0.86
33:Ba:387:TRP:HE1	33:Ba:404:ILE:HD11	1.41	0.86
12:BA:1230:U:H5'	12:BA:1231:U:H5'	1.56	0.85
51:Bu:52:SER:HB2	51:Bu:57:THR:HG21	1.56	0.85
33:Ba:350:ARG:NH1	33:Ba:384:GLN:O	2.10	0.85
53:Bw:97:THR:HG22	53:Bw:99:ALA:H	1.40	0.85
14:BC:543:GLU:HB3	14:BC:614:LEU:HD11	1.59	0.84
22:BO:72:ARG:HB2	22:BO:72:ARG:HH11	1.40	0.84
40:Bh:259:ARG:HG3	40:Bh:259:ARG:HH11	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:748:A:OP1	53:Bw:307:LYS:NZ	2.11	0.84
26:BS:85:ARG:HB3	26:BS:120:ARG:NH1	1.92	0.83
12:BA:529:G:H4'	49:Bq:122:ARG:NH1	1.93	0.83
20:BK:43:GLY:HA3	20:BK:76:ARG:HH11	1.43	0.82
8:B6:59:GLN:HG2	8:B6:60:LYS:HG3	1.60	0.82
12:BA:548:A:H5''	49:Bq:126:ILE:HD11	1.60	0.82
12:BA:546:C:O2'	49:Bq:136:ARG:NH2	2.13	0.82
12:BA:79:U:O2'	18:BI:61:LYS:NZ	2.13	0.81
36:Bd:164:ARG:NH1	43:Bk:88:TYR:HB3	1.95	0.81
26:BS:86:THR:HG22	26:BS:88:HIS:H	1.44	0.81
12:BA:1213:A:H2	12:BA:1220:A:H62	1.28	0.81
16:BE:76:LYS:NZ	16:BE:168:LEU:O	2.13	0.81
12:BA:69:C:H4'	12:BA:70:A:H5'	1.62	0.80
12:BA:142:U:H5''	32:BY:100:LYS:HZ1	1.46	0.80
20:BK:124:LYS:NZ	20:BK:127:ASP:OD2	2.13	0.80
36:Bd:164:ARG:HH12	43:Bk:91:LEU:HD11	1.44	0.80
2:B0:39:SER:N	12:BA:1156:A:HO2'	1.80	0.79
12:BA:62:C:OP1	18:BI:76:ARG:NH1	2.16	0.79
12:BA:1216:C:H42	26:BS:173:ARG:HH22	1.25	0.79
11:B9:71:LYS:NZ	12:BA:496:C:OP1	2.13	0.78
12:BA:169:U:OP2	39:Bg:114:ARG:NH2	2.16	0.78
20:BK:159:LEU:O	20:BK:163:GLU:N	2.15	0.78
33:Ba:333:SER:HB3	33:Ba:363:ASP:HB3	1.63	0.78
12:BA:477:A:H2'	12:BA:478:G:H5''	1.63	0.78
37:Be:44:ARG:NH1	53:Bw:157:ALA:HB3	1.99	0.78
38:Bf:122:ARG:HH11	38:Bf:122:ARG:HG3	1.47	0.78
10:B8:183:ARG:NH1	34:Bb:354:GLN:HE21	1.82	0.78
5:B3:72:ILE:HD11	5:B3:118:ARG:NH1	1.98	0.78
39:Bg:17:ASN:HD21	39:Bg:23:VAL:H	1.28	0.78
29:BV:136:LYS:NZ	47:Bo:48:ASP:HB3	1.99	0.78
39:Bg:144:ARG:NH1	40:Bh:260:GLN:OE1	2.17	0.78
34:Bb:286:ARG:NH1	34:Bb:295:GLN:O	2.16	0.78
40:Bh:259:ARG:HH11	40:Bh:259:ARG:CG	1.97	0.77
12:BA:142:U:H5''	32:BY:100:LYS:NZ	1.97	0.77
29:BV:131:ARG:NH1	29:BV:161:GLU:OE1	2.17	0.77
7:B5:181:ARG:HH11	7:B5:187:GLN:HG2	1.49	0.77
20:BK:156:VAL:HG11	20:BK:159:LEU:HD13	1.67	0.77
7:B5:152:PRO:HG3	7:B5:173:ARG:NH1	2.00	0.76
41:Bi:267:PRO:HG2	41:Bi:270:ALA:HB2	1.68	0.76
5:B3:134:MET:HE1	47:Bo:78:VAL:HG21	1.67	0.76
12:BA:515:A:C8	12:BA:541:A:H4'	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BU:112:THR:H	39:Bg:127:GLN:HE22	1.32	0.76
32:BY:122:LEU:HD23	32:BY:133:VAL:HG21	1.67	0.76
23:BP:137:GLY:HA3	23:BP:157:GLN:HG3	1.67	0.76
9:B7:74:ARG:NH2	12:BA:31:A:O2'	2.16	0.76
17:BF:287:ARG:HD2	52:Bv:33:ARG:NH1	2.00	0.76
24:BQ:118:MET:HE2	24:BQ:163:MET:HE1	1.68	0.76
26:BS:130:ARG:HH11	34:Bb:129:ARG:HH11	1.28	0.75
42:Bj:187:THR:HG23	42:Bj:190:ARG:HH21	1.52	0.75
12:BA:889:C:H41	12:BA:1082:U:H4'	1.51	0.75
12:BA:171:A:OP1	38:Bf:135:LYS:NZ	2.15	0.75
16:BE:341:GLY:HA2	27:BT:105:ILE:HD11	1.69	0.75
2:B0:76:HIS:CD2	26:BS:70:THR:HG21	2.21	0.75
37:Be:25:ARG:HG2	37:Be:25:ARG:NH1	1.99	0.75
26:BS:130:ARG:HH11	34:Bb:129:ARG:NH1	1.84	0.75
15:BD:111:ARG:HH11	15:BD:182:ALA:HB2	1.51	0.75
4:B2:220:ARG:NH2	46:Bn:105:ASP:OD2	2.20	0.74
4:B2:93:ARG:NH1	37:Be:82:THR:O	2.20	0.74
15:BD:247:ARG:HH12	15:BD:251:VAL:HG11	1.53	0.74
23:BP:97:SER:HB2	23:BP:143:GLU:HB2	1.69	0.74
3:B1:100:ARG:NH2	18:BI:75:ARG:HE	1.86	0.74
11:B9:65:THR:HG23	11:B9:100:MET:HB3	1.70	0.74
17:BF:83:HIS:HD2	17:BF:85:ASP:H	1.34	0.74
38:Bf:122:ARG:HG3	38:Bf:122:ARG:NH1	2.01	0.74
41:Bi:165:THR:HG23	41:Bi:167:ASN:H	1.53	0.73
14:BC:392:CYS:HB3	14:BC:423:ASP:HB2	1.69	0.73
34:Bb:308:GLN:HE22	47:Bo:111:LYS:H	1.37	0.73
35:Bc:111:ASP:N	35:Bc:111:ASP:OD1	2.18	0.73
3:B1:163:ARG:HD3	3:B1:205:GLY:H	1.54	0.73
12:BA:1549:A:H2	38:Bf:104:GLU:HG2	1.54	0.73
12:BA:482:G:OP1	47:Bo:23:ALA:N	2.21	0.72
24:BQ:50:LEU:H	24:BQ:110:ASN:HD21	1.37	0.72
40:Bh:105:ARG:HB2	40:Bh:112:LYS:HD2	1.71	0.72
1:CL:31:LEU:HD22	1:DL:67:LEU:HD12	1.71	0.72
40:Bh:105:ARG:HD2	40:Bh:112:LYS:HB2	1.72	0.72
53:Bw:213:ARG:HB2	53:Bw:213:ARG:NH1	2.04	0.72
12:BA:1287:G:H1	12:BA:1309:U:H3	1.35	0.72
46:Bn:35:ARG:HH12	46:Bn:39:PRO:CA	2.02	0.72
53:Bw:310:CYS:HB3	53:Bw:313:GLN:HG3	1.71	0.72
23:BP:47:ARG:HH11	29:BV:183:ASN:HB2	1.53	0.72
25:BR:38:ARG:HB2	25:BR:38:ARG:HH11	1.53	0.72
27:BT:233:TRP:HB3	27:BT:240:ILE:HD12	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:AV:49:G:H1	56:AV:56:C:H42	1.38	0.72
41:Bi:186:VAL:HG22	41:Bi:187:GLU:HG3	1.70	0.72
47:Bo:63:GLN:HE21	47:Bo:66:ARG:NH1	1.88	0.72
50:Bt:24:PRO:HG2	54:Bx:169:TRP:HB2	1.71	0.72
25:BR:91:GLN:NE2	53:Bw:44:TYR:OH	2.23	0.72
10:B8:172:TYR:HB2	10:B8:175:ASP:HB2	1.71	0.71
27:BT:76:LEU:HD21	27:BT:282:ILE:HD11	1.71	0.71
14:BC:182:VAL:HG12	14:BC:252:THR:HG22	1.72	0.71
41:Bi:80:CYS:SG	41:Bi:165:THR:OG1	2.46	0.71
16:BE:317:PRO:HG2	16:BE:320:PHE:HE2	1.54	0.71
29:BV:126:VAL:HG11	29:BV:132:ILE:HD11	1.72	0.71
32:BY:130:PRO:O	32:BY:149:ARG:NH1	2.23	0.71
14:BC:363:PHE:HB3	14:BC:524:VAL:HG13	1.71	0.71
39:Bg:73:PRO:HB2	39:Bg:89:ILE:HG13	1.73	0.71
7:B5:94:ARG:NH1	12:BA:644:G:OP2	2.23	0.71
20:BK:159:LEU:HB3	20:BK:163:GLU:HG2	1.72	0.71
21:BN:15:ALA:HB1	40:Bh:269:VAL:HG21	1.72	0.71
20:BK:43:GLY:HA3	20:BK:76:ARG:NH1	2.05	0.70
38:Bf:74:PRO:HD3	40:Bh:256:ARG:HH21	1.55	0.70
46:Bn:69:HIS:CD2	46:Bn:71:LYS:HG3	2.26	0.70
12:BA:58:C:H2'	12:BA:59:A:H5''	1.73	0.70
12:BA:429:G:OP1	23:BP:62:ARG:NH2	2.24	0.70
21:BN:80:HIS:HD2	21:BN:82:GLY:H	1.36	0.70
12:BA:696:A:H3'	12:BA:697:C:H5''	1.72	0.70
12:BA:554:U:O2'	54:Bx:102:ARG:NH1	2.24	0.70
53:Bw:278:ILE:HD11	53:Bw:333:GLN:HG2	1.72	0.70
19:BJ:148:VAL:HG11	48:Bp:28:GLU:HG2	1.73	0.70
40:Bh:278:ARG:HB2	40:Bh:278:ARG:HH11	1.57	0.70
53:Bw:201:HIS:CD2	53:Bw:228:ASN:HD22	2.09	0.70
3:B1:196:ILE:HG12	3:B1:197:PRO:HD2	1.72	0.69
12:BA:515:A:H8	12:BA:541:A:H4'	1.55	0.69
17:BF:262:THR:HG22	17:BF:264:PRO:HD2	1.74	0.69
19:BJ:95:MET:HE2	19:BJ:161:VAL:HG22	1.73	0.69
12:BA:975:G:O2'	12:BA:977:G:OP2	2.09	0.69
23:BP:47:ARG:NH1	29:BV:183:ASN:HB2	2.07	0.69
5:B3:119:ILE:H	50:Bt:45:ASN:HD21	1.37	0.69
14:BC:215:GLN:HE22	14:BC:598:ILE:HA	1.57	0.69
23:BP:264:GLN:NE2	23:BP:269:LEU:O	2.21	0.69
39:Bg:131:HIS:HD2	39:Bg:133:PHE:H	1.40	0.69
53:Bw:51:LEU:HD23	53:Bw:61:ARG:NH1	2.07	0.69
16:BE:96:ARG:NH2	16:BE:197:HIS:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EL:76:LEU:HA	1:EL:79:ILE:HD12	1.74	0.69
12:BA:229:A:H4'	12:BA:230:G:H5'	1.75	0.69
28:BU:92:LYS:HB3	28:BU:123:ARG:NH1	2.07	0.69
6:B4:58:VAL:HG22	6:B4:64:THR:HG22	1.75	0.68
12:BA:260:C:H42	12:BA:317:A:H61	1.41	0.68
29:BV:136:LYS:HZ2	47:Bo:48:ASP:HB3	1.59	0.68
12:BA:138:A:OP2	32:BY:34:LYS:NZ	2.26	0.68
13:BB:26:C:OP1	34:Bb:59:ARG:NH1	2.19	0.68
23:BP:14:ASP:OD1	23:BP:17:ARG:NH1	2.26	0.68
12:BA:888:A:O2'	12:BA:891:A:N6	2.27	0.68
15:BD:111:ARG:NH1	15:BD:182:ALA:HB2	2.07	0.68
39:Bg:28:ARG:HB3	39:Bg:28:ARG:NH1	2.08	0.68
12:BA:502:U:H2'	12:BA:503:A:H5''	1.76	0.68
41:Bi:88:TYR:OH	41:Bi:108:ARG:NH1	2.26	0.68
12:BA:148:A:H4'	12:BA:149:A:H5''	1.73	0.68
33:Ba:144:ARG:O	33:Ba:194:LYS:NZ	2.27	0.68
34:Bb:290:CYS:SG	34:Bb:296:ARG:NH2	2.67	0.67
39:Bg:28:ARG:HB3	39:Bg:28:ARG:HH11	1.59	0.67
48:Bp:15:GLN:HE22	48:Bp:52:ILE:HD12	1.59	0.67
42:Bj:162:ARG:HH21	42:Bj:164:LYS:HE2	1.58	0.67
7:B5:90:ASN:OD1	7:B5:93:ARG:NH2	2.26	0.67
12:BA:1548:A:H3'	12:BA:1549:A:H5'	1.76	0.67
26:BS:42:GLU:HA	34:Bb:337:MET:HE3	1.75	0.67
36:Bd:164:ARG:HH11	43:Bk:88:TYR:HB3	1.56	0.67
14:BC:562:ASN:OD1	14:BC:589:LYS:NZ	2.28	0.67
8:B6:24:ALA:HB2	8:B6:54:VAL:HG11	1.77	0.67
14:BC:163:LYS:HB3	14:BC:439:ARG:HH12	1.59	0.67
46:Bn:77:PRO:HG2	46:Bn:80:LEU:HB2	1.76	0.67
30:BW:77:GLN:H	30:BW:171:HIS:HD2	1.43	0.67
34:Bb:308:GLN:NE2	47:Bo:111:LYS:H	1.92	0.67
12:BA:529:G:H4'	49:Bq:122:ARG:HH12	1.58	0.67
33:Ba:207:ASN:HD21	33:Ba:229:ARG:HD2	1.60	0.66
21:BN:8:PRO:HB2	40:Bh:285:PRO:HG2	1.76	0.66
30:BW:53:ASN:ND2	30:BW:72:TYR:O	2.27	0.66
32:BY:126:THR:HB	32:BY:152:ARG:NH1	2.10	0.66
24:BQ:124:VAL:HA	24:BQ:158:ARG:HH21	1.59	0.66
26:BS:130:ARG:NH1	34:Bb:129:ARG:NH1	2.43	0.66
21:BN:140:ASN:HB3	40:Bh:262:GLY:HA2	1.77	0.66
42:Bj:257:LYS:NZ	42:Bj:273:ARG:HB2	2.10	0.66
12:BA:539:U:O4	12:BA:540:A:N6	2.29	0.66
15:BD:177:ALA:HB1	15:BD:245:VAL:HG11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Ba:207:ASN:HB3	53:Bw:151:LEU:HD11	1.77	0.66
42:Bj:53:LEU:HG	42:Bj:238:LEU:HD11	1.77	0.66
45:Bm:114:PRO:HG2	45:Bm:117:ARG:HG3	1.77	0.66
1:EL:76:LEU:HG	1:HL:79:ILE:HD13	1.76	0.66
12:BA:1216:C:OP2	12:BA:1219:A:N6	2.28	0.66
17:BF:83:HIS:CD2	17:BF:85:ASP:H	2.13	0.66
17:BF:221:LEU:HD22	17:BF:264:PRO:HB2	1.77	0.66
12:BA:164:A:HO2'	12:BA:1016:C:H5	1.42	0.66
41:Bi:196:GLN:HE22	41:Bi:198:ARG:HE	1.45	0.65
21:BN:74:GLN:HB2	54:Bx:174:MET:HE3	1.79	0.65
16:BE:43:GLY:H	35:Bc:98:ARG:HH12	1.44	0.65
35:Bc:190:MET:HE3	35:Bc:291:ARG:HH11	1.59	0.65
1:CL:40:LEU:HA	1:CL:43:ILE:HD12	1.79	0.65
2:B0:124:ALA:O	34:Bb:51:TYR:OH	2.15	0.65
12:BA:666:G:H5''	12:BA:779:G:O2'	1.97	0.65
36:Bd:97:LYS:HA	36:Bd:99:ARG:NH1	2.12	0.65
10:B8:156:LYS:NZ	12:BA:427:G:OP2	2.27	0.65
17:BF:192:SER:OG	17:BF:193:LEU:N	2.30	0.65
25:BR:142:ASN:O	25:BR:148:GLN:NE2	2.30	0.65
21:BN:109:TYR:HD2	21:BN:122:MET:HE3	1.61	0.65
12:BA:188:C:H3'	29:BV:181:ARG:NH2	2.12	0.65
14:BC:721:THR:HG22	14:BC:723:TRP:H	1.61	0.65
12:BA:516:G:O2'	12:BA:533:A:OP2	2.14	0.64
19:BJ:162:LYS:NZ	19:BJ:196:LYS:HA	2.12	0.64
12:BA:697:C:OP2	31:BX:78:ARG:NH2	2.29	0.64
14:BC:344:MET:HE3	1:BL:158:LEU:HD11	1.80	0.64
35:Bc:156:LYS:HB2	38:Bf:89:ASP:H	1.63	0.64
42:Bj:53:LEU:HD11	42:Bj:238:LEU:HD21	1.80	0.64
42:Bj:51:LEU:HD22	42:Bj:192:LEU:HD21	1.77	0.64
3:B1:100:ARG:HH12	18:Bl:75:ARG:HH21	1.45	0.64
22:BO:93:GLY:O	22:BO:95:ARG:NH1	2.21	0.64
12:BA:143:A:H2'	12:BA:144:A:C8	2.33	0.64
42:Bj:123:MET:HE3	42:Bj:127:LYS:HZ1	1.62	0.64
1:HL:76:LEU:HA	1:HL:79:ILE:HD12	1.79	0.64
5:B3:43:ASP:OD1	5:B3:43:ASP:N	2.30	0.64
19:BJ:89:VAL:HG22	19:BJ:124:LYS:HZ2	1.63	0.64
26:BS:39:VAL:HG12	26:BS:41:ASN:H	1.63	0.64
23:BP:20:PRO:HD3	50:Bt:99:ARG:HH12	1.62	0.64
42:Bj:257:LYS:HZ3	42:Bj:273:ARG:HB2	1.63	0.64
16:BE:113:ASP:N	16:BE:113:ASP:OD1	2.30	0.63
22:BO:99:ARG:HH12	27:BT:191:ARG:NH2	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BX:140:ARG:NH1	35:Bc:63:GLU:OE2	2.31	0.63
53:Bw:244:PHE:HE2	53:Bw:365:CYS:HB3	1.62	0.63
6:B4:38:ARG:NH1	36:Bd:128:GLU:HG2	2.12	0.63
21:BN:71:LYS:NZ	54:Bx:196:HIS:CD2	2.66	0.63
26:BS:59:LEU:HB3	26:BS:61:VAL:HG23	1.80	0.63
16:BE:129:VAL:HG23	16:BE:189:PRO:HA	1.80	0.63
53:Bw:118:LEU:HG	53:Bw:119:PRO:HD2	1.79	0.63
3:B1:189:ASP:HA	3:B1:192:LYS:HE3	1.79	0.63
1:BL:134:LEU:HB2	1:BL:172:ILE:HD11	1.80	0.63
32:BY:19:TYR:OH	32:BY:31:ASP:OD1	2.16	0.63
8:B6:36:ARG:HH22	8:B6:64:SER:HB3	1.64	0.63
12:BA:166:A:H5''	39:Bg:2:THR:HG21	1.80	0.63
14:BC:319:GLN:HE22	1:BL:159:VAL:HG23	1.64	0.63
33:Ba:391:VAL:HG13	33:Ba:399:GLU:HB2	1.81	0.63
15:BD:73:THR:HG22	15:BD:75:MET:H	1.64	0.62
41:Bi:235:GLN:HB2	41:Bi:238:VAL:HG12	1.80	0.62
3:B1:85:TRP:CD1	3:B1:107:PRO:HD2	2.34	0.62
14:BC:515:VAL:HG13	14:BC:545:GLU:HB2	1.81	0.62
36:Bd:169:PHE:HB2	36:Bd:170:PRO:HD3	1.81	0.62
38:Bf:134:ARG:HB3	38:Bf:134:ARG:HH11	1.62	0.62
53:Bw:77:ASP:OD1	53:Bw:77:ASP:N	2.31	0.62
1:CL:36:ALA:HB1	1:FL:77:LEU:HG	1.81	0.62
10:B8:137:THR:HG22	10:B8:139:ALA:H	1.64	0.62
12:BA:1182:G:H4'	12:BA:1230:U:O2'	1.99	0.62
23:BP:191:VAL:HG13	23:BP:277:MET:HE1	1.81	0.62
48:Bp:73:ARG:HB3	54:Bx:46:THR:HG22	1.81	0.62
12:BA:468:A:C2	50:Bt:18:ILE:HD11	2.35	0.62
12:BA:1548:A:H5'	12:BA:1549:A:OP2	2.00	0.62
17:BF:192:SER:O	17:BF:193:LEU:HB2	1.99	0.62
20:BK:166:ALA:O	20:BK:169:LYS:N	2.32	0.62
43:Bk:147:ASP:N	43:Bk:147:ASP:OD1	2.30	0.62
2:B0:100:THR:HG23	34:Bb:73:THR:HA	1.81	0.62
12:BA:477:A:C2'	12:BA:478:G:H5''	2.29	0.62
12:BA:1552:C:H5'	12:BA:1553:A:OP1	1.99	0.62
5:B3:65:LYS:HG2	47:Bo:84:MET:HE3	1.80	0.62
28:BU:33:GLY:O	28:BU:36:ASN:ND2	2.32	0.62
12:BA:1317:A:O2'	24:BQ:137:GLY:HA2	2.00	0.62
12:BA:909:U:H5'	12:BA:910:U:OP2	1.99	0.61
27:BT:152:ARG:HH12	27:BT:191:ARG:HA	1.65	0.61
40:Bh:258:THR:HG22	40:Bh:259:ARG:HG2	1.82	0.61
46:Bn:69:HIS:HD2	46:Bn:71:LYS:H	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:707:A:N1	53:Bw:97:THR:HG23	2.15	0.61
16:BE:195:ALA:H	16:BE:281:ASN:HD22	1.48	0.61
14:BC:572:TYR:HB3	14:BC:602:LEU:HD11	1.82	0.61
23:BP:11:ARG:HG2	23:BP:11:ARG:HH11	1.66	0.61
34:Bb:157:LEU:HD13	34:Bb:221:LEU:HD11	1.81	0.61
12:BA:1463:A:H5''	14:BC:266:MET:HE2	1.82	0.61
41:Bi:90:PRO:HB2	41:Bi:269:TRP:HH2	1.64	0.61
17:BF:249:ASN:ND2	17:BF:252:SER:H	1.97	0.61
30:BW:131:ASN:O	41:Bi:230:ARG:NH2	2.34	0.61
33:Ba:193:LEU:HD13	53:Bw:184:VAL:HA	1.83	0.61
43:Bk:106:TYR:OH	43:Bk:174:ILE:O	2.17	0.61
53:Bw:140:VAL:HG21	53:Bw:412:LEU:HD21	1.82	0.61
12:BA:32:C:O2'	12:BA:36:A:N6	2.34	0.61
31:BX:37:GLU:HB3	31:BX:104:THR:HG23	1.83	0.61
41:Bi:111:ARG:O	41:Bi:115:ASN:ND2	2.34	0.61
23:BP:211:VAL:O	23:BP:215:THR:OG1	2.18	0.61
36:Bd:100:GLN:HG2	42:Bj:84:TYR:HA	1.81	0.61
29:BV:99:LEU:HD23	29:BV:142:ALA:HB2	1.83	0.61
17:BF:71:GLY:H	17:BF:74:GLN:HE21	1.49	0.60
22:BO:64:THR:HG22	22:BO:66:VAL:H	1.67	0.60
14:BC:396:VAL:HG11	14:BC:399:MET:HE2	1.84	0.60
5:B3:119:ILE:N	50:Bt:45:ASN:HD21	2.00	0.60
16:BE:90:TRP:CH2	16:BE:92:PRO:HA	2.36	0.60
34:Bb:224:HIS:CD2	34:Bb:227:GLU:H	2.19	0.60
15:BD:115:GLU:HA	15:BD:148:ARG:HH12	1.65	0.60
24:BQ:36:VAL:HG23	49:Bq:128:ARG:HD2	1.82	0.60
32:BY:127:ASP:OD1	32:BY:152:ARG:NH1	2.29	0.60
12:BA:292:G:O2'	12:BA:295:G:O2'	2.18	0.60
32:BY:105:ARG:HG3	41:Bi:174:TRP:CH2	2.36	0.60
5:B3:74:SER:HB3	12:BA:472:U:OP2	2.02	0.60
35:Bc:294:GLN:HE22	35:Bc:320:VAL:N	1.94	0.60
27:BT:80:PHE:HB3	27:BT:282:ILE:HD12	1.83	0.60
47:Bo:31:GLN:HB3	47:Bo:33:PHE:CE1	2.37	0.60
12:BA:1215:C:H42	12:BA:1219:A:H3'	1.66	0.60
19:BJ:97:ALA:HB1	19:BJ:176:LEU:HD11	1.84	0.60
28:BU:112:THR:H	39:Bg:127:GLN:NE2	1.99	0.59
48:Bp:14:LYS:NZ	48:Bp:69:GLY:HA2	2.17	0.59
3:B1:85:TRP:HD1	3:B1:107:PRO:HD2	1.65	0.59
12:BA:145:A:H2'	12:BA:146:A:C8	2.36	0.59
14:BC:233:LEU:HD21	14:BC:375:ILE:HD11	1.85	0.59
32:BY:98:VAL:HG21	32:BY:109:ILE:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B0:54:LYS:HE2	2:B0:69:THR:HG22	1.83	0.59
12:BA:63:A:H3'	12:BA:64:C:O2	2.02	0.59
12:BA:1253:G:O6	23:BP:77:ARG:NH2	2.34	0.59
53:Bw:96:GLN:HE21	53:Bw:321:ASN:HD21	1.48	0.59
6:B4:61:ASP:HB3	6:B4:63:SER:H	1.66	0.59
12:BA:1241:U:H4'	12:BA:1242:U:OP1	2.02	0.59
22:BO:69:VAL:HG23	22:BO:89:HIS:CE1	2.37	0.59
53:Bw:213:ARG:HB2	53:Bw:213:ARG:HH11	1.65	0.59
10:B8:183:ARG:NH1	34:Bb:354:GLN:NE2	2.48	0.59
26:BS:115:HIS:HD2	34:Bb:135:VAL:HG22	1.67	0.59
34:Bb:284:ASP:N	34:Bb:284:ASP:OD1	2.35	0.59
39:Bg:28:ARG:HD2	40:Bh:60:ARG:HH21	1.67	0.59
42:Bj:55:ARG:NH2	42:Bj:152:LYS:O	2.33	0.59
12:BA:574:A:H2'	54:Bx:192:LEU:HD22	1.85	0.59
15:BD:247:ARG:HH12	15:BD:251:VAL:CG1	2.16	0.59
21:BN:27:PRO:HG2	21:BN:30:LYS:HB2	1.84	0.59
48:Bp:8:LEU:HD13	48:Bp:95:GLN:HG3	1.85	0.59
14:BC:161:LYS:HB2	14:BC:163:LYS:HE2	1.83	0.59
36:Bd:147:LEU:HD21	42:Bj:209:PRO:HD2	1.83	0.59
38:Bf:69:TYR:CZ	40:Bh:256:ARG:NH1	2.71	0.59
1:BL:134:LEU:HD21	1:BL:145:LEU:HD21	1.85	0.59
33:Ba:108:HIS:HD2	33:Ba:110:ARG:H	1.51	0.59
43:Bk:111:HIS:CE1	43:Bk:121:VAL:HG11	2.37	0.58
53:Bw:201:HIS:HD2	53:Bw:228:ASN:HA	1.67	0.58
3:B1:100:ARG:NH1	18:BI:75:ARG:HH21	2.01	0.58
13:BB:44:U:H2'	13:BB:45:A:C8	2.38	0.58
36:Bd:151:ARG:HG2	36:Bd:158:HIS:HB3	1.85	0.58
42:Bj:159:LEU:HD23	42:Bj:174:PRO:HG3	1.85	0.58
14:BC:673:LEU:HD23	14:BC:696:LEU:HD23	1.85	0.58
28:BU:97:LEU:HA	29:BV:109:GLN:HE22	1.67	0.58
34:Bb:238:THR:HG21	34:Bb:281:PHE:CZ	2.38	0.58
6:B4:38:ARG:HH22	36:Bd:129:HIS:HA	1.68	0.58
12:BA:1522:A:H5''	48:Bp:84:GLN:HE22	1.68	0.58
30:BW:202:ARG:NH1	40:Bh:287:GLU:OE2	2.34	0.58
1:FL:76:LEU:HA	1:FL:79:ILE:HD12	1.86	0.58
3:B1:87:LEU:HD23	3:B1:104:VAL:HB	1.84	0.58
4:B2:128:MET:HE3	4:B2:131:PRO:HA	1.86	0.58
36:Bd:142:ALA:HA	42:Bj:274:ARG:HH21	1.69	0.58
1:CL:46:LEU:HD21	1:DL:67:LEU:HD23	1.85	0.58
6:B4:55:VAL:HG21	6:B4:69:TYR:HB3	1.86	0.58
12:BA:1442:U:O2	16:BE:257:MET:HE1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BX:35:GLN:HG3	31:BX:36:PRO:HD2	1.86	0.58
33:Ba:149:ASN:OD1	33:Ba:149:ASN:N	2.35	0.58
56:AV:3:U:H3	56:AV:65:A:H61	1.52	0.58
20:BK:142:ARG:HG3	49:Bq:99:MET:HE3	1.85	0.58
3:B1:156:LYS:NZ	3:B1:205:GLY:O	2.32	0.58
14:BC:310:VAL:HB	14:BC:316:GLY:HA3	1.85	0.58
53:Bw:251:ILE:HG22	53:Bw:253:ILE:H	1.68	0.58
12:BA:1302:U:OP1	12:BA:1360:U:O2'	2.19	0.57
34:Bb:72:ARG:HH11	34:Bb:72:ARG:N	2.02	0.57
50:Bt:99:ARG:HB2	50:Bt:99:ARG:HH11	1.69	0.57
12:BA:743:U:H3'	12:BA:744:A:H5''	1.85	0.57
15:BD:133:ASP:OD2	15:BD:136:ARG:NH1	2.37	0.57
22:BO:72:ARG:HB2	22:BO:72:ARG:NH1	2.16	0.57
36:Bd:143:GLN:HE22	42:Bj:210:CYS:HA	1.68	0.57
39:Bg:34:SER:OG	39:Bg:70:CYS:O	2.22	0.57
2:B0:100:THR:HB	2:B0:132:HIS:HE2	1.69	0.57
5:B3:46:PHE:O	50:Bt:50:SER:OG	2.15	0.57
5:B3:73:LYS:NZ	12:BA:471:U:OP1	2.37	0.57
13:BB:43:C:H2'	13:BB:44:U:H5'	1.86	0.57
43:Bk:86:TYR:HE1	43:Bk:88:TYR:HD1	1.49	0.57
12:BA:407:A:OP2	43:Bk:49:ARG:NH1	2.37	0.57
16:BE:197:HIS:CD2	16:BE:318:THR:HG22	2.40	0.57
20:BK:140:VAL:O	20:BK:144:ILE:HG12	2.05	0.57
12:BA:58:C:C2'	12:BA:59:A:H5''	2.33	0.57
12:BA:993:U:OP2	16:BE:238:ARG:NH2	2.38	0.57
42:Bj:57:PRO:HD3	42:Bj:156:ASN:HB3	1.86	0.57
12:BA:1093:A:H4'	12:BA:1094:A:OP1	2.03	0.57
14:BC:180:SER:OG	14:BC:229:LYS:O	2.21	0.57
19:BJ:89:VAL:HG22	19:BJ:124:LYS:NZ	2.19	0.57
33:Ba:153:ARG:HH11	33:Ba:187:LEU:HD22	1.69	0.57
41:Bi:215:ARG:HG3	41:Bi:245:TYR:CE1	2.39	0.57
53:Bw:158:PRO:HB2	53:Bw:160:ILE:HG22	1.87	0.57
16:BE:53:LEU:HA	25:BR:147:ASN:HD21	1.69	0.57
22:BO:75:LEU:HD23	22:BO:77:ILE:HD11	1.86	0.57
40:Bh:227:GLU:HB2	40:Bh:230:GLU:HB2	1.86	0.57
11:B9:99:GLN:HE21	12:BA:560:A:H2'	1.70	0.57
19:BJ:89:VAL:HG13	19:BJ:93:ASN:HD21	1.70	0.57
43:Bk:90:VAL:HB	43:Bk:189:HIS:HB3	1.86	0.57
53:Bw:235:ILE:HB	53:Bw:290:HIS:HB3	1.86	0.57
1:GL:64:ILE:HD11	1:HL:85:LEU:HD12	1.87	0.57
12:BA:831:U:OP2	12:BA:836:A:N6	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BT:96:ARG:NH1	27:BT:285:GLU:OE1	2.38	0.57
5:B3:59:ASP:O	50:Bt:51:ARG:NH2	2.37	0.56
12:BA:590:U:OP1	47:Bo:66:ARG:NH2	2.37	0.56
24:BQ:101:HIS:O	24:BQ:105:MET:HG3	2.04	0.56
28:BU:146:VAL:HG11	38:Bf:56:ARG:HG2	1.87	0.56
34:Bb:304:TYR:CE2	34:Bb:313:PRO:HD3	2.40	0.56
12:BA:660:C:O3'	25:BR:81:THR:HG21	2.05	0.56
25:BR:108:LEU:HD11	25:BR:136:LEU:HD22	1.88	0.56
11:B9:82:ARG:N	12:BA:1527:U:OP1	2.34	0.56
12:BA:80:A:H5'	18:BI:61:LYS:HZ1	1.70	0.56
14:BC:522:GLY:HA2	14:BC:574:PHE:HB3	1.88	0.56
36:Bd:136:ILE:HG13	43:Bk:173:ILE:HD11	1.87	0.56
40:Bh:278:ARG:HB2	40:Bh:278:ARG:NH1	2.20	0.56
42:Bj:47:LEU:HB3	42:Bj:178:TRP:NE1	2.20	0.56
46:Bn:81:ARG:HG2	46:Bn:81:ARG:HH11	1.70	0.56
48:Bp:76:MET:HE1	48:Bp:86:MET:HA	1.87	0.56
25:BR:41:ARG:NH1	25:BR:134:LEU:HD13	2.21	0.56
28:BU:65:ARG:HH12	28:BU:99:ARG:NH1	2.03	0.56
32:BY:109:ILE:HD13	41:Bi:76:ILE:HG21	1.87	0.56
42:Bj:123:MET:HE3	42:Bj:127:LYS:NZ	2.20	0.56
19:BJ:89:VAL:O	19:BJ:93:ASN:ND2	2.38	0.56
21:BN:15:ALA:CB	40:Bh:269:VAL:HG21	2.35	0.56
51:Bu:177:SER:O	51:Bu:181:ASN:HB2	2.05	0.56
12:BA:30:U:H5'	12:BA:31:A:OP1	2.06	0.56
29:BV:209:CYS:C	38:Bf:52:THR:HG23	2.31	0.56
35:Bc:207:ILE:HA	35:Bc:269:THR:HG22	1.87	0.56
53:Bw:195:ASP:HB2	53:Bw:234:GLN:HB2	1.86	0.56
12:BA:142:U:OP2	32:BY:100:LYS:NZ	2.33	0.56
20:BK:66:LEU:HA	20:BK:85:PRO:HA	1.87	0.56
33:Ba:215:ARG:HH11	33:Ba:215:ARG:HG3	1.69	0.56
20:BK:160:SER:O	20:BK:163:GLU:HB2	2.06	0.56
1:BL:185:LYS:HD3	1:BL:197:LEU:HG	1.88	0.56
23:BP:247:ILE:HD13	51:Bu:59:TRP:HB3	1.87	0.56
32:BY:189:PRO:O	37:Be:93:THR:OG1	2.24	0.56
39:Bg:35:ARG:HG2	45:Bm:159:TYR:CZ	2.41	0.56
44:Bl:77:ASP:HB2	44:Bl:78:PRO:HD3	1.87	0.56
10:B8:124:ARG:NH2	12:BA:1204:A:OP1	2.36	0.56
12:BA:1399:G:O2'	12:BA:1402:C:OP2	2.22	0.56
14:BC:285:LEU:HD13	14:BC:304:LEU:HD11	1.86	0.56
16:BE:181:VAL:HG13	16:BE:185:ALA:HB3	1.87	0.56
19:BJ:162:LYS:HZ1	19:BJ:196:LYS:HA	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B3:121:PRO:HG3	50:Bt:48:TRP:CH2	2.41	0.56
12:BA:811:A:H1'	16:BE:230:THR:CG2	2.35	0.56
12:BA:1569:A:H4'	16:BE:62:LYS:HG2	1.87	0.56
15:BD:128:ILE:HD11	33:Ba:114:LEU:HD21	1.88	0.56
39:Bg:26:LEU:HD21	39:Bg:29:LEU:HD13	1.87	0.56
12:BA:745:A:OP2	37:Be:44:ARG:NH2	2.39	0.55
28:BU:111:LYS:HB2	39:Bg:127:GLN:NE2	2.20	0.55
33:Ba:229:ARG:HG3	33:Ba:291:LEU:HD23	1.87	0.55
34:Bb:240:ILE:HD13	34:Bb:248:GLY:HA3	1.87	0.55
42:Bj:170:ILE:HG22	42:Bj:172:MET:HB2	1.86	0.55
12:BA:728:C:H5	33:Ba:300:ARG:HH21	1.53	0.55
35:Bc:145:MET:HE2	35:Bc:254:PHE:HD1	1.71	0.55
36:Bd:83:ILE:HB	55:Bz:302:ALA:HB1	1.88	0.55
12:BA:1050:C:H2'	12:BA:1327:U:H4'	1.88	0.55
32:BY:199:MET:HG2	32:BY:204:ILE:HB	1.88	0.55
41:Bi:186:VAL:HG13	41:Bi:219:ARG:HB3	1.88	0.55
13:BB:9:A:H5'	13:BB:47:A:H1'	1.88	0.55
30:BW:77:GLN:H	30:BW:171:HIS:CD2	2.24	0.55
35:Bc:48:GLU:O	35:Bc:52:GLN:HG2	2.07	0.55
17:BF:211:ARG:HD2	45:Bm:59:ARG:CZ	2.36	0.55
30:BW:165:MET:HE3	30:BW:167:LYS:HE3	1.87	0.55
34:Bb:47:ARG:HE	43:Bk:120:LYS:HZ1	1.55	0.55
12:BA:129:A:OP1	17:BF:142:ARG:NH2	2.39	0.55
32:BY:131:THR:HG21	32:BY:147:SER:HB3	1.89	0.55
33:Ba:153:ARG:HH11	33:Ba:187:LEU:CD2	2.20	0.55
33:Ba:387:TRP:NE1	33:Ba:404:ILE:HD11	2.17	0.55
34:Bb:169:PRO:HA	34:Bb:314:ALA:O	2.06	0.55
42:Bj:44:PRO:HG2	42:Bj:227:LEU:HA	1.89	0.55
42:Bj:273:ARG:HA	42:Bj:276:LEU:HB3	1.87	0.55
12:BA:1227:U:H5	12:BA:1230:U:O4	1.90	0.55
12:BA:1530:C:H1'	54:Bx:133:PRO:HD2	1.88	0.55
14:BC:255:VAL:HG13	14:BC:281:VAL:HG11	1.89	0.55
16:BE:90:TRP:HA	16:BE:316:PHE:HE2	1.71	0.55
31:BX:145:PRO:HB3	41:Bi:175:ASP:HB2	1.88	0.55
37:Be:25:ARG:HH11	37:Be:25:ARG:CG	2.08	0.55
3:B1:144:TYR:O	3:B1:148:THR:OG1	2.17	0.55
12:BA:97:A:O2'	52:Bv:38:ARG:NH1	2.40	0.55
12:BA:219:A:P	23:BP:109:ARG:HH22	2.30	0.55
41:Bi:170:PRO:O	41:Bi:174:TRP:HB2	2.06	0.55
54:Bx:135:LEU:H	54:Bx:139:PHE:HE1	1.55	0.55
12:BA:163:C:H42	12:BA:1013:A:H61	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BC:394:ALA:HB2	14:BC:421:TRP:HA	1.88	0.55
21:BN:155:LEU:HD13	54:Bx:86:VAL:HG12	1.89	0.55
41:Bi:88:TYR:CG	41:Bi:195:VAL:HG11	2.42	0.55
10:B8:112:TYR:HD2	23:BP:80:LYS:HZ3	1.54	0.55
15:BD:213:THR:O	15:BD:248:VAL:HG23	2.07	0.55
34:Bb:197:GLU:OE1	34:Bb:197:GLU:N	2.40	0.55
36:Bd:180:PRO:HD3	42:Bj:59:VAL:HG21	1.87	0.55
41:Bi:88:TYR:CD2	41:Bi:195:VAL:HG11	2.42	0.55
3:B1:80:TRP:CZ2	3:B1:109:LEU:HD11	2.42	0.54
3:B1:96:LYS:O	12:BA:60:U:O2'	2.21	0.54
7:B5:83:ASN:ND2	12:BA:1015:C:H41	2.05	0.54
12:BA:173:C:H1'	38:Bf:126:ARG:NH2	2.22	0.54
12:BA:937:C:H3'	12:BA:938:U:H5''	1.89	0.54
14:BC:183:VAL:HG22	14:BC:254:ILE:HB	1.88	0.54
22:BO:99:ARG:HH12	27:BT:191:ARG:HH21	1.55	0.54
26:BS:163:HIS:O	26:BS:167:GLU:HG2	2.07	0.54
31:BX:7:TYR:CE2	37:Be:37:LYS:HG3	2.42	0.54
32:BY:144:VAL:HG11	32:BY:153:ILE:HD12	1.88	0.54
34:Bb:120:GLU:HG2	34:Bb:124:ARG:HE	1.72	0.54
34:Bb:217:LEU:HD13	34:Bb:236:LEU:HD13	1.88	0.54
32:BY:29:LEU:HD12	41:Bi:68:PRO:HG3	1.90	0.54
33:Ba:192:ILE:HD11	33:Ba:199:ALA:HB2	1.88	0.54
13:BB:8:U:H5'	13:BB:9:A:OP2	2.08	0.54
16:BE:108:PRO:HG2	27:BT:145:LEU:HB3	1.88	0.54
42:Bj:202:ALA:HB2	42:Bj:238:LEU:HD23	1.89	0.54
53:Bw:156:ARG:HH11	53:Bw:161:GLN:HA	1.72	0.54
4:B2:175:PHE:O	4:B2:214:ARG:NH2	2.39	0.54
20:BK:95:ALA:HB1	20:BK:110:GLY:HA3	1.90	0.54
31:BX:50:ARG:NH1	31:BX:69:ARG:HA	2.22	0.54
34:Bb:322:ARG:NH1	51:Bu:180:GLU:OE2	2.39	0.54
7:B5:90:ASN:O	7:B5:94:ARG:HG2	2.07	0.54
1:BL:142:LYS:NZ	1:BL:166:GLU:HG2	2.22	0.54
31:BX:26:ILE:HG12	31:BX:44:ILE:HG22	1.89	0.54
39:Bg:93:SER:O	39:Bg:97:ILE:HG12	2.07	0.54
42:Bj:265:LYS:HG3	42:Bj:266:PRO:HD3	1.90	0.54
3:B1:133:ASP:OD1	18:BI:120:ARG:NH2	2.40	0.54
10:B8:113:ARG:NH2	12:BA:84:G:OP2	2.40	0.54
34:Bb:124:ARG:HH12	36:Bd:115:ALA:HB3	1.73	0.54
39:Bg:77:ALA:HB2	39:Bg:104:LEU:HD13	1.89	0.54
51:Bu:108:ASP:OD1	51:Bu:108:ASP:N	2.40	0.54
7:B5:179:ARG:HE	7:B5:182:PRO:HG3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Bc:109:PRO:HB2	35:Bc:264:PRO:HG3	1.90	0.54
44:Bl:94:ILE:HD11	44:Bl:162:LEU:HG	1.89	0.54
6:B4:51:ARG:HB2	42:Bj:84:TYR:O	2.07	0.54
7:B5:127:TYR:OH	25:BR:43:GLU:OE1	2.26	0.54
16:BE:208:ALA:HB3	16:BE:290:PRO:O	2.07	0.54
17:BF:62:VAL:HG13	45:Bm:119:HIS:HB3	1.89	0.54
21:BN:11:TRP:HE1	40:Bh:269:VAL:HG22	1.73	0.54
31:BX:150:LEU:HD13	41:Bi:240:ARG:HG2	1.89	0.54
36:Bd:147:LEU:O	36:Bd:151:ARG:HG3	2.08	0.54
11:B9:69:LEU:HB2	12:BA:560:A:H62	1.72	0.54
13:BB:21:C:H1'	34:Bb:143:CYS:HB3	1.90	0.54
16:BE:187:ILE:HG22	16:BE:188:LYS:H	1.71	0.54
17:BF:76:ARG:NH1	45:Bm:112:ALA:HB2	2.23	0.54
29:BV:176:MET:HE2	29:BV:187:LYS:HB2	1.89	0.54
40:Bh:59:ARG:NH1	40:Bh:181:SER:O	2.41	0.54
30:BW:78:ILE:HG22	30:BW:80:TYR:H	1.72	0.54
31:BX:46:MET:HG3	37:Be:34:ARG:HB3	1.90	0.54
35:Bc:190:MET:HE3	35:Bc:291:ARG:NH1	2.23	0.54
40:Bh:184:PHE:O	40:Bh:186:VAL:HG23	2.08	0.54
48:Bp:76:MET:HE3	54:Bx:49:ILE:HD12	1.90	0.54
1:DL:76:LEU:HD21	19:BJ:200:LEU:HA	1.89	0.53
12:BA:1458:G:O2'	12:BA:1467:G:O6	2.19	0.53
27:BT:278:ILE:O	27:BT:282:ILE:HG23	2.08	0.53
35:Bc:61:LYS:NZ	35:Bc:79:ASN:OD1	2.35	0.53
39:Bg:92:LYS:HB2	39:Bg:97:ILE:HD11	1.90	0.53
53:Bw:401:ASP:O	53:Bw:402:ASN:ND2	2.36	0.53
15:BD:82:SER:O	15:BD:82:SER:OG	2.24	0.53
34:Bb:304:TYR:HE2	34:Bb:313:PRO:HD3	1.72	0.53
56:AV:49:G:H1	56:AV:56:C:N4	2.05	0.53
12:BA:1238:A:H5'	12:BA:1239:A:OP2	2.08	0.53
18:BI:130:VAL:HB	18:BI:136:ASN:HD21	1.73	0.53
40:Bh:121:ASP:N	40:Bh:121:ASP:OD1	2.41	0.53
52:Bv:48:PRO:HB2	52:Bv:50:TRP:CD1	2.43	0.53
7:B5:108:ASP:OD2	35:Bc:99:LYS:NZ	2.42	0.53
12:BA:486:A:H61	12:BA:582:C:H42	1.57	0.53
12:BA:1008:A:O2'	30:BW:157:HIS:HE1	1.91	0.53
26:BS:117:TYR:OH	34:Bb:120:GLU:OE1	2.20	0.53
32:BY:133:VAL:HG13	32:BY:145:ARG:HB3	1.89	0.53
33:Ba:124:THR:HG23	33:Ba:318:PHE:CG	2.44	0.53
33:Ba:280:GLN:HG2	53:Bw:152:ARG:HE	1.73	0.53
33:Ba:380:GLN:HB3	33:Ba:410:THR:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Bb:262:GLY:HA3	34:Bb:342:PHE:HB2	1.91	0.53
35:Bc:165:ARG:HD3	35:Bc:236:PHE:HE2	1.74	0.53
41:Bi:165:THR:HG23	41:Bi:167:ASN:N	2.22	0.53
43:Bk:132:MET:HE1	55:Bz:104:ALA:HB2	1.90	0.53
53:Bw:363:PHE:HB3	53:Bw:418:PHE:CZ	2.44	0.53
53:Bw:393:LYS:HB2	53:Bw:393:LYS:NZ	2.23	0.53
14:BC:635:THR:O	56:AV:70:C:N4	2.37	0.53
16:BE:200:PRO:HA	16:BE:273:VAL:HG22	1.91	0.53
43:Bk:171:LEU:HA	43:Bk:174:ILE:HD12	1.90	0.53
7:B5:161:SER:OG	7:B5:178:GLU:O	2.24	0.53
16:BE:195:ALA:H	16:BE:281:ASN:ND2	2.06	0.53
19:BJ:163:GLU:N	19:BJ:163:GLU:OE1	2.42	0.53
20:BK:155:VAL:HB	49:Bq:101:VAL:HG13	1.90	0.53
3:B1:162:LYS:O	3:B1:166:LEU:HB2	2.09	0.53
4:B2:95:LYS:NZ	32:BY:181:ASP:O	2.40	0.53
12:BA:1399:G:H8	12:BA:1404:G:O6	1.92	0.53
12:BA:1414:C:H2'	12:BA:1415:G:C8	2.44	0.53
14:BC:426:SER:O	14:BC:429:GLU:HB2	2.08	0.53
46:Bn:105:ASP:OD1	46:Bn:105:ASP:N	2.27	0.53
53:Bw:53:ALA:O	53:Bw:62:ARG:NH2	2.41	0.53
53:Bw:175:VAL:HG12	53:Bw:194:LEU:HD21	1.91	0.53
20:BK:122:ARG:HB3	20:BK:137:LEU:HD21	1.90	0.53
22:BO:55:PRO:HB3	22:BO:77:ILE:HG23	1.91	0.53
23:BP:247:ILE:H	23:BP:247:ILE:HD12	1.73	0.53
33:Ba:211:ALA:HB3	33:Ba:222:VAL:HG13	1.91	0.53
2:B0:125:VAL:HG21	34:Bb:64:GLU:HG3	1.91	0.53
12:BA:1213:A:N1	12:BA:1220:A:N7	2.57	0.53
19:BJ:119:HIS:CE1	19:BJ:160:LYS:HB2	2.44	0.53
20:BK:20:ILE:HD11	20:BK:42:ARG:HE	1.73	0.53
20:BK:86:THR:HG22	20:BK:88:SER:H	1.73	0.53
30:BW:66:ARG:NH1	41:Bi:230:ARG:NH1	2.57	0.53
31:BX:144:VAL:HG11	41:Bi:233:TYR:CD1	2.44	0.53
34:Bb:35:MET:HG3	34:Bb:36:PRO:HD2	1.90	0.53
12:BA:1092:A:H3'	12:BA:1093:A:H5''	1.91	0.53
33:Ba:67:MET:HE3	33:Ba:68:PRO:HD2	1.91	0.53
40:Bh:270:TYR:O	40:Bh:285:PRO:HA	2.08	0.53
43:Bk:94:HIS:HB2	43:Bk:185:SER:HB3	1.89	0.53
2:B0:118:THR:HG23	34:Bb:52:ARG:HA	1.90	0.52
12:BA:1375:U:C2	12:BA:1377:U:H5''	2.44	0.52
23:BP:141:VAL:HG11	34:Bb:377:TYR:CZ	2.44	0.52
31:BX:138:ASP:HB3	31:BX:141:ARG:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Bb:261:ARG:NH1	34:Bb:341:VAL:HG21	2.24	0.52
40:Bh:60:ARG:HG2	40:Bh:177:GLN:HE21	1.74	0.52
43:Bk:81:ASN:HB3	43:Bk:86:TYR:CE2	2.45	0.52
12:BA:509:C:O2'	20:BK:102:ARG:HG3	2.09	0.52
21:BN:178:LEU:HD21	54:Bx:100:LEU:HD11	1.91	0.52
23:BP:238:ARG:HH22	51:Bu:69:ASN:HA	1.75	0.52
33:Ba:174:GLU:HA	33:Ba:296:SER:HB2	1.92	0.52
34:Bb:194:THR:HB	34:Bb:197:GLU:OE1	2.09	0.52
53:Bw:128:GLU:O	53:Bw:130:THR:N	2.42	0.52
5:B3:68:ILE:HD11	5:B3:122:LEU:HD13	1.91	0.52
12:BA:130:A:H2'	12:BA:131:A:O4'	2.09	0.52
12:BA:173:C:H1'	38:Bf:126:ARG:HH21	1.73	0.52
12:BA:1510:A:O3'	54:Bx:160:LYS:NZ	2.42	0.52
16:BE:99:LEU:HD21	16:BE:193:LEU:HB3	1.91	0.52
3:B1:16:LEU:HD21	3:B1:29:LEU:HD22	1.91	0.52
14:BC:176:LEU:HB3	14:BC:348:LYS:HB3	1.90	0.52
14:BC:632:PHE:HB2	14:BC:643:VAL:HB	1.91	0.52
17:BF:249:ASN:HD21	17:BF:252:SER:H	1.56	0.52
26:BS:61:VAL:HG11	34:Bb:344:PHE:CE2	2.43	0.52
32:BY:170:TRP:O	37:Be:75:ARG:NH2	2.42	0.52
12:BA:443:G:O6	19:BJ:31:LYS:NZ	2.35	0.52
12:BA:1230:U:H5'	12:BA:1231:U:C5'	2.34	0.52
14:BC:655:LYS:HZ3	14:BC:674:THR:C	2.18	0.52
15:BD:133:ASP:OD1	15:BD:134:PRO:HD2	2.10	0.52
31:BX:66:ALA:HB2	31:BX:100:ALA:HA	1.91	0.52
34:Bb:96:LYS:HE3	47:Bo:118:GLN:HB2	1.91	0.52
34:Bb:108:GLN:HA	34:Bb:111:ARG:HD2	1.91	0.52
42:Bj:198:ASN:HB2	42:Bj:243:PHE:HA	1.92	0.52
42:Bj:209:PRO:HB2	42:Bj:212:HIS:NE2	2.23	0.52
3:B1:6:VAL:HB	52:Bv:46:LEU:HD21	1.92	0.52
4:B2:185:GLN:HB3	32:BY:213:VAL:HG11	1.92	0.52
7:B5:181:ARG:NH1	7:B5:187:GLN:HA	2.25	0.52
12:BA:1486:A:N1	12:BA:1499:G:O2'	2.40	0.52
41:Bi:196:GLN:NE2	41:Bi:198:ARG:HE	2.07	0.52
41:Bi:254:ASP:OD2	41:Bi:257:GLY:N	2.42	0.52
43:Bk:122:GLU:HG2	43:Bk:160:SER:HB2	1.90	0.52
54:Bx:90:SER:HA	54:Bx:93:ILE:HD11	1.90	0.52
34:Bb:124:ARG:HH12	36:Bd:115:ALA:CB	2.23	0.52
36:Bd:99:ARG:H	36:Bd:99:ARG:HD3	1.75	0.52
43:Bk:127:MET:HE2	43:Bk:128:PRO:HD2	1.92	0.52
53:Bw:265:LEU:HD23	53:Bw:267:LEU:HG	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BC:598:ILE:HB	14:BC:601:ARG:HG2	1.92	0.52
26:BS:149:THR:HG21	26:BS:151:TRP:CZ2	2.45	0.52
37:Be:129:TYR:HB3	37:Be:130:PRO:HD3	1.92	0.52
40:Bh:259:ARG:HB2	40:Bh:271:PHE:HB2	1.92	0.52
53:Bw:101:ASN:O	53:Bw:105:TRP:HD1	1.93	0.52
18:BI:115:LYS:HE3	18:BI:117:SER:HB2	1.91	0.52
19:BJ:95:MET:HB3	19:BJ:156:SER:HB2	1.92	0.52
21:BN:65:ILE:HD11	21:BN:104:VAL:HG23	1.92	0.52
21:BN:71:LYS:HZ3	54:Bx:196:HIS:HD2	1.58	0.52
23:BP:179:TYR:CE2	23:BP:187:LEU:HD22	2.45	0.52
27:BT:74:ARG:HB3	27:BT:283:TRP:CH2	2.45	0.52
36:Bd:168:LEU:HG	42:Bj:205:LEU:O	2.10	0.52
41:Bi:150:LEU:HD23	41:Bi:153:ASN:HD22	1.75	0.52
6:B4:72:PRO:HG2	42:Bj:87:HIS:CG	2.45	0.52
14:BC:184:THR:OG1	14:BC:255:VAL:HG12	2.10	0.52
21:BN:74:GLN:HE22	54:Bx:175:PRO:HD2	1.74	0.52
25:BR:139:ARG:HH11	25:BR:139:ARG:HG3	1.75	0.52
29:BV:165:ILE:HD11	29:BV:198:ARG:HB2	1.92	0.52
33:Ba:136:VAL:HG22	33:Ba:420:HIS:CD2	2.45	0.52
34:Bb:187:VAL:HG13	34:Bb:319:PHE:HB3	1.91	0.52
41:Bi:141:ALA:HB1	41:Bi:248:PHE:CZ	2.45	0.52
1:CL:49:LEU:HD12	1:DL:64:ILE:HG21	1.91	0.51
12:BA:1351:U:H2'	12:BA:1353:C:H5''	1.92	0.51
24:BQ:72:ILE:HD11	24:BQ:96:TYR:CZ	2.44	0.51
26:BS:169:GLY:O	51:Bu:183:ASN:ND2	2.40	0.51
32:BY:22:GLY:C	32:BY:24:SER:H	2.18	0.51
35:Bc:60:GLU:HB3	35:Bc:80:LYS:HB3	1.91	0.51
53:Bw:339:PHE:CD1	53:Bw:345:VAL:HA	2.45	0.51
1:FL:83:ASN:O	1:FL:87:LYS:HG3	2.11	0.51
8:B6:42:THR:HG23	8:B6:57:VAL:HG22	1.92	0.51
17:BF:276:HIS:O	44:Bl:90:ARG:NH2	2.43	0.51
19:BJ:103:ALA:HB3	48:Bp:39:SER:HA	1.92	0.51
19:BJ:162:LYS:HG3	19:BJ:195:SER:HB2	1.92	0.51
27:BT:268:ASP:O	27:BT:270:MET:N	2.43	0.51
53:Bw:372:ALA:HB1	53:Bw:377:ALA:HB1	1.92	0.51
3:B1:92:VAL:HG22	3:B1:98:SER:HB3	1.92	0.51
13:BB:35:G:H1'	36:Bd:88:PHE:CZ	2.45	0.51
14:BC:179:ARG:NE	14:BC:413:SER:OG	2.39	0.51
15:BD:202:GLY:O	33:Ba:30:ALA:N	2.44	0.51
17:BF:83:HIS:CD2	17:BF:85:ASP:HB2	2.45	0.51
33:Ba:115:GLU:O	33:Ba:119:GLN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Bc:105:VAL:HG22	35:Bc:122:ILE:HG12	1.93	0.51
41:Bi:293:PHE:CE2	41:Bi:295:GLU:HG2	2.45	0.51
45:Bm:74:HIS:HA	45:Bm:77:GLU:HG2	1.93	0.51
53:Bw:244:PHE:CE2	53:Bw:365:CYS:HB3	2.45	0.51
2:B0:88:CYS:SG	12:BA:1207:C:O2'	2.69	0.51
2:B0:102:GLU:HB2	2:B0:130:PHE:CD2	2.45	0.51
12:BA:71:U:H3	12:BA:94:U:H3	1.57	0.51
12:BA:1009:A:H2'	12:BA:1010:A:C8	2.45	0.51
21:BN:177:ARG:NH1	54:Bx:38:VAL:HG11	2.25	0.51
34:Bb:224:HIS:HD2	34:Bb:227:GLU:H	1.57	0.51
15:BD:83:GLY:O	15:BD:85:ARG:HG2	2.11	0.51
21:BN:152:PRO:HB3	54:Bx:84:GLU:HG3	1.93	0.51
26:BS:72:TRP:CG	26:BS:73:PRO:HA	2.46	0.51
38:Bf:126:ARG:HB2	38:Bf:126:ARG:HH11	1.75	0.51
42:Bj:185:ARG:NH1	42:Bj:204:PHE:HB3	2.24	0.51
51:Bu:56:ASP:OD1	51:Bu:56:ASP:N	2.39	0.51
54:Bx:54:THR:HG22	54:Bx:55:GLU:H	1.76	0.51
12:BA:137:A:OP1	32:BY:83:ARG:NH2	2.44	0.51
12:BA:392:U:H2'	12:BA:393:A:C8	2.45	0.51
12:BA:1537:A:H2'	12:BA:1538:A:O4'	2.11	0.51
16:BE:228:PRO:O	16:BE:233:GLN:HG3	2.11	0.51
16:BE:316:PHE:CG	16:BE:316:PHE:O	2.64	0.51
26:BS:130:ARG:HG2	26:BS:164:ALA:HB1	1.92	0.51
39:Bg:35:ARG:HG2	45:Bm:159:TYR:CE1	2.45	0.51
44:Bl:117:ILE:HD12	44:Bl:142:GLU:HA	1.93	0.51
47:Bo:23:ALA:O	47:Bo:28:ARG:NH2	2.43	0.51
1:DL:90:LEU:HD22	19:BJ:214:LEU:HD13	1.93	0.51
4:B2:232:LYS:NZ	12:BA:10:A:OP1	2.43	0.51
17:BF:287:ARG:CD	52:Bv:33:ARG:HH12	2.13	0.51
21:BN:4:PHE:CE2	40:Bh:285:PRO:HD3	2.44	0.51
30:BW:152:LYS:HD3	30:BW:164:ILE:HD11	1.92	0.51
43:Bk:111:HIS:HE1	43:Bk:121:VAL:HG11	1.71	0.51
10:B8:97:PHE:H	46:Bn:122:ASN:HD21	1.59	0.51
12:BA:175:C:H5''	21:BN:115:ASN:HB2	1.93	0.51
12:BA:950:U:O4	12:BA:1379:C:N4	2.44	0.51
22:BO:32:ILE:HD12	22:BO:86:ILE:HD13	1.93	0.51
27:BT:268:ASP:HB3	27:BT:271:ARG:HB2	1.93	0.51
1:FL:87:LYS:HG2	19:BJ:221:MET:HE3	1.92	0.51
3:B1:238:LEU:HD13	37:Be:102:PHE:HD2	1.75	0.51
12:BA:808:G:H2'	12:BA:809:G:H5''	1.91	0.51
14:BC:407:ILE:HD11	14:BC:416:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:BF:59:ARG:HH21	23:BP:10:PRO:HD3	1.76	0.51
35:Bc:149:CYS:HB2	35:Bc:257:PHE:CD2	2.46	0.51
39:Bg:81:ASN:HD21	39:Bg:110:LEU:HD23	1.76	0.51
45:Bm:115:ASN:ND2	45:Bm:115:ASN:H	2.08	0.51
53:Bw:326:LEU:O	53:Bw:330:THR:OG1	2.29	0.51
12:BA:138:A:C2	12:BA:141:A:H5'	2.45	0.51
14:BC:660:LYS:HD3	14:BC:670:LYS:NZ	2.26	0.51
16:BE:248:VAL:HG12	16:BE:250:ARG:HG2	1.92	0.51
19:BJ:100:GLN:OE1	48:Bp:31:ARG:HD3	2.11	0.51
35:Bc:145:MET:HE2	35:Bc:254:PHE:CD1	2.46	0.51
12:BA:575:C:H5	54:Bx:186:SER:HA	1.74	0.50
12:BA:725:C:H5	33:Ba:389:LEU:H	1.57	0.50
12:BA:1321:C:O2'	12:BA:1322:C:H5'	2.11	0.50
15:BD:163:THR:HG22	15:BD:178:ARG:HH22	1.75	0.50
16:BE:99:LEU:HD13	16:BE:124:VAL:HG21	1.94	0.50
19:BJ:111:LEU:O	19:BJ:115:GLN:HG2	2.11	0.50
42:Bj:179:GLN:HG2	42:Bj:181:GLY:H	1.76	0.50
50:Bt:12:ILE:HD13	50:Bt:23:ARG:HB2	1.92	0.50
1:DL:77:LEU:HD12	19:BJ:184:THR:HG21	1.92	0.50
12:BA:295:G:H2'	12:BA:297:A:N7	2.26	0.50
12:BA:748:A:C8	53:Bw:308:GLN:HG2	2.46	0.50
60:BA:3205:SPM:N1	30:BW:157:HIS:O	2.43	0.50
14:BC:188:HIS:HA	14:BC:268:GLN:HB2	1.93	0.50
42:Bj:235:LYS:NZ	43:Bk:172:GLU:HG2	2.15	0.50
54:Bx:92:PHE:O	54:Bx:93:ILE:HG23	2.12	0.50
14:BC:330:ASN:O	14:BC:333:ALA:N	2.42	0.50
24:BQ:47:LYS:NZ	24:BQ:51:ARG:HH21	2.09	0.50
24:BQ:144:LYS:HG3	24:BQ:145:GLY:H	1.74	0.50
41:Bi:293:PHE:HE2	41:Bi:295:GLU:HG2	1.76	0.50
1:HL:87:LYS:HG3	19:BJ:232:LEU:HD11	1.93	0.50
4:B2:204:MET:HB3	4:B2:205:PRO:HD2	1.94	0.50
5:B3:119:ILE:H	50:Bt:45:ASN:ND2	2.07	0.50
12:BA:377:G:O2'	23:BP:56:GLU:OE1	2.28	0.50
12:BA:505:U:H4'	12:BA:506:A:OP1	2.12	0.50
17:BF:280:TYR:OH	23:BP:109:ARG:HD3	2.11	0.50
19:BJ:225:GLN:HB2	19:BJ:226:PRO:HD3	1.92	0.50
40:Bh:105:ARG:CZ	40:Bh:113:GLU:HG3	2.42	0.50
41:Bi:165:THR:HG21	41:Bi:262:HIS:ND1	2.26	0.50
45:Bm:86:ASN:OD1	45:Bm:86:ASN:N	2.42	0.50
4:B2:90:GLN:NE2	4:B2:93:ARG:NH1	2.59	0.50
12:BA:142:U:H3'	12:BA:143:A:C5'	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BC:253:ASP:O	14:BC:281:VAL:HG13	2.11	0.50
20:BK:54:ASN:HB3	20:BK:58:LYS:HE3	1.92	0.50
42:Bj:198:ASN:HB2	42:Bj:242:ASP:O	2.11	0.50
44:Bl:96:VAL:HG22	44:Bl:110:ILE:HG12	1.93	0.50
53:Bw:156:ARG:NH1	53:Bw:161:GLN:HA	2.26	0.50
3:B1:25:PRO:HB2	3:B1:27:HIS:CE1	2.46	0.50
20:BK:19:MET:HG2	20:BK:71:PHE:HD1	1.77	0.50
25:BR:77:ASP:HA	25:BR:86:ILE:HD11	1.93	0.50
30:BW:95:MET:HE1	30:BW:103:GLN:HG3	1.94	0.50
31:BX:16:GLN:OE1	37:Be:53:GLU:HA	2.12	0.50
1:CL:38:LEU:HD12	1:CL:46:LEU:HD12	1.93	0.50
10:B8:142:ARG:HB2	10:B8:142:ARG:CZ	2.41	0.50
12:BA:392:U:H2'	12:BA:393:A:H8	1.77	0.50
33:Ba:288:PRO:HD2	33:Ba:324:GLN:CD	2.37	0.50
51:Bu:78:ILE:HD13	51:Bu:146:LEU:HD21	1.94	0.50
14:BC:253:ASP:N	14:BC:253:ASP:OD1	2.45	0.50
32:BY:129:LYS:HD3	32:BY:149:ARG:HH21	1.77	0.50
46:Bn:35:ARG:HH12	46:Bn:39:PRO:N	2.09	0.50
12:BA:343:C:H2'	12:BA:344:U:C6	2.46	0.50
12:BA:749:C:N3	31:BX:51:VAL:HG13	2.27	0.50
12:BA:1145:C:H4'	12:BA:1146:G:O5'	2.12	0.50
28:BU:149:ARG:HB2	38:Bf:56:ARG:HH21	1.76	0.50
12:BA:811:A:H1'	16:BE:230:THR:HG23	1.95	0.49
17:BF:92:ARG:HG2	17:BF:95:ILE:HD12	1.94	0.49
23:BP:287:ASP:OD1	23:BP:288:GLU:N	2.45	0.49
35:Bc:78:MET:HE1	35:Bc:88:CYS:HA	1.92	0.49
53:Bw:86:MET:HB3	53:Bw:88:PHE:CE2	2.47	0.49
53:Bw:393:LYS:HG3	53:Bw:394:PRO:HD2	1.94	0.49
5:B3:36:PHE:CE1	24:BQ:228:LYS:HA	2.48	0.49
5:B3:71:ARG:HH22	12:BA:473:G:P	2.36	0.49
6:B4:60:GLN:HB3	55:Bz:702:ALA:HB1	1.93	0.49
12:BA:447:A:H5''	12:BA:448:G:OP2	2.13	0.49
21:BN:112:LEU:HD13	21:BN:121:MET:HG3	1.93	0.49
21:BN:177:ARG:HB2	54:Bx:36:ARG:O	2.11	0.49
23:BP:238:ARG:NH2	51:Bu:69:ASN:HA	2.27	0.49
33:Ba:212:THR:HG21	33:Ba:273:VAL:HG22	1.94	0.49
35:Bc:206:LEU:HD11	35:Bc:254:PHE:HE2	1.76	0.49
41:Bi:189:LEU:HB2	41:Bi:217:HIS:HD2	1.77	0.49
41:Bi:208:ILE:HB	41:Bi:252:LEU:HD12	1.93	0.49
46:Bn:35:ARG:HH12	46:Bn:39:PRO:CB	2.25	0.49
1:GL:67:LEU:HD22	1:HL:67:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B9:69:LEU:HB2	12:BA:560:A:N6	2.26	0.49
12:BA:138:A:C4	12:BA:141:A:H2	2.30	0.49
26:BS:107:THR:HB	26:BS:119:THR:HG23	1.94	0.49
31:BX:15:PRO:HA	32:BY:208:ARG:HH11	1.78	0.49
33:Ba:173:ARG:HA	33:Ba:176:TYR:CD2	2.48	0.49
35:Bc:67:VAL:HG22	35:Bc:121:GLU:HB2	1.94	0.49
40:Bh:259:ARG:HG3	40:Bh:259:ARG:NH1	2.13	0.49
45:Bm:77:GLU:HG3	45:Bm:104:ARG:HH11	1.76	0.49
2:B0:90:TYR:CZ	12:BA:1208:A:H4'	2.46	0.49
14:BC:388:VAL:HG11	14:BC:443:VAL:HG11	1.93	0.49
28:BU:88:ILE:HG13	28:BU:89:ASN:N	2.26	0.49
34:Bb:261:ARG:HB3	34:Bb:341:VAL:HG13	1.93	0.49
53:Bw:97:THR:HG22	53:Bw:99:ALA:N	2.20	0.49
54:Bx:89:LEU:HD11	54:Bx:118:CYS:HB3	1.94	0.49
6:B4:57:LEU:HD23	6:B4:65:ILE:HD12	1.94	0.49
10:B8:118:HIS:HE1	12:BA:227:U:OP1	1.96	0.49
21:BN:4:PHE:CD2	40:Bh:285:PRO:HD3	2.47	0.49
21:BN:112:LEU:HB2	21:BN:118:ARG:HD2	1.94	0.49
34:Bb:238:THR:HG21	34:Bb:281:PHE:CE1	2.48	0.49
35:Bc:253:ARG:HG3	35:Bc:258:ILE:HG12	1.93	0.49
36:Bd:102:PRO:HG2	36:Bd:103:PRO:HD3	1.94	0.49
42:Bj:116:LEU:N	42:Bj:119:ASP:OD2	2.45	0.49
53:Bw:158:PRO:C	53:Bw:160:ILE:H	2.20	0.49
54:Bx:144:LYS:H	54:Bx:144:LYS:HD2	1.76	0.49
12:BA:1549:A:C2	38:Bf:104:GLU:HG2	2.41	0.49
21:BN:26:GLN:NE2	21:BN:147:GLN:OE1	2.45	0.49
23:BP:51:ARG:NH1	23:BP:57:ARG:O	2.46	0.49
36:Bd:146:ALA:HB2	42:Bj:211:GLY:HA2	1.94	0.49
12:BA:1215:C:H3'	12:BA:1219:A:H62	1.77	0.49
16:BE:105:GLY:HA3	27:BT:91:LYS:HD2	1.94	0.49
21:BN:71:LYS:HZ1	54:Bx:196:HIS:CD2	2.29	0.49
31:BX:71:ARG:NH1	31:BX:96:TYR:OH	2.46	0.49
45:Bm:77:GLU:HG3	45:Bm:104:ARG:NH1	2.28	0.49
4:B2:66:LEU:HD13	31:BX:63:VAL:HG21	1.92	0.49
4:B2:230:ARG:NH2	12:BA:101:U:O2'	2.45	0.49
14:BC:309:VAL:HG13	14:BC:318:VAL:HG21	1.94	0.49
16:BE:148:GLY:HA3	16:BE:173:LYS:HG3	1.95	0.49
17:BF:59:ARG:NH1	17:BF:59:ARG:HG2	2.28	0.49
26:BS:57:GLU:HG2	26:BS:78:TRP:CD1	2.48	0.49
26:BS:91:GLU:HG2	26:BS:93:LEU:HD21	1.94	0.49
33:Ba:140:ALA:HB2	33:Ba:416:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:Bw:335:MET:HG2	53:Bw:371:LEU:HD21	1.95	0.49
1:EL:70:ASP:HB2	1:FL:67:LEU:HD21	1.95	0.49
5:B3:38:ARG:HB2	12:BA:410:U:OP1	2.13	0.49
12:BA:801:G:H4'	22:BO:36:THR:HG22	1.95	0.49
33:Ba:329:TYR:HB3	33:Ba:334:LYS:NZ	2.28	0.49
7:B5:140:GLN:NE2	7:B5:176:GLU:O	2.42	0.49
12:BA:562:A:N6	12:BA:1286:U:O2	2.46	0.49
12:BA:788:A:H3'	25:BR:10:SER:HB2	1.94	0.49
33:Ba:63:LYS:HD3	33:Ba:67:MET:HG3	1.94	0.49
33:Ba:96:HIS:CD2	33:Ba:97:PRO:HD2	2.48	0.49
6:B4:72:PRO:HG2	42:Bj:87:HIS:CD2	2.47	0.48
8:B6:59:GLN:HE21	8:B6:60:LYS:HE3	1.78	0.48
12:BA:468:A:N1	50:Bt:18:ILE:HD11	2.27	0.48
14:BC:660:LYS:HD3	14:BC:670:LYS:HZ3	1.78	0.48
31:BX:36:PRO:HD3	53:Bw:260:CYS:SG	2.53	0.48
33:Ba:162:ARG:HA	33:Ba:162:ARG:HD2	1.63	0.48
34:Bb:99:ARG:H	34:Bb:99:ARG:HD2	1.78	0.48
35:Bc:45:PHE:CD2	35:Bc:253:ARG:NH1	2.81	0.48
35:Bc:112:MET:HE1	35:Bc:124:PHE:HD1	1.78	0.48
43:Bk:81:ASN:HB3	43:Bk:86:TYR:CZ	2.48	0.48
8:B6:35:SER:HB3	8:B6:38:ARG:HB2	1.94	0.48
12:BA:13:U:H4'	12:BA:112:A:OP1	2.13	0.48
12:BA:225:C:H5'	23:BP:133:LYS:HE2	1.94	0.48
12:BA:620:A:H2'	12:BA:621:U:C6	2.47	0.48
17:BF:190:VAL:HG13	17:BF:191:ASP:O	2.13	0.48
20:BK:67:PRO:HD2	20:BK:85:PRO:HA	1.94	0.48
21:BN:170:TRP:CH2	21:BN:172:PRO:HB3	2.48	0.48
26:BS:89:HIS:HA	26:BS:119:THR:HG22	1.95	0.48
26:BS:177:ARG:HD3	26:BS:180:GLU:HG3	1.95	0.48
27:BT:76:LEU:HB2	27:BT:283:TRP:HZ3	1.78	0.48
2:B0:62:HIS:H	2:B0:65:ASN:ND2	2.12	0.48
5:B3:79:PRO:HD2	5:B3:82:GLU:OE2	2.13	0.48
5:B3:101:LYS:HG3	47:Bo:80:LEU:HD13	1.96	0.48
7:B5:179:ARG:NE	7:B5:182:PRO:HG3	2.28	0.48
12:BA:525:A:C2'	12:BA:526:A:H5''	2.43	0.48
12:BA:1386:U:H1'	12:BA:1389:A:N6	2.28	0.48
14:BC:677:LYS:HE3	14:BC:680:LYS:HA	1.95	0.48
22:BO:42:ASP:OD2	22:BO:44:SER:OG	2.25	0.48
40:Bh:308:THR:H	40:Bh:311:ARG:HD3	1.77	0.48
44:Bl:85:PHE:HA	44:Bl:166:PHE:CE1	2.48	0.48
12:BA:526:A:O2'	20:BK:135:VAL:HG11	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:692:A:H2'	12:BA:693:U:H5'	1.94	0.48
23:BP:52:GLY:O	23:BP:58:GLN:HG3	2.14	0.48
33:Ba:213:TRP:HZ3	33:Ba:222:VAL:HG12	1.78	0.48
53:Bw:321:ASN:HB3	53:Bw:355:ILE:HD13	1.95	0.48
54:Bx:108:CYS:SG	54:Bx:111:GLU:HB2	2.54	0.48
8:B6:62:ILE:HG21	12:BA:1244:U:H4'	1.96	0.48
12:BA:1234:U:H5'	23:BP:79:PRO:HB3	1.96	0.48
13:BB:30:G:H1'	36:Bd:122:SER:HB2	1.96	0.48
17:BF:284:TYR:HB2	17:BF:285:PRO:HD2	1.94	0.48
19:BJ:146:LEU:HA	48:Bp:31:ARG:HH22	1.78	0.48
23:BP:62:ARG:HG3	46:Bn:128:ARG:HH21	1.79	0.48
24:BQ:98:HIS:HD2	24:BQ:100:GLY:H	1.61	0.48
24:BQ:247:THR:OG1	24:BQ:250:ARG:HG2	2.13	0.48
33:Ba:351:LEU:HD11	33:Ba:379:ASP:HA	1.96	0.48
34:Bb:251:THR:HG23	34:Bb:285:THR:HA	1.95	0.48
35:Bc:300:VAL:HG23	35:Bc:301:HIS:CD2	2.47	0.48
53:Bw:278:ILE:HG22	53:Bw:280:SER:H	1.78	0.48
12:BA:274:A:H1'	12:BA:309:A:O2'	2.14	0.48
15:BD:68:SER:CB	33:Ba:38:THR:HG21	2.43	0.48
17:BF:71:GLY:H	17:BF:74:GLN:NE2	2.12	0.48
21:BN:75:LYS:HB2	54:Bx:174:MET:HE1	1.94	0.48
27:BT:188:LEU:HB3	27:BT:191:ARG:NH1	2.28	0.48
32:BY:80:ILE:HB	32:BY:85:TRP:HB2	1.95	0.48
10:B8:96:TYR:H	46:Bn:122:ASN:HD22	1.60	0.48
12:BA:1199:A:H2'	12:BA:1200:A:O4'	2.14	0.48
12:BA:1404:G:H4'	12:BA:1405:A:C8	2.48	0.48
19:BJ:139:LYS:HE3	19:BJ:140:TYR:CE2	2.48	0.48
29:BV:98:ARG:HH11	29:BV:113:THR:HG21	1.77	0.48
51:Bu:103:HIS:HD2	51:Bu:106:SER:H	1.62	0.48
10:B8:116:ARG:NH1	10:B8:120:GLY:HA2	2.29	0.48
12:BA:203:A:H5'	17:BF:152:ALA:CB	2.44	0.48
12:BA:659:U:OP2	53:Bw:55:SER:HB2	2.14	0.48
12:BA:1326:A:H61	41:Bi:40:ARG:HH22	1.61	0.48
20:BK:17:SER:N	20:BK:72:VAL:O	2.46	0.48
24:BQ:250:ARG:HD2	24:BQ:250:ARG:HA	1.48	0.48
42:Bj:85:SER:HB3	42:Bj:88:GLU:HB2	1.96	0.48
43:Bk:96:ILE:HG12	43:Bk:154:GLU:HG2	1.95	0.48
53:Bw:369:ASN:H	53:Bw:385:ASN:HD22	1.62	0.48
1:EL:71:ILE:HG22	1:HL:76:LEU:HD12	1.95	0.48
3:B1:5:LYS:HD2	12:BA:18:A:N7	2.29	0.48
3:B1:160:ASP:OD1	3:B1:163:ARG:NH2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:532:A:OP1	49:Bq:123:LYS:HE3	2.14	0.48
12:BA:1292:A:N6	12:BA:1304:G:O2'	2.43	0.48
14:BC:171:ALA:HB3	14:BC:176:LEU:HD21	1.96	0.48
33:Ba:117:VAL:O	33:Ba:121:LEU:HG	2.14	0.48
33:Ba:318:PHE:HZ	33:Ba:364:LEU:HD11	1.78	0.48
33:Ba:373:LEU:HD12	33:Ba:373:LEU:HA	1.69	0.48
34:Bb:72:ARG:N	34:Bb:72:ARG:NH1	2.62	0.48
40:Bh:141:PHE:CE2	40:Bh:156:LEU:HB3	2.49	0.48
41:Bi:169:PHE:HB3	41:Bi:170:PRO:HD3	1.96	0.48
53:Bw:171:LEU:HD23	53:Bw:232:HIS:CD2	2.48	0.48
12:BA:119:A:H5''	12:BA:120:C:OP2	2.14	0.48
12:BA:140:A:OP2	32:BY:94:HIS:NE2	2.47	0.48
12:BA:218:A:C5	34:Bb:379:ILE:HG21	2.49	0.48
21:BN:59:ILE:HB	21:BN:127:LEU:HD23	1.95	0.48
33:Ba:240:ALA:HB2	33:Ba:375:TRP:HH2	1.79	0.48
41:Bi:180:THR:HB	41:Bi:225:TYR:HB2	1.96	0.48
42:Bj:182:GLU:OE1	42:Bj:187:THR:OG1	2.32	0.48
7:B5:81:PRO:HA	12:BA:1438:U:C2	2.49	0.47
12:BA:221:A:H5''	12:BA:222:G:OP2	2.14	0.47
12:BA:1290:C:N4	12:BA:1291:U:O4	2.47	0.47
14:BC:179:ARG:HE	14:BC:413:SER:HG	1.58	0.47
16:BE:54:SER:O	16:BE:58:VAL:HG23	2.13	0.47
17:BF:211:ARG:NH1	45:Bm:59:ARG:HD2	2.29	0.47
34:Bb:216:LEU:HB3	34:Bb:237:VAL:HG12	1.96	0.47
53:Bw:213:ARG:HH11	53:Bw:213:ARG:CB	2.27	0.47
53:Bw:221:ASP:OD1	53:Bw:222:ALA:N	2.47	0.47
3:B1:100:ARG:HH22	18:BI:75:ARG:HE	1.61	0.47
6:B4:59:LYS:HE2	6:B4:65:ILE:HD11	1.96	0.47
10:B8:142:ARG:NH1	12:BA:1193:C:OP2	2.47	0.47
12:BA:527:U:O2'	19:BJ:113:ARG:NH1	2.45	0.47
15:BD:111:ARG:NH1	15:BD:111:ARG:HG3	2.29	0.47
26:BS:94:VAL:HG11	26:BS:141:ILE:HD11	1.96	0.47
14:BC:240:ALA:HB1	14:BC:534:ILE:HD11	1.94	0.47
14:BC:289:LYS:HG2	61:BC:901:GSP:C6	2.50	0.47
15:BD:170:ILE:HG22	15:BD:171:GLY:H	1.78	0.47
21:BN:39:LEU:HD21	21:BN:125:LEU:HD13	1.96	0.47
21:BN:71:LYS:HZ3	54:Bx:196:HIS:CD2	2.32	0.47
26:BS:81:LEU:HB2	26:BS:144:MET:SD	2.55	0.47
31:BX:3:ARG:O	31:BX:23:ASN:ND2	2.46	0.47
31:BX:40:VAL:HB	31:BX:97:VAL:HG22	1.95	0.47
35:Bc:181:VAL:HG22	35:Bc:290:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:Bx:43:ASP:O	54:Bx:46:THR:OG1	2.28	0.47
7:B5:138:ARG:HA	7:B5:141:MET:HG2	1.97	0.47
17:BF:70:ARG:O	17:BF:202:TYR:OH	2.32	0.47
22:BO:110:ASP:OD1	22:BO:110:ASP:N	2.35	0.47
23:BP:281:LYS:HD3	44:Bl:42:VAL:HG22	1.97	0.47
25:BR:145:LEU:HB2	35:Bc:136:ASN:OD1	2.13	0.47
28:BU:90:LEU:HD12	28:BU:90:LEU:HA	1.68	0.47
41:Bi:177:ARG:HG2	41:Bi:177:ARG:NH1	2.30	0.47
3:B1:119:LEU:HA	3:B1:168:ARG:HH11	1.79	0.47
3:B1:139:CYS:SG	18:BI:133:SER:HB2	2.55	0.47
9:B7:74:ARG:HA	9:B7:74:ARG:HD3	1.63	0.47
12:BA:320:U:OP1	15:BD:61:ALA:N	2.47	0.47
12:BA:978:G:H2'	12:BA:979:G:H5''	1.97	0.47
12:BA:1005:G:H1'	25:BR:116:GLN:HE22	1.79	0.47
13:BB:67:A:H2'	13:BB:68:A:O4'	2.14	0.47
28:BU:137:GLU:HB2	28:BU:138:PRO:HD3	1.96	0.47
30:BW:154:ILE:HG12	41:Bi:52:SER:CB	2.45	0.47
39:Bg:17:ASN:HD21	39:Bg:23:VAL:N	2.05	0.47
43:Bk:175:HIS:HA	43:Bk:178:LEU:HG	1.97	0.47
53:Bw:163:ARG:HD3	53:Bw:163:ARG:HA	1.67	0.47
12:BA:477:A:O2'	29:BV:192:ASN:ND2	2.43	0.47
12:BA:646:A:H2'	12:BA:647:A:O4'	2.14	0.47
16:BE:197:HIS:NE2	16:BE:318:THR:HG22	2.30	0.47
21:BN:140:ASN:CB	40:Bh:262:GLY:HA2	2.45	0.47
23:BP:246:ASP:OD1	23:BP:246:ASP:N	2.48	0.47
41:Bi:288:LYS:HD2	41:Bi:290:TRP:CZ2	2.50	0.47
53:Bw:59:ARG:HA	53:Bw:62:ARG:NH1	2.28	0.47
53:Bw:267:LEU:HA	53:Bw:267:LEU:HD23	1.60	0.47
1:CL:28:ILE:HG21	1:DL:85:LEU:HD12	1.97	0.47
2:B0:120:LEU:HD11	2:B0:126:LEU:HD23	1.97	0.47
8:B6:16:ILE:HD11	8:B6:61:LYS:HG3	1.96	0.47
10:B8:116:ARG:NE	10:B8:167:LYS:HG2	2.30	0.47
12:BA:187:G:H2'	12:BA:1025:A:N7	2.29	0.47
12:BA:478:G:H5'	12:BA:478:G:H8	1.79	0.47
12:BA:574:A:OP1	54:Bx:150:TYR:OH	2.26	0.47
12:BA:644:G:O2'	12:BA:1007:G:O6	2.32	0.47
12:BA:788:A:C2	25:BR:17:ARG:NH1	2.82	0.47
12:BA:1047:A:O4'	16:BE:244:SER:HB3	2.15	0.47
12:BA:1521:U:H3'	12:BA:1522:A:C5'	2.45	0.47
23:BP:154:ILE:HG22	23:BP:174:VAL:HG13	1.97	0.47
24:BQ:33:LEU:HD12	49:Bq:118:TRP:HE3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BS:109:GLU:OE2	26:BS:135:ARG:NH2	2.47	0.47
27:BT:115:SER:HB3	27:BT:180:GLU:H	1.80	0.47
29:BV:115:GLU:HG2	39:Bg:19:LEU:HD11	1.96	0.47
33:Ba:313:MET:HE1	33:Ba:346:GLY:HA3	1.97	0.47
33:Ba:337:GLU:CD	33:Ba:337:GLU:H	2.23	0.47
38:Bf:67:ILE:HD12	40:Bh:258:THR:CG2	2.45	0.47
39:Bg:131:HIS:HB2	39:Bg:132:PRO:HD2	1.95	0.47
41:Bi:177:ARG:HG2	41:Bi:177:ARG:HH11	1.80	0.47
42:Bj:46:ARG:HB3	42:Bj:229:ALA:HB2	1.97	0.47
42:Bj:63:LEU:HB2	42:Bj:68:GLU:HG2	1.96	0.47
54:Bx:99:MET:HE1	54:Bx:119:VAL:HB	1.95	0.47
54:Bx:99:MET:CE	54:Bx:116:GLU:HA	2.45	0.47
3:B1:159:MET:HE3	3:B1:205:GLY:HA2	1.97	0.47
4:B2:88:THR:HB	4:B2:91:GLN:HG3	1.97	0.47
12:BA:122:G:H5'	12:BA:123:U:OP2	2.15	0.47
16:BE:98:GLY:HA3	16:BE:179:PHE:CE1	2.50	0.47
17:BF:113:LYS:HG3	17:BF:157:GLY:H	1.79	0.47
19:BJ:54:ILE:HD12	24:BQ:211:ASN:HB3	1.97	0.47
20:BK:149:ARG:HH12	49:Bq:104:PRO:HB3	1.79	0.47
37:Be:88:GLN:O	37:Be:92:GLU:HG2	2.14	0.47
38:Bf:74:PRO:HA	40:Bh:256:ARG:HE	1.79	0.47
42:Bj:185:ARG:HH12	42:Bj:204:PHE:HB3	1.80	0.47
46:Bn:46:ARG:HA	46:Bn:51:ARG:HD2	1.97	0.47
47:Bo:63:GLN:NE2	47:Bo:66:ARG:NH1	2.61	0.47
5:B3:71:ARG:HH21	5:B3:74:SER:HA	1.80	0.47
7:B5:144:GLN:HE22	7:B5:175:ILE:HA	1.79	0.47
12:BA:678:A:H5'	53:Bw:213:ARG:HG2	1.97	0.47
12:BA:688:A:H3'	12:BA:689:A:H4'	1.95	0.47
12:BA:995:C:H5''	25:BR:13:ARG:HH22	1.79	0.47
13:BB:24:A:H2'	13:BB:25:G:H8	1.79	0.47
17:BF:69:LEU:HD13	17:BF:190:VAL:HG21	1.96	0.47
22:BO:58:ILE:HD11	22:BO:76:ALA:HB2	1.97	0.47
24:BQ:188:LYS:NZ	24:BQ:198:MET:HE1	2.30	0.47
35:Bc:267:PRO:HG2	35:Bc:271:ILE:HD11	1.97	0.47
36:Bd:171:PHE:HD1	42:Bj:203:LYS:HE2	1.79	0.47
42:Bj:51:LEU:HD13	42:Bj:192:LEU:HG	1.95	0.47
42:Bj:173:LEU:HD23	42:Bj:233:PHE:CE2	2.50	0.47
42:Bj:176:SER:HB3	42:Bj:187:THR:HG22	1.97	0.47
46:Bn:117:LEU:HD23	46:Bn:117:LEU:HA	1.77	0.47
12:BA:196:U:O2'	12:BA:1014:A:OP1	2.29	0.47
12:BA:744:A:OP1	12:BA:744:A:H4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:1131:U:O2'	18:BI:87:LYS:NZ	2.48	0.47
15:BD:90:GLN:H	15:BD:90:GLN:HG2	1.47	0.47
16:BE:104:LEU:HB2	16:BE:121:LEU:HB2	1.97	0.47
27:BT:188:LEU:HD22	27:BT:191:ARG:HH12	1.79	0.47
33:Ba:244:GLU:O	33:Ba:248:THR:OG1	2.26	0.47
39:Bg:28:ARG:HH11	39:Bg:28:ARG:CB	2.26	0.47
45:Bm:139:SER:OG	45:Bm:140:LYS:N	2.48	0.47
1:GL:70:ASP:O	1:GL:74:LEU:HG	2.15	0.46
12:BA:80:A:H5'	18:BI:61:LYS:NZ	2.30	0.46
12:BA:721:A:H5''	33:Ba:301:PRO:HB3	1.97	0.46
12:BA:798:A:O2'	12:BA:1489:U:H4'	2.16	0.46
12:BA:1420:A:H5'	15:BD:278:ARG:NH2	2.30	0.46
12:BA:1531:C:O2'	54:Bx:138:GLY:HA3	2.15	0.46
14:BC:298:GLU:O	14:BC:302:LYS:HG2	2.15	0.46
16:BE:329:PRO:HD2	16:BE:332:LEU:HD21	1.97	0.46
1:BL:142:LYS:HZ3	1:BL:166:GLU:HG2	1.79	0.46
30:BW:101:LEU:HD23	30:BW:101:LEU:HA	1.73	0.46
1:HL:76:LEU:O	1:HL:80:SER:OG	2.32	0.46
11:B9:74:ARG:NH1	12:BA:545:U:O2'	2.48	0.46
11:B9:92:ASN:OD1	11:B9:92:ASN:N	2.49	0.46
12:BA:1544:A:H5''	16:BE:300:LYS:NZ	2.31	0.46
15:BD:83:GLY:HA2	15:BD:96:ILE:HG22	1.96	0.46
15:BD:159:LYS:O	15:BD:162:ASP:HB2	2.16	0.46
20:BK:137:LEU:O	20:BK:141:VAL:HG23	2.15	0.46
33:Ba:240:ALA:HB3	33:Ba:358:GLN:HE22	1.78	0.46
39:Bg:27:GLN:O	39:Bg:61:VAL:HA	2.14	0.46
42:Bj:149:LEU:HD13	42:Bj:254:TRP:CE2	2.50	0.46
2:B0:76:HIS:HE1	2:B0:128:LYS:HD2	1.81	0.46
4:B2:236:LEU:HD13	32:BY:48:PRO:HG3	1.96	0.46
12:BA:573:A:H5'	21:BN:29:GLY:HA3	1.98	0.46
14:BC:365:ASP:OD1	14:BC:366:LYS:N	2.48	0.46
15:BD:111:ARG:HH11	15:BD:111:ARG:HG3	1.80	0.46
15:BD:258:ILE:HG23	15:BD:263:ARG:HB3	1.97	0.46
19:BJ:33:VAL:HB	24:BQ:69:LEU:HB3	1.98	0.46
26:BS:171:VAL:HG21	51:Bu:179:ILE:HD13	1.97	0.46
33:Ba:215:ARG:HG3	33:Ba:215:ARG:NH1	2.31	0.46
42:Bj:178:TRP:HB3	42:Bj:187:THR:HG21	1.96	0.46
48:Bp:89:ALA:O	48:Bp:93:HIS:HB2	2.16	0.46
4:B2:105:TYR:HE1	31:BX:60:ILE:HD13	1.80	0.46
4:B2:193:ASN:O	4:B2:197:ASN:HB2	2.15	0.46
12:BA:223:A:H5'	17:BF:285:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:1026:A:C6	12:BA:1321:C:H1'	2.51	0.46
17:BF:283:LEU:HB2	23:BP:125:ARG:HH12	1.80	0.46
22:BO:107:LEU:HA	22:BO:107:LEU:HD23	1.61	0.46
29:BV:150:LYS:HE3	38:Bf:58:ILE:HD11	1.97	0.46
35:Bc:190:MET:CE	35:Bc:291:ARG:HH11	2.27	0.46
40:Bh:223:MET:HE2	40:Bh:223:MET:HB3	1.86	0.46
43:Bk:166:PHE:O	43:Bk:170:PHE:HB2	2.15	0.46
48:Bp:16:VAL:HG22	48:Bp:66:VAL:HG13	1.98	0.46
54:Bx:190:ARG:HB3	54:Bx:190:ARG:NH1	2.30	0.46
10:B8:183:ARG:NH2	34:Bb:355:LYS:O	2.48	0.46
12:BA:220:G:H1'	12:BA:231:C:O2'	2.15	0.46
12:BA:302:A:H2'	12:BA:303:G:O4'	2.16	0.46
12:BA:435:C:H2'	12:BA:436:U:H6	1.80	0.46
12:BA:547:A:H3'	12:BA:548:A:H5'	1.97	0.46
12:BA:1226:C:H3'	12:BA:1227:U:O2	2.16	0.46
12:BA:1294:A:H5'	12:BA:1295:G:OP2	2.15	0.46
14:BC:435:GLU:OE1	14:BC:439:ARG:HG2	2.15	0.46
16:BE:225:LYS:HB3	16:BE:225:LYS:HE2	1.72	0.46
18:BI:91:LYS:HE2	18:BI:116:LYS:HD2	1.97	0.46
23:BP:26:ASN:OD1	23:BP:26:ASN:N	2.49	0.46
23:BP:142:GLU:CD	23:BP:142:GLU:H	2.23	0.46
23:BP:208:GLU:HG2	52:Bv:99:MET:HE3	1.98	0.46
25:BR:101:ASN:O	25:BR:104:TYR:OH	2.22	0.46
51:Bu:44:SER:OG	51:Bu:45:LEU:N	2.48	0.46
53:Bw:204:TRP:HZ3	53:Bw:227:ILE:HG13	1.79	0.46
12:BA:131:A:H8	12:BA:131:A:OP2	1.99	0.46
12:BA:311:A:H5'	15:BD:262:GLY:HA2	1.98	0.46
12:BA:1464:A:H2'	12:BA:1465:A:C8	2.51	0.46
25:BR:46:TRP:CD1	25:BR:122:ALA:HB2	2.51	0.46
33:Ba:202:ILE:HA	33:Ba:202:ILE:HD13	1.63	0.46
36:Bd:143:GLN:NE2	42:Bj:210:CYS:O	2.49	0.46
40:Bh:51:LEU:HD22	40:Bh:51:LEU:HA	1.77	0.46
40:Bh:102:GLU:HA	40:Bh:105:ARG:HB3	1.96	0.46
53:Bw:166:ILE:HA	53:Bw:166:ILE:HD13	1.78	0.46
3:B1:176:LEU:HD23	3:B1:184:ARG:HG3	1.97	0.46
12:BA:130:A:OP1	17:BF:147:ARG:NH2	2.49	0.46
12:BA:1072:A:N3	12:BA:1257:A:O2'	2.46	0.46
12:BA:1127:A:H2'	12:BA:1128:A:C8	2.51	0.46
20:BK:66:LEU:HD13	20:BK:82:ILE:HG23	1.98	0.46
1:BL:148:GLU:HG3	1:BL:152:HIS:HD2	1.80	0.46
53:Bw:96:GLN:HE21	53:Bw:321:ASN:ND2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:705:U:H5'	31:BX:71:ARG:HB3	1.97	0.46
14:BC:516:LEU:HG	14:BC:518:VAL:HG23	1.97	0.46
16:BE:279:LYS:HB2	16:BE:330:GLU:OE2	2.16	0.46
33:Ba:384:GLN:HB2	33:Ba:404:ILE:O	2.16	0.46
41:Bi:90:PRO:HB2	41:Bi:269:TRP:CH2	2.46	0.46
42:Bj:257:LYS:HD3	42:Bj:276:LEU:HD21	1.97	0.46
3:B1:75:SER:HB2	3:B1:80:TRP:CE3	2.51	0.46
5:B3:105:SER:HB3	12:BA:416:U:H1'	1.97	0.46
14:BC:179:ARG:HG2	14:BC:180:SER:H	1.80	0.46
14:BC:570:VAL:HG13	14:BC:592:LYS:HG3	1.97	0.46
24:BQ:166:ARG:NH1	24:BQ:166:ARG:HB3	2.31	0.46
24:BQ:216:GLU:HG2	24:BQ:238:LYS:HG2	1.98	0.46
26:BS:90:ILE:HD11	26:BS:120:ARG:NH1	2.31	0.46
29:BV:99:LEU:O	29:BV:113:THR:HG23	2.16	0.46
53:Bw:182:LEU:HD11	53:Bw:416:VAL:HG22	1.98	0.46
8:B6:36:ARG:NH2	8:B6:64:SER:HB3	2.30	0.46
12:BA:172:C:OP1	38:Bf:135:LYS:HE2	2.16	0.46
12:BA:416:U:H2'	12:BA:417:G:C8	2.51	0.46
16:BE:236:THR:O	16:BE:238:ARG:N	2.49	0.46
17:BF:283:LEU:HB2	23:BP:125:ARG:NH1	2.31	0.46
35:Bc:206:LEU:HD21	35:Bc:254:PHE:CE2	2.51	0.46
36:Bd:164:ARG:HH22	43:Bk:91:LEU:HD21	1.81	0.46
39:Bg:35:ARG:O	39:Bg:44:ARG:NH1	2.49	0.46
3:B1:20:ILE:HA	3:B1:23:ARG:NH1	2.31	0.45
5:B3:75:THR:HB	5:B3:83:LYS:HG2	1.98	0.45
7:B5:95:ARG:HG2	30:BW:86:TRP:CH2	2.51	0.45
12:BA:719:C:O2'	33:Ba:112:ARG:HG3	2.16	0.45
12:BA:1530:C:H4'	54:Bx:132:ARG:HD3	1.98	0.45
16:BE:275:ARG:HD2	16:BE:333:TYR:CE1	2.51	0.45
18:BI:99:THR:C	18:BI:108:ARG:HG2	2.41	0.45
1:BL:185:LYS:HB3	1:BL:185:LYS:HE2	1.77	0.45
21:BN:10:GLN:NE2	30:BW:202:ARG:HA	2.31	0.45
22:BO:56:ARG:HG2	22:BO:56:ARG:HH11	1.81	0.45
22:BO:98:PRO:HA	27:BT:162:ILE:HD13	1.97	0.45
24:BQ:209:ASN:HD22	24:BQ:210:GLN:N	2.14	0.45
28:BU:42:ALA:O	28:BU:46:VAL:HG23	2.16	0.45
28:BU:90:LEU:HD21	28:BU:116:LEU:HD22	1.97	0.45
32:BY:91:LEU:HD23	32:BY:91:LEU:HA	1.61	0.45
33:Ba:209:LEU:O	33:Ba:223:HIS:HA	2.16	0.45
35:Bc:163:LEU:HB3	35:Bc:178:TYR:HE2	1.81	0.45
41:Bi:160:LEU:O	41:Bi:164:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:Bw:157:ALA:N	53:Bw:158:PRO:HD2	2.31	0.45
54:Bx:70:CYS:SG	54:Bx:108:CYS:HB3	2.55	0.45
1:CL:36:ALA:HA	1:FL:76:LEU:HB3	1.98	0.45
2:B0:61:VAL:HG12	2:B0:65:ASN:HD22	1.81	0.45
12:BA:548:A:H5''	49:Bq:126:ILE:CD1	2.38	0.45
14:BC:176:LEU:HB3	14:BC:348:LYS:HD2	1.98	0.45
17:BF:211:ARG:HD2	45:Bm:59:ARG:NH1	2.31	0.45
24:BQ:64:ARG:NH1	24:BQ:144:LYS:HB3	2.31	0.45
26:BS:146:TYR:CE2	26:BS:148:PRO:HB3	2.50	0.45
27:BT:225:LYS:HB3	27:BT:226:PRO:HD2	1.98	0.45
31:BX:7:TYR:HD2	37:Be:37:LYS:HE3	1.81	0.45
39:Bg:28:ARG:HH21	40:Bh:177:GLN:HE21	1.64	0.45
40:Bh:161:THR:HG23	40:Bh:196:PHE:CZ	2.51	0.45
40:Bh:191:LEU:HD23	40:Bh:191:LEU:HA	1.80	0.45
46:Bn:35:ARG:NH1	46:Bn:39:PRO:HB3	2.31	0.45
50:Bt:99:ARG:HH11	50:Bt:99:ARG:CB	2.29	0.45
8:B6:16:ILE:HG22	8:B6:34:ARG:O	2.15	0.45
9:B7:85:ARG:NH1	37:Be:17:ARG:HH12	2.14	0.45
12:BA:479:A:H8	12:BA:479:A:OP1	1.98	0.45
14:BC:570:VAL:HG22	14:BC:592:LYS:HE3	1.98	0.45
14:BC:654:GLU:HG2	14:BC:685:ILE:HG12	1.97	0.45
26:BS:149:THR:HG22	26:BS:150:PRO:HD2	1.98	0.45
27:BT:142:GLY:HA3	27:BT:147:ALA:HA	1.97	0.45
51:Bu:153:LEU:HD12	51:Bu:156:MET:HE2	1.99	0.45
2:B0:67:LEU:N	2:B0:89:LEU:O	2.42	0.45
8:B6:54:VAL:HG12	8:B6:55:LEU:H	1.82	0.45
14:BC:184:THR:CG2	14:BC:233:LEU:HB2	2.46	0.45
14:BC:288:ASN:HA	14:BC:323:VAL:O	2.17	0.45
17:BF:211:ARG:HB2	45:Bm:59:ARG:NH2	2.32	0.45
21:BN:176:TYR:CE2	54:Bx:104:ILE:HG13	2.51	0.45
23:BP:54:LYS:HB3	23:BP:55:GLY:H	1.54	0.45
51:Bu:132:LEU:HD21	51:Bu:156:MET:HE1	1.98	0.45
55:Bz:702:ALA:HA	55:Bz:705:ALA:HB3	1.98	0.45
12:BA:304:U:H2'	12:BA:305:G:O4'	2.17	0.45
12:BA:1466:G:OP1	14:BC:601:ARG:NH2	2.49	0.45
14:BC:361:GLU:HB3	14:BC:524:VAL:HG11	1.98	0.45
31:BX:3:ARG:O	31:BX:5:VAL:HG23	2.17	0.45
34:Bb:72:ARG:HD3	34:Bb:72:ARG:HA	1.71	0.45
53:Bw:352:GLN:HB3	53:Bw:418:PHE:CD2	2.51	0.45
12:BA:39:A:H4'	12:BA:40:C:OP1	2.15	0.45
12:BA:1329:U:O2'	12:BA:1330:U:H5'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BD:76:PRO:HB2	15:BD:103:ARG:HD2	1.99	0.45
23:BP:11:ARG:HG2	23:BP:11:ARG:NH1	2.30	0.45
30:BW:154:ILE:HG12	41:Bi:52:SER:HB3	1.98	0.45
33:Ba:42:GLU:H	33:Ba:42:GLU:HG3	1.54	0.45
33:Ba:207:ASN:ND2	33:Ba:229:ARG:HD2	2.28	0.45
34:Bb:238:THR:HG22	34:Bb:239:ASN:H	1.81	0.45
34:Bb:265:PHE:CZ	34:Bb:322:ARG:HD2	2.51	0.45
38:Bf:129:TYR:O	38:Bf:133:ARG:HG2	2.17	0.45
53:Bw:91:TYR:CE2	53:Bw:269:LYS:HE3	2.52	0.45
53:Bw:113:VAL:HG21	53:Bw:384:LYS:HD3	1.97	0.45
54:Bx:190:ARG:HB3	54:Bx:190:ARG:HH11	1.82	0.45
12:BA:513:A:H2'	12:BA:514:A:H5''	1.97	0.45
12:BA:724:A:H2	12:BA:728:C:H42	1.65	0.45
12:BA:1050:C:H5'	12:BA:1051:G:OP1	2.17	0.45
14:BC:410:ALA:HB2	14:BC:416:VAL:HG21	1.99	0.45
15:BD:137:SER:C	15:BD:211:ALA:HB2	2.42	0.45
16:BE:42:HIS:HA	35:Bc:98:ARG:HH22	1.82	0.45
21:BN:62:THR:HG21	21:BN:101:VAL:HA	1.99	0.45
27:BT:118:ARG:NH1	27:BT:175:GLN:OE1	2.47	0.45
30:BW:88:LEU:HB3	30:BW:115:ILE:HD12	1.98	0.45
33:Ba:181:VAL:O	33:Ba:185:ILE:HG12	2.16	0.45
54:Bx:164:ASN:O	54:Bx:166:GLY:N	2.49	0.45
5:B3:65:LYS:NZ	47:Bo:81:SER:OG	2.43	0.45
15:BD:185:LEU:HA	15:BD:185:LEU:HD23	1.83	0.45
17:BF:263:LEU:HD23	17:BF:263:LEU:HA	1.81	0.45
25:BR:41:ARG:NH1	25:BR:125:GLU:OE2	2.50	0.45
26:BS:127:SER:O	26:BS:131:VAL:HG23	2.17	0.45
28:BU:98:ASN:H	29:BV:109:GLN:NE2	2.15	0.45
38:Bf:74:PRO:CD	40:Bh:256:ARG:HH21	2.28	0.45
6:B4:63:SER:HA	36:Bd:179:THR:O	2.16	0.45
7:B5:97:PRO:HA	7:B5:100:LEU:HD12	1.98	0.45
12:BA:1000:A:H2'	12:BA:1001:A:C8	2.51	0.45
12:BA:1092:A:H5'	12:BA:1093:A:OP2	2.16	0.45
12:BA:1531:C:H3'	12:BA:1532:U:H5''	1.99	0.45
12:BA:1542:A:H5'	12:BA:1543:U:OP2	2.15	0.45
17:BF:275:TRP:CZ3	17:BF:279:ARG:HD3	2.51	0.45
19:BJ:93:ASN:CG	19:BJ:155:VAL:HG13	2.42	0.45
19:BJ:163:GLU:HG3	19:BJ:166:ARG:NH1	2.32	0.45
20:BK:64:ILE:HG21	20:BK:90:PHE:HE1	1.82	0.45
27:BT:112:TYR:CE2	27:BT:215:VAL:HG11	2.51	0.45
28:BU:94:GLN:NE2	28:BU:145:VAL:HG13	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Ba:361:THR:HG22	33:Ba:363:ASP:H	1.82	0.45
40:Bh:238:MET:O	40:Bh:242:VAL:HG23	2.17	0.45
52:Bv:79:GLN:O	52:Bv:83:ARG:HG3	2.16	0.45
1:GL:76:LEU:HD21	19:BJ:240:GLN:HB2	1.98	0.45
12:BA:438:A:OP2	19:BJ:38:ARG:NH2	2.50	0.45
12:BA:931:U:H5	12:BA:938:U:O4	2.00	0.45
14:BC:381:LEU:HG	14:BC:399:MET:HE1	1.97	0.45
20:BK:124:LYS:HE3	20:BK:124:LYS:HB3	1.82	0.45
24:BQ:135:GLY:O	24:BQ:138:GLN:HG2	2.17	0.45
25:BR:62:TYR:HD2	27:BT:269:MET:HE3	1.81	0.45
27:BT:99:MET:HB2	27:BT:167:TYR:CE1	2.52	0.45
27:BT:196:GLU:H	27:BT:196:GLU:CD	2.24	0.45
31:BX:63:VAL:HA	31:BX:64:PRO:HD3	1.75	0.45
34:Bb:79:GLY:C	34:Bb:81:GLU:H	2.25	0.45
34:Bb:162:PHE:HB2	34:Bb:165:ALA:HB3	1.99	0.45
36:Bd:154:SER:HB3	36:Bd:157:LEU:HD12	1.99	0.45
5:B3:81:TRP:CD1	5:B3:82:GLU:HG2	2.52	0.44
12:BA:101:U:H4'	12:BA:102:G:O5'	2.17	0.44
12:BA:745:A:H3'	12:BA:746:U:H5''	1.99	0.44
14:BC:611:SER:HB2	14:BC:720:LYS:HA	1.99	0.44
22:BO:95:ARG:NH1	22:BO:95:ARG:N	2.64	0.44
23:BP:234:LEU:HB3	51:Bu:66:LYS:NZ	2.32	0.44
35:Bc:99:LYS:O	35:Bc:126:THR:HG23	2.17	0.44
38:Bf:67:ILE:HD12	40:Bh:258:THR:HG21	1.99	0.44
53:Bw:294:HIS:HB2	53:Bw:355:ILE:HG12	1.99	0.44
1:CL:28:ILE:O	1:CL:32:VAL:HG23	2.16	0.44
1:EL:79:ILE:HD13	1:HL:76:LEU:HG	2.00	0.44
13:BB:26:C:OP2	26:BS:86:THR:HG23	2.17	0.44
16:BE:342:ALA:H	27:BT:105:ILE:HD11	1.82	0.44
33:Ba:121:LEU:O	33:Ba:125:LYS:N	2.51	0.44
33:Ba:136:VAL:HG22	33:Ba:420:HIS:HD2	1.82	0.44
34:Bb:66:ARG:O	34:Bb:75:ARG:NH1	2.44	0.44
35:Bc:218:VAL:HG12	35:Bc:222:VAL:HG23	1.97	0.44
35:Bc:274:GLN:NE2	35:Bc:303:ARG:HB2	2.32	0.44
42:Bj:158:ILE:HG21	42:Bj:260:LEU:HD13	1.99	0.44
53:Bw:356:THR:HG23	53:Bw:357:ASP:O	2.17	0.44
3:B1:102:ARG:NH1	12:BA:48:U:C5	2.86	0.44
22:BO:61:TYR:HB2	22:BO:72:ARG:HB3	2.00	0.44
22:BO:127:LEU:HD23	22:BO:127:LEU:HA	1.78	0.44
23:BP:68:GLU:HG3	23:BP:73:PRO:HA	1.99	0.44
29:BV:102:VAL:HA	29:BV:110:TRP:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Bb:233:VAL:HG23	34:Bb:298:PHE:CG	2.52	0.44
34:Bb:360:ARG:HG2	34:Bb:360:ARG:NH1	2.32	0.44
36:Bd:117:LEU:HD23	42:Bj:73:LEU:HD22	2.00	0.44
38:Bf:84:ILE:HA	38:Bf:92:LEU:CB	2.48	0.44
41:Bi:289:PRO:HG2	41:Bi:290:TRP:CE3	2.51	0.44
2:B0:56:MET:HE2	2:B0:56:MET:HB2	1.76	0.44
6:B4:50:ALA:H	36:Bd:94:PHE:HE2	1.65	0.44
7:B5:140:GLN:HE22	7:B5:176:GLU:C	2.24	0.44
12:BA:670:A:H5''	37:Be:28:ARG:HD2	1.99	0.44
12:BA:938:U:OP1	12:BA:938:U:H6	2.00	0.44
12:BA:947:A:N3	12:BA:1383:G:O2'	2.47	0.44
16:BE:206:VAL:HG22	16:BE:299:ILE:HG23	1.98	0.44
17:BF:204:ILE:HD11	17:BF:237:LEU:HD21	2.00	0.44
30:BW:157:HIS:HB2	30:BW:161:ARG:O	2.17	0.44
32:BY:75:LYS:HE2	32:BY:159:PHE:HE1	1.81	0.44
33:Ba:279:PHE:CE1	53:Bw:151:LEU:HD13	2.51	0.44
36:Bd:106:LEU:HB3	36:Bd:110:GLU:HB2	1.98	0.44
37:Be:127:GLN:H	37:Be:127:GLN:HG2	1.62	0.44
41:Bi:102:LYS:HD2	41:Bi:102:LYS:HA	1.57	0.44
45:Bm:141:PHE:CE2	45:Bm:145:ILE:HD11	2.53	0.44
53:Bw:237:ILE:HD11	53:Bw:290:HIS:HB2	2.00	0.44
7:B5:138:ARG:HB3	12:BA:655:C:C6	2.52	0.44
7:B5:140:GLN:HG3	7:B5:143:LYS:HZ2	1.81	0.44
9:B7:58:PRO:HB2	12:BA:672:G:H4'	1.99	0.44
12:BA:96:U:N3	52:Bv:34:SER:O	2.51	0.44
12:BA:218:A:H4'	12:BA:219:A:H5'	1.99	0.44
12:BA:486:A:N6	50:Bt:30:GLN:HE22	2.15	0.44
12:BA:720:C:OP1	12:BA:720:C:H6	2.01	0.44
12:BA:801:G:OP1	22:BO:90:ARG:HD3	2.18	0.44
14:BC:489:ARG:O	14:BC:493:ARG:HB2	2.16	0.44
16:BE:152:VAL:HG21	16:BE:157:LYS:NZ	2.33	0.44
20:BK:64:ILE:HG21	20:BK:90:PHE:CE1	2.52	0.44
22:BO:95:ARG:HA	22:BO:95:ARG:HH11	1.82	0.44
23:BP:153:ASN:HB2	23:BP:256:LEU:HD23	2.00	0.44
31:BX:7:TYR:CD2	37:Be:37:LYS:HG3	2.53	0.44
35:Bc:128:LYS:HE3	35:Bc:128:LYS:HB2	1.88	0.44
39:Bg:35:ARG:HD3	45:Bm:157:TRP:CH2	2.52	0.44
42:Bj:243:PHE:HE1	42:Bj:248:LYS:HE2	1.82	0.44
54:Bx:99:MET:HE3	54:Bx:116:GLU:HG3	1.98	0.44
7:B5:85:ARG:HH11	12:BA:642:G:H5''	1.83	0.44
7:B5:156:THR:HG21	7:B5:173:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B8:188:VAL:HG11	12:BA:424:U:H4'	1.99	0.44
12:BA:508:G:H4'	20:BK:151:LEU:HD13	2.00	0.44
16:BE:205:ASP:OD1	16:BE:269:PHE:HA	2.18	0.44
17:BF:107:LYS:HA	46:Bn:74:ILE:HD12	2.00	0.44
18:BI:61:LYS:HB3	18:BI:61:LYS:HE2	1.66	0.44
20:BK:23:ILE:HG12	20:BK:67:PRO:HB3	1.99	0.44
20:BK:160:SER:HA	20:BK:163:GLU:HB2	2.00	0.44
38:Bf:56:ARG:CB	38:Bf:56:ARG:HH11	2.30	0.44
52:Bv:29:PRO:HA	52:Bv:30:PRO:HD3	1.88	0.44
54:Bx:100:LEU:HD12	54:Bx:100:LEU:HA	1.90	0.44
12:BA:379:U:OP2	23:BP:62:ARG:NH1	2.51	0.44
16:BE:221:ARG:HA	16:BE:261:LEU:HD22	1.99	0.44
19:BJ:41:HIS:CD2	19:BJ:43:GLU:H	2.35	0.44
23:BP:281:LYS:HD2	44:Bl:40:GLU:HG2	1.99	0.44
26:BS:90:ILE:O	26:BS:107:THR:OG1	2.35	0.44
27:BT:254:MET:HE2	27:BT:254:MET:HA	2.00	0.44
33:Ba:213:TRP:CD1	33:Ba:364:LEU:HD12	2.53	0.44
36:Bd:158:HIS:O	36:Bd:162:THR:OG1	2.25	0.44
39:Bg:117:LYS:HA	39:Bg:118:PRO:HD3	1.77	0.44
40:Bh:278:ARG:HH11	40:Bh:278:ARG:CB	2.25	0.44
46:Bn:65:ASN:O	46:Bn:67:GLU:HG3	2.17	0.44
50:Bt:82:PHE:CG	50:Bt:83:PRO:HD2	2.53	0.44
54:Bx:138:GLY:C	54:Bx:141:PRO:HD2	2.43	0.44
56:AV:15:A:O2'	56:AV:16:A:O4'	2.35	0.44
3:B1:42:HIS:CE1	3:B1:83:GLU:HB2	2.52	0.44
7:B5:140:GLN:HG3	7:B5:143:LYS:NZ	2.33	0.44
12:BA:769:A:H5'	12:BA:770:G:OP1	2.18	0.44
15:BD:164:VAL:HG22	15:BD:180:GLY:HA3	1.99	0.44
21:BN:3:SER:OG	40:Bh:309:GLU:HG2	2.17	0.44
26:BS:115:HIS:CD2	34:Bb:135:VAL:HG22	2.50	0.44
30:BW:117:GLU:O	30:BW:121:GLU:HG3	2.17	0.44
32:BY:191:LEU:HG	37:Be:93:THR:HG21	2.00	0.44
34:Bb:308:GLN:O	47:Bo:113:LYS:NZ	2.37	0.44
40:Bh:227:GLU:OE1	40:Bh:302:ARG:HD3	2.18	0.44
10:B8:125:ARG:HG2	10:B8:129:TYR:CE1	2.53	0.44
12:BA:442:G:OP1	24:BQ:144:LYS:HE3	2.18	0.44
12:BA:494:U:C2	12:BA:560:A:C2	3.06	0.44
17:BF:74:GLN:O	17:BF:210:ARG:NH2	2.51	0.44
17:BF:195:LEU:O	17:BF:229:ASN:ND2	2.50	0.44
20:BK:33:PRO:HA	20:BK:37:PRO:HD2	2.00	0.44
24:BQ:55:ARG:HD3	24:BQ:99:TRP:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Ba:180:ILE:O	33:Ba:184:LEU:HG	2.17	0.44
33:Ba:195:HIS:O	33:Ba:197:SER:N	2.50	0.44
37:Be:68:LEU:HD12	37:Be:68:LEU:HA	1.87	0.44
48:Bp:16:VAL:HG13	48:Bp:66:VAL:HG22	2.00	0.44
51:Bu:182:MET:HE2	51:Bu:182:MET:HB3	1.67	0.44
3:B1:128:THR:HG22	3:B1:129:MET:H	1.83	0.43
5:B3:67:HIS:O	5:B3:99:VAL:HA	2.18	0.43
12:BA:222:G:H1	46:Bn:61:GLY:HA3	1.83	0.43
12:BA:391:A:O2'	12:BA:392:U:O4'	2.27	0.43
12:BA:894:U:H4'	15:BD:285:ARG:O	2.18	0.43
12:BA:1033:G:H2'	12:BA:1034:G:O4'	2.18	0.43
16:BE:69:ASN:OD1	16:BE:171:PRO:HB3	2.18	0.43
25:BR:65:LEU:HD23	25:BR:65:LEU:HA	1.76	0.43
33:Ba:351:LEU:HD13	33:Ba:381:LEU:HD12	1.99	0.43
35:Bc:266:ILE:HD12	35:Bc:271:ILE:HB	2.00	0.43
40:Bh:90:THR:HG23	40:Bh:120:LYS:O	2.18	0.43
53:Bw:103:ASP:N	53:Bw:103:ASP:OD1	2.51	0.43
12:BA:341:G:H2'	12:BA:342:C:C6	2.53	0.43
12:BA:717:A:H1'	33:Ba:266:GLN:HE21	1.83	0.43
12:BA:889:C:N4	12:BA:1082:U:H4'	2.26	0.43
13:BB:69:C:H3'	13:BB:70:A:H5''	2.00	0.43
14:BC:197:LEU:HD23	14:BC:197:LEU:HA	1.74	0.43
14:BC:538:TYR:HA	14:BC:723:TRP:CD1	2.54	0.43
16:BE:98:GLY:O	16:BE:99:LEU:HD23	2.19	0.43
16:BE:175:LYS:HD2	16:BE:296:LEU:HB3	2.00	0.43
21:BN:173:PRO:HG2	21:BN:176:TYR:HB2	1.99	0.43
26:BS:152:GLU:HB3	26:BS:158:ILE:HD12	2.00	0.43
41:Bi:126:ARG:HH12	41:Bi:134:ILE:HG12	1.83	0.43
48:Bp:12:ALA:O	48:Bp:68:PHE:HB2	2.17	0.43
48:Bp:62:PRO:HG2	48:Bp:78:GLY:O	2.18	0.43
56:AV:16:A:H4'	56:AV:17:U:OP1	2.18	0.43
6:B4:71:GLU:HA	6:B4:72:PRO:HD3	1.77	0.43
12:BA:572:A:O3'	21:BN:29:GLY:HA3	2.18	0.43
12:BA:935:C:H2'	12:BA:936:A:O4'	2.18	0.43
12:BA:1326:A:H61	41:Bi:40:ARG:NH2	2.16	0.43
16:BE:45:SER:O	35:Bc:303:ARG:NH2	2.52	0.43
16:BE:201:GLY:O	16:BE:202:GLN:HB2	2.17	0.43
18:BI:57:GLU:HG2	18:BI:58:ARG:N	2.32	0.43
24:BQ:166:ARG:HB3	24:BQ:166:ARG:HH11	1.84	0.43
33:Ba:355:LEU:HD13	33:Ba:376:VAL:HG22	2.00	0.43
39:Bg:35:ARG:HD3	45:Bm:157:TRP:HH2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:Bh:244:GLU:O	40:Bh:248:ARG:HG2	2.17	0.43
53:Bw:370:THR:HG22	53:Bw:372:ALA:H	1.83	0.43
4:B2:194:LYS:HG3	12:BA:42:C:OP1	2.18	0.43
12:BA:479:A:N1	30:BW:208:HIS:HA	2.33	0.43
12:BA:803:A:H5''	22:BO:35:MET:HE2	1.99	0.43
12:BA:1328:G:N2	12:BA:1329:U:O4	2.46	0.43
19:BJ:161:VAL:HG21	19:BJ:181:ILE:HD13	1.99	0.43
20:BK:141:VAL:HG12	49:Bq:99:MET:HE1	1.99	0.43
21:BN:99:ASP:HA	21:BN:100:PRO:HD3	1.90	0.43
28:BU:86:PHE:HE2	28:BU:102:LEU:HD13	1.83	0.43
35:Bc:100:SER:HB3	35:Bc:112:MET:HE3	2.00	0.43
38:Bf:68:PRO:HG2	38:Bf:71:HIS:CG	2.54	0.43
41:Bi:173:VAL:O	41:Bi:176:ILE:HG22	2.18	0.43
43:Bk:168:GLU:O	43:Bk:172:GLU:HG3	2.19	0.43
53:Bw:159:VAL:O	53:Bw:161:GLN:HG2	2.18	0.43
56:AV:15:A:H2'	56:AV:16:A:C2	2.54	0.43
4:B2:93:ARG:HH12	37:Be:82:THR:C	2.27	0.43
12:BA:276:G:O2'	12:BA:310:G:H4'	2.18	0.43
12:BA:1522:A:H5''	48:Bp:84:GLN:NE2	2.32	0.43
14:BC:449:TYR:O	14:BC:453:GLN:HG2	2.19	0.43
16:BE:55:GLU:H	16:BE:55:GLU:CD	2.27	0.43
16:BE:244:SER:OG	16:BE:245:THR:N	2.50	0.43
22:BO:32:ILE:HG23	22:BO:36:THR:OG1	2.19	0.43
23:BP:118:LEU:HD12	23:BP:118:LEU:HA	1.80	0.43
32:BY:178:SER:OG	32:BY:181:ASP:OD2	2.35	0.43
33:Ba:72:ARG:HA	33:Ba:73:PRO:HD3	1.85	0.43
33:Ba:144:ARG:HB3	33:Ba:194:LYS:NZ	2.33	0.43
34:Bb:71:TRP:C	34:Bb:72:ARG:NH1	2.76	0.43
34:Bb:266:HIS:CD2	34:Bb:266:HIS:N	2.85	0.43
40:Bh:231:MET:HE2	40:Bh:231:MET:HB3	1.63	0.43
42:Bj:157:LEU:HD23	42:Bj:254:TRP:HB3	1.99	0.43
54:Bx:190:ARG:H	54:Bx:190:ARG:HG2	1.55	0.43
5:B3:41:ILE:HA	5:B3:42:PRO:HD2	1.88	0.43
12:BA:329:A:C2	15:BD:275:LEU:HD13	2.54	0.43
12:BA:626:G:O4'	17:BF:154:GLY:HA2	2.18	0.43
12:BA:1425:A:H5''	12:BA:1425:A:N3	2.33	0.43
12:BA:1521:U:H3'	12:BA:1522:A:H5'	2.01	0.43
14:BC:305:LEU:HD11	14:BC:314:TYR:CD1	2.53	0.43
14:BC:341:LEU:O	14:BC:345:LEU:HG	2.19	0.43
16:BE:96:ARG:NH1	16:BE:301:ASP:OD2	2.51	0.43
20:BK:103:HIS:HB3	20:BK:106:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BS:65:GLU:OE2	34:Bb:74:TYR:OH	2.31	0.43
32:BY:65:LEU:HD11	32:BY:121:LYS:HG3	1.99	0.43
33:Ba:283:TYR:CD1	33:Ba:284:PRO:HD2	2.53	0.43
34:Bb:351:HIS:HA	34:Bb:352:PRO:HD3	1.93	0.43
36:Bd:132:GLU:O	36:Bd:136:ILE:HG22	2.18	0.43
36:Bd:173:ARG:NH2	42:Bj:56:PRO:HB3	2.34	0.43
53:Bw:347:ARG:H	53:Bw:347:ARG:HG3	1.64	0.43
1:EL:75:THR:HA	1:HL:75:THR:HA	2.01	0.43
4:B2:157:LEU:HD23	4:B2:157:LEU:HA	1.85	0.43
12:BA:901:C:H5'	12:BA:902:C:OP1	2.18	0.43
12:BA:1316:U:H2'	12:BA:1317:A:O4'	2.19	0.43
16:BE:146:THR:HG23	16:BE:178:ILE:HG12	2.01	0.43
18:BI:84:GLU:HG3	18:BI:85:ASP:N	2.34	0.43
19:BJ:36:HIS:O	19:BJ:37:ARG:HB3	2.18	0.43
1:BL:131:THR:HG22	1:BL:133:ARG:HG3	1.98	0.43
26:BS:106:SER:O	26:BS:112:ILE:HD12	2.19	0.43
31:BX:75:GLY:O	31:BX:88:LYS:NZ	2.51	0.43
32:BY:127:ASP:OD1	32:BY:127:ASP:N	2.49	0.43
33:Ba:147:ILE:HG22	33:Ba:148:GLU:H	1.84	0.43
36:Bd:151:ARG:HG2	36:Bd:158:HIS:CB	2.48	0.43
51:Bu:152:LYS:O	51:Bu:156:MET:HG3	2.18	0.43
3:B1:42:HIS:O	18:BI:55:ILE:HA	2.19	0.43
3:B1:190:ARG:H	3:B1:190:ARG:HG2	1.45	0.43
4:B2:100:LEU:HD23	4:B2:100:LEU:HA	1.82	0.43
7:B5:131:ARG:HA	7:B5:131:ARG:HD2	1.81	0.43
7:B5:140:GLN:HA	7:B5:143:LYS:HE3	2.00	0.43
12:BA:1295:G:H2'	12:BA:1298:C:H42	1.83	0.43
14:BC:555:ASP:HA	14:BC:576:VAL:HB	2.01	0.43
17:BF:249:ASN:HA	46:Bn:59:ASN:ND2	2.34	0.43
1:BL:153:ILE:HD11	1:BL:172:ILE:HG23	2.00	0.43
23:BP:156:VAL:O	23:BP:176:THR:HA	2.17	0.43
1:CL:15:ALA:HB2	19:BJ:185:ILE:HG22	1.99	0.43
4:B2:190:TRP:HB3	32:BY:216:TYR:CD1	2.54	0.43
9:B7:56:TYR:CE2	9:B7:58:PRO:HG3	2.53	0.43
12:BA:925:G:N2	12:BA:964:A:OP2	2.47	0.43
12:BA:1205:G:H5'	12:BA:1206:U:OP2	2.18	0.43
12:BA:1207:C:H5'	12:BA:1208:A:OP2	2.19	0.43
14:BC:183:VAL:HA	14:BC:254:ILE:O	2.18	0.43
14:BC:401:ASP:OD1	14:BC:402:GLU:N	2.49	0.43
1:BL:148:GLU:HG3	1:BL:152:HIS:CD2	2.54	0.43
22:BO:41:VAL:HG13	22:BO:121:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:BP:276:ASN:ND2	23:BP:279:ASP:OD2	2.52	0.43
29:BV:60:LEU:HD23	29:BV:60:LEU:HA	1.78	0.43
32:BY:105:ARG:H	32:BY:105:ARG:HD3	1.84	0.43
33:Ba:329:TYR:OH	33:Ba:338:GLN:HB3	2.18	0.43
39:Bg:29:LEU:HD21	39:Bg:101:VAL:HG13	2.01	0.43
42:Bj:51:LEU:HD12	42:Bj:188:ALA:HB1	2.00	0.43
42:Bj:264:LEU:HD12	42:Bj:264:LEU:HA	1.88	0.43
46:Bn:81:ARG:HG2	46:Bn:81:ARG:NH1	2.32	0.43
52:Bv:41:ASP:HB2	52:Bv:44:ASP:HB2	2.01	0.43
56:AV:35:C:H2'	56:AV:36:C:O4'	2.19	0.43
3:B1:96:LYS:HG2	12:BA:60:U:O2'	2.19	0.43
11:B9:87:ILE:HB	11:B9:97:GLN:HB2	2.01	0.43
12:BA:287:U:H2'	12:BA:288:C:C6	2.54	0.43
12:BA:1326:A:H4'	12:BA:1327:U:OP1	2.19	0.43
12:BA:1418:G:N2	12:BA:1421:A:OP2	2.45	0.43
12:BA:1508:A:H2	12:BA:1538:A:N7	2.17	0.43
21:BN:20:LEU:HB2	21:BN:141:LEU:HD13	2.01	0.43
21:BN:140:ASN:HD22	40:Bh:262:GLY:HA2	1.83	0.43
23:BP:114:GLN:HB3	23:BP:115:PRO:HD2	2.01	0.43
25:BR:38:ARG:HB2	25:BR:38:ARG:NH1	2.28	0.43
28:BU:17:ARG:HA	28:BU:20:ARG:HG3	2.01	0.43
34:Bb:73:THR:HG23	34:Bb:76:GLU:H	1.84	0.43
34:Bb:93:PRO:HA	34:Bb:94:PRO:HD2	1.85	0.43
34:Bb:153:GLU:HG2	34:Bb:158:TYR:HD2	1.83	0.43
35:Bc:206:LEU:HD21	35:Bc:254:PHE:CZ	2.54	0.43
42:Bj:264:LEU:HG	42:Bj:269:LEU:HB3	2.01	0.43
46:Bn:32:PHE:C	46:Bn:32:PHE:HD1	2.27	0.43
12:BA:104:C:C4	17:BF:108:ARG:HD2	2.53	0.42
12:BA:600:C:H5''	23:BP:50:GLY:HA2	2.01	0.42
12:BA:901:C:H3'	12:BA:925:G:C8	2.54	0.42
12:BA:990:U:H3'	12:BA:991:C:H2'	2.00	0.42
12:BA:993:U:H2'	12:BA:994:A:C8	2.53	0.42
17:BF:290:TYR:HB2	17:BF:293:PHE:HB3	2.01	0.42
19:BJ:164:MET:HE2	19:BJ:164:MET:HB3	1.92	0.42
20:BK:80:ILE:HG13	20:BK:82:ILE:HD12	2.01	0.42
21:BN:20:LEU:HD22	21:BN:141:LEU:HD13	2.01	0.42
24:BQ:47:LYS:HE3	24:BQ:47:LYS:HB2	1.68	0.42
27:BT:250:THR:HG22	27:BT:252:GLU:H	1.83	0.42
29:BV:60:LEU:HB2	54:Bx:80:LYS:O	2.18	0.42
34:Bb:252:CYS:HA	34:Bb:253:PRO:HD3	1.90	0.42
40:Bh:178:LEU:HD12	40:Bh:178:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Bi:89:VAL:HA	41:Bi:90:PRO:HD3	1.52	0.42
46:Bn:32:PHE:C	46:Bn:32:PHE:CD1	2.97	0.42
47:Bo:76:ARG:HH11	47:Bo:76:ARG:HG3	1.84	0.42
1:CL:25:PRO:HD2	1:CL:28:ILE:HD12	2.00	0.42
12:BA:337:A:N3	12:BA:337:A:H2'	2.34	0.42
12:BA:435:C:H2'	12:BA:436:U:C6	2.55	0.42
12:BA:1201:A:H61	23:BP:71:GLN:HE22	1.66	0.42
17:BF:59:ARG:HG2	17:BF:59:ARG:HH11	1.84	0.42
17:BF:167:MET:HB3	17:BF:167:MET:HE2	1.70	0.42
19:BJ:37:ARG:HG3	19:BJ:37:ARG:O	2.19	0.42
23:BP:55:GLY:O	23:BP:59:ARG:HG3	2.19	0.42
30:BW:151:LEU:HD12	30:BW:151:LEU:HA	1.86	0.42
32:BY:166:VAL:HA	32:BY:167:PRO:HD3	1.87	0.42
40:Bh:166:VAL:HG13	40:Bh:195:PHE:CD2	2.54	0.42
51:Bu:173:GLU:HA	51:Bu:176:ARG:HH21	1.84	0.42
8:B6:20:MET:HG2	8:B6:58:GLU:HA	2.01	0.42
14:BC:564:ALA:O	14:BC:569:GLY:N	2.42	0.42
16:BE:341:GLY:CA	27:BT:105:ILE:HD11	2.46	0.42
22:BO:94:PRO:C	22:BO:95:ARG:NH1	2.77	0.42
25:BR:92:VAL:C	25:BR:95:PRO:HD2	2.44	0.42
30:BW:70:GLU:HG2	30:BW:177:VAL:HG22	2.00	0.42
35:Bc:140:TRP:CE3	35:Bc:140:TRP:HA	2.54	0.42
40:Bh:92:PHE:HE1	40:Bh:175:VAL:HG13	1.84	0.42
53:Bw:274:ASN:OD1	53:Bw:274:ASN:N	2.45	0.42
12:BA:573:A:N6	54:Bx:196:HIS:HB3	2.34	0.42
12:BA:805:C:C5	12:BA:806:U:C4	3.07	0.42
16:BE:227:GLN:CD	16:BE:227:GLN:N	2.78	0.42
24:BQ:240:ARG:HG2	24:BQ:240:ARG:HH11	1.84	0.42
30:BW:133:GLU:HG2	41:Bi:278:LYS:HB2	2.00	0.42
35:Bc:63:GLU:O	35:Bc:119:SER:OG	2.36	0.42
37:Be:22:THR:HG21	37:Be:34:ARG:NH2	2.34	0.42
37:Be:95:ALA:HB3	37:Be:96:PRO:HD3	2.01	0.42
38:Bf:49:LEU:HD23	38:Bf:49:LEU:HA	1.80	0.42
38:Bf:122:ARG:NH1	38:Bf:122:ARG:CG	2.75	0.42
40:Bh:119:LEU:HD23	40:Bh:119:LEU:HA	1.83	0.42
42:Bj:46:ARG:HB3	42:Bj:229:ALA:CB	2.50	0.42
53:Bw:412:LEU:HD23	53:Bw:412:LEU:HA	1.81	0.42
3:B1:119:LEU:HA	3:B1:168:ARG:NH1	2.35	0.42
3:B1:146:LEU:HD21	3:B1:165:MET:HG3	2.01	0.42
6:B4:37:ASN:HA	6:B4:40:LEU:HD12	2.01	0.42
8:B6:55:LEU:H	52:Bv:128:MET:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BA:100:C:N4	46:Bn:75:LYS:NZ	2.68	0.42
12:BA:125:A:P	37:Be:17:ARG:HH22	2.42	0.42
12:BA:1466:G:H5'	12:BA:1467:G:OP2	2.18	0.42
15:BD:128:ILE:HD13	33:Ba:114:LEU:HD11	2.02	0.42
17:BF:48:LEU:HD22	45:Bm:95:VAL:HG12	2.02	0.42
22:BO:77:ILE:HD11	22:BO:107:LEU:HD21	2.00	0.42
32:BY:35:ASN:HA	32:BY:36:PRO:HD2	1.77	0.42
35:Bc:112:MET:HB2	35:Bc:267:PRO:HB3	2.00	0.42
36:Bd:168:LEU:HD23	36:Bd:168:LEU:HA	1.88	0.42
44:Bl:60:PRO:HA	44:Bl:61:PRO:HD3	1.86	0.42
44:Bl:110:ILE:HD11	44:Bl:157:LEU:HD13	2.01	0.42
44:Bl:140:VAL:H	50:Bt:85:HIS:CD2	2.37	0.42
46:Bn:38:LEU:HD23	46:Bn:38:LEU:HA	1.86	0.42
2:B0:148:LEU:C	34:Bb:338:ARG:HB3	2.45	0.42
12:BA:178:C:H1'	28:BU:55:ARG:NH2	2.34	0.42
12:BA:525:A:H2'	12:BA:526:A:H5''	2.01	0.42
12:BA:835:A:H5''	12:BA:1431:G:H4'	2.00	0.42
13:BB:9:A:O2'	13:BB:10:G:N7	2.53	0.42
14:BC:221:LEU:HD12	14:BC:221:LEU:HA	1.90	0.42
14:BC:519:ILE:HG12	14:BC:549:VAL:HG23	2.01	0.42
16:BE:271:LEU:HB3	16:BE:285:VAL:HG12	2.01	0.42
18:BI:86:THR:HG23	18:BI:89:ARG:NH1	2.33	0.42
27:BT:96:ARG:HA	27:BT:99:MET:HG2	2.02	0.42
30:BW:200:GLU:OE1	38:Bf:122:ARG:NH2	2.53	0.42
37:Be:73:ASN:OD1	37:Be:74:TYR:N	2.52	0.42
40:Bh:56:PRO:HA	40:Bh:57:PRO:HD3	1.89	0.42
42:Bj:191:THR:O	42:Bj:195:LEU:HB2	2.19	0.42
46:Bn:69:HIS:CD2	46:Bn:71:LYS:H	2.32	0.42
53:Bw:399:ILE:H	53:Bw:399:ILE:HG13	1.53	0.42
2:B0:134:VAL:HA	2:B0:135:PRO:HD3	1.83	0.42
12:BA:379:U:P	23:BP:62:ARG:HH11	2.43	0.42
12:BA:746:U:O4	37:Be:44:ARG:HG3	2.20	0.42
12:BA:1242:U:H2'	12:BA:1243:U:O4'	2.20	0.42
16:BE:199:ARG:HA	16:BE:199:ARG:HD3	1.68	0.42
23:BP:247:ILE:H	23:BP:247:ILE:CD1	2.31	0.42
26:BS:55:ASN:ND2	34:Bb:264:GLY:O	2.53	0.42
34:Bb:355:LYS:HB2	34:Bb:355:LYS:HE3	1.76	0.42
35:Bc:158:GLU:HB3	35:Bc:185:ARG:NH2	2.34	0.42
42:Bj:161:VAL:HA	42:Bj:251:HIS:O	2.19	0.42
42:Bj:214:LYS:HZ2	42:Bj:230:LYS:HB3	1.85	0.42
44:Bl:57:ILE:HD13	44:Bl:91:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Bn:35:ARG:HH12	46:Bn:39:PRO:HA	1.83	0.42
53:Bw:326:LEU:HD23	53:Bw:326:LEU:HA	1.85	0.42
12:BA:14:C:O2'	17:BF:111:TYR:HB3	2.20	0.42
12:BA:379:U:OP1	23:BP:62:ARG:HD3	2.19	0.42
12:BA:995:C:H2'	12:BA:996:U:H6	1.85	0.42
16:BE:264:ILE:HG12	16:BE:265:ASP:N	2.35	0.42
25:BR:107:MET:O	25:BR:108:LEU:HD23	2.20	0.42
26:BS:116:LEU:HD12	26:BS:116:LEU:HA	1.89	0.42
29:BV:199:ILE:O	29:BV:199:ILE:HG13	2.16	0.42
31:BX:136:SER:HA	31:BX:137:PRO:HD3	1.89	0.42
32:BY:101:THR:HG22	32:BY:104:TYR:HB3	2.02	0.42
34:Bb:45:LEU:HD12	43:Bk:64:LYS:HG3	2.02	0.42
34:Bb:203:GLU:CD	51:Bu:194:SER:HB3	2.44	0.42
34:Bb:373:HIS:O	34:Bb:374:GLU:HG2	2.19	0.42
47:Bo:101:GLU:O	47:Bo:105:LYS:HG2	2.20	0.42
53:Bw:231:PRO:HG2	53:Bw:234:GLN:HE21	1.83	0.42
3:B1:163:ARG:NH1	33:Ba:55:LEU:HD11	2.35	0.42
6:B4:40:LEU:HD23	43:Bk:102:LEU:HD11	2.02	0.42
10:B8:106:THR:OG1	10:B8:162:THR:HA	2.20	0.42
12:BA:551:A:H2'	12:BA:552:A:O4'	2.20	0.42
15:BD:154:ALA:O	15:BD:249:SER:OG	2.26	0.42
18:BI:60:TRP:CE3	18:BI:76:ARG:HD2	2.55	0.42
20:BK:22:ALA:O	20:BK:68:THR:HG22	2.20	0.42
20:BK:145:ILE:HD12	49:Bq:99:MET:HE2	2.02	0.42
25:BR:79:TRP:NE1	27:BT:267:PHE:O	2.41	0.42
28:BU:65:ARG:HA	28:BU:68:TRP:CE3	2.55	0.42
32:BY:77:VAL:HG21	32:BY:89:GLU:HB3	2.01	0.42
34:Bb:99:ARG:H	34:Bb:99:ARG:CD	2.32	0.42
34:Bb:116:ASN:HB3	34:Bb:118:GLU:HG3	2.01	0.42
40:Bh:105:ARG:HH11	40:Bh:116:LEU:HD23	1.85	0.42
42:Bj:197:GLU:O	42:Bj:244:SER:HB3	2.19	0.42
4:B2:66:LEU:HD21	31:BX:40:VAL:HG21	2.01	0.42
7:B5:84:ARG:HG2	7:B5:84:ARG:HH11	1.85	0.42
8:B6:20:MET:HE2	8:B6:20:MET:HB3	1.75	0.42
12:BA:160:A:O2'	12:BA:161:A:H2'	2.19	0.42
14:BC:579:GLY:O	14:BC:583:GLN:HG3	2.19	0.42
27:BT:74:ARG:HB3	27:BT:283:TRP:CZ2	2.54	0.42
34:Bb:258:PHE:N	34:Bb:258:PHE:CD1	2.88	0.42
41:Bi:215:ARG:HE	41:Bi:243:LEU:HD11	1.85	0.42
45:Bm:76:LYS:HG2	45:Bm:83:VAL:HG23	2.02	0.42
54:Bx:69:GLN:HB3	54:Bx:70:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B2:135:GLU:OE2	32:BY:11:SER:N	2.53	0.41
6:B4:50:ALA:HA	42:Bj:83:LEU:O	2.20	0.41
7:B5:81:PRO:HA	12:BA:1438:U:N1	2.34	0.41
12:BA:984:A:H2'	12:BA:985:C:O4'	2.21	0.41
15:BD:66:TRP:CZ3	15:BD:79:MET:HB3	2.54	0.41
22:BO:38:VAL:HG21	22:BO:75:LEU:HD11	2.02	0.41
23:BP:12:ALA:HB2	50:Bt:88:LEU:HD21	2.02	0.41
28:BU:149:ARG:HD2	38:Bf:56:ARG:HH21	1.84	0.41
33:Ba:351:LEU:HD13	33:Ba:381:LEU:CD1	2.50	0.41
39:Bg:28:ARG:HG2	39:Bg:78:GLU:HB3	2.02	0.41
42:Bj:120:LEU:HB3	42:Bj:124:TRP:CH2	2.55	0.41
43:Bk:150:LEU:HD13	43:Bk:150:LEU:HA	1.92	0.41
4:B2:184:LYS:HB3	4:B2:186:TRP:NE1	2.35	0.41
6:B4:79:PRO:HB3	55:Bz:700:ALA:N	2.35	0.41
9:B7:74:ARG:HH22	12:BA:31:A:HO2'	1.61	0.41
12:BA:949:A:N3	12:BA:1374:U:H5'	2.36	0.41
14:BC:282:PRO:HG2	14:BC:345:LEU:HD11	2.02	0.41
16:BE:209:LYS:HA	16:BE:264:ILE:O	2.20	0.41
16:BE:285:VAL:HG12	16:BE:286:ASN:H	1.85	0.41
21:BN:128:PHE:HA	21:BN:129:PRO:HD3	1.82	0.41
27:BT:152:ARG:HH12	27:BT:191:ARG:CA	2.32	0.41
30:BW:58:PRO:HA	30:BW:59:PRO:HD3	1.95	0.41
33:Ba:313:MET:HE2	33:Ba:313:MET:HB3	1.81	0.41
33:Ba:393:LYS:HE3	33:Ba:394:LYS:HE3	2.02	0.41
35:Bc:285:THR:HG22	35:Bc:286:GLN:H	1.85	0.41
41:Bi:69:HIS:O	41:Bi:72:LEU:HG	2.20	0.41
12:BA:71:U:OP2	46:Bn:96:ARG:NH2	2.53	0.41
12:BA:193:U:H2'	12:BA:194:G:C8	2.55	0.41
12:BA:494:U:H2'	12:BA:560:A:H2	1.85	0.41
12:BA:1028:A:H1'	12:BA:1030:G:OP2	2.21	0.41
19:BJ:65:LEU:HD23	19:BJ:65:LEU:HA	1.94	0.41
21:BN:74:GLN:HB2	54:Bx:174:MET:CE	2.48	0.41
26:BS:90:ILE:HD11	26:BS:120:ARG:HH11	1.86	0.41
29:BV:140:VAL:HG23	29:BV:153:LEU:HD23	2.01	0.41
29:BV:178:PHE:HD1	29:BV:185:GLN:HG2	1.85	0.41
32:BY:105:ARG:O	32:BY:105:ARG:NH1	2.52	0.41
35:Bc:186:LEU:HD12	35:Bc:186:LEU:HA	1.89	0.41
42:Bj:208:ALA:HA	42:Bj:209:PRO:HD3	1.78	0.41
50:Bt:55:THR:HG22	50:Bt:56:ALA:H	1.85	0.41
52:Bv:30:PRO:HA	52:Bv:31:PRO:HD3	1.92	0.41
54:Bx:173:ARG:HB3	54:Bx:195:TYR:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B1:2:PRO:HG2	46:Bn:103:PHE:CE2	2.55	0.41
12:BA:164:A:O2'	12:BA:1016:C:H5	2.02	0.41
12:BA:230:G:H2'	12:BA:231:C:C6	2.56	0.41
14:BC:273:ILE:HD13	14:BC:273:ILE:HA	1.83	0.41
19:BJ:186:LEU:HD22	19:BJ:190:GLY:HA3	2.03	0.41
21:BN:74:GLN:HA	54:Bx:161:PRO:HA	2.03	0.41
22:BO:75:LEU:HD22	22:BO:84:ALA:HB2	2.01	0.41
26:BS:72:TRP:CD1	26:BS:73:PRO:HA	2.55	0.41
32:BY:73:GLN:H	41:Bi:256:TYR:HH	1.61	0.41
33:Ba:124:THR:HG23	33:Ba:318:PHE:CD1	2.56	0.41
33:Ba:194:LYS:HB3	33:Ba:195:HIS:HD2	1.85	0.41
36:Bd:147:LEU:CD2	42:Bj:209:PRO:HD2	2.48	0.41
40:Bh:194:THR:O	40:Bh:198:VAL:HG23	2.20	0.41
46:Bn:80:LEU:HD23	46:Bn:80:LEU:HA	1.66	0.41
50:Bt:42:GLU:HA	50:Bt:45:ASN:HB2	2.02	0.41
51:Bu:45:LEU:HD12	51:Bu:45:LEU:HA	1.88	0.41
52:Bv:65:GLY:H	52:Bv:68:SER:HB2	1.86	0.41
3:B1:42:HIS:HD2	18:BI:54:VAL:O	2.04	0.41
8:B6:63:ARG:NH2	12:BA:1246:A:OP1	2.53	0.41
12:BA:160:A:N6	38:Bf:119:THR:HG21	2.34	0.41
12:BA:421:U:H2'	12:BA:422:U:C6	2.56	0.41
14:BC:667:VAL:HG11	14:BC:670:LYS:HE2	2.01	0.41
19:BJ:42:PHE:CE2	19:BJ:46:LYS:HD2	2.55	0.41
33:Ba:67:MET:HB3	33:Ba:67:MET:HE2	1.77	0.41
33:Ba:174:GLU:HG3	33:Ba:298:ASN:OD1	2.20	0.41
53:Bw:330:THR:HG22	53:Bw:349:PHE:HB3	2.03	0.41
54:Bx:170:ASN:O	54:Bx:170:ASN:CG	2.63	0.41
4:B2:113:MET:HE2	4:B2:114:LEU:HG	2.03	0.41
12:BA:271:U:H5'	12:BA:272:A:OP2	2.21	0.41
12:BA:1136:U:H2'	12:BA:1137:A:O4'	2.20	0.41
16:BE:95:SER:HB2	16:BE:303:LYS:NZ	2.35	0.41
16:BE:208:ALA:HB2	16:BE:297:VAL:HG22	2.02	0.41
21:BN:3:SER:O	40:Bh:299:VAL:HG22	2.19	0.41
22:BO:57:CYS:HA	22:BO:75:LEU:HD12	2.02	0.41
23:BP:151:LYS:NZ	23:BP:250:ASP:OD2	2.52	0.41
26:BS:125:CYS:SG	26:BS:157:SER:HB2	2.60	0.41
26:BS:141:ILE:O	26:BS:141:ILE:HG12	2.21	0.41
34:Bb:92:LEU:HD23	34:Bb:92:LEU:HA	1.82	0.41
35:Bc:159:TYR:CE1	35:Bc:186:LEU:HD13	2.56	0.41
39:Bg:45:GLU:HB2	39:Bg:94:VAL:HG22	2.01	0.41
40:Bh:35:PHE:CE2	40:Bh:39:TYR:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Bi:122:ILE:CG2	41:Bi:126:ARG:HH11	2.33	0.41
45:Bm:58:SER:C	45:Bm:60:THR:H	2.29	0.41
45:Bm:78:VAL:HG21	45:Bm:101:PHE:HA	2.02	0.41
51:Bu:101:ARG:HG2	51:Bu:133:ILE:HG12	2.02	0.41
7:B5:132:LYS:HE3	41:Bi:290:TRP:CZ3	2.56	0.41
7:B5:181:ARG:HA	7:B5:182:PRO:HD3	1.84	0.41
12:BA:242:G:H2'	12:BA:351:A:H61	1.85	0.41
12:BA:554:U:H2'	12:BA:555:C:O4'	2.21	0.41
16:BE:175:LYS:HB3	16:BE:296:LEU:HD23	2.03	0.41
17:BF:92:ARG:HG2	17:BF:92:ARG:NH1	2.36	0.41
17:BF:291:CYS:SG	17:BF:292:ASP:N	2.93	0.41
21:BN:13:THR:OG1	39:Bg:129:GLN:NE2	2.50	0.41
22:BO:70:GLY:HA2	22:BO:85:LEU:HD11	2.03	0.41
23:BP:233:ARG:HD3	23:BP:244:LEU:HD21	2.02	0.41
24:BQ:218:ILE:HG23	24:BQ:223:MET:HB2	2.02	0.41
25:BR:26:ILE:HD13	25:BR:26:ILE:HA	1.87	0.41
26:BS:48:PHE:CZ	34:Bb:223:GLY:HA2	2.56	0.41
27:BT:168:ASN:HA	27:BT:169:PRO:HD2	1.87	0.41
29:BV:138:LEU:HD23	29:BV:152:LEU:HD23	2.02	0.41
34:Bb:27:ARG:HD2	34:Bb:27:ARG:HA	1.84	0.41
39:Bg:44:ARG:NH1	50:Bt:100:LYS:HA	2.36	0.41
40:Bh:88:LEU:HD23	40:Bh:88:LEU:HA	1.90	0.41
41:Bi:109:ALA:HB1	41:Bi:113:LYS:HE3	2.03	0.41
43:Bk:122:GLU:CG	43:Bk:160:SER:HB2	2.49	0.41
10:B8:179:LYS:HG2	34:Bb:370:ARG:NH2	2.35	0.41
12:BA:792:G:P	16:BE:238:ARG:HB2	2.60	0.41
12:BA:1240:A:C8	12:BA:1241:U:C5	3.09	0.41
12:BA:1465:A:C5	12:BA:1466:G:H1'	2.55	0.41
12:BA:1483:C:H5'	16:BE:290:PRO:HA	2.03	0.41
16:BE:79:PRO:HD2	16:BE:322:ASP:OD2	2.21	0.41
17:BF:79:LEU:HD22	17:BF:79:LEU:HA	1.78	0.41
17:BF:84:PRO:O	17:BF:88:SER:HB3	2.21	0.41
21:BN:117:HIS:O	21:BN:121:MET:HG2	2.21	0.41
22:BO:45:ALA:O	22:BO:49:THR:HG22	2.21	0.41
35:Bc:240:LYS:HD2	35:Bc:240:LYS:HA	1.85	0.41
35:Bc:281:HIS:CD2	35:Bc:319:MET:HG2	2.55	0.41
39:Bg:85:ARG:NH1	39:Bg:104:LEU:HD21	2.36	0.41
42:Bj:187:THR:HG23	42:Bj:190:ARG:NH2	2.28	0.41
48:Bp:80:HIS:HB3	54:Bx:36:ARG:HD2	2.02	0.41
53:Bw:105:TRP:CE2	53:Bw:258:MET:HE2	2.55	0.41
7:B5:129:LYS:HG2	41:Bi:289:PRO:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B7:57:GLN:HA	9:B7:58:PRO:HD3	1.90	0.41
12:BA:503:A:C8	12:BA:526:A:C5	3.09	0.41
12:BA:877:U:H5''	12:BA:878:G:H5'	2.02	0.41
12:BA:1129:C:H5'	12:BA:1130:A:OP2	2.21	0.41
12:BA:1192:U:H2'	12:BA:1193:C:O4'	2.21	0.41
15:BD:68:SER:HB3	33:Ba:38:THR:OG1	2.21	0.41
15:BD:195:ASN:OD1	15:BD:244:THR:HB	2.20	0.41
16:BE:99:LEU:HD23	16:BE:99:LEU:HA	1.75	0.41
16:BE:157:LYS:HA	16:BE:157:LYS:HD3	1.67	0.41
16:BE:296:LEU:HD12	16:BE:296:LEU:HA	1.74	0.41
17:BF:85:ASP:OD1	44:Bl:87:ARG:NH2	2.54	0.41
19:BJ:123:MET:HB2	19:BJ:152:LEU:HD11	2.03	0.41
19:BJ:128:ASN:ND2	19:BJ:147:PHE:O	2.48	0.41
20:BK:30:ARG:HA	20:BK:31:PRO:HD3	1.80	0.41
23:BP:255:MET:HE3	23:BP:255:MET:HB3	1.89	0.41
23:BP:260:LYS:HG3	23:BP:267:PHE:CE1	2.56	0.41
24:BQ:92:LEU:HD23	24:BQ:92:LEU:HA	1.83	0.41
24:BQ:117:ASN:HB3	24:BQ:166:ARG:HG3	2.01	0.41
27:BT:201:ASP:HB3	27:BT:204:MET:HB3	2.03	0.41
28:BU:50:PHE:O	28:BU:53:CYS:HB3	2.21	0.41
29:BV:63:PRO:HA	29:BV:64:PRO:HD3	1.76	0.41
30:BW:144:THR:HG23	30:BW:173:PHE:HD2	1.85	0.41
33:Ba:125:LYS:HE3	33:Ba:364:LEU:HA	2.02	0.41
33:Ba:142:ASP:OD2	33:Ba:144:ARG:HB2	2.21	0.41
35:Bc:112:MET:HE1	35:Bc:124:PHE:CD1	2.55	0.41
36:Bd:100:GLN:CG	42:Bj:84:TYR:HA	2.50	0.41
37:Be:67:LYS:H	37:Be:67:LYS:HG3	1.76	0.41
40:Bh:87:LEU:HA	40:Bh:87:LEU:HD23	1.84	0.41
42:Bj:266:PRO:O	42:Bj:270:ALA:HB2	2.21	0.41
43:Bk:96:ILE:HG23	43:Bk:154:GLU:HG2	2.03	0.41
45:Bm:113:VAL:HG22	45:Bm:130:PHE:CE2	2.56	0.41
49:Bq:122:ARG:O	49:Bq:126:ILE:HG12	2.20	0.41
50:Bt:49:LEU:HD12	50:Bt:49:LEU:HA	1.92	0.41
51:Bu:39:PHE:O	51:Bu:40:GLN:HG2	2.21	0.41
53:Bw:105:TRP:CD1	53:Bw:265:LEU:HD13	2.56	0.41
53:Bw:206:ARG:O	53:Bw:223:LEU:HB2	2.20	0.41
53:Bw:296:LEU:HD22	53:Bw:297:PRO:HD2	2.03	0.41
4:B2:66:LEU:HD12	4:B2:66:LEU:HA	1.77	0.41
7:B5:85:ARG:NH1	12:BA:642:G:OP1	2.54	0.41
8:B6:18:VAL:O	8:B6:31:ASN:HA	2.20	0.41
11:B9:84:ARG:NH1	11:B9:99:GLN:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B9:99:GLN:NE2	12:BA:560:A:H2'	2.35	0.41
12:BA:360:U:H2'	12:BA:361:C:C6	2.56	0.41
15:BD:108:ASP:OD1	15:BD:113:ARG:NH1	2.54	0.41
18:BI:138:LYS:HA	18:BI:141:GLU:CD	2.46	0.41
21:BN:11:TRP:NE1	40:Bh:269:VAL:HG22	2.34	0.41
29:BV:90:LEU:HA	29:BV:90:LEU:HD23	1.84	0.41
33:Ba:63:LYS:HB3	33:Ba:63:LYS:HE2	1.87	0.41
34:Bb:240:ILE:HG23	34:Bb:244:ARG:O	2.21	0.41
37:Be:114:LYS:HE3	37:Be:115:TYR:CE2	2.56	0.41
37:Be:118:GLU:HA	37:Be:119:PRO:HD3	1.90	0.41
41:Bi:277:LEU:HD23	41:Bi:277:LEU:HA	1.92	0.41
53:Bw:105:TRP:O	53:Bw:108:SER:HB3	2.21	0.41
53:Bw:209:GLU:N	53:Bw:221:ASP:O	2.54	0.41
56:AV:46:U:H2'	56:AV:47:U:H5'	2.03	0.41
3:B1:197:PRO:HG2	3:B1:200:GLU:HG3	2.03	0.40
7:B5:141:MET:HE3	7:B5:173:ARG:HH22	1.86	0.40
12:BA:36:A:C4	37:Be:32:LYS:HG3	2.56	0.40
12:BA:146:A:H2'	12:BA:146:A:N3	2.36	0.40
12:BA:763:C:O3'	60:BA:3205:SPM:H131	2.21	0.40
12:BA:1548:A:C2	16:BE:176:VAL:HG21	2.56	0.40
13:BB:44:U:H2'	13:BB:45:A:H8	1.86	0.40
15:BD:127:VAL:HG21	15:BD:158:MET:HE3	2.03	0.40
16:BE:102:LEU:HD23	16:BE:296:LEU:HD13	2.03	0.40
17:BF:211:ARG:HB2	45:Bm:59:ARG:HH22	1.87	0.40
17:BF:249:ASN:HA	46:Bn:59:ASN:HD22	1.87	0.40
17:BF:283:LEU:HD12	17:BF:283:LEU:HA	1.82	0.40
19:BJ:119:HIS:CD2	19:BJ:163:GLU:HG2	2.56	0.40
22:BO:99:ARG:NH1	27:BT:191:ARG:HH21	2.19	0.40
27:BT:83:PRO:HD2	27:BT:92:PHE:CZ	2.56	0.40
41:Bi:148:ALA:O	41:Bi:151:CYS:HB2	2.21	0.40
42:Bj:98:LEU:HD23	42:Bj:101:LYS:HD2	2.02	0.40
42:Bj:162:ARG:HD3	42:Bj:171:TRP:HE3	1.86	0.40
47:Bo:73:PHE:O	47:Bo:77:VAL:HG23	2.21	0.40
53:Bw:92:VAL:HG23	53:Bw:92:VAL:O	2.21	0.40
53:Bw:306:LEU:HD23	53:Bw:306:LEU:HA	1.78	0.40
54:Bx:63:PRO:HA	54:Bx:64:PRO:HD3	1.75	0.40
54:Bx:176:VAL:HG21	54:Bx:196:HIS:NE2	2.36	0.40
1:GL:76:LEU:HD22	19:BJ:237:VAL:HA	2.03	0.40
3:B1:136:ASP:OD1	18:BI:131:TYR:HE2	2.03	0.40
5:B3:81:TRP:O	5:B3:85:ILE:HG12	2.21	0.40
12:BA:1465:A:C4	12:BA:1466:G:H1'	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:BF:120:VAL:HG12	17:BF:121:ARG:H	1.86	0.40
26:BS:61:VAL:HG13	34:Bb:346:ARG:HH22	1.86	0.40
32:BY:69:ASP:HB3	32:BY:72:LYS:HD2	2.03	0.40
33:Ba:153:ARG:NH2	53:Bw:191:ALA:HA	2.36	0.40
33:Ba:173:ARG:HA	33:Ba:176:TYR:CE2	2.56	0.40
33:Ba:236:LEU:HD12	33:Ba:236:LEU:HA	1.94	0.40
34:Bb:210:GLU:HA	34:Bb:212:SER:H	1.86	0.40
40:Bh:89:LYS:O	40:Bh:93:VAL:HG23	2.21	0.40
40:Bh:274:LEU:HG	40:Bh:296:ALA:HB1	2.03	0.40
46:Bn:35:ARG:NH1	46:Bn:39:PRO:CB	2.84	0.40
53:Bw:195:ASP:O	53:Bw:233:ASN:HA	2.21	0.40
1:CL:43:ILE:CD1	1:FL:76:LEU:HD12	2.52	0.40
3:B1:226:LEU:HD12	4:B2:157:LEU:HB3	2.03	0.40
6:B4:51:ARG:HA	42:Bj:82:SER:HB2	2.03	0.40
12:BA:746:U:O2'	12:BA:747:U:OP2	2.32	0.40
12:BA:913:G:H21	12:BA:914:A:N6	2.19	0.40
16:BE:202:GLN:HB3	16:BE:273:VAL:HG13	2.03	0.40
17:BF:226:MET:HA	17:BF:227:PRO:HD2	1.80	0.40
17:BF:237:LEU:O	52:Bv:25:TYR:N	2.54	0.40
18:BI:94:LEU:HB2	18:BI:116:LYS:HG2	2.01	0.40
24:BQ:172:VAL:HA	24:BQ:175:PHE:CE2	2.56	0.40
25:BR:62:TYR:CD2	27:BT:269:MET:HE3	2.56	0.40
26:BS:116:LEU:HD22	34:Bb:130:ILE:HG12	2.02	0.40
40:Bh:105:ARG:HB2	40:Bh:112:LYS:CD	2.47	0.40
41:Bi:168:CYS:HB2	41:Bi:262:HIS:O	2.20	0.40
43:Bk:127:MET:HB2	43:Bk:154:GLU:HB2	2.03	0.40
53:Bw:310:CYS:HB3	53:Bw:313:GLN:CG	2.47	0.40
2:B0:57:GLU:HB3	12:BA:400:A:H1'	2.03	0.40
3:B1:179:ASP:OD1	3:B1:179:ASP:N	2.54	0.40
3:B1:202:GLU:HG3	3:B1:203:TRP:CD1	2.56	0.40
12:BA:145:A:H2'	12:BA:146:A:H8	1.81	0.40
12:BA:1341:A:N3	12:BA:1341:A:H2'	2.37	0.40
14:BC:311:CYS:HB2	14:BC:314:TYR:HD2	1.86	0.40
20:BK:171:ARG:O	20:BK:175:LEU:HG	2.21	0.40
24:BQ:133:ARG:HG3	24:BQ:148:ASP:OD2	2.19	0.40
25:BR:16:ARG:HG2	25:BR:51:GLU:OE1	2.21	0.40
27:BT:77:SER:HA	27:BT:78:PRO:HD3	1.86	0.40
27:BT:96:ARG:NH1	27:BT:285:GLU:CD	2.79	0.40
30:BW:161:ARG:HD3	41:Bi:44:PRO:HB3	2.04	0.40
33:Ba:309:LEU:O	33:Ba:313:MET:HG2	2.22	0.40
35:Bc:207:ILE:HA	35:Bc:269:THR:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Bd:100:GLN:O	36:Bd:100:GLN:HG3	2.21	0.40
39:Bg:139:THR:OG1	39:Bg:140:LEU:N	2.54	0.40
42:Bj:203:LYS:HB3	42:Bj:239:LEU:HD21	2.03	0.40
43:Bk:92:ASN:ND2	43:Bk:189:HIS:HA	2.37	0.40
45:Bm:133:VAL:HA	45:Bm:134:PRO:HD3	1.82	0.40
45:Bm:157:TRP:NE1	45:Bm:159:TYR:HB2	2.37	0.40
48:Bp:19:GLN:HG2	48:Bp:54:ASP:HB3	2.03	0.40
48:Bp:93:HIS:CE1	54:Bx:47:THR:HG21	2.57	0.40
50:Bt:99:ARG:HH11	50:Bt:99:ARG:CG	2.35	0.40
4:B2:120:GLU:HG2	31:BX:110:LEU:HD12	2.04	0.40
12:BA:517:C:H5'	12:BA:518:A:OP1	2.22	0.40
12:BA:551:A:OP1	19:BJ:128:ASN:HB2	2.21	0.40
12:BA:734:A:OP2	15:BD:105:ARG:NH2	2.51	0.40
12:BA:877:U:O2'	12:BA:965:A:OP2	2.34	0.40
14:BC:264:GLY:HA2	14:BC:300:VAL:HG22	2.03	0.40
14:BC:629:LEU:O	14:BC:705:VAL:HG13	2.21	0.40
17:BF:293:PHE:HA	17:BF:294:PRO:HD3	1.92	0.40
22:BO:41:VAL:HG12	22:BO:119:ILE:HG23	2.02	0.40
23:BP:45:ARG:HH11	23:BP:45:ARG:HG3	1.86	0.40
23:BP:107:LEU:HD23	23:BP:107:LEU:HA	1.89	0.40
27:BT:139:GLN:HG2	27:BT:150:ILE:HD12	2.04	0.40
34:Bb:153:GLU:HG2	34:Bb:158:TYR:CD2	2.57	0.40
37:Be:66:PHE:CD1	37:Be:66:PHE:C	2.99	0.40
41:Bi:218:THR:HG21	41:Bi:220:GLN:HE21	1.85	0.40
43:Bk:86:TYR:CE1	43:Bk:88:TYR:HD1	2.35	0.40
53:Bw:91:TYR:HE2	53:Bw:223:LEU:HD22	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BL	68/198 (34%)	65 (96%)	3 (4%)	0	100	100
1	CL	43/198 (22%)	41 (95%)	1 (2%)	1 (2%)	5	29
1	DL	25/198 (13%)	25 (100%)	0	0	100	100
1	EL	26/198 (13%)	25 (96%)	1 (4%)	0	100	100
1	FL	25/198 (13%)	25 (100%)	0	0	100	100
1	GL	25/198 (13%)	25 (100%)	0	0	100	100
1	HL	24/198 (12%)	24 (100%)	0	0	100	100
2	B0	108/148 (73%)	105 (97%)	3 (3%)	0	100	100
3	B1	242/256 (94%)	238 (98%)	4 (2%)	0	100	100
4	B2	177/252 (70%)	171 (97%)	6 (3%)	0	100	100
5	B3	116/161 (72%)	114 (98%)	2 (2%)	0	100	100
6	B4	43/126 (34%)	40 (93%)	3 (7%)	0	100	100
7	B5	108/188 (57%)	107 (99%)	1 (1%)	0	100	100
8	B6	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
9	B7	44/95 (46%)	43 (98%)	1 (2%)	0	100	100
10	B8	93/188 (50%)	91 (98%)	2 (2%)	0	100	100
11	B9	36/100 (36%)	36 (100%)	0	0	100	100
14	BC	569/657 (87%)	545 (96%)	23 (4%)	1 (0%)	43	73
15	BD	238/306 (78%)	225 (94%)	13 (6%)	0	100	100
16	BE	305/348 (88%)	282 (92%)	20 (7%)	3 (1%)	12	45
17	BF	248/294 (84%)	237 (96%)	11 (4%)	0	100	100
18	BI	96/268 (36%)	91 (95%)	5 (5%)	0	100	100
19	BJ	210/262 (80%)	203 (97%)	7 (3%)	0	100	100
20	BK	174/192 (91%)	164 (94%)	9 (5%)	1 (1%)	21	56
21	BN	175/178 (98%)	172 (98%)	3 (2%)	0	100	100
22	BO	113/145 (78%)	108 (96%)	5 (4%)	0	100	100
23	BP	286/296 (97%)	276 (96%)	10 (4%)	0	100	100
24	BQ	220/251 (88%)	218 (99%)	2 (1%)	0	100	100
25	BR	151/169 (89%)	146 (97%)	5 (3%)	0	100	100
26	BS	141/180 (78%)	128 (91%)	12 (8%)	1 (1%)	18	52
27	BT	221/292 (76%)	214 (97%)	7 (3%)	0	100	100
28	BU	138/149 (93%)	134 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BV	153/209 (73%)	147 (96%)	6 (4%)	0	100	100
30	BW	164/210 (78%)	159 (97%)	5 (3%)	0	100	100
31	BX	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
32	BY	204/216 (94%)	192 (94%)	12 (6%)	0	100	100
33	Ba	391/423 (92%)	375 (96%)	16 (4%)	0	100	100
34	Bb	352/380 (93%)	330 (94%)	22 (6%)	0	100	100
35	Bc	293/334 (88%)	279 (95%)	14 (5%)	0	100	100
36	Bd	97/206 (47%)	89 (92%)	7 (7%)	1 (1%)	12	45
37	Be	120/135 (89%)	114 (95%)	6 (5%)	0	100	100
38	Bf	106/142 (75%)	102 (96%)	2 (2%)	2 (2%)	6	33
39	Bg	146/159 (92%)	137 (94%)	9 (6%)	0	100	100
40	Bh	287/332 (86%)	274 (96%)	13 (4%)	0	100	100
41	Bi	258/306 (84%)	250 (97%)	8 (3%)	0	100	100
42	Bj	211/279 (76%)	200 (95%)	10 (5%)	1 (0%)	24	59
43	Bk	132/212 (62%)	126 (96%)	6 (4%)	0	100	100
44	Bl	131/166 (79%)	127 (97%)	4 (3%)	0	100	100
45	Bm	107/159 (67%)	103 (96%)	4 (4%)	0	100	100
46	Bn	95/128 (74%)	89 (94%)	6 (6%)	0	100	100
47	Bo	95/124 (77%)	91 (96%)	4 (4%)	0	100	100
48	Bp	95/112 (85%)	89 (94%)	6 (6%)	0	100	100
49	Bq	66/138 (48%)	64 (97%)	1 (2%)	1 (2%)	8	37
50	Bt	92/102 (90%)	86 (94%)	6 (6%)	0	100	100
51	Bu	147/205 (72%)	137 (93%)	9 (6%)	1 (1%)	18	52
52	Bv	133/222 (60%)	132 (99%)	1 (1%)	0	100	100
53	Bw	385/433 (89%)	364 (94%)	20 (5%)	1 (0%)	36	68
54	Bx	160/196 (82%)	156 (98%)	3 (2%)	1 (1%)	21	56
55	Bz	70/82 (85%)	70 (100%)	0	0	100	100
All	All	9175/12712 (72%)	8795 (96%)	365 (4%)	15 (0%)	44	73

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CL	21	PRO

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Mol	Chain	Res	Type
38	Bf	78	PRO
38	Bf	80	PRO
51	Bu	167	PRO
16	BE	202	GLN
53	Bw	159	VAL
54	Bx	93	ILE
14	BC	502	PRO
16	BE	317	PRO
20	BK	157	LYS
49	Bq	101	VAL
42	Bj	151	ARG
16	BE	264	ILE
36	Bd	170	PRO
26	BS	45	ALA

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	BL	59/157 (38%)	59 (100%)	0	100	100
1	CL	30/157 (19%)	29 (97%)	1 (3%)	33	65
1	DL	26/157 (17%)	24 (92%)	2 (8%)	12	41
1	EL	27/157 (17%)	25 (93%)	2 (7%)	13	43
1	FL	26/157 (17%)	24 (92%)	2 (8%)	12	41
1	GL	26/157 (17%)	25 (96%)	1 (4%)	29	62
1	HL	25/157 (16%)	23 (92%)	2 (8%)	11	40
2	B0	90/115 (78%)	77 (86%)	13 (14%)	3	16
3	B1	219/229 (96%)	189 (86%)	30 (14%)	3	18
4	B2	164/228 (72%)	146 (89%)	18 (11%)	6	26
5	B3	110/147 (75%)	99 (90%)	11 (10%)	7	30
6	B4	42/114 (37%)	34 (81%)	8 (19%)	1	9
7	B5	99/163 (61%)	87 (88%)	12 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	B6	49/60 (82%)	47 (96%)	2 (4%)	27	60
9	B7	41/78 (53%)	38 (93%)	3 (7%)	13	43
10	B8	87/162 (54%)	77 (88%)	10 (12%)	5	24
11	B9	36/77 (47%)	30 (83%)	6 (17%)	2	11
14	BC	464/556 (84%)	445 (96%)	19 (4%)	27	60
15	BD	193/248 (78%)	169 (88%)	24 (12%)	4	21
16	BE	263/290 (91%)	234 (89%)	29 (11%)	6	26
17	BF	217/251 (86%)	192 (88%)	25 (12%)	5	24
18	BI	88/228 (39%)	85 (97%)	3 (3%)	32	64
19	BJ	192/230 (84%)	179 (93%)	13 (7%)	14	46
20	BK	129/151 (85%)	119 (92%)	10 (8%)	11	41
21	BN	156/157 (99%)	137 (88%)	19 (12%)	5	22
22	BO	99/123 (80%)	88 (89%)	11 (11%)	6	25
23	BP	245/249 (98%)	216 (88%)	29 (12%)	5	23
24	BQ	190/210 (90%)	176 (93%)	14 (7%)	13	43
25	BR	132/143 (92%)	118 (89%)	14 (11%)	6	27
26	BS	123/153 (80%)	113 (92%)	10 (8%)	11	39
27	BT	204/258 (79%)	179 (88%)	25 (12%)	4	22
28	BU	118/127 (93%)	109 (92%)	9 (8%)	12	42
29	BV	136/178 (76%)	119 (88%)	17 (12%)	4	21
30	BW	144/180 (80%)	130 (90%)	14 (10%)	8	32
31	BX	116/134 (87%)	103 (89%)	13 (11%)	6	25
32	BY	185/192 (96%)	160 (86%)	25 (14%)	4	19
33	Ba	348/365 (95%)	305 (88%)	43 (12%)	4	21
34	Bb	310/328 (94%)	272 (88%)	38 (12%)	4	22
35	Bc	271/299 (91%)	254 (94%)	17 (6%)	16	48
36	Bd	92/181 (51%)	86 (94%)	6 (6%)	15	47
37	Be	100/108 (93%)	86 (86%)	14 (14%)	3	17
38	Bf	80/133 (60%)	66 (82%)	14 (18%)	2	10
39	Bg	128/136 (94%)	112 (88%)	16 (12%)	4	21
40	Bh	251/284 (88%)	223 (89%)	28 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	Bi	236/275 (86%)	219 (93%)	17 (7%)	13	44
42	Bj	190/242 (78%)	172 (90%)	18 (10%)	8	32
43	Bk	119/181 (66%)	112 (94%)	7 (6%)	18	50
44	Bl	122/147 (83%)	106 (87%)	16 (13%)	4	19
45	Bm	103/145 (71%)	94 (91%)	9 (9%)	9	36
46	Bn	88/113 (78%)	77 (88%)	11 (12%)	4	21
47	Bo	77/97 (79%)	68 (88%)	9 (12%)	5	23
48	Bp	79/88 (90%)	72 (91%)	7 (9%)	9	34
49	Bq	50/114 (44%)	47 (94%)	3 (6%)	17	50
50	Bt	75/82 (92%)	56 (75%)	19 (25%)	0	3
51	Bu	126/177 (71%)	116 (92%)	10 (8%)	11	40
52	Bv	115/183 (63%)	111 (96%)	4 (4%)	32	64
53	Bw	340/373 (91%)	298 (88%)	42 (12%)	4	21
54	Bx	149/173 (86%)	133 (89%)	16 (11%)	6	27
All	All	7999/10754 (74%)	7189 (90%)	810 (10%)	9	30

All (810) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CL	40	LEU
1	DL	75	THR
1	DL	86	LEU
1	EL	76	LEU
1	EL	82	LEU
1	FL	76	LEU
1	FL	79	ILE
1	GL	82	LEU
1	HL	76	LEU
1	HL	79	ILE
2	B0	49	LYS
2	B0	50	ARG
2	B0	53	ILE
2	B0	56	MET
2	B0	61	VAL
2	B0	66	ILE
2	B0	117	VAL
2	B0	118	THR

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Mol	Chain	Res	Type
2	B0	122	GLN
2	B0	126	LEU
2	B0	131	VAL
2	B0	141	THR
2	B0	147	MET
3	B1	6	VAL
3	B1	31	SER
3	B1	32	LEU
3	B1	46	HIS
3	B1	61	ARG
3	B1	64	ASP
3	B1	69	VAL
3	B1	75	SER
3	B1	77	LEU
3	B1	79	LEU
3	B1	100	ARG
3	B1	101	VAL
3	B1	104	VAL
3	B1	112	ARG
3	B1	120	ASP
3	B1	126	THR
3	B1	128	THR
3	B1	136	ASP
3	B1	155	SER
3	B1	161	LEU
3	B1	166	LEU
3	B1	169	LEU
3	B1	172	GLN
3	B1	173	ASP
3	B1	177	HIS
3	B1	179	ASP
3	B1	190	ARG
3	B1	204	VAL
3	B1	224	ILE
3	B1	238	LEU
4	B2	66	LEU
4	B2	67	GLU
4	B2	72	ASP
4	B2	79	GLU
4	B2	126	LEU
4	B2	133	ARG
4	B2	144	LEU

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Mol	Chain	Res	Type
4	B2	145	ASP
4	B2	153	ASP
4	B2	158	LEU
4	B2	171	ARG
4	B2	174	ILE
4	B2	177	ARG
4	B2	197	ASN
4	B2	204	MET
4	B2	218	GLN
4	B2	228	LEU
4	B2	230	ARG
5	B3	38	ARG
5	B3	43	ASP
5	B3	69	VAL
5	B3	72	ILE
5	B3	73	LYS
5	B3	82	GLU
5	B3	86	ILE
5	B3	144	GLU
5	B3	147	VAL
5	B3	150	LEU
5	B3	151	LEU
6	B4	42	THR
6	B4	44	LEU
6	B4	49	TYR
6	B4	52	LEU
6	B4	57	LEU
6	B4	60	GLN
6	B4	65	ILE
6	B4	78	MET
7	B5	85	ARG
7	B5	87	ILE
7	B5	92	CYS
7	B5	94	ARG
7	B5	108	ASP
7	B5	109	VAL
7	B5	136	GLU
7	B5	153	THR
7	B5	156	THR
7	B5	158	VAL
7	B5	175	ILE
7	B5	186	THR

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Mol	Chain	Res	Type
8	B6	22	SER
8	B6	54	VAL
9	B7	65	HIS
9	B7	75	THR
9	B7	92	SER
10	B8	106	THR
10	B8	111	ILE
10	B8	113	ARG
10	B8	142	ARG
10	B8	162	THR
10	B8	163	THR
10	B8	169	ARG
10	B8	182	ASP
10	B8	183	ARG
10	B8	184	THR
11	B9	63	PHE
11	B9	65	THR
11	B9	74	ARG
11	B9	75	ASP
11	B9	79	VAL
11	B9	92	ASN
14	BC	163	LYS
14	BC	184	THR
14	BC	185	ILE
14	BC	226	SER
14	BC	251	VAL
14	BC	252	THR
14	BC	253	ASP
14	BC	283	ILE
14	BC	304	LEU
14	BC	330	ASN
14	BC	472	GLU
14	BC	484	LEU
14	BC	515	VAL
14	BC	520	ILE
14	BC	524	VAL
14	BC	568	ASP
14	BC	570	VAL
14	BC	628	ILE
14	BC	679	HIS
15	BD	62	THR
15	BD	64	VAL

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Mol	Chain	Res	Type
15	BD	69	ARG
15	BD	74	VAL
15	BD	75	MET
15	BD	90	GLN
15	BD	103	ARG
15	BD	105	ARG
15	BD	111	ARG
15	BD	117	GLU
15	BD	124	GLU
15	BD	148	ARG
15	BD	150	ARG
15	BD	153	ILE
15	BD	155	THR
15	BD	158	MET
15	BD	163	THR
15	BD	170	ILE
15	BD	190	VAL
15	BD	224	THR
15	BD	240	THR
15	BD	251	VAL
15	BD	285	ARG
15	BD	288	ARG
16	BE	53	LEU
16	BE	55	GLU
16	BE	80	LEU
16	BE	96	ARG
16	BE	97	VAL
16	BE	109	LEU
16	BE	113	ASP
16	BE	146	THR
16	BE	168	LEU
16	BE	181	VAL
16	BE	187	ILE
16	BE	218	VAL
16	BE	227	GLN
16	BE	231	HIS
16	BE	236	THR
16	BE	239	ARG
16	BE	251	VAL
16	BE	264	ILE
16	BE	273	VAL
16	BE	284	TYR

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Mol	Chain	Res	Type
16	BE	285	VAL
16	BE	289	VAL
16	BE	296	LEU
16	BE	297	VAL
16	BE	299	ILE
16	BE	301	ASP
16	BE	311	CYS
16	BE	313	ASN
16	BE	326	GLU
17	BF	47	VAL
17	BF	59	ARG
17	BF	76	ARG
17	BF	77	VAL
17	BF	79	LEU
17	BF	80	THR
17	BF	89	THR
17	BF	94	ASP
17	BF	101	ILE
17	BF	114	THR
17	BF	116	THR
17	BF	125	ARG
17	BF	129	VAL
17	BF	143	SER
17	BF	165	LEU
17	BF	167	MET
17	BF	172	GLN
17	BF	190	VAL
17	BF	193	LEU
17	BF	203	LEU
17	BF	224	GLU
17	BF	239	THR
17	BF	263	LEU
17	BF	281	THR
17	BF	291	CYS
18	BI	56	VAL
18	BI	75	ARG
18	BI	99	THR
19	BJ	34	THR
19	BJ	60	ILE
19	BJ	63	ARG
19	BJ	76	THR
19	BJ	78	LEU

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Mol	Chain	Res	Type
19	BJ	81	LEU
19	BJ	93	ASN
19	BJ	95	MET
19	BJ	121	ILE
19	BJ	128	ASN
19	BJ	150	HIS
19	BJ	152	LEU
19	BJ	229	LEU
20	BK	57	THR
20	BK	64	ILE
20	BK	111	LEU
20	BK	113	THR
20	BK	117	VAL
20	BK	137	LEU
20	BK	145	ILE
20	BK	158	ASP
20	BK	163	GLU
20	BK	164	LEU
21	BN	10	GLN
21	BN	24	LYS
21	BN	31	LEU
21	BN	39	LEU
21	BN	65	ILE
21	BN	67	PHE
21	BN	78	SER
21	BN	91	THR
21	BN	101	VAL
21	BN	104	VAL
21	BN	118	ARG
21	BN	123	GLN
21	BN	124	ARG
21	BN	131	GLU
21	BN	136	ASP
21	BN	137	ILE
21	BN	140	ASN
21	BN	153	ARG
21	BN	177	ARG
22	BO	60	VAL
22	BO	72	ARG
22	BO	73	ILE
22	BO	77	ILE
22	BO	91	MET

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Mol	Chain	Res	Type
22	BO	95	ARG
22	BO	101	ASP
22	BO	110	ASP
22	BO	111	ASN
22	BO	121	THR
22	BO	138	LEU
23	BP	11	ARG
23	BP	43	ARG
23	BP	44	ARG
23	BP	45	ARG
23	BP	58	GLN
23	BP	61	THR
23	BP	62	ARG
23	BP	65	LEU
23	BP	71	GLN
23	BP	125	ARG
23	BP	127	VAL
23	BP	130	GLN
23	BP	140	LEU
23	BP	141	VAL
23	BP	152	VAL
23	BP	154	ILE
23	BP	158	MET
23	BP	176	THR
23	BP	211	VAL
23	BP	215	THR
23	BP	233	ARG
23	BP	234	LEU
23	BP	246	ASP
23	BP	247	ILE
23	BP	248	THR
23	BP	251	GLU
23	BP	257	SER
23	BP	261	ASP
23	BP	286	THR
24	BQ	55	ARG
24	BQ	68	ASN
24	BQ	77	THR
24	BQ	132	THR
24	BQ	140	MET
24	BQ	161	VAL
24	BQ	166	ARG

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Mol	Chain	Res	Type
24	BQ	171	GLU
24	BQ	209	ASN
24	BQ	214	THR
24	BQ	224	LEU
24	BQ	226	ILE
24	BQ	247	THR
24	BQ	250	ARG
25	BR	17	ARG
25	BR	24	SER
25	BR	30	GLN
25	BR	38	ARG
25	BR	67	ASP
25	BR	84	ASP
25	BR	93	LEU
25	BR	98	GLN
25	BR	110	ILE
25	BR	124	ILE
25	BR	134	LEU
25	BR	139	ARG
25	BR	142	ASN
25	BR	148	GLN
26	BS	44	VAL
26	BS	61	VAL
26	BS	80	ARG
26	BS	107	THR
26	BS	116	LEU
26	BS	141	ILE
26	BS	149	THR
26	BS	161	LEU
26	BS	163	HIS
26	BS	171	VAL
27	BT	77	SER
27	BT	79	GLU
27	BT	90	LEU
27	BT	94	ILE
27	BT	130	THR
27	BT	138	ILE
27	BT	145	LEU
27	BT	162	ILE
27	BT	165	GLU
27	BT	170	ARG
27	BT	177	VAL

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Mol	Chain	Res	Type
27	BT	187	LEU
27	BT	202	VAL
27	BT	224	MET
27	BT	234	GLU
27	BT	239	ASN
27	BT	243	ILE
27	BT	246	ASP
27	BT	254	MET
27	BT	272	GLU
27	BT	274	ASP
27	BT	275	THR
27	BT	282	ILE
27	BT	284	ASP
27	BT	289	SER
28	BU	43	VAL
28	BU	54	THR
28	BU	77	GLN
28	BU	78	GLU
28	BU	87	ILE
28	BU	101	VAL
28	BU	109	GLU
28	BU	123	ARG
28	BU	126	GLU
29	BV	91	ILE
29	BV	103	VAL
29	BV	111	LYS
29	BV	117	LEU
29	BV	120	ILE
29	BV	126	VAL
29	BV	133	ARG
29	BV	153	LEU
29	BV	160	VAL
29	BV	164	VAL
29	BV	169	GLU
29	BV	174	ILE
29	BV	176	MET
29	BV	179	GLN
29	BV	186	ARG
29	BV	190	THR
29	BV	199	ILE
30	BW	50	GLU
30	BW	60	GLN

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Mol	Chain	Res	Type
30	BW	75	ARG
30	BW	77	GLN
30	BW	80	TYR
30	BW	119	LEU
30	BW	131	ASN
30	BW	133	GLU
30	BW	136	SER
30	BW	147	ARG
30	BW	151	LEU
30	BW	154	ILE
30	BW	164	ILE
30	BW	199	GLN
31	BX	6	LEU
31	BX	26	ILE
31	BX	28	LEU
31	BX	35	GLN
31	BX	47	GLU
31	BX	49	THR
31	BX	50	ARG
31	BX	52	ASP
31	BX	57	LEU
31	BX	60	ILE
31	BX	79	ARG
31	BX	97	VAL
31	BX	104	THR
32	BY	30	SER
32	BY	31	ASP
32	BY	39	THR
32	BY	40	ARG
32	BY	43	ARG
32	BY	44	VAL
32	BY	46	VAL
32	BY	66	GLU
32	BY	78	GLN
32	BY	86	VAL
32	BY	96	ARG
32	BY	107	THR
32	BY	116	LEU
32	BY	131	THR
32	BY	137	PHE
32	BY	138	THR
32	BY	144	VAL

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Mol	Chain	Res	Type
32	BY	145	ARG
32	BY	149	ARG
32	BY	153	ILE
32	BY	163	ASP
32	BY	166	VAL
32	BY	181	ASP
32	BY	200	GLU
32	BY	208	ARG
33	Ba	42	GLU
33	Ba	47	ASP
33	Ba	51	GLU
33	Ba	58	ILE
33	Ba	63	LYS
33	Ba	67	MET
33	Ba	113	LEU
33	Ba	137	LEU
33	Ba	139	LEU
33	Ba	147	ILE
33	Ba	149	ASN
33	Ba	150	GLN
33	Ba	162	ARG
33	Ba	163	LEU
33	Ba	167	THR
33	Ba	175	THR
33	Ba	189	LYS
33	Ba	193	LEU
33	Ba	195	HIS
33	Ba	202	ILE
33	Ba	207	ASN
33	Ba	210	SER
33	Ba	212	THR
33	Ba	215	ARG
33	Ba	222	VAL
33	Ba	234	ASP
33	Ba	256	PHE
33	Ba	259	ILE
33	Ba	262	THR
33	Ba	270	VAL
33	Ba	277	THR
33	Ba	322	LEU
33	Ba	335	VAL
33	Ba	337	GLU

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Mol	Chain	Res	Type
33	Ba	345	VAL
33	Ba	347	THR
33	Ba	348	ASP
33	Ba	373	LEU
33	Ba	381	LEU
33	Ba	391	VAL
33	Ba	396	VAL
33	Ba	398	VAL
33	Ba	415	LEU
34	Bb	32	LEU
34	Bb	35	MET
34	Bb	40	ILE
34	Bb	50	LYS
34	Bb	51	TYR
34	Bb	52	ARG
34	Bb	72	ARG
34	Bb	88	VAL
34	Bb	90	ILE
34	Bb	99	ARG
34	Bb	118	GLU
34	Bb	120	GLU
34	Bb	130	ILE
34	Bb	135	VAL
34	Bb	141	ARG
34	Bb	173	LEU
34	Bb	179	VAL
34	Bb	210	GLU
34	Bb	222	ASP
34	Bb	229	ASP
34	Bb	233	VAL
34	Bb	237	VAL
34	Bb	238	THR
34	Bb	245	VAL
34	Bb	252	CYS
34	Bb	258	PHE
34	Bb	261	ARG
34	Bb	267	ARG
34	Bb	272	LEU
34	Bb	276	ASP
34	Bb	281	PHE
34	Bb	284	ASP
34	Bb	288	SER

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Mol	Chain	Res	Type
34	Bb	324	ASP
34	Bb	343	GLU
34	Bb	356	ARG
34	Bb	360	ARG
34	Bb	376	THR
35	Bc	67	VAL
35	Bc	87	SER
35	Bc	106	ASP
35	Bc	111	ASP
35	Bc	122	ILE
35	Bc	140	TRP
35	Bc	171	VAL
35	Bc	186	LEU
35	Bc	190	MET
35	Bc	218	VAL
35	Bc	222	VAL
35	Bc	256	ASP
35	Bc	260	VAL
35	Bc	280	VAL
35	Bc	285	THR
35	Bc	300	VAL
35	Bc	319	MET
36	Bd	83	ILE
36	Bd	89	ILE
36	Bd	106	LEU
36	Bd	136	ILE
36	Bd	150	LEU
36	Bd	168	LEU
37	Be	23	SER
37	Be	25	ARG
37	Be	28	ARG
37	Be	29	THR
37	Be	60	VAL
37	Be	66	PHE
37	Be	68	LEU
37	Be	78	GLU
37	Be	106	THR
37	Be	110	GLU
37	Be	111	HIS
37	Be	120	THR
37	Be	122	GLU
37	Be	127	GLN

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Mol	Chain	Res	Type
38	Bf	44	ASN
38	Bf	45	CYS
38	Bf	56	ARG
38	Bf	58	ILE
38	Bf	59	VAL
38	Bf	60	CYS
38	Bf	67	ILE
38	Bf	70	GLU
38	Bf	75	ILE
38	Bf	114	LYS
38	Bf	122	ARG
38	Bf	126	ARG
38	Bf	133	ARG
38	Bf	134	ARG
39	Bg	6	THR
39	Bg	12	THR
39	Bg	14	VAL
39	Bg	21	ARG
39	Bg	33	LEU
39	Bg	47	VAL
39	Bg	52	THR
39	Bg	61	VAL
39	Bg	68	ARG
39	Bg	80	LEU
39	Bg	88	SER
39	Bg	93	SER
39	Bg	113	ILE
39	Bg	125	SER
39	Bg	126	ILE
39	Bg	148	VAL
40	Bh	45	LEU
40	Bh	51	LEU
40	Bh	52	ARG
40	Bh	78	ARG
40	Bh	82	THR
40	Bh	96	CYS
40	Bh	98	ILE
40	Bh	110	ILE
40	Bh	121	ASP
40	Bh	148	LEU
40	Bh	154	THR
40	Bh	177	GLN

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Mol	Chain	Res	Type
40	Bh	178	LEU
40	Bh	191	LEU
40	Bh	192	ARG
40	Bh	216	ARG
40	Bh	231	MET
40	Bh	233	THR
40	Bh	254	GLU
40	Bh	259	ARG
40	Bh	263	SER
40	Bh	264	THR
40	Bh	265	THR
40	Bh	267	LEU
40	Bh	288	THR
40	Bh	289	VAL
40	Bh	301	LEU
40	Bh	307	PHE
41	Bi	57	VAL
41	Bi	74	ARG
41	Bi	76	ILE
41	Bi	85	PHE
41	Bi	102	LYS
41	Bi	112	LEU
41	Bi	165	THR
41	Bi	176	ILE
41	Bi	181	VAL
41	Bi	186	VAL
41	Bi	196	GLN
41	Bi	221	THR
41	Bi	238	VAL
41	Bi	242	VAL
41	Bi	244	GLU
41	Bi	246	VAL
41	Bi	281	MET
42	Bj	51	LEU
42	Bj	55	ARG
42	Bj	60	THR
42	Bj	64	THR
42	Bj	119	ASP
42	Bj	136	ARG
42	Bj	137	LEU
42	Bj	145	ASP
42	Bj	169	ASP

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Mol	Chain	Res	Type
42	Bj	179	GLN
42	Bj	195	LEU
42	Bj	210	CYS
42	Bj	230	LYS
42	Bj	255	VAL
42	Bj	264	LEU
42	Bj	265	LYS
42	Bj	276	LEU
42	Bj	279	LEU
43	Bk	50	SER
43	Bk	53	THR
43	Bk	56	ILE
43	Bk	132	MET
43	Bk	147	ASP
43	Bk	150	LEU
43	Bk	165	THR
44	Bl	42	VAL
44	Bl	89	SER
44	Bl	90	ARG
44	Bl	98	ARG
44	Bl	100	ILE
44	Bl	101	THR
44	Bl	107	MET
44	Bl	117	ILE
44	Bl	128	LEU
44	Bl	137	VAL
44	Bl	138	THR
44	Bl	141	ASN
44	Bl	143	VAL
44	Bl	154	ASP
44	Bl	155	GLN
44	Bl	156	GLN
45	Bm	52	VAL
45	Bm	67	LEU
45	Bm	71	LEU
45	Bm	86	ASN
45	Bm	115	ASN
45	Bm	121	MET
45	Bm	128	LEU
45	Bm	135	VAL
45	Bm	142	ASP
46	Bn	32	PHE

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Mol	Chain	Res	Type
46	Bn	34	VAL
46	Bn	35	ARG
46	Bn	41	ARG
46	Bn	44	VAL
46	Bn	48	ASN
46	Bn	53	MET
46	Bn	56	VAL
46	Bn	71	LYS
46	Bn	92	ILE
46	Bn	105	ASP
47	Bo	31	GLN
47	Bo	40	TYR
47	Bo	43	LEU
47	Bo	44	THR
47	Bo	53	ASP
47	Bo	55	ARG
47	Bo	64	LEU
47	Bo	84	MET
47	Bo	110	LEU
48	Bp	15	GLN
48	Bp	28	GLU
48	Bp	55	VAL
48	Bp	75	ILE
48	Bp	76	MET
48	Bp	82	THR
48	Bp	84	GLN
49	Bq	95	TRP
49	Bq	96	LEU
49	Bq	137	LYS
50	Bt	9	ARG
50	Bt	10	ASN
50	Bt	16	GLN
50	Bt	25	ARG
50	Bt	27	VAL
50	Bt	35	MET
50	Bt	37	ARG
50	Bt	41	THR
50	Bt	45	ASN
50	Bt	49	LEU
50	Bt	55	THR
50	Bt	57	GLU
50	Bt	60	ARG

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Mol	Chain	Res	Type
50	Bt	81	ARG
50	Bt	88	LEU
50	Bt	90	GLU
50	Bt	97	VAL
50	Bt	98	THR
50	Bt	99	ARG
51	Bu	81	CYS
51	Bu	94	VAL
51	Bu	97	LYS
51	Bu	104	LEU
51	Bu	110	ILE
51	Bu	123	LYS
51	Bu	135	THR
51	Bu	146	LEU
51	Bu	177	SER
51	Bu	182	MET
52	Bv	38	ARG
52	Bv	47	THR
52	Bv	90	ARG
52	Bv	108	LEU
53	Bw	43	ARG
53	Bw	51	LEU
53	Bw	77	ASP
53	Bw	81	ARG
53	Bw	100	LEU
53	Bw	118	LEU
53	Bw	147	GLU
53	Bw	151	LEU
53	Bw	153	ARG
53	Bw	162	ASP
53	Bw	166	ILE
53	Bw	173	GLN
53	Bw	194	LEU
53	Bw	196	CYS
53	Bw	200	VAL
53	Bw	220	VAL
53	Bw	248	ASP
53	Bw	260	CYS
53	Bw	271	GLN
53	Bw	274	ASN
53	Bw	278	ILE
53	Bw	280	SER

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Mol	Chain	Res	Type
53	Bw	291	THR
53	Bw	306	LEU
53	Bw	330	THR
53	Bw	345	VAL
53	Bw	347	ARG
53	Bw	356	THR
53	Bw	370	THR
53	Bw	376	GLN
53	Bw	393	LYS
53	Bw	395	LEU
53	Bw	399	ILE
53	Bw	402	ASN
53	Bw	404	VAL
53	Bw	405	LYS
53	Bw	410	ASP
53	Bw	414	GLN
53	Bw	415	LEU
53	Bw	416	VAL
53	Bw	420	LEU
53	Bw	421	ASN
54	Bx	38	VAL
54	Bx	54	THR
54	Bx	70	CYS
54	Bx	90	SER
54	Bx	92	PHE
54	Bx	93	ILE
54	Bx	100	LEU
54	Bx	115	ILE
54	Bx	121	MET
54	Bx	128	LEU
54	Bx	152	THR
54	Bx	157	ARG
54	Bx	183	ASP
54	Bx	185	VAL
54	Bx	190	ARG
54	Bx	193	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (191) such sidechains are listed below:

Mol	Chain	Res	Type
2	B0	41	ASN
2	B0	65	ASN

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Mol	Chain	Res	Type
2	B0	76	HIS
3	B1	27	HIS
3	B1	42	HIS
3	B1	70	HIS
3	B1	172	GLN
4	B2	75	ASN
4	B2	90	GLN
4	B2	91	GLN
5	B3	67	HIS
5	B3	142	ASN
6	B4	37	ASN
6	B4	47	GLN
7	B5	83	ASN
7	B5	144	GLN
7	B5	170	GLN
7	B5	188	ASN
9	B7	65	HIS
9	B7	87	HIS
10	B8	118	HIS
14	BC	215	GLN
14	BC	268	GLN
14	BC	319	GLN
14	BC	330	ASN
14	BC	475	GLN
14	BC	596	HIS
16	BE	72	GLN
16	BE	174	GLN
16	BE	197	HIS
16	BE	231	HIS
16	BE	281	ASN
16	BE	336	ASN
17	BF	74	GLN
17	BF	83	HIS
17	BF	103	GLN
17	BF	105	ASN
17	BF	249	ASN
18	BI	88	HIS
18	BI	121	ASN
18	BI	126	GLN
18	BI	136	ASN
19	BJ	93	ASN
19	BJ	217	GLN

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Mol	Chain	Res	Type
19	BJ	224	HIS
20	BK	84	GLN
20	BK	103	HIS
1	BL	152	HIS
21	BN	40	GLN
21	BN	74	GLN
21	BN	80	HIS
21	BN	94	GLN
22	BO	89	HIS
22	BO	103	ASN
23	BP	30	ASN
23	BP	71	GLN
23	BP	84	ASN
23	BP	87	HIS
23	BP	91	HIS
23	BP	94	GLN
23	BP	170	ASN
23	BP	219	ASN
23	BP	276	ASN
24	BQ	68	ASN
24	BQ	98	HIS
24	BQ	110	ASN
24	BQ	138	GLN
24	BQ	181	HIS
24	BQ	209	ASN
25	BR	27	HIS
25	BR	30	GLN
25	BR	91	GLN
25	BR	98	GLN
25	BR	112	ASN
25	BR	116	GLN
25	BR	147	ASN
26	BS	52	ASN
26	BS	79	HIS
26	BS	115	HIS
26	BS	147	HIS
27	BT	153	ASN
27	BT	239	ASN
27	BT	258	GLN
28	BU	77	GLN
28	BU	79	HIS
29	BV	79	HIS

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Mol	Chain	Res	Type
29	BV	108	HIS
29	BV	109	GLN
29	BV	144	ASN
30	BW	73	HIS
30	BW	157	HIS
30	BW	171	HIS
30	BW	199	GLN
30	BW	203	ASN
31	BX	77	ASN
32	BY	35	ASN
32	BY	78	GLN
32	BY	84	ASN
32	BY	210	HIS
33	Ba	65	HIS
33	Ba	108	HIS
33	Ba	156	ASN
33	Ba	195	HIS
33	Ba	223	HIS
33	Ba	266	GLN
33	Ba	305	GLN
33	Ba	358	GLN
33	Ba	360	ASN
34	Bb	163	HIS
34	Bb	220	ASN
34	Bb	224	HIS
34	Bb	239	ASN
34	Bb	266	HIS
34	Bb	275	GLN
34	Bb	308	GLN
34	Bb	354	GLN
35	Bc	66	HIS
35	Bc	243	GLN
35	Bc	252	HIS
35	Bc	274	GLN
35	Bc	294	GLN
35	Bc	301	HIS
35	Bc	310	ASN
36	Bd	143	GLN
38	Bf	44	ASN
38	Bf	62	HIS
38	Bf	121	HIS
38	Bf	137	ASN

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Mol	Chain	Res	Type
39	Bg	17	ASN
39	Bg	102	GLN
39	Bg	127	GLN
39	Bg	129	GLN
39	Bg	131	HIS
39	Bg	135	ASN
40	Bh	94	ASN
40	Bh	118	ASN
40	Bh	172	ASN
40	Bh	177	GLN
41	Bi	69	HIS
41	Bi	115	ASN
41	Bi	167	ASN
41	Bi	196	GLN
41	Bi	207	ASN
42	Bj	87	HIS
42	Bj	150	HIS
42	Bj	175	GLN
42	Bj	251	HIS
43	Bk	54	HIS
43	Bk	92	ASN
43	Bk	111	HIS
43	Bk	138	GLN
43	Bk	175	HIS
44	Bl	46	HIS
44	Bl	92	HIS
44	Bl	141	ASN
44	Bl	155	GLN
45	Bm	111	HIS
45	Bm	115	ASN
45	Bm	136	GLN
46	Bn	33	HIS
46	Bn	48	ASN
46	Bn	59	ASN
46	Bn	69	HIS
46	Bn	120	HIS
46	Bn	122	ASN
47	Bo	31	GLN
47	Bo	63	GLN
48	Bp	15	GLN
48	Bp	84	GLN
48	Bp	93	HIS

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Mol	Chain	Res	Type
49	Bq	129	HIS
50	Bt	30	GLN
50	Bt	34	ASN
50	Bt	45	ASN
50	Bt	85	HIS
50	Bt	94	HIS
51	Bu	145	ASN
51	Bu	151	GLN
52	Bv	107	GLN
53	Bw	96	GLN
53	Bw	146	GLN
53	Bw	173	GLN
53	Bw	201	HIS
53	Bw	234	GLN
53	Bw	271	GLN
53	Bw	385	ASN
54	Bx	112	HIS
54	Bx	164	ASN
54	Bx	170	ASN
54	Bx	184	ASN
54	Bx	196	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	BA	1547/1571 (98%)	509 (32%)	10 (0%)
13	BB	65/73 (89%)	25 (38%)	1 (1%)
56	AV	70/71 (98%)	31 (44%)	0
All	All	1682/1715 (98%)	565 (33%)	11 (0%)

All (565) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	BA	4	A
12	BA	6	A
12	BA	7	G
12	BA	11	G
12	BA	15	A
12	BA	16	A
12	BA	19	U
12	BA	20	A

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Mol	Chain	Res	Type
12	BA	21	C
12	BA	22	U
12	BA	23	A
12	BA	25	A
12	BA	26	C
12	BA	31	A
12	BA	32	C
12	BA	33	A
12	BA	36	A
12	BA	37	A
12	BA	39	A
12	BA	40	C
12	BA	41	A
12	BA	42	C
12	BA	45	A
12	BA	46	A
12	BA	47	A
12	BA	48	U
12	BA	49	A
12	BA	50	A
12	BA	56	A
12	BA	57	A
12	BA	59	A
12	BA	60	U
12	BA	63	A
12	BA	66	U
12	BA	67	A
12	BA	68	A
12	BA	82	G
12	BA	83	A
12	BA	84	G
12	BA	96	U
12	BA	97	A
12	BA	99	C
12	BA	101	U
12	BA	102	G
12	BA	104	C
12	BA	105	G
12	BA	108	A
12	BA	109	U
12	BA	115	U
12	BA	118	U

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Mol	Chain	Res	Type
12	BA	119	A
12	BA	122	G
12	BA	129	A
12	BA	132	G
12	BA	139	G
12	BA	140	A
12	BA	141	A
12	BA	142	U
12	BA	143	A
12	BA	146	A
12	BA	147	U
12	BA	148	A
12	BA	149	A
12	BA	153	U
12	BA	157	A
12	BA	163	C
12	BA	164	A
12	BA	165	A
12	BA	168	A
12	BA	172	C
12	BA	179	U
12	BA	180	A
12	BA	182	C
12	BA	188	C
12	BA	190	U
12	BA	192	A
12	BA	203	A
12	BA	205	A
12	BA	218	A
12	BA	219	A
12	BA	221	A
12	BA	223	A
12	BA	224	A
12	BA	225	C
12	BA	228	U
12	BA	229	A
12	BA	231	C
12	BA	237	A
12	BA	238	C
12	BA	239	C
12	BA	243	A
12	BA	245	A

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Mol	Chain	Res	Type
12	BA	252	G
12	BA	254	G
12	BA	260	C
12	BA	263	G
12	BA	265	G
12	BA	271	U
12	BA	272	A
12	BA	273	A
12	BA	274	A
12	BA	275	A
12	BA	276	G
12	BA	277	A
12	BA	295	G
12	BA	303	G
12	BA	305	G
12	BA	306	A
12	BA	309	A
12	BA	311	A
12	BA	312	C
12	BA	313	U
12	BA	318	G
12	BA	322	G
12	BA	324	G
12	BA	329	A
12	BA	330	A
12	BA	331	A
12	BA	336	A
12	BA	337	A
12	BA	338	C
12	BA	339	G
12	BA	340	A
12	BA	352	G
12	BA	359	G
12	BA	364	A
12	BA	366	A
12	BA	367	A
12	BA	368	A
12	BA	369	G
12	BA	371	A
12	BA	373	U
12	BA	374	U
12	BA	381	A

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Mol	Chain	Res	Type
12	BA	389	A
12	BA	390	A
12	BA	392	U
12	BA	393	A
12	BA	394	C
12	BA	397	C
12	BA	398	A
12	BA	402	A
12	BA	403	C
12	BA	404	C
12	BA	409	A
12	BA	414	A
12	BA	417	G
12	BA	418	U
12	BA	419	A
12	BA	420	U
12	BA	427	G
12	BA	428	A
12	BA	440	A
12	BA	441	A
12	BA	446	C
12	BA	447	A
12	BA	448	G
12	BA	449	C
12	BA	459	A
12	BA	460	C
12	BA	467	A
12	BA	468	A
12	BA	472	U
12	BA	473	G
12	BA	474	A
12	BA	478	G
12	BA	479	A
12	BA	480	G
12	BA	488	U
12	BA	489	C
12	BA	490	U
12	BA	491	U
12	BA	492	A
12	BA	493	A
12	BA	494	U
12	BA	497	U

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Mol	Chain	Res	Type
12	BA	500	C
12	BA	501	A
12	BA	503	A
12	BA	504	G
12	BA	505	U
12	BA	506	A
12	BA	515	A
12	BA	516	G
12	BA	518	A
12	BA	526	A
12	BA	532	A
12	BA	533	A
12	BA	545	U
12	BA	547	A
12	BA	548	A
12	BA	550	A
12	BA	552	A
12	BA	553	U
12	BA	554	U
12	BA	557	C
12	BA	560	A
12	BA	561	C
12	BA	562	A
12	BA	563	U
12	BA	566	U
12	BA	570	A
12	BA	574	A
12	BA	575	C
12	BA	576	U
12	BA	578	A
12	BA	579	U
12	BA	580	A
12	BA	583	A
12	BA	584	A
12	BA	585	A
12	BA	586	C
12	BA	592	G
12	BA	593	C
12	BA	595	C
12	BA	596	A
12	BA	614	U
12	BA	617	A

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Mol	Chain	Res	Type
12	BA	618	A
12	BA	619	C
12	BA	625	A
12	BA	628	A
12	BA	631	A
12	BA	634	G
12	BA	640	A
12	BA	643	A
12	BA	648	C
12	BA	649	A
12	BA	650	A
12	BA	656	C
12	BA	657	U
12	BA	661	U
12	BA	673	C
12	BA	674	U
12	BA	684	A
12	BA	689	A
12	BA	690	U
12	BA	691	A
12	BA	694	A
12	BA	695	U
12	BA	696	A
12	BA	697	C
12	BA	704	U
12	BA	705	U
12	BA	707	A
12	BA	708	C
12	BA	713	A
12	BA	715	U
12	BA	718	A
12	BA	719	C
12	BA	720	C
12	BA	722	A
12	BA	723	A
12	BA	724	A
12	BA	725	C
12	BA	727	A
12	BA	728	C
12	BA	736	C
12	BA	737	G
12	BA	744	A

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Mol	Chain	Res	Type
12	BA	745	A
12	BA	746	U
12	BA	747	U
12	BA	748	A
12	BA	753	G
12	BA	761	A
12	BA	764	A
12	BA	766	A
12	BA	774	A
12	BA	775	C
12	BA	777	A
12	BA	778	A
12	BA	779	G
12	BA	780	G
12	BA	782	A
12	BA	783	A
12	BA	784	G
12	BA	789	A
12	BA	795	G
12	BA	809	G
12	BA	814	C
12	BA	818	A
12	BA	819	A
12	BA	824	G
12	BA	825	C
12	BA	834	C
12	BA	835	A
12	BA	847	U
12	BA	848	C
12	BA	850	A
12	BA	852	C
12	BA	853	A
12	BA	854	U
12	BA	855	U
12	BA	859	A
12	BA	860	G
12	BA	864	U
12	BA	872	A
12	BA	876	C
12	BA	883	G
12	BA	887	C
12	BA	888	A

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Mol	Chain	Res	Type
12	BA	889	C
12	BA	890	C
12	BA	892	G
12	BA	895	U
12	BA	897	A
12	BA	899	G
12	BA	901	C
12	BA	902	C
12	BA	908	A
12	BA	909	U
12	BA	910	U
12	BA	922	A
12	BA	923	A
12	BA	924	G
12	BA	925	G
12	BA	931	U
12	BA	932	A
12	BA	933	A
12	BA	935	C
12	BA	938	U
12	BA	939	U
12	BA	948	A
12	BA	950	U
12	BA	958	U
12	BA	959	G
12	BA	960	U
12	BA	961	A
12	BA	964	A
12	BA	965	A
12	BA	967	G
12	BA	970	C
12	BA	977	G
12	BA	979	G
12	BA	981	U
12	BA	982	U
12	BA	983	U
12	BA	986	U
12	BA	988	U
12	BA	992	U
12	BA	1015	C
12	BA	1016	C
12	BA	1018	U

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Mol	Chain	Res	Type
12	BA	1022	G
12	BA	1026	A
12	BA	1027	G
12	BA	1028	A
12	BA	1034	G
12	BA	1038	A
12	BA	1041	A
12	BA	1045	U
12	BA	1050	C
12	BA	1051	G
12	BA	1055	A
12	BA	1056	G
12	BA	1057	A
12	BA	1063	U
12	BA	1064	G
12	BA	1071	U
12	BA	1072	A
12	BA	1075	U
12	BA	1080	A
12	BA	1089	G
12	BA	1092	A
12	BA	1093	A
12	BA	1094	A
12	BA	1123	A
12	BA	1127	A
12	BA	1129	C
12	BA	1137	A
12	BA	1138	G
12	BA	1140	A
12	BA	1145	C
12	BA	1146	G
12	BA	1166	A
12	BA	1167	C
12	BA	1168	A
12	BA	1169	A
12	BA	1178	C
12	BA	1183	U
12	BA	1188	U
12	BA	1190	A
12	BA	1195	A
12	BA	1205	G
12	BA	1206	U

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Mol	Chain	Res	Type
12	BA	1207	C
12	BA	1215	C
12	BA	1216	C
12	BA	1217	A
12	BA	1218	U
12	BA	1219	A
12	BA	1220	A
12	BA	1221	C
12	BA	1222	A
12	BA	1226	C
12	BA	1231	U
12	BA	1234	U
12	BA	1238	A
12	BA	1239	A
12	BA	1240	A
12	BA	1241	U
12	BA	1242	U
12	BA	1246	A
12	BA	1247	U
12	BA	1248	C
12	BA	1249	A
12	BA	1253	G
12	BA	1254	A
12	BA	1255	A
12	BA	1258	A
12	BA	1259	G
12	BA	1264	C
12	BA	1268	G
12	BA	1270	G
12	BA	1271	A
12	BA	1287	G
12	BA	1288	U
12	BA	1291	U
12	BA	1294	A
12	BA	1296	U
12	BA	1297	U
12	BA	1299	C
12	BA	1303	C
12	BA	1307	A
12	BA	1311	G
12	BA	1314	U
12	BA	1317	A

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Mol	Chain	Res	Type
12	BA	1324	C
12	BA	1325	G
12	BA	1326	A
12	BA	1328	G
12	BA	1331	G
12	BA	1341	A
12	BA	1342	C
12	BA	1348	U
12	BA	1352	G
12	BA	1353	C
12	BA	1357	C
12	BA	1358	G
12	BA	1377	U
12	BA	1385	U
12	BA	1387	A
12	BA	1388	A
12	BA	1389	A
12	BA	1390	G
12	BA	1396	C
12	BA	1399	G
12	BA	1404	G
12	BA	1406	G
12	BA	1409	C
12	BA	1410	A
12	BA	1420	A
12	BA	1426	G
12	BA	1427	G
12	BA	1428	U
12	BA	1429	C
12	BA	1432	U
12	BA	1433	U
12	BA	1436	U
12	BA	1438	U
12	BA	1444	A
12	BA	1445	U
12	BA	1448	A
12	BA	1458	G
12	BA	1459	U
12	BA	1465	A
12	BA	1466	G
12	BA	1467	G
12	BA	1468	A

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Mol	Chain	Res	Type
12	BA	1474	G
12	BA	1476	A
12	BA	1492	C
12	BA	1493	A
12	BA	1494	A
12	BA	1498	C
12	BA	1504	A
12	BA	1505	G
12	BA	1508	A
12	BA	1509	U
12	BA	1510	A
12	BA	1514	A
12	BA	1518	A
12	BA	1521	U
12	BA	1522	A
12	BA	1525	C
12	BA	1526	U
12	BA	1527	U
12	BA	1528	A
12	BA	1529	A
12	BA	1531	C
12	BA	1532	U
12	BA	1533	A
12	BA	1536	U
12	BA	1548	A
12	BA	1549	A
12	BA	1550	U
12	BA	1551	C
12	BA	1552	C
12	BA	1553	A
12	BA	1554	G
12	BA	1555	C
12	BA	1556	C
12	BA	1558	U
12	BA	1559	A
12	BA	1560	G
12	BA	1561	A
12	BA	1570	C
12	BA	1571	A
13	BB	3	U
13	BB	5	A
13	BB	7	G

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Mol	Chain	Res	Type
13	BB	8	U
13	BB	9	A
13	BB	13	U
13	BB	21	C
13	BB	22	A
13	BB	23	A
13	BB	24	A
13	BB	25	G
13	BB	29	G
13	BB	30	G
13	BB	34	U
13	BB	35	G
13	BB	43	C
13	BB	44	U
13	BB	45	A
13	BB	46	G
13	BB	47	A
13	BB	48	U
13	BB	55	C
13	BB	67	A
13	BB	69	C
13	BB	70	A
56	AV	6	G
56	AV	7	G
56	AV	9	C
56	AV	13	U
56	AV	14	A
56	AV	15	A
56	AV	16	A
56	AV	17	U
56	AV	18	A
56	AV	19	A
56	AV	22	U
56	AV	28	G
56	AV	39	G
56	AV	40	A
56	AV	43	A
56	AV	44	U
56	AV	45	G
56	AV	46	U
56	AV	51	U
56	AV	52	A

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Mol	Chain	Res	Type
56	AV	53	U
56	AV	54	A
56	AV	55	C
56	AV	56	C
56	AV	62	C
56	AV	63	G
56	AV	64	U
56	AV	65	A
56	AV	67	U
56	AV	68	A
56	AV	71	A

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	BA	39	A
12	BA	48	U
12	BA	101	U
12	BA	553	U
12	BA	1093	A
12	BA	1145	C
12	BA	1219	A
12	BA	1220	A
12	BA	1240	A
12	BA	1241	U
13	BB	20	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 226 ligands modelled in this entry, 220 are monoatomic - leaving 6 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
61	GSP	BC	901	57,62	30,34,34	1.92	2 (6%)	41,54,54	1.76	9 (21%)
63	FME	AV	101	56	8,9,10	0.96	0	7,9,11	0.67	0
60	SPM	BA	3205	-	13,13,13	0.37	0	12,12,12	0.81	0
59	5GP	BA	3204	-	26,26,26	0.85	1 (3%)	40,40,40	1.74	9 (22%)
60	SPM	BR	201	-	13,13,13	0.48	0	12,12,12	0.77	0
59	5GP	BA	3203	-	26,26,26	0.96	1 (3%)	40,40,40	2.09	9 (22%)

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
61	GSP	BC	901	57,62	-	0/21/38/38	0/3/3/3
63	FME	AV	101	56	-	4/7/9/11	-
60	SPM	BA	3205	-	-	6/11/11/11	-
59	5GP	BA	3204	-	-	5/10/26/26	0/3/3/3
60	SPM	BR	201	-	-	7/11/11/11	-
59	5GP	BA	3203	-	-	6/10/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	BC	901	GSP	PG-S1G	-9.35	1.70	1.90
59	BA	3203	5GP	C6-N1	-2.71	1.33	1.38
61	BC	901	GSP	C2-N3	2.40	1.38	1.33
59	BA	3204	5GP	C6-N1	-2.12	1.34	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	BA	3203	5GP	C5-C4-N3	-7.46	116.36	128.46
59	BA	3204	5GP	C5-C4-N3	-5.92	118.86	128.46
59	BA	3203	5GP	C2-N3-C4	5.45	122.01	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	BC	901	GSP	C5-C4-N3	-4.97	120.40	128.46
59	BA	3203	5GP	N9-C4-N3	4.69	135.37	125.94
61	BC	901	GSP	C2-N3-C4	4.55	120.41	112.30
59	BA	3204	5GP	C2-N3-C4	4.43	120.19	112.30
59	BA	3204	5GP	N9-C4-N3	3.48	132.93	125.94
61	BC	901	GSP	N9-C4-N3	3.34	132.65	125.94
59	BA	3203	5GP	C4-C5-N7	-2.94	106.06	110.72
59	BA	3203	5GP	C5-C6-N1	2.85	120.42	113.19
61	BC	901	GSP	PA-O3A-PB	-2.84	123.07	132.83
59	BA	3203	5GP	C2-N1-C6	-2.82	119.96	125.10
61	BC	901	GSP	C2-N1-C6	-2.76	120.06	125.10
59	BA	3203	5GP	C8-N7-C5	2.66	109.06	104.24
61	BC	901	GSP	N9-C8-N7	-2.65	108.40	113.39
59	BA	3204	5GP	C2-N1-C6	-2.54	120.47	125.10
61	BC	901	GSP	C8-N7-C5	2.52	108.80	104.24
61	BC	901	GSP	C5-C6-N1	2.47	119.46	113.19
59	BA	3204	5GP	C5-C6-N1	2.39	119.25	113.19
59	BA	3204	5GP	C4-C5-N7	-2.38	106.95	110.72
61	BC	901	GSP	O6-C6-C5	-2.34	120.40	126.60
59	BA	3204	5GP	O6-C6-C5	-2.20	120.77	126.60
59	BA	3203	5GP	N9-C8-N7	-2.18	109.29	113.39
59	BA	3204	5GP	N9-C8-N7	-2.11	109.41	113.39
59	BA	3204	5GP	C8-N7-C5	2.07	107.98	104.24
59	BA	3203	5GP	C6-C5-N7	2.04	134.05	130.25

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	BA	3203	5GP	C5'-O5'-P-OP1
59	BA	3203	5GP	C5'-O5'-P-OP3
59	BA	3203	5GP	C5'-O5'-P-OP2
59	BA	3204	5GP	C5'-O5'-P-OP1
59	BA	3204	5GP	C5'-O5'-P-OP3
59	BA	3204	5GP	C5'-O5'-P-OP2
59	BA	3204	5GP	O4'-C4'-C5'-O5'
59	BA	3204	5GP	C3'-C4'-C5'-O5'
63	AV	101	FME	C-CA-CB-CG
63	AV	101	FME	CA-CB-CG-SD
60	BR	201	SPM	N5-C6-C7-C8
60	BA	3205	SPM	C7-C8-C9-N10
60	BA	3205	SPM	C2-C3-C4-N5

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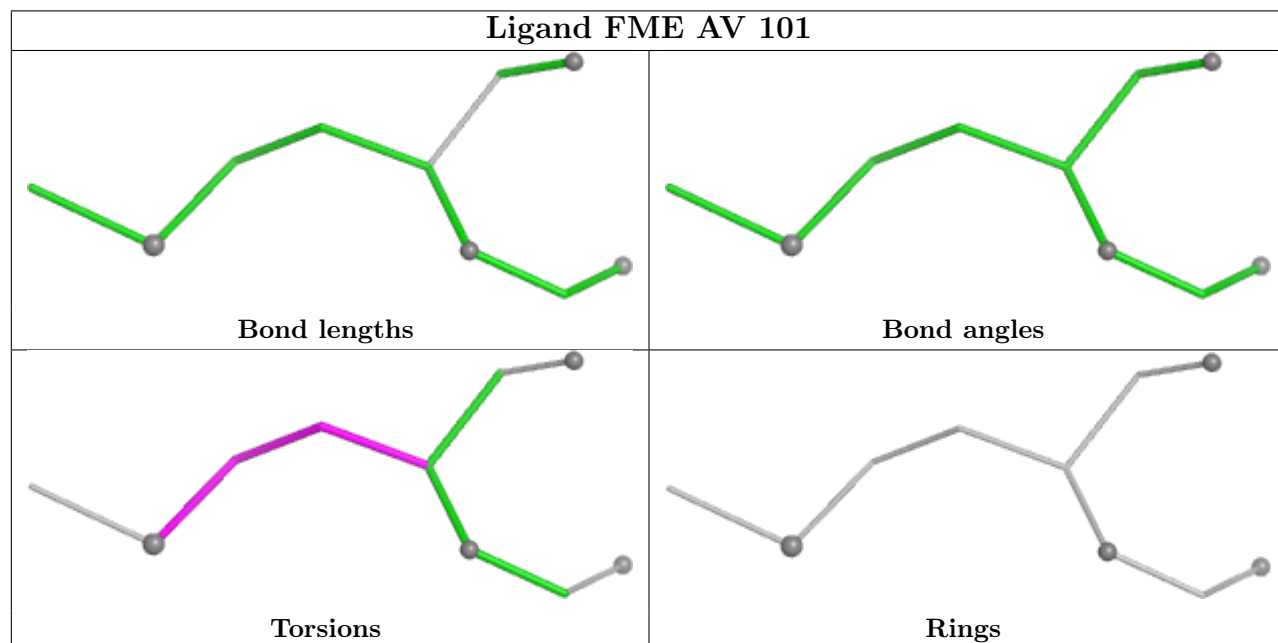
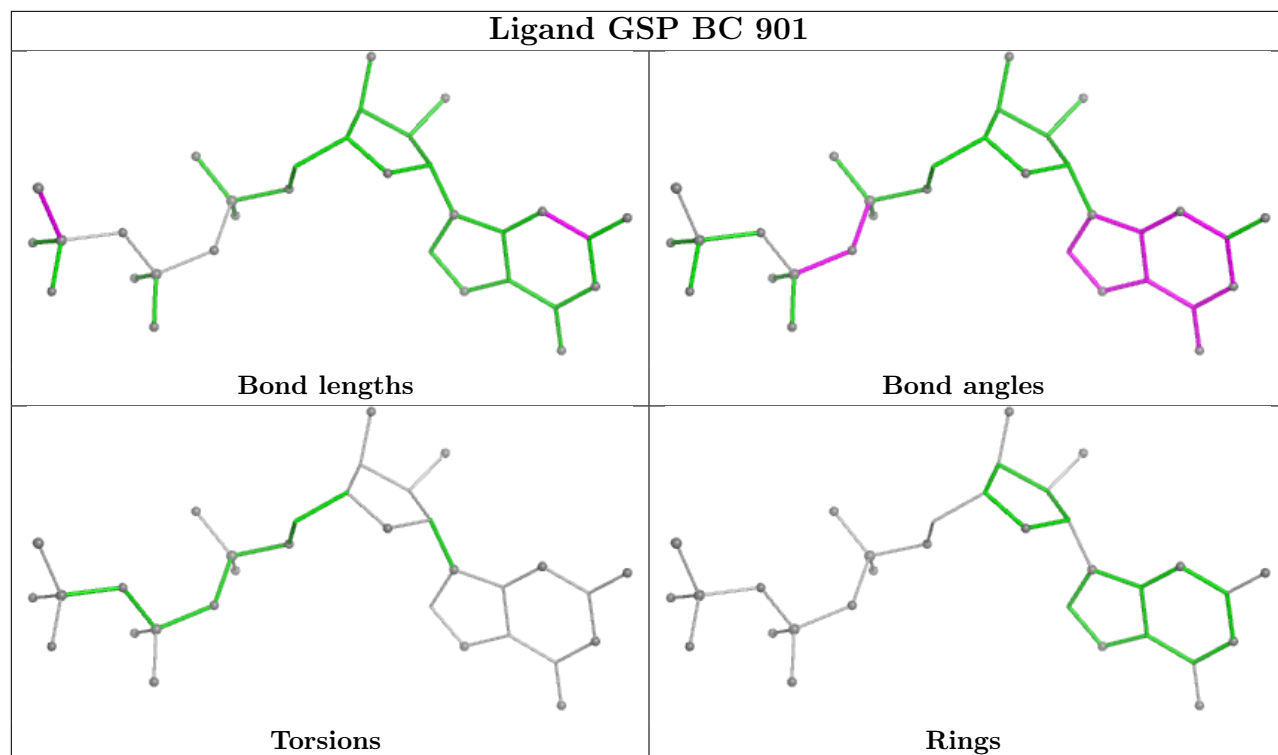
Mol	Chain	Res	Type	Atoms
60	BR	201	SPM	C2-C3-C4-N5
63	AV	101	FME	N-CA-CB-CG
60	BR	201	SPM	C8-C9-N10-C11
63	AV	101	FME	CB-CG-SD-CE
60	BR	201	SPM	N1-C2-C3-C4
60	BA	3205	SPM	C6-C7-C8-C9
60	BR	201	SPM	C6-C7-C8-C9
59	BA	3203	5GP	C4'-C5'-O5'-P
60	BA	3205	SPM	N1-C2-C3-C4
60	BA	3205	SPM	C7-C6-N5-C4
60	BR	201	SPM	N10-C11-C12-C13
60	BR	201	SPM	C12-C11-N10-C9
60	BA	3205	SPM	N5-C6-C7-C8
59	BA	3203	5GP	O4'-C4'-C5'-O5'
59	BA	3203	5GP	C2'-C1'-N9-C8

There are no ring outliers.

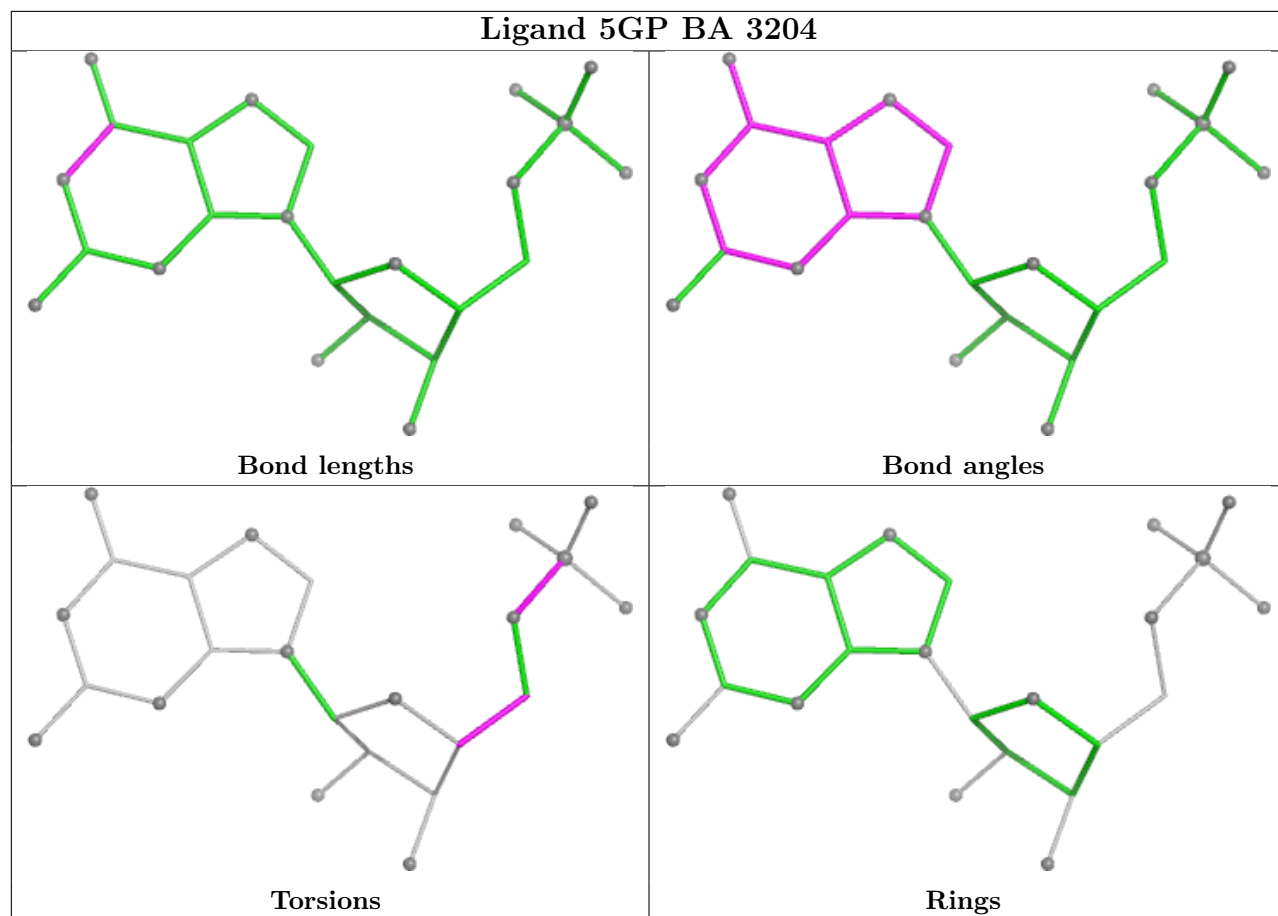
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	BC	901	GSP	1	0
60	BA	3205	SPM	2	0

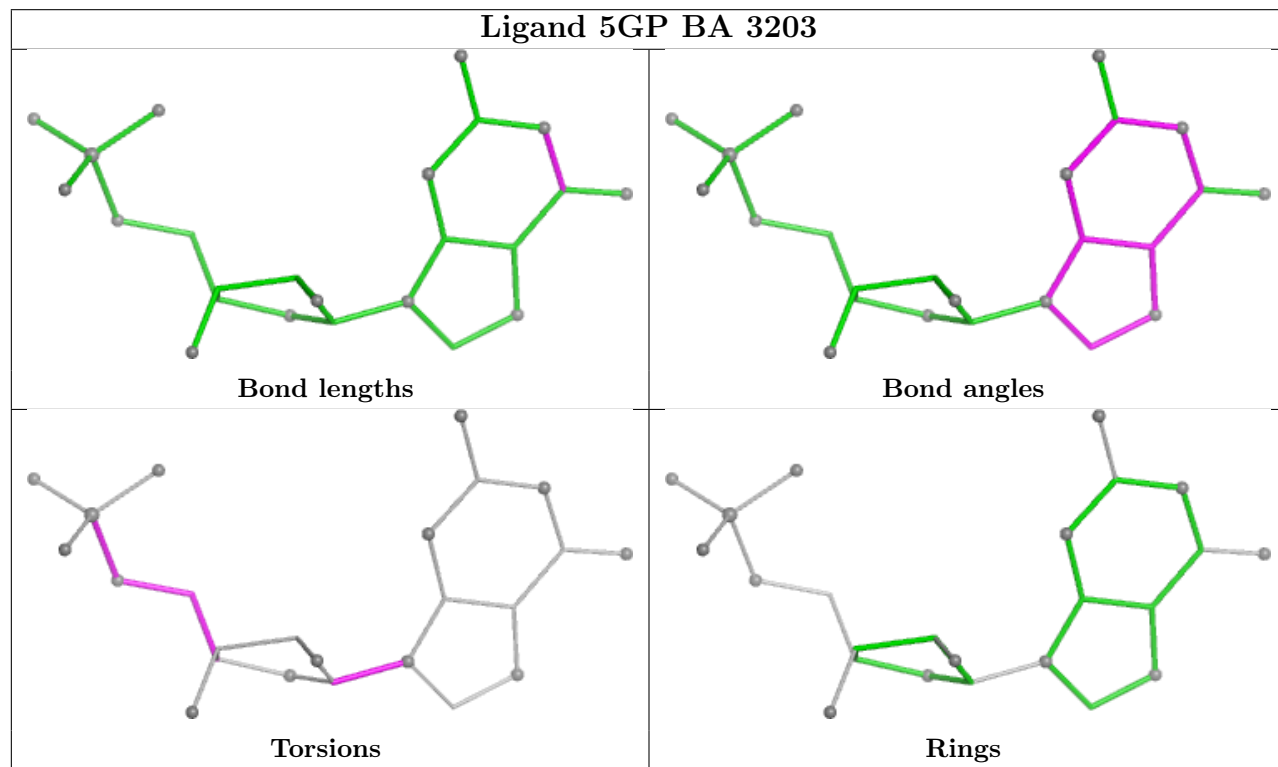
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand 5GP BA 3204



Ligand 5GP BA 3203



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
55	Bz	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bz	710:ALA	C	1001:ALA	N	60.04
1	Bz	415:ALA	C	601:ALA	N	51.34
1	Bz	106:ALA	C	301:ALA	N	30.40
1	Bz	615:ALA	C	700:ALA	N	17.65
1	Bz	315:ALA	C	399:ALA	N	16.53

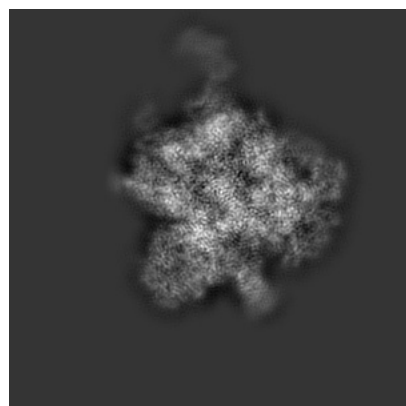
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4370. These allow visual inspection of the internal detail of the map and identification of artifacts.

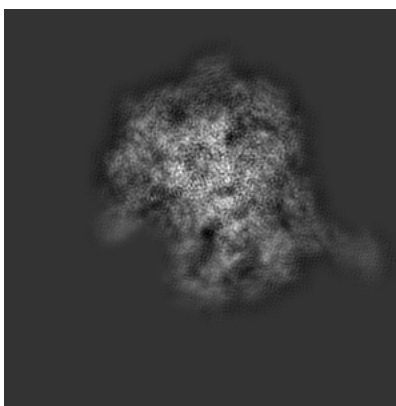
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

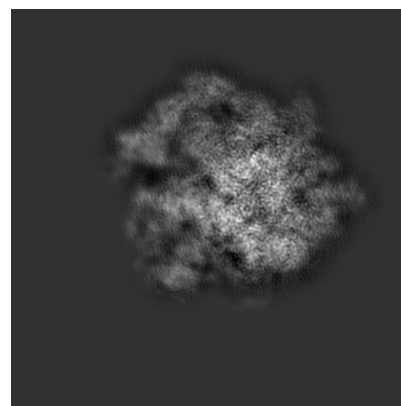
6.1.1 Primary map



X

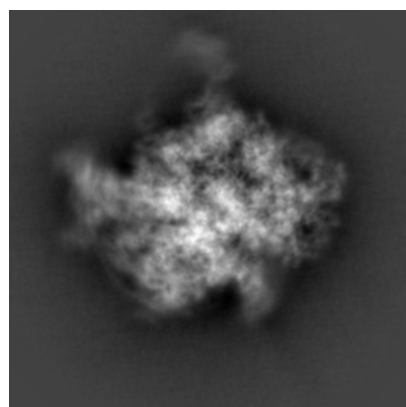


Y

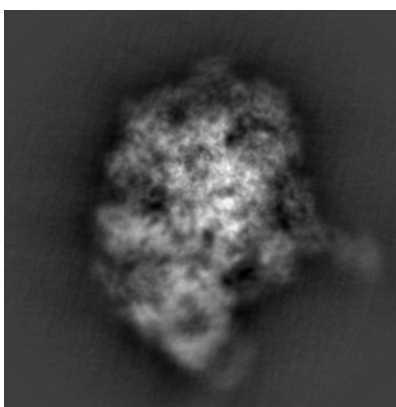


Z

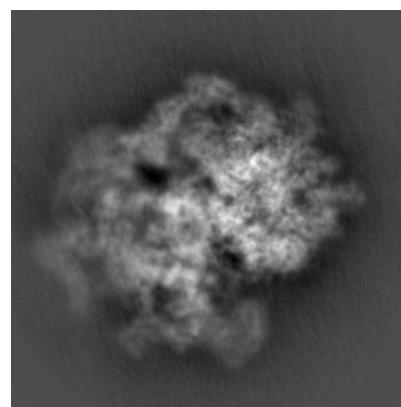
6.1.2 Raw map



X



Y

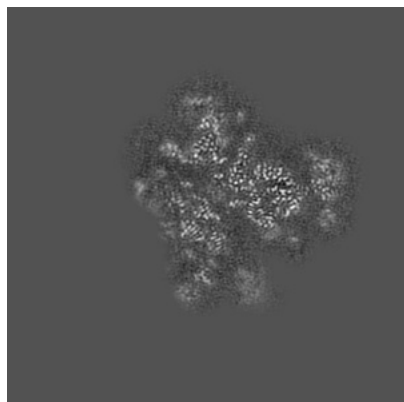


Z

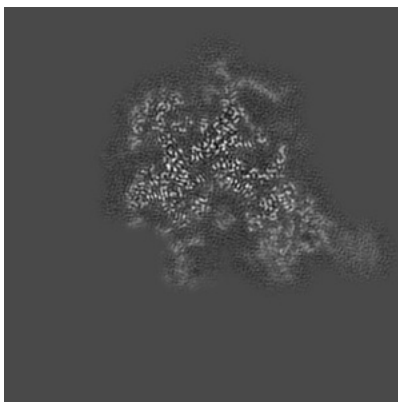
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

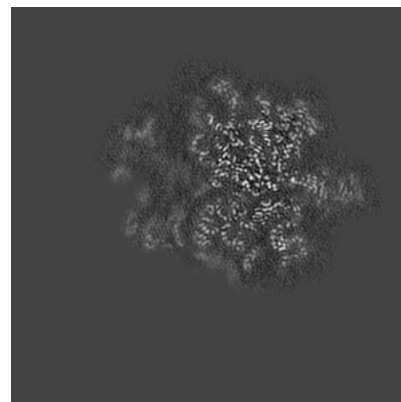
6.2.1 Primary map



X Index: 140

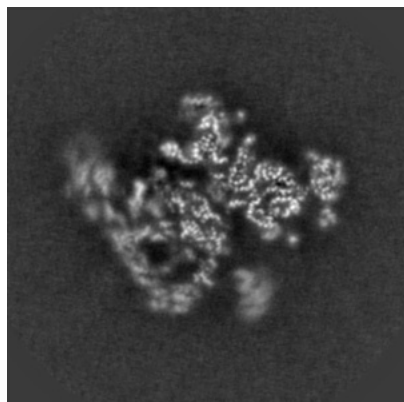


Y Index: 140

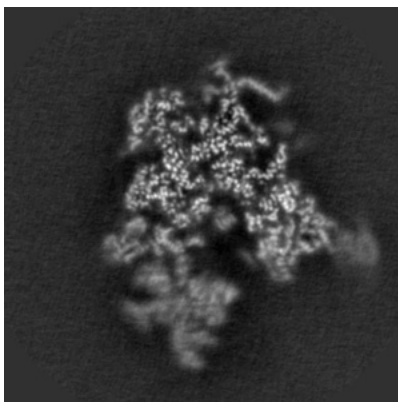


Z Index: 140

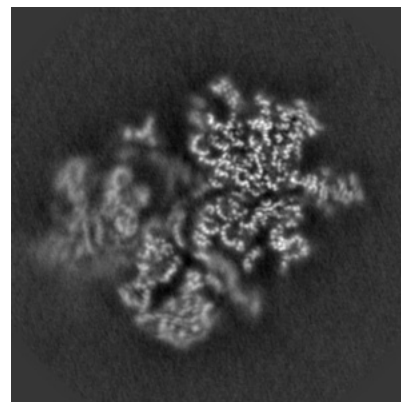
6.2.2 Raw map



X Index: 140



Y Index: 140

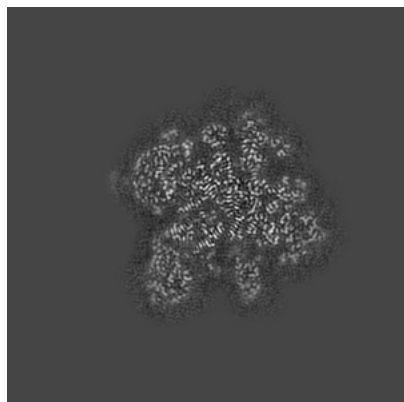


Z Index: 140

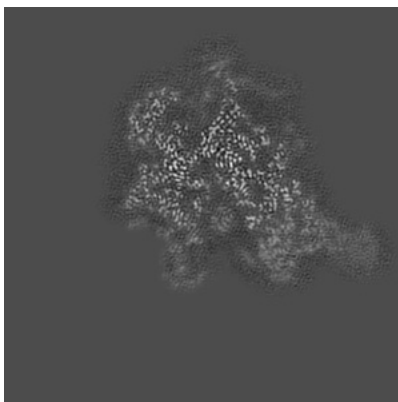
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

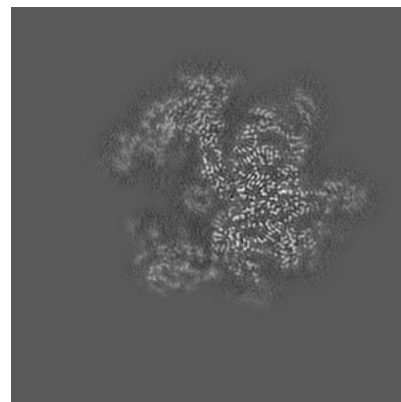
6.3.1 Primary map



X Index: 169

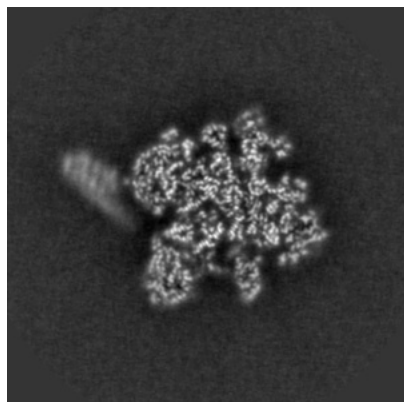


Y Index: 142

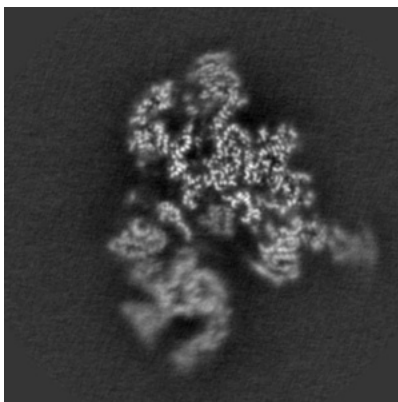


Z Index: 153

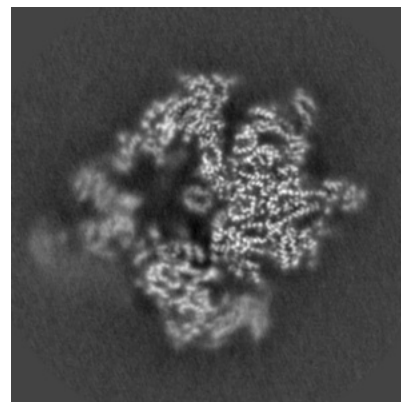
6.3.2 Raw map



X Index: 169



Y Index: 148

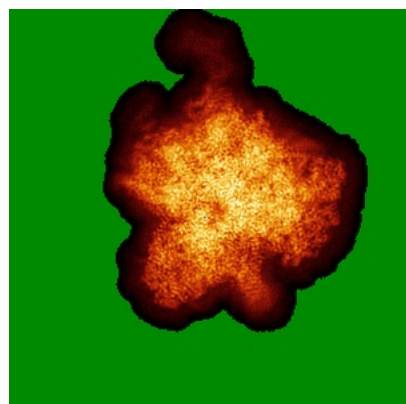


Z Index: 153

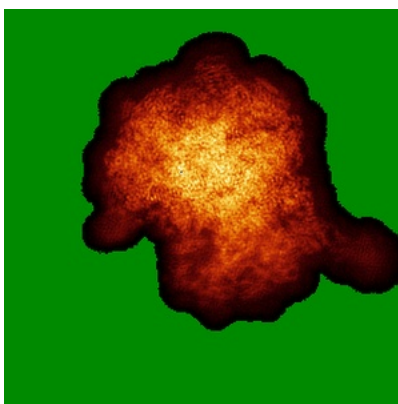
The images above show the largest variance slices of the map in three orthogonal directions.

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

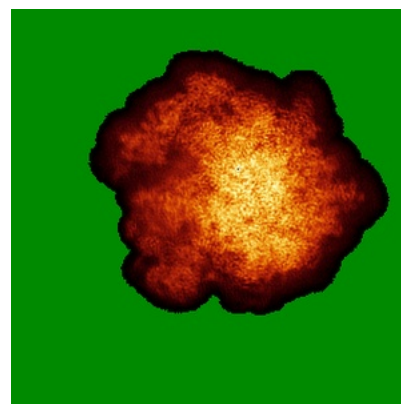
6.4.1 Primary map



X

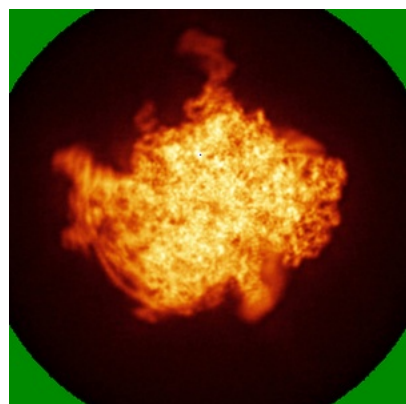


Y

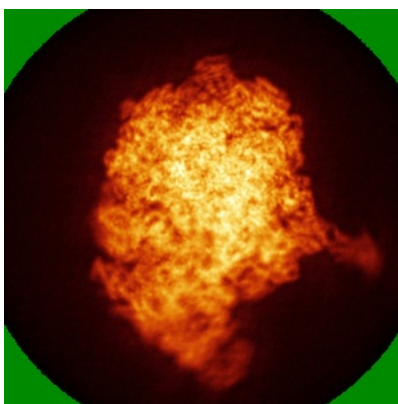


Z

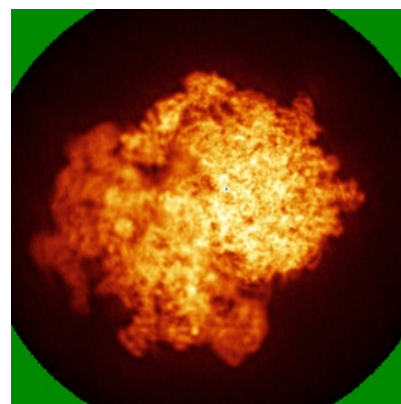
6.4.2 Raw map



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

6.5.2 Raw map



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

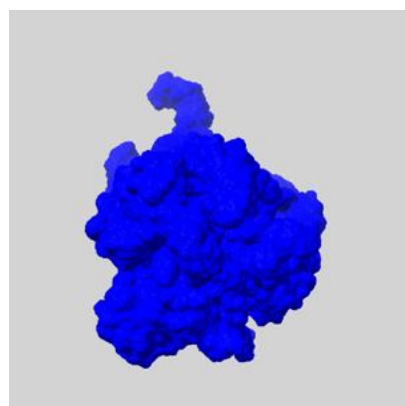
6.6 Mask visualisation [i](#)

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

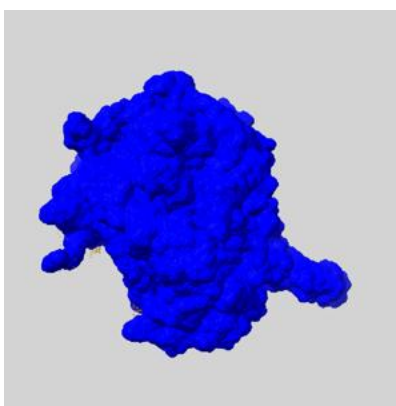
A mask typically either:

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

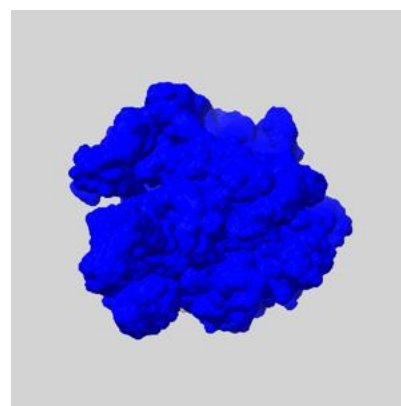
6.6.1 emd_4370_msk_1.map [i](#)



X



Y

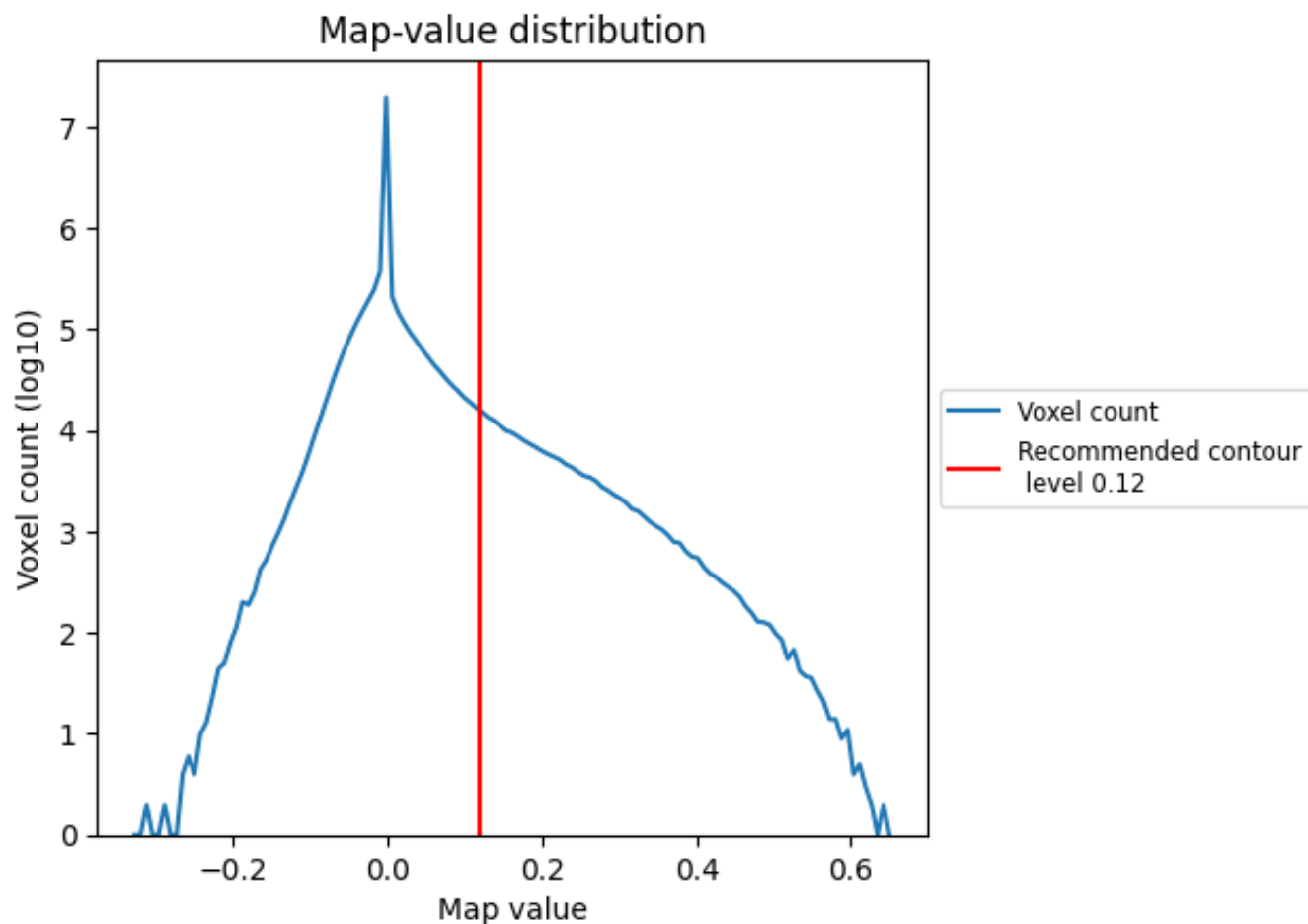


Z

7 Map analysis [i](#)

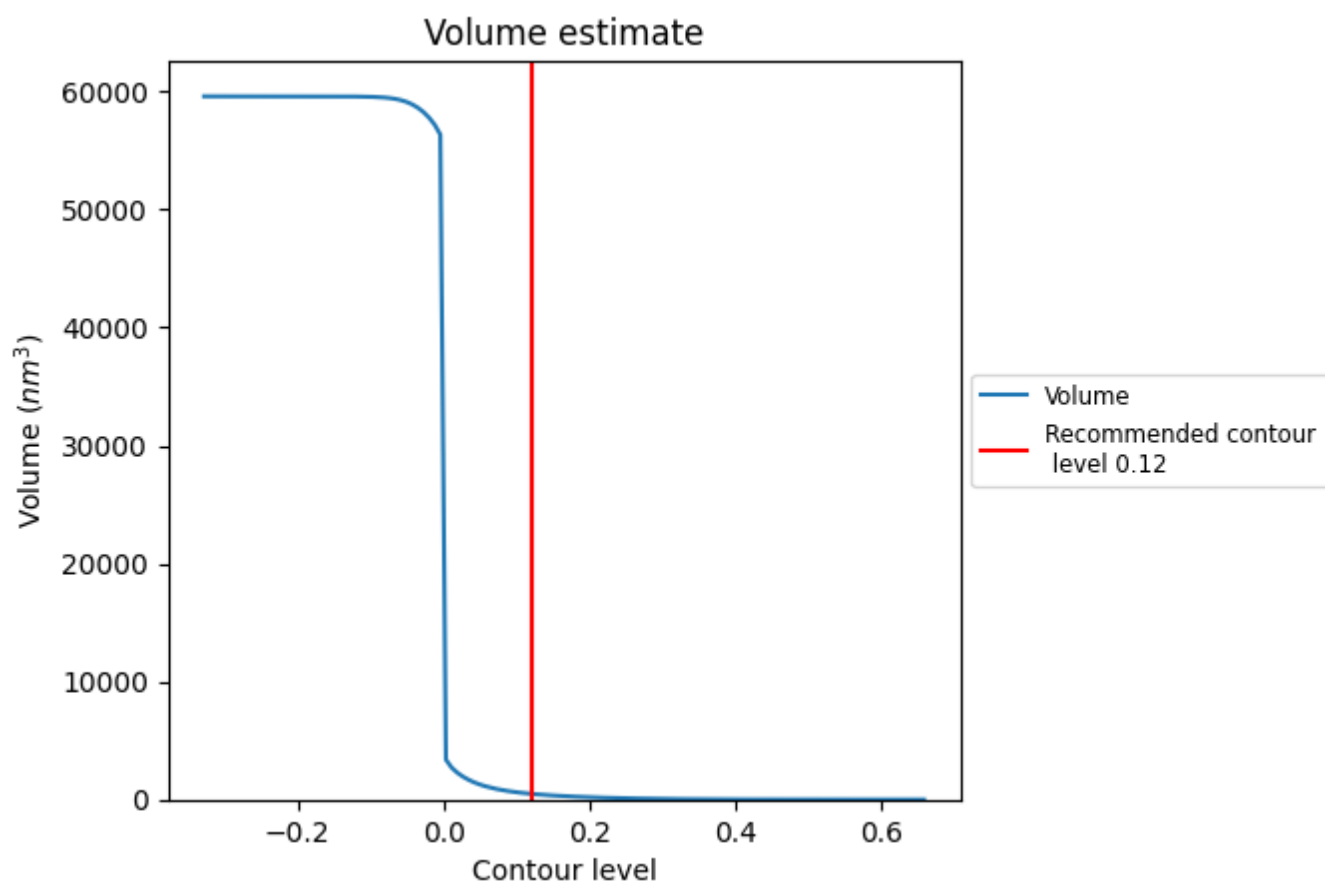
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

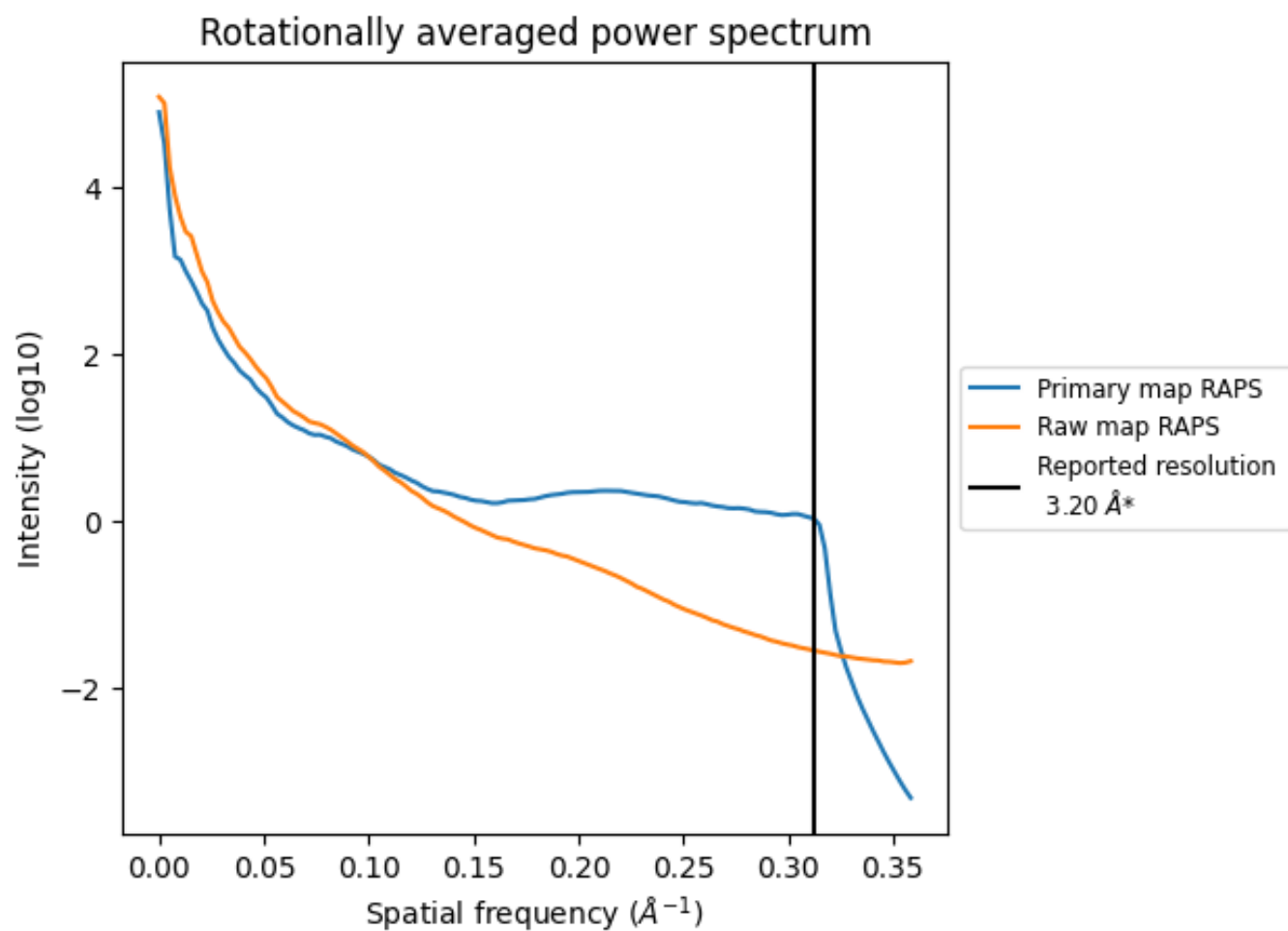
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 485 nm^3 ; this corresponds to an approximate mass of 438 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 ⓘ

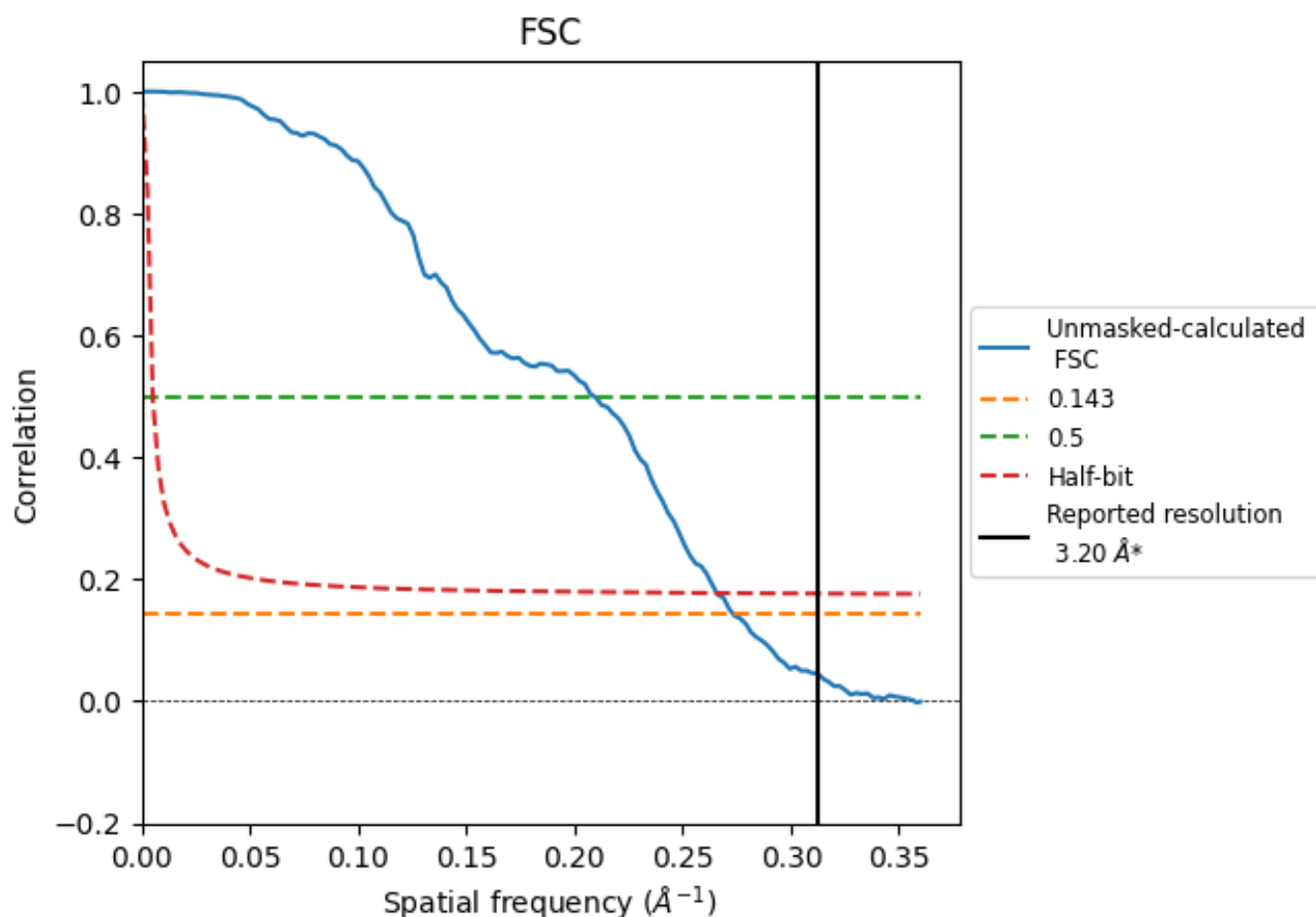


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

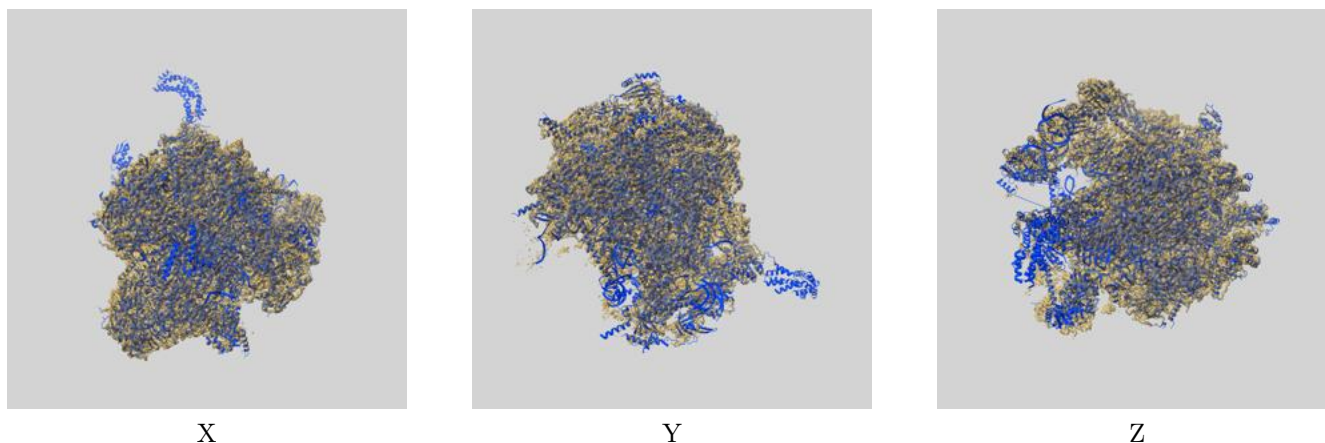
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.66	4.78	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.66 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

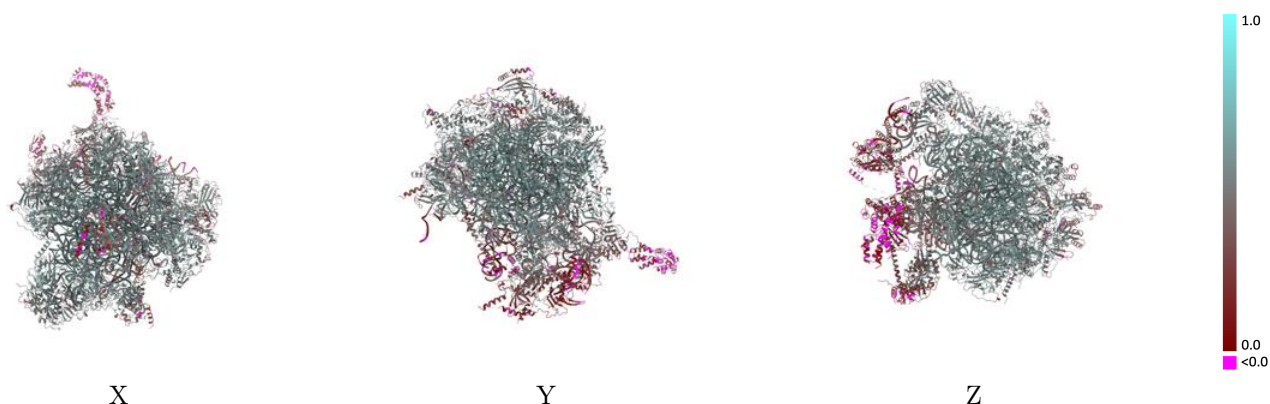
This section contains information regarding the fit between EMDB map EMD-4370 and PDB model 6GB2. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

9.1 Map-model overlay [i](#)



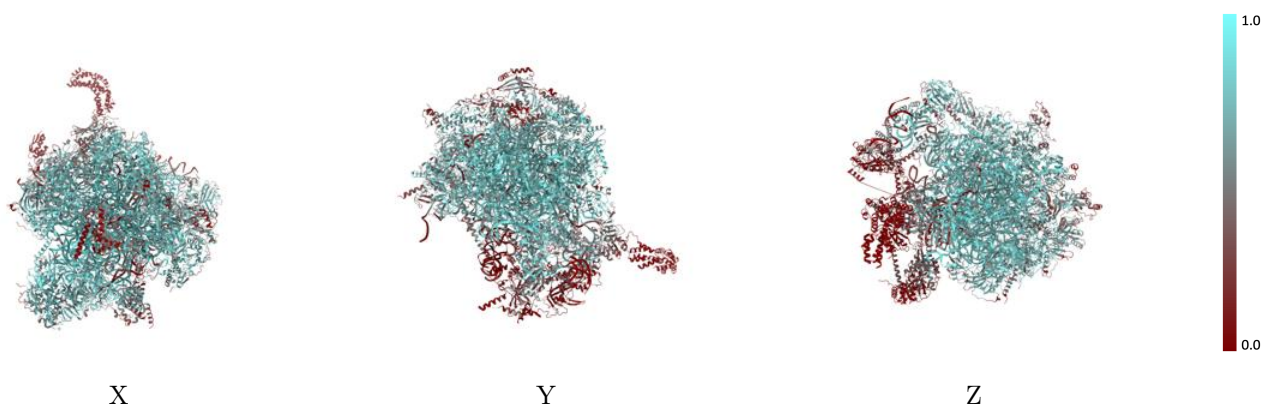
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



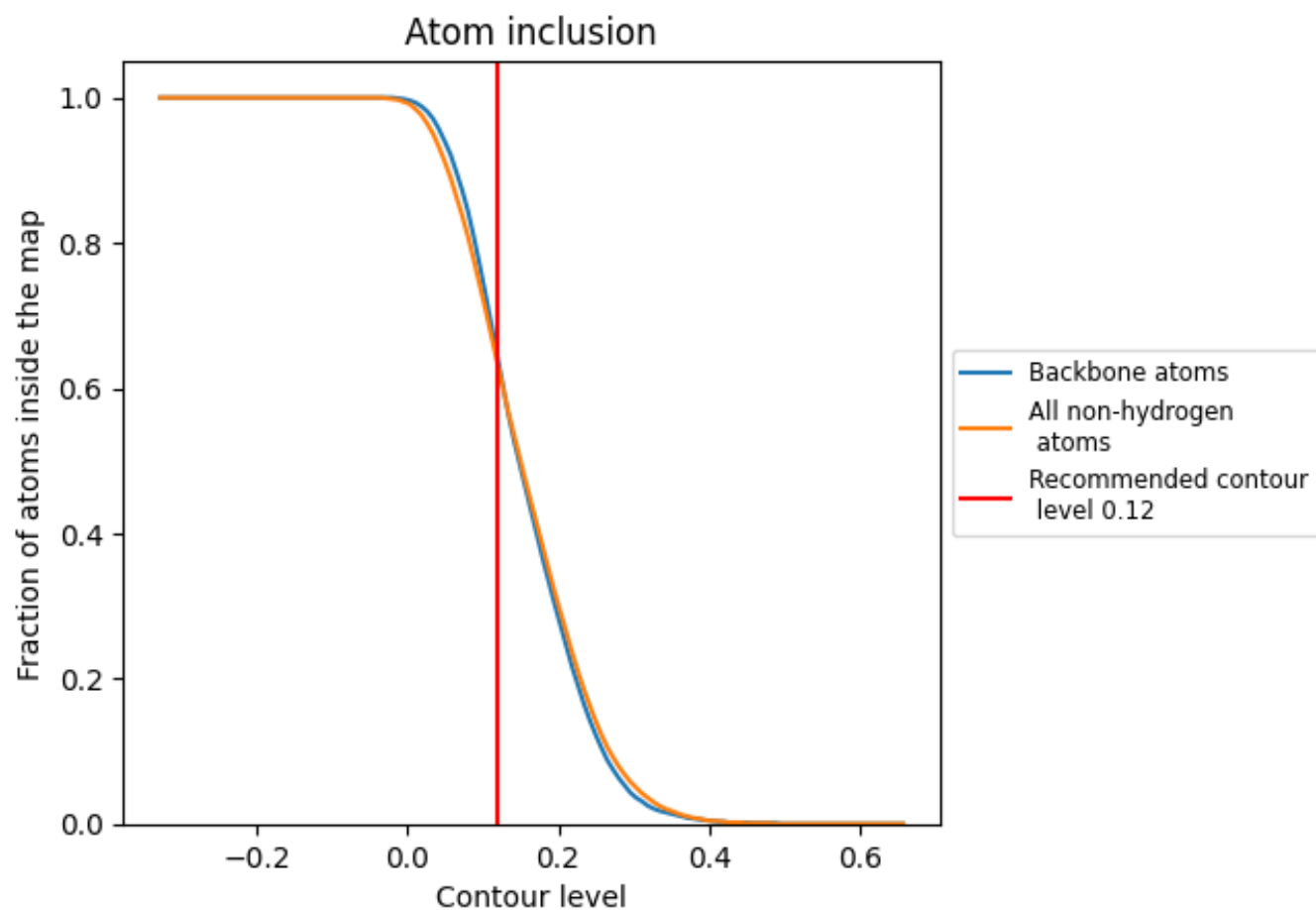
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 63% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6310	 0.4810
AV	 0.0440	 0.1900
B0	 0.7590	 0.5630
B1	 0.6000	 0.4850
B2	 0.7180	 0.5260
B3	 0.7270	 0.5410
B4	 0.3340	 0.2940
B5	 0.6980	 0.5220
B6	 0.4810	 0.4760
B7	 0.8020	 0.5900
B8	 0.7720	 0.5710
B9	 0.7820	 0.5530
BA	 0.8420	 0.5520
BB	 0.4940	 0.2870
BC	 0.2590	 0.3620
BD	 0.6690	 0.5360
BE	 0.7180	 0.5320
BF	 0.7370	 0.5480
BI	 0.4800	 0.4340
BJ	 0.3390	 0.3300
BK	 0.1670	 0.2330
BL	 0.0040	 0.1550
BN	 0.7750	 0.5590
BO	 0.6180	 0.5250
BP	 0.7330	 0.5470
BQ	 0.6820	 0.5310
BR	 0.7360	 0.5470
BS	 0.6810	 0.5090
BT	 0.6410	 0.5130
BU	 0.7540	 0.5500
BV	 0.7220	 0.5330
BW	 0.7250	 0.5520
BX	 0.6800	 0.5080
BY	 0.4290	 0.4340
Ba	 0.6580	 0.4990



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Chain	Atom inclusion	Q-score
Bb	 0.6590	 0.4740
Bc	 0.6020	 0.4660
Bd	 0.2790	 0.2660
Be	 0.5850	 0.4820
Bf	 0.6390	 0.4810
Bg	 0.7220	 0.5470
Bh	 0.6650	 0.4940
Bi	 0.3580	 0.3980
Bj	 0.1740	 0.1960
Bk	 0.3150	 0.3150
Bl	 0.7220	 0.5250
Bm	 0.2810	 0.3950
Bn	 0.7640	 0.5620
Bo	 0.6580	 0.5030
Bp	 0.3790	 0.3700
Bq	 0.3300	 0.3570
Bt	 0.7460	 0.5540
Bu	 0.4530	 0.3870
Bv	 0.4930	 0.4090
Bw	 0.6910	 0.5090
Bx	 0.6750	 0.5040
Bz	 0.0150	 0.0900
CL	 0.0090	 0.1490
DL	 0.0050	 0.1210
EL	 0.0000	 0.0300
FL	 0.0050	 0.0730
GL	 0.0000	 0.0360
HL	 0.0000	 0.0780