



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 06:21 AM UTC

PDB ID : 6YXY / pdb_00006yxy
EMDB ID : EMD-11000
Title : State B of the Trypanosoma brucei mitoribosomal large subunit assembly intermediate
Authors : Jaskolowski, M.; Ramrath, D.J.F.; Bieri, P.; Niemann, M.; Mattei, S.; Calderaro, S.; Leibundgut, M.A.; Horn, E.K.; Boehringer, D.; Schneider, A.; Ban, N.
Deposited on : 2020-05-04
Resolution : 3.10 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:

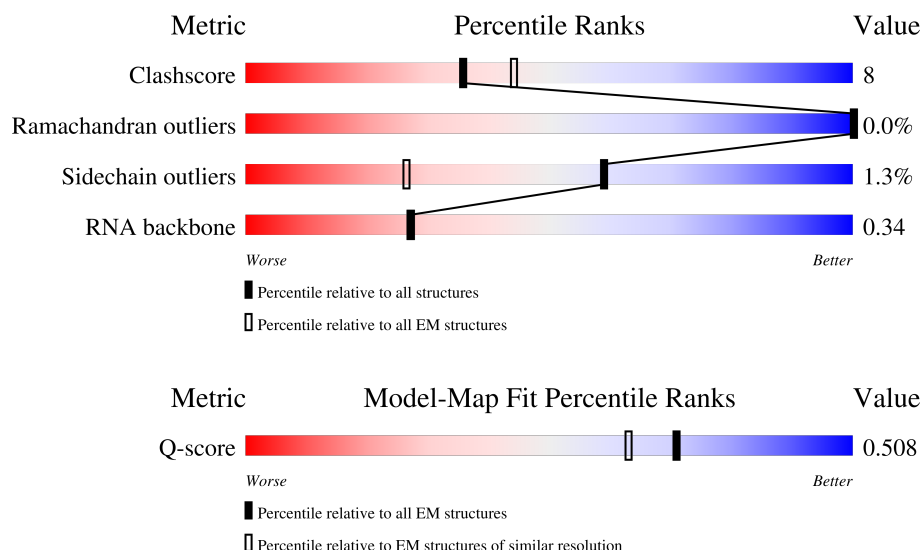
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 3.10 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.



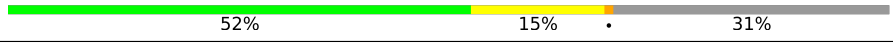
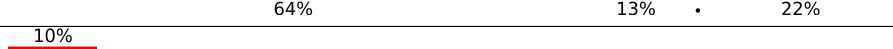
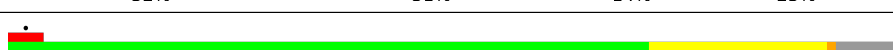
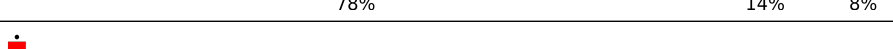
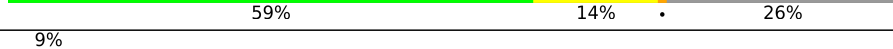
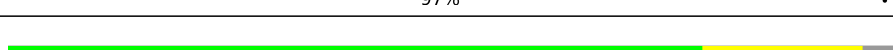
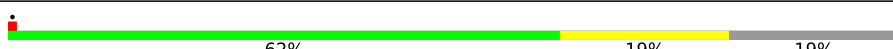
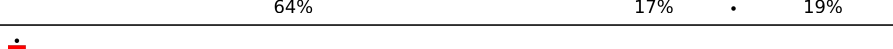
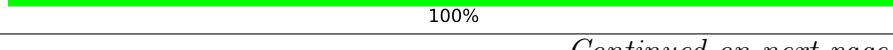
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	A1	241	
2	A2	471	

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Mol	Chain	Length	Quality of chain
3	A3	218	
4	A5	80	
5	A8	181	
6	AA	1176	
7	BA	831	
8	EA	576	
9	BB	541	
10	EB	754	
11	EC	406	
12	BD	547	
13	ED	616	
14	AE	473	
15	BE	449	
16	EE	586	
17	UE	33	
18	AF	459	
19	BF	426	
20	EF	373	
21	EG	156	
22	BH	349	
23	EH	634	
24	AI	263	
25	BI	342	
26	EI	349	
27	UI	23	

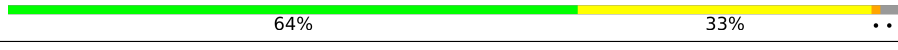
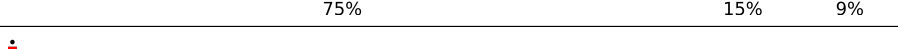
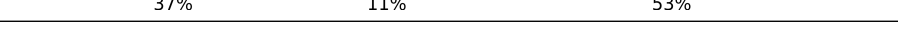
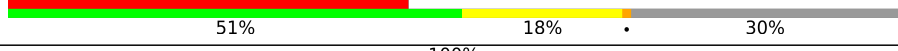
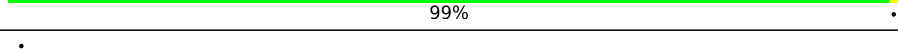
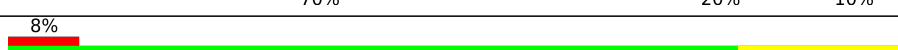
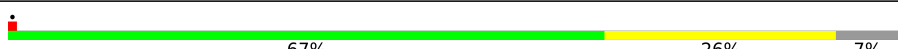
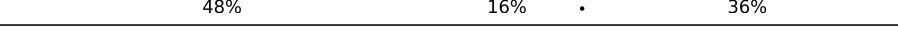
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Mol	Chain	Length	Quality of chain
28	BJ	333	
29	EJ	116	
30	AK	342	
31	BK	386	
32	EK	148	
32	ER	148	
33	UK	25	
34	BL	312	
35	EL	691	
36	UL	72	
37	EM	451	
38	UM	8	
39	AN	202	
40	BN	302	
41	EN	731	
42	AO	217	
43	BO	262	
44	EO	319	
44	EP	319	
45	AP	374	
46	BQ	231	
47	EQ	655	
48	AR	301	
49	BR	205	
50	BS	198	

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Mol	Chain	Length	Quality of chain
51	ES	524	
52	AT	144	
53	BT	191	
54	ET	102	
55	AU	213	
56	BU	185	
57	EU	56	
58	AV	188	
59	BV	190	
60	AW	278	
61	BW	188	
62	AX	246	
63	BX	190	
64	UX	180	
65	AY	378	
66	BZ	190	
67	Ba	153	
68	Bb	162	
69	Bc	146	
70	Ae	197	
71	Af	189	
72	Bf	113	
73	Ag	260	
74	Bg	105	
75	Bh	92	

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Mol	Chain	Length	Quality of chain
76	Bi	245	
77	Al	218	
78	Ao	1520	
79	Ap	309	
80	At	154	
81	Av	242	

2 Entry composition [i](#)

There are 90 unique types of molecules in this entry. The entry contains 177224 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 bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	217	Total	C	N	O	S	0	0
			1788	1138	324	317	9		

- Molecule 2 is a protein called uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	452	Total	C	N	O	S	0	0
			3661	2337	635	676	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	238	GLY	ALA	conflict	UNP Q38EM7

- Molecule 3 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A3	150	Total	C	N	O	S	0	0
			1226	781	236	203	6		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A3	22	VAL	GLY	conflict	UNP Q38ED8
A3	26	SER	LEU	conflict	UNP Q38ED8
A3	35	ASN	SER	conflict	UNP Q38ED8
A3	198	UNK	ALA	conflict	UNP Q38ED8

- Molecule 4 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A5	55	Total	C	N	O	S	0	0
			483	311	90	76	6		

- Molecule 5 is a protein called bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A8	142	Total	C	N	O	S	0	0
			1203	753	243	198	9		

- Molecule 6 is a RNA chain called 12S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AA	903	Total	C	N	O	P	0	0
			18833	8482	3157	6291	903		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1032	N	A	conflict	GB 343546
AA	1033	N	U	conflict	GB 343546
AA	1034	N	U	conflict	GB 343546
AA	1035	N	G	conflict	GB 343546
AA	1036	N	U	conflict	GB 343546
AA	1037	N	U	conflict	GB 343546
AA	1038	N	C	conflict	GB 343546
AA	1039	N	A	conflict	GB 343546
AA	1040	N	U	conflict	GB 343546
AA	1041	N	C	conflict	GB 343546
AA	1042	N	A	conflict	GB 343546
AA	1043	N	A	conflict	GB 343546
AA	1044	N	A	conflict	GB 343546
AA	1045	N	A	conflict	GB 343546
AA	1046	N	U	conflict	GB 343546
AA	1047	N	A	conflict	GB 343546
AA	1048	N	G	conflict	GB 343546
AA	1049	N	U	conflict	GB 343546

- Molecule 7 is a protein called mL67.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BA	769	Total	C	N	O	S	0	0
			6059	3847	1074	1104	34		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	359	CYS	GLY	conflict	UNP Q386Z1

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Chain	Residue	Modelled	Actual	Comment	Reference
BA	385	PRO	SER	conflict	UNP Q386Z1
BA	387	SER	GLY	conflict	UNP Q386Z1
BA	456	ALA	VAL	conflict	UNP Q386Z1
BA	520	LEU	ARG	conflict	UNP Q386Z1

- Molecule 8 is a protein called mt-EngA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	EA	532	Total	C	N	O	S	0	0
			4263	2672	785	785	21		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EA	12	UNK	ARG	conflict	UNP Q57TZ4

- Molecule 9 is a protein called mL68.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BB	412	Total	C	N	O	S	0	0
			3365	2142	595	607	21		

- Molecule 10 is a protein called mt-LAF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	EB	663	Total	C	N	O	S	0	0
			5308	3344	1017	920	27		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EB	301	ALA	THR	conflict	UNP D0A9G9

- Molecule 11 is a protein called mt-LAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	EC	373	Total	C	N	O	S	0	0
			3005	1923	540	524	18		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EC	25	UNK	HIS	conflict	UNP Q38FJ3

- Molecule 12 is a protein called mL70.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BD	419	Total	C	N	O	S	0	0
			3349	2134	586	609	20		

- Molecule 13 is a protein called mt-LAF4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	ED	598	Total	C	N	O	S	0	0
			4764	3026	850	865	23		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ED	252	ARG	LYS	conflict	UNP Q385G9
ED	326	UNK	GLY	conflict	UNP Q385G9

- Molecule 14 is a protein called uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AE	434	Total	C	N	O	S	0	0
			3461	2215	598	630	18		

- Molecule 15 is a protein called mL71.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BE	407	Total	C	N	O	S	0	0
			3223	2044	558	608	13		

- Molecule 16 is a protein called mt-LAF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	EE	433	Total	C	N	O	S	0	0
			3444	2144	649	638	13		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EE	20	VAL	MET	conflict	UNP Q38DC9

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Chain	Residue	Modelled	Actual	Comment	Reference
EE	27	ARG	LYS	conflict	UNP Q38DC9
EE	337	ASP	GLY	conflict	UNP Q38DC9
EE	546	VAL	ALA	conflict	UNP Q38DC9

- Molecule 17 is a protein called UNK.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	UE	33	Total	C	N	O		0	0
			165	99	33	33			

- Molecule 18 is a protein called uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AF	442	Total	C	N	O	S	0	0
			3597	2294	624	654	25		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AF	12	THR	ALA	conflict	UNP D0A7A6

- Molecule 19 is a protein called mL72.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BF	346	Total	C	N	O	S	0	0
			2847	1803	519	512	13		

- Molecule 20 is a protein called mt-LAF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	EF	302	Total	C	N	O	S	0	0
			2290	1451	406	425	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EF	47	UNK	GLU	conflict	UNP C9ZWD9
EF	48	UNK	VAL	conflict	UNP C9ZWD9
EF	49	UNK	ALA	conflict	UNP C9ZWD9
EF	50	UNK	GLN	conflict	UNP C9ZWD9
EF	51	UNK	VAL	conflict	UNP C9ZWD9

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Chain	Residue	Modelled	Actual	Comment	Reference
EF	52	UNK	THR	conflict	UNP C9ZWD9

- Molecule 21 is a protein called mt-LAF7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	EG	154	Total	C	N	O	S	0	0
			1295	812	256	218	9		

- Molecule 22 is a protein called mL74.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BH	282	Total	C	N	O	S	0	0
			2293	1457	423	409	4		

- Molecule 23 is a protein called mt-LAF8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	EH	438	Total	C	N	O	S	0	0
			3471	2193	627	632	19		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EH	166	UNK	GLY	conflict	UNP Q57ZS6
EH	485	PRO	SER	conflict	UNP Q57ZS6
EH	495	ARG	LYS	conflict	UNP Q57ZS6

- Molecule 24 is a protein called bL9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AI	240	Total	C	N	O	S	0	0
			1967	1260	345	353	9		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	249	UNK	LYS	conflict	UNP Q57UC5
AI	250	UNK	GLY	conflict	UNP Q57UC5
AI	251	UNK	PRO	conflict	UNP Q57UC5
AI	252	UNK	VAL	conflict	UNP Q57UC5
AI	253	UNK	LYS	conflict	UNP Q57UC5

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Chain	Residue	Modelled	Actual	Comment	Reference
AI	254	UNK	GLN	conflict	UNP Q57UC5
AI	255	UNK	ARG	conflict	UNP Q57UC5
AI	256	UNK	LYS	conflict	UNP Q57UC5
AI	257	UNK	ALA	conflict	UNP Q57UC5
AI	258	UNK	ARG	conflict	UNP Q57UC5

- Molecule 25 is a protein called mL75.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BI	323	Total	C	N	O	S	0	0
			2641	1681	483	461	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BI	227	ASN	ASP	conflict	UNP D0A108

- Molecule 26 is a protein called MALSU1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	EI	275	Total	C	N	O	S	0	0
			2101	1307	372	412	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EI	12	TYR	CYS	conflict	UNP Q584Y2
EI	70	PRO	LEU	conflict	UNP Q584Y2
EI	129	HIS	ARG	conflict	UNP Q584Y2
EI	144	SER	LEU	conflict	UNP Q584Y2

- Molecule 27 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	UI	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 28 is a protein called mL76.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BJ	293	Total	C	N	O	S	0	0
			2433	1527	463	435	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BJ	329	GLU	ALA	conflict	UNP Q383M2

- Molecule 29 is a protein called L0R8F8.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	EJ	95	Total	C	N	O	S	0	0
			765	475	156	131	3		

- Molecule 30 is a protein called uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AK	301	Total	C	N	O	S	0	0
			2499	1593	456	433	17		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AK	327	UNK	ALA	conflict	UNP Q586R9

- Molecule 31 is a protein called mL77.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BK	228	Total	C	N	O	S	0	0
			1855	1153	353	341	8		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	33	UNK	HIS	conflict	UNP C9ZQR6
BK	60	UNK	PRO	conflict	UNP C9ZQR6
BK	348	VAL	LEU	conflict	UNP C9ZQR6

- Molecule 32 is a protein called mt-ACP.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	EK	84	Total	C	N	O	S	0	0
			669	427	106	135	1		
32	ER	84	Total	C	N	O	S	0	0
			669	427	106	135	1		

- Molecule 33 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	UK	25	Total	C	N	O	0	0
			125	75	25	25		

- Molecule 34 is a protein called mL78.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BL	259	Total	C	N	O	S	0	0
			2023	1241	397	375	10		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BL	77	TYR	HIS	conflict	UNP Q389N4
BL	218	ALA	THR	conflict	UNP Q389N4
BL	292	SER	ASN	conflict	UNP Q389N4

- Molecule 35 is a protein called mt-LAF12.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	EL	559	Total	C	N	O	S	0	0
			4484	2876	781	798	29		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EL	104	UNK	ILE	conflict	UNP C9ZVC0
EL	108	GLU	GLY	conflict	UNP C9ZVC0
EL	126	VAL	LEU	conflict	UNP C9ZVC0
EL	188	SER	PHE	conflict	UNP C9ZVC0

- Molecule 36 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	UL	72	Total	C	N	O	0	0
			360	216	72	72		

- Molecule 37 is a protein called Mtg1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	EM	330	Total	C	N	O	S	0	0
			2606	1646	476	469	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EM	407	UNK	PRO	conflict	UNP Q38E75

- Molecule 38 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	UM	8	Total	C	N	O	0	0
			40	24	8	8		

- Molecule 39 is a protein called uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	AN	193	Total	C	N	O	S	0	0
			1639	1059	301	269	10		

- Molecule 40 is a protein called mL80.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BN	214	Total	C	N	O	S	0	0
			1714	1077	320	312	5		

- Molecule 41 is a protein called mt-LAF14.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	EN	638	Total	C	N	O	S	0	0
			5025	3152	909	936	28		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EN	18	GLU	GLY	conflict	UNP C9ZPS0

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Chain	Residue	Modelled	Actual	Comment	Reference
EN	310	LYS	ASN	conflict	UNP C9ZPS0
EN	676	CYS	TYR	conflict	UNP C9ZPS0

- Molecule 42 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AO	165	Total	C	N	O	S	0	0
			1339	843	272	215	9		

- Molecule 43 is a protein called mL81.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BO	215	Total	C	N	O	S	0	0
			1686	1058	294	321	13		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	30	THR	ILE	conflict	UNP Q385L5
BO	123	LEU	MET	conflict	UNP Q385L5
BO	134	PRO	SER	conflict	UNP Q385L5
BO	196	ASN	SER	conflict	UNP Q385L5
BO	238	ALA	GLU	conflict	UNP Q385L5

- Molecule 44 is a protein called mt-LAF15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	EO	275	Total	C	N	O	S	0	0
			2141	1348	396	387	10		
44	EP	245	Total	C	N	O	S	0	0
			1919	1212	349	349	9		

- Molecule 45 is a protein called uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AP	325	Total	C	N	O	S	0	0
			2691	1713	499	466	13		

- Molecule 46 is a protein called mL83.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BQ	218	Total	C	N	O	S	0	0
			1651	1049	288	306	8		

- Molecule 47 is a protein called mt-EngB.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	EQ	471	Total	C	N	O	S	0	0
			3628	2286	657	666	19		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EQ	26	CYS	ARG	conflict	UNP Q380Y8
EQ	272	SER	ASN	conflict	UNP Q380Y8
EQ	325	ALA	THR	conflict	UNP Q380Y8
EQ	326	ALA	THR	conflict	UNP Q380Y8
EQ	379	UNK	PRO	conflict	UNP Q380Y8
EQ	400	SER	PRO	conflict	UNP Q380Y8
EQ	426	ARG	GLN	conflict	UNP Q380Y8
EQ	447	GLU	LYS	conflict	UNP Q380Y8
EQ	448	UNK	SER	conflict	UNP Q380Y8
EQ	468	SER	PRO	conflict	UNP Q380Y8
EQ	472	SER	PRO	conflict	UNP Q380Y8

- Molecule 48 is a protein called bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AR	257	Total	C	N	O	S	0	0
			2146	1359	399	374	14		

- Molecule 49 is a protein called mL84.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BR	196	Total	C	N	O	S	0	0
			1659	1064	299	287	9		

- Molecule 50 is a protein called mL85.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BS	151	Total	C	N	O	S	0	0
			1218	753	232	226	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BS	45	ILE	VAL	conflict	UNP Q38FG8
BS	173	UNK	LEU	conflict	UNP Q38FG8

- Molecule 51 is a protein called mt-LAF18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	ES	152	Total	C	N	O	S	0	0
			1259	779	246	230	4		

- Molecule 52 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AT	141	Total	C	N	O	S	0	0
			1163	732	221	204	6		

- Molecule 53 is a protein called mL86.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BT	173	Total	C	N	O	S	0	0
			1435	884	278	267	6		

- Molecule 54 is a protein called mt-LAF19.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	ET	101	Total	C	N	O	S	0	0
			839	529	166	140	4		

- Molecule 55 is a protein called bL20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AU	175	Total	C	N	O	S	0	0
			1423	895	280	243	5		

- Molecule 56 is a protein called mL87.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BU	83	Total	C	N	O	S	0	0
			705	442	143	116	4		

- Molecule 57 is a protein called mt-LAF20.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	EU	47	Total	C	N	O	S	0	0
			407	250	90	61	6		

- Molecule 58 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AV	181	Total	C	N	O	S	0	0
			1424	909	257	252	6		

- Molecule 59 is a protein called mL88.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BV	90	Total	C	N	O	S	0	0
			763	492	133	136	2		

- Molecule 60 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AW	278	Total	C	N	O	S	0	0
			2251	1427	417	393	14		

- Molecule 61 is a protein called mL89.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BW	187	Total	C	N	O	S	0	0
			1557	987	298	264	8		

- Molecule 62 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AX	166	Total	C	N	O	S	0	0
			1400	904	247	244	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AX	126	TYR	HIS	conflict	UNP Q387G3

- Molecule 63 is a protein called mL90.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BX	133	Total	C	N	O	S	0	0
			1088	695	201	183	9		

- Molecule 64 is a protein called UNK.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	UX	180	Total	C	N	O	S	0	0
			900	540	180	180			

- Molecule 65 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AY	340	Total	C	N	O	S	0	0
			2790	1741	497	537	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	345	GLU	VAL	conflict	UNP C9ZK52

- Molecule 66 is a protein called mL92.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	BZ	190	Total	C	N	O	S	0	0
			1420	897	247	269	7		

- Molecule 67 is a protein called mL93.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Ba	142	Total	C	N	O	S	0	0
			1245	800	226	212	7		

- Molecule 68 is a protein called mL94.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Bb	128	Total	C	N	O	S	0	0
			1011	637	191	181	2		

- Molecule 69 is a protein called mL95.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bc	137	Total	C	N	O	S	0	0
			1194	776	216	201	1		

- Molecule 70 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Ae	127	Total	C	N	O	S	0	0
			1031	667	190	169	5		

- Molecule 71 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Af	139	Total	C	N	O	S	0	0
			1107	692	210	200	5		

- Molecule 72 is a protein called mL98.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bf	87	Total	C	N	O		0	0
			725	462	131	132			

- Molecule 73 is a protein called mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Ag	186	Total	C	N	O	S	0	0
			1564	979	295	283	7		

- Molecule 74 is a protein called mL99.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bg	83	Total	C	N	O	S	0	0
			667	418	130	117	2		

- Molecule 75 is a protein called mL100.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bh	91	Total	C	N	O	S	0	0
			730	466	129	125	10		

- Molecule 76 is a protein called mL101.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bi	192	Total	C	N	O	S	0	0
			1502	958	277	263	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bi	143	MET	ILE	conflict	UNP Q4GZ80
Bi	163	VAL	LEU	conflict	UNP Q4GZ80
Bi	213	ILE	PRO	conflict	UNP Q4GZ80

- Molecule 77 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Al	181	Total	C	N	O	S	0	0
			1440	936	250	247	7		

- Molecule 78 is a protein called mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ao	184	Total	C	N	O	S	0	0
			1443	903	263	270	7		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ao	-1239	GLN	ARG	conflict	UNP Q385V2
Ao	-1157	ALA	GLU	conflict	UNP Q385V2
Ao	-1105	ALA	VAL	conflict	UNP Q385V2
Ao	-1062	GLY	SER	conflict	UNP Q385V2
Ao	-879	HIS	TYR	conflict	UNP Q385V2
Ao	-776	UNK	HIS	conflict	UNP Q385V2
Ao	-742	UNK	LYS	conflict	UNP Q385V2
Ao	-724	GLU	LYS	conflict	UNP Q385V2
Ao	-707	UNK	SER	conflict	UNP Q385V2
Ao	-521	GLU	GLY	conflict	UNP Q385V2
Ao	-515	ARG	GLN	conflict	UNP Q385V2
Ao	-481	LEU	VAL	conflict	UNP Q385V2
Ao	-214	ALA	VAL	conflict	UNP Q385V2
Ao	-175	LEU	VAL	conflict	UNP Q385V2
Ao	?	-	LEU	deletion	UNP Q385V2
Ao	?	-	LYS	deletion	UNP Q385V2

- Molecule 79 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Ap	297	Total	C	N	O	S	0	0
			2428	1572	428	416	12		

- Molecule 80 is a protein called mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	At	138	Total	C	N	O	S	0	0
			1149	722	223	200	4		

- Molecule 81 is a protein called mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Av	196	Total	C	N	O	S	0	0
			1668	1062	309	285	12		

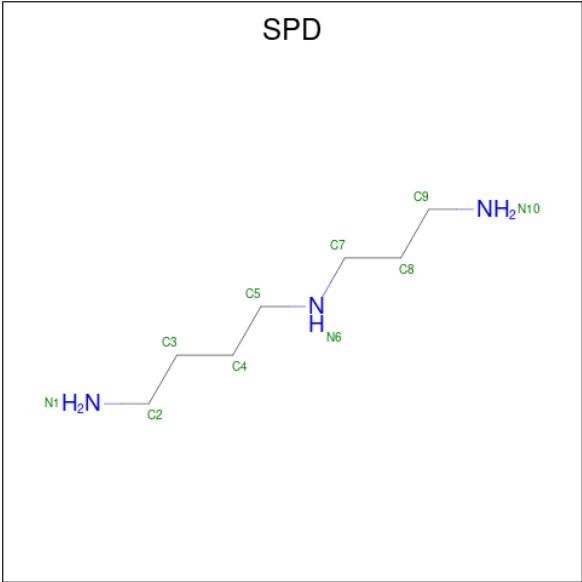
- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
82	A5	1	Total	Zn	0
			1	1	
82	EG	1	Total	Zn	0
			1	1	
82	BX	2	Total	Zn	0
			2	2	
82	Bh	1	Total	Zn	0
			1	1	

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

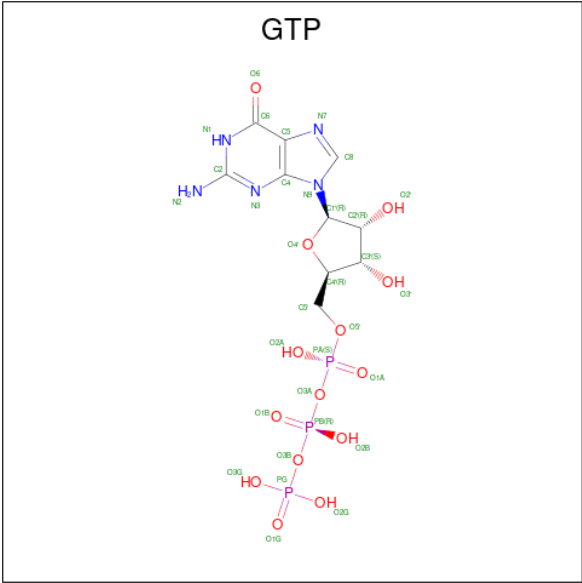
Mol	Chain	Residues	Atoms		AltConf
83	AA	29	Total	Mg	0
			29	29	
83	EA	2	Total	Mg	0
			2	2	
83	EB	1	Total	Mg	0
			1	1	
83	EQ	1	Total	Mg	0
			1	1	

- Molecule 84 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms			AltConf
84	AA	1	Total	C	N	0
			10	7	3	

- Molecule 85 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

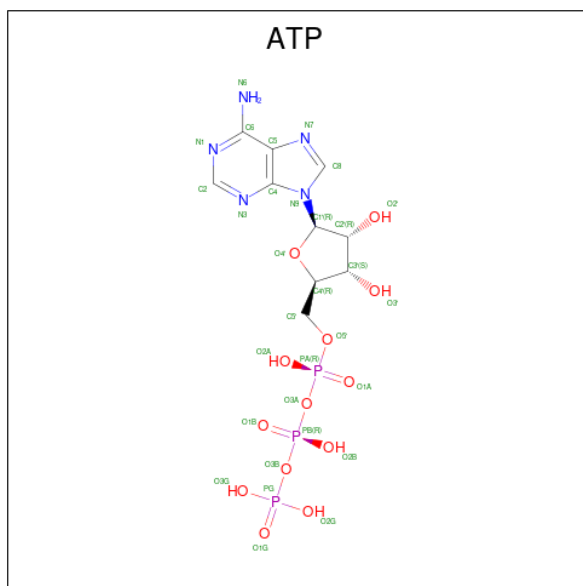


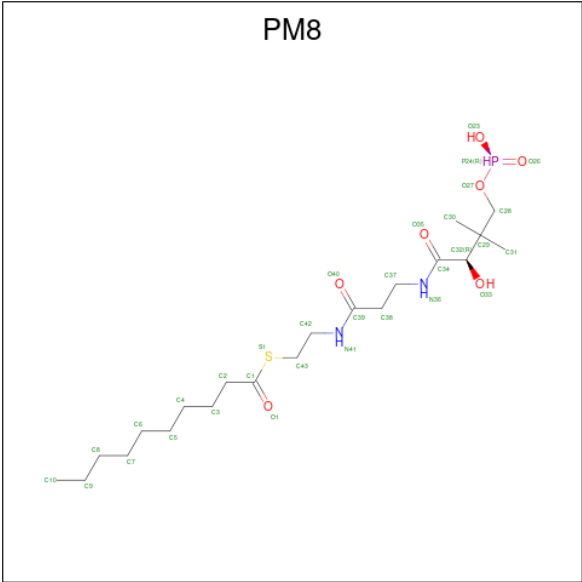
Mol	Chain	Residues	Atoms					AltConf
85	EA	1	Total	C	N	O	P	0
			32	10	5	14	3	
85	EA	1	Total	C	N	O	P	0
			32	10	5	14	3	
85	EQ	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 86 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
86	EA	2	Total	Na	0
			2	2	

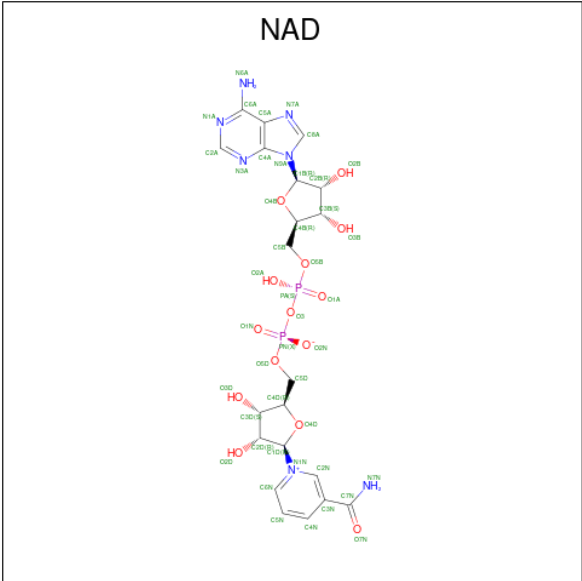
- Molecule 87 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).





Mol	Chain	Residues	Atoms					AltConf
88	EK	1	Total	C	N	O	P	S
			32	21	2	7	1	1
88	ER	1	Total	C	N	O	P	S
			32	21	2	7	1	1

- Molecule 89 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
89	Av	1	Total	C	N	O	P	
			44	21	7	14	2	0

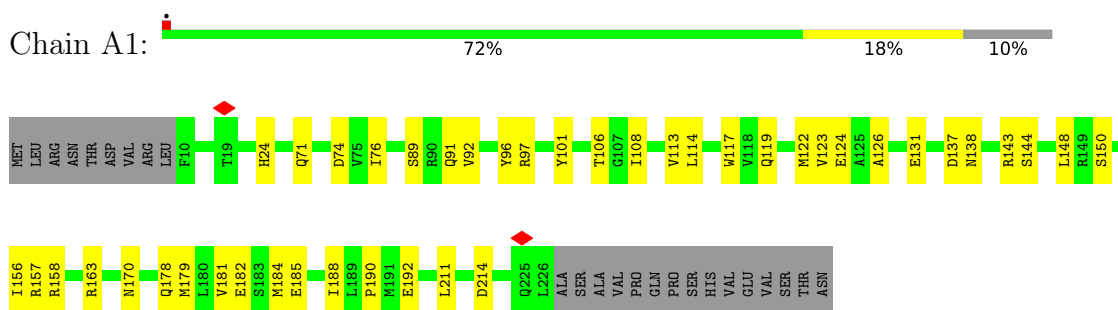
- Molecule 90 is water.

Mol	Chain	Residues	Atoms		AltConf
90	EA	2	Total 2	O 2	0
90	EA	2	Total 2	O 2	0
90	EB	4	Total 4	O 4	0
90	EQ	2	Total 2	O 2	0

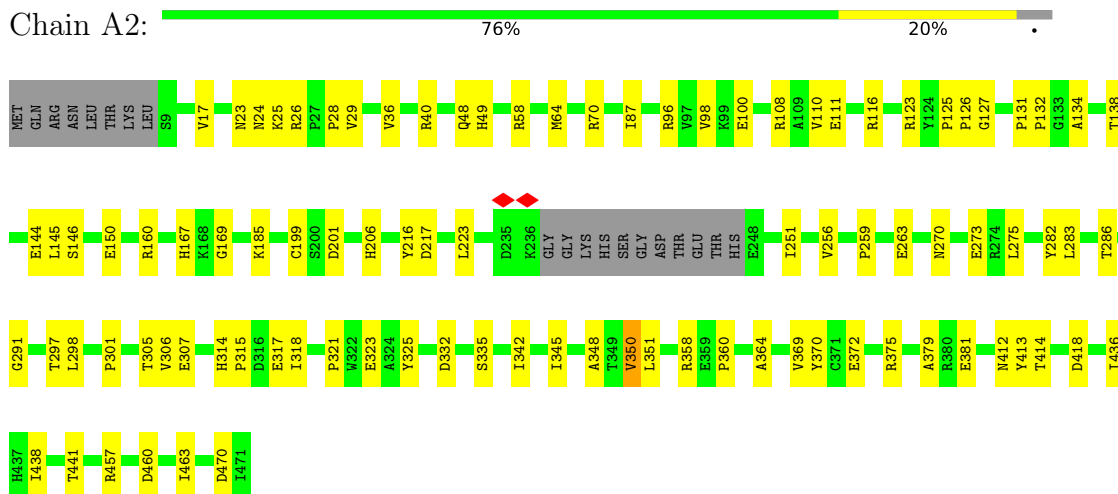
3 Residue-property plots

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.

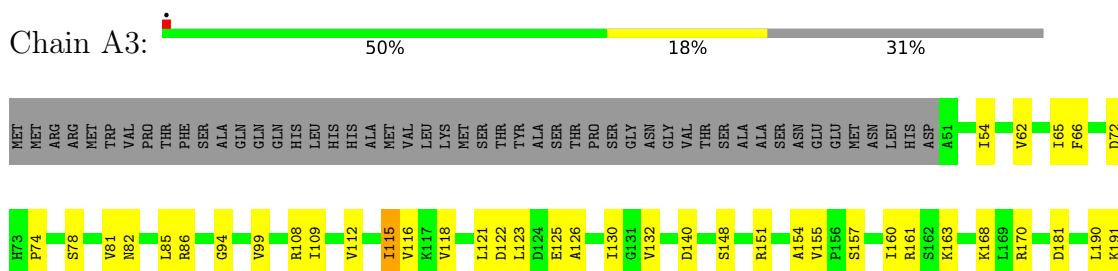
• Molecule 1: bL28m

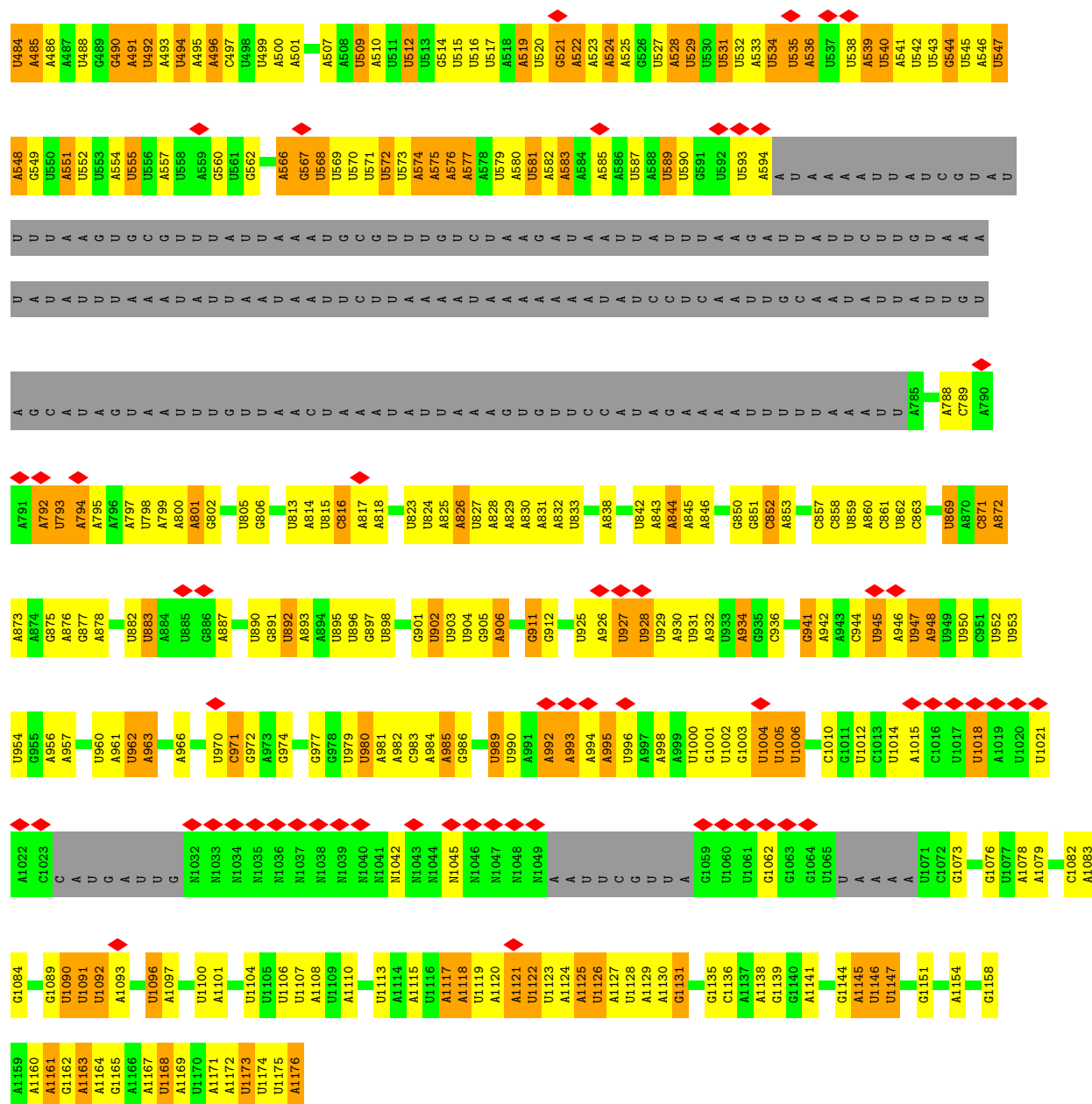


• Molecule 2: uL29m



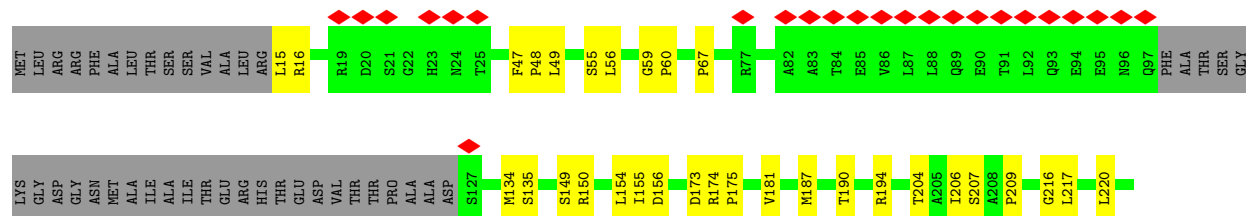
• Molecule 3: uL30m

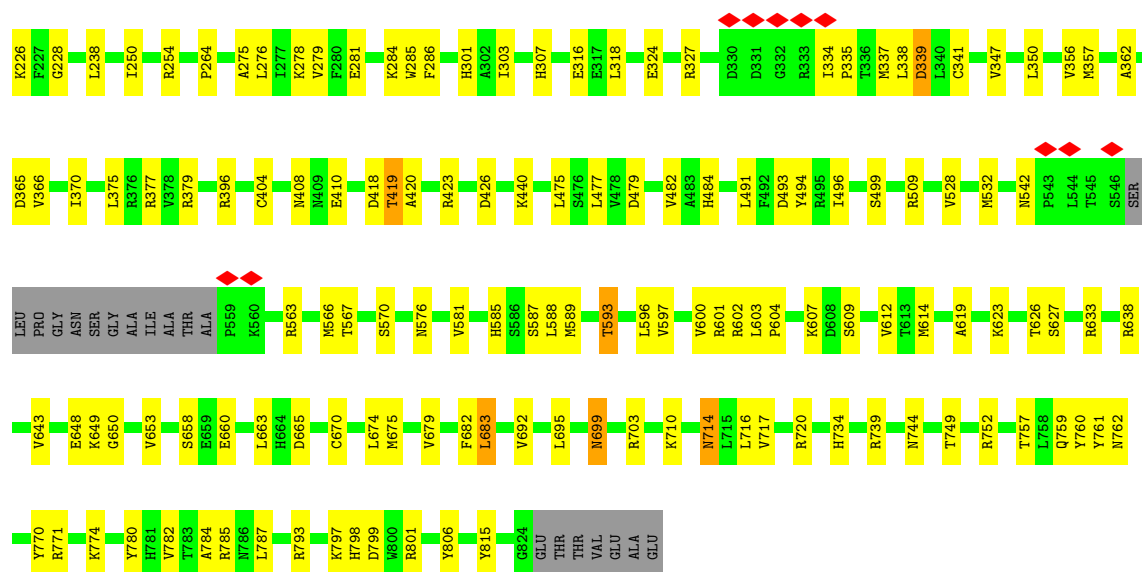




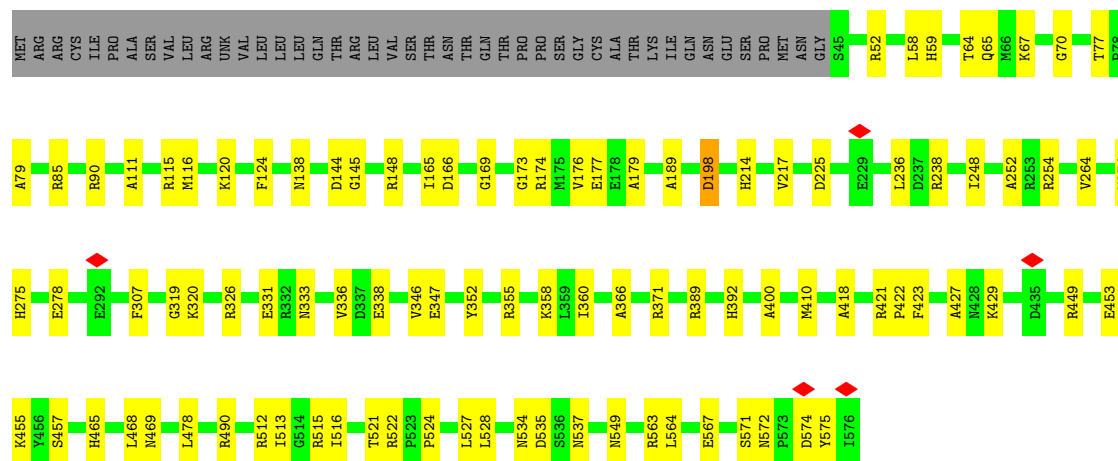
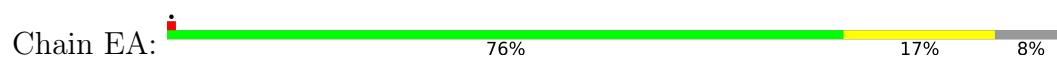
• Molecule 7: mL67

Chain BA: 72% 20% 7%

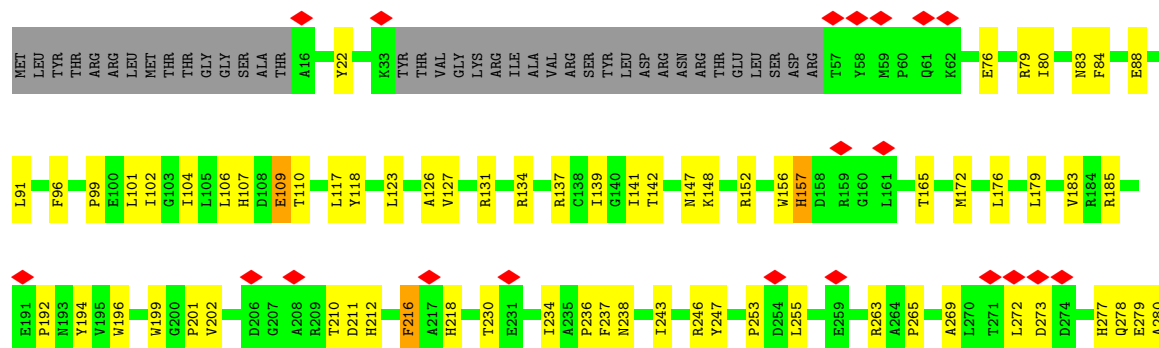




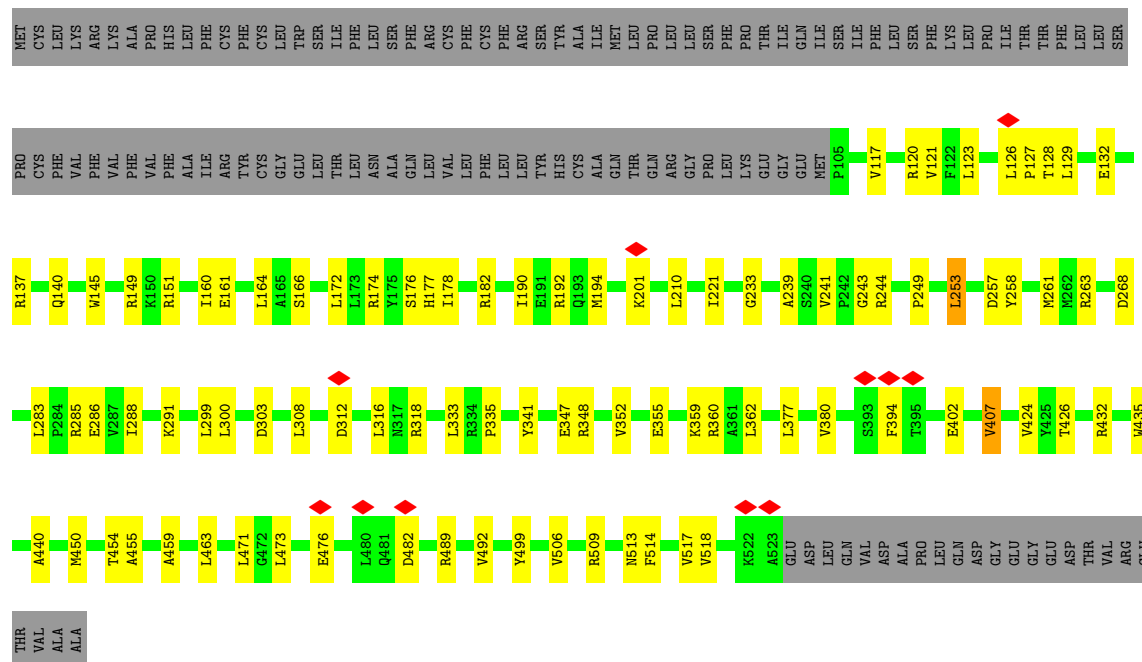
• Molecule 8: mt-EngA



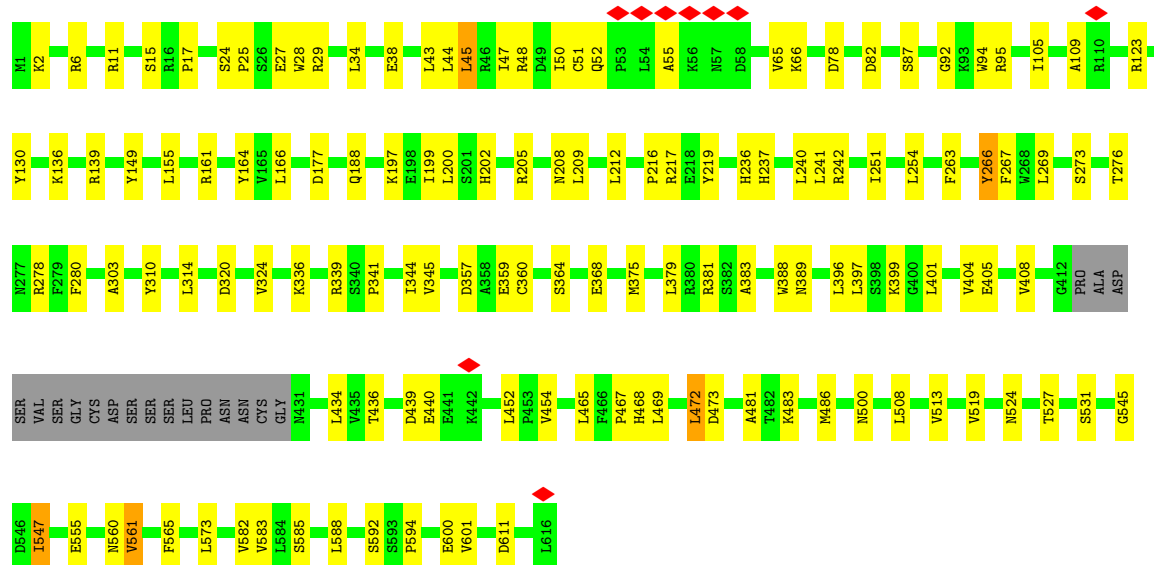
• Molecule 9: mL68



Chain BD:

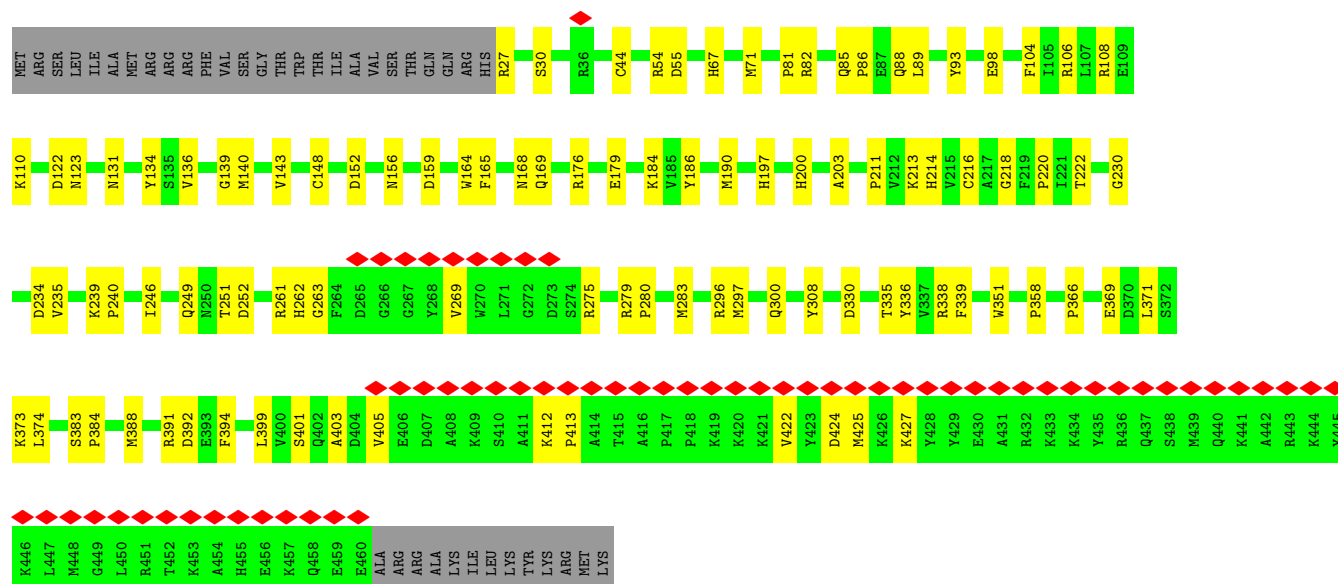


Chain ED:

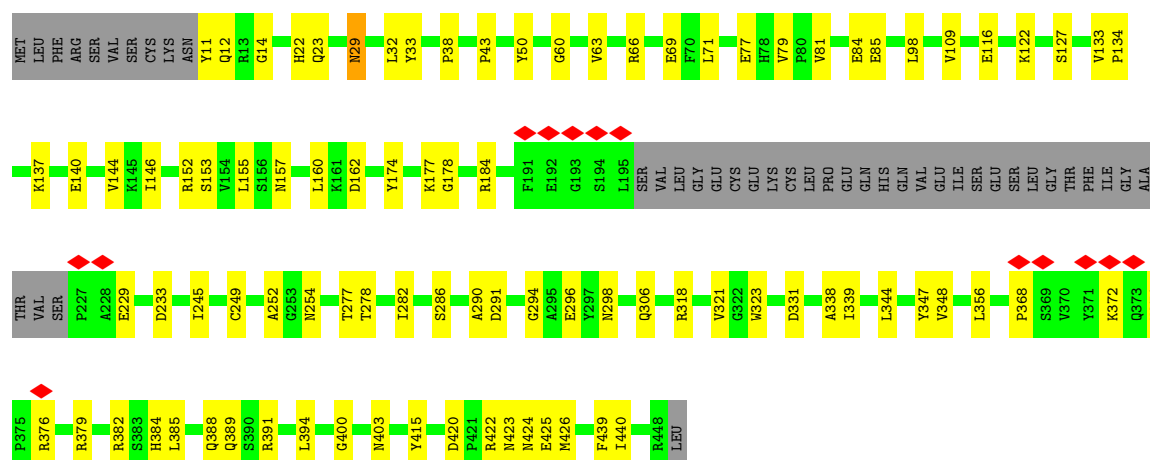


Chain AE:

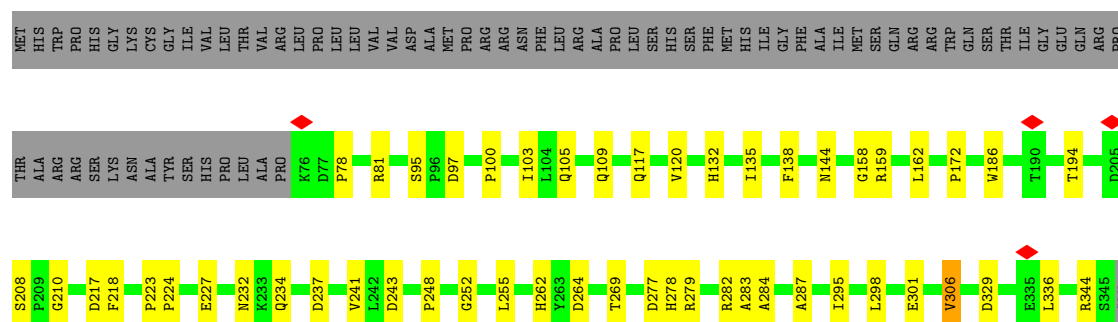


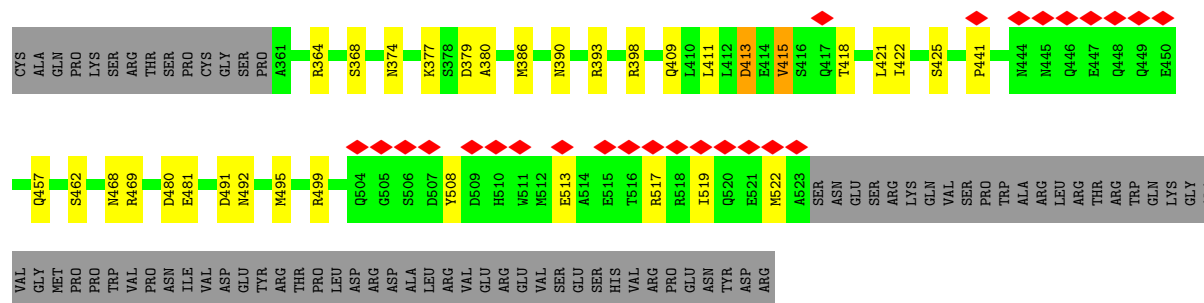


• Molecule 15: mL71

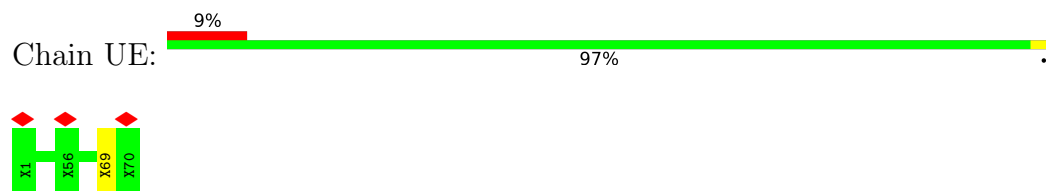


• Molecule 16: mt-LAF5

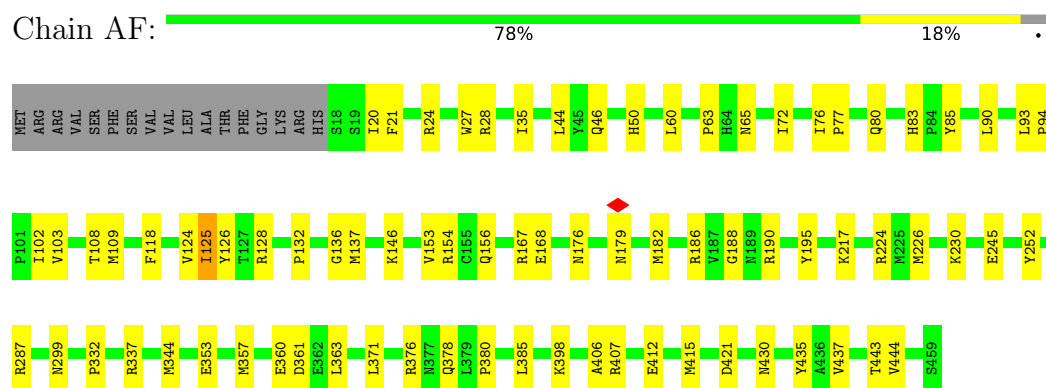




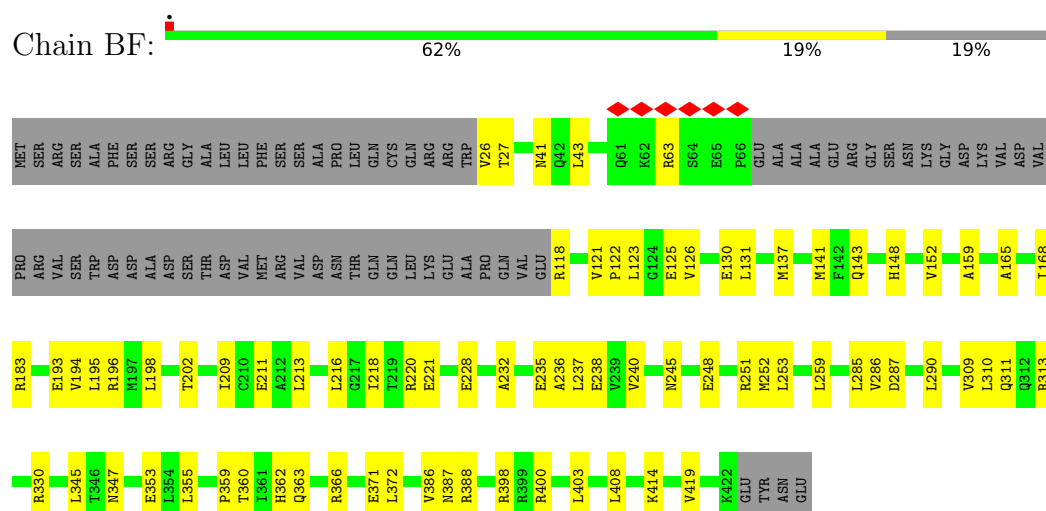
• Molecule 17: UNK



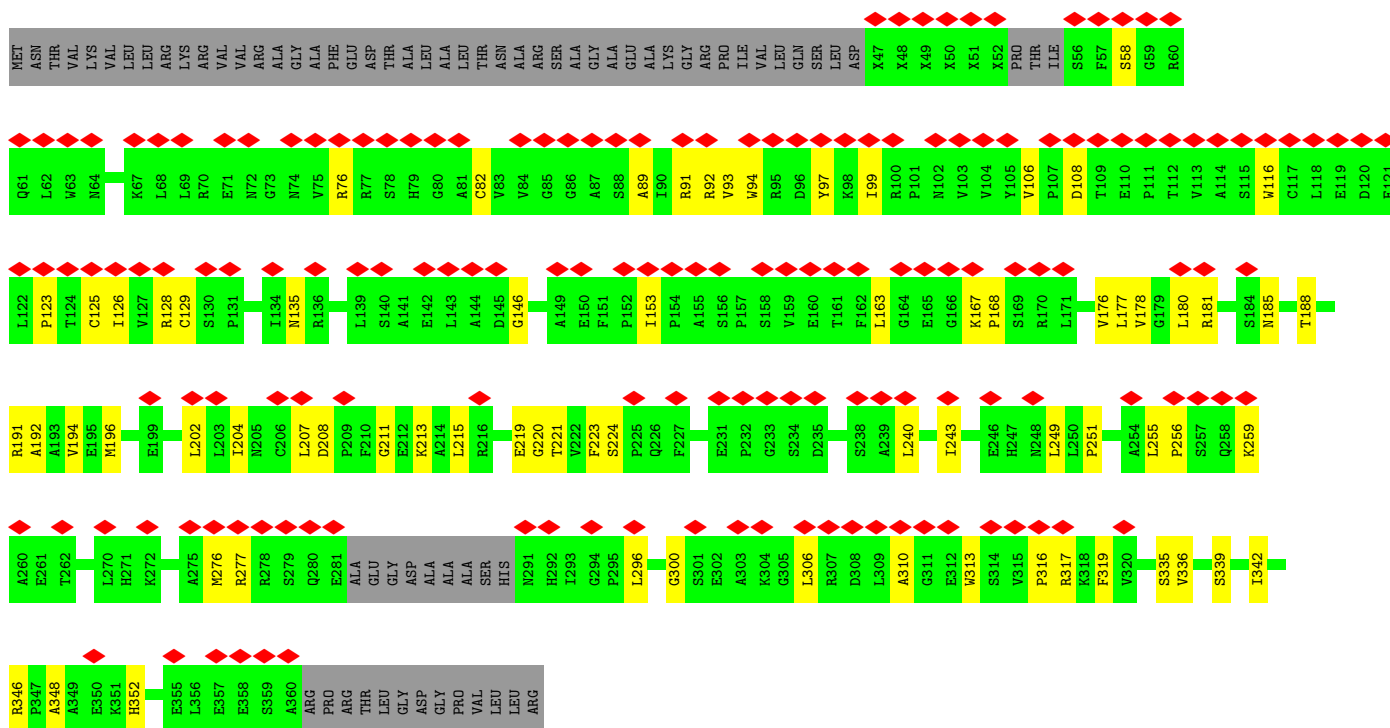
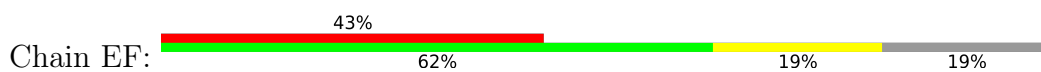
• Molecule 18: uL4m



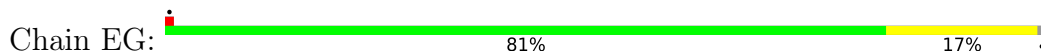
• Molecule 19: mL72



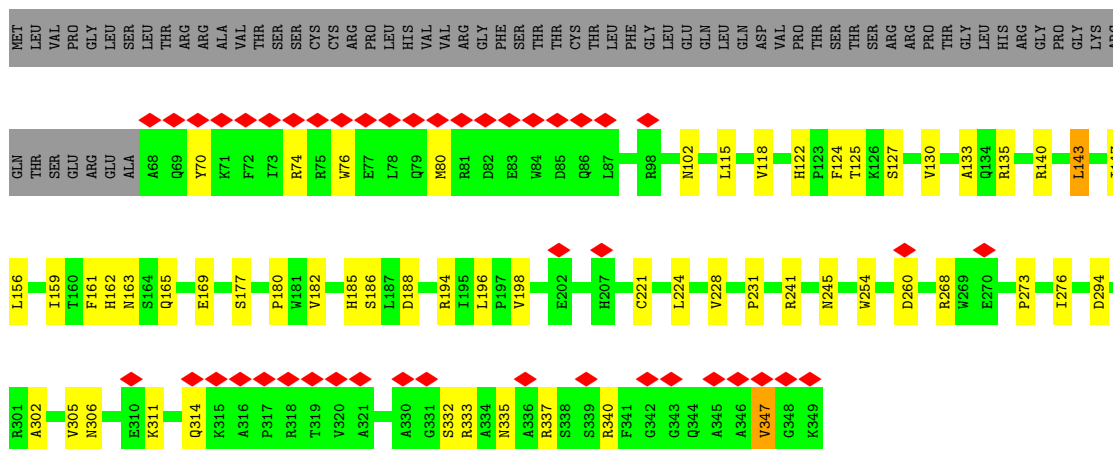
• Molecule 20: mt-LAF6



- Molecule 21: mt-LAF7



- Molecule 22: mL74

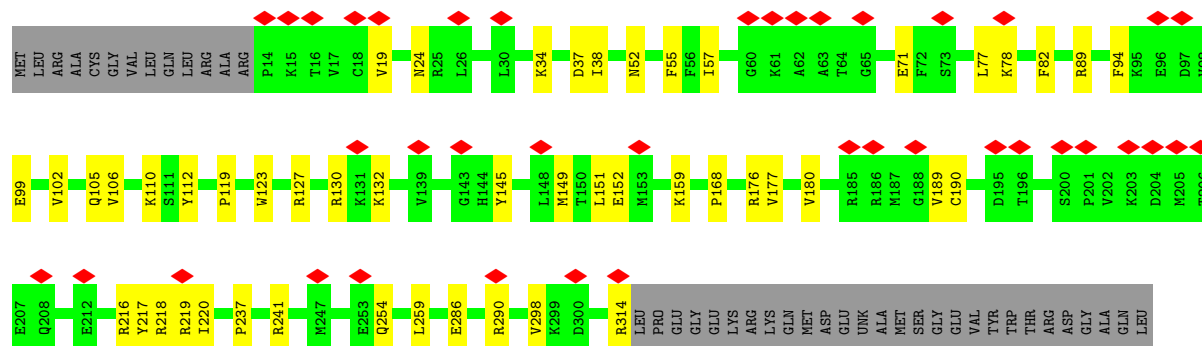
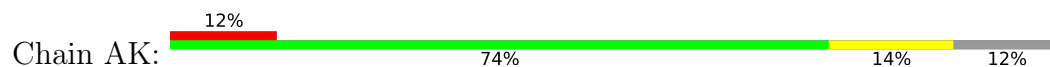


- Molecule 23: mt-LAF8

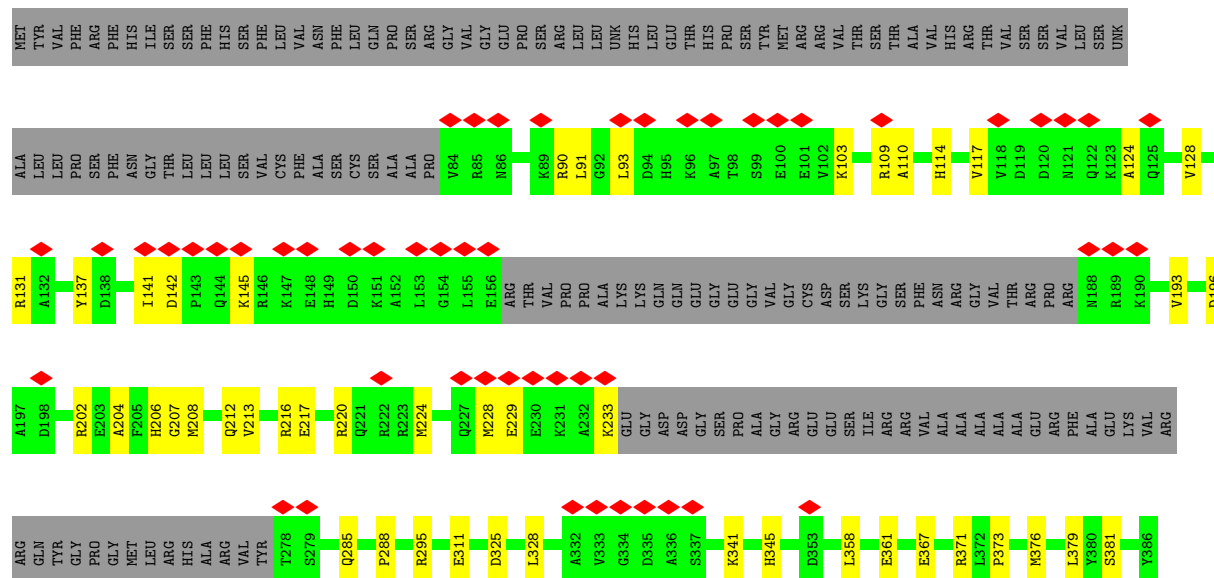




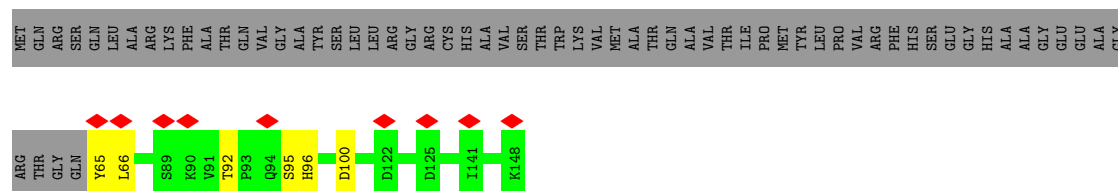
• Molecule 30: uL11m



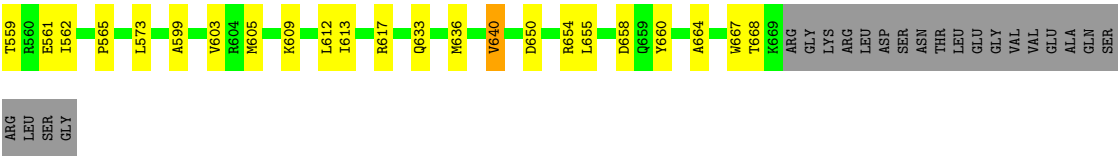
• Molecule 31: mL77



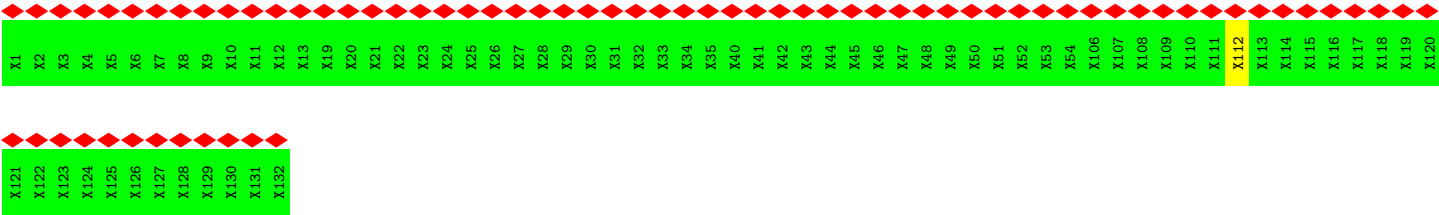
• Molecule 32: mt-ACP



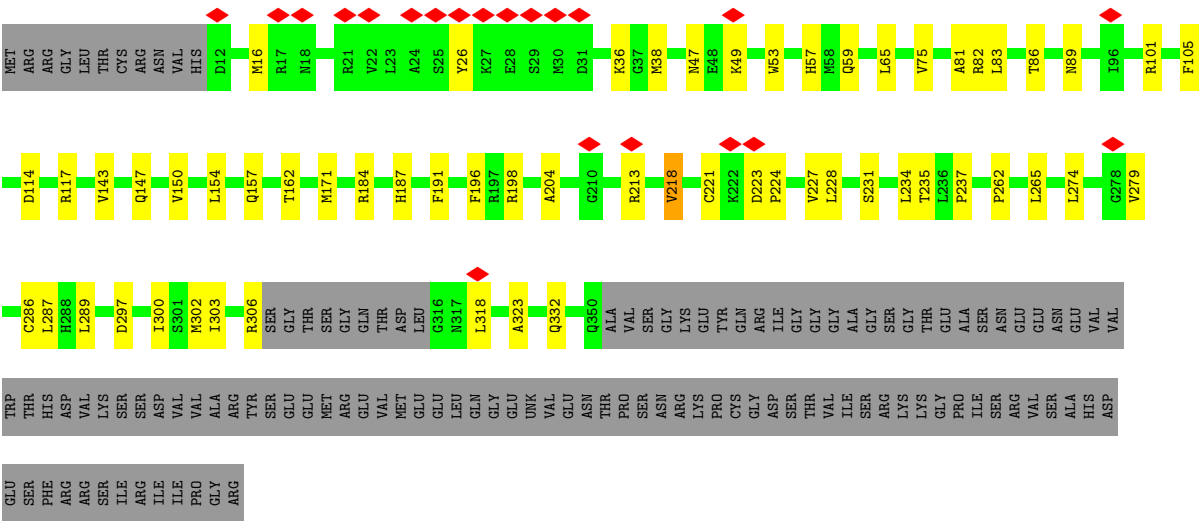
• Molecule 32: mt-ACP



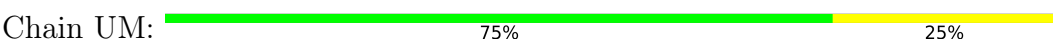
• Molecule 36: UNK



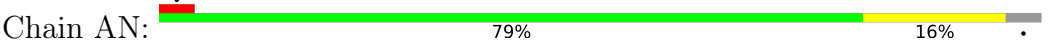
• Molecule 37: Mtg1

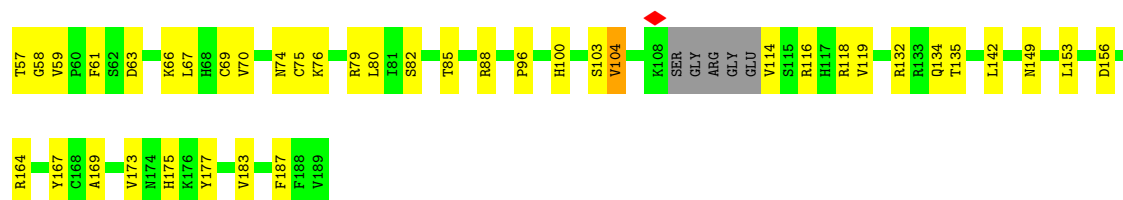


• Molecule 38: UNK

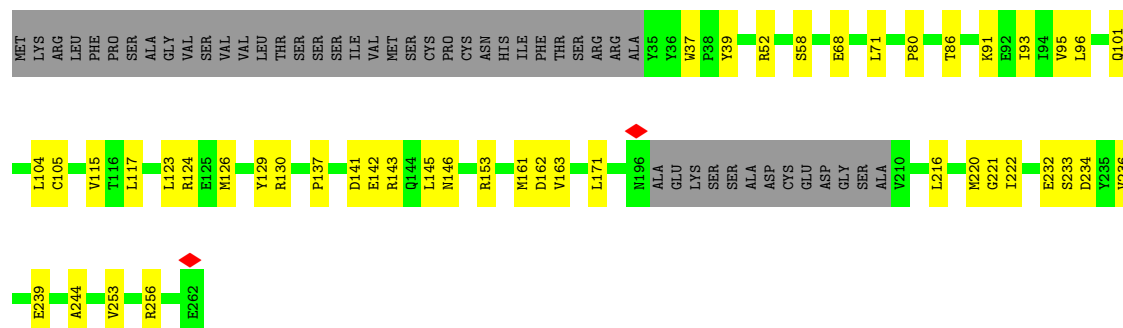


• Molecule 39: uL13m

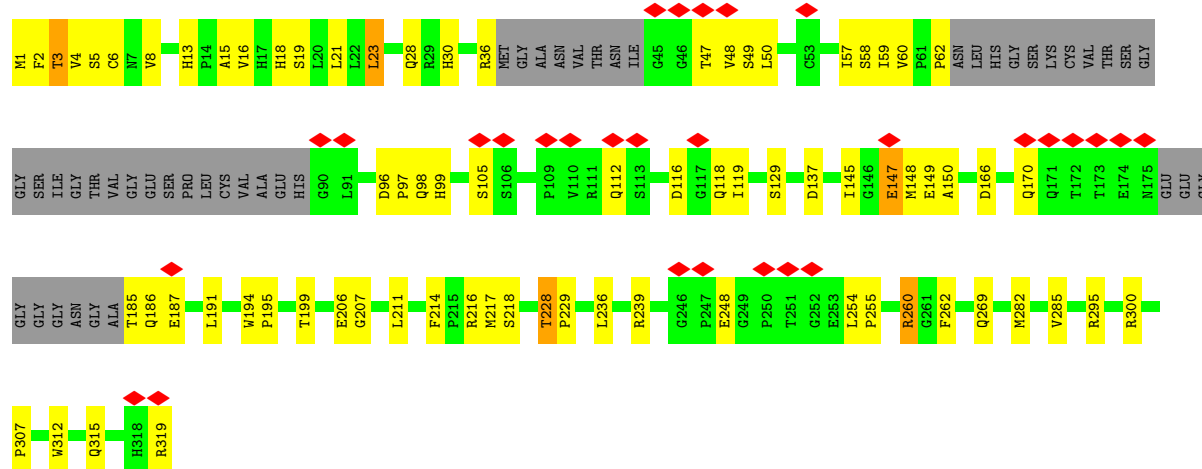




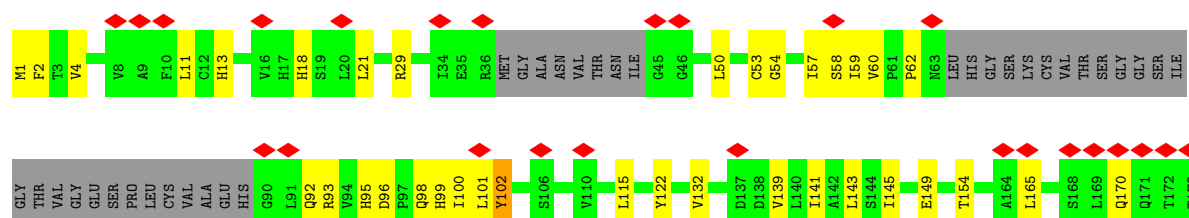
• Molecule 43: mL81

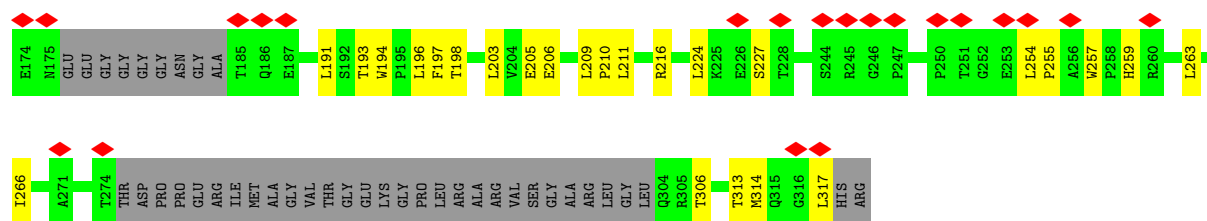


• Molecule 44: mt-LAF15a

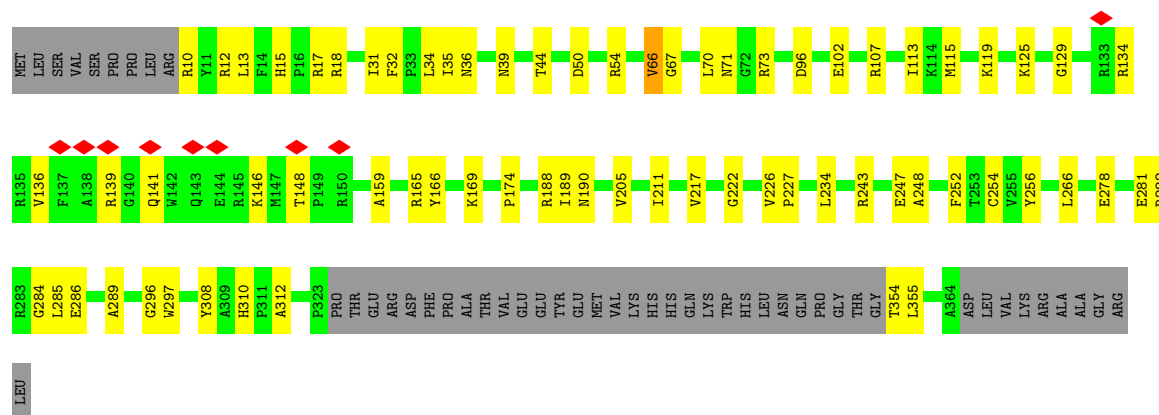


• Molecule 44: mt-LAF15a

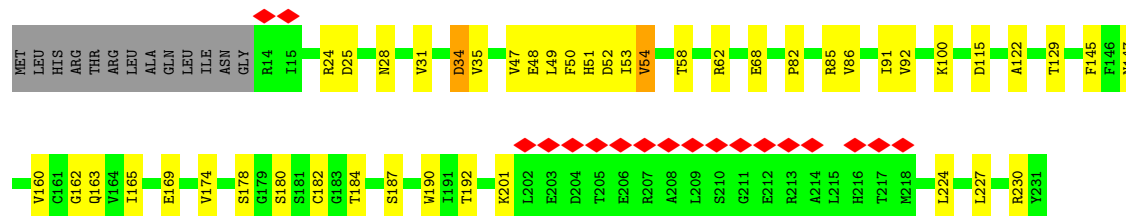
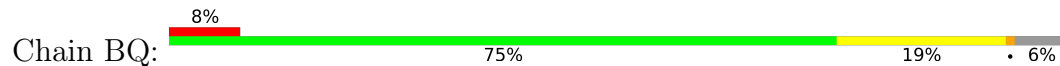




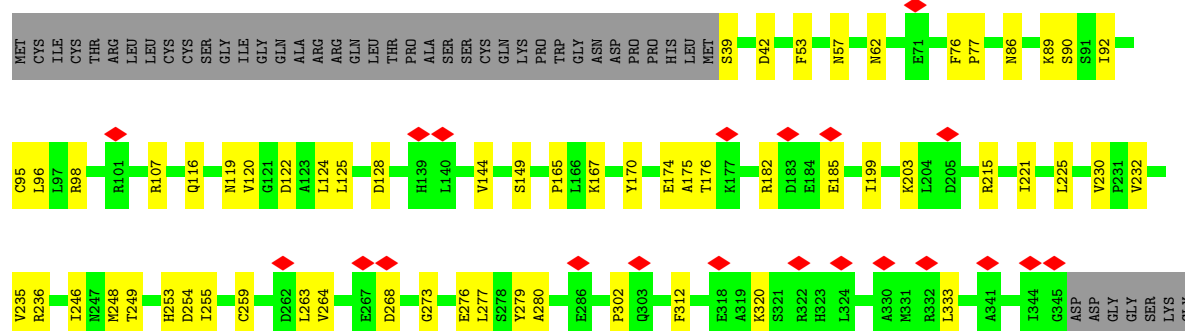
• Molecule 45: uL15m

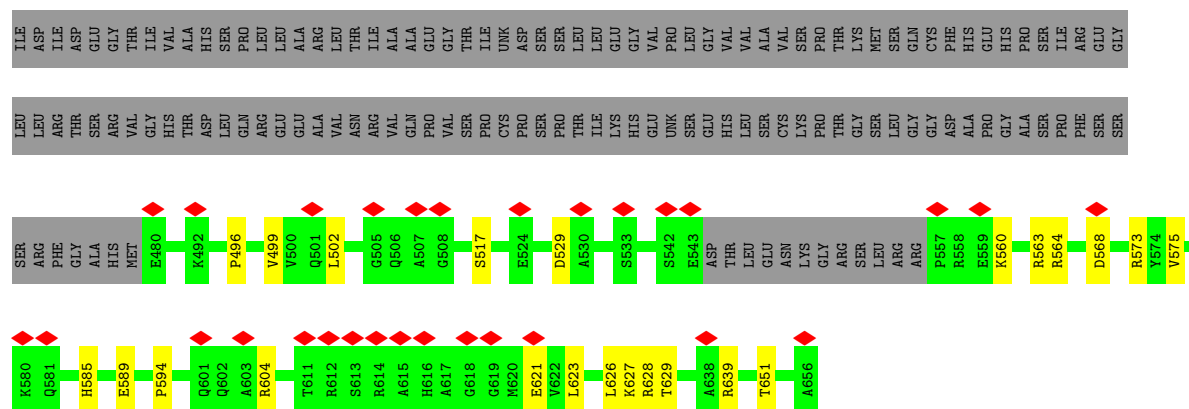


• Molecule 46: mL83

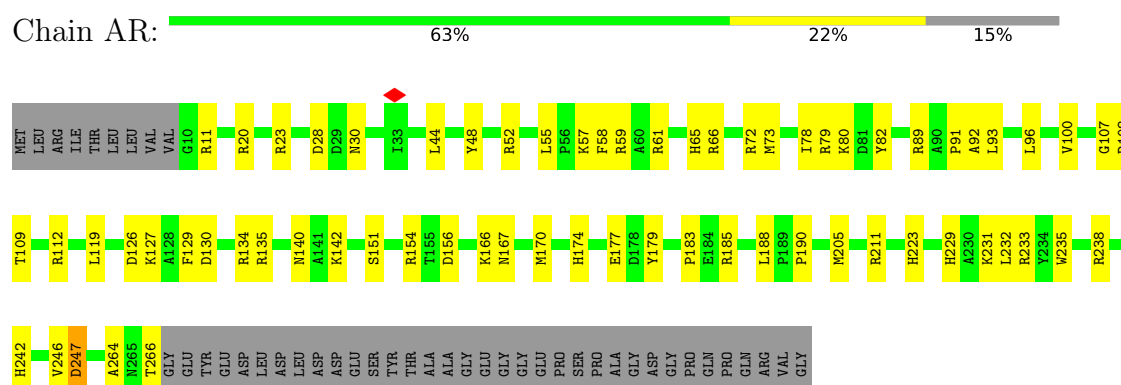


• Molecule 47: mt-EngB

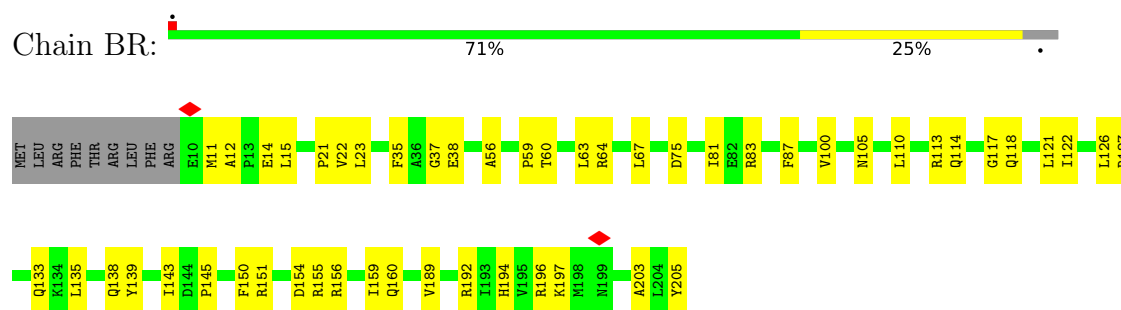




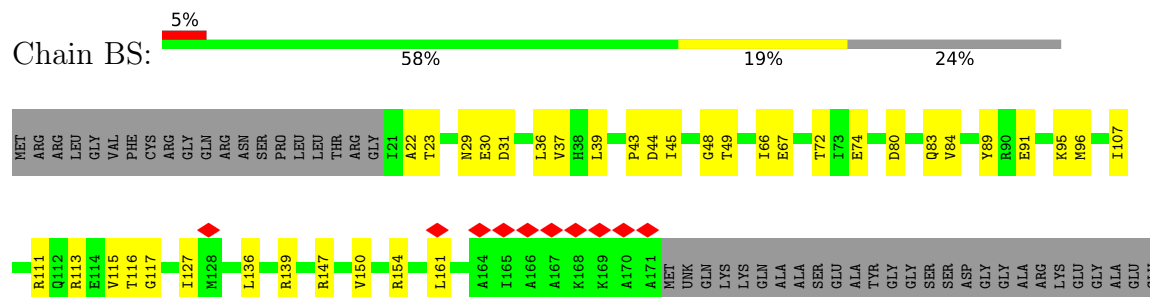
• Molecule 48: bL17m



• Molecule 49: mL84



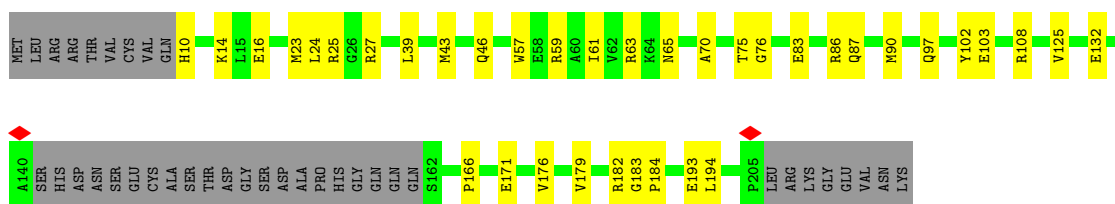
• Molecule 50: mL85



• Molecule 51: mt-LAF18

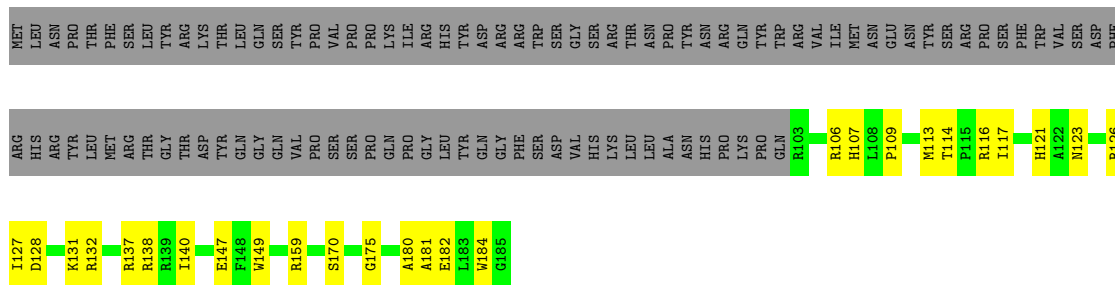


Chain AU:  65% 17% 18%



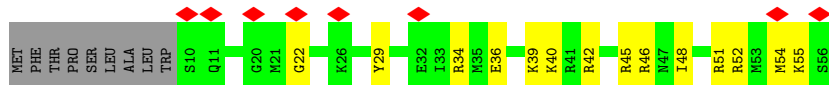
• Molecule 56: mL87

Chain BU:  31% 14% 55%



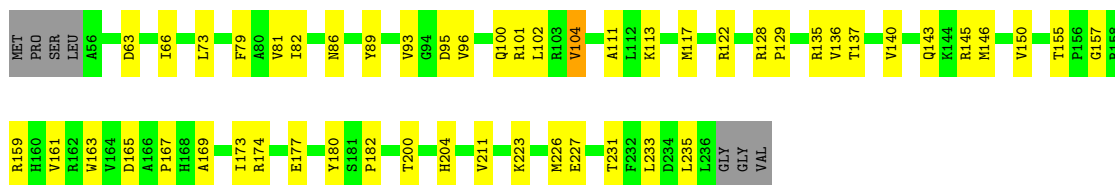
• Molecule 57: mt-LAF20

Chain EU:  14% 59% 25% 16%



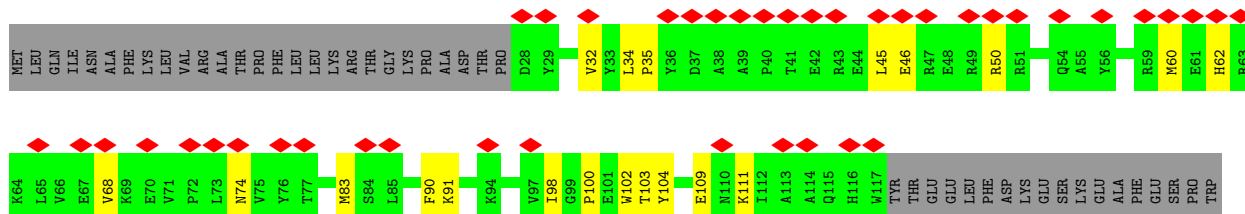
• Molecule 58: bL21m

Chain AV:  69% 27% 4%



• Molecule 59: mL88

Chain BV:  22% 37% 11% 53%



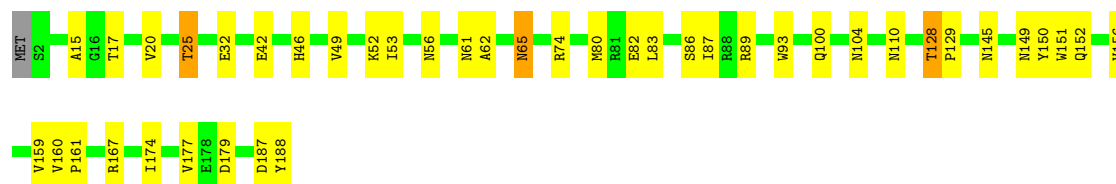
- Molecule 60: uL22m

Chain AW:  76% 24%

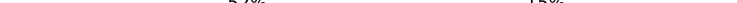


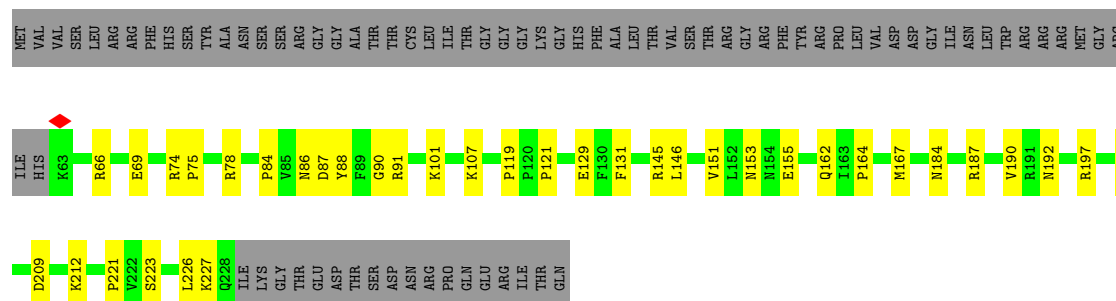
- Molecule 61: mL89

Chain BW:  77% 21% 2%



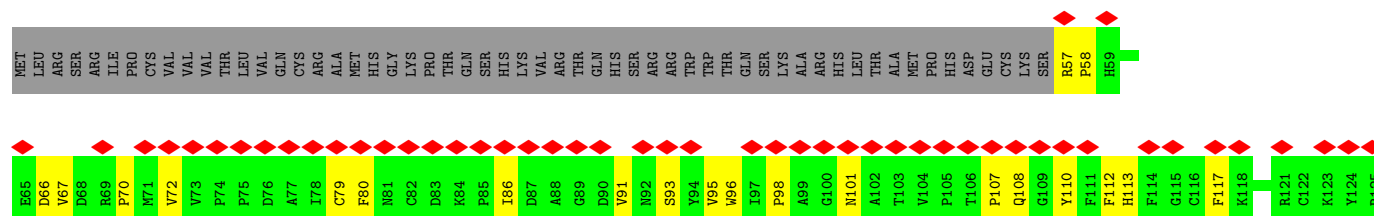
- Molecule 62: uL23m

Chain AX: 

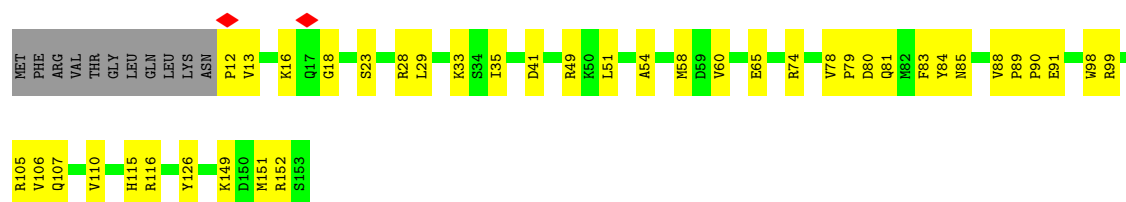


- Molecule 63: mL90

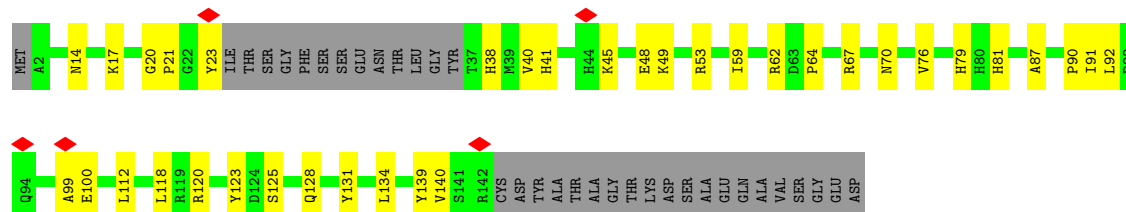
Chain BX:



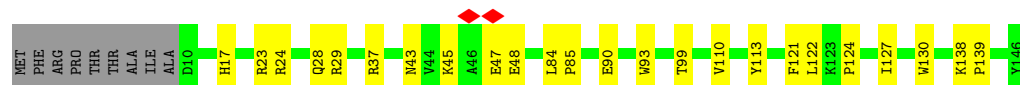
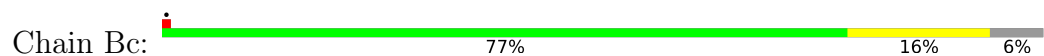




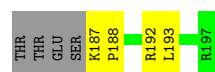
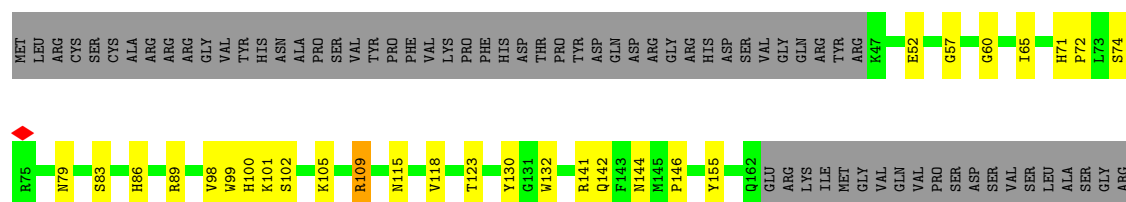
• Molecule 68: mL94



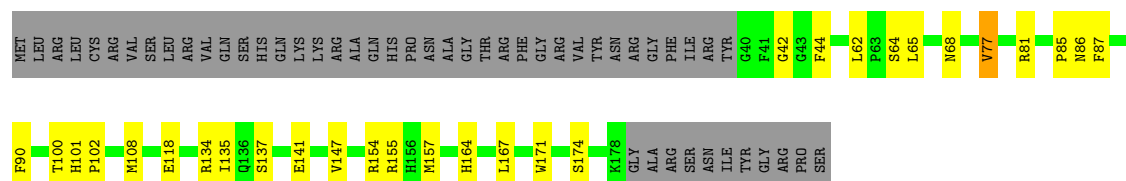
• Molecule 69: mL95



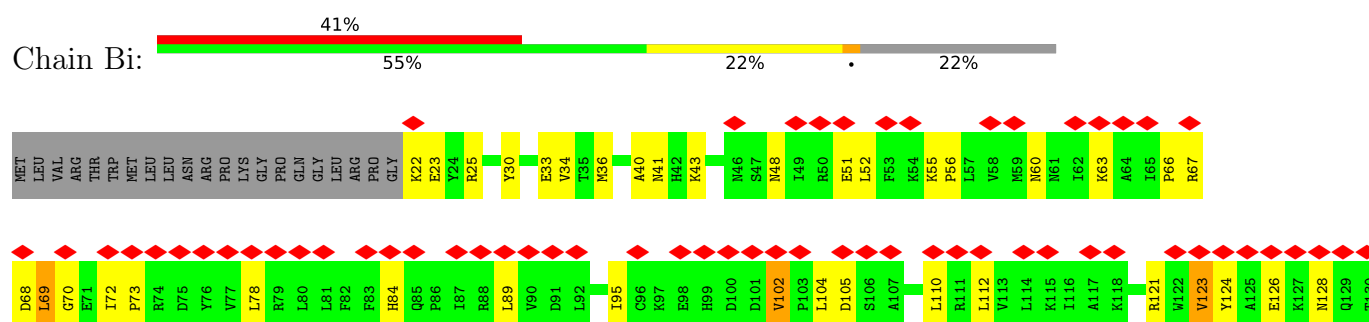
• Molecule 70: mL41



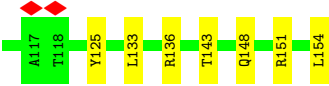
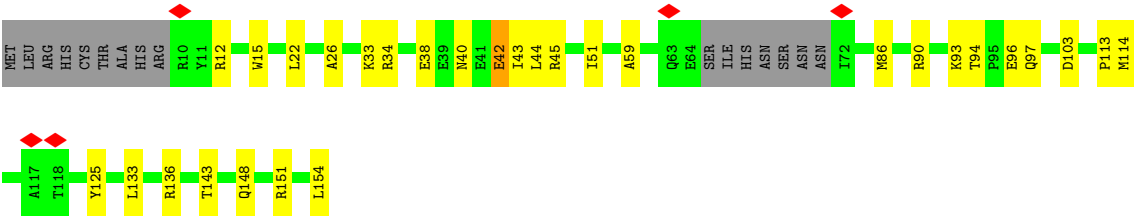
• Molecule 71: mL42



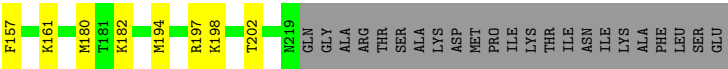
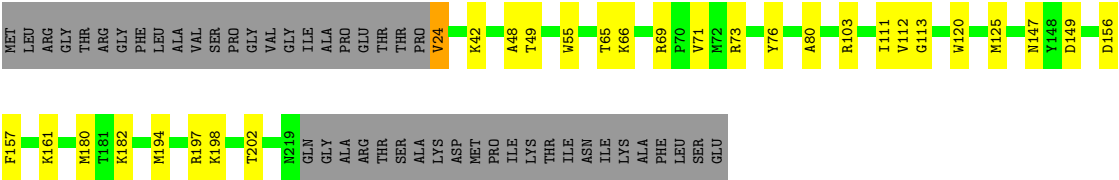
• Molecule 72: mL98







• Molecule 81: mL64



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	98508	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 ($e^-/\text{\AA}^2$)	75	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	0.210	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	434.0, 434.0, 434.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.085, 1.085, 1.085	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PM8, NA, NAD, GTP, ATP, MG, SPD

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	A1	0.11	0/1828	0.29	0/2466
2	A2	0.11	0/3763	0.27	0/5124
3	A3	0.13	0/1246	0.31	0/1678
4	A5	0.12	0/498	0.30	0/663
5	A8	0.12	0/1231	0.33	0/1648
6	AA	0.11	0/20700	0.24	0/32183
7	BA	0.11	0/6192	0.29	0/8401
8	EA	0.10	0/4337	0.26	0/5856
9	BB	0.10	0/3456	0.27	0/4684
10	EB	0.10	0/5426	0.27	0/7340
11	EC	0.11	0/3090	0.28	0/4190
12	BD	0.10	0/3418	0.29	0/4629
13	ED	0.11	0/4872	0.29	0/6599
14	AE	0.12	0/3570	0.30	1/4849 (0.0%)
15	BE	0.11	0/3306	0.29	0/4476
16	EE	0.10	0/3510	0.29	1/4751 (0.0%)
18	AF	0.11	0/3706	0.27	0/5029
19	BF	0.12	0/2909	0.31	0/3920
20	EF	0.10	0/2308	0.29	0/3137
21	EG	0.11	0/1331	0.29	0/1784
22	BH	0.10	0/2356	0.28	0/3203
23	EH	0.10	0/3548	0.28	0/4814
24	AI	0.10	0/1980	0.28	0/2693
25	BI	0.11	0/2717	0.28	0/3674
26	EI	0.10	0/2133	0.28	1/2894 (0.0%)
28	BJ	0.10	0/2494	0.28	0/3373
29	EJ	0.12	0/778	0.32	0/1047
30	AK	0.11	0/2565	0.30	0/3465
31	BK	0.10	0/1897	0.28	0/2556
32	EK	0.06	0/679	0.19	0/923
32	ER	0.08	0/679	0.21	0/923
34	BL	0.11	0/2064	0.29	0/2794

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	EL	0.10	0/4615	0.27	0/6282
37	EM	0.10	0/2658	0.27	0/3594
39	AN	0.11	0/1698	0.29	0/2308
40	BN	0.10	0/1755	0.27	0/2381
41	EN	0.10	0/5115	0.28	0/6936
42	AO	0.10	0/1371	0.29	0/1846
43	BO	0.10	0/1715	0.26	0/2322
44	EO	0.11	0/2188	0.29	0/2976
44	EP	0.10	0/1961	0.28	0/2669
45	AP	0.11	0/2774	0.28	0/3761
46	BQ	0.10	0/1691	0.27	0/2293
47	EQ	0.08	0/3701	0.25	0/4994
48	AR	0.12	0/2211	0.30	0/2988
49	BR	0.11	0/1702	0.29	0/2296
50	BS	0.11	0/1235	0.30	0/1665
51	ES	0.11	0/1276	0.28	0/1715
52	AT	0.11	0/1193	0.30	0/1611
53	BT	0.13	0/1465	0.29	0/1970
54	ET	0.11	0/858	0.29	0/1148
55	AU	0.12	0/1456	0.31	0/1971
56	BU	0.12	0/722	0.31	0/969
57	EU	0.12	0/412	0.34	0/538
58	AV	0.12	0/1454	0.30	0/1973
59	BV	0.09	0/786	0.25	0/1063
60	AW	0.11	0/2307	0.28	0/3119
61	BW	0.12	0/1604	0.31	0/2167
62	AX	0.11	0/1445	0.29	0/1963
63	BX	0.13	0/1131	0.34	0/1539
65	AY	0.11	0/2846	0.27	0/3847
66	BZ	0.09	0/1446	0.25	0/1956
67	Ba	0.11	0/1289	0.32	0/1742
68	Bb	0.10	0/1035	0.26	0/1402
69	Bc	0.11	0/1238	0.32	0/1685
70	Ae	0.11	0/1068	0.29	0/1447
71	Af	0.10	0/1134	0.26	0/1536
72	Bf	0.11	0/749	0.34	0/1012
73	Ag	0.12	0/1608	0.31	0/2180
74	Bg	0.11	0/682	0.30	0/919
75	Bh	0.10	0/752	0.32	0/1015
76	Bi	0.13	0/1530	0.28	0/2076
77	Al	0.11	0/1484	0.27	0/2019
78	Ao	0.11	0/1486	0.26	0/2022
79	Ap	0.10	0/2506	0.27	0/3404

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
80	At	0.11	0/1179	0.29	0/1596
81	Av	0.10	0/1714	0.27	0/2311
All	All	0.11	0/180832	0.28	3/248992 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	EE	441	PRO	N-CA-CB	7.05	110.65	103.25
14	AE	413	PRO	N-CA-CB	6.79	110.37	103.25
26	EI	156	PRO	N-CA-CB	5.99	110.14	103.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	1788	0	1814	32	0
2	A2	3661	0	3623	68	0
3	A3	1226	0	1282	32	0
4	A5	483	0	493	13	0
5	A8	1203	0	1226	21	0
6	AA	18833	0	9384	388	0
7	BA	6059	0	6051	122	0
8	EA	4263	0	4306	62	0
9	BB	3365	0	3284	78	0
10	EB	5308	0	5428	90	0
11	EC	3005	0	3010	42	0
12	BD	3349	0	3368	53	0
13	ED	4764	0	4768	87	0
14	AE	3461	0	3244	72	0
15	BE	3223	0	3143	59	0
16	EE	3444	0	3386	65	0
17	UE	165	0	37	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	AF	3597	0	3509	69	0
19	BF	2847	0	2832	63	0
20	EF	2290	0	2296	43	0
21	EG	1295	0	1250	19	0
22	BH	2293	0	2258	43	0
23	EH	3471	0	3499	49	0
24	AI	1967	0	1885	31	0
25	BI	2641	0	2577	42	0
26	EI	2101	0	1986	53	0
27	UI	115	0	25	0	0
28	BJ	2433	0	2368	41	0
29	EJ	765	0	781	14	0
30	AK	2499	0	2519	36	0
31	BK	1855	0	1827	35	0
32	EK	669	0	663	3	0
32	ER	669	0	663	4	0
33	UK	125	0	27	0	0
34	BL	2023	0	1911	29	0
35	EL	4484	0	4426	82	0
36	UL	360	0	82	1	0
37	EM	2606	0	2645	39	0
38	UM	40	0	10	2	0
39	AN	1639	0	1612	23	0
40	BN	1714	0	1593	23	0
41	EN	5025	0	5101	75	0
42	AO	1339	0	1363	33	0
43	BO	1686	0	1661	37	0
44	EO	2141	0	2147	49	0
44	EP	1919	0	1910	47	0
45	AP	2691	0	2642	57	0
46	BQ	1651	0	1571	33	0
47	EQ	3628	0	3624	56	0
48	AR	2146	0	2089	59	0
49	BR	1659	0	1638	37	0
50	BS	1218	0	1219	26	0
51	ES	1259	0	1265	25	0
52	AT	1163	0	1148	44	0
53	BT	1435	0	1397	25	0
54	ET	839	0	858	16	0
55	AU	1423	0	1447	40	0
56	BU	705	0	710	26	0
57	EU	407	0	434	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	AV	1424	0	1457	36	0
59	BV	763	0	747	15	0
60	AW	2251	0	2292	58	0
61	BW	1557	0	1517	34	0
62	AX	1400	0	1380	32	0
63	BX	1088	0	1013	27	0
64	UX	900	0	208	1	0
65	AY	2790	0	2726	66	0
66	BZ	1420	0	1405	21	0
67	Ba	1245	0	1195	37	0
68	Bb	1011	0	1010	28	0
69	Bc	1194	0	1169	21	0
70	Ae	1031	0	1024	25	0
71	Af	1107	0	1087	23	0
72	Bf	725	0	687	15	0
73	Ag	1564	0	1507	28	0
74	Bg	667	0	662	24	0
75	Bh	730	0	708	18	0
76	Bi	1502	0	1455	45	0
77	Al	1440	0	1448	31	0
78	Ao	1443	0	1376	24	0
79	Ap	2428	0	2429	41	0
80	At	1149	0	1164	28	0
81	Av	1668	0	1648	26	0
82	A5	1	0	0	0	0
82	BX	2	0	0	0	0
82	Bh	1	0	0	0	0
82	EG	1	0	0	0	0
83	AA	29	0	0	0	0
83	EA	2	0	0	0	0
83	EB	1	0	0	0	0
83	EQ	1	0	0	0	0
84	AA	10	0	19	2	0
85	EA	64	0	24	5	0
85	EQ	32	0	12	1	0
86	EA	2	0	0	0	0
87	EB	31	0	12	1	0
88	EK	32	0	39	2	0
88	ER	32	0	39	4	0
89	Av	44	0	26	0	0
90	EA	4	0	0	0	0
90	EB	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	EQ	2	0	0	0	0
All	All	177224	0	164800	2666	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 8.

All (2666) 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)
6:AA:871:C:O2	6:AA:901:G:N2	2.12	0.83
6:AA:1018:U:H3	6:AA:1062:G:H1	1.27	0.82
20:EF:300:GLY:HA3	20:EF:306:LEU:HD21	1.61	0.81
65:AY:118:GLU:HG2	65:AY:128:ARG:HG2	1.61	0.81
55:AU:83:GLU:HG3	71:Af:77:VAL:HG12	1.64	0.78
6:AA:871:C:N3	6:AA:901:G:N1	2.31	0.78
29:EJ:65:GLY:O	29:EJ:69:LEU:HB2	1.82	0.78
55:AU:108:ARG:HH22	71:Af:81:ARG:HB2	1.49	0.77
19:BF:213:LEU:HD11	19:BF:236:ALA:HB2	1.67	0.76
79:Ap:187:PRO:HG3	79:Ap:223:TYR:HB3	1.66	0.76
18:AF:156:GLN:NE2	60:AW:9:ALA:O	2.19	0.75
6:AA:575:A:H1'	48:AR:23:ARG:HD2	1.67	0.75
11:EC:233:MET:SD	14:AE:279:ARG:NH1	2.61	0.74
6:AA:1073:G:H21	11:EC:179:MET:HE1	1.53	0.73
7:BA:532:MET:SD	7:BA:576:ASN:ND2	2.62	0.73
62:AX:74:ARG:HH11	62:AX:75:PRO:HD2	1.52	0.73
6:AA:310:A:H5'	10:EB:70:VAL:HG23	1.70	0.73
15:BE:66:ARG:HD2	31:BK:381:SER:HA	1.70	0.72
6:AA:9:A:N7	65:AY:6:ARG:NH2	2.37	0.72
72:Bf:99:ILE:HG22	72:Bf:100:TYR:H	1.55	0.71
19:BF:125:GLU:HB3	55:AU:179:VAL:HG22	1.73	0.71
7:BA:563:ARG:NH1	7:BA:650:GLY:O	2.23	0.71
68:Bb:53:ARG:HH22	68:Bb:100:GLU:H	1.37	0.71
13:ED:547:ILE:HG23	13:ED:585:SER:HB2	1.71	0.71
20:EF:94:TRP:HE1	20:EF:123:PRO:HG3	1.56	0.71
54:ET:17:MET:HA	54:ET:20:MET:HG2	1.73	0.71
5:A8:144:ASN:OD1	45:AP:165:ARG:NH2	2.23	0.70
34:BL:51:SER:O	65:AY:27:ASN:ND2	2.23	0.70
6:AA:1115:A:OP2	25:BI:26:ASN:ND2	2.24	0.70
57:EU:52:ARG:HD2	57:EU:55:LYS:HB2	1.73	0.70
6:AA:575:A:OP1	48:AR:59:ARG:NH2	2.24	0.70
79:Ap:66:CYS:HB2	79:Ap:70:GLU:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BD:241:VAL:HG22	12:BD:243:GLY:H	1.57	0.70
22:BH:165:GLN:O	22:BH:241:ARG:NH1	2.25	0.70
73:Ag:131:GLN:O	73:Ag:134:ARG:NH1	2.24	0.70
5:A8:79:PRO:HG2	5:A8:82:SER:HB2	1.74	0.70
6:AA:552:U:OP2	6:AA:554:A:N6	2.25	0.70
7:BA:49:LEU:O	35:EL:352:ARG:NH2	2.25	0.70
22:BH:305:VAL:HG13	28:BJ:51:PRO:HB3	1.74	0.69
34:BL:264:LEU:HD21	34:BL:287:ARG:HH12	1.56	0.69
37:EM:171:MET:HE3	37:EM:237:PRO:HD3	1.73	0.69
25:BI:151:MET:HE3	25:BI:185:MET:HE3	1.74	0.69
7:BA:749:THR:O	60:AW:197:ARG:NH2	2.25	0.69
2:A2:126:PRO:O	66:BZ:84:GLN:NE2	2.24	0.69
6:AA:234:U:O2	60:AW:215:ARG:NH1	2.26	0.69
28:BJ:175:GLU:HB2	28:BJ:178:ILE:HG22	1.73	0.69
9:BB:354:MET:HE1	9:BB:410:ALA:HA	1.74	0.69
15:BE:423:ASN:HD21	15:BE:425:GLU:HB2	1.58	0.69
66:BZ:76:ARG:HB3	66:BZ:84:GLN:HB3	1.73	0.69
77:Al:135:PRO:HG2	77:Al:175:ARG:HE	1.58	0.69
12:BD:362:LEU:HD23	12:BD:492:VAL:HG23	1.74	0.69
28:BJ:122:ASN:HB3	28:BJ:125:GLU:HB3	1.72	0.68
6:AA:386:U:H2'	25:BI:311:PRO:HG2	1.75	0.68
6:AA:548:A:OP2	57:EU:46:ARG:NH2	2.26	0.68
7:BA:784:ALA:HB1	7:BA:787:LEU:HB3	1.74	0.68
22:BH:102:ASN:HD21	22:BH:169:GLU:HG3	1.58	0.68
43:BO:126:MET:HE3	43:BO:129:TYR:HA	1.76	0.68
55:AU:125:VAL:O	78:Ao:25:ASN:ND2	2.27	0.68
68:Bb:17:LYS:HG3	78:Ao:209:MET:HE2	1.75	0.68
6:AA:823:U:H5''	21:EG:51:SER:HB3	1.76	0.68
26:EI:223:LYS:NZ	26:EI:296:TRP:O	2.27	0.68
28:BJ:40:ILE:HG12	47:EQ:651:THR:HG22	1.74	0.68
6:AA:393:A:OP1	25:BI:299:ARG:NH2	2.26	0.68
49:BR:110:LEU:H	49:BR:138:GLN:HE22	1.40	0.68
6:AA:485:A:N1	60:AW:50:GLN:NE2	2.40	0.68
67:Ba:80:ASP:O	67:Ba:84:TYR:HA	1.94	0.68
6:AA:1129:A:H5''	6:AA:1130:A:H2'	1.75	0.68
35:EL:130:SER:HB2	35:EL:136:PRO:HG3	1.76	0.68
49:BR:122:ILE:HG22	49:BR:160:GLN:HG3	1.74	0.68
1:A1:143:ARG:HB3	1:A1:148:LEU:HB2	1.76	0.67
4:A5:78:ILE:HG21	60:AW:259:ALA:HB2	1.76	0.67
6:AA:188:A:O2'	6:AA:189:A:O4'	2.10	0.67
52:AT:62:PHE:HB2	52:AT:69:VAL:HG13	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:EB:641:LEU:HG	14:AE:283:MET:HE1	1.75	0.67
24:AI:236:VAL:HG21	51:ES:50:GLU:HG3	1.76	0.67
25:BI:217:ARG:HD2	79:Ap:149:GLU:HA	1.75	0.67
60:AW:39:LYS:HB2	65:AY:21:ALA:HB2	1.77	0.67
6:AA:1131:G:N2	26:EI:260:ILE:O	2.24	0.67
81:Av:66:LYS:NZ	81:Av:69:ARG:O	2.28	0.67
14:AE:424:ASP:HB3	14:AE:427:LYS:HG2	1.76	0.67
16:EE:508:TYR:HB3	23:EH:475:PRO:HG3	1.77	0.67
6:AA:152:A:OP2	45:AP:107:ARG:NH1	2.28	0.67
12:BD:347:GLU:OE1	12:BD:348:ARG:NH2	2.28	0.67
79:Ap:69:GLY:H	79:Ap:73:THR:HG21	1.60	0.67
35:EL:650:ASP:OD2	35:EL:654:ARG:NH1	2.28	0.67
6:AA:509:U:H2'	6:AA:510:A:H8	1.61	0.66
10:EB:69:LEU:O	10:EB:305:ARG:NH2	2.28	0.66
23:EH:542:LEU:HD12	23:EH:600:LEU:HD21	1.76	0.66
25:BI:48:PHE:CG	25:BI:49:PRO:HA	2.30	0.66
35:EL:372:PRO:HD2	35:EL:482:PRO:HA	1.78	0.66
47:EQ:560:LYS:HE3	47:EQ:564:ARG:HG2	1.76	0.66
6:AA:445:U:H2'	6:AA:446:A:H8	1.60	0.66
6:AA:892:U:H1'	8:EA:70:GLY:H	1.61	0.66
8:EA:236:LEU:HD12	41:EN:399:ARG:HB3	1.77	0.66
35:EL:559:THR:HG22	35:EL:561:GLU:H	1.60	0.66
41:EN:412:LEU:HD21	41:EN:417:LYS:HE3	1.78	0.66
63:BX:79:CYS:SG	63:BX:80:PHE:N	2.68	0.66
35:EL:383:ASP:HA	35:EL:471:MET:HB3	1.75	0.66
63:BX:155:ARG:HE	63:BX:158:THR:HG23	1.59	0.66
15:BE:331:ASP:O	15:BE:379:ARG:NH1	2.28	0.66
65:AY:315:SER:OG	65:AY:321:GLN:NE2	2.29	0.66
58:AV:140:VAL:HA	58:AV:173:ILE:HG22	1.77	0.66
40:BN:10:GLN:H	40:BN:14:HIS:HD2	1.44	0.66
55:AU:70:ALA:HB1	55:AU:75:THR:HG23	1.76	0.66
14:AE:275:ARG:NH2	21:EG:108:SER:O	2.26	0.66
15:BE:79:VAL:O	70:Ae:192:ARG:NH2	2.29	0.65
20:EF:76:ARG:NH2	20:EF:208:ASP:OD2	2.28	0.65
51:ES:31:LEU:HA	51:ES:116:GLN:HE22	1.62	0.65
68:Bb:59:ILE:HG22	68:Bb:76:VAL:HB	1.79	0.65
6:AA:1163:A:O2'	6:AA:1165:G:N2	2.29	0.65
19:BF:118:ARG:NH2	78:Ao:90:ASP:OD2	2.29	0.65
21:EG:142:ARG:NH2	49:BR:118:GLN:OE1	2.29	0.65
66:BZ:96:GLN:NE2	66:BZ:124:ALA:O	2.29	0.65
6:AA:348:A:H61	21:EG:38:GLN:HE22	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:Bh:17:VAL:HG22	75:Bh:28:ARG:HH21	1.60	0.65
6:AA:67:C:N4	13:ED:109:ALA:O	2.29	0.65
16:EE:269:THR:HG22	16:EE:298:LEU:HB2	1.79	0.65
22:BH:127:SER:HB2	22:BH:185:HIS:HB2	1.79	0.65
5:A8:74:PHE:HD1	5:A8:87:ALA:HB2	1.62	0.65
6:AA:516:U:OP1	48:AR:61:ARG:NH2	2.29	0.65
12:BD:352:VAL:HG11	12:BD:359:LYS:HB3	1.79	0.65
13:ED:242:ARG:NH1	13:ED:527:THR:O	2.30	0.65
35:EL:371:PHE:HB2	35:EL:480:VAL:HG12	1.79	0.65
16:EE:499:ARG:NH2	25:BI:304:ALA:O	2.29	0.65
23:EH:190:PHE:HB3	23:EH:192:MET:HE3	1.76	0.65
6:AA:119:A:H5'	6:AA:120:A:C8	2.32	0.65
6:AA:141:U:O2'	55:AU:27:ARG:NH2	2.30	0.65
7:BA:627:SER:O	7:BA:633:ARG:NH1	2.29	0.65
19:BF:63:ARG:NH2	19:BF:238:GLU:OE1	2.28	0.65
77:Al:75:ARG:H	77:Al:211:HIS:CE1	2.14	0.65
15:BE:368:PRO:HA	15:BE:372:LYS:HA	1.79	0.65
31:BK:373:PRO:HG2	31:BK:376:MET:HB2	1.77	0.65
66:BZ:2:ARG:HH12	66:BZ:28:ARG:HE	1.43	0.65
6:AA:802:G:N2	48:AR:156:ASP:O	2.30	0.65
9:BB:131:ARG:HE	9:BB:390:LEU:HD21	1.62	0.64
9:BB:253:PRO:HB2	9:BB:387:ALA:HB2	1.80	0.64
41:EN:692:VAL:HA	41:EN:695:THR:HG22	1.78	0.64
47:EQ:276:GLU:HG3	47:EQ:628:ARG:HH22	1.62	0.64
49:BR:59:PRO:HB2	49:BR:64:ARG:HE	1.61	0.64
9:BB:348:VAL:HG23	9:BB:430:TYR:HB2	1.79	0.64
16:EE:243:ASP:OD1	16:EE:398:ARG:NH2	2.30	0.64
67:Ba:116:ARG:NH1	67:Ba:126:TYR:OH	2.30	0.64
6:AA:298:U:N3	18:AF:21:PHE:O	2.24	0.64
63:BX:67:VAL:HG12	75:Bh:12:MET:HE1	1.79	0.64
12:BD:174:ARG:O	12:BD:263:ARG:NH1	2.30	0.64
13:ED:92:GLY:O	13:ED:202:HIS:NE2	2.29	0.64
50:BS:48:GLY:HA2	50:BS:72:THR:HG23	1.80	0.64
12:BD:140:GLN:OE1	22:BH:135:ARG:NH2	2.30	0.64
6:AA:549:G:N2	10:EB:716:ALA:O	2.29	0.64
13:ED:276:THR:O	46:BQ:230:ARG:NH1	2.31	0.64
35:EL:70:ARG:NH2	35:EL:554:LYS:O	2.26	0.64
6:AA:275:C:OP1	22:BH:340:ARG:NH1	2.31	0.64
6:AA:577:A:OP1	48:AR:20:ARG:NH2	2.30	0.64
6:AA:1131:G:O6	26:EI:242:HIS:NE2	2.29	0.64
7:BA:56:LEU:HD13	7:BA:60:PRO:HD3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:EE:262:HIS:O	30:AK:78:LYS:NZ	2.29	0.64
5:A8:114:GLU:HB2	5:A8:117:TYR:HD2	1.62	0.64
6:AA:307:A:O2'	6:AA:317:A:N3	2.27	0.64
17:UE:69:UNK:O	47:EQ:215:ARG:NH2	2.31	0.64
19:BF:347:ASN:HD21	73:Ag:77:MET:HB2	1.62	0.64
42:AO:61:PHE:HB2	42:AO:85:THR:HB	1.79	0.64
6:AA:125:U:H2'	6:AA:126:A:H8	1.63	0.64
6:AA:356:A:O2'	49:BR:196:ARG:NH1	2.30	0.64
10:EB:184:PRO:HD2	10:EB:188:LEU:HD23	1.78	0.64
44:EO:1:MET:HB2	44:EO:62:PRO:HG3	1.80	0.64
62:AX:167:MET:HG2	70:Ae:141:ARG:HH21	1.63	0.64
6:AA:995:A:H61	10:EB:353:HIS:CE1	2.15	0.64
29:EJ:25:ARG:NH1	52:AT:130:ASP:OD2	2.31	0.64
41:EN:416:SER:HA	41:EN:557:ARG:HH22	1.62	0.64
50:BS:67:GLU:OE2	56:BU:175:GLY:N	2.30	0.64
7:BA:601:ARG:NH2	15:BE:122:LYS:O	2.31	0.63
14:AE:136:VAL:HG21	79:Ap:41:LEU:HD11	1.80	0.63
44:EO:3:THR:HG23	44:EO:60:VAL:HB	1.80	0.63
6:AA:562:G:H4'	56:BU:127:ILE:HG12	1.81	0.63
14:AE:401:SER:OG	26:EI:275:GLY:O	2.17	0.63
19:BF:363:GLN:HB2	61:BW:174:ILE:HG23	1.79	0.63
20:EF:93:VAL:HA	20:EF:97:TYR:HD2	1.63	0.63
25:BI:73:ILE:HD11	73:Ag:144:TYR:HB3	1.81	0.63
44:EP:13:HIS:HE1	44:EP:50:LEU:HA	1.64	0.63
62:AX:155:GLU:HG2	62:AX:221:PRO:HB2	1.80	0.63
1:A1:143:ARG:O	1:A1:157:ARG:NH1	2.31	0.63
7:BA:324:GLU:OE2	7:BA:327:ARG:NH1	2.30	0.63
8:EA:52:ARG:NH2	8:EA:58:LEU:O	2.28	0.63
72:Bf:103:ASN:OD1	72:Bf:112:ARG:NH1	2.31	0.63
6:AA:1006:U:H4'	11:EC:40:PRO:HG3	1.80	0.63
48:AR:28:ASP:OD2	48:AR:30:ASN:ND2	2.30	0.63
58:AV:63:ASP:HB3	58:AV:66:ILE:HG22	1.79	0.63
7:BA:567:THR:HG1	7:BA:570:SER:HG	1.44	0.63
10:EB:65:ARG:NH2	10:EB:625:GLU:OE2	2.32	0.63
41:EN:673:SER:HB3	41:EN:676:CYS:HB2	1.79	0.63
62:AX:155:GLU:HA	62:AX:223:SER:HB2	1.81	0.63
10:EB:725:GLY:HA2	67:Ba:18:GLY:HA2	1.81	0.63
23:EH:593:ASP:OD1	23:EH:596:ARG:NH2	2.32	0.63
25:BI:130:ASP:OD1	25:BI:162:ARG:NH2	2.30	0.63
26:EI:221:SER:O	52:AT:67:ARG:NH2	2.31	0.63
64:UX:180:UNK:O	64:UX:203:UNK:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BB:102:ILE:HG21	9:BB:393:LEU:HD11	1.80	0.63
41:EN:258:LEU:O	41:EN:262:ASN:ND2	2.31	0.63
47:EQ:277:LEU:O	47:EQ:627:LYS:NZ	2.30	0.63
49:BR:127:ARG:NH2	80:At:38:GLU:OE2	2.31	0.63
7:BA:341:CYS:O	7:BA:377:ARG:NH1	2.32	0.63
20:EF:249:LEU:HD23	20:EF:296:LEU:HB2	1.80	0.63
35:EL:228:TYR:O	35:EL:233:ARG:NH1	2.32	0.63
43:BO:126:MET:HE2	43:BO:137:PRO:HD2	1.80	0.63
6:AA:50:A:H4'	81:Av:48:ALA:HB2	1.80	0.62
6:AA:77:A:OP1	81:Av:73:ARG:NH1	2.31	0.62
6:AA:155:U:OP1	18:AF:146:LYS:NZ	2.31	0.62
6:AA:377:A:OP2	55:AU:59:ARG:NH2	2.32	0.62
9:BB:110:THR:HG23	9:BB:117:LEU:HD12	1.81	0.62
31:BK:91:LEU:HB2	31:BK:93:LEU:HD22	1.81	0.62
41:EN:592:THR:OG1	41:EN:618:TYR:OH	2.17	0.62
46:BQ:24:ARG:NH1	46:BQ:25:ASP:O	2.33	0.62
6:AA:461:U:OP1	55:AU:59:ARG:NH1	2.32	0.62
6:AA:571:U:H3'	48:AR:61:ARG:HH21	1.64	0.62
9:BB:273:ASP:HB2	9:BB:299:ASN:HB2	1.79	0.62
14:AE:81:PRO:HG3	25:BI:241:TYR:HB3	1.81	0.62
66:BZ:141:LYS:HG2	66:BZ:142:GLU:HG3	1.82	0.62
9:BB:141:ILE:HG12	9:BB:172:MET:HE2	1.80	0.62
14:AE:140:MET:HE1	14:AE:235:VAL:HA	1.81	0.62
50:BS:72:THR:HG22	50:BS:74:GLU:H	1.64	0.62
58:AV:211:VAL:HG22	73:Ag:125:ARG:HG2	1.82	0.62
19:BF:287:ASP:OD1	19:BF:313:ARG:NE	2.32	0.62
75:Bh:46:VAL:HG21	76:Bi:34:VAL:HG13	1.81	0.62
44:EO:145:ILE:HG21	44:EP:145:ILE:HG21	1.81	0.62
6:AA:570:U:OP1	57:EU:42:ARG:NH1	2.33	0.62
6:AA:1015:A:N3	11:EC:270:LYS:NZ	2.46	0.62
14:AE:136:VAL:HG22	14:AE:222:THR:HG23	1.82	0.62
51:ES:3:VAL:O	51:ES:8:ARG:NH1	2.33	0.62
7:BA:720:ARG:NH2	73:Ag:103:HIS:O	2.32	0.62
19:BF:388:ARG:HG2	60:AW:93:GLU:HG2	1.82	0.62
25:BI:70:PRO:HD2	25:BI:73:ILE:HD12	1.81	0.62
39:AN:30:ASN:O	39:AN:39:ARG:NH1	2.33	0.62
59:BV:46:GLU:HG3	59:BV:50:ARG:HE	1.65	0.62
62:AX:121:PRO:HG3	65:AY:259:MET:HE3	1.81	0.62
6:AA:48:U:OP1	67:Ba:105:ARG:NH2	2.33	0.61
6:AA:296:A:OP2	55:AU:10:HIS:N	2.33	0.61
37:EM:114:ASP:OD1	37:EM:117:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BQ:53:ILE:HG23	46:BQ:54:VAL:HG23	1.82	0.61
48:AR:135:ARG:NE	48:AR:167:ASN:O	2.29	0.61
16:EE:78:PRO:O	16:EE:81:ARG:NE	2.32	0.61
44:EP:54:GLY:HA2	44:EP:95:HIS:HB3	1.83	0.61
6:AA:529:U:N3	62:AX:197:ARG:O	2.34	0.61
20:EF:191:ARG:HA	20:EF:221:THR:HG21	1.81	0.61
44:EO:116:ASP:OD2	44:EP:92:GLN:NE2	2.33	0.61
63:BX:129:ASN:ND2	63:BX:160:TYR:O	2.34	0.61
4:A5:79:LYS:O	7:BA:785:ARG:NH2	2.33	0.61
5:A8:104:LYS:NZ	6:AA:952:U:O2'	2.33	0.61
9:BB:376:ASP:HB3	9:BB:379:ARG:HB2	1.81	0.61
16:EE:425:SER:HB2	20:EF:336:VAL:HG13	1.82	0.61
20:EF:82:CYS:HB3	20:EF:153:ILE:HD11	1.82	0.61
43:BO:101:GLN:HG2	43:BO:117:LEU:HD13	1.82	0.61
75:Bh:8:ARG:NH1	75:Bh:37:GLN:OE1	2.33	0.61
45:AP:36:ASN:ND2	55:AU:171:GLU:OE2	2.32	0.61
6:AA:294:U:O2'	60:AW:19:ASN:OD1	2.19	0.61
16:EE:469:ARG:NH1	79:Ap:210:ALA:O	2.33	0.61
77:Al:153:MET:HE2	77:Al:199:TYR:HD2	1.66	0.61
81:Av:147:ASN:ND2	81:Av:149:ASP:OD2	2.33	0.61
31:BK:208:MET:SD	31:BK:216:ARG:NH1	2.74	0.61
58:AV:227:GLU:O	73:Ag:124:ARG:NH1	2.28	0.61
67:Ba:105:ARG:O	67:Ba:107:GLN:NE2	2.33	0.61
1:A1:178:GLN:HG2	65:AY:299:MET:HE1	1.83	0.61
6:AA:1104:U:H2'	7:BA:226:LYS:HG3	1.83	0.61
15:BE:420:ASP:OD1	15:BE:422:ARG:NH2	2.34	0.61
18:AF:176:ASN:ND2	18:AF:188:GLY:O	2.32	0.61
22:BH:180:PRO:HG2	22:BH:198:VAL:HB	1.81	0.61
26:EI:298:VAL:HG13	29:EJ:103:ARG:HG2	1.83	0.61
51:ES:21:VAL:HG21	51:ES:99:ALA:HB1	1.83	0.61
56:BU:113:MET:HG2	70:Ae:60:GLY:HA3	1.83	0.61
81:Av:71:VAL:HG21	81:Av:120:TRP:HB3	1.82	0.61
1:A1:185:GLU:HA	1:A1:188:ILE:HG22	1.83	0.61
9:BB:99:PRO:HD2	56:BU:106:ARG:HH21	1.65	0.61
20:EF:185:ASN:ND2	20:EF:335:SER:OG	2.33	0.61
43:BO:52:ARG:HB2	52:AT:118:THR:HG22	1.83	0.61
6:AA:522:A:N6	6:AA:560:G:O4'	2.34	0.60
30:AK:177:VAL:HA	30:AK:180:VAL:HG22	1.82	0.60
6:AA:116:U:H1'	55:AU:23:MET:HE1	1.82	0.60
35:EL:339:GLU:O	35:EL:342:ARG:NH1	2.34	0.60
41:EN:608:LEU:HD22	41:EN:643:GLY:HA2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BT:83:GLU:OE2	53:BT:86:ARG:NH2	2.35	0.60
80:At:94:THR:HG23	80:At:97:GLN:H	1.66	0.60
19:BF:398:ARG:NH2	60:AW:60:LEU:O	2.32	0.60
20:EF:58:SER:O	20:EF:128:ARG:NH2	2.34	0.60
24:AI:67:ASN:HB3	81:Av:112:VAL:HB	1.83	0.60
26:EI:79:VAL:HG11	35:EL:281:VAL:HG22	1.83	0.60
44:EO:228:THR:HG23	44:EO:229:PRO:HD3	1.83	0.60
76:Bi:128:ASN:HD21	76:Bi:131:ASN:HB2	1.65	0.60
1:A1:131:GLU:OE2	24:AI:145:ARG:NH2	2.34	0.60
10:EB:71:SER:HB2	10:EB:304:THR:HB	1.83	0.60
13:ED:34:LEU:HD23	13:ED:269:LEU:HD12	1.83	0.60
48:AR:183:PRO:HG3	48:AR:190:PRO:HA	1.83	0.60
2:A2:414:THR:HG21	31:BK:373:PRO:HG3	1.84	0.60
7:BA:156:ASP:OD1	14:AE:169:GLN:NE2	2.35	0.60
11:EC:87:LYS:NZ	21:EG:155:ASP:O	2.34	0.60
13:ED:166:LEU:HD22	13:ED:199:ILE:HG12	1.84	0.60
18:AF:154:ARG:HD2	18:AF:332:PRO:HB2	1.82	0.60
19:BF:195:LEU:HD11	19:BF:216:LEU:HD22	1.83	0.60
37:EM:157:GLN:NE2	37:EM:162:THR:O	2.33	0.60
44:EO:16:VAL:HG12	44:EO:57:ILE:HG21	1.84	0.60
66:BZ:19:ARG:HD2	66:BZ:162:VAL:HG22	1.82	0.60
6:AA:1151:G:O6	48:AR:11:ARG:NH1	2.35	0.60
8:EA:59:HIS:H	8:EA:65:GLN:HE21	1.49	0.60
11:EC:242:SER:HB2	11:EC:361:HIS:HE1	1.65	0.60
18:AF:103:VAL:HG11	18:AF:371:LEU:HD11	1.83	0.60
25:BI:163:CYS:HB3	25:BI:185:MET:HE1	1.83	0.60
40:BN:9:TRP:N	56:BU:180:ALA:O	2.35	0.60
59:BV:60:MET:HE3	59:BV:62:HIS:HB2	1.83	0.60
35:EL:257:ARG:NH1	35:EL:395:CYS:O	2.35	0.60
50:BS:80:ASP:OD1	50:BS:83:GLN:NE2	2.34	0.60
79:Ap:238:ASP:H	79:Ap:270:MET:HE1	1.66	0.60
6:AA:103:U:OP2	65:AY:10:LYS:NZ	2.35	0.60
6:AA:1129:A:HO2'	69:Bc:130:TRP:CD1	2.19	0.60
7:BA:479:ASP:HB3	7:BA:482:VAL:HG22	1.83	0.60
7:BA:638:ARG:NH2	60:AW:239:GLU:OE1	2.35	0.60
55:AU:65:ASN:HD22	55:AU:97:GLN:HE21	1.49	0.60
13:ED:200:LEU:HD23	13:ED:216:PRO:HG3	1.82	0.60
45:AP:12:ARG:HE	80:At:33:LYS:HB2	1.67	0.60
45:AP:31:ILE:HD12	45:AP:44:THR:HG22	1.84	0.60
1:A1:138:ASN:HD21	28:BJ:299:ARG:HH22	1.48	0.60
74:Bg:92:LYS:HA	74:Bg:96:ARG:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:275:LEU:HD22	31:BK:328:LEU:HG	1.83	0.59
5:A8:61:TYR:HB3	5:A8:64:GLN:HB2	1.84	0.59
6:AA:318:A:H2'	6:AA:319:A:C8	2.37	0.59
6:AA:1172:A:OP1	43:BO:124:ARG:NH1	2.34	0.59
15:BE:376:ARG:HD3	15:BE:379:ARG:HE	1.66	0.59
35:EL:443:HIS:HB2	35:EL:474:PRO:HG2	1.84	0.59
65:AY:282:ALA:HA	67:Ba:58:MET:HE1	1.82	0.59
2:A2:270:ASN:HB3	2:A2:273:GLU:HG2	1.82	0.59
2:A2:457:ARG:NH1	2:A2:460:ASP:OD1	2.35	0.59
6:AA:318:A:H2'	6:AA:319:A:H8	1.67	0.59
14:AE:169:GLN:HE21	14:AE:230:GLY:HA2	1.66	0.59
16:EE:413:ASP:OD1	16:EE:413:ASP:N	2.34	0.59
22:BH:125:THR:HG21	22:BH:221:CYS:HB3	1.83	0.59
39:AN:156:ALA:O	69:Bc:23:ARG:NH1	2.34	0.59
65:AY:117:VAL:HG12	65:AY:177:HIS:HA	1.84	0.59
70:Ae:142:GLN:O	70:Ae:144:ASN:ND2	2.35	0.59
6:AA:1090:U:H5'	47:EQ:563:ARG:HD2	1.84	0.59
14:AE:249:GLN:OE1	52:AT:16:ARG:NH2	2.35	0.59
21:EG:91:ARG:HB3	21:EG:108:SER:HB3	1.84	0.59
26:EI:307:VAL:O	52:AT:94:ARG:NH1	2.35	0.59
52:AT:25:PRO:HB2	52:AT:28:ARG:HB2	1.84	0.59
79:Ap:266:ALA:O	79:Ap:270:MET:HG2	2.02	0.59
14:AE:384:PRO:HG2	69:Bc:99:THR:HG23	1.83	0.59
19:BF:330:ARG:NH1	45:AP:102:GLU:O	2.35	0.59
20:EF:135:ASN:ND2	20:EF:146:GLY:O	2.34	0.59
47:EQ:76:PHE:HB2	47:EQ:125:LEU:HG	1.84	0.59
49:BR:14:GLU:HG2	49:BR:15:LEU:HD12	1.83	0.59
52:AT:44:ARG:NH1	52:AT:114:GLU:OE2	2.36	0.59
6:AA:334:U:OP1	19:BF:27:THR:OG1	2.19	0.59
6:AA:801:A:H3'	6:AA:802:G:H8	1.66	0.59
6:AA:1173:U:OP2	43:BO:124:ARG:NH2	2.32	0.59
7:BA:714:ASN:HD22	7:BA:716:LEU:H	1.49	0.59
13:ED:105:ILE:HD12	13:ED:123:ARG:HD2	1.85	0.59
14:AE:261:ARG:NH1	14:AE:300:GLN:O	2.36	0.59
19:BF:171:ARG:HG3	19:BF:194:VAL:HG22	1.84	0.59
41:EN:357:LEU:HD12	41:EN:448:ALA:HB1	1.85	0.59
2:A2:70:ARG:NH2	6:AA:531:U:O2'	2.35	0.59
6:AA:1168:U:OP1	48:AR:52:ARG:NH1	2.34	0.59
47:EQ:95:CYS:HB3	47:EQ:248:MET:HE2	1.85	0.59
51:ES:7:ILE:HG23	51:ES:88:ILE:HG21	1.83	0.59
79:Ap:61:ASN:O	79:Ap:92:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:199:CYS:HB2	2:A2:306:VAL:HG13	1.84	0.59
16:EE:234:GLN:NE2	30:AK:110:LYS:O	2.35	0.59
19:BF:43:LEU:HA	61:BW:188:TYR:HB3	1.84	0.59
41:EN:346:GLU:HB3	41:EN:386:ARG:HD2	1.83	0.59
66:BZ:96:GLN:HE21	66:BZ:134:GLN:HB2	1.67	0.59
14:AE:27:ARG:N	52:AT:5:ARG:O	2.36	0.59
19:BF:123:LEU:HA	19:BF:126:VAL:HG22	1.84	0.59
34:BL:158:ARG:NH2	34:BL:221:CYS:O	2.36	0.59
37:EM:184:ARG:NH2	47:EQ:517:SER:O	2.36	0.59
45:AP:227:PRO:HD3	77:Al:118:ALA:HB2	1.84	0.59
52:AT:57:PRO:HD2	52:AT:117:SER:HB2	1.83	0.59
6:AA:946:A:N7	13:ED:336:LYS:NZ	2.51	0.59
7:BA:16:ARG:NH2	35:EL:215:TYR:OH	2.36	0.59
20:EF:167:LYS:HB2	20:EF:168:PRO:HD3	1.85	0.59
41:EN:499:LEU:O	41:EN:503:HIS:ND1	2.35	0.59
50:BS:84:VAL:HG13	50:BS:96:MET:HG3	1.84	0.59
6:AA:453:U:H5	49:BR:156:ARG:HD2	1.68	0.59
14:AE:55:ASP:HB2	79:Ap:84:ALA:HB1	1.84	0.59
16:EE:81:ARG:NH1	37:EM:286:CYS:SG	2.75	0.59
30:AK:77:LEU:HD21	30:AK:110:LYS:HB3	1.85	0.59
31:BK:142:ASP:HB3	31:BK:145:LYS:HB2	1.85	0.59
46:BQ:48:GLU:HB2	46:BQ:165:ILE:HD11	1.84	0.59
8:EA:572:ASN:ND2	8:EA:574:ASP:O	2.36	0.58
15:BE:66:ARG:NH1	15:BE:69:GLU:OE2	2.35	0.58
24:AI:257:UNK:O	41:EN:158:GLN:NE2	2.36	0.58
41:EN:625:LEU:HD23	41:EN:671:VAL:HG21	1.85	0.58
8:EA:549:ASN:ND2	47:EQ:589:GLU:OE2	2.36	0.58
25:BI:96:ASN:HD22	25:BI:101:PHE:HZ	1.51	0.58
47:EQ:92:ILE:HG23	47:EQ:248:MET:HE1	1.85	0.58
57:EU:34:ARG:HG2	57:EU:51:ARG:HB2	1.84	0.58
60:AW:203:CYS:O	65:AY:8:ARG:NH2	2.37	0.58
73:Ag:12:VAL:HB	73:Ag:45:ILE:HG12	1.84	0.58
13:ED:6:ARG:NH2	46:BQ:230:ARG:O	2.37	0.58
13:ED:436:THR:OG1	13:ED:439:ASP:OD1	2.20	0.58
16:EE:468:ASN:HD22	44:EP:314:MET:HA	1.68	0.58
19:BF:355:LEU:HD23	61:BW:160:VAL:HG13	1.84	0.58
44:EP:209:LEU:HD12	44:EP:210:PRO:HD2	1.84	0.58
2:A2:96:ARG:HB2	31:BK:358:LEU:HD11	1.85	0.58
6:AA:150:A:OP2	45:AP:134:ARG:NH2	2.36	0.58
6:AA:303:U:O2'	54:ET:33:ARG:NH2	2.36	0.58
6:AA:384:U:N3	6:AA:451:A:N1	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:813:U:O2	6:AA:816:C:N4	2.36	0.58
6:AA:1045:N:H4'	20:EF:207:LEU:HD12	1.86	0.58
13:ED:208:ASN:OD1	13:ED:209:LEU:N	2.36	0.58
60:AW:46:PRO:HB2	60:AW:49:ILE:HB	1.86	0.58
65:AY:85:LEU:HB3	65:AY:89:GLN:HE21	1.67	0.58
18:AF:24:ARG:NH1	55:AU:16:GLU:OE2	2.35	0.58
18:AF:226:MET:HE1	18:AF:344:MET:HE2	1.85	0.58
53:BT:77:ARG:NH1	53:BT:85:GLU:OE2	2.36	0.58
63:BX:72:VAL:O	63:BX:108:GLN:NE2	2.37	0.58
72:Bf:86:ILE:HB	72:Bf:91:LYS:HB3	1.85	0.58
12:BD:172:LEU:O	12:BD:176:SER:OG	2.15	0.58
15:BE:294:GLY:O	15:BE:298:ASN:ND2	2.31	0.58
20:EF:106:VAL:HG23	20:EF:108:ASP:H	1.69	0.58
40:BN:67:LEU:HD13	40:BN:109:VAL:HG11	1.85	0.58
44:EP:170:GLN:HB2	44:EP:216:ARG:HD3	1.85	0.58
47:EQ:149:SER:HB2	47:EQ:502:LEU:HD21	1.86	0.58
76:Bi:56:PRO:O	76:Bi:60:ASN:ND2	2.36	0.58
6:AA:851:G:H5''	10:EB:684:ARG:HH21	1.68	0.58
13:ED:251:ILE:HG21	13:ED:582:VAL:HG11	1.86	0.58
14:AE:71:MET:HG2	79:Ap:110:LYS:HB2	1.85	0.58
23:EH:459:PRO:HG3	23:EH:490:PRO:HD3	1.85	0.58
42:AO:175:HIS:HD2	42:AO:177:TYR:H	1.52	0.58
44:EO:5:SER:HG	44:EO:58:SER:HG	1.41	0.58
54:ET:59:LYS:HB2	77:Al:60:LEU:HD11	1.86	0.58
16:EE:336:LEU:HD21	35:EL:544:LEU:HB3	1.85	0.58
77:Al:72:ARG:NH2	77:Al:144:GLY:O	2.36	0.58
6:AA:88:G:H4'	19:BF:403:LEU:HD23	1.86	0.58
15:BE:385:LEU:H	15:BE:388:GLN:HE21	1.52	0.58
16:EE:422:ILE:HG21	20:EF:192:ALA:HB2	1.85	0.58
30:AK:37:ASP:O	30:AK:89:ARG:NH2	2.37	0.58
34:BL:169:GLU:OE1	34:BL:245:ARG:NH2	2.32	0.58
41:EN:361:VAL:HG21	41:EN:451:LEU:HD22	1.86	0.58
45:AP:139:ARG:HH12	45:AP:141:GLN:HG3	1.68	0.58
65:AY:251:LEU:O	65:AY:255:ARG:HG2	2.04	0.58
7:BA:135:SER:O	43:BO:153:ARG:NH1	2.37	0.58
8:EA:64:THR:HA	8:EA:67:LYS:HE2	1.86	0.58
13:ED:341:PRO:HD2	13:ED:344:ILE:HD12	1.86	0.58
16:EE:492:ASN:OD1	25:BI:299:ARG:NH1	2.36	0.58
20:EF:220:GLY:HA2	20:EF:223:PHE:HD2	1.68	0.58
53:BT:14:LYS:O	61:BW:74:ARG:NH2	2.30	0.58
7:BA:134:MET:HB2	43:BO:145:LEU:HD13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:EA:455:LYS:O	47:EQ:604:ARG:NH2	2.37	0.57
13:ED:273:SER:HB3	13:ED:278:ARG:HG2	1.86	0.57
14:AE:176:ARG:NH2	14:AE:179:GLU:OE1	2.37	0.57
20:EF:310:ALA:O	20:EF:317:ARG:NH1	2.37	0.57
22:BH:149:ARG:HH21	22:BH:153:ARG:HH22	1.50	0.57
26:EI:81:LEU:HG	35:EL:492:GLY:HA3	1.85	0.57
66:BZ:1:MET:N	66:BZ:1:MET:SD	2.74	0.57
15:BE:440:ILE:O	48:AR:211:ARG:NH1	2.36	0.57
35:EL:469:PRO:HG3	35:EL:565:PRO:HB2	1.86	0.57
41:EN:380:THR:HG23	41:EN:470:THR:HG21	1.85	0.57
45:AP:34:LEU:HD22	45:AP:39:ASN:HD22	1.69	0.57
9:BB:380:THR:HG23	9:BB:385:ILE:HD11	1.86	0.57
37:EM:191:PHE:HA	37:EM:198:ARG:HH12	1.69	0.57
9:BB:237:PHE:HB3	9:BB:243:ILE:HG22	1.86	0.57
15:BE:162:ASP:OD1	34:BL:283:ARG:NH2	2.36	0.57
26:EI:295:LYS:HB2	42:AO:164:ARG:HH21	1.68	0.57
28:BJ:138:ILE:HD11	28:BJ:168:ILE:HD12	1.86	0.57
48:AR:235:TRP:NE1	57:EU:48:ILE:O	2.36	0.57
48:AR:238:ARG:NH1	65:AY:60:GLU:OE1	2.34	0.57
6:AA:1139:G:OP1	26:EI:239:ARG:NH1	2.37	0.57
40:BN:104:ARG:NH1	75:Bh:79:ALA:O	2.37	0.57
41:EN:666:ALA:HA	41:EN:682:LEU:HD23	1.86	0.57
50:BS:31:ASP:OD1	52:AT:28:ARG:NH1	2.34	0.57
1:A1:163:ARG:HH22	28:BJ:286:ARG:HD2	1.70	0.57
2:A2:116:ARG:NH1	65:AY:260:GLU:OE2	2.37	0.57
18:AF:99:THR:HG21	18:AF:357:MET:HG3	1.85	0.57
42:AO:58:GLY:O	42:AO:88:ARG:NH2	2.38	0.57
45:AP:189:ILE:HD11	45:AP:205:VAL:HG21	1.86	0.57
59:BV:45:LEU:HD11	59:BV:74:ASN:HA	1.87	0.57
60:AW:81:ARG:NH1	60:AW:94:ASP:OD1	2.37	0.57
68:Bb:41:HIS:NE2	68:Bb:128:GLN:O	2.37	0.57
6:AA:861:C:O3'	10:EB:615:LYS:NZ	2.37	0.57
7:BA:734:HIS:O	39:AN:35:GLN:NE2	2.35	0.57
18:AF:108:THR:HB	18:AF:132:PRO:HB2	1.87	0.57
32:EK:65:TYR:HD1	32:EK:66:LEU:HG	1.70	0.57
57:EU:54:MET:HE1	60:AW:214:ILE:HD12	1.85	0.57
6:AA:465:A:N3	58:AV:86:ASN:ND2	2.52	0.57
6:AA:484:U:H1'	6:AA:485:A:H5''	1.87	0.57
16:EE:210:GLY:O	16:EE:282:ARG:NH2	2.38	0.57
16:EE:284:ALA:HB1	16:EE:287:ALA:HB3	1.87	0.57
19:BF:130:GLU:HB2	19:BF:152:VAL:HG11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BI:120:GLN:HG2	25:BI:236:LYS:HE2	1.87	0.57
7:BA:588:LEU:HD22	7:BA:695:LEU:HB3	1.87	0.57
7:BA:699:ASN:O	7:BA:699:ASN:ND2	2.37	0.57
10:EB:281:GLN:HG2	10:EB:285:MET:HE3	1.86	0.57
20:EF:106:VAL:HG22	20:EF:129:CYS:HA	1.87	0.57
34:BL:73:GLY:HA2	34:BL:78:ARG:HH21	1.70	0.57
34:BL:254:VAL:HG21	34:BL:304:VAL:HG21	1.86	0.57
35:EL:447:GLU:O	35:EL:609:LYS:NZ	2.35	0.57
76:Bi:128:ASN:HD22	76:Bi:133:LEU:HD11	1.69	0.57
6:AA:1127:A:OP2	26:EI:261:ARG:NH1	2.38	0.57
16:EE:100:PRO:HD2	16:EE:103:ILE:HD12	1.87	0.56
30:AK:24:ASN:OD1	30:AK:159:LYS:NZ	2.38	0.56
49:BR:105:ASN:OD1	49:BR:192:ARG:NH1	2.38	0.56
61:BW:149:ASN:ND2	61:BW:152:GLN:OE1	2.35	0.56
65:AY:115:ASP:OD2	65:AY:205:ARG:NH1	2.38	0.56
2:A2:145:LEU:O	2:A2:321:PRO:HA	2.05	0.56
6:AA:1096:U:H2'	6:AA:1097:A:H8	1.69	0.56
8:EA:77:THR:OG1	8:EA:148:ARG:NH2	2.38	0.56
10:EB:94:LYS:NZ	10:EB:96:LYS:O	2.38	0.56
30:AK:94:PHE:O	59:BV:91:LYS:NZ	2.32	0.56
49:BR:37:GLY:O	49:BR:83:ARG:NH1	2.39	0.56
2:A2:108:ARG:NH1	2:A2:111:GLU:OE2	2.39	0.56
2:A2:123:ARG:HG2	2:A2:125:PRO:HD2	1.85	0.56
2:A2:146:SER:OG	2:A2:348:ALA:O	2.17	0.56
6:AA:521:G:C6	56:BU:126:ARG:HG2	2.40	0.56
7:BA:806:TYR:OH	43:BO:143:ARG:NH2	2.36	0.56
8:EA:449:ARG:NH1	37:EM:196:PHE:O	2.38	0.56
13:ED:149:TYR:HH	13:ED:531:SER:HG	1.47	0.56
26:EI:214:ASP:O	26:EI:287:ARG:NH2	2.38	0.56
39:AN:47:LEU:HD13	39:AN:174:LEU:HD23	1.87	0.56
40:BN:10:GLN:HB2	40:BN:13:VAL:HG12	1.85	0.56
41:EN:365:GLU:HG3	41:EN:366:LYS:HG3	1.85	0.56
45:AP:282:ARG:HE	81:Av:180:MET:HG2	1.70	0.56
53:BT:104:ARG:NH1	53:BT:107:GLU:OE2	2.38	0.56
6:AA:159:U:O2'	45:AP:205:VAL:O	2.22	0.56
8:EA:198:ASP:OD1	8:EA:238:ARG:NH1	2.39	0.56
8:EA:418:ALA:O	8:EA:563:ARG:NH2	2.37	0.56
29:EJ:25:ARG:NH2	52:AT:127:ASP:OD1	2.37	0.56
35:EL:130:SER:OG	35:EL:134:LYS:O	2.24	0.56
45:AP:286:GLU:HG3	81:Av:182:LYS:HD3	1.88	0.56
49:BR:21:PRO:HB2	49:BR:59:PRO:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Bc:124:PRO:HG2	69:Bc:127:ILE:HD13	1.86	0.56
1:A1:101:TYR:OH	81:Av:24:VAL:O	2.22	0.56
10:EB:733:ALA:HB3	70:Ae:100:HIS:HA	1.88	0.56
13:ED:434:LEU:HG	13:ED:465:LEU:HD21	1.87	0.56
41:EN:466:LYS:NZ	41:EN:470:THR:OG1	2.38	0.56
44:EP:59:ILE:HD13	44:EP:100:ILE:HD11	1.87	0.56
76:Bi:55:LYS:O	76:Bi:60:ASN:ND2	2.38	0.56
77:Al:75:ARG:H	77:Al:211:HIS:HE1	1.51	0.56
3:A3:78:SER:O	3:A3:82:ASN:ND2	2.33	0.56
8:EA:355:ARG:HD2	8:EA:478:LEU:HD13	1.87	0.56
8:EA:389:ARG:O	8:EA:421:ARG:NH2	2.39	0.56
10:EB:549:ASP:OD2	87:EB:1001:ATP:O3'	2.21	0.56
45:AP:50:ASP:HB2	80:At:148:GLN:HB2	1.88	0.56
46:BQ:34:ASP:N	46:BQ:34:ASP:OD1	2.39	0.56
52:AT:88:GLY:H	52:AT:106:PRO:HD3	1.68	0.56
11:EC:64:GLU:HB2	23:EH:485:PRO:HB3	1.87	0.56
72:Bf:71:PRO:HB2	72:Bf:72:LEU:HD23	1.87	0.56
8:EA:528:LEU:HD11	8:EA:564:LEU:HD22	1.88	0.56
10:EB:674:HIS:HD2	10:EB:676:GLY:H	1.51	0.56
18:AF:398:LYS:O	53:BT:113:ARG:NH2	2.38	0.56
79:Ap:242:TYR:CZ	79:Ap:262:GLU:HG3	2.41	0.56
6:AA:850:G:N1	6:AA:1091:U:OP2	2.32	0.56
20:EF:177:LEU:HB3	20:EF:180:LEU:HD13	1.88	0.56
34:BL:165:LEU:HD23	34:BL:239:VAL:HG11	1.88	0.56
48:AR:61:ARG:H	48:AR:65:HIS:HD2	1.53	0.56
9:BB:118:TYR:OH	9:BB:358:ARG:NH1	2.39	0.56
34:BL:37:ARG:NH1	34:BL:170:GLU:OE2	2.37	0.56
7:BA:418:ASP:O	7:BA:423:ARG:NH2	2.38	0.55
20:EF:213:LYS:H	20:EF:213:LYS:HD2	1.71	0.55
44:EO:129:SER:HB2	44:EO:199:THR:HG21	1.86	0.55
69:Bc:84:LEU:HD12	69:Bc:85:PRO:HD2	1.88	0.55
8:EA:535:ASP:OD1	10:EB:337:ARG:NH1	2.39	0.55
10:EB:254:ARG:HG2	10:EB:292:VAL:HG23	1.88	0.55
13:ED:65:VAL:HG12	13:ED:241:LEU:HD22	1.88	0.55
14:AE:152:ASP:OD1	14:AE:156:ASN:N	2.39	0.55
15:BE:439:PHE:HB3	74:Bg:26:PHE:HB3	1.87	0.55
21:EG:29:PRO:HB3	21:EG:118:ARG:HA	1.88	0.55
26:EI:79:VAL:HG21	35:EL:281:VAL:HG13	1.86	0.55
44:EP:197:PHE:HB2	44:EP:224:LEU:HD13	1.88	0.55
1:A1:190:PRO:HB2	1:A1:192:GLU:HG2	1.88	0.55
6:AA:330:U:OP1	46:BQ:100:LYS:NZ	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:EA:527:LEU:HD11	8:EA:567:GLU:HB2	1.88	0.55
15:BE:33:TYR:O	65:AY:77:HIS:NE2	2.38	0.55
30:AK:152:GLU:HG3	59:BV:104:TYR:HE2	1.71	0.55
35:EL:219:PRO:HG2	35:EL:221:ARG:HE	1.72	0.55
51:ES:52:ASN:ND2	51:ES:91:GLU:OE1	2.39	0.55
79:Ap:33:PRO:O	79:Ap:37:ASN:ND2	2.35	0.55
81:Av:156:ASP:HB3	81:Av:161:LYS:HD2	1.88	0.55
6:AA:266:C:C6	47:EQ:62:ASN:HB2	2.41	0.55
6:AA:519:A:O2'	6:AA:568:U:O4	2.22	0.55
6:AA:950:U:O2'	13:ED:94:TRP:NE1	2.40	0.55
20:EF:92:ARG:HD2	20:EF:219:GLU:HG3	1.87	0.55
48:AR:73:MET:HE3	48:AR:93:LEU:HB2	1.89	0.55
68:Bb:79:HIS:HD2	68:Bb:81:HIS:H	1.53	0.55
6:AA:890:U:O2'	24:AI:104:GLU:O	2.24	0.55
7:BA:149:SER:OG	7:BA:155:ILE:O	2.24	0.55
7:BA:375:LEU:HD11	7:BA:408:ASN:HD21	1.71	0.55
13:ED:469:LEU:HD23	13:ED:472:LEU:HD22	1.88	0.55
15:BE:32:LEU:HD23	15:BE:32:LEU:H	1.71	0.55
16:EE:95:SER:OG	16:EE:97:ASP:OD1	2.25	0.55
19:BF:211:GLU:OE2	80:At:136:ARG:NH1	2.38	0.55
23:EH:273:PRO:O	23:EH:300:ARG:NH2	2.40	0.55
67:Ba:58:MET:HG2	67:Ba:65:GLU:HA	1.89	0.55
2:A2:470:ASP:OD2	19:BF:414:LYS:NZ	2.39	0.55
6:AA:130:U:OP1	10:EB:667:HIS:NE2	2.39	0.55
19:BF:131:LEU:HD22	80:At:143:THR:HB	1.87	0.55
23:EH:315:ASN:ND2	39:AN:190:GLN:OE1	2.37	0.55
39:AN:154:GLU:O	69:Bc:23:ARG:NH2	2.35	0.55
65:AY:141:ILE:HG13	65:AY:172:VAL:HG22	1.88	0.55
70:Ae:100:HIS:HD2	70:Ae:102:SER:H	1.55	0.55
2:A2:131:PRO:HG2	2:A2:134:ALA:HB2	1.89	0.55
6:AA:490:G:H1	18:AF:27:TRP:HE1	1.53	0.55
8:EA:90:ARG:NH2	8:EA:177:GLU:OE2	2.36	0.55
10:EB:572:GLY:O	10:EB:573:ARG:NH2	2.40	0.55
14:AE:218:GLY:O	14:AE:338:ARG:NH2	2.32	0.55
15:BE:157:ASN:HB3	15:BE:160:LEU:HB2	1.87	0.55
18:AF:421:ASP:OD1	53:BT:94:TYR:OH	2.23	0.55
19:BF:26:VAL:HG22	54:ET:24:GLU:HG2	1.88	0.55
44:EO:96:ASP:HB3	44:EO:99:HIS:HD2	1.72	0.55
45:AP:190:ASN:ND2	61:BW:100:GLN:OE1	2.37	0.55
48:AR:73:MET:HB3	48:AR:93:LEU:HD13	1.89	0.55
60:AW:164:CYS:HB3	60:AW:176:PHE:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:536:A:H1'	74:Bg:89:ARG:HH21	1.72	0.55
6:AA:953:U:OP1	13:ED:130:TYR:OH	2.21	0.55
6:AA:995:A:H61	10:EB:353:HIS:HE1	1.53	0.55
11:EC:310:THR:OG1	11:EC:315:GLN:NE2	2.40	0.55
19:BF:220:ARG:HD3	19:BF:228:GLU:HB3	1.89	0.55
44:EP:115:LEU:HD21	44:EP:191:LEU:HD11	1.87	0.55
6:AA:202:U:O2'	6:AA:265:U:OP2	2.24	0.55
6:AA:202:U:H2'	6:AA:203:A:C8	2.42	0.55
12:BD:424:VAL:HG21	12:BD:440:ALA:HB2	1.88	0.55
37:EM:83:LEU:HB3	37:EM:86:THR:HB	1.89	0.55
42:AO:187:PHE:HZ	52:AT:71:LEU:HD21	1.72	0.55
51:ES:108:ASN:ND2	51:ES:142:GLU:OE2	2.40	0.55
63:BX:91:VAL:HG12	63:BX:93:SER:H	1.72	0.55
63:BX:95:VAL:N	63:BX:112:PHE:O	2.36	0.55
73:Ag:171:GLU:O	73:Ag:175:ARG:NH1	2.40	0.55
3:A3:140:ASP:N	3:A3:140:ASP:OD1	2.38	0.55
6:AA:871:C:N4	6:AA:901:G:O6	2.38	0.55
6:AA:1076:G:H5''	11:EC:224:ARG:HE	1.71	0.55
15:BE:81:VAL:HA	15:BE:84:GLU:HG2	1.88	0.55
49:BR:150:PHE:HB3	49:BR:154:ASP:HB2	1.89	0.55
2:A2:342:ILE:HG13	2:A2:350:VAL:HG11	1.90	0.54
2:A2:375:ARG:NH1	67:Ba:85:ASN:O	2.40	0.54
7:BA:509:ARG:NH1	7:BA:648:GLU:O	2.38	0.54
25:BI:293:THR:HG22	25:BI:295:TYR:H	1.72	0.54
31:BK:379:LEU:HD11	62:AX:200:ASN:HA	1.88	0.54
61:BW:110:ASN:ND2	77:Al:108:GLU:OE2	2.37	0.54
1:A1:97:ARG:NH1	22:BH:294:ASP:OD2	2.34	0.54
6:AA:512:U:H5'	57:EU:52:ARG:HG3	1.88	0.54
6:AA:521:G:C5	74:Bg:95:PHE:HD2	2.25	0.54
9:BB:307:ASP:OD1	9:BB:334:ARG:NH2	2.41	0.54
14:AE:234:ASP:OD1	14:AE:235:VAL:N	2.40	0.54
14:AE:263:GLY:H	42:AO:43:SER:HB3	1.72	0.54
15:BE:277:THR:HG23	15:BE:318:ARG:HH22	1.72	0.54
43:BO:141:ASP:OD2	43:BO:146:ASN:ND2	2.39	0.54
65:AY:25:ASP:HB3	65:AY:28:VAL:HG23	1.89	0.54
75:Bh:27:LEU:HB3	75:Bh:40:LEU:HD11	1.89	0.54
77:Al:132:ASP:OD1	77:Al:133:THR:N	2.40	0.54
16:EE:364:ARG:HD3	16:EE:411:LEU:HD11	1.89	0.54
18:AF:80:GLN:NE2	61:BW:161:PRO:O	2.40	0.54
35:EL:459:LYS:O	35:EL:463:LYS:HB2	2.08	0.54
46:BQ:180:SER:OG	46:BQ:184:THR:O	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:291:GLY:O	18:AF:287:ARG:NH1	2.40	0.54
6:AA:527:U:O2	62:AX:91:ARG:NH1	2.40	0.54
6:AA:871:C:H2'	6:AA:872:A:C8	2.43	0.54
6:AA:952:U:O4	10:EB:221:SER:OG	2.25	0.54
7:BA:649:LYS:NZ	15:BE:116:GLU:OE1	2.39	0.54
7:BA:660:GLU:HG3	7:BA:675:MET:HE3	1.90	0.54
18:AF:337:ARG:NH2	53:BT:25:ASP:OD1	2.40	0.54
29:EJ:50:THR:H	29:EJ:53:GLN:HE21	1.54	0.54
34:BL:241:ASP:OD1	34:BL:241:ASP:N	2.41	0.54
44:EO:13:HIS:HD2	44:EO:15:ALA:H	1.56	0.54
61:BW:177:VAL:HG12	61:BW:179:ASP:H	1.71	0.54
3:A3:130:ILE:HG13	3:A3:132:VAL:HG12	1.90	0.54
7:BA:589:MET:SD	7:BA:589:MET:N	2.80	0.54
7:BA:626:THR:HA	71:Af:167:LEU:HB3	1.89	0.54
10:EB:114:LEU:HD21	10:EB:155:LEU:HD11	1.90	0.54
16:EE:159:ARG:HH22	16:EE:186:TRP:HE1	1.55	0.54
26:EI:225:SER:O	52:AT:67:ARG:NH1	2.40	0.54
35:EL:286:LEU:HB2	35:EL:290:ILE:HD12	1.90	0.54
41:EN:224:LEU:HA	41:EN:227:VAL:HG23	1.88	0.54
44:EP:18:HIS:HB2	44:EP:198:THR:HG21	1.88	0.54
58:AV:223:LYS:HD2	58:AV:226:MET:HE1	1.88	0.54
4:A5:50:LYS:O	6:AA:1161:A:N6	2.41	0.54
6:AA:525:A:OP1	10:EB:725:GLY:N	2.30	0.54
6:AA:528:A:N1	6:AA:547:U:O2'	2.29	0.54
7:BA:493:ASP:HB3	7:BA:614:MET:HE1	1.89	0.54
20:EF:194:VAL:HG21	20:EF:221:THR:HB	1.88	0.54
6:AA:115:A:OP1	55:AU:25:ARG:NH2	2.41	0.54
9:BB:269:ALA:O	9:BB:440:LYS:NZ	2.34	0.54
14:AE:159:ASP:N	14:AE:159:ASP:OD1	2.41	0.54
35:EL:441:GLN:NE2	69:Bc:113:TYR:OH	2.41	0.54
44:EO:285:VAL:HG11	79:Ap:247:LEU:HD11	1.89	0.54
49:BR:100:VAL:HG11	78:Ao:210:PHE:HE2	1.72	0.54
61:BW:25:THR:HB	77:Al:109:ALA:HB3	1.89	0.54
61:BW:42:GLU:OE2	61:BW:89:ARG:NH2	2.40	0.54
6:AA:102:A:N6	65:AY:43:TYR:O	2.36	0.54
6:AA:286:U:H2'	6:AA:287:A:H5''	1.89	0.54
6:AA:891:G:H1'	24:AI:105:PRO:HB3	1.90	0.54
13:ED:208:ASN:ND2	54:ET:102:ARG:O	2.41	0.54
14:AE:351:TRP:HB3	14:AE:358:PRO:HD3	1.90	0.54
22:BH:335:ASN:HD22	22:BH:347:VAL:HB	1.73	0.54
25:BI:294:VAL:HG21	79:Ap:167:ARG:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:EI:181:VAL:HG21	50:BS:136:LEU:HB2	1.90	0.54
35:EL:613:ILE:HG12	69:Bc:122:LEU:HD11	1.90	0.54
40:BN:106:GLU:O	75:Bh:34:ARG:NH1	2.41	0.54
43:BO:39:TYR:O	52:AT:129:ARG:NH2	2.33	0.54
44:EO:236:LEU:HA	44:EO:239:ARG:HE	1.73	0.54
51:ES:36:GLY:HA2	51:ES:119:SER:HB2	1.90	0.54
9:BB:84:PHE:O	9:BB:88:GLU:HB2	2.08	0.54
9:BB:91:LEU:HD11	9:BB:126:ALA:HA	1.90	0.54
19:BF:240:VAL:HG11	19:BF:286:VAL:HG11	1.90	0.54
23:EH:214:ILE:HG22	23:EH:321:GLU:HG2	1.89	0.54
35:EL:237:CYS:HA	35:EL:292:PRO:HG2	1.90	0.54
44:EP:205:GLU:HG3	44:EP:206:GLU:HG3	1.88	0.54
58:AV:101:ARG:HD3	58:AV:169:ALA:HB1	1.88	0.54
79:Ap:138:PRO:HA	79:Ap:141:TRP:HD1	1.72	0.54
6:AA:309:U:H6	10:EB:309:PHE:HB3	1.73	0.54
8:EA:347:GLU:HG3	8:EA:360:ILE:HG12	1.89	0.54
10:EB:130:VAL:HG13	10:EB:156:PRO:HG3	1.90	0.54
23:EH:213:ASP:HB2	23:EH:324:ARG:HA	1.90	0.54
35:EL:419:ILE:HD11	35:EL:605:MET:HE3	1.90	0.54
47:EQ:564:ARG:NH1	47:EQ:568:ASP:OD1	2.41	0.54
80:At:94:THR:OG1	80:At:96:GLU:OE1	2.26	0.54
6:AA:380:G:H3'	6:AA:381:U:H5''	1.88	0.53
7:BA:15:LEU:N	35:EL:209:LEU:O	2.41	0.53
9:BB:152:ARG:NH2	74:Bg:105:GLU:OE1	2.40	0.53
13:ED:469:LEU:HB3	13:ED:472:LEU:HB3	1.91	0.53
14:AE:108:ARG:NH1	14:AE:122:ASP:OD1	2.41	0.53
15:BE:286:SER:HB3	15:BE:291:ASP:HB3	1.91	0.53
18:AF:126:TYR:OH	18:AF:353:GLU:OE2	2.22	0.53
22:BH:260:ASP:OD1	22:BH:268:ARG:NH1	2.41	0.53
49:BR:23:LEU:HG	49:BR:59:PRO:HB3	1.90	0.53
6:AA:455:G:H5'	78:Ao:54:GLN:HB3	1.91	0.53
7:BA:278:LYS:HD2	7:BA:284:LYS:HD2	1.91	0.53
9:BB:183:VAL:HG11	9:BB:246:ARG:HD2	1.89	0.53
14:AE:85:GLN:HB2	14:AE:88:GLN:HB2	1.91	0.53
30:AK:34:LYS:O	30:AK:38:ILE:HG22	2.08	0.53
31:BK:206:HIS:HB2	31:BK:208:MET:HE3	1.90	0.53
44:EO:166:ASP:HB2	44:EO:217:MET:HE3	1.90	0.53
77:Al:89:TYR:HB2	77:Al:216:LEU:HD11	1.89	0.53
6:AA:92:U:OP2	19:BF:400:ARG:NH2	2.35	0.53
6:AA:952:U:OP1	10:EB:247:ARG:NH2	2.40	0.53
13:ED:468:HIS:HA	13:ED:473:ASP:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:366:PRO:HG2	14:AE:369:GLU:HB2	1.90	0.53
25:BI:303:TRP:HB2	72:Bf:78:GLN:HB2	1.89	0.53
28:BJ:175:GLU:N	28:BJ:175:GLU:OE1	2.42	0.53
39:AN:125:ASP:HB3	39:AN:128:MET:HG3	1.91	0.53
6:AA:361:U:OP2	21:EG:146:ASN:ND2	2.41	0.53
6:AA:365:C:H2'	6:AA:366:U:H4'	1.91	0.53
8:EA:252:ALA:N	85:EA:1001:GTP:O6	2.42	0.53
9:BB:439:ASP:OD1	28:BJ:181:ARG:NH2	2.42	0.53
10:EB:54:TYR:HD2	10:EB:671:THR:HG21	1.72	0.53
44:EO:105:SER:HA	44:EO:112:GLN:HG3	1.89	0.53
44:EO:300:ARG:HH11	73:Ag:159:ILE:HG21	1.74	0.53
44:EP:58:SER:HB2	44:EP:93:ARG:HH21	1.73	0.53
76:Bi:128:ASN:OD1	76:Bi:131:ASN:N	2.37	0.53
6:AA:193:A:H4'	81:Av:42:LYS:HE3	1.90	0.53
6:AA:284:U:H5''	18:AF:167:ARG:HH11	1.73	0.53
9:BB:399:ILE:O	9:BB:403:THR:OG1	2.27	0.53
10:EB:463:GLU:HG2	11:EC:98:TYR:CG	2.43	0.53
12:BD:166:SER:OG	12:BD:318:ARG:O	2.23	0.53
18:AF:65:ASN:HD22	61:BW:174:ILE:HD11	1.73	0.53
23:EH:208:ILE:HG13	23:EH:273:PRO:HB3	1.90	0.53
44:EP:53:CYS:HB2	44:EP:57:ILE:HD13	1.90	0.53
55:AU:87:GLN:OE1	58:AV:128:ARG:NH1	2.41	0.53
55:AU:176:VAL:HG13	55:AU:194:LEU:HD23	1.89	0.53
62:AX:129:GLU:OE1	65:AY:255:ARG:NH1	2.42	0.53
77:Al:79:TYR:OH	77:Al:92:HIS:O	2.22	0.53
6:AA:278:A:H2'	6:AA:279:A:H8	1.73	0.53
6:AA:545:U:O4'	70:Ae:109:ARG:NH2	2.40	0.53
6:AA:1172:A:C8	7:BA:774:LYS:HG2	2.44	0.53
13:ED:51:CYS:SG	13:ED:52:GLN:N	2.82	0.53
16:EE:232:ASN:ND2	16:EE:234:GLN:O	2.41	0.53
37:EM:26:TYR:HB2	47:EQ:333:LEU:HD21	1.90	0.53
41:EN:161:VAL:HG13	41:EN:222:LEU:HD11	1.90	0.53
42:AO:175:HIS:CD2	42:AO:177:TYR:H	2.26	0.53
43:BO:52:ARG:HG3	50:BS:43:PRO:HG2	1.89	0.53
3:A3:66:PHE:HB2	3:A3:99:VAL:HG23	1.91	0.53
6:AA:115:A:N7	55:AU:46:GLN:NE2	2.56	0.53
7:BA:475:LEU:HD13	7:BA:670:CYS:HB2	1.91	0.53
10:EB:641:LEU:HD11	10:EB:647:ILE:HD11	1.91	0.53
19:BF:143:GLN:HE22	19:BF:183:ARG:HH12	1.56	0.53
23:EH:106:ARG:HH21	23:EH:110:MET:HB2	1.73	0.53
35:EL:216:HIS:HB2	35:EL:247:HIS:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BU:128:ASP:OD2	56:BU:132:ARG:NH2	2.40	0.53
2:A2:463:ILE:HD11	53:BT:42:MET:HE2	1.91	0.53
47:EQ:302:PRO:HG3	47:EQ:312:PHE:CG	2.43	0.53
57:EU:51:ARG:HG2	57:EU:52:ARG:HG2	1.90	0.53
63:BX:170:LEU:HD23	63:BX:170:LEU:H	1.72	0.53
7:BA:228:GLY:HA3	39:AN:16:LEU:HD22	1.90	0.53
8:EA:116:MET:HG3	8:EA:169:GLY:HA3	1.91	0.53
19:BF:259:LEU:HD11	19:BF:345:LEU:HD21	1.90	0.53
28:BJ:251:GLY:HA3	67:Ba:54:ALA:HA	1.89	0.53
41:EN:380:THR:HG21	41:EN:452:LEU:HD22	1.91	0.53
49:BR:143:ILE:HG22	78:Ao:210:PHE:HB2	1.91	0.53
60:AW:138:VAL:HG13	60:AW:174:ILE:HD13	1.91	0.53
3:A3:62:VAL:HG13	3:A3:123:LEU:HB2	1.91	0.53
14:AE:169:GLN:HE22	14:AE:211:PRO:HD2	1.73	0.53
19:BF:169:GLY:O	80:At:136:ARG:NH2	2.42	0.53
19:BF:366:ARG:NE	19:BF:371:GLU:OE2	2.34	0.53
28:BJ:77:TRP:CE3	47:EQ:98:ARG:HD2	2.44	0.53
37:EM:147:GLN:NE2	37:EM:221:CYS:SG	2.82	0.53
37:EM:287:LEU:O	37:EM:306:ARG:NH1	2.39	0.53
44:EP:132:VAL:HG21	44:EP:165:LEU:HD22	1.91	0.53
50:BS:113:ARG:HA	50:BS:117:GLY:HA2	1.90	0.53
76:Bi:55:LYS:HG3	76:Bi:60:ASN:HD22	1.74	0.53
3:A3:72:ASP:HB3	3:A3:115:ILE:HG23	1.91	0.52
9:BB:101:LEU:HD22	9:BB:104:ILE:HD12	1.91	0.52
9:BB:201:PRO:HB3	56:BU:106:ARG:HD3	1.91	0.52
16:EE:227:GLU:OE1	16:EE:227:GLU:N	2.42	0.52
16:EE:329:ASP:OD1	16:EE:390:ASN:ND2	2.42	0.52
16:EE:491:ASP:OD2	25:BI:295:TYR:OH	2.23	0.52
18:AF:137:MET:HE3	18:AF:224:ARG:HH12	1.74	0.52
21:EG:118:ARG:HD3	21:EG:143:CYS:HB3	1.90	0.52
25:BI:276:ILE:HG23	73:Ag:159:ILE:HD13	1.89	0.52
37:EM:150:VAL:HG13	37:EM:154:LEU:HD12	1.89	0.52
41:EN:580:GLU:OE1	41:EN:618:TYR:OH	2.26	0.52
68:Bb:62:ARG:NH2	68:Bb:70:ASN:O	2.42	0.52
2:A2:127:GLY:HA2	66:BZ:124:ALA:HB1	1.90	0.52
7:BA:665:ASP:OD1	7:BA:665:ASP:N	2.39	0.52
9:BB:147:ASN:OD1	9:BB:148:LYS:N	2.40	0.52
18:AF:132:PRO:O	18:AF:136:GLY:CA	2.58	0.52
23:EH:24:ARG:NH2	23:EH:534:ASP:OD2	2.41	0.52
31:BK:131:ARG:NH2	48:AR:264:ALA:O	2.42	0.52
40:BN:54:ASP:O	40:BN:95:HIS:NE2	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:EN:45:VAL:HB	41:EN:48:ASP:HB2	1.91	0.52
61:BW:100:GLN:NE2	61:BW:104:ASN:OD1	2.34	0.52
6:AA:575:A:H62	6:AA:576:A:H2	1.55	0.52
7:BA:187:MET:SD	7:BA:206:ILE:HD11	2.49	0.52
7:BA:220:LEU:HD21	7:BA:286:PHE:HA	1.91	0.52
8:EA:189:ALA:HB3	8:EA:217:VAL:HG22	1.90	0.52
9:BB:439:ASP:OD2	9:BB:442:ARG:NH2	2.43	0.52
12:BD:120:ARG:NE	12:BD:161:GLU:OE2	2.41	0.52
35:EL:257:ARG:NH1	35:EL:398:LEU:O	2.42	0.52
42:AO:76:LYS:HD3	42:AO:103:SER:HB2	1.92	0.52
50:BS:74:GLU:HG2	50:BS:107:ILE:HD11	1.91	0.52
6:AA:941:G:H2'	6:AA:942:A:C8	2.45	0.52
14:AE:186:TYR:HB3	14:AE:216:CYS:SG	2.49	0.52
20:EF:163:LEU:HD13	20:EF:243:ILE:HD12	1.91	0.52
61:BW:56:ASN:HB2	61:BW:65:ASN:HD21	1.74	0.52
63:BX:66:ASP:HB3	63:BX:70:PRO:HA	1.91	0.52
73:Ag:12:VAL:HG13	73:Ag:57:ILE:HD11	1.91	0.52
6:AA:157:U:OP2	18:AF:217:LYS:NZ	2.39	0.52
10:EB:236:PRO:HA	10:EB:239:VAL:HG12	1.90	0.52
12:BD:300:LEU:HB3	12:BD:303:ASP:HB3	1.92	0.52
16:EE:377:LYS:HE2	16:EE:380:ALA:HA	1.92	0.52
23:EH:35:GLU:HA	23:EH:106:ARG:HH12	1.75	0.52
31:BK:202:ARG:HG3	31:BK:207:GLY:HA2	1.91	0.52
39:AN:93:MET:HG3	39:AN:97:GLN:HB2	1.92	0.52
50:BS:37:VAL:HG21	52:AT:35:MET:HE1	1.90	0.52
55:AU:57:TRP:O	55:AU:61:ILE:HG12	2.09	0.52
55:AU:108:ARG:NH2	73:Ag:121:GLU:OE2	2.42	0.52
75:Bh:74:ARG:HG3	75:Bh:75:GLU:HG2	1.91	0.52
2:A2:216:TYR:CZ	18:AF:406:ALA:HB1	2.45	0.52
5:A8:155:GLU:HG2	5:A8:156:TRP:CD1	2.45	0.52
6:AA:539:A:O2'	6:AA:540:U:O4'	2.26	0.52
6:AA:1012:U:H5	11:EC:313:ARG:HH12	1.57	0.52
6:AA:1096:U:H2'	6:AA:1097:A:C8	2.44	0.52
6:AA:1108:A:OP2	14:AE:200:HIS:NE2	2.37	0.52
15:BE:400:GLY:O	48:AR:154:ARG:HD3	2.09	0.52
19:BF:41:ASN:HA	19:BF:253:LEU:HD11	1.92	0.52
34:BL:33:GLY:O	34:BL:88:ASN:ND2	2.42	0.52
43:BO:239:GLU:HG2	43:BO:244:ALA:HA	1.91	0.52
65:AY:64:HIS:HD2	65:AY:66:ARG:H	1.57	0.52
12:BD:244:ARG:NH2	12:BD:268:ASP:OD1	2.43	0.52
13:ED:280:PHE:HB2	13:ED:486:MET:HE1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:ED:524:ASN:HA	13:ED:573:LEU:HD21	1.91	0.52
16:EE:301:GLU:N	16:EE:301:GLU:OE1	2.43	0.52
23:EH:479:ASP:O	49:BR:151:ARG:NH2	2.43	0.52
28:BJ:61:GLU:OE1	28:BJ:61:GLU:N	2.43	0.52
35:EL:64:PRO:HA	35:EL:73:SER:HA	1.90	0.52
35:EL:250:ASP:HB2	35:EL:268:PRO:HB2	1.92	0.52
35:EL:633:GLN:HA	35:EL:636:MET:HG2	1.91	0.52
1:A1:124:GLU:OE2	24:AI:106:ARG:NH2	2.39	0.52
15:BE:296:GLU:HG3	15:BE:323:TRP:CD1	2.45	0.52
18:AF:128:ARG:NH2	18:AF:360:GLU:OE2	2.43	0.52
26:EI:138:ARG:NH1	26:EI:180:GLU:OE1	2.42	0.52
31:BK:328:LEU:HD23	65:AY:191:VAL:HG12	1.92	0.52
39:AN:119:THR:HG23	79:Ap:65:VAL:HG11	1.92	0.52
48:AR:232:LEU:HD23	48:AR:235:TRP:HE3	1.75	0.52
55:AU:76:GLY:HA3	71:Af:62:LEU:HD11	1.91	0.52
65:AY:289:GLN:HE22	67:Ba:60:VAL:HG11	1.74	0.52
11:EC:187:MET:HE3	16:EE:117:GLN:HG2	1.92	0.52
13:ED:136:LYS:HD2	41:EN:525:ARG:HH12	1.74	0.52
24:AI:204:GLU:OE1	24:AI:204:GLU:N	2.42	0.52
31:BK:361:GLU:OE1	31:BK:361:GLU:N	2.43	0.52
43:BO:91:LYS:NZ	50:BS:89:TYR:O	2.42	0.52
44:EP:141:ILE:O	44:EP:145:ILE:HG12	2.10	0.52
47:EQ:86:ASN:ND2	47:EQ:107:ARG:O	2.39	0.52
4:A5:26:PRO:HG2	6:AA:1096:U:C2	2.45	0.51
9:BB:202:VAL:HB	9:BB:378:MET:HB3	1.91	0.51
13:ED:336:LYS:HE2	13:ED:345:VAL:HG11	1.92	0.51
34:BL:38:GLY:HA3	34:BL:167:LEU:HD11	1.93	0.51
35:EL:521:MET:HE2	35:EL:530:PHE:HB2	1.91	0.51
39:AN:46:LEU:HB2	39:AN:171:PRO:HB2	1.92	0.51
41:EN:31:ARG:NH1	41:EN:39:ASP:OD1	2.43	0.51
48:AR:55:LEU:HD23	48:AR:92:ALA:HA	1.93	0.51
6:AA:236:A:O4'	57:EU:52:ARG:NH2	2.43	0.51
6:AA:793:U:H4'	6:AA:794:A:O5'	2.10	0.51
6:AA:911:G:H5''	10:EB:516:ALA:HB2	1.91	0.51
10:EB:208:ILE:HD11	10:EB:223:LEU:HD13	1.91	0.51
16:EE:421:LEU:HD23	20:EF:188:THR:HG21	1.93	0.51
19:BF:171:ARG:NE	19:BF:193:GLU:OE1	2.44	0.51
19:BF:193:GLU:O	19:BF:196:ARG:HG3	2.10	0.51
25:BI:195:PRO:HD2	25:BI:198:GLN:HG3	1.91	0.51
26:EI:179:MET:HE2	26:EI:185:LEU:HD11	1.92	0.51
35:EL:289:ASP:HB2	35:EL:397:LEU:HD21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:AN:172:ARG:NH1	73:Ag:119:ASN:O	2.40	0.51
41:EN:180:PRO:HB3	81:Av:202:THR:HG23	1.92	0.51
41:EN:696:ILE:HG23	41:EN:698:GLY:H	1.75	0.51
45:AP:165:ARG:HA	45:AP:169:LYS:HD2	1.91	0.51
44:EP:143:LEU:HD21	44:EP:266:ILE:HG12	1.91	0.51
48:AR:48:TYR:HB3	48:AR:57:LYS:HB3	1.91	0.51
3:A3:54:ILE:HG21	68:Bb:76:VAL:HG21	1.92	0.51
6:AA:869:U:H5'	8:EA:410:MET:HB2	1.92	0.51
7:BA:752:ARG:NH2	60:AW:151:VAL:O	2.43	0.51
15:BE:344:LEU:O	15:BE:347:TYR:O	2.28	0.51
58:AV:81:VAL:HB	58:AV:117:MET:HB3	1.92	0.51
70:Ae:57:GLY:H	70:Ae:65:ILE:HD11	1.74	0.51
6:AA:555:U:OP1	57:EU:52:ARG:NH1	2.35	0.51
9:BB:272:LEU:HD21	9:BB:303:ILE:HD13	1.93	0.51
18:AF:63:PRO:O	19:BF:366:ARG:NH1	2.41	0.51
40:BN:54:ASP:OD2	40:BN:216:TYR:OH	2.26	0.51
41:EN:500:GLU:OE2	41:EN:537:HIS:NE2	2.21	0.51
44:EP:13:HIS:CE1	44:EP:50:LEU:HA	2.45	0.51
67:Ba:41:ASP:O	67:Ba:99:ARG:NH2	2.36	0.51
79:Ap:22:GLN:O	79:Ap:30:ARG:NH2	2.43	0.51
5:A8:99:ARG:NH2	6:AA:911:G:OP2	2.38	0.51
6:AA:13:A:H61	65:AY:39:LEU:HB2	1.75	0.51
6:AA:59:U:OP1	38:UM:1:UNK:N	2.38	0.51
7:BA:181:VAL:HG11	14:AE:203:ALA:HB1	1.93	0.51
11:EC:69:ARG:NH2	11:EC:71:ASP:OD2	2.38	0.51
13:ED:481:ALA:O	13:ED:486:MET:N	2.41	0.51
18:AF:224:ARG:HD3	18:AF:363:LEU:HD13	1.92	0.51
6:AA:934:A:OP1	41:EN:53:ARG:NE	2.41	0.51
14:AE:388:MET:O	79:Ap:14:ARG:NH1	2.38	0.51
22:BH:335:ASN:HD21	22:BH:337:ARG:HD2	1.76	0.51
30:AK:99:GLU:O	30:AK:119:PRO:HG3	2.11	0.51
41:EN:468:LEU:HD13	41:EN:513:ARG:HH12	1.74	0.51
55:AU:102:TYR:O	73:Ag:108:SER:OG	2.22	0.51
58:AV:145:ARG:HB3	58:AV:167:PRO:HB2	1.91	0.51
59:BV:83:MET:HB2	59:BV:98:ILE:HD12	1.92	0.51
76:Bi:140:GLN:OE1	76:Bi:140:GLN:N	2.41	0.51
2:A2:160:ARG:NH1	2:A2:332:ASP:OD1	2.43	0.51
6:AA:871:C:H2'	6:AA:872:A:H8	1.74	0.51
7:BA:264:PRO:HA	7:BA:337:MET:HE1	1.93	0.51
7:BA:597:VAL:HG11	60:AW:239:GLU:HG3	1.91	0.51
9:BB:201:PRO:HG2	9:BB:378:MET:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AK:55:PHE:HZ	30:AK:71:GLU:HG3	1.76	0.51
41:EN:235:ALA:HB1	41:EN:242:CYS:HB3	1.93	0.51
47:EQ:628:ARG:HG3	47:EQ:629:THR:HG23	1.92	0.51
48:AR:80:LYS:NZ	48:AR:82:TYR:O	2.42	0.51
60:AW:6:PRO:HG2	60:AW:9:ALA:HB3	1.91	0.51
70:Ae:79:ASN:O	70:Ae:89:ARG:NH2	2.35	0.51
72:Bf:92:HIS:NE2	79:Ap:261:GLU:OE1	2.43	0.51
6:AA:534:U:H2'	6:AA:535:U:C5	2.46	0.51
6:AA:862:U:H2'	6:AA:863:C:H6	1.76	0.51
8:EA:333:ASN:HD21	8:EA:346:VAL:HG11	1.75	0.51
9:BB:263:ARG:HH12	9:BB:346:GLU:HG3	1.76	0.51
18:AF:77:PRO:HG2	19:BF:360:THR:HG21	1.92	0.51
31:BK:325:ASP:OD1	31:BK:325:ASP:N	2.44	0.51
44:EP:11:LEU:HD23	44:EP:255:PRO:HG3	1.92	0.51
49:BR:114:GLN:HG3	49:BR:203:ALA:HB1	1.93	0.51
69:Bc:48:GLU:HG3	79:Ap:108:LEU:HB2	1.92	0.51
71:Af:108:MET:HE3	71:Af:135:ILE:HG23	1.92	0.51
2:A2:24:ASN:ND2	62:AX:227:LYS:O	2.43	0.51
6:AA:187:A:H3'	6:AA:287:A:H61	1.76	0.51
22:BH:133:ALA:HB2	22:BH:177:SER:HB3	1.91	0.51
28:BJ:138:ILE:HD11	28:BJ:168:ILE:HG23	1.93	0.51
34:BL:103:ASN:HD22	34:BL:105:SER:H	1.59	0.51
63:BX:107:PRO:O	63:BX:108:GLN:HG3	2.11	0.51
2:A2:379:ALA:HB2	67:Ba:84:TYR:HB2	1.92	0.51
6:AA:51:A:OP2	81:Av:48:ALA:N	2.43	0.51
6:AA:1078:A:O2'	11:EC:132:ALA:O	2.27	0.51
19:BF:232:ALA:O	19:BF:235:GLU:HG2	2.11	0.51
40:BN:186:THR:HG23	76:Bi:197:ASN:HD22	1.75	0.51
47:EQ:119:ASN:HD21	47:EQ:122:ASP:HA	1.76	0.51
4:A5:61:ALA:HB1	15:BE:389:GLN:HA	1.92	0.50
6:AA:843:A:H2'	6:AA:844:A:C8	2.46	0.50
9:BB:414:THR:HG23	9:BB:417:GLU:H	1.76	0.50
11:EC:299:GLU:OE2	42:AO:79:ARG:NH2	2.44	0.50
12:BD:137:ARG:HH22	24:AI:220:ARG:HE	1.59	0.50
16:EE:132:HIS:HB3	16:EE:135:ILE:HG12	1.92	0.50
18:AF:154:ARG:HH21	18:AF:332:PRO:HB2	1.76	0.50
19:BF:362:HIS:HD2	61:BW:177:VAL:H	1.59	0.50
37:EM:65:LEU:HB2	37:EM:234:LEU:HD12	1.94	0.50
37:EM:287:LEU:HD13	37:EM:303:ILE:HD11	1.93	0.50
38:UM:1:UNK:O	38:UM:3:UNK:N	2.44	0.50
39:AN:82:HIS:HD2	39:AN:157:TRP:HE1	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AP:297:TRP:HA	61:BW:15:ALA:HB2	1.92	0.50
76:Bi:69:LEU:HD23	76:Bi:70:GLY:H	1.76	0.50
2:A2:259:PRO:HG2	2:A2:297:THR:HG21	1.93	0.50
6:AA:929:U:H2'	6:AA:930:A:C8	2.46	0.50
18:AF:437:VAL:HG22	18:AF:444:VAL:HG22	1.92	0.50
20:EF:181:ARG:HA	20:EF:207:LEU:HD22	1.93	0.50
23:EH:466:THR:N	23:EH:469:SER:OG	2.44	0.50
35:EL:253:ALA:HA	35:EL:268:PRO:HA	1.94	0.50
35:EL:323:HIS:NE2	35:EL:370:GLU:OE2	2.41	0.50
48:AR:127:LYS:HD2	48:AR:205:MET:HE2	1.94	0.50
63:BX:162:ASN:ND2	76:Bi:63:LYS:H	2.08	0.50
65:AY:64:HIS:CD2	65:AY:66:ARG:H	2.29	0.50
2:A2:345:ILE:HG13	2:A2:348:ALA:HB3	1.93	0.50
7:BA:714:ASN:HB3	7:BA:717:VAL:HG22	1.93	0.50
8:EA:366:ALA:O	8:EA:371:ARG:NH1	2.43	0.50
12:BD:123:LEU:HG	12:BD:132:GLU:HB2	1.93	0.50
14:AE:123:ASN:H	79:Ap:109:GLN:HE22	1.57	0.50
25:BI:180:GLN:NE2	25:BI:184:ASN:OD1	2.43	0.50
25:BI:281:GLN:HA	25:BI:284:VAL:HG22	1.93	0.50
44:EP:224:LEU:O	44:EP:227:SER:OG	2.24	0.50
60:AW:116:ARG:NH2	60:AW:120:GLU:OE1	2.44	0.50
61:BW:32:GLU:HG3	61:BW:93:TRP:HZ3	1.77	0.50
76:Bi:139:HIS:O	76:Bi:143:MET:N	2.39	0.50
7:BA:316:GLU:OE1	69:Bc:29:ARG:NH1	2.44	0.50
9:BB:96:PHE:O	9:BB:137:ARG:NH2	2.43	0.50
23:EH:104:VAL:HG13	23:EH:192:MET:HE1	1.93	0.50
35:EL:77:VAL:HG13	35:EL:467:VAL:HG13	1.93	0.50
46:BQ:48:GLU:O	46:BQ:162:GLY:HA3	2.11	0.50
69:Bc:17:HIS:CD2	69:Bc:24:ARG:HH22	2.30	0.50
76:Bi:123:VAL:HG12	76:Bi:136:TYR:HE1	1.76	0.50
76:Bi:128:ASN:N	76:Bi:131:ASN:O	2.41	0.50
79:Ap:55:HIS:HD2	79:Ap:57:LYS:HB2	1.76	0.50
6:AA:962:U:H5'	6:AA:963:A:H5''	1.93	0.50
6:AA:980:U:H3	21:EG:34:ARG:H	1.59	0.50
22:BH:161:PHE:HA	22:BH:245:ASN:HD22	1.75	0.50
28:BJ:198:ALA:HA	28:BJ:201:ARG:HD3	1.93	0.50
35:EL:471:MET:HG3	35:EL:473:ILE:HG13	1.94	0.50
48:AR:107:GLY:HA2	48:AR:129:PHE:HE1	1.76	0.50
52:AT:10:ARG:HB2	52:AT:13:PHE:HD2	1.75	0.50
77:Al:147:PRO:HB2	77:Al:166:ILE:HG23	1.94	0.50
79:Ap:180:LYS:HG2	79:Ap:235:THR:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:19:A:N6	6:AA:97:A:O4'	2.44	0.50
6:AA:266:C:O2'	47:EQ:639:ARG:O	2.29	0.50
23:EH:228:PRO:HG3	25:BI:321:PRO:HD2	1.93	0.50
40:BN:201:LEU:HD12	40:BN:202:PRO:HD2	1.94	0.50
66:BZ:69:TYR:OH	66:BZ:133:SER:O	2.24	0.50
68:Bb:38:HIS:HB3	68:Bb:41:HIS:HE1	1.75	0.50
68:Bb:99:ALA:O	68:Bb:125:SER:OG	2.30	0.50
73:Ag:13:ILE:HB	73:Ag:58:THR:HB	1.94	0.50
3:A3:157:SER:HB3	3:A3:160:ILE:HG12	1.94	0.50
6:AA:883:U:H5'	24:AI:110:SER:HB3	1.93	0.50
34:BL:241:ASP:HB2	34:BL:244:GLU:HB2	1.93	0.50
35:EL:451:PRO:HB3	72:Bf:66:SER:HB3	1.94	0.50
43:BO:233:SER:HB3	50:BS:30:GLU:HB2	1.94	0.50
74:Bg:60:TYR:H	74:Bg:63:GLN:HE21	1.58	0.50
80:At:90:ARG:O	80:At:93:LYS:NZ	2.38	0.50
1:A1:113:VAL:HG12	1:A1:163:ARG:HG3	1.94	0.50
2:A2:206:HIS:HE1	2:A2:301:PRO:HG2	1.75	0.50
11:EC:325:ARG:HG2	37:EM:36:LYS:HG3	1.93	0.50
18:AF:44:LEU:HD21	34:BL:229:SER:HB3	1.94	0.50
25:BI:79:GLY:O	25:BI:268:LYS:NZ	2.44	0.50
31:BK:367:GLU:OE1	31:BK:371:ARG:NE	2.45	0.50
41:EN:387:ILE:HD12	41:EN:445:LEU:HD22	1.93	0.50
32:ER:103:LEU:HB3	32:ER:107:ASP:HB3	1.94	0.50
52:AT:26:ILE:O	52:AT:30:GLN:HG2	2.12	0.50
77:Al:87:LEU:HD21	77:Al:183:ILE:HD11	1.94	0.50
6:AA:509:U:H2'	6:AA:510:A:C8	2.43	0.50
6:AA:931:U:O2'	41:EN:418:PRO:O	2.27	0.50
13:ED:452:LEU:HD12	13:ED:508:LEU:HD21	1.94	0.50
14:AE:165:PHE:HD2	14:AE:168:ASN:HD21	1.59	0.50
19:BF:122:PRO:HG2	55:AU:179:VAL:HG13	1.94	0.50
19:BF:325:ARG:NH1	77:Al:178:GLU:OE2	2.45	0.50
22:BH:188:ASP:HB2	22:BH:228:VAL:HG23	1.94	0.50
26:EI:210:LEU:HD11	26:EI:247:ALA:HB3	1.94	0.50
37:EM:289:LEU:HD13	37:EM:302:MET:HE3	1.93	0.50
43:BO:71:LEU:HB2	43:BO:253:VAL:HG11	1.93	0.50
53:BT:173:LEU:HD23	53:BT:173:LEU:H	1.76	0.50
54:ET:55:PHE:HA	54:ET:92:GLN:HE22	1.77	0.50
55:AU:24:LEU:HD11	55:AU:39:LEU:HG	1.93	0.50
55:AU:75:THR:OG1	55:AU:76:GLY:N	2.45	0.50
81:Av:76:TYR:HB3	81:Av:80:ALA:HB3	1.94	0.50
3:A3:151:ARG:NH1	6:AA:333:U:OP1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:528:A:O2'	74:Bg:64:LYS:NZ	2.34	0.49
14:AE:104:PHE:CZ	14:AE:108:ARG:HD2	2.47	0.49
44:EO:148:MET:HE1	44:EO:269:GLN:HB3	1.94	0.49
66:BZ:89:VAL:HG21	66:BZ:95:GLU:HB3	1.94	0.49
70:Ae:83:SER:HB2	70:Ae:86:HIS:HD2	1.77	0.49
1:A1:89:SER:HB3	1:A1:96:TYR:HE1	1.76	0.49
6:AA:262:U:H2'	6:AA:263:G:H8	1.77	0.49
6:AA:281:A:H2'	6:AA:282:A:H8	1.77	0.49
9:BB:185:ARG:HE	9:BB:192:PRO:HA	1.76	0.49
18:AF:380:PRO:HD3	18:AF:385:LEU:HD12	1.93	0.49
20:EF:251:PRO:HD2	20:EF:316:PRO:O	2.12	0.49
37:EM:318:LEU:HD23	37:EM:318:LEU:H	1.76	0.49
43:BO:123:LEU:HD13	43:BO:137:PRO:HA	1.93	0.49
46:BQ:50:PHE:CZ	46:BQ:163:GLN:HG3	2.47	0.49
58:AV:163:TRP:NE1	58:AV:165:ASP:OD1	2.44	0.49
61:BW:128:THR:HG22	61:BW:129:PRO:HD2	1.94	0.49
73:Ag:29:LEU:HD22	73:Ag:33:LEU:HD22	1.94	0.49
2:A2:28:PRO:HG2	65:AY:227:ASP:HB3	1.95	0.49
6:AA:857:C:H2'	6:AA:858:C:C6	2.47	0.49
8:EA:400:ALA:HB2	8:EA:427:ALA:HB1	1.94	0.49
10:EB:529:ASP:HA	10:EB:534:ARG:HH11	1.77	0.49
13:ED:87:SER:HB3	13:ED:217:ARG:HH12	1.76	0.49
13:ED:267:PHE:HB2	13:ED:389:ASN:HD21	1.78	0.49
16:EE:368:SER:HB2	20:EF:352:HIS:CD2	2.48	0.49
32:EK:96:HIS:H	32:EK:100:ASP:HB2	1.77	0.49
37:EM:75:VAL:HB	37:EM:101:ARG:HB3	1.93	0.49
45:AP:66:VAL:N	61:BW:187:ASP:OD2	2.42	0.49
47:EQ:236:ARG:HG2	47:EQ:246:ILE:HG22	1.95	0.49
79:Ap:270:MET:HB2	79:Ap:277:LEU:HD11	1.93	0.49
6:AA:125:U:H2'	6:AA:126:A:C8	2.43	0.49
6:AA:830:A:H2'	6:AA:831:A:H8	1.77	0.49
6:AA:989:U:OP1	8:EA:512:ARG:NH1	2.46	0.49
13:ED:263:PHE:HB2	13:ED:600:GLU:HG3	1.94	0.49
21:EG:129:ALA:HB3	21:EG:139:MET:HB2	1.94	0.49
23:EH:366:ASP:OD1	23:EH:366:ASP:N	2.45	0.49
26:EI:134:ARG:HG3	26:EI:137:SER:HB3	1.95	0.49
49:BR:12:ALA:HB3	49:BR:15:LEU:HD13	1.94	0.49
75:Bh:14:GLU:OE2	75:Bh:71:ARG:NH2	2.36	0.49
75:Bh:46:VAL:HG23	76:Bi:33:GLU:HB2	1.94	0.49
78:Ao:36:ALA:HB3	78:Ao:39:LYS:HD3	1.93	0.49
6:AA:296:A:OP1	6:AA:494:U:O2'	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:927:U:H5'	6:AA:928:U:H2'	1.95	0.49
6:AA:1001:G:H2'	6:AA:1002:U:C6	2.47	0.49
6:AA:1004:U:H4'	6:AA:1005:U:C5'	2.42	0.49
9:BB:142:THR:HG23	56:BU:107:HIS:HE1	1.76	0.49
12:BD:299:LEU:O	12:BD:489:ARG:NE	2.45	0.49
23:EH:217:ILE:HG12	23:EH:318:TYR:HB2	1.93	0.49
28:BJ:121:MET:HG3	28:BJ:122:ASN:H	1.78	0.49
32:EK:92:THR:HG23	32:EK:95:SER:HB3	1.94	0.49
39:AN:182:LYS:HD3	71:Af:64:SER:HB3	1.95	0.49
44:EO:96:ASP:HB3	44:EO:99:HIS:CD2	2.47	0.49
50:BS:115:VAL:HG13	50:BS:116:THR:HG22	1.95	0.49
52:AT:46:TRP:CE2	52:AT:83:THR:HA	2.48	0.49
60:AW:28:GLN:HE21	60:AW:34:SER:HA	1.77	0.49
69:Bc:90:GLU:HA	69:Bc:93:TRP:CD1	2.48	0.49
6:AA:577:A:H61	57:EU:22:GLY:HA2	1.77	0.49
6:AA:944:C:H2'	6:AA:945:U:H4'	1.94	0.49
19:BF:408:LEU:HD23	53:BT:39:ARG:NH2	2.28	0.49
20:EF:259:LYS:HD2	20:EF:319:PHE:HB2	1.94	0.49
22:BH:300:HIS:CD2	22:BH:302:ALA:H	2.31	0.49
28:BJ:104:SER:HB2	28:BJ:223:THR:HG23	1.93	0.49
44:EP:4:VAL:HG13	44:EP:59:ILE:HG12	1.95	0.49
48:AR:223:HIS:CE1	74:Bg:83:LEU:H	2.30	0.49
54:ET:94:GLU:OE2	54:ET:102:ARG:NH1	2.42	0.49
2:A2:305:THR:HG22	2:A2:307:GLU:H	1.77	0.49
7:BA:347:VAL:HG11	7:BA:396:ARG:HG3	1.94	0.49
7:BA:566:MET:HB3	7:BA:653:VAL:HG12	1.95	0.49
9:BB:263:ARG:HH21	9:BB:398:ARG:HG2	1.78	0.49
13:ED:303:ALA:HB1	13:ED:310:TYR:HA	1.93	0.49
19:BF:319:LYS:HA	61:BW:159:VAL:HG13	1.93	0.49
25:BI:240:GLY:O	25:BI:243:SER:OG	2.30	0.49
43:BO:68:GLU:OE2	43:BO:256:ARG:NH1	2.45	0.49
44:EP:165:LEU:HD11	44:EP:196:LEU:HG	1.95	0.49
58:AV:146:MET:HG3	73:Ag:97:PHE:HB2	1.93	0.49
63:BX:172:GLY:HA2	76:Bi:105:ASP:HB2	1.94	0.49
71:Af:65:LEU:HB3	71:Af:68:ASN:HD22	1.78	0.49
79:Ap:52:ARG:NH1	79:Ap:55:HIS:O	2.46	0.49
16:EE:248:PRO:HB2	16:EE:279:ARG:HB2	1.94	0.49
58:AV:82:ILE:HD11	58:AV:136:VAL:HG21	1.93	0.49
68:Bb:112:LEU:HD22	68:Bb:128:GLN:HE22	1.78	0.49
9:BB:324:ALA:HB1	9:BB:333:VAL:HG13	1.95	0.49
14:AE:262:HIS:CD2	14:AE:296:ARG:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BH:118:VAL:HG22	22:BH:162:HIS:CE1	2.48	0.49
23:EH:403:ARG:HH22	30:AK:314:ARG:HH22	1.60	0.49
26:EI:271:VAL:HG21	42:AO:183:VAL:HG21	1.94	0.49
41:EN:337:GLU:HG3	41:EN:338:ASN:H	1.78	0.49
43:BO:37:TRP:CE2	52:AT:129:ARG:HG3	2.48	0.49
1:A1:123:VAL:HG23	1:A1:126:ALA:H	1.78	0.49
6:AA:35:G:C5	62:AX:84:PRO:HD2	2.48	0.49
6:AA:135:G:O2'	6:AA:826:A:H2'	2.13	0.49
7:BA:278:LYS:HB3	7:BA:281:GLU:HG2	1.95	0.49
8:EA:248:ILE:HD11	8:EA:264:VAL:HG21	1.95	0.49
8:EA:513:ILE:HD13	8:EA:528:LEU:HD23	1.95	0.49
10:EB:388:LEU:HD22	10:EB:481:PHE:HB3	1.95	0.49
13:ED:177:ASP:OD1	13:ED:500:ASN:ND2	2.44	0.49
14:AE:131:ASN:HB3	14:AE:134:TYR:HB3	1.94	0.49
34:BL:42:TYR:CE1	60:AW:100:GLU:HG3	2.47	0.49
35:EL:612:LEU:HD21	35:EL:640:VAL:HG13	1.95	0.49
44:EO:206:GLU:OE1	44:EO:260:ARG:NH2	2.45	0.49
44:EP:203:LEU:HG	44:EP:209:LEU:HB2	1.95	0.49
48:AR:185:ARG:HB2	48:AR:188:LEU:HG	1.94	0.49
65:AY:316:PHE:O	65:AY:321:GLN:NE2	2.46	0.49
66:BZ:118:PRO:HG3	66:BZ:141:LYS:HA	1.95	0.49
74:Bg:38:ASN:HB3	74:Bg:41:TYR:HB3	1.94	0.49
6:AA:310:A:H5''	45:AP:146:LYS:HD2	1.94	0.48
6:AA:581:U:O4	6:AA:582:A:N6	2.45	0.48
7:BA:207:SER:HB3	7:BA:276:LEU:HD23	1.95	0.48
7:BA:607:LYS:HE3	34:BL:36:GLY:HA3	1.95	0.48
13:ED:408:VAL:HG23	13:ED:467:PRO:HG3	1.94	0.48
13:ED:561:VAL:HG13	13:ED:565:PHE:HB3	1.95	0.48
15:BE:85:GLU:HG2	31:BK:288:PRO:HG3	1.95	0.48
26:EI:269:TRP:HE1	26:EI:280:ASN:HD22	1.60	0.48
30:AK:151:LEU:HD23	30:AK:151:LEU:H	1.78	0.48
35:EL:454:ASP:OD1	35:EL:454:ASP:N	2.46	0.48
42:AO:114:VAL:O	42:AO:118:ARG:HD3	2.13	0.48
55:AU:103:GLU:HG2	58:AV:79:PHE:CE1	2.48	0.48
63:BX:98:PRO:HG3	63:BX:165:ARG:HD2	1.95	0.48
6:AA:94:U:H2'	6:AA:95:U:C6	2.48	0.48
6:AA:984:A:H2'	11:EC:40:PRO:HB2	1.96	0.48
9:BB:314:LEU:HD23	9:BB:320:ARG:HG2	1.93	0.48
29:EJ:65:GLY:O	29:EJ:69:LEU:CB	2.58	0.48
29:EJ:100:MET:HE2	88:EK:200:PM8:H22	1.94	0.48
65:AY:64:HIS:HD2	65:AY:66:ARG:HB2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:Al:129:ASP:OD1	77:Al:129:ASP:N	2.46	0.48
1:A1:76:ILE:HD12	1:A1:122:MET:HG2	1.96	0.48
2:A2:369:VAL:HG13	65:AY:270:SER:HB2	1.94	0.48
5:A8:181:VAL:HB	81:Av:103:ARG:HD3	1.94	0.48
6:AA:41:U:OP1	62:AX:107:LYS:NZ	2.46	0.48
6:AA:184:U:H2'	6:AA:185:U:C6	2.47	0.48
6:AA:234:U:H3	15:BE:23:GLN:HE22	1.61	0.48
12:BD:194:MET:HE1	12:BD:432:ARG:HA	1.95	0.48
13:ED:240:LEU:HD13	13:ED:583:VAL:HG22	1.95	0.48
14:AE:54:ARG:HD2	79:Ap:97:PHE:HE1	1.79	0.48
15:BE:153:SER:OG	15:BE:252:ALA:HB2	2.13	0.48
15:BE:403:ASN:HD22	48:AR:151:SER:HB3	1.78	0.48
16:EE:241:VAL:HB	16:EE:386:MET:HG2	1.96	0.48
18:AF:90:LEU:HD12	18:AF:93:LEU:HD12	1.94	0.48
26:EI:210:LEU:HD13	26:EI:244:ALA:HA	1.94	0.48
44:EO:96:ASP:O	44:EO:98:GLN:N	2.46	0.48
47:EQ:182:ARG:NH2	47:EQ:185:GLU:OE1	2.46	0.48
60:AW:42:PHE:HE1	65:AY:18:PRO:HB3	1.77	0.48
76:Bi:89:LEU:HD23	76:Bi:89:LEU:H	1.78	0.48
7:BA:154:LEU:HD12	69:Bc:84:LEU:HD21	1.95	0.48
7:BA:279:VAL:HA	7:BA:285:TRP:HZ2	1.78	0.48
11:EC:276:ALA:HB3	37:EM:53:TRP:HB2	1.96	0.48
31:BK:103:LYS:HD3	31:BK:137:TYR:HE1	1.79	0.48
31:BK:128:VAL:HG12	31:BK:131:ARG:HH12	1.78	0.48
45:AP:281:GLU:HG3	45:AP:284:GLY:H	1.77	0.48
67:Ba:18:GLY:HA3	67:Ba:23:SER:HB3	1.96	0.48
76:Bi:43:LYS:HG2	76:Bi:52:LEU:HD11	1.95	0.48
2:A2:167:HIS:HD2	2:A2:169:GLY:H	1.61	0.48
3:A3:74:PRO:HB3	3:A3:85:LEU:HD13	1.96	0.48
6:AA:202:U:H2'	6:AA:203:A:H8	1.79	0.48
6:AA:903:U:O2'	6:AA:966:A:OP2	2.25	0.48
19:BF:148:HIS:O	19:BF:152:VAL:HG23	2.14	0.48
21:EG:45:ARG:HG3	21:EG:47:HIS:CD2	2.49	0.48
23:EH:457:LYS:HB2	23:EH:493:PHE:HE1	1.77	0.48
39:AN:19:HIS:CD2	39:AN:21:HIS:H	2.31	0.48
45:AP:115:MET:HE1	54:ET:6:LEU:HB3	1.95	0.48
60:AW:207:PRO:O	60:AW:227:SER:OG	2.23	0.48
63:BX:162:ASN:HB3	63:BX:166:THR:HB	1.95	0.48
6:AA:275:C:H5''	22:BH:340:ARG:HH12	1.78	0.48
6:AA:589:U:H2'	6:AA:590:U:C6	2.48	0.48
20:EF:176:VAL:HG22	20:EF:202:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:EF:221:THR:O	20:EF:224:SER:OG	2.31	0.48
24:AI:27:PRO:HG3	24:AI:76:HIS:NE2	2.29	0.48
28:BJ:150:ARG:HB3	28:BJ:160:THR:HG22	1.96	0.48
44:EO:2:PHE:HA	44:EO:62:PRO:HD3	1.96	0.48
44:EO:170:GLN:HB2	44:EO:216:ARG:HD2	1.95	0.48
48:AR:108:ASP:OD1	48:AR:109:THR:N	2.46	0.48
49:BR:145:PRO:HD2	78:Ao:217:ALA:HB1	1.96	0.48
62:AX:87:ASP:HB2	65:AY:82:ARG:HG2	1.95	0.48
78:Ao:82:GLU:OE1	78:Ao:107:GLN:NE2	2.47	0.48
2:A2:223:LEU:HB3	53:BT:120:ALA:HA	1.95	0.48
6:AA:445:U:H4'	44:EO:319:ARG:HD2	1.96	0.48
9:BB:107:HIS:HB2	9:BB:358:ARG:HB2	1.95	0.48
18:AF:124:VAL:O	53:BT:160:HIS:NE2	2.45	0.48
26:EI:112:ASP:OD1	26:EI:113:ILE:N	2.46	0.48
62:AX:153:ASN:HD21	62:AX:226:LEU:HB3	1.79	0.48
77:Al:181:LEU:HD23	77:Al:189:ILE:HD13	1.95	0.48
81:Av:194:MET:HG3	81:Av:198:LYS:HE3	1.94	0.48
2:A2:48:GLN:HG3	70:Ae:146:PRO:HG2	1.96	0.48
2:A2:412:ASN:HD21	2:A2:438:ILE:HG23	1.78	0.48
6:AA:37:G:H5''	6:AA:38:U:C5	2.49	0.48
6:AA:154:A:C2	60:AW:2:PRO:HA	2.49	0.48
6:AA:280:U:N3	6:AA:281:A:N7	2.61	0.48
6:AA:470:G:H5''	45:AP:70:LEU:HD22	1.96	0.48
6:AA:1117:A:H2'	6:AA:1118:A:H5''	1.95	0.48
7:BA:528:VAL:HG12	7:BA:532:MET:HE3	1.95	0.48
13:ED:381:ARG:HH12	13:ED:500:ASN:HB2	1.78	0.48
26:EI:166:PRO:O	29:EJ:36:ARG:NH1	2.46	0.48
28:BJ:141:GLU:HB3	28:BJ:178:ILE:HD11	1.95	0.48
40:BN:220:ASP:OD1	40:BN:220:ASP:N	2.45	0.48
45:AP:285:LEU:HA	45:AP:289:ALA:HB3	1.95	0.48
46:BQ:91:ILE:HD13	80:At:113:PRO:HG2	1.96	0.48
46:BQ:122:ALA:HA	46:BQ:160:VAL:HB	1.95	0.48
49:BR:63:LEU:HD22	49:BR:67:LEU:HD13	1.94	0.48
65:AY:192:LYS:HG2	65:AY:203:GLU:HG3	1.96	0.48
4:A5:69:TRP:CD1	4:A5:79:LYS:HB2	2.48	0.48
5:A8:181:VAL:HG12	24:AI:94:ILE:HG12	1.94	0.48
6:AA:264:U:OP2	28:BJ:67:ARG:NH2	2.46	0.48
7:BA:350:LEU:HB2	7:BA:370:ILE:HG21	1.96	0.48
9:BB:134:ARG:HB2	9:BB:386:THR:HG21	1.96	0.48
10:EB:254:ARG:HD2	10:EB:290:TRP:HH2	1.78	0.48
13:ED:139:ARG:NH2	41:EN:176:TYR:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:EE:344:ARG:NH2	35:EL:542:ASP:OD1	2.47	0.48
25:BI:334:ASN:HA	73:Ag:134:ARG:HG3	1.95	0.48
37:EM:297:ASP:HB2	42:AO:104:VAL:HG23	1.96	0.48
42:AO:48:TRP:HB3	42:AO:59:VAL:HG22	1.95	0.48
42:AO:58:GLY:H	42:AO:88:ARG:HH21	1.62	0.48
42:AO:75:CYS:HB2	42:AO:119:VAL:HG11	1.96	0.48
44:EP:21:LEU:HB3	44:EP:194:TRP:CD1	2.49	0.48
51:ES:35:GLU:CD	51:ES:35:GLU:H	2.22	0.48
77:Al:139:HIS:NE2	77:Al:170:GLU:OE1	2.39	0.48
80:At:59:ALA:HB2	80:At:86:MET:HB3	1.95	0.48
2:A2:413:TYR:OH	2:A2:418:ASP:OD2	2.31	0.48
3:A3:190:LEU:HD12	19:BF:310:LEU:HD12	1.96	0.48
6:AA:195:U:H2'	6:AA:196:G:C8	2.49	0.48
6:AA:531:U:C5	74:Bg:76:SER:HB2	2.49	0.48
6:AA:579:U:H2'	6:AA:580:A:C8	2.47	0.48
6:AA:947:U:H4'	54:ET:82:ARG:HG2	1.95	0.48
6:AA:1127:A:H4'	26:EI:258:CYS:SG	2.53	0.48
7:BA:674:LEU:HD11	71:Af:147:VAL:HG11	1.96	0.48
15:BE:424:ASN:HD21	48:AR:79:ARG:HH22	1.60	0.48
22:BH:186:SER:HB2	22:BH:224:LEU:HG	1.94	0.48
41:EN:227:VAL:HG13	41:EN:231:LEU:HD13	1.96	0.48
46:BQ:86:VAL:HG13	46:BQ:92:VAL:HG22	1.96	0.48
49:BR:194:HIS:CD2	49:BR:196:ARG:HE	2.32	0.48
63:BX:140:CYS:SG	63:BX:143:CYS:HB2	2.53	0.48
65:AY:316:PHE:HB2	65:AY:321:GLN:HG3	1.95	0.48
6:AA:449:U:H4'	25:BI:320:ARG:HH21	1.79	0.47
6:AA:815:U:H5	55:AU:25:ARG:HH21	1.61	0.47
6:AA:934:A:O2'	41:EN:522:SER:O	2.31	0.47
6:AA:1001:G:H2'	6:AA:1002:U:H6	1.79	0.47
13:ED:399:LYS:HG2	13:ED:404:VAL:HG21	1.96	0.47
15:BE:249:CYS:SG	15:BE:254:ASN:HB3	2.54	0.47
18:AF:245:GLU:OE1	18:AF:245:GLU:N	2.43	0.47
26:EI:77:ASP:OD1	35:EL:307:ARG:NH2	2.47	0.47
28:BJ:176:GLU:HA	28:BJ:179:ARG:HG2	1.96	0.47
37:EM:16:MET:HE1	47:EQ:320:LYS:HB2	1.96	0.47
44:EO:185:THR:OG1	44:EO:186:GLN:OE1	2.32	0.47
44:EP:21:LEU:HB3	44:EP:194:TRP:NE1	2.30	0.47
65:AY:171:SER:HB3	65:AY:174:ARG:HG2	1.96	0.47
68:Bb:38:HIS:HB3	68:Bb:41:HIS:CE1	2.49	0.47
2:A2:23:ASN:O	2:A2:25:LYS:NZ	2.45	0.47
7:BA:496:ILE:O	7:BA:499:SER:OG	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:ED:555:GLU:O	13:ED:560:ASN:ND2	2.47	0.47
16:EE:237:ASP:N	16:EE:264:ASP:OD2	2.43	0.47
21:EG:109:GLY:O	21:EG:126:GLN:NE2	2.47	0.47
22:BH:115:LEU:HD13	81:Av:157:PHE:HA	1.96	0.47
22:BH:149:ARG:HH21	22:BH:153:ARG:NH2	2.12	0.47
22:BH:231:PRO:HB2	45:AP:308:TYR:HB2	1.95	0.47
23:EH:217:ILE:HD12	23:EH:263:PHE:HB3	1.96	0.47
26:EI:213:ARG:NH2	26:EI:236:GLU:OE1	2.45	0.47
34:BL:178:ASP:N	34:BL:178:ASP:OD1	2.48	0.47
37:EM:231:SER:HB2	37:EM:234:LEU:HD23	1.96	0.47
44:EO:207:GLY:HA2	44:EO:262:PHE:CE1	2.49	0.47
48:AR:223:HIS:HE1	74:Bg:83:LEU:H	1.61	0.47
51:ES:35:GLU:HG2	51:ES:36:GLY:H	1.78	0.47
61:BW:46:HIS:CD2	61:BW:82:GLU:HB3	2.49	0.47
6:AA:149:U:H5'	60:AW:17:ARG:HD2	1.96	0.47
12:BD:499:TYR:HA	12:BD:506:VAL:HG21	1.96	0.47
19:BF:290:LEU:HD22	19:BF:309:VAL:HG13	1.97	0.47
26:EI:342:LYS:NZ	52:AT:97:GLU:OE2	2.40	0.47
35:EL:543:LEU:HD13	35:EL:573:LEU:HA	1.97	0.47
37:EM:223:ASP:HB3	37:EM:224:PRO:HD3	1.96	0.47
42:AO:74:ASN:O	42:AO:103:SER:N	2.40	0.47
44:EO:21:LEU:HD23	44:EO:194:TRP:HD1	1.79	0.47
51:ES:26:THR:HG23	51:ES:31:LEU:HB2	1.95	0.47
58:AV:104:VAL:O	58:AV:143:GLN:NE2	2.47	0.47
76:Bi:202:GLN:HG2	76:Bi:206:PRO:HB3	1.96	0.47
6:AA:798:U:OP1	48:AR:66:ARG:NH2	2.36	0.47
7:BA:335:PRO:HB2	7:BA:338:LEU:HB2	1.96	0.47
14:AE:394:PHE:H	14:AE:399:LEU:HD21	1.78	0.47
16:EE:162:LEU:HD22	16:EE:218:PHE:HE1	1.79	0.47
35:EL:655:LEU:HD11	35:EL:658:ASP:HA	1.96	0.47
39:AN:198:ASN:HA	39:AN:202:HIS:HB3	1.96	0.47
45:AP:254:CYS:HB3	45:AP:296:GLY:HA2	1.96	0.47
46:BQ:169:GLU:N	46:BQ:169:GLU:OE1	2.47	0.47
56:BU:147:GLU:OE2	74:Bg:26:PHE:N	2.46	0.47
56:BU:182:GLU:OE2	75:Bh:92:TRP:NE1	2.47	0.47
74:Bg:49:LEU:HB3	74:Bg:55:ILE:HD12	1.97	0.47
81:Av:65:THR:O	81:Av:69:ARG:NH2	2.35	0.47
1:A1:144:SER:HA	1:A1:157:ARG:HH12	1.79	0.47
2:A2:314:HIS:HB3	2:A2:317:GLU:HG3	1.97	0.47
6:AA:172:U:OP2	45:AP:222:GLY:N	2.48	0.47
6:AA:1084:G:OP1	11:EC:286:VAL:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:1131:G:O2'	26:EI:262:ARG:NH2	2.46	0.47
8:EA:326:ARG:NH1	8:EA:465:HIS:O	2.47	0.47
8:EA:521:THR:HA	8:EA:524:PRO:HA	1.97	0.47
9:BB:265:PRO:HB3	9:BB:309:ARG:HD2	1.97	0.47
15:BE:29:ASN:O	60:AW:220:TYR:OH	2.22	0.47
22:BH:149:ARG:NH2	24:AI:211:GLU:O	2.46	0.47
26:EI:315:GLY:HA3	52:AT:138:THR:HG23	1.96	0.47
28:BJ:60:PRO:HA	28:BJ:63:VAL:HG22	1.95	0.47
39:AN:121:MET:HE3	39:AN:128:MET:HB3	1.97	0.47
41:EN:173:SER:HB2	41:EN:176:TYR:HD2	1.78	0.47
44:EO:28:GLN:O	44:EO:30:HIS:ND1	2.44	0.47
45:AP:310:HIS:HD2	45:AP:312:ALA:HB3	1.79	0.47
44:EP:257:TRP:CD1	44:EP:259:HIS:H	2.32	0.47
49:BR:22:VAL:HG13	49:BR:56:ALA:HB1	1.97	0.47
49:BR:151:ARG:O	49:BR:155:ARG:HG2	2.13	0.47
58:AV:111:ALA:N	78:Ao:87:GLU:O	2.39	0.47
68:Bb:49:LYS:O	68:Bb:53:ARG:HG3	2.15	0.47
76:Bi:124:TYR:CE1	76:Bi:135:TYR:HB2	2.49	0.47
5:A8:134:LEU:HA	77:Al:155:PRO:HG2	1.96	0.47
6:AA:859:U:H2'	6:AA:860:A:C8	2.49	0.47
6:AA:936:C:O2'	13:ED:95:ARG:NH2	2.47	0.47
6:AA:1004:U:H4'	6:AA:1005:U:O5'	2.14	0.47
8:EA:111:ALA:HA	8:EA:165:ILE:HB	1.97	0.47
10:EB:674:HIS:CD2	10:EB:676:GLY:H	2.31	0.47
11:EC:63:GLN:O	49:BR:192:ARG:NH2	2.46	0.47
13:ED:483:LYS:NZ	46:BQ:224:LEU:O	2.33	0.47
23:EH:225:ALA:O	23:EH:234:ARG:NH2	2.42	0.47
41:EN:363:LEU:O	41:EN:367:GLY:N	2.46	0.47
43:BO:171:LEU:HD23	43:BO:171:LEU:H	1.78	0.47
47:EQ:116:GLN:HB2	47:EQ:128:ASP:HB3	1.96	0.47
53:BT:109:VAL:O	53:BT:113:ARG:HG2	2.15	0.47
2:A2:26:ARG:N	70:Ae:187:LYS:O	2.48	0.47
5:A8:95:ARG:NH1	6:AA:911:G:O6	2.44	0.47
6:AA:496:A:OP2	55:AU:14:LYS:NZ	2.46	0.47
6:AA:792:A:H4'	42:AO:49:GLY:H	1.79	0.47
7:BA:440:LYS:HD3	7:BA:477:LEU:HD23	1.95	0.47
8:EA:116:MET:HE2	8:EA:144:ASP:HB3	1.95	0.47
9:BB:83:ASN:OD1	9:BB:84:PHE:N	2.48	0.47
9:BB:165:THR:HG23	9:BB:238:ASN:HB2	1.96	0.47
14:AE:197:HIS:NE2	14:AE:213:LYS:O	2.41	0.47
15:BE:321:VAL:HG13	15:BE:356:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BE:415:TYR:HE2	48:AR:229:HIS:HE1	1.63	0.47
16:EE:277:ASP:OD1	16:EE:278:HIS:N	2.48	0.47
16:EE:336:LEU:HD13	35:EL:548:GLN:HE21	1.80	0.47
16:EE:390:ASN:HB3	16:EE:393:ARG:HA	1.97	0.47
16:EE:415:VAL:HG12	16:EE:418:THR:HB	1.97	0.47
19:BF:193:GLU:OE2	19:BF:196:ARG:NH2	2.46	0.47
24:AI:39:SER:HB3	24:AI:89:PRO:HG3	1.97	0.47
24:AI:226:ASP:HB2	24:AI:229:GLU:HB2	1.97	0.47
31:BK:371:ARG:NH1	62:AX:209:ASP:OD1	2.42	0.47
41:EN:264:ILE:HD12	41:EN:269:GLU:HG3	1.96	0.47
42:AO:132:ARG:NH2	42:AO:134:GLN:OE1	2.47	0.47
47:EQ:89:LYS:NZ	85:EQ:1000:GTP:O1B	2.42	0.47
47:EQ:268:ASP:HA	47:EQ:273:GLY:HA3	1.95	0.47
49:BR:126:LEU:HB2	49:BR:159:ILE:HB	1.97	0.47
53:BT:118:LYS:O	53:BT:121:GLU:HG3	2.14	0.47
63:BX:182:MET:HE2	63:BX:182:MET:HA	1.96	0.47
6:AA:93:A:H5'	60:AW:54:GLY:O	2.14	0.47
6:AA:521:G:OP1	57:EU:45:ARG:NH1	2.38	0.47
6:AA:857:C:H2'	6:AA:858:C:H6	1.80	0.47
6:AA:1100:U:O2	14:AE:297:MET:HE1	2.15	0.47
7:BA:491:LEU:HG	7:BA:494:TYR:HB3	1.97	0.47
7:BA:714:ASN:ND2	7:BA:716:LEU:H	2.12	0.47
7:BA:720:ARG:NH1	73:Ag:95:GLN:OE1	2.47	0.47
26:EI:138:ARG:HD3	50:BS:139:ARG:HD2	1.97	0.47
40:BN:86:PRO:HG3	76:Bi:193:ALA:HB1	1.96	0.47
45:AP:113:ILE:HD11	45:AP:129:GLY:HA3	1.96	0.47
44:EP:209:LEU:HG	44:EP:211:LEU:H	1.80	0.47
58:AV:113:LYS:HD2	78:Ao:84:ALA:HB3	1.96	0.47
63:BX:168:SER:HB3	76:Bi:66:PRO:HG2	1.96	0.47
67:Ba:74:ARG:NH2	67:Ba:91:GLU:OE2	2.48	0.47
81:Av:156:ASP:OD1	81:Av:156:ASP:N	2.47	0.47
2:A2:132:PRO:HB2	2:A2:360:PRO:HB2	1.97	0.47
6:AA:188:A:H2'	6:AA:189:A:C8	2.50	0.47
6:AA:557:A:H5'	57:EU:40:LYS:HB3	1.96	0.47
6:AA:977:G:OP1	10:EB:626:TRP:NE1	2.35	0.47
12:BD:471:LEU:HD23	12:BD:473:LEU:HD11	1.96	0.47
13:ED:24:SER:HB3	13:ED:25:PRO:HD3	1.97	0.47
23:EH:19:ASP:OD1	23:EH:20:GLY:N	2.48	0.47
23:EH:48:GLU:HB2	23:EH:374:THR:HG23	1.97	0.47
34:BL:177:LEU:HA	34:BL:180:LEU:HD12	1.97	0.47
35:EL:374:GLN:HA	35:EL:479:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:AN:70:ARG:NH1	39:AN:72:ASP:OD1	2.48	0.47
42:AO:142:LEU:HB2	52:AT:111:LEU:HD21	1.96	0.47
45:AP:354:THR:OG1	45:AP:355:LEU:N	2.46	0.47
47:EQ:199:ILE:HB	47:EQ:232:VAL:HG22	1.95	0.47
65:AY:131:ILE:HG23	65:AY:141:ILE:HG23	1.96	0.47
68:Bb:79:HIS:CD2	68:Bb:81:HIS:H	2.31	0.47
69:Bc:47:GLU:O	79:Ap:106:LYS:N	2.46	0.47
6:AA:37:G:H5''	6:AA:38:U:C6	2.50	0.47
9:BB:137:ARG:HG3	56:BU:107:HIS:HA	1.97	0.47
13:ED:2:LYS:HE2	13:ED:324:VAL:HG21	1.97	0.47
14:AE:190:MET:O	14:AE:214:HIS:N	2.48	0.47
58:AV:95:ASP:HA	73:Ag:105:GLN:HE21	1.80	0.47
74:Bg:90:LEU:HA	74:Bg:93:GLU:HG2	1.96	0.47
75:Bh:25:LEU:HD22	76:Bi:36:MET:HE3	1.97	0.47
2:A2:256:VAL:HG11	53:BT:111:LEU:HB3	1.98	0.46
6:AA:1172:A:N6	7:BA:782:VAL:O	2.48	0.46
7:BA:683:LEU:HD13	7:BA:692:VAL:HG21	1.96	0.46
10:EB:45:ILE:HD11	47:EQ:575:VAL:HA	1.97	0.46
11:EC:332:ALA:HA	11:EC:336:GLY:HA2	1.96	0.46
14:AE:335:THR:OG1	52:AT:16:ARG:NH1	2.48	0.46
25:BI:28:ALA:HB2	79:Ap:57:LYS:HE3	1.97	0.46
41:EN:502:LEU:HD13	41:EN:514:HIS:CD2	2.49	0.46
32:ER:69:LYS:HA	32:ER:72:VAL:HG12	1.96	0.46
76:Bi:72:ILE:HB	76:Bi:73:PRO:HD3	1.96	0.46
81:Av:147:ASN:OD1	81:Av:147:ASN:N	2.48	0.46
6:AA:159:U:OP1	77:Al:143:ASN:ND2	2.48	0.46
9:BB:157:HIS:HA	70:Ae:130:TYR:HE2	1.80	0.46
10:EB:161:MET:HE3	10:EB:178:ARG:HB2	1.96	0.46
13:ED:66:LYS:NZ	13:ED:611:ASP:OD2	2.37	0.46
28:BJ:241:MET:HE1	65:AY:289:GLN:HG2	1.98	0.46
35:EL:337:MET:HE1	72:Bf:27:LEU:HD11	1.96	0.46
37:EM:218:VAL:HG23	37:EM:228:LEU:HB2	1.98	0.46
40:BN:197:GLU:OE2	40:BN:219:ARG:NE	2.48	0.46
44:EO:36:ARG:HH22	44:EO:248:GLU:HG2	1.80	0.46
50:BS:45:ILE:HG23	50:BS:49:THR:HG21	1.96	0.46
66:BZ:43:GLY:HA3	66:BZ:68:THR:HG22	1.98	0.46
69:Bc:138:LYS:HG2	69:Bc:139:PRO:HD2	1.97	0.46
75:Bh:47:SER:N	76:Bi:33:GLU:OE1	2.41	0.46
2:A2:217:ASP:OD1	18:AF:407:ARG:NH2	2.37	0.46
6:AA:1000:U:H2'	6:AA:1001:G:C8	2.50	0.46
7:BA:528:VAL:O	7:BA:532:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:EA:392:HIS:O	8:EA:422:PRO:HD2	2.14	0.46
9:BB:277:HIS:ND1	9:BB:279:GLU:OE1	2.39	0.46
14:AE:184:LYS:HB3	14:AE:220:PRO:HA	1.97	0.46
16:EE:374:ASN:O	16:EE:377:LYS:NZ	2.47	0.46
26:EI:213:ARG:NH1	26:EI:284:GLU:OE2	2.49	0.46
44:EO:19:SER:HB3	44:EO:97:PRO:HB3	1.96	0.46
44:EP:257:TRP:HD1	44:EP:259:HIS:H	1.62	0.46
53:BT:152:ASN:OD1	53:BT:155:ARG:NH2	2.48	0.46
6:AA:882:U:H1'	24:AI:106:ARG:O	2.15	0.46
10:EB:208:ILE:HB	10:EB:229:VAL:HG11	1.97	0.46
13:ED:161:ARG:HA	13:ED:164:TYR:CE2	2.49	0.46
15:BE:14:GLY:HA3	15:BE:22:HIS:HB2	1.98	0.46
15:BE:38:PRO:HB3	15:BE:43:PRO:HA	1.95	0.46
18:AF:83:HIS:HD2	18:AF:85:TYR:HB2	1.80	0.46
41:EN:223:LEU:HD22	41:EN:230:LEU:HD22	1.98	0.46
44:EO:147:GLU:HB3	44:EO:150:ALA:HB3	1.97	0.46
46:BQ:35:VAL:HG11	46:BQ:174:VAL:HG21	1.97	0.46
51:ES:104:ARG:NH1	51:ES:143:GLU:OE2	2.44	0.46
70:Ae:123:THR:HG23	70:Ae:132:TRP:HE1	1.79	0.46
77:Al:177:GLU:O	77:Al:181:LEU:HG	2.14	0.46
6:AA:544:G:P	62:AX:192:ASN:HD22	2.39	0.46
6:AA:902:U:H5'	28:BJ:26:LYS:HB2	1.97	0.46
11:EC:287:ALA:HB2	11:EC:312:ARG:HG3	1.97	0.46
18:AF:252:TYR:OH	18:AF:299:ASN:ND2	2.40	0.46
21:EG:62:ARG:NH1	39:AN:102:PRO:HG3	2.31	0.46
35:EL:392:VAL:HG22	35:EL:520:VAL:HG11	1.98	0.46
39:AN:61:ALA:HB3	39:AN:134:LEU:HD21	1.97	0.46
49:BR:117:GLY:O	49:BR:197:LYS:NZ	2.41	0.46
57:EU:45:ARG:NH2	74:Bg:56:ARG:O	2.34	0.46
58:AV:102:LEU:O	58:AV:143:GLN:NE2	2.49	0.46
74:Bg:52:THR:HA	74:Bg:86:ARG:HA	1.98	0.46
76:Bi:68:ASP:OD1	76:Bi:68:ASP:N	2.44	0.46
6:AA:830:A:H2'	6:AA:831:A:C8	2.51	0.46
6:AA:843:A:H2'	6:AA:844:A:H8	1.80	0.46
10:EB:135:GLN:NE2	78:Ao:200:GLU:OE2	2.41	0.46
12:BD:253:LEU:HD21	12:BD:258:TYR:HE1	1.81	0.46
13:ED:241:LEU:HB2	13:ED:582:VAL:HG22	1.97	0.46
19:BF:285:LEU:HD23	80:At:133:LEU:HD21	1.98	0.46
31:BK:295:ARG:NH1	31:BK:311:GLU:OE1	2.44	0.46
47:EQ:53:PHE:HZ	47:EQ:255:ILE:HD11	1.81	0.46
60:AW:269:ASP:OD1	60:AW:269:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:BW:49:VAL:HA	61:BW:52:LYS:HD3	1.98	0.46
2:A2:17:VAL:HA	2:A2:64:MET:HE3	1.98	0.46
7:BA:423:ARG:HA	7:BA:423:ARG:HD3	1.81	0.46
7:BA:585:HIS:HD2	7:BA:587:SER:H	1.63	0.46
9:BB:277:HIS:CD2	9:BB:315:SER:HB2	2.51	0.46
11:EC:352:ASN:OD1	11:EC:353:LYS:N	2.49	0.46
12:BD:283:LEU:HD21	12:BD:377:LEU:HD11	1.96	0.46
13:ED:45:LEU:HD22	13:ED:397:LEU:HG	1.98	0.46
13:ED:280:PHE:HB3	13:ED:383:ALA:HA	1.98	0.46
13:ED:405:GLU:HG3	13:ED:436:THR:HA	1.98	0.46
16:EE:422:ILE:HG22	20:EF:339:SER:HB3	1.97	0.46
18:AF:154:ARG:NH1	53:BT:32:THR:HG21	2.30	0.46
20:EF:346:ARG:HE	20:EF:348:ALA:HB3	1.80	0.46
30:AK:19:VAL:HG13	59:BV:102:TRP:HE1	1.81	0.46
30:AK:145:TYR:HB2	59:BV:68:VAL:HA	1.98	0.46
43:BO:216:LEU:HD23	43:BO:220:MET:HG3	1.98	0.46
44:EO:13:HIS:CD2	44:EO:15:ALA:H	2.34	0.46
48:AR:247:ASP:OD1	48:AR:247:ASP:N	2.49	0.46
55:AU:75:THR:HB	71:Af:77:VAL:HG23	1.98	0.46
60:AW:70:TRP:HB2	65:AY:24:VAL:HG22	1.97	0.46
63:BX:57:ARG:HB3	63:BX:58:PRO:HD3	1.98	0.46
71:Af:154:ARG:HH21	71:Af:157:MET:HE3	1.80	0.46
16:EE:513:GLU:O	16:EE:517:ARG:HG2	2.16	0.46
26:EI:257:VAL:HG13	26:EI:258:CYS:SG	2.56	0.46
28:BJ:106:ARG:HB3	28:BJ:110:TRP:HE1	1.80	0.46
62:AX:190:VAL:HB	62:AX:212:LYS:HD3	1.97	0.46
63:BX:160:TYR:HB3	76:Bi:63:LYS:HD2	1.97	0.46
66:BZ:113:SER:OG	66:BZ:147:ASN:O	2.33	0.46
68:Bb:100:GLU:HG2	68:Bb:125:SER:HB2	1.95	0.46
6:AA:458:U:H5'	78:Ao:58:ARG:HB3	1.96	0.46
6:AA:983:C:OP1	10:EB:604:LYS:NZ	2.43	0.46
12:BD:145:TRP:CD1	12:BD:149:ARG:HH11	2.34	0.46
13:ED:78:ASP:OD1	13:ED:82:ASP:N	2.48	0.46
18:AF:72:ILE:HD11	18:AF:118:PHE:CZ	2.51	0.46
24:AI:251:UNK:N	41:EN:344:GLU:O	2.49	0.46
25:BI:189:ALA:HB1	25:BI:194:LYS:HB2	1.98	0.46
31:BK:137:TYR:CE1	31:BK:141:ILE:HG13	2.50	0.46
35:EL:124:TRP:CE2	35:EL:135:PRO:HG3	2.51	0.46
41:EN:658:ASP:OD1	41:EN:658:ASP:N	2.44	0.46
47:EQ:167:LYS:NZ	47:EQ:279:TYR:OH	2.36	0.46
48:AR:112:ARG:NH2	48:AR:126:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:AV:73:LEU:HD22	58:AV:122:ARG:HG2	1.97	0.46
65:AY:221:ASP:OD1	65:AY:221:ASP:N	2.46	0.46
6:AA:178:A:O2'	60:AW:3:ARG:NH2	2.48	0.46
6:AA:355:A:OP1	78:Ao:199:HIS:HE1	1.99	0.46
10:EB:732:VAL:HG13	70:Ae:99:TRP:HD1	1.81	0.46
14:AE:89:LEU:HD21	72:Bf:94:ARG:HH22	1.80	0.46
20:EF:276:MET:HE1	20:EF:277:ARG:HH11	1.80	0.46
21:EG:69:HIS:HB2	71:Af:42:GLY:HA3	1.98	0.46
22:BH:122:HIS:HD2	22:BH:124:PHE:H	1.63	0.46
22:BH:254:TRP:HA	24:AI:187:LYS:HB3	1.98	0.46
28:BJ:180:GLU:HA	28:BJ:183:ILE:HG12	1.97	0.46
30:AK:149:MET:SD	30:AK:189:VAL:HG11	2.56	0.46
35:EL:411:HIS:CD2	79:Ap:131:TRP:HB2	2.51	0.46
37:EM:221:CYS:HB3	37:EM:224:PRO:HD2	1.98	0.46
43:BO:216:LEU:HD22	43:BO:222:ILE:HD12	1.97	0.46
66:BZ:27:PRO:HG3	66:BZ:34:VAL:HG11	1.98	0.46
70:Ae:100:HIS:CD2	70:Ae:102:SER:H	2.34	0.46
2:A2:314:HIS:CG	53:BT:86:ARG:HG3	2.51	0.45
6:AA:260:G:C2	6:AA:278:A:C8	3.04	0.45
6:AA:971:C:H2'	6:AA:972:G:H8	1.81	0.45
26:EI:234:THR:OG1	26:EI:287:ARG:NE	2.41	0.45
50:BS:147:ARG:HA	50:BS:150:VAL:HG12	1.98	0.45
58:AV:137:THR:HB	58:AV:177:GLU:HG2	1.98	0.45
67:Ba:80:ASP:OD1	67:Ba:81:GLN:N	2.49	0.45
6:AA:354:U:H4'	10:EB:92:ASN:HB2	1.98	0.45
6:AA:805:U:H2'	6:AA:806:G:O4'	2.17	0.45
6:AA:1173:U:H3	50:BS:95:LYS:NZ	2.14	0.45
9:BB:179:LEU:HB3	9:BB:247:TYR:CD1	2.51	0.45
10:EB:334:LEU:HD11	10:EB:583:VAL:HG23	1.98	0.45
10:EB:515:HIS:HD2	10:EB:517:ALA:H	1.64	0.45
14:AE:93:TYR:CE1	14:AE:98:GLU:HG3	2.51	0.45
16:EE:158:GLY:O	16:EE:162:LEU:HG	2.16	0.45
18:AF:430:ASN:OD1	18:AF:435:TYR:OH	2.34	0.45
21:EG:63:GLU:HB2	21:EG:94:PHE:HE2	1.82	0.45
21:EG:146:ASN:O	21:EG:150:ARG:HG2	2.16	0.45
37:EM:81:ALA:HB2	37:EM:105:PHE:HB3	1.99	0.45
48:AR:79:ARG:O	48:AR:127:LYS:NZ	2.49	0.45
88:ER:200:PM8:H312	51:ES:11:THR:HG21	1.98	0.45
60:AW:126:GLU:OE1	65:AY:43:TYR:OH	2.33	0.45
65:AY:148:VAL:HG22	65:AY:167:GLU:HG3	1.96	0.45
77:Al:164:LEU:HD21	77:Al:209:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:317:A:H2'	6:AA:318:A:C8	2.51	0.45
7:BA:204:THR:HG23	71:Af:164:HIS:HB2	1.98	0.45
9:BB:109:GLU:HB3	9:BB:117:LEU:HD11	1.99	0.45
9:BB:313:HIS:O	9:BB:320:ARG:NH1	2.40	0.45
12:BD:177:HIS:CE1	12:BD:244:ARG:HB2	2.51	0.45
13:ED:310:TYR:CZ	13:ED:314:LEU:HD11	2.52	0.45
19:BF:213:LEU:CD1	19:BF:236:ALA:HB2	2.43	0.45
23:EH:255:GLU:OE2	23:EH:318:TYR:OH	2.31	0.45
23:EH:335:LEU:HB3	23:EH:338:CYS:SG	2.55	0.45
30:AK:34:LYS:HD2	59:BV:90:PHE:CG	2.51	0.45
35:EL:439:PHE:HB3	35:EL:478:ARG:HB3	1.99	0.45
35:EL:496:ARG:HA	35:EL:499:ARG:HG2	1.98	0.45
46:BQ:178:SER:OG	46:BQ:187:SER:O	2.28	0.45
46:BQ:182:CYS:HB2	80:At:103:ASP:HA	1.99	0.45
47:EQ:120:VAL:HG23	47:EQ:124:LEU:HB2	1.98	0.45
47:EQ:175:ALA:HB2	47:EQ:203:LYS:HB2	1.99	0.45
48:AR:78:ILE:HD12	48:AR:119:LEU:HD11	1.97	0.45
48:AR:177:GLU:OE1	48:AR:179:TYR:OH	2.30	0.45
74:Bg:80:MET:HG3	74:Bg:81:PHE:CD2	2.51	0.45
79:Ap:233:GLU:OE2	79:Ap:241:SER:HB3	2.16	0.45
5:A8:52:ARG:HG2	62:AX:75:PRO:HG3	1.98	0.45
7:BA:619:ALA:O	7:BA:623:LYS:HG2	2.15	0.45
9:BB:80:ILE:HA	9:BB:83:ASN:HD21	1.81	0.45
14:AE:373:LYS:HA	43:BO:232:GLU:HG3	1.99	0.45
14:AE:422:VAL:HG21	14:AE:425:MET:HE3	1.97	0.45
15:BE:344:LEU:O	15:BE:347:TYR:C	2.60	0.45
18:AF:94:PRO:O	18:AF:126:TYR:HB2	2.17	0.45
19:BF:387:ASN:HB3	60:AW:81:ARG:HH12	1.82	0.45
41:EN:475:LEU:HD13	41:EN:494:PHE:HE2	1.80	0.45
42:AO:53:GLU:HB2	42:AO:57:THR:HG21	1.99	0.45
44:EO:23:LEU:HB3	44:EO:30:HIS:ND1	2.31	0.45
45:AP:234:LEU:HB2	45:AP:252:PHE:HE1	1.82	0.45
46:BQ:129:THR:HG23	46:BQ:160:VAL:HG13	1.99	0.45
47:EQ:170:TYR:OH	47:EQ:254:ASP:OD1	2.26	0.45
47:EQ:174:GLU:HG3	47:EQ:203:LYS:HG3	1.99	0.45
55:AU:10:HIS:HE1	58:AV:161:VAL:HG23	1.81	0.45
63:BX:101:ASN:HB3	76:Bi:102:VAL:C	2.41	0.45
65:AY:275:GLU:OE2	65:AY:278:ARG:NH2	2.48	0.45
66:BZ:1:MET:HE2	66:BZ:35:LYS:HB2	1.99	0.45
66:BZ:78:GLU:HG3	66:BZ:81:TYR:HB3	1.97	0.45
2:A2:58:ARG:HB2	2:A2:87:ILE:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:1:A:N6	7:BA:209:PRO:HB2	2.32	0.45
7:BA:585:HIS:CD2	7:BA:587:SER:H	2.35	0.45
7:BA:597:VAL:O	7:BA:601:ARG:HG2	2.16	0.45
8:EA:174:ARG:HH12	22:BH:76:TRP:HB3	1.81	0.45
10:EB:164:ASP:OD2	10:EB:255:TYR:OH	2.27	0.45
10:EB:563:ASN:HD21	10:EB:566:THR:HG23	1.81	0.45
11:EC:186:GLU:HA	16:EE:117:GLN:HE22	1.81	0.45
12:BD:239:ALA:HB3	12:BD:249:PRO:HB3	1.97	0.45
20:EF:91:ARG:HD2	20:EF:116:TRP:CD1	2.52	0.45
44:EO:295:ARG:NH1	72:Bf:112:ARG:HH21	2.15	0.45
56:BU:131:LYS:HB3	56:BU:131:LYS:HE2	1.83	0.45
2:A2:150:GLU:OE1	2:A2:150:GLU:N	2.47	0.45
3:A3:191:LYS:HE2	19:BF:311:GLN:HE21	1.81	0.45
4:A5:64:LYS:NZ	4:A5:69:TRP:HD1	2.14	0.45
6:AA:239:U:H5''	10:EB:708:ARG:HG2	1.98	0.45
6:AA:486:A:H5'	19:BF:372:LEU:HD12	1.99	0.45
6:AA:1165:G:O3'	48:AR:52:ARG:NH2	2.50	0.45
7:BA:623:LYS:O	7:BA:627:SER:OG	2.26	0.45
7:BA:663:LEU:HD11	7:BA:682:PHE:CG	2.51	0.45
9:BB:255:LEU:HD23	9:BB:255:LEU:H	1.80	0.45
12:BD:132:GLU:OE2	12:BD:151:ARG:NH2	2.49	0.45
12:BD:257:ASP:O	12:BD:261:MET:HG2	2.16	0.45
16:EE:105:GLN:O	16:EE:109:GLN:HG2	2.16	0.45
20:EF:125:CYS:SG	20:EF:126:ILE:N	2.89	0.45
23:EH:45:PHE:HB2	23:EH:379:LEU:HD13	1.98	0.45
24:AI:28:PRO:HB2	24:AI:83:ILE:HD11	1.98	0.45
30:AK:123:TRP:CH2	30:AK:127:ARG:HG3	2.52	0.45
35:EL:664:ALA:O	35:EL:668:THR:OG1	2.23	0.45
41:EN:546:LEU:HD12	41:EN:547:PRO:HD2	1.98	0.45
42:AO:51:GLY:HA3	42:AO:135:THR:O	2.17	0.45
43:BO:86:THR:OG1	43:BO:221:GLY:O	2.34	0.45
47:EQ:77:PRO:HA	47:EQ:165:PRO:HB2	1.98	0.45
60:AW:98:PHE:HB3	60:AW:105:MET:HE3	1.98	0.45
60:AW:179:LEU:HD23	60:AW:232:LEU:HD21	1.97	0.45
70:Ae:115:ASN:HB3	70:Ae:118:VAL:HG22	1.97	0.45
76:Bi:202:GLN:HA	76:Bi:206:PRO:HA	1.98	0.45
7:BA:357:MET:HG3	7:BA:362:ALA:HA	1.98	0.45
9:BB:199:TRP:CH2	56:BU:109:PRO:HG3	2.51	0.45
10:EB:174:GLU:HA	10:EB:228:LEU:HD11	1.99	0.45
10:EB:246:ARG:HD3	54:ET:102:ARG:NH2	2.31	0.45
11:EC:365:GLN:HE21	11:EC:375:PHE:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AE:240:PRO:O	14:AE:383:SER:HB3	2.17	0.45
15:BE:339:ILE:HG13	31:BK:212:GLN:HE21	1.80	0.45
30:AK:145:TYR:CG	30:AK:190:CYS:HB2	2.52	0.45
30:AK:151:LEU:HD11	59:BV:111:LYS:HG2	1.97	0.45
35:EL:458:PHE:HD1	35:EL:562:ILE:HG23	1.81	0.45
43:BO:130:ARG:HD3	52:AT:19:ALA:O	2.16	0.45
44:EP:54:GLY:O	44:EP:95:HIS:ND1	2.50	0.45
46:BQ:50:PHE:HZ	46:BQ:163:GLN:HG3	1.82	0.45
52:AT:79:HIS:HB3	52:AT:87:GLY:O	2.16	0.45
62:AX:84:PRO:HA	67:Ba:28:ARG:O	2.17	0.45
63:BX:86:ILE:HG22	63:BX:113:HIS:NE2	2.32	0.45
65:AY:243:ASP:OD1	65:AY:243:ASP:N	2.44	0.45
76:Bi:84:HIS:NE2	76:Bi:95:ILE:HD13	2.32	0.45
2:A2:144:GLU:HB2	2:A2:351:LEU:HB2	1.98	0.45
3:A3:65:ILE:HG13	3:A3:121:LEU:O	2.17	0.45
6:AA:531:U:H5	74:Bg:76:SER:HB2	1.82	0.45
6:AA:862:U:H2'	6:AA:863:C:C6	2.52	0.45
15:BE:109:VAL:HG13	15:BE:155:LEU:HD21	1.99	0.45
16:EE:462:SER:OG	44:EP:313:THR:O	2.34	0.45
18:AF:376:ARG:HH12	45:AP:188:ARG:HE	1.65	0.45
24:AI:11:PRO:HB2	67:Ba:84:TYR:HD2	1.82	0.45
35:EL:217:VAL:HG22	35:EL:246:VAL:HG22	1.98	0.45
41:EN:207:VAL:HG12	41:EN:210:THR:H	1.82	0.45
44:EP:254:LEU:HG	44:EP:255:PRO:HD2	1.98	0.45
47:EQ:263:LEU:HD22	47:EQ:268:ASP:HB3	1.99	0.45
49:BR:11:MET:HE2	49:BR:15:LEU:HB3	1.99	0.45
49:BR:133:GLN:HG2	78:Ao:144:PRO:HD3	1.99	0.45
51:ES:153:GLU:HA	51:ES:156:THR:HG22	1.98	0.45
52:AT:58:VAL:HG22	52:AT:115:VAL:HG22	1.98	0.45
54:ET:22:ARG:HH22	54:ET:28:PRO:C	2.25	0.45
55:AU:132:GLU:OE1	55:AU:132:GLU:N	2.46	0.45
62:AX:66:ARG:NE	62:AX:69:GLU:OE2	2.44	0.45
63:BX:96:TRP:HB3	63:BX:165:ARG:HB3	1.99	0.45
79:Ap:283:ASP:N	79:Ap:283:ASP:OD1	2.47	0.45
2:A2:372:GLU:OE2	67:Ba:49:ARG:NH1	2.38	0.45
6:AA:1129:A:OP2	6:AA:1130:A:O2'	2.25	0.45
8:EA:336:VAL:HG23	8:EA:338:GLU:H	1.82	0.45
13:ED:11:ARG:HH22	13:ED:15:SER:HA	1.81	0.45
16:EE:298:LEU:HD13	16:EE:306:VAL:HA	1.99	0.45
37:EM:262:PRO:HD2	37:EM:265:LEU:HB2	1.99	0.45
41:EN:203:ARG:O	41:EN:206:SER:OG	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:AP:67:GLY:HA3	73:Ag:81:LEU:HD13	1.98	0.45
47:EQ:90:SER:OG	47:EQ:128:ASP:OD2	2.35	0.45
65:AY:118:GLU:OE2	65:AY:128:ARG:NE	2.47	0.45
76:Bi:180:LYS:O	76:Bi:183:LEU:HG	2.17	0.45
6:AA:187:A:H3'	6:AA:287:A:N6	2.31	0.45
6:AA:296:A:O4'	6:AA:476:G:N2	2.49	0.45
6:AA:813:U:H5''	55:AU:27:ARG:NH1	2.32	0.45
12:BD:221:ILE:HG12	12:BD:514:PHE:HZ	1.82	0.45
12:BD:233:GLY:HA2	12:BD:253:LEU:HD13	1.99	0.45
20:EF:211:GLY:O	20:EF:215:LEU:HG	2.17	0.45
21:EG:26:GLN:HA	21:EG:30:GLN:HE22	1.82	0.45
22:BH:273:PRO:HA	22:BH:276:ILE:HB	1.98	0.45
23:EH:571:ARG:CZ	68:Bb:40:VAL:HG12	2.47	0.45
28:BJ:139:PHE:HA	28:BJ:142:THR:HG22	1.99	0.45
30:AK:259:LEU:HD23	44:EP:306:THR:HG21	1.99	0.45
59:BV:83:MET:HE2	59:BV:98:ILE:HD12	1.99	0.45
6:AA:40:U:H1'	70:Ae:72:PRO:HG3	1.99	0.44
6:AA:281:A:H2'	6:AA:282:A:C8	2.52	0.44
6:AA:574:A:H61	6:AA:1167:A:N6	2.16	0.44
7:BA:379:ARG:HH21	7:BA:410:GLU:CD	2.25	0.44
7:BA:426:ASP:OD1	71:Af:171:TRP:NE1	2.49	0.44
7:BA:581:VAL:HG22	7:BA:609:SER:HB3	1.99	0.44
10:EB:499:ALA:O	10:EB:503:ARG:HG2	2.17	0.44
15:BE:137:LYS:HA	15:BE:140:GLU:HG2	1.99	0.44
15:BE:306:GLN:OE1	15:BE:347:TYR:OH	2.25	0.44
19:BF:245:ASN:ND2	19:BF:248:GLU:HB2	2.32	0.44
24:AI:12:TRP:HE3	67:Ba:79:PRO:HB3	1.81	0.44
29:EJ:48:ASP:HB3	50:BS:161:LEU:HD11	1.97	0.44
31:BK:224:MET:O	31:BK:228:MET:HG2	2.16	0.44
35:EL:412:ALA:O	35:EL:416:ILE:HG13	2.17	0.44
44:EP:96:ASP:HB2	44:EP:99:HIS:HD2	1.82	0.44
2:A2:70:ARG:NH2	6:AA:531:U:HO2'	2.15	0.44
3:A3:94:GLY:HA3	6:AA:463:U:H1'	1.99	0.44
6:AA:198:A:C6	67:Ba:16:LYS:HD3	2.52	0.44
6:AA:276:C:H4'	6:AA:277:A:H5'	2.00	0.44
6:AA:322:U:H2'	6:AA:323:U:C6	2.52	0.44
6:AA:1163:A:H8	7:BA:771:ARG:HH22	1.63	0.44
6:AA:1163:A:HO2'	6:AA:1165:G:H21	1.60	0.44
9:BB:357:THR:HA	9:BB:364:VAL:HG22	1.99	0.44
12:BD:308:LEU:HG	12:BD:312:ASP:HB2	1.98	0.44
14:AE:371:LEU:HD23	14:AE:374:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BE:63:VAL:HB	65:AY:85:LEU:HD23	1.99	0.44
25:BI:291:VAL:HG21	79:Ap:254:ASP:HB3	1.99	0.44
37:EM:300:ILE:HG23	37:EM:323:ALA:HB3	1.99	0.44
43:BO:115:VAL:HG13	43:BO:163:VAL:HG13	1.98	0.44
44:EO:118:GLN:HE21	44:EO:191:LEU:H	1.65	0.44
48:AR:44:LEU:HD23	48:AR:96:LEU:HD22	2.00	0.44
75:Bh:45:SER:HG	75:Bh:67:THR:HG1	1.58	0.44
2:A2:381:GLU:HG2	62:AX:119:PRO:HG2	1.99	0.44
6:AA:500:A:H2'	6:AA:501:A:C8	2.52	0.44
6:AA:974:G:OP1	47:EQ:573:ARG:NH2	2.35	0.44
6:AA:1000:U:H2'	6:AA:1001:G:H8	1.82	0.44
6:AA:1174:U:OP2	48:AR:140:ASN:ND2	2.50	0.44
13:ED:155:LEU:HD21	13:ED:188:GLN:HE22	1.83	0.44
15:BE:382:ARG:NH1	60:AW:256:MET:HE1	2.32	0.44
18:AF:76:ILE:HB	53:BT:148:PRO:HG2	1.97	0.44
22:BH:118:VAL:HA	22:BH:162:HIS:CD2	2.52	0.44
22:BH:130:VAL:HG22	22:BH:182:VAL:HG12	1.99	0.44
22:BH:152:ALA:HA	22:BH:156:LEU:HG	2.00	0.44
26:EI:77:ASP:HA	35:EL:299:LYS:HE2	1.99	0.44
28:BJ:157:LYS:N	28:BJ:158:PRO:HD3	2.32	0.44
31:BK:217:GLU:OE1	31:BK:220:ARG:NH2	2.45	0.44
41:EN:502:LEU:HD13	41:EN:514:HIS:HD2	1.83	0.44
52:AT:50:LYS:HA	52:AT:53:ILE:HG22	1.99	0.44
62:AX:146:LEU:HD21	62:AX:151:VAL:HG21	1.98	0.44
68:Bb:59:ILE:HD11	68:Bb:118:LEU:HD11	2.00	0.44
6:AA:97:A:H2	65:AY:91:GLN:HE22	1.66	0.44
6:AA:1129:A:HO2'	69:Bc:130:TRP:CG	2.36	0.44
8:EA:534:ASN:HB3	8:EA:537:ASN:HD22	1.81	0.44
11:EC:178:MET:HE1	11:EC:218:VAL:HG21	2.00	0.44
11:EC:242:SER:HB2	11:EC:361:HIS:CE1	2.50	0.44
11:EC:335:GLY:HA3	37:EM:38:MET:HE1	1.99	0.44
13:ED:364:SER:O	13:ED:368:GLU:HG2	2.18	0.44
14:AE:82:ARG:HD3	25:BI:77:ASN:HB2	1.99	0.44
14:AE:143:VAL:N	14:AE:164:TRP:O	2.47	0.44
15:BE:146:ILE:HG23	15:BE:245:ILE:HG21	1.99	0.44
22:BH:70:TYR:O	22:BH:74:ARG:HG2	2.18	0.44
25:BI:225:TRP:CZ2	72:Bf:106:PRO:HD3	2.53	0.44
37:EM:57:HIS:HD2	37:EM:59:GLN:HB2	1.83	0.44
40:BN:97:ARG:NH1	75:Bh:83:LEU:O	2.50	0.44
41:EN:357:LEU:HD21	41:EN:376:ALA:HB1	2.00	0.44
42:AO:63:ASP:OD1	42:AO:63:ASP:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:EO:147:GLU:OE1	44:EO:149:GLU:N	2.47	0.44
45:AP:15:HIS:O	45:AP:17:ARG:NH1	2.50	0.44
45:AP:31:ILE:HG23	45:AP:44:THR:HG22	1.99	0.44
32:ER:108:VAL:HA	32:ER:111:VAL:HG22	1.99	0.44
60:AW:123:VAL:O	60:AW:127:ARG:HG2	2.18	0.44
60:AW:137:ALA:H	60:AW:229:HIS:CD2	2.36	0.44
61:BW:56:ASN:ND2	61:BW:61:ASN:O	2.43	0.44
66:BZ:89:VAL:HG23	66:BZ:90:THR:HG22	1.99	0.44
74:Bg:38:ASN:O	74:Bg:41:TYR:N	2.50	0.44
2:A2:364:ALA:HB1	2:A2:370:TYR:CD1	2.53	0.44
3:A3:86:ARG:NH2	19:BF:27:THR:O	2.48	0.44
5:A8:100:GLN:OE1	6:AA:912:G:N2	2.32	0.44
6:AA:465:A:H2'	6:AA:466:G:C8	2.53	0.44
7:BA:250:ILE:HD13	7:BA:254:ARG:HD2	2.00	0.44
22:BH:302:ALA:O	22:BH:306:ASN:ND2	2.36	0.44
40:BN:183:VAL:HA	40:BN:186:THR:HG22	1.99	0.44
42:AO:156:ASP:OD1	42:AO:156:ASP:N	2.44	0.44
50:BS:22:ALA:O	50:BS:23:THR:OG1	2.31	0.44
57:EU:42:ARG:HG3	57:EU:48:ILE:HD11	1.98	0.44
58:AV:122:ARG:NH1	71:Af:101:HIS:O	2.50	0.44
60:AW:169:ARG:HB2	60:AW:172:HIS:HD2	1.81	0.44
6:AA:126:A:H2'	6:AA:127:A:C8	2.52	0.44
7:BA:190:THR:O	7:BA:194:ARG:HG3	2.18	0.44
13:ED:38:GLU:HB3	13:ED:43:LEU:HB2	1.99	0.44
18:AF:60:LEU:HD11	19:BF:359:PRO:HB3	1.99	0.44
25:BI:94:LYS:HD3	25:BI:94:LYS:HA	1.85	0.44
26:EI:253:ALA:HA	26:EI:256:ARG:HG2	1.99	0.44
35:EL:257:ARG:NH2	35:EL:393:ASP:O	2.35	0.44
42:AO:114:VAL:HG23	42:AO:116:ARG:HG2	1.98	0.44
43:BO:104:LEU:HD12	43:BO:117:LEU:HD11	2.00	0.44
49:BR:205:TYR:HE1	80:At:34:ARG:HG3	1.82	0.44
32:ER:86:VAL:HG22	32:ER:103:LEU:HD21	2.00	0.44
50:BS:39:LEU:O	50:BS:113:ARG:NH2	2.49	0.44
51:ES:129:GLN:HE21	51:ES:133:ARG:HE	1.66	0.44
60:AW:100:GLU:HG2	60:AW:105:MET:SD	2.57	0.44
67:Ba:115:HIS:HD2	67:Ba:116:ARG:HD3	1.83	0.44
3:A3:126:ALA:O	3:A3:130:ILE:HG12	2.18	0.44
4:A5:64:LYS:HZ2	4:A5:80:PRO:HG2	1.83	0.44
6:AA:579:U:H2'	6:AA:580:A:H8	1.83	0.44
6:AA:992:A:H5''	6:AA:993:A:C8	2.53	0.44
8:EA:85:ARG:NH1	8:EA:331:GLU:OE1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:EB:501:TYR:CZ	10:EB:505:ARG:HD2	2.53	0.44
14:AE:246:ILE:HG12	14:AE:308:TYR:HB2	2.00	0.44
15:BE:77:GLU:HG3	70:Ae:193:LEU:HD11	2.00	0.44
44:EO:214:PHE:HB3	44:EO:217:MET:HB3	2.00	0.44
45:AP:166:TYR:CE2	45:AP:169:LYS:HG3	2.53	0.44
53:BT:75:THR:HG21	67:Ba:151:MET:HG2	2.00	0.44
62:AX:78:ARG:HA	62:AX:78:ARG:HD2	1.82	0.44
76:Bi:78:LEU:HA	76:Bi:136:TYR:OH	2.18	0.44
1:A1:71:GLN:HG2	67:Ba:98:TRP:CD2	2.52	0.44
6:AA:149:U:OP2	60:AW:17:ARG:NH1	2.51	0.44
6:AA:1127:A:H2'	6:AA:1128:U:C6	2.52	0.44
84:AA:1250:SPD:H32	52:AT:15:ALA:HA	2.00	0.44
7:BA:275:ALA:HB2	7:BA:356:VAL:HG23	2.00	0.44
13:ED:236:HIS:CD2	13:ED:545:GLY:HA2	2.53	0.44
14:AE:86:PRO:HB3	44:EO:307:PRO:HB3	1.99	0.44
22:BH:122:HIS:CD2	22:BH:124:PHE:H	2.36	0.44
26:EI:184:SER:HB3	43:BO:58:SER:HA	1.99	0.44
41:EN:704:GLU:O	41:EN:708:GLN:HG2	2.17	0.44
44:EP:21:LEU:HB3	44:EP:194:TRP:HE1	1.81	0.44
48:AR:58:PHE:CG	48:AR:89:ARG:HG2	2.53	0.44
48:AR:134:ARG:NH2	48:AR:170:MET:O	2.51	0.44
51:ES:105:ALA:HB2	51:ES:135:TYR:OH	2.18	0.44
52:AT:60:CYS:SG	52:AT:71:LEU:HB2	2.58	0.44
54:ET:99:THR:HG22	54:ET:101:PHE:H	1.83	0.44
56:BU:140:ILE:HG21	74:Bg:28:MET:HE1	2.00	0.44
59:BV:100:PRO:HG2	59:BV:103:THR:HB	1.99	0.44
60:AW:169:ARG:HB2	60:AW:172:HIS:CD2	2.53	0.44
61:BW:151:TRP:CD1	61:BW:152:GLN:HG3	2.52	0.44
72:Bf:99:ILE:HG13	72:Bf:104:VAL:HG21	2.00	0.44
73:Ag:32:HIS:HB3	73:Ag:80:PHE:CD1	2.53	0.44
2:A2:375:ARG:HB3	67:Ba:83:PHE:O	2.18	0.44
5:A8:66:ARG:NH2	5:A8:139:ARG:O	2.51	0.44
6:AA:5:U:H2'	6:AA:6:A:H8	1.83	0.44
6:AA:185:U:H2'	6:AA:186:A:O4'	2.18	0.44
6:AA:384:U:H4'	6:AA:385:A:C8	2.52	0.44
6:AA:490:G:C6	18:AF:28:ARG:HD2	2.52	0.44
6:AA:582:A:H2'	6:AA:583:A:C8	2.53	0.44
6:AA:993:A:H61	8:EA:490:ARG:HH11	1.65	0.44
6:AA:1042:N:O2'	16:EE:210:GLY:HA3	2.18	0.44
9:BB:216:PHE:HB3	56:BU:121:HIS:CE1	2.53	0.44
10:EB:557:ASN:HB2	10:EB:585:SER:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:EE:462:SER:HB3	44:EP:317:LEU:HD11	2.00	0.44
19:BF:325:ARG:HD2	77:AI:174:PHE:CG	2.53	0.44
23:EH:306:PRO:O	23:EH:311:ARG:NH1	2.46	0.44
40:BN:14:HIS:NE2	56:BU:181:ALA:O	2.48	0.44
46:BQ:82:PRO:HA	46:BQ:190:TRP:HA	1.98	0.44
46:BQ:145:PHE:HE2	46:BQ:147:ASN:HD21	1.65	0.44
49:BR:194:HIS:HD2	49:BR:196:ARG:HE	1.66	0.44
73:Ag:82:ARG:HA	73:Ag:82:ARG:HD2	1.72	0.44
3:A3:151:ARG:NH2	6:AA:334:U:OP2	2.51	0.43
6:AA:302:G:OP1	54:ET:8:LYS:NZ	2.47	0.43
7:BA:484:HIS:CD2	7:BA:658:SER:HB3	2.53	0.43
7:BA:703:ARG:HG3	7:BA:744:ASN:ND2	2.33	0.43
22:BH:194:ARG:HH22	22:BH:196:LEU:HD21	1.82	0.43
35:EL:331:HIS:CE1	35:EL:350:ILE:HG21	2.52	0.43
40:BN:9:TRP:HA	40:BN:14:HIS:CD2	2.53	0.43
47:EQ:623:LEU:HD12	47:EQ:626:LEU:HD11	2.00	0.43
48:AR:242:HIS:O	48:AR:246:VAL:HG13	2.17	0.43
49:BR:133:GLN:HA	78:Ao:144:PRO:HG3	1.99	0.43
6:AA:484:U:H4'	6:AA:485:A:OP1	2.17	0.43
6:AA:514:G:O2'	6:AA:570:U:O2	2.32	0.43
6:AA:852:C:N4	47:EQ:563:ARG:O	2.51	0.43
6:AA:1100:U:H2'	6:AA:1101:A:C8	2.54	0.43
6:AA:1165:G:C8	6:AA:1167:A:H1'	2.53	0.43
7:BA:602:ARG:HA	34:BL:98:CYS:SG	2.57	0.43
7:BA:759:GLN:NE2	60:AW:247:CYS:SG	2.77	0.43
13:ED:519:VAL:HG22	13:ED:582:VAL:HG12	2.00	0.43
15:BE:338:ALA:HB3	31:BK:212:GLN:HE22	1.83	0.43
23:EH:217:ILE:HG22	23:EH:265:VAL:HG22	2.00	0.43
23:EH:476:MET:HE1	80:At:15:TRP:CD1	2.53	0.43
23:EH:509:ASN:ND2	49:BR:75:ASP:OD2	2.51	0.43
35:EL:298:VAL:HG11	35:EL:305:VAL:HG22	1.99	0.43
41:EN:258:LEU:HD12	41:EN:313:CYS:HB3	1.99	0.43
41:EN:539:PHE:HZ	41:EN:597:LEU:HB2	1.82	0.43
43:BO:93:ILE:HG21	43:BO:161:MET:HE1	1.99	0.43
49:BR:35:PHE:CE1	49:BR:38:GLU:HB2	2.52	0.43
51:ES:37:LEU:HD11	51:ES:115:LEU:HB3	2.00	0.43
60:AW:149:ILE:HD11	60:AW:230:LEU:HD13	2.00	0.43
68:Bb:45:LYS:O	68:Bb:48:GLU:HG3	2.18	0.43
76:Bi:121:ARG:HB3	76:Bi:138:VAL:HG11	1.98	0.43
2:A2:412:ASN:ND2	2:A2:438:ILE:HG23	2.34	0.43
6:AA:562:G:OP1	63:BX:155:ARG:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:948:A:C2	13:ED:339:ARG:HD3	2.54	0.43
84:AA:1250:SPD:H82	52:AT:16:ARG:HG3	2.01	0.43
8:EA:319:GLY:HA2	85:EA:2001:GTP:H5'	2.01	0.43
11:EC:127:TRP:CD2	11:EC:133:PRO:HB3	2.53	0.43
11:EC:388:LYS:O	11:EC:392:LYS:HG2	2.19	0.43
12:BD:210:LEU:HD22	12:BD:455:ALA:HB1	2.01	0.43
18:AF:412:GLU:O	18:AF:415:MET:HG2	2.19	0.43
26:EI:189:TRP:CE2	52:AT:70:ARG:HB3	2.54	0.43
34:BL:182:GLY:HA2	34:BL:185:ARG:HB2	2.00	0.43
47:EQ:144:VAL:HG11	47:EQ:496:PRO:HG3	2.00	0.43
58:AV:231:THR:HG21	71:Af:85:PRO:HG2	2.01	0.43
62:AX:164:PRO:HG2	62:AX:167:MET:HG3	1.98	0.43
68:Bb:134:LEU:HG	68:Bb:139:TYR:HB3	2.01	0.43
2:A2:201:ASP:OD2	67:Ba:152:ARG:NH1	2.51	0.43
2:A2:332:ASP:O	2:A2:335:SER:OG	2.26	0.43
3:A3:168:LYS:NZ	80:At:151:ARG:O	2.45	0.43
3:A3:181:ASP:HB3	77:Al:88:ARG:HG3	1.99	0.43
6:AA:20:A:H62	60:AW:68:SER:HA	1.84	0.43
6:AA:392:A:H5'	16:EE:495:MET:SD	2.58	0.43
6:AA:823:U:H2'	6:AA:824:U:C6	2.53	0.43
6:AA:983:C:H5''	10:EB:603:GLN:NE2	2.34	0.43
7:BA:593:THR:HG22	7:BA:596:LEU:HB3	2.00	0.43
11:EC:172:LYS:NZ	11:EC:214:THR:O	2.41	0.43
12:BD:514:PHE:HA	12:BD:517:VAL:HG22	1.99	0.43
20:EF:346:ARG:HG2	20:EF:348:ALA:H	1.82	0.43
25:BI:90:TYR:CZ	25:BI:128:LEU:HD22	2.54	0.43
26:EI:326:LEU:HD13	26:EI:349:VAL:HG13	1.99	0.43
31:BK:213:VAL:O	31:BK:217:GLU:HG2	2.18	0.43
37:EM:204:ALA:HB1	47:EQ:585:HIS:HB3	2.00	0.43
43:BO:95:VAL:HG23	43:BO:96:LEU:HG	1.99	0.43
43:BO:142:GLU:HB3	43:BO:145:LEU:HG	2.00	0.43
44:EO:282:MET:HG2	79:Ap:247:LEU:HD22	2.00	0.43
45:AP:211:ILE:HG21	45:AP:266:LEU:HD11	2.00	0.43
46:BQ:85:ARG:HH22	80:At:114:MET:HG2	1.84	0.43
56:BU:114:THR:HB	56:BU:117:ILE:HG12	2.01	0.43
67:Ba:18:GLY:HA3	67:Ba:23:SER:CB	2.48	0.43
1:A1:181:VAL:HG21	65:AY:299:MET:HB2	2.00	0.43
3:A3:108:ARG:O	3:A3:112:VAL:HG22	2.18	0.43
3:A3:170:ARG:CZ	77:Al:181:LEU:HD22	2.48	0.43
4:A5:47:LYS:HE2	6:AA:802:G:H5''	1.99	0.43
7:BA:217:LEU:HD23	7:BA:238:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:EB:642:ILE:HA	14:AE:283:MET:HE3	1.99	0.43
13:ED:27:GLU:HG3	13:ED:28:TRP:CD1	2.54	0.43
13:ED:48:ARG:HB2	13:ED:55:ALA:HB1	2.00	0.43
15:BE:60:GLY:HA3	65:AY:75:THR:HG21	1.99	0.43
20:EF:178:VAL:HG22	20:EF:204:ILE:HB	2.00	0.43
26:EI:245:ALA:HB2	26:EI:270:GLU:HG2	2.00	0.43
31:BK:114:HIS:HB3	31:BK:117:VAL:HG22	2.01	0.43
31:BK:229:GLU:O	31:BK:233:LYS:HG2	2.17	0.43
35:EL:384:ASP:OD1	35:EL:384:ASP:N	2.49	0.43
35:EL:399:PHE:CE2	35:EL:432:ILE:HA	2.53	0.43
40:BN:70:HIS:HB2	40:BN:73:CYS:SG	2.58	0.43
54:ET:94:GLU:OE1	54:ET:102:ARG:NH2	2.52	0.43
63:BX:112:PHE:CG	63:BX:117:PHE:HD1	2.37	0.43
65:AY:87:LYS:HA	65:AY:90:LYS:HZ2	1.83	0.43
79:Ap:286:LYS:HD2	79:Ap:286:LYS:HA	1.86	0.43
6:AA:11:U:H1'	6:AA:12:U:O4'	2.18	0.43
6:AA:1123:U:H2'	6:AA:1124:A:H8	1.83	0.43
7:BA:174:ARG:HD3	7:BA:815:TYR:CZ	2.53	0.43
9:BB:106:LEU:HD22	9:BB:117:LEU:HB3	2.01	0.43
9:BB:309:ARG:O	9:BB:313:HIS:ND1	2.51	0.43
9:BB:438:LEU:HD13	28:BJ:181:ARG:HG3	1.99	0.43
11:EC:206:VAL:HG22	11:EC:220:LEU:HD22	1.99	0.43
15:BE:384:HIS:H	15:BE:388:GLN:NE2	2.16	0.43
18:AF:132:PRO:O	18:AF:136:GLY:N	2.51	0.43
24:AI:190:GLU:OE1	24:AI:201:TYR:OH	2.36	0.43
28:BJ:177:THR:O	28:BJ:180:GLU:HG3	2.18	0.43
41:EN:212:SER:HB3	41:EN:215:ALA:HB3	2.00	0.43
43:BO:130:ARG:HE	43:BO:130:ARG:H	1.66	0.43
43:BO:234:ASP:HB2	50:BS:29:ASN:HB3	2.00	0.43
45:AP:226:VAL:HB	45:AP:248:ALA:HB2	1.99	0.43
50:BS:107:ILE:O	50:BS:111:ARG:HG2	2.17	0.43
60:AW:52:HIS:ND1	60:AW:57:PRO:HB3	2.34	0.43
62:AX:86:ASN:HB2	67:Ba:29:LEU:HD21	1.99	0.43
65:AY:273:PHE:HD2	65:AY:274:HIS:HD2	1.66	0.43
68:Bb:90:PRO:HG2	80:At:51:ILE:O	2.19	0.43
2:A2:49:HIS:HE1	70:Ae:155:TYR:HB2	1.83	0.43
3:A3:121:LEU:HD21	45:AP:18:ARG:HE	1.83	0.43
5:A8:61:TYR:OH	6:AA:61:A:OP2	2.34	0.43
6:AA:127:A:O2'	58:AV:159:ARG:NH2	2.49	0.43
6:AA:325:A:H5''	77:Al:200:ASN:OD1	2.18	0.43
6:AA:461:U:OP1	55:AU:63:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:912:G:H21	10:EB:237:LYS:NZ	2.16	0.43
6:AA:1126:U:H5'	26:EI:261:ARG:HH12	1.83	0.43
7:BA:301:HIS:CD2	7:BA:303:ILE:HG12	2.54	0.43
8:EA:173:GLY:HA3	22:BH:80:MET:HE2	2.01	0.43
9:BB:418:ARG:O	9:BB:422:MET:HB3	2.19	0.43
10:EB:134:MET:HG3	10:EB:156:PRO:HB3	2.01	0.43
10:EB:208:ILE:HD11	10:EB:223:LEU:HB3	2.01	0.43
10:EB:593:VAL:HG21	10:EB:615:LYS:HB2	1.99	0.43
13:ED:357:ASP:HB2	13:ED:360:CYS:HB3	2.01	0.43
14:AE:139:GLY:HA3	14:AE:339:PHE:O	2.18	0.43
34:BL:230:ARG:NH2	60:AW:102:GLU:O	2.48	0.43
35:EL:599:ALA:HB1	35:EL:603:VAL:HB	2.00	0.43
35:EL:612:LEU:HD23	69:Bc:121:PHE:HE1	1.83	0.43
37:EM:303:ILE:O	37:EM:306:ARG:HG2	2.18	0.43
47:EQ:96:LEU:HG	47:EQ:248:MET:HE3	1.99	0.43
48:AR:130:ASP:OD1	56:BU:170:SER:HB3	2.19	0.43
58:AV:66:ILE:HD11	71:Af:90:PHE:CD2	2.53	0.43
67:Ba:12:PRO:HB2	67:Ba:13:VAL:H	1.63	0.43
3:A3:109:ILE:HG22	80:At:44:LEU:HD11	2.01	0.43
6:AA:481:G:H1'	6:AA:482:U:OP2	2.18	0.43
6:AA:883:U:H1'	24:AI:106:ARG:HH22	1.82	0.43
6:AA:960:U:O2	10:EB:503:ARG:NH1	2.44	0.43
7:BA:67:PRO:HG3	35:EL:396:PRO:HG3	2.00	0.43
22:BH:143:LEU:O	22:BH:147:ILE:HG12	2.18	0.43
34:BL:238:GLN:NE2	60:AW:100:GLU:OE1	2.33	0.43
37:EM:82:ARG:HH22	37:EM:332:GLN:HA	1.83	0.43
41:EN:447:ARG:O	41:EN:450:THR:OG1	2.32	0.43
43:BO:52:ARG:NE	50:BS:44:ASP:OD1	2.51	0.43
44:EP:139:VAL:HG12	44:EP:154:THR:HG23	2.00	0.43
47:EQ:280:ALA:HB3	47:EQ:621:GLU:H	1.84	0.43
67:Ba:80:ASP:O	67:Ba:84:TYR:CA	2.64	0.43
80:At:42:GLU:HG2	80:At:45:ARG:HH21	1.83	0.43
1:A1:163:ARG:NH2	28:BJ:286:ARG:HD2	2.32	0.43
5:A8:88:LEU:HD23	5:A8:88:LEU:H	1.83	0.43
6:AA:256:U:O4	6:AA:257:A:N6	2.51	0.43
6:AA:296:A:C5	6:AA:476:G:C6	3.07	0.43
6:AA:572:U:O2'	48:AR:156:ASP:OD2	2.35	0.43
6:AA:593:U:H2'	6:AA:594:A:C8	2.54	0.43
6:AA:906:A:H3'	10:EB:562:THR:HG21	2.01	0.43
7:BA:55:SER:OG	14:AE:106:ARG:NH1	2.50	0.43
7:BA:600:VAL:HA	7:BA:603:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:EA:115:ARG:O	8:EA:120:LYS:NZ	2.43	0.43
8:EA:176:VAL:HG23	8:EA:179:ALA:H	1.83	0.43
9:BB:309:ARG:HG3	9:BB:313:HIS:CE1	2.53	0.43
10:EB:478:ARG:HA	10:EB:532:SER:HA	2.00	0.43
10:EB:735:MET:HA	70:Ae:101:LYS:HG3	2.01	0.43
13:ED:237:HIS:CG	13:ED:594:PRO:HG3	2.54	0.43
41:EN:251:HIS:ND1	41:EN:313:CYS:SG	2.85	0.43
42:AO:69:CYS:SG	42:AO:153:LEU:HG	2.58	0.43
43:BO:80:PRO:HB3	43:BO:162:ASP:HB3	1.99	0.43
44:EO:236:LEU:HB3	44:EO:239:ARG:HH21	1.83	0.43
58:AV:155:THR:HG22	58:AV:157:GLY:H	1.84	0.43
66:BZ:128:PRO:O	66:BZ:131:HIS:NE2	2.52	0.43
70:Ae:71:HIS:HB3	70:Ae:74:SER:HB2	2.00	0.43
74:Bg:76:SER:O	74:Bg:80:MET:HG2	2.19	0.43
76:Bi:104:LEU:HD23	76:Bi:110:LEU:HB2	2.00	0.43
3:A3:163:LYS:HE2	3:A3:163:LYS:HB3	1.82	0.43
4:A5:36:ARG:HD2	6:AA:8:C:OP1	2.18	0.43
6:AA:466:G:H21	58:AV:100:GLN:NE2	2.16	0.43
6:AA:1136:C:H1'	16:EE:144:ASN:ND2	2.34	0.43
8:EA:571:SER:HB2	8:EA:575:TYR:HE2	1.83	0.43
10:EB:673:VAL:HG13	28:BJ:32:ARG:HD2	2.00	0.43
19:BF:43:LEU:HD13	19:BF:252:MET:HG3	2.01	0.43
22:BH:153:ARG:NH2	24:AI:210:TYR:O	2.42	0.43
22:BH:311:LYS:HD2	22:BH:314:GLN:HE21	1.84	0.43
31:BK:341:LYS:HE2	31:BK:341:LYS:HB3	1.88	0.43
35:EL:414:HIS:CD2	35:EL:415:MET:HG3	2.53	0.43
37:EM:187:HIS:CE1	47:EQ:594:PRO:HG3	2.54	0.43
42:AO:67:LEU:HD22	42:AO:149:ASN:HB3	2.00	0.43
52:AT:46:TRP:CZ2	52:AT:83:THR:HA	2.54	0.43
54:ET:79:ILE:HG23	81:Av:197:ARG:HD2	2.00	0.43
56:BU:114:THR:HG22	56:BU:116:ARG:H	1.84	0.43
61:BW:62:ALA:HA	61:BW:65:ASN:ND2	2.33	0.43
77:Al:40:ASP:HB3	77:Al:43:ALA:HB3	2.01	0.43
6:AA:102:A:C8	65:AY:42:THR:HG23	2.53	0.42
7:BA:339:ASP:O	7:BA:377:ARG:NH2	2.52	0.42
7:BA:710:LYS:NZ	39:AN:35:GLN:O	2.43	0.42
8:EA:278:GLU:OE1	51:ES:137:ARG:NH2	2.52	0.42
9:BB:431:ARG:HA	9:BB:434:GLU:HG2	2.00	0.42
12:BD:316:LEU:HD13	12:BD:341:TYR:CE2	2.54	0.42
13:ED:50:ILE:HD11	13:ED:396:LEU:HB3	2.01	0.42
15:BE:415:TYR:HE2	48:AR:229:HIS:CE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BE:426:MET:HE3	48:AR:72:ARG:HD2	2.00	0.42
20:EF:89:ALA:HA	20:EF:219:GLU:OE1	2.19	0.42
30:AK:106:VAL:HG22	30:AK:112:TYR:HB3	2.01	0.42
35:EL:497:PHE:HZ	35:EL:518:LEU:HG	1.84	0.42
44:EP:2:PHE:HA	44:EP:62:PRO:HD3	2.01	0.42
47:EQ:57:ASN:HB3	47:EQ:120:VAL:HA	2.01	0.42
52:AT:5:ARG:NH1	52:AT:9:ASN:OD1	2.51	0.42
67:Ba:51:LEU:HB2	67:Ba:88:VAL:HG12	2.00	0.42
76:Bi:67:ARG:HD2	76:Bi:112:LEU:HD12	2.01	0.42
1:A1:170:ASN:HD22	28:BJ:289:GLU:CD	2.27	0.42
6:AA:88:G:O2'	6:AA:91:U:OP1	2.38	0.42
6:AA:154:A:O2'	6:AA:176:A:H1'	2.19	0.42
6:AA:524:A:C8	6:AA:525:A:C8	3.06	0.42
6:AA:542:U:H2'	6:AA:543:U:C6	2.54	0.42
6:AA:931:U:H1'	41:EN:418:PRO:HD2	2.01	0.42
6:AA:1117:A:H5''	14:AE:30:SER:HA	2.00	0.42
6:AA:1167:A:C6	48:AR:91:PRO:HG3	2.54	0.42
14:AE:336:TYR:CZ	52:AT:17:ALA:HB2	2.54	0.42
15:BE:278:THR:O	15:BE:282:ILE:HG13	2.19	0.42
18:AF:179:ASN:HB2	18:AF:186:ARG:HD2	2.01	0.42
19:BF:141:MET:SD	45:AP:34:LEU:HD23	2.59	0.42
19:BF:198:LEU:HD22	19:BF:209:ILE:HG22	2.02	0.42
20:EF:255:LEU:HD12	20:EF:256:PRO:HD2	2.02	0.42
23:EH:309:VAL:HB	39:AN:193:ARG:HD2	2.00	0.42
25:BI:160:PHE:N	25:BI:161:PRO:HD2	2.34	0.42
40:BN:179:LEU:HD22	76:Bi:190:LEU:HB3	2.01	0.42
41:EN:446:THR:O	41:EN:450:THR:HG23	2.20	0.42
41:EN:611:TRP:CZ2	41:EN:637:ARG:HB2	2.54	0.42
44:EO:47:THR:OG1	44:EO:48:VAL:N	2.50	0.42
45:AP:256:TYR:CE2	45:AP:284:GLY:HA3	2.53	0.42
47:EQ:496:PRO:HG2	47:EQ:499:VAL:HG23	2.01	0.42
48:AR:231:LYS:HG2	74:Bg:60:TYR:CZ	2.54	0.42
51:ES:150:GLU:O	51:ES:153:GLU:HG2	2.18	0.42
55:AU:65:ASN:ND2	55:AU:97:GLN:HE21	2.15	0.42
58:AV:135:ARG:NH2	78:Ao:89:ALA:O	2.50	0.42
68:Bb:79:HIS:HD2	68:Bb:81:HIS:HB2	1.84	0.42
2:A2:263:GLU:OE1	2:A2:263:GLU:N	2.52	0.42
3:A3:81:VAL:HG13	3:A3:112:VAL:HG12	2.00	0.42
3:A3:148:SER:HB3	80:At:154:LEU:HA	2.00	0.42
4:A5:78:ILE:HG23	7:BA:780:TYR:CD2	2.54	0.42
6:AA:53:A:N6	81:Av:55:TRP:HE1	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:290:A:H61	18:AF:186:ARG:NH1	2.17	0.42
6:AA:478:A:N7	6:AA:491:A:N6	2.68	0.42
7:BA:799:ASP:OD2	7:BA:801:ARG:NE	2.52	0.42
8:EA:274:MET:HE1	51:ES:134:ASN:HB3	2.02	0.42
11:EC:254:VAL:HG23	11:EC:291:PHE:HZ	1.85	0.42
12:BD:121:VAL:HB	12:BD:160:ILE:HG13	2.01	0.42
12:BD:352:VAL:O	12:BD:360:ARG:NH1	2.52	0.42
18:AF:99:THR:OG1	18:AF:360:GLU:OE1	2.33	0.42
30:AK:130:ARG:O	30:AK:132:LYS:NZ	2.51	0.42
35:EL:337:MET:HE1	72:Bf:27:LEU:HD21	2.01	0.42
44:EP:1:MET:N	44:EP:29:ARG:HG3	2.34	0.42
65:AY:99:TYR:CE1	65:AY:138:LYS:HE2	2.55	0.42
5:A8:84:VAL:HA	5:A8:118:GLN:HE22	1.83	0.42
6:AA:492:U:OP2	60:AW:45:ARG:HD2	2.18	0.42
9:BB:194:TYR:CE2	9:BB:196:TRP:HB2	2.54	0.42
10:EB:646:THR:HB	42:AO:23:ALA:HB3	2.00	0.42
12:BD:402:GLU:H	12:BD:402:GLU:CD	2.27	0.42
13:ED:43:LEU:HD22	13:ED:266:TYR:CG	2.54	0.42
13:ED:44:LEU:HD21	46:BQ:227:LEU:HD21	2.00	0.42
13:ED:47:ILE:HG23	13:ED:401:LEU:HD11	2.00	0.42
13:ED:405:GLU:N	13:ED:440:GLU:OE2	2.53	0.42
18:AF:100:LYS:NZ	18:AF:361:ASP:OD1	2.45	0.42
18:AF:125:ILE:H	18:AF:125:ILE:HG12	1.62	0.42
18:AF:176:ASN:ND2	18:AF:190:ARG:HG2	2.34	0.42
23:EH:221:GLU:HG3	23:EH:222:PRO:HD2	2.01	0.42
31:BK:90:ARG:O	31:BK:109:ARG:NH1	2.52	0.42
35:EL:247:HIS:HB2	35:EL:272:TYR:CE2	2.54	0.42
44:EO:312:TRP:HA	44:EO:315:GLN:HG2	2.00	0.42
48:AR:78:ILE:HD11	48:AR:100:VAL:HG11	2.01	0.42
68:Bb:64:PRO:HA	68:Bb:67:ARG:HG2	2.01	0.42
4:A5:64:LYS:HE3	4:A5:68:GLU:O	2.19	0.42
6:AA:954:U:H5	41:EN:65:TRP:H	1.66	0.42
6:AA:1176:A:N6	48:AR:166:LYS:HD3	2.34	0.42
7:BA:770:TYR:HE1	7:BA:787:LEU:HD22	1.83	0.42
10:EB:206:HIS:CD2	10:EB:229:VAL:HG12	2.55	0.42
14:AE:251:THR:N	14:AE:330:ASP:O	2.48	0.42
16:EE:480:ASP:OD1	16:EE:481:GLU:N	2.47	0.42
26:EI:79:VAL:HG12	26:EI:80:ASP:H	1.84	0.42
37:EM:184:ARG:HH21	37:EM:213:ARG:HB3	1.85	0.42
41:EN:481:ALA:O	41:EN:523:ARG:NH2	2.52	0.42
45:AP:13:LEU:HD21	78:Ao:62:THR:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:AW:116:ARG:HD2	60:AW:116:ARG:HA	1.78	0.42
67:Ba:110:VAL:HG11	81:Av:49:THR:HG21	2.02	0.42
2:A2:185:LYS:NZ	2:A2:315:PRO:O	2.40	0.42
6:AA:5:U:H2'	6:AA:6:A:C8	2.54	0.42
6:AA:1005:U:C2'	6:AA:1006:U:H5'	2.49	0.42
8:EA:274:MET:HE3	8:EA:275:HIS:CE1	2.54	0.42
11:EC:64:GLU:HG3	11:EC:65:TRP:CD1	2.55	0.42
12:BD:291:LYS:HG3	12:BD:380:VAL:HB	2.00	0.42
13:ED:6:ARG:NH1	46:BQ:201:LYS:HG2	2.35	0.42
13:ED:25:PRO:O	13:ED:29:ARG:HG3	2.20	0.42
13:ED:375:MET:O	13:ED:379:LEU:HG	2.19	0.42
20:EF:240:LEU:HB3	20:EF:313:TRP:CH2	2.54	0.42
29:EJ:91:GLN:O	36:UL:112:UNK:HA	2.19	0.42
30:AK:152:GLU:HG3	59:BV:104:TYR:CE2	2.54	0.42
35:EL:526:HIS:HB3	35:EL:529:ASP:HB2	2.01	0.42
37:EM:47:ASN:HD22	37:EM:49:LYS:H	1.67	0.42
55:AU:43:MET:HE1	58:AV:150:VAL:HB	2.01	0.42
68:Bb:91:ILE:HG13	80:At:51:ILE:HG22	2.02	0.42
69:Bc:24:ARG:O	69:Bc:28:GLN:HG2	2.18	0.42
79:Ap:45:LEU:HD12	79:Ap:46:PRO:HD2	2.01	0.42
3:A3:122:ASP:OD1	3:A3:125:GLU:N	2.46	0.42
3:A3:160:ILE:HA	3:A3:163:LYS:HG2	2.00	0.42
5:A8:151:SER:HB3	6:AA:59:U:O4	2.20	0.42
6:AA:128:A:H5'	45:AP:125:LYS:HB3	2.00	0.42
6:AA:832:A:H2'	6:AA:833:U:C6	2.55	0.42
6:AA:984:A:C8	11:EC:42:SER:HB3	2.55	0.42
8:EA:468:LEU:HG	8:EA:469:ASN:ND2	2.35	0.42
9:BB:123:LEU:HB3	9:BB:397:GLN:HG2	2.01	0.42
9:BB:211:ASP:OD1	9:BB:212:HIS:N	2.52	0.42
12:BD:117:VAL:HB	12:BD:164:LEU:HB2	2.01	0.42
18:AF:65:ASN:ND2	61:BW:174:ILE:HD11	2.35	0.42
25:BI:58:GLU:OE2	25:BI:62:HIS:NE2	2.53	0.42
29:EJ:47:VAL:HG13	29:EJ:98:GLY:HA3	2.00	0.42
30:AK:237:PRO:HA	30:AK:254:GLN:CD	2.44	0.42
42:AO:66:LYS:HE2	42:AO:100:HIS:CD2	2.55	0.42
43:BO:105:CYS:SG	43:BO:115:VAL:HB	2.60	0.42
44:EO:13:HIS:CE1	44:EO:50:LEU:HA	2.54	0.42
48:AR:233:ARG:NH1	65:AY:73:ASP:OD2	2.53	0.42
88:ER:200:PM8:H382	51:ES:52:ASN:HB2	2.01	0.42
58:AV:180:TYR:CZ	58:AV:182:PRO:HB3	2.55	0.42
60:AW:12:HIS:CE1	60:AW:13:MET:HE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:BW:83:LEU:O	61:BW:87:ILE:HG13	2.20	0.42
65:AY:149:GLN:HB2	65:AY:168:HIS:CD2	2.55	0.42
66:BZ:81:TYR:OH	66:BZ:145:HIS:NE2	2.39	0.42
68:Bb:120:ARG:CZ	78:Ao:147:PRO:HG3	2.50	0.42
73:Ag:25:THR:O	73:Ag:29:LEU:HG	2.19	0.42
77:Al:75:ARG:HB3	77:Al:77:ASP:OD1	2.18	0.42
1:A1:179:MET:HA	1:A1:182:GLU:HG2	2.01	0.42
4:A5:78:ILE:O	4:A5:80:PRO:HD3	2.20	0.42
6:AA:280:U:C2	6:AA:281:A:C8	3.07	0.42
6:AA:350:A:H2	6:AA:359:A:H61	1.68	0.42
7:BA:761:TYR:HE1	7:BA:793:ARG:HG3	1.83	0.42
8:EA:320:LYS:HG2	85:EA:2001:GTP:O2B	2.19	0.42
9:BB:230:THR:O	9:BB:234:ILE:HG13	2.19	0.42
11:EC:78:TYR:HD1	11:EC:80:GLN:HE22	1.68	0.42
12:BD:117:VAL:HG12	12:BD:192:ARG:HH11	1.85	0.42
12:BD:288:ILE:HD13	12:BD:288:ILE:HA	1.88	0.42
14:AE:405:VAL:HG21	26:EI:193:ARG:HG2	2.01	0.42
15:BE:133:VAL:HB	15:BE:134:PRO:HD3	2.02	0.42
28:BJ:123:ASP:OD1	28:BJ:124:ALA:N	2.53	0.42
28:BJ:155:GLU:OE1	28:BJ:155:GLU:N	2.53	0.42
30:AK:286:GLU:O	30:AK:290:ARG:HG3	2.20	0.42
35:EL:617:ARG:NH1	35:EL:667:TRP:HA	2.35	0.42
41:EN:31:ARG:HB3	41:EN:35:GLU:HB2	2.02	0.42
55:AU:132:GLU:HB3	55:AU:166:PRO:HB2	2.01	0.42
68:Bb:87:ALA:O	80:At:51:ILE:N	2.43	0.42
2:A2:110:VAL:HA	65:AY:259:MET:HE1	2.02	0.42
6:AA:201:G:H2'	6:AA:202:U:C6	2.55	0.42
6:AA:479:A:N6	45:AP:96:ASP:OD1	2.40	0.42
6:AA:566:A:N7	56:BU:137:ARG:NH1	2.68	0.42
6:AA:985:A:C8	8:EA:575:TYR:HB2	2.55	0.42
6:AA:1145:A:H2'	6:AA:1146:U:C6	2.55	0.42
8:EA:423:PHE:CE1	8:EA:457:SER:HB3	2.55	0.42
8:EA:521:THR:HG23	8:EA:522:ARG:HG2	2.02	0.42
10:EB:144:PRO:HD2	10:EB:147:GLU:OE1	2.19	0.42
15:BE:290:ALA:HB3	15:BE:391:ARG:HH22	1.85	0.42
18:AF:153:VAL:HA	18:AF:156:GLN:HE21	1.85	0.42
18:AF:443:THR:HG22	45:AP:278:GLU:HA	2.02	0.42
88:EK:200:PM8:O35	88:EK:200:PM8:H311	2.20	0.42
34:BL:183:TRP:CD1	34:BL:253:THR:HG21	2.55	0.42
34:BL:226:HIS:O	34:BL:230:ARG:HG3	2.19	0.42
46:BQ:52:ASP:OD1	46:BQ:52:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:AU:86:ARG:O	78:Ao:68:HIS:NE2	2.49	0.42
60:AW:10:MET:HB3	60:AW:12:HIS:HD2	1.85	0.42
63:BX:129:ASN:O	76:Bi:66:PRO:HA	2.20	0.42
1:A1:131:GLU:OE1	24:AI:141:ARG:NE	2.51	0.42
6:AA:523:A:O3'	70:Ae:105:LYS:HD2	2.20	0.42
7:BA:799:ASP:OD1	7:BA:801:ARG:HG2	2.19	0.42
9:BB:360:ASP:O	9:BB:364:VAL:HG23	2.19	0.42
12:BD:182:ARG:NE	12:BD:257:ASP:HB3	2.35	0.42
12:BD:308:LEU:HD12	12:BD:308:LEU:HA	1.94	0.42
12:BD:450:MET:O	12:BD:454:THR:HG22	2.20	0.42
14:AE:44:CYS:O	79:Ap:50:MET:HG3	2.20	0.42
14:AE:239:LYS:HD3	14:AE:351:TRP:HZ3	1.84	0.42
15:BE:178:GLY:O	15:BE:184:ARG:NH2	2.39	0.42
16:EE:252:GLY:HA3	16:EE:283:ALA:HB3	2.02	0.42
18:AF:98:THR:HG21	18:AF:102:ILE:HD11	2.02	0.42
18:AF:126:TYR:CD2	53:BT:124:LEU:HD21	2.55	0.42
23:EH:3:SER:O	23:EH:7:ILE:HG12	2.20	0.42
24:AI:87:PRO:HD3	81:Av:103:ARG:O	2.19	0.42
26:EI:326:LEU:HD22	26:EI:349:VAL:HG22	2.00	0.42
41:EN:376:ALA:O	41:EN:380:THR:HG22	2.19	0.42
52:AT:50:LYS:O	52:AT:54:LEU:HG	2.20	0.42
58:AV:89:TYR:HE2	73:Ag:102:LEU:HB3	1.85	0.42
68:Bb:20:GLY:HA3	68:Bb:23:TYR:HE2	1.84	0.42
80:At:22:LEU:HB3	80:At:26:ALA:HB3	2.01	0.42
1:A1:74:ASP:O	1:A1:150:SER:OG	2.27	0.41
6:AA:130:U:N3	6:AA:134:U:OP2	2.41	0.41
6:AA:269:U:H2'	6:AA:270:A:O4'	2.20	0.41
6:AA:1092:U:H3	10:EB:692:LYS:NZ	2.18	0.41
9:BB:347:LYS:HG2	9:BB:405:TRP:CH2	2.54	0.41
10:EB:220:LEU:HD21	10:EB:242:LEU:HD11	2.02	0.41
12:BD:126:LEU:HD12	12:BD:127:PRO:HA	2.01	0.41
13:ED:254:LEU:HB3	13:ED:601:VAL:HG21	2.02	0.41
16:EE:208:SER:OG	16:EE:282:ARG:NH2	2.52	0.41
20:EF:196:MET:HG3	20:EF:342:ILE:HG22	2.02	0.41
30:AK:82:PHE:HZ	30:AK:102:VAL:HG11	1.85	0.41
51:ES:34:THR:OG1	51:ES:35:GLU:OE1	2.39	0.41
55:AU:90:MET:HE2	58:AV:129:PRO:HB2	2.02	0.41
59:BV:34:LEU:HD12	59:BV:35:PRO:HD2	2.00	0.41
65:AY:273:PHE:HD2	65:AY:274:HIS:CD2	2.38	0.41
1:A1:137:ASP:OD1	1:A1:137:ASP:N	2.52	0.41
6:AA:9:A:OP2	65:AY:6:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:43:U:H2'	6:AA:44:A:N7	2.35	0.41
6:AA:161:G:C2	45:AP:174:PRO:HG3	2.56	0.41
6:AA:291:A:OP1	10:EB:667:HIS:ND1	2.35	0.41
6:AA:543:U:H2'	6:AA:544:G:C8	2.55	0.41
6:AA:573:U:OP1	48:AR:89:ARG:NH2	2.53	0.41
7:BA:603:LEU:N	7:BA:604:PRO:HD2	2.35	0.41
7:BA:739:ARG:NH2	7:BA:744:ASN:OD1	2.53	0.41
7:BA:785:ARG:HG2	60:AW:251:SER:HB2	2.02	0.41
8:EA:79:ALA:HB2	8:EA:145:GLY:HA3	2.01	0.41
8:EA:225:ASP:HB3	8:EA:254:ARG:HD2	2.02	0.41
11:EC:105:LYS:HE3	11:EC:107:THR:HG22	2.01	0.41
12:BD:394:PHE:CD1	22:BH:140:ARG:HD3	2.55	0.41
12:BD:459:ALA:O	12:BD:463:LEU:HG	2.19	0.41
12:BD:482:ASP:OD1	12:BD:482:ASP:N	2.52	0.41
16:EE:138:PHE:CZ	16:EE:217:ASP:HB2	2.55	0.41
24:AI:12:TRP:HB2	67:Ba:84:TYR:CE2	2.55	0.41
24:AI:250:UNK:HA	41:EN:344:GLU:HB2	2.02	0.41
30:AK:55:PHE:HB2	30:AK:57:ILE:HD11	2.03	0.41
34:BL:33:GLY:HA2	34:BL:91:CYS:SG	2.60	0.41
41:EN:554:ASP:N	41:EN:554:ASP:OD1	2.50	0.41
42:AO:169:ALA:HB1	42:AO:173:VAL:HG21	2.02	0.41
44:EP:96:ASP:HB3	44:EP:98:GLN:HG2	2.01	0.41
46:BQ:50:PHE:HE1	46:BQ:163:GLN:HE21	1.68	0.41
50:BS:150:VAL:O	50:BS:154:ARG:HG3	2.20	0.41
55:AU:108:ARG:HG2	71:Af:87:PHE:CZ	2.55	0.41
58:AV:96:VAL:HG22	58:AV:174:ARG:HB2	2.02	0.41
62:AX:121:PRO:HG2	65:AY:259:MET:HG2	2.02	0.41
66:BZ:75:HIS:CD2	66:BZ:76:ARG:HB2	2.55	0.41
1:A1:211:LEU:HA	1:A1:214:ASP:OD2	2.20	0.41
2:A2:36:VAL:O	2:A2:40:ARG:HG3	2.20	0.41
6:AA:15:G:O6	6:AA:100:U:O2'	2.33	0.41
6:AA:358:A:H2'	49:BR:196:ARG:HG2	2.02	0.41
6:AA:1124:A:H2'	6:AA:1125:A:H8	1.84	0.41
6:AA:1135:G:N2	6:AA:1138:A:OP2	2.46	0.41
7:BA:759:GLN:HB2	7:BA:797:LYS:HG3	2.01	0.41
16:EE:379:ASP:OD1	16:EE:379:ASP:N	2.47	0.41
19:BF:251:ARG:NH2	19:BF:353:GLU:OE1	2.36	0.41
21:EG:116:CYS:HB3	21:EG:119:CYS:SG	2.60	0.41
25:BI:300:ARG:NH2	79:Ap:79:GLN:OE1	2.51	0.41
28:BJ:253:VAL:HG21	65:AY:280:LYS:HE3	2.01	0.41
41:EN:200:ASP:HA	41:EN:203:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:BS:66:ILE:HD12	56:BU:184:TRP:HH2	1.84	0.41
65:AY:118:GLU:HB2	65:AY:185:ILE:HD11	2.01	0.41
67:Ba:89:PRO:HA	67:Ba:90:PRO:HD3	1.95	0.41
71:Af:134:ARG:HA	71:Af:134:ARG:HD2	1.94	0.41
76:Bi:23:GLU:HG3	76:Bi:25:ARG:H	1.86	0.41
76:Bi:41:ASN:ND2	76:Bi:51:GLU:HG3	2.35	0.41
1:A1:158:ARG:HD3	1:A1:158:ARG:HA	1.92	0.41
2:A2:323:GLU:OE1	2:A2:325:TYR:OH	2.23	0.41
6:AA:97:A:OP1	60:AW:33:ARG:NH1	2.37	0.41
6:AA:957:A:N3	10:EB:519:PRO:HA	2.35	0.41
6:AA:1147:U:P	14:AE:391:ARG:HH22	2.43	0.41
7:BA:612:VAL:HG11	7:BA:643:VAL:HG11	2.02	0.41
7:BA:757:THR:HA	7:BA:760:TYR:HD2	1.85	0.41
8:EA:124:PHE:CD1	8:EA:166:ASP:HB2	2.55	0.41
9:BB:142:THR:HG23	56:BU:107:HIS:CE1	2.56	0.41
10:EB:334:LEU:HD21	10:EB:571:ALA:HB1	2.02	0.41
10:EB:542:ASP:OD1	10:EB:570:ARG:NH2	2.45	0.41
11:EC:169:VAL:HG21	11:EC:378:VAL:HG21	2.02	0.41
11:EC:261:MET:HE2	11:EC:276:ALA:HB1	2.03	0.41
14:AE:392:ASP:OD2	52:AT:64:TYR:OH	2.27	0.41
19:BF:121:VAL:HG21	19:BF:159:ALA:HB2	2.01	0.41
22:BH:159:ILE:O	22:BH:163:ASN:ND2	2.37	0.41
23:EH:35:GLU:HG2	23:EH:106:ARG:NH1	2.35	0.41
23:EH:543:ARG:HG2	23:EH:606:LEU:HD11	2.02	0.41
28:BJ:135:THR:HG23	28:BJ:168:ILE:HG13	2.02	0.41
31:BK:110:ALA:O	31:BK:114:HIS:HB2	2.21	0.41
35:EL:357:ASP:OD1	72:Bf:30:ARG:NH2	2.54	0.41
41:EN:689:TRP:HA	41:EN:692:VAL:HG12	2.01	0.41
43:BO:130:ARG:HD2	52:AT:22:SER:OG	2.20	0.41
44:EO:4:VAL:HG22	44:EO:59:ILE:HD12	2.02	0.41
46:BQ:62:ARG:HH12	46:BQ:68:GLU:CD	2.28	0.41
48:AR:130:ASP:CG	56:BU:159:ARG:HH21	2.28	0.41
49:BR:113:ARG:CB	49:BR:122:ILE:HD11	2.50	0.41
56:BU:123:ASN:O	56:BU:127:ILE:HG13	2.20	0.41
62:AX:88:TYR:CZ	62:AX:90:GLY:HA3	2.55	0.41
68:Bb:14:ASN:HA	68:Bb:21:PRO:HD3	2.02	0.41
76:Bi:178:ARG:HA	76:Bi:181:VAL:HG12	2.03	0.41
77:Al:159:MET:HA	77:Al:160:PRO:HD3	1.88	0.41
2:A2:138:THR:HG23	2:A2:358:ARG:HH12	1.85	0.41
2:A2:283:LEU:O	2:A2:286:THR:OG1	2.33	0.41
6:AA:144:U:OP1	60:AW:41:TYR:OH	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:156:U:O4	18:AF:224:ARG:NH2	2.37	0.41
7:BA:59:GLY:HA2	14:AE:110:LYS:HE2	2.03	0.41
9:BB:127:VAL:HG12	9:BB:393:LEU:HB3	2.01	0.41
9:BB:356:ASN:HD22	9:BB:367:PHE:HD1	1.68	0.41
12:BD:335:PRO:HG3	12:BD:407:VAL:HG21	2.02	0.41
14:AE:403:ALA:O	26:EI:193:ARG:NH2	2.48	0.41
15:BE:50:TYR:OH	65:AY:69:ASP:HB2	2.20	0.41
18:AF:46:GLN:HB2	18:AF:50:HIS:HB2	2.02	0.41
18:AF:378:GLN:NE2	61:BW:128:THR:OG1	2.54	0.41
19:BF:137:MET:HE3	80:At:125:TYR:HE1	1.86	0.41
23:EH:476:MET:HE2	80:At:12:ARG:HH21	1.85	0.41
25:BI:160:PHE:HB2	25:BI:192:THR:HG21	2.02	0.41
28:BJ:74:TRP:CZ2	47:EQ:53:PHE:HB3	2.55	0.41
28:BJ:296:THR:HA	28:BJ:299:ARG:HD2	2.02	0.41
28:BJ:312:GLN:O	28:BJ:315:GLU:HG3	2.20	0.41
30:AK:237:PRO:O	30:AK:241:ARG:HG2	2.20	0.41
41:EN:417:LYS:HB3	41:EN:418:PRO:C	2.45	0.41
41:EN:664:LEU:O	41:EN:668:LEU:HG	2.20	0.41
44:EO:50:LEU:H	44:EO:137:ASP:CG	2.27	0.41
45:AP:70:LEU:HD23	61:BW:188:TYR:OH	2.20	0.41
45:AP:243:ARG:O	45:AP:247:GLU:HG2	2.20	0.41
44:EP:4:VAL:HG22	44:EP:59:ILE:HG23	2.02	0.41
46:BQ:31:VAL:HG23	46:BQ:47:VAL:HB	2.02	0.41
47:EQ:39:SER:HB3	47:EQ:42:ASP:HB2	2.02	0.41
47:EQ:167:LYS:HG3	47:EQ:259:CYS:HA	2.02	0.41
6:AA:528:A:OP1	65:AY:78:ASN:ND2	2.40	0.41
6:AA:539:A:H61	62:AX:187:ARG:HD3	1.85	0.41
7:BA:150:ARG:NH1	7:BA:150:ARG:HA	2.36	0.41
7:BA:206:ILE:O	7:BA:209:PRO:HD2	2.21	0.41
8:EA:138:ASN:ND2	8:EA:166:ASP:OD2	2.52	0.41
8:EA:429:LYS:HG2	85:EA:2001:GTP:C5	2.55	0.41
9:BB:76:GLU:CD	9:BB:79:ARG:HH21	2.28	0.41
9:BB:176:LEU:HD23	9:BB:179:LEU:HD12	2.01	0.41
9:BB:280:ALA:O	9:BB:283:LEU:HG	2.21	0.41
10:EB:50:GLN:HG2	10:EB:686:MET:HE1	2.03	0.41
10:EB:177:PRO:HG3	10:EB:232:MET:SD	2.60	0.41
12:BD:190:ILE:HD12	12:BD:435:TRP:HB3	2.02	0.41
12:BD:509:ARG:O	12:BD:513:ASN:ND2	2.54	0.41
13:ED:205:ARG:HB2	13:ED:212:LEU:HB3	2.02	0.41
16:EE:223:PRO:HA	16:EE:224:PRO:HD3	1.95	0.41
16:EE:468:ASN:ND2	44:EP:313:THR:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AK:168:PRO:O	30:AK:176:ARG:NH2	2.46	0.41
45:AP:10:ARG:NH1	45:AP:12:ARG:O	2.53	0.41
45:AP:119:LYS:HE3	45:AP:119:LYS:HB2	1.80	0.41
46:BQ:28:ASN:HB3	46:BQ:49:LEU:O	2.21	0.41
49:BR:81:ILE:HG21	49:BR:87:PHE:CZ	2.55	0.41
57:EU:29:TYR:CE1	76:Bi:22:LYS:HD2	2.56	0.41
63:BX:66:ASP:HB2	75:Bh:44:MET:HE1	2.02	0.41
73:Ag:24:ASN:OD1	73:Ag:25:THR:N	2.52	0.41
73:Ag:152:MET:O	73:Ag:156:GLU:HG2	2.21	0.41
76:Bi:185:GLU:HA	76:Bi:188:VAL:HG12	2.02	0.41
78:Ao:136:THR:O	78:Ao:140:ARG:HG3	2.21	0.41
1:A1:108:ILE:HG12	1:A1:119:GLN:HB3	2.02	0.41
2:A2:282:TYR:O	2:A2:286:THR:HG23	2.21	0.41
2:A2:441:THR:HG22	31:BK:345:HIS:HD2	1.85	0.41
3:A3:154:ALA:HB2	6:AA:333:U:OP2	2.20	0.41
6:AA:189:A:H61	6:AA:285:A:N6	2.18	0.41
6:AA:491:A:O2'	60:AW:45:ARG:NH1	2.54	0.41
7:BA:327:ARG:NH1	69:Bc:37:ARG:HE	2.18	0.41
7:BA:365:ASP:OD1	7:BA:366:VAL:N	2.53	0.41
9:BB:236:PRO:O	9:BB:238:ASN:ND2	2.53	0.41
10:EB:491:THR:HG22	10:EB:558:PHE:HB3	2.02	0.41
13:ED:197:LYS:HE3	13:ED:219:TYR:CE2	2.56	0.41
13:ED:205:ARG:N	13:ED:212:LEU:O	2.32	0.41
14:AE:106:ARG:O	14:AE:110:LYS:HG2	2.19	0.41
16:EE:457:GLN:HE21	30:AK:89:ARG:HD3	1.85	0.41
16:EE:519:ILE:HA	16:EE:522:MET:HG2	2.01	0.41
18:AF:230:LYS:HA	18:AF:230:LYS:HD3	1.84	0.41
19:BF:237:LEU:HD13	19:BF:290:LEU:HD11	2.03	0.41
23:EH:5:PHE:CE1	23:EH:385:GLU:HB3	2.55	0.41
23:EH:9:ARG:HH21	30:AK:298:VAL:HG21	1.84	0.41
23:EH:193:SER:HB2	23:EH:249:ARG:CZ	2.50	0.41
23:EH:270:TYR:CZ	23:EH:301:ARG:HD3	2.55	0.41
23:EH:609:PRO:HA	23:EH:610:PRO:HD3	1.96	0.41
25:BI:50:ARG:HD3	25:BI:50:ARG:HA	1.83	0.41
40:BN:78:LEU:HD23	40:BN:100:LEU:HD11	2.03	0.41
53:BT:144:GLU:OE2	61:BW:167:ARG:NH2	2.30	0.41
67:Ba:105:ARG:HG2	67:Ba:106:VAL:N	2.36	0.41
75:Bh:80:SER:O	75:Bh:84:ASP:N	2.54	0.41
78:Ao:143:ASP:OD2	80:At:45:ARG:NH1	2.45	0.41
79:Ap:211:ARG:NH2	79:Ap:281:ALA:O	2.54	0.41
2:A2:298:LEU:HD11	53:BT:103:MET:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:1:A:H2'	6:AA:2:U:C6	2.56	0.41
6:AA:321:A:H2'	6:AA:322:U:C6	2.56	0.41
8:EA:571:SER:HB2	8:EA:575:TYR:CE2	2.56	0.41
9:BB:278:GLN:HA	9:BB:281:VAL:HG12	2.02	0.41
9:BB:415:ASP:O	9:BB:418:ARG:HG2	2.21	0.41
10:EB:743:GLY:HA2	70:Ae:52:GLU:OE1	2.21	0.41
13:ED:388:TRP:CG	13:ED:454:VAL:HG12	2.56	0.41
13:ED:588:LEU:HB3	13:ED:592:SER:OG	2.21	0.41
14:AE:252:ASP:OD1	14:AE:300:GLN:NE2	2.53	0.41
15:BE:11:TYR:HD2	18:AF:182:MET:HB3	1.85	0.41
15:BE:174:TYR:HD1	15:BE:177:LYS:HE2	1.84	0.41
16:EE:255:LEU:HD22	16:EE:295:ILE:HD13	2.02	0.41
26:EI:117:GLN:OE1	26:EI:126:ILE:N	2.48	0.41
26:EI:335:ASP:OD1	26:EI:335:ASP:N	2.53	0.41
29:EJ:65:GLY:HA2	29:EJ:112:LEU:HD11	2.03	0.41
29:EJ:83:HIS:O	29:EJ:87:VAL:HG22	2.21	0.41
30:AK:218:ARG:HH21	59:BV:109:GLU:HG3	1.85	0.41
31:BK:124:ALA:HA	48:AR:264:ALA:HB2	2.02	0.41
41:EN:211:MET:HG3	41:EN:212:SER:H	1.86	0.41
42:AO:70:VAL:HG11	42:AO:167:TYR:HB2	2.03	0.41
44:EO:254:LEU:HD12	44:EO:255:PRO:HD2	2.01	0.41
62:AX:184:ASN:OD1	62:AX:184:ASN:N	2.52	0.41
74:Bg:41:TYR:HB2	74:Bg:90:LEU:HD11	2.03	0.41
1:A1:24:HIS:HB2	45:AP:159:ALA:HB3	2.02	0.41
1:A1:117:TRP:HZ3	1:A1:119:GLN:HG2	1.85	0.41
3:A3:155:VAL:HG21	3:A3:161:ARG:HB2	2.03	0.41
6:AA:14:A:O4'	6:AA:15:G:N2	2.53	0.41
6:AA:16:A:OP1	65:AY:33:LYS:NZ	2.52	0.41
6:AA:196:G:H4'	22:BH:332:SER:HB2	2.03	0.41
6:AA:521:G:N1	74:Bg:95:PHE:HB3	2.36	0.41
6:AA:551:A:N1	60:AW:220:TYR:HB3	2.36	0.41
7:BA:679:VAL:O	7:BA:683:LEU:HG	2.21	0.41
7:BA:761:TYR:H	7:BA:798:HIS:HE1	1.69	0.41
8:EA:307:PHE:CG	8:EA:358:LYS:HE3	2.56	0.41
10:EB:106:LEU:HD23	10:EB:159:GLN:HE22	1.86	0.41
10:EB:143:ALA:O	10:EB:301:ALA:HA	2.21	0.41
10:EB:182:LEU:HD12	10:EB:258:VAL:HG22	2.02	0.41
10:EB:218:HIS:NE2	10:EB:222:ARG:HD2	2.36	0.41
10:EB:286:PHE:CZ	10:EB:288:HIS:HB2	2.56	0.41
10:EB:340:PRO:HB3	10:EB:587:TYR:CZ	2.56	0.41
11:EC:99:ARG:NH1	11:EC:114:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:BD:129:LEU:HD13	12:BD:132:GLU:OE1	2.21	0.41
12:BD:178:ILE:O	12:BD:182:ARG:HG2	2.21	0.41
13:ED:6:ARG:NH1	46:BQ:201:LYS:HZ2	2.18	0.41
13:ED:139:ARG:NH2	41:EN:179:THR:OG1	2.53	0.41
16:EE:364:ARG:HG2	16:EE:409:GLN:HG2	2.03	0.41
18:AF:20:ILE:HG22	45:AP:73:ARG:HD3	2.02	0.41
18:AF:35:ILE:O	73:Ag:11:LYS:NZ	2.52	0.41
18:AF:261:TRP:HB3	18:AF:270:VAL:HG21	2.03	0.41
20:EF:93:VAL:HG12	20:EF:99:ILE:HG21	2.02	0.41
23:EH:337:GLU:HG3	23:EH:340:CYS:SG	2.60	0.41
23:EH:591:GLU:HG3	23:EH:625:ILE:HD13	2.03	0.41
26:EI:189:TRP:NE1	52:AT:70:ARG:HB3	2.36	0.41
29:EJ:89:ALA:HB1	29:EJ:97:ARG:HG2	2.01	0.41
34:BL:181:LEU:HD13	34:BL:295:VAL:HG22	2.02	0.41
35:EL:232:GLN:HE22	35:EL:522:GLN:CD	2.28	0.41
37:EM:89:ASN:ND2	37:EM:235:THR:OG1	2.51	0.41
40:BN:58:ILE:HB	40:BN:59:PRO:HD3	2.03	0.41
44:EO:47:THR:HG23	44:EO:49:SER:H	1.86	0.41
45:AP:32:PHE:HB2	45:AP:35:ILE:HB	2.02	0.41
44:EP:101:LEU:HD21	44:EP:122:TYR:CE2	2.56	0.41
44:EP:203:LEU:HD11	44:EP:263:LEU:HD22	2.03	0.41
47:EQ:62:ASN:ND2	47:EQ:116:GLN:HG2	2.35	0.41
49:BR:135:LEU:O	49:BR:139:TYR:HB2	2.20	0.41
88:ER:200:PM8:H431	51:ES:45:PHE:CE2	2.56	0.41
54:ET:76:GLY:HA3	54:ET:84:PHE:CE2	2.55	0.41
55:AU:182:ARG:NH2	78:Ao:21:GLU:HG3	2.36	0.41
58:AV:204:HIS:CE1	58:AV:233:LEU:HD23	2.56	0.41
68:Bb:70:ASN:HB3	68:Bb:131:TYR:CZ	2.56	0.41
76:Bi:40:ALA:HB3	76:Bi:48:ASN:HB2	2.02	0.41
79:Ap:178:MET:HG2	79:Ap:236:TRP:CZ3	2.56	0.41
1:A1:156:ILE:HD12	1:A1:156:ILE:HA	1.98	0.41
1:A1:184:MET:SD	65:AY:300:LEU:HD22	2.61	0.41
2:A2:96:ARG:NE	2:A2:100:GLU:OE2	2.53	0.41
2:A2:98:VAL:HG12	62:AX:131:PHE:HE1	1.85	0.41
5:A8:52:ARG:O	18:AF:168:GLU:HG2	2.20	0.41
6:AA:33:G:H2'	67:Ba:33:LYS:HD3	2.03	0.41
6:AA:108:G:O6	39:AN:10:ALA:N	2.54	0.41
6:AA:517:U:H3'	6:AA:567:G:N2	2.36	0.41
6:AA:519:A:H62	6:AA:568:U:H2'	1.85	0.41
6:AA:1168:U:O4	48:AR:142:LYS:NZ	2.36	0.41
7:BA:47:PHE:CG	7:BA:48:PRO:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:EA:320:LYS:NZ	85:EA:2001:GTP:O2B	2.49	0.41
9:BB:22:TYR:OH	24:AI:147:GLU:OE2	2.37	0.41
10:EB:563:ASN:ND2	10:EB:566:THR:H	2.18	0.41
10:EB:607:PRO:HB2	10:EB:609:GLU:HG3	2.03	0.41
16:EE:97:ASP:OD1	16:EE:97:ASP:N	2.46	0.41
19:BF:218:ILE:O	19:BF:221:GLU:HG3	2.21	0.41
24:AI:36:PHE:CD1	24:AI:91:PRO:HD3	2.56	0.41
26:EI:179:MET:HE3	52:AT:116:THR:HB	2.02	0.41
35:EL:290:ILE:HG23	35:EL:294:MET:HB2	2.03	0.41
44:EO:6:CYS:HA	44:EO:57:ILE:HD12	2.03	0.41
45:AP:54:ARG:HG2	78:Ao:96:ILE:O	2.21	0.41
44:EP:29:ARG:HD2	44:EP:29:ARG:HA	1.84	0.41
44:EP:149:GLU:H	44:EP:149:GLU:CD	2.29	0.41
55:AU:183:GLY:HA2	55:AU:184:PRO:HD3	1.95	0.41
58:AV:235:LEU:HD21	71:Af:100:THR:HG21	2.03	0.41
62:AX:101:LYS:HA	67:Ba:35:ILE:HD13	2.03	0.41
67:Ba:149:LYS:O	67:Ba:152:ARG:NE	2.46	0.41
68:Bb:92:LEU:HD13	68:Bb:123:TYR:CE1	2.56	0.41
71:Af:137:SER:O	71:Af:141:GLU:HB3	2.20	0.41
5:A8:66:ARG:HH21	5:A8:138:MET:HG2	1.86	0.40
6:AA:158:A:OP2	45:AP:188:ARG:NH2	2.54	0.40
6:AA:189:A:H5''	6:AA:277:A:N7	2.35	0.40
6:AA:499:U:H4'	18:AF:195:TYR:CD2	2.56	0.40
7:BA:173:ASP:O	7:BA:175:PRO:HD3	2.21	0.40
10:EB:142:ALA:HB3	10:EB:322:ILE:HB	2.03	0.40
13:ED:17:PRO:HD2	77:Al:43:ALA:HB1	2.02	0.40
13:ED:375:MET:HE2	13:ED:375:MET:HB3	1.91	0.40
15:BE:127:SER:HA	15:BE:152:ARG:HH12	1.85	0.40
16:EE:172:PRO:O	16:EE:194:THR:OG1	2.27	0.40
18:AF:109:MET:HG2	18:AF:136:GLY:O	2.21	0.40
25:BI:73:ILE:HA	25:BI:88:ALA:HB2	2.03	0.40
26:EI:226:ASN:O	52:AT:66:PRO:HG2	2.21	0.40
30:AK:217:TYR:HD1	30:AK:220:ILE:HD11	1.86	0.40
31:BK:137:TYR:CZ	31:BK:204:ALA:HB2	2.57	0.40
35:EL:655:LEU:HD13	35:EL:660:TYR:CZ	2.56	0.40
40:BN:206:LEU:HD12	56:BU:149:TRP:CE2	2.56	0.40
41:EN:497:MET:HE2	41:EN:497:MET:HB3	1.99	0.40
61:BW:83:LEU:O	61:BW:86:SER:OG	2.39	0.40
71:Af:86:ASN:HB3	71:Af:102:PRO:HD3	2.03	0.40
76:Bi:124:TYR:CE2	76:Bi:126:GLU:HB2	2.56	0.40
81:Av:111:ILE:HD11	81:Av:125:MET:SD	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:179:MET:HE2	1:A1:179:MET:HB3	1.97	0.40
6:AA:267:U:C2	6:AA:268:A:C8	3.09	0.40
6:AA:351:A:H4'	11:EC:105:LYS:NZ	2.37	0.40
6:AA:797:A:OP1	48:AR:57:LYS:NZ	2.42	0.40
7:BA:588:LEU:HD23	7:BA:589:MET:HE1	2.03	0.40
8:EA:352:TYR:HD2	8:EA:478:LEU:HD11	1.85	0.40
10:EB:213:ARG:HH11	10:EB:219:ARG:HH12	1.69	0.40
10:EB:587:TYR:CG	10:EB:595:VAL:HG21	2.55	0.40
11:EC:69:ARG:HG3	11:EC:112:ARG:NH1	2.36	0.40
12:BD:285:ARG:HG3	12:BD:333:LEU:HD11	2.03	0.40
13:ED:136:LYS:HD2	41:EN:525:ARG:NH1	2.36	0.40
19:BF:165:ALA:O	19:BF:168:ILE:HG12	2.22	0.40
30:AK:52:ASN:HD21	30:AK:105:GLN:HE21	1.67	0.40
35:EL:236:LEU:HD22	35:EL:291:PRO:HG3	2.02	0.40
40:BN:71:GLN:HA	40:BN:72:PRO:HA	1.81	0.40
41:EN:378:LEU:HG	41:EN:382:MET:HE3	2.03	0.40
42:AO:82:SER:OG	42:AO:96:PRO:HD2	2.22	0.40
44:EO:18:HIS:NE2	44:EO:195:PRO:HG3	2.36	0.40
63:BX:173:HIS:HD2	63:BX:177:ARG:HD3	1.86	0.40
71:Af:155:ARG:HA	71:Af:155:ARG:HD3	1.90	0.40
79:Ap:55:HIS:CD2	79:Ap:57:LYS:H	2.40	0.40
3:A3:116:VAL:O	80:At:40:ASN:ND2	2.48	0.40
3:A3:196:LYS:HE3	3:A3:196:LYS:HB3	1.96	0.40
6:AA:842:U:H2'	6:AA:843:A:C8	2.57	0.40
6:AA:981:A:N6	6:AA:1083:A:C8	2.89	0.40
6:AA:1108:A:H4'	52:AT:11:HIS:CD2	2.56	0.40
7:BA:216:GLY:HA3	7:BA:278:LYS:H	1.86	0.40
12:BD:426:THR:HA	12:BD:454:THR:HG23	2.03	0.40
14:AE:148:CYS:HB2	52:AT:85:ILE:HD12	2.03	0.40
14:AE:283:MET:HE3	14:AE:283:MET:HB2	1.90	0.40
15:BE:174:TYR:CE2	15:BE:233:ASP:HB3	2.56	0.40
22:BH:300:HIS:HD2	22:BH:302:ALA:H	1.69	0.40
23:EH:100:LEU:HD13	23:EH:102:TRP:CZ2	2.56	0.40
23:EH:230:PHE:O	23:EH:234:ARG:HG3	2.22	0.40
28:BJ:164:GLU:O	28:BJ:168:ILE:HG12	2.21	0.40
41:EN:682:LEU:O	41:EN:689:TRP:NE1	2.54	0.40
42:AO:67:LEU:HD11	42:AO:80:LEU:HD11	2.04	0.40
44:EO:211:LEU:HD22	44:EO:218:SER:HB3	2.02	0.40
45:AP:71:ASN:ND2	61:BW:187:ASP:HA	2.36	0.40
45:AP:139:ARG:HA	45:AP:139:ARG:HH11	1.86	0.40
57:EU:36:GLU:HA	57:EU:39:LYS:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:BW:80:MET:HA	61:BW:80:MET:HE2	2.03	0.40
61:BW:145:ASN:HD21	61:BW:150:TYR:HB2	1.86	0.40
62:AX:145:ARG:HG3	62:AX:162:GLN:HB2	2.03	0.40
65:AY:144:GLN:HG2	65:AY:145:ASN:HD22	1.86	0.40
70:Ae:187:LYS:N	70:Ae:188:PRO:HD2	2.37	0.40
72:Bf:49:ALA:O	72:Bf:53:THR:HG23	2.21	0.40
2:A2:251:ILE:HD11	53:BT:119:ARG:CZ	2.51	0.40
6:AA:372:A:H2'	6:AA:373:C:C6	2.57	0.40
6:AA:979:U:H5'	6:AA:980:U:H2'	2.04	0.40
6:AA:982:A:H2'	6:AA:983:C:C6	2.56	0.40
6:AA:1121:A:H4'	6:AA:1122:U:OP2	2.22	0.40
7:BA:281:GLU:OE1	7:BA:281:GLU:N	2.54	0.40
7:BA:419:THR:HG22	7:BA:420:ALA:H	1.87	0.40
7:BA:499:SER:O	71:Af:174:SER:HB2	2.21	0.40
9:BB:80:ILE:HA	9:BB:83:ASN:ND2	2.37	0.40
19:BF:408:LEU:HD23	53:BT:39:ARG:HH22	1.85	0.40
25:BI:265:THR:HG21	25:BI:305:LYS:HE3	2.03	0.40
26:EI:302:MET:HE2	26:EI:302:MET:HB3	1.97	0.40
28:BJ:196:THR:HG23	28:BJ:199:ASP:H	1.86	0.40
30:AK:216:ARG:HA	30:AK:219:ARG:HG2	2.04	0.40
34:BL:107:LEU:HD22	34:BL:164:ARG:HD2	2.03	0.40
34:BL:143:THR:O	34:BL:147:ARG:HG3	2.22	0.40
35:EL:457:ALA:HB1	35:EL:562:ILE:HD11	2.04	0.40
35:EL:551:GLU:OE1	35:EL:551:GLU:N	2.38	0.40
37:EM:143:VAL:O	37:EM:147:GLN:HG3	2.21	0.40
37:EM:187:HIS:HE1	47:EQ:594:PRO:HG3	1.87	0.40
42:AO:52:ALA:HB2	42:AO:135:THR:HG21	2.03	0.40
44:EO:119:ILE:HD11	44:EP:102:TYR:HE2	1.86	0.40
44:EP:170:GLN:HG2	44:EP:216:ARG:NH1	2.36	0.40
60:AW:85:VAL:HA	60:AW:89:ARG:O	2.22	0.40
65:AY:305:LEU:O	65:AY:309:ASN:ND2	2.54	0.40
69:Bc:43:ASN:HD21	69:Bc:45:LYS:HE2	1.86	0.40
75:Bh:19:ASN:HD21	76:Bi:30:TYR:HA	1.86	0.40
77:Al:122:LEU:HD23	77:Al:122:LEU:HA	1.96	0.40
6:AA:538:U:H2'	6:AA:539:A:O4'	2.22	0.40
8:EA:214:HIS:HA	51:ES:126:HIS:CE1	2.57	0.40
9:BB:141:ILE:HG23	9:BB:152:ARG:HD2	2.03	0.40
9:BB:418:ARG:HA	9:BB:421:VAL:HG22	2.03	0.40
12:BD:300:LEU:HD22	12:BD:303:ASP:HB3	2.02	0.40
13:ED:320:ASP:O	13:ED:324:VAL:HG23	2.22	0.40
14:AE:279:ARG:HG2	14:AE:280:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:AI:68:ALA:HA	81:Av:113:GLY:O	2.22	0.40
26:EI:75:GLU:OE1	26:EI:75:GLU:N	2.54	0.40
35:EL:309:LEU:HD13	35:EL:309:LEU:HA	1.93	0.40
35:EL:612:LEU:HD23	69:Bc:121:PHE:CE1	2.56	0.40
46:BQ:51:HIS:HB2	46:BQ:58:THR:HG21	2.03	0.40
46:BQ:115:ASP:OD1	46:BQ:115:ASP:N	2.54	0.40
47:EQ:221:ILE:HG23	47:EQ:225:LEU:HD23	2.03	0.40
47:EQ:249:THR:O	47:EQ:253:HIS:ND1	2.55	0.40
48:AR:174:HIS:HA	48:AR:177:GLU:CD	2.46	0.40
88:ER:200:PM8:S1	51:ES:91:GLU:HB3	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	215/241 (89%)	205 (95%)	10 (5%)	0	100	100
2	A2	448/471 (95%)	438 (98%)	10 (2%)	0	100	100
3	A3	147/218 (67%)	143 (97%)	4 (3%)	0	100	100
4	A5	53/80 (66%)	53 (100%)	0	0	100	100
5	A8	140/181 (77%)	134 (96%)	6 (4%)	0	100	100
7	BA	763/831 (92%)	738 (97%)	25 (3%)	0	100	100
8	EA	530/576 (92%)	514 (97%)	16 (3%)	0	100	100
9	BB	408/541 (75%)	394 (97%)	14 (3%)	0	100	100
10	EB	659/754 (87%)	646 (98%)	13 (2%)	0	100	100
11	EC	371/406 (91%)	360 (97%)	11 (3%)	0	100	100
12	BD	417/547 (76%)	401 (96%)	16 (4%)	0	100	100
13	ED	593/616 (96%)	574 (97%)	19 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	AE	432/473 (91%)	414 (96%)	17 (4%)	1 (0%)	43	73
15	BE	403/449 (90%)	381 (94%)	21 (5%)	1 (0%)	43	73
16	EE	429/586 (73%)	415 (97%)	14 (3%)	0	100	100
18	AF	440/459 (96%)	425 (97%)	15 (3%)	0	100	100
19	BF	342/426 (80%)	335 (98%)	7 (2%)	0	100	100
20	EF	292/373 (78%)	278 (95%)	14 (5%)	0	100	100
21	EG	152/156 (97%)	150 (99%)	2 (1%)	0	100	100
22	BH	280/349 (80%)	272 (97%)	8 (3%)	0	100	100
23	EH	424/634 (67%)	423 (100%)	1 (0%)	0	100	100
24	AI	228/263 (87%)	226 (99%)	2 (1%)	0	100	100
25	BI	321/342 (94%)	310 (97%)	11 (3%)	0	100	100
26	EI	273/349 (78%)	270 (99%)	3 (1%)	0	100	100
28	BJ	289/333 (87%)	278 (96%)	11 (4%)	0	100	100
29	EJ	93/116 (80%)	89 (96%)	3 (3%)	1 (1%)	11	39
30	AK	299/342 (87%)	289 (97%)	10 (3%)	0	100	100
31	BK	222/386 (58%)	218 (98%)	4 (2%)	0	100	100
32	EK	82/148 (55%)	82 (100%)	0	0	100	100
32	ER	82/148 (55%)	81 (99%)	1 (1%)	0	100	100
34	BL	255/312 (82%)	247 (97%)	8 (3%)	0	100	100
35	EL	553/691 (80%)	541 (98%)	12 (2%)	0	100	100
37	EM	326/451 (72%)	319 (98%)	7 (2%)	0	100	100
39	AN	191/202 (95%)	184 (96%)	7 (4%)	0	100	100
40	BN	212/302 (70%)	210 (99%)	2 (1%)	0	100	100
41	EN	632/731 (86%)	614 (97%)	18 (3%)	0	100	100
42	AO	161/217 (74%)	156 (97%)	5 (3%)	0	100	100
43	BO	211/262 (80%)	209 (99%)	2 (1%)	0	100	100
44	EO	267/319 (84%)	257 (96%)	10 (4%)	0	100	100
44	EP	235/319 (74%)	227 (97%)	8 (3%)	0	100	100
45	AP	321/374 (86%)	309 (96%)	12 (4%)	0	100	100
46	BQ	216/231 (94%)	204 (94%)	12 (6%)	0	100	100
47	EQ	465/655 (71%)	460 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	AR	255/301 (85%)	250 (98%)	5 (2%)	0	100	100
49	BR	194/205 (95%)	185 (95%)	9 (5%)	0	100	100
50	BS	149/198 (75%)	146 (98%)	3 (2%)	0	100	100
51	ES	148/524 (28%)	145 (98%)	3 (2%)	0	100	100
52	AT	139/144 (96%)	134 (96%)	5 (4%)	0	100	100
53	BT	171/191 (90%)	165 (96%)	6 (4%)	0	100	100
54	ET	99/102 (97%)	95 (96%)	4 (4%)	0	100	100
55	AU	171/213 (80%)	165 (96%)	6 (4%)	0	100	100
56	BU	81/185 (44%)	81 (100%)	0	0	100	100
57	EU	45/56 (80%)	45 (100%)	0	0	100	100
58	AV	179/188 (95%)	174 (97%)	5 (3%)	0	100	100
59	BV	88/190 (46%)	86 (98%)	2 (2%)	0	100	100
60	AW	276/278 (99%)	273 (99%)	3 (1%)	0	100	100
61	BW	185/188 (98%)	183 (99%)	2 (1%)	0	100	100
62	AX	164/246 (67%)	162 (99%)	2 (1%)	0	100	100
63	BX	131/190 (69%)	122 (93%)	9 (7%)	0	100	100
65	AY	338/378 (89%)	334 (99%)	4 (1%)	0	100	100
66	BZ	188/190 (99%)	178 (95%)	10 (5%)	0	100	100
67	Ba	140/153 (92%)	134 (96%)	6 (4%)	0	100	100
68	Bb	124/162 (76%)	120 (97%)	4 (3%)	0	100	100
69	Bc	135/146 (92%)	131 (97%)	4 (3%)	0	100	100
70	Ae	123/197 (62%)	119 (97%)	4 (3%)	0	100	100
71	Af	137/189 (72%)	136 (99%)	1 (1%)	0	100	100
72	Bf	85/113 (75%)	79 (93%)	6 (7%)	0	100	100
73	Ag	184/260 (71%)	178 (97%)	6 (3%)	0	100	100
74	Bg	81/105 (77%)	77 (95%)	4 (5%)	0	100	100
75	Bh	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
76	Bi	190/245 (78%)	183 (96%)	7 (4%)	0	100	100
77	Al	179/218 (82%)	175 (98%)	4 (2%)	0	100	100
78	Ao	180/1520 (12%)	179 (99%)	1 (1%)	0	100	100
79	Ap	295/309 (96%)	290 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	At	134/154 (87%)	129 (96%)	5 (4%)	0	100	100
81	Av	194/242 (80%)	190 (98%)	4 (2%)	0	100	100
All	All	19143/24932 (77%)	18599 (97%)	541 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	BE	348	VAL
29	EJ	46	PRO
14	AE	412	LYS

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	A1	195/217 (90%)	191 (98%)	4 (2%)	47	71
2	A2	397/413 (96%)	393 (99%)	4 (1%)	68	79
3	A3	134/193 (69%)	132 (98%)	2 (2%)	57	75
4	A5	52/73 (71%)	49 (94%)	3 (6%)	18	48
5	A8	126/161 (78%)	123 (98%)	3 (2%)	43	69
7	BA	662/727 (91%)	650 (98%)	12 (2%)	51	73
8	EA	463/502 (92%)	459 (99%)	4 (1%)	70	80
9	BB	356/470 (76%)	344 (97%)	12 (3%)	32	63
10	EB	573/649 (88%)	568 (99%)	5 (1%)	70	80
11	EC	327/354 (92%)	326 (100%)	1 (0%)	86	87
12	BD	356/472 (75%)	348 (98%)	8 (2%)	45	71
13	ED	529/544 (97%)	522 (99%)	7 (1%)	61	77
14	AE	349/406 (86%)	347 (99%)	2 (1%)	78	83
15	BE	348/386 (90%)	340 (98%)	8 (2%)	44	70
16	EE	367/514 (71%)	363 (99%)	4 (1%)	65	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AF	394/409 (96%)	393 (100%)	1 (0%)	86	87
19	BF	300/368 (82%)	297 (99%)	3 (1%)	68	79
20	EF	249/302 (82%)	249 (100%)	0	100	100
21	EG	134/136 (98%)	133 (99%)	1 (1%)	76	82
22	BH	238/297 (80%)	235 (99%)	3 (1%)	61	77
23	EH	385/527 (73%)	383 (100%)	2 (0%)	81	85
24	AI	205/225 (91%)	201 (98%)	4 (2%)	48	72
25	BI	271/288 (94%)	265 (98%)	6 (2%)	45	71
26	EI	217/310 (70%)	216 (100%)	1 (0%)	81	85
28	BJ	255/298 (86%)	252 (99%)	3 (1%)	63	78
29	EJ	77/95 (81%)	76 (99%)	1 (1%)	61	77
30	AK	269/301 (89%)	269 (100%)	0	100	100
31	BK	200/329 (61%)	197 (98%)	3 (2%)	57	75
32	EK	78/127 (61%)	78 (100%)	0	100	100
32	ER	78/127 (61%)	77 (99%)	1 (1%)	61	77
34	BL	203/262 (78%)	198 (98%)	5 (2%)	42	69
35	EL	485/598 (81%)	477 (98%)	8 (2%)	55	75
37	EM	284/386 (74%)	280 (99%)	4 (1%)	59	76
39	AN	173/182 (95%)	170 (98%)	3 (2%)	53	74
40	BN	167/265 (63%)	162 (97%)	5 (3%)	36	65
41	EN	564/640 (88%)	562 (100%)	2 (0%)	84	86
42	AO	143/185 (77%)	142 (99%)	1 (1%)	76	82
43	BO	181/225 (80%)	180 (99%)	1 (1%)	78	83
44	EO	233/263 (89%)	226 (97%)	7 (3%)	36	65
44	EP	211/263 (80%)	208 (99%)	3 (1%)	59	76
45	AP	287/330 (87%)	283 (99%)	4 (1%)	59	76
46	BQ	172/195 (88%)	169 (98%)	3 (2%)	53	74
47	EQ	382/539 (71%)	377 (99%)	5 (1%)	61	77
48	AR	222/256 (87%)	220 (99%)	2 (1%)	70	80
49	BR	172/181 (95%)	169 (98%)	3 (2%)	53	74
50	BS	127/164 (77%)	124 (98%)	3 (2%)	43	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	ES	134/437 (31%)	134 (100%)	0	100	100
52	AT	121/124 (98%)	118 (98%)	3 (2%)	42	69
53	BT	151/163 (93%)	150 (99%)	1 (1%)	76	82
54	ET	87/88 (99%)	87 (100%)	0	100	100
55	AU	151/184 (82%)	150 (99%)	1 (1%)	76	82
56	BU	72/168 (43%)	71 (99%)	1 (1%)	59	76
57	EU	43/51 (84%)	43 (100%)	0	100	100
58	AV	153/158 (97%)	150 (98%)	3 (2%)	48	72
59	BV	79/163 (48%)	78 (99%)	1 (1%)	61	77
60	AW	246/246 (100%)	245 (100%)	1 (0%)	84	86
61	BW	163/164 (99%)	156 (96%)	7 (4%)	26	57
62	AX	154/221 (70%)	154 (100%)	0	100	100
63	BX	117/170 (69%)	114 (97%)	3 (3%)	40	68
65	AY	305/337 (90%)	303 (99%)	2 (1%)	76	82
66	BZ	152/160 (95%)	148 (97%)	4 (3%)	40	68
67	Ba	134/144 (93%)	133 (99%)	1 (1%)	76	82
68	Bb	109/135 (81%)	108 (99%)	1 (1%)	70	80
69	Bc	127/134 (95%)	126 (99%)	1 (1%)	73	81
70	Ae	110/172 (64%)	108 (98%)	2 (2%)	51	73
71	Af	120/162 (74%)	117 (98%)	3 (2%)	42	69
72	Bf	77/98 (79%)	76 (99%)	1 (1%)	61	77
73	Ag	170/239 (71%)	170 (100%)	0	100	100
74	Bg	66/87 (76%)	65 (98%)	1 (2%)	57	75
75	Bh	79/80 (99%)	77 (98%)	2 (2%)	42	69
76	Bi	147/217 (68%)	143 (97%)	4 (3%)	39	67
77	Al	155/186 (83%)	155 (100%)	0	100	100
78	Ao	151/1258 (12%)	149 (99%)	2 (1%)	61	77
79	Ap	259/267 (97%)	258 (100%)	1 (0%)	84	86
80	At	125/140 (89%)	123 (98%)	2 (2%)	55	75
81	Av	174/210 (83%)	173 (99%)	1 (1%)	78	83
All	All	16721/21517 (78%)	16505 (99%)	216 (1%)	59	77

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	91	GLN
1	A1	92	VAL
1	A1	106	THR
1	A1	114	LEU
2	A2	29	VAL
2	A2	318	ILE
2	A2	350	VAL
2	A2	436	ILE
3	A3	115	ILE
3	A3	118	VAL
4	A5	31	ASN
4	A5	49	LEU
4	A5	78	ILE
5	A8	44	CYS
5	A8	74	PHE
5	A8	114	GLU
7	BA	307	HIS
7	BA	318	LEU
7	BA	334	ILE
7	BA	339	ASP
7	BA	404	CYS
7	BA	419	THR
7	BA	542	ASN
7	BA	593	THR
7	BA	683	LEU
7	BA	699	ASN
7	BA	714	ASN
7	BA	762	ASN
8	EA	198	ASP
8	EA	453	GLU
8	EA	515	ARG
8	EA	516	ILE
9	BB	109	GLU
9	BB	139	ILE
9	BB	156	TRP
9	BB	157	HIS
9	BB	210	THR
9	BB	216	PHE
9	BB	218	HIS
9	BB	286	ASP
9	BB	303	ILE
9	BB	326	GLU

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Mol	Chain	Res	Type
9	BB	413	LEU
9	BB	439	ASP
10	EB	228	LEU
10	EB	292	VAL
10	EB	467	THR
10	EB	562	THR
10	EB	671	THR
11	EC	205	VAL
12	BD	128	THR
12	BD	201	LYS
12	BD	253	LEU
12	BD	286	GLU
12	BD	355	GLU
12	BD	407	VAL
12	BD	476	GLU
12	BD	518	VAL
13	ED	45	LEU
13	ED	266	TYR
13	ED	359	GLU
13	ED	472	LEU
13	ED	513	VAL
13	ED	547	ILE
13	ED	561	VAL
14	AE	67	HIS
14	AE	269	VAL
15	BE	12	GLN
15	BE	29	ASN
15	BE	71	LEU
15	BE	98	LEU
15	BE	144	VAL
15	BE	229	GLU
15	BE	374	VAL
15	BE	394	LEU
16	EE	120	VAL
16	EE	306	VAL
16	EE	413	ASP
16	EE	415	VAL
18	AF	125	ILE
19	BF	202	THR
19	BF	386	VAL
19	BF	419	VAL
21	EG	8	VAL

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Mol	Chain	Res	Type
22	BH	143	LEU
22	BH	333	ARG
22	BH	347	VAL
23	EH	262	THR
23	EH	374	THR
24	AI	38	VAL
24	AI	170	VAL
24	AI	190	GLU
24	AI	211	GLU
25	BI	50	ARG
25	BI	103	THR
25	BI	112	ILE
25	BI	119	GLU
25	BI	215	VAL
25	BI	216	MET
26	EI	79	VAL
28	BJ	126	ILE
28	BJ	139	PHE
28	BJ	180	GLU
29	EJ	87	VAL
31	BK	193	VAL
31	BK	196	ASP
31	BK	285	GLN
34	BL	103	ASN
34	BL	123	LEU
34	BL	290	GLU
34	BL	296	GLU
34	BL	306	LEU
35	EL	62	THR
35	EL	91	VAL
35	EL	114	VAL
35	EL	227	THR
35	EL	339	GLU
35	EL	418	THR
35	EL	531	LEU
35	EL	640	VAL
37	EM	218	VAL
37	EM	227	VAL
37	EM	274	LEU
37	EM	279	VAL
39	AN	92	VAL
39	AN	119	THR

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Mol	Chain	Res	Type
39	AN	181	VAL
40	BN	40	PHE
40	BN	57	THR
40	BN	179	LEU
40	BN	211	ASN
40	BN	221	VAL
41	EN	287	THR
41	EN	425	VAL
42	AO	104	VAL
43	BO	236	VAL
44	EO	3	THR
44	EO	8	VAL
44	EO	23	LEU
44	EO	147	GLU
44	EO	187	GLU
44	EO	228	THR
44	EO	260	ARG
45	AP	66	VAL
45	AP	136	VAL
45	AP	148	THR
45	AP	217	VAL
44	EP	60	VAL
44	EP	102	TYR
44	EP	193	THR
46	BQ	34	ASP
46	BQ	54	VAL
46	BQ	192	THR
47	EQ	176	THR
47	EQ	230	VAL
47	EQ	235	VAL
47	EQ	264	VAL
47	EQ	529	ASP
48	AR	247	ASP
48	AR	266	THR
49	BR	60	THR
49	BR	121	LEU
49	BR	189	VAL
32	ER	121	LEU
50	BS	36	LEU
50	BS	91	GLU
50	BS	127	ILE
52	AT	51	GLU

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Mol	Chain	Res	Type
52	AT	69	VAL
52	AT	97	GLU
53	BT	126	GLU
55	AU	193	GLU
56	BU	138	ARG
58	AV	93	VAL
58	AV	104	VAL
58	AV	200	THR
59	BV	32	VAL
60	AW	133	LEU
61	BW	17	THR
61	BW	20	VAL
61	BW	25	THR
61	BW	53	ILE
61	BW	65	ASN
61	BW	128	THR
61	BW	156	VAL
63	BX	110	TYR
63	BX	158	THR
63	BX	173	HIS
65	AY	86	GLU
65	AY	219	VAL
66	BZ	45	VAL
66	BZ	77	VAL
66	BZ	151	ILE
66	BZ	172	ASP
67	Ba	78	VAL
68	Bb	140	VAL
69	Bc	110	VAL
70	Ae	98	VAL
70	Ae	109	ARG
71	Af	44	PHE
71	Af	77	VAL
71	Af	118	GLU
72	Bf	72	LEU
74	Bg	104	THR
75	Bh	38	LEU
75	Bh	86	VAL
76	Bi	69	LEU
76	Bi	102	VAL
76	Bi	123	VAL
76	Bi	133	LEU

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Mol	Chain	Res	Type
78	Ao	90	ASP
78	Ao	187	THR
79	Ap	194	HIS
80	At	42	GLU
80	At	43	ILE
81	Av	24	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (351) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	62	GLN
1	A1	98	GLN
1	A1	116	HIS
1	A1	138	ASN
1	A1	225	GLN
2	A2	23	ASN
2	A2	67	HIS
2	A2	71	HIS
2	A2	72	GLN
2	A2	135	HIS
2	A2	167	HIS
2	A2	194	GLN
2	A2	206	HIS
2	A2	389	HIS
2	A2	412	ASN
3	A3	200	GLN
5	A8	118	GLN
5	A8	130	HIS
5	A8	132	ASN
5	A8	136	GLN
7	BA	39	HIS
7	BA	159	HIS
7	BA	256	GLN
7	BA	283	ASN
7	BA	301	HIS
7	BA	389	HIS
7	BA	408	ASN
7	BA	490	ASN
7	BA	502	HIS
7	BA	531	GLN
7	BA	585	HIS
7	BA	714	ASN

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Mol	Chain	Res	Type
7	BA	798	HIS
8	EA	65	GLN
8	EA	172	GLN
8	EA	208	GLN
8	EA	275	HIS
8	EA	289	GLN
8	EA	333	ASN
8	EA	392	HIS
8	EA	450	GLN
8	EA	537	ASN
8	EA	549	ASN
9	BB	170	GLN
9	BB	218	HIS
9	BB	242	GLN
9	BB	420	ASN
10	EB	159	GLN
10	EB	193	HIS
10	EB	268	GLN
10	EB	269	HIS
10	EB	336	HIS
10	EB	353	HIS
10	EB	502	HIS
10	EB	515	HIS
10	EB	563	ASN
10	EB	577	GLN
10	EB	603	GLN
10	EB	683	GLN
11	EC	174	HIS
11	EC	208	HIS
11	EC	209	ASN
11	EC	225	ASN
11	EC	262	HIS
11	EC	315	GLN
11	EC	322	HIS
11	EC	361	HIS
11	EC	365	GLN
12	BD	513	ASN
13	ED	52	GLN
13	ED	75	ASN
13	ED	178	GLN
13	ED	235	HIS
13	ED	277	ASN

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Mol	Chain	Res	Type
13	ED	318	ASN
13	ED	402	ASN
13	ED	543	GLN
13	ED	560	ASN
14	AE	85	GLN
14	AE	131	ASN
14	AE	157	GLN
14	AE	168	ASN
14	AE	169	GLN
14	AE	262	HIS
14	AE	437	GLN
15	BE	12	GLN
15	BE	22	HIS
15	BE	23	GLN
15	BE	41	HIS
15	BE	76	GLN
15	BE	78	HIS
15	BE	100	ASN
15	BE	251	ASN
15	BE	388	GLN
16	EE	82	ASN
16	EE	90	HIS
16	EE	109	GLN
16	EE	117	GLN
16	EE	118	GLN
16	EE	136	GLN
16	EE	174	HIS
16	EE	181	GLN
16	EE	182	GLN
16	EE	189	ASN
16	EE	288	HIS
16	EE	342	GLN
16	EE	409	GLN
16	EE	429	HIS
16	EE	434	HIS
16	EE	457	GLN
16	EE	520	GLN
18	AF	33	HIS
18	AF	46	GLN
18	AF	56	HIS
18	AF	80	GLN
18	AF	83	HIS

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Mol	Chain	Res	Type
18	AF	193	HIS
18	AF	223	ASN
18	AF	249	GLN
18	AF	321	GLN
18	AF	331	ASN
18	AF	346	HIS
18	AF	378	GLN
19	BF	132	GLN
19	BF	143	GLN
19	BF	148	HIS
19	BF	250	HIS
19	BF	311	GLN
19	BF	337	HIS
19	BF	362	HIS
19	BF	405	ASN
20	EF	61	GLN
20	EF	64	ASN
20	EF	74	ASN
20	EF	185	ASN
20	EF	280	GLN
21	EG	3	ASN
21	EG	38	GLN
21	EG	43	HIS
21	EG	68	HIS
21	EG	69	HIS
22	BH	99	GLN
22	BH	122	HIS
22	BH	191	GLN
22	BH	282	HIS
22	BH	296	ASN
23	EH	11	HIS
23	EH	392	ASN
23	EH	509	ASN
23	EH	602	HIS
25	BI	54	ASN
25	BI	81	ASN
25	BI	113	HIS
25	BI	263	HIS
26	EI	226	ASN
26	EI	280	ASN
28	BJ	49	HIS
28	BJ	272	HIS

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Mol	Chain	Res	Type
29	EJ	53	GLN
29	EJ	66	HIS
30	AK	51	HIS
30	AK	105	GLN
30	AK	144	HIS
30	AK	254	GLN
30	AK	273	HIS
30	AK	279	HIS
31	BK	212	GLN
31	BK	298	HIS
32	EK	126	HIS
34	BL	83	HIS
34	BL	103	ASN
34	BL	112	HIS
34	BL	144	GLN
34	BL	163	GLN
34	BL	226	HIS
34	BL	307	GLN
35	EL	232	GLN
35	EL	277	GLN
35	EL	285	GLN
35	EL	374	GLN
35	EL	382	HIS
35	EL	441	GLN
35	EL	548	GLN
35	EL	576	HIS
37	EM	18	ASN
37	EM	47	ASN
37	EM	106	ASN
37	EM	120	GLN
37	EM	128	ASN
37	EM	147	GLN
37	EM	152	HIS
37	EM	181	ASN
37	EM	187	HIS
37	EM	329	HIS
37	EM	350	GLN
39	AN	19	HIS
39	AN	63	GLN
39	AN	82	HIS
39	AN	164	HIS
40	BN	102	GLN

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Mol	Chain	Res	Type
40	BN	118	ASN
41	EN	71	GLN
41	EN	76	GLN
41	EN	158	GLN
41	EN	168	HIS
41	EN	338	ASN
41	EN	411	GLN
41	EN	544	ASN
41	EN	596	HIS
42	AO	100	HIS
42	AO	145	ASN
42	AO	175	HIS
43	BO	186	GLN
44	EO	13	HIS
44	EO	52	GLN
44	EO	118	GLN
44	EO	131	GLN
44	EO	170	GLN
44	EO	201	GLN
44	EO	304	GLN
44	EO	315	GLN
45	AP	76	GLN
45	AP	89	GLN
45	AP	143	GLN
45	AP	199	HIS
45	AP	202	GLN
45	AP	259	HIS
45	AP	310	HIS
44	EP	52	GLN
44	EP	92	GLN
44	EP	130	ASN
44	EP	131	GLN
44	EP	186	GLN
46	BQ	147	ASN
46	BQ	196	GLN
47	EQ	62	ASN
47	EQ	310	GLN
47	EQ	323	HIS
47	EQ	342	ASN
47	EQ	501	GLN
47	EQ	581	GLN
47	EQ	585	HIS

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Mol	Chain	Res	Type
48	AR	65	HIS
48	AR	113	GLN
48	AR	223	HIS
48	AR	259	HIS
49	BR	96	GLN
49	BR	138	GLN
49	BR	160	GLN
32	ER	99	ASN
51	ES	54	GLN
51	ES	77	GLN
51	ES	116	GLN
51	ES	126	HIS
51	ES	129	GLN
51	ES	134	ASN
51	ES	166	HIS
52	AT	65	ASN
52	AT	99	ASN
53	BT	26	HIS
53	BT	52	GLN
54	ET	92	GLN
55	AU	10	HIS
55	AU	73	HIS
55	AU	79	HIS
55	AU	82	ASN
55	AU	97	GLN
55	AU	165	HIS
56	BU	156	GLN
58	AV	87	HIS
58	AV	100	GLN
58	AV	143	GLN
58	AV	206	ASN
60	AW	12	HIS
60	AW	30	HIS
60	AW	40	HIS
60	AW	195	HIS
61	BW	19	ASN
61	BW	37	HIS
61	BW	65	ASN
61	BW	145	ASN
63	BX	64	ASN
63	BX	162	ASN
63	BX	173	HIS

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Mol	Chain	Res	Type
63	BX	178	HIS
65	AY	64	HIS
65	AY	89	GLN
65	AY	91	GLN
65	AY	145	ASN
65	AY	168	HIS
65	AY	195	ASN
65	AY	235	GLN
65	AY	248	GLN
65	AY	287	GLN
65	AY	289	GLN
65	AY	321	GLN
66	BZ	44	ASN
66	BZ	66	GLN
66	BZ	96	GLN
67	Ba	31	GLN
67	Ba	81	GLN
67	Ba	129	GLN
67	Ba	147	ASN
68	Bb	3	GLN
68	Bb	38	HIS
68	Bb	70	ASN
68	Bb	79	HIS
68	Bb	81	HIS
69	Bc	43	ASN
69	Bc	91	ASN
69	Bc	97	GLN
69	Bc	126	ASN
70	Ae	56	ASN
70	Ae	71	HIS
70	Ae	86	HIS
70	Ae	96	GLN
70	Ae	162	GLN
71	Af	68	ASN
71	Af	86	ASN
71	Af	101	HIS
71	Af	104	HIS
71	Af	106	GLN
71	Af	136	GLN
71	Af	142	ASN
71	Af	168	GLN
72	Bf	93	HIS

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Mol	Chain	Res	Type
73	Ag	27	GLN
73	Ag	84	ASN
73	Ag	105	GLN
73	Ag	151	GLN
73	Ag	160	GLN
74	Bg	63	GLN
76	Bi	41	ASN
76	Bi	60	ASN
76	Bi	192	ASN
76	Bi	197	ASN
77	Al	101	GLN
77	Al	211	HIS
78	Ao	70	HIS
78	Ao	199	HIS
79	Ap	55	HIS
79	Ap	78	HIS
79	Ap	109	GLN
79	Ap	132	HIS
79	Ap	194	HIS
79	Ap	289	GLN
80	At	20	HIS
80	At	63	GLN
80	At	147	HIS
81	Av	102	GLN
81	Av	128	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	AA	879/1176 (74%)	318 (36%)	11 (1%)

All (318) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	AA	2	U
6	AA	4	U
6	AA	5	U
6	AA	11	U
6	AA	12	U
6	AA	13	A
6	AA	15	G

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Mol	Chain	Res	Type
6	AA	16	A
6	AA	18	G
6	AA	19	A
6	AA	20	A
6	AA	21	U
6	AA	29	U
6	AA	30	A
6	AA	34	G
6	AA	38	U
6	AA	40	U
6	AA	41	U
6	AA	43	U
6	AA	44	A
6	AA	45	U
6	AA	50	A
6	AA	53	A
6	AA	54	A
6	AA	59	U
6	AA	60	U
6	AA	66	C
6	AA	67	C
6	AA	68	G
6	AA	69	U
6	AA	70	G
6	AA	73	G
6	AA	75	A
6	AA	77	A
6	AA	79	U
6	AA	80	U
6	AA	84	A
6	AA	85	U
6	AA	88	G
6	AA	89	U
6	AA	93	A
6	AA	97	A
6	AA	99	A
6	AA	104	A
6	AA	105	G
6	AA	106	G
6	AA	107	U
6	AA	111	U
6	AA	113	A

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Mol	Chain	Res	Type
6	AA	115	A
6	AA	116	U
6	AA	119	A
6	AA	120	A
6	AA	123	U
6	AA	124	U
6	AA	125	U
6	AA	133	U
6	AA	134	U
6	AA	135	G
6	AA	136	U
6	AA	146	A
6	AA	149	U
6	AA	155	U
6	AA	156	U
6	AA	164	U
6	AA	168	A
6	AA	172	U
6	AA	173	U
6	AA	176	A
6	AA	177	U
6	AA	183	U
6	AA	188	A
6	AA	190	U
6	AA	191	U
6	AA	197	A
6	AA	198	A
6	AA	203	A
6	AA	232	G
6	AA	234	U
6	AA	250	A
6	AA	260	G
6	AA	261	U
6	AA	262	U
6	AA	265	U
6	AA	274	A
6	AA	275	C
6	AA	276	C
6	AA	277	A
6	AA	278	A
6	AA	282	A
6	AA	284	U

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Mol	Chain	Res	Type
6	AA	285	A
6	AA	286	U
6	AA	287	A
6	AA	288	G
6	AA	289	U
6	AA	290	A
6	AA	293	A
6	AA	296	A
6	AA	297	U
6	AA	299	U
6	AA	302	G
6	AA	309	U
6	AA	310	A
6	AA	313	A
6	AA	315	A
6	AA	317	A
6	AA	319	A
6	AA	323	U
6	AA	327	U
6	AA	330	U
6	AA	341	A
6	AA	342	U
6	AA	345	U
6	AA	346	G
6	AA	347	A
6	AA	355	A
6	AA	357	A
6	AA	358	A
6	AA	362	A
6	AA	363	A
6	AA	366	U
6	AA	369	U
6	AA	371	A
6	AA	378	A
6	AA	379	U
6	AA	380	G
6	AA	381	U
6	AA	385	A
6	AA	387	A
6	AA	388	U
6	AA	389	A
6	AA	449	U

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Mol	Chain	Res	Type
6	AA	451	A
6	AA	452	A
6	AA	454	G
6	AA	455	G
6	AA	456	U
6	AA	461	U
6	AA	462	U
6	AA	463	U
6	AA	464	U
6	AA	468	A
6	AA	470	G
6	AA	473	A
6	AA	476	G
6	AA	478	A
6	AA	481	G
6	AA	482	U
6	AA	483	A
6	AA	484	U
6	AA	485	A
6	AA	488	U
6	AA	490	G
6	AA	491	A
6	AA	492	U
6	AA	493	A
6	AA	494	U
6	AA	495	A
6	AA	496	A
6	AA	497	C
6	AA	507	A
6	AA	509	U
6	AA	512	U
6	AA	515	U
6	AA	519	A
6	AA	520	U
6	AA	521	G
6	AA	522	A
6	AA	524	A
6	AA	528	A
6	AA	529	U
6	AA	531	U
6	AA	532	U
6	AA	533	A

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Mol	Chain	Res	Type
6	AA	535	U
6	AA	536	A
6	AA	540	U
6	AA	541	A
6	AA	544	G
6	AA	546	A
6	AA	547	U
6	AA	548	A
6	AA	551	A
6	AA	555	U
6	AA	566	A
6	AA	567	G
6	AA	568	U
6	AA	569	U
6	AA	572	U
6	AA	574	A
6	AA	575	A
6	AA	576	A
6	AA	577	A
6	AA	581	U
6	AA	583	A
6	AA	585	A
6	AA	587	U
6	AA	589	U
6	AA	788	A
6	AA	789	C
6	AA	792	A
6	AA	793	U
6	AA	794	A
6	AA	795	A
6	AA	799	A
6	AA	800	A
6	AA	801	A
6	AA	814	A
6	AA	816	C
6	AA	817	A
6	AA	818	A
6	AA	825	A
6	AA	826	A
6	AA	827	U
6	AA	828	A
6	AA	829	A

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Mol	Chain	Res	Type
6	AA	838	A
6	AA	844	A
6	AA	845	A
6	AA	846	A
6	AA	852	C
6	AA	853	A
6	AA	869	U
6	AA	871	C
6	AA	872	A
6	AA	873	A
6	AA	875	G
6	AA	876	A
6	AA	877	G
6	AA	878	A
6	AA	883	U
6	AA	887	A
6	AA	892	U
6	AA	893	A
6	AA	895	U
6	AA	896	U
6	AA	897	G
6	AA	898	U
6	AA	902	U
6	AA	904	U
6	AA	905	G
6	AA	906	A
6	AA	911	G
6	AA	925	U
6	AA	926	A
6	AA	927	U
6	AA	928	U
6	AA	932	A
6	AA	934	A
6	AA	941	G
6	AA	945	U
6	AA	947	U
6	AA	948	A
6	AA	956	A
6	AA	961	A
6	AA	962	U
6	AA	963	A
6	AA	970	U

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Mol	Chain	Res	Type
6	AA	971	C
6	AA	980	U
6	AA	985	A
6	AA	986	G
6	AA	989	U
6	AA	990	U
6	AA	992	A
6	AA	993	A
6	AA	994	A
6	AA	995	A
6	AA	996	U
6	AA	998	A
6	AA	1003	G
6	AA	1004	U
6	AA	1005	U
6	AA	1006	U
6	AA	1010	C
6	AA	1014	U
6	AA	1018	U
6	AA	1021	U
6	AA	1079	A
6	AA	1082	C
6	AA	1089	G
6	AA	1090	U
6	AA	1091	U
6	AA	1092	U
6	AA	1093	A
6	AA	1096	U
6	AA	1106	U
6	AA	1107	U
6	AA	1110	A
6	AA	1113	U
6	AA	1117	A
6	AA	1118	A
6	AA	1119	U
6	AA	1120	A
6	AA	1121	A
6	AA	1122	U
6	AA	1125	A
6	AA	1126	U
6	AA	1131	G
6	AA	1141	A

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Mol	Chain	Res	Type
6	AA	1144	G
6	AA	1145	A
6	AA	1146	U
6	AA	1147	U
6	AA	1154	A
6	AA	1158	G
6	AA	1160	A
6	AA	1161	A
6	AA	1162	G
6	AA	1163	A
6	AA	1164	A
6	AA	1168	U
6	AA	1169	A
6	AA	1171	A
6	AA	1173	U
6	AA	1175	U
6	AA	1176	A

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	AA	69	U
6	AA	379	U
6	AA	481	G
6	AA	484	U
6	AA	493	A
6	AA	534	U
6	AA	539	A
6	AA	793	U
6	AA	895	U
6	AA	994	A
6	AA	1004	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

Of 48 ligands modelled in this entry, 40 are monoatomic - leaving 8 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
84	SPD	AA	1250	-	9,9,9	0.32	0	8,8,8	0.87	0
89	NAD	Av	301	-	46,48,48	0.57	1 (2%)	64,73,73	0.58	1 (1%)
87	ATP	EB	1001	83	32,33,33	1.42	5 (15%)	48,52,52	1.72	9 (18%)
88	PM8	ER	200	32	26,31,31	0.77	1 (3%)	30,38,38	1.04	1 (3%)
88	PM8	EK	200	32	26,31,31	0.73	1 (3%)	30,38,38	0.98	2 (6%)
85	GTP	EA	2001	86,83	33,34,34	0.93	2 (6%)	50,54,54	1.66	11 (22%)
85	GTP	EQ	1000	83	33,34,34	0.90	1 (3%)	50,54,54	1.55	9 (18%)
85	GTP	EA	1001	86,83	33,34,34	0.95	2 (6%)	50,54,54	1.64	10 (20%)

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
84	SPD	AA	1250	-	-	2/7/7/7	-
89	NAD	Av	301	-	-	2/30/62/62	0/5/5/5
87	ATP	EB	1001	83	-	2/22/38/38	0/3/3/3
88	PM8	ER	200	32	-	17/36/38/38	-
88	PM8	EK	200	32	-	13/36/38/38	-
85	GTP	EA	2001	86,83	-	4/22/38/38	0/3/3/3
85	GTP	EQ	1000	83	-	2/22/38/38	0/3/3/3
85	GTP	EA	1001	86,83	-	8/22/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	EB	1001	ATP	C5-C4	4.62	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	EB	1001	ATP	C5-C6	2.71	1.48	1.41
88	EK	200	PM8	C1-S1	-2.55	1.70	1.76
88	ER	200	PM8	C2-C1	2.53	1.53	1.50
89	Av	301	NAD	C2N-N1N	2.36	1.37	1.35
87	EB	1001	ATP	PB-O3B	2.33	1.62	1.59
85	EA	1001	GTP	PB-O3B	2.30	1.62	1.59
87	EB	1001	ATP	C5-N7	-2.30	1.34	1.39
87	EB	1001	ATP	C8-N7	2.28	1.36	1.31
85	EA	2001	GTP	C2-N3	2.15	1.38	1.33
85	EA	1001	GTP	C2-N3	2.14	1.38	1.33
85	EA	2001	GTP	PB-O3B	2.13	1.61	1.59
85	EQ	1000	GTP	C2-N3	2.12	1.38	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	EB	1001	ATP	C5-C4-N3	-5.82	118.70	126.72
85	EA	1001	GTP	C2-N3-C4	5.16	121.19	112.30
85	EA	2001	GTP	C2-N3-C4	5.15	121.17	112.30
85	EA	1001	GTP	C5-C4-N3	-5.05	120.35	128.39
85	EA	2001	GTP	C5-C4-N3	-5.03	120.38	128.39
85	EQ	1000	GTP	C5-C4-N3	-4.81	120.74	128.39
87	EB	1001	ATP	N3-C4-N9	4.60	135.00	127.17
85	EQ	1000	GTP	C2-N3-C4	4.38	119.85	112.30
87	EB	1001	ATP	C2-N3-C4	3.72	120.91	111.83
87	EB	1001	ATP	C4-C5-N7	-3.46	106.63	110.58
87	EB	1001	ATP	N3-C2-N1	-3.26	123.65	128.58
85	EA	2001	GTP	N9-C4-N3	3.13	132.21	125.95
85	EA	1001	GTP	N9-C4-N3	3.12	132.20	125.95
85	EQ	1000	GTP	N9-C4-N3	3.08	132.12	125.95
88	EK	200	PM8	C37-C38-C39	-2.89	107.58	112.39
85	EA	1001	GTP	C2-N1-C6	-2.85	119.95	125.11
85	EA	2001	GTP	C2-N1-C6	-2.84	119.97	125.11
88	ER	200	PM8	O1-C1-C2	-2.83	120.71	123.98
85	EQ	1000	GTP	C2-N1-C6	-2.80	120.04	125.11
85	EA	1001	GTP	C5-C6-N1	2.66	120.01	113.25
85	EQ	1000	GTP	N9-C8-N7	-2.65	108.49	113.40
85	EA	2001	GTP	C5-C6-N1	2.64	119.98	113.25
87	EB	1001	ATP	C4-N9-C8	2.63	108.50	105.74
85	EQ	1000	GTP	O6-C6-C5	-2.53	119.84	126.53
85	EA	1001	GTP	N9-C8-N7	-2.53	108.72	113.40
87	EB	1001	ATP	C5-N7-C8	2.50	107.38	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	EA	2001	GTP	O6-C6-C5	-2.50	119.93	126.53
85	EA	1001	GTP	O6-C6-C5	-2.49	119.95	126.53
85	EA	2001	GTP	N9-C8-N7	-2.48	108.80	113.40
88	EK	200	PM8	C42-N41-C39	-2.48	118.21	122.82
89	Av	301	NAD	C6N-N1N-C2N	-2.45	119.79	121.88
85	EQ	1000	GTP	C8-N7-C5	2.45	108.62	104.26
85	EA	2001	GTP	C8-N7-C5	2.42	108.57	104.26
85	EA	1001	GTP	C8-N7-C5	2.42	108.56	104.26
85	EQ	1000	GTP	C5-C6-N1	2.37	119.30	113.25
85	EA	1001	GTP	N2-C2-N1	2.27	121.54	116.76
85	EA	2001	GTP	N2-C2-N1	2.25	121.52	116.76
85	EA	1001	GTP	N1-C2-N3	-2.21	119.28	123.32
85	EA	2001	GTP	N1-C2-N3	-2.20	119.29	123.32
87	EB	1001	ATP	C6-C5-N7	2.13	136.19	132.09
85	EQ	1000	GTP	C3'-C2'-C1'	2.12	105.47	101.46
85	EA	2001	GTP	O2A-PA-O3A	2.09	112.91	107.27
87	EB	1001	ATP	C3'-C2'-C1'	2.04	105.32	101.46

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	EA	1001	GTP	PB-O3B-PG-O3G
85	EA	1001	GTP	C5'-O5'-PA-O3A
85	EA	1001	GTP	C5'-O5'-PA-O1A
85	EA	1001	GTP	C5'-O5'-PA-O2A
85	EA	1001	GTP	O4'-C4'-C5'-O5'
85	EA	2001	GTP	C5'-O5'-PA-O1A
88	EK	200	PM8	N41-C42-C43-S1
88	EK	200	PM8	C42-C43-S1-C1
88	EK	200	PM8	O1-C1-S1-C43
88	EK	200	PM8	C2-C1-S1-C43
88	EK	200	PM8	C1-C2-C3-C4
88	ER	200	PM8	O27-C28-C29-C30
88	ER	200	PM8	O27-C28-C29-C32
88	ER	200	PM8	N41-C42-C43-S1
88	ER	200	PM8	O1-C1-S1-C43
88	ER	200	PM8	C2-C1-S1-C43
85	EA	1001	GTP	C3'-C4'-C5'-O5'
85	EA	2001	GTP	O4'-C4'-C5'-O5'
88	EK	200	PM8	C3-C4-C5-C6
89	Av	301	NAD	O4D-C4D-C5D-O5D

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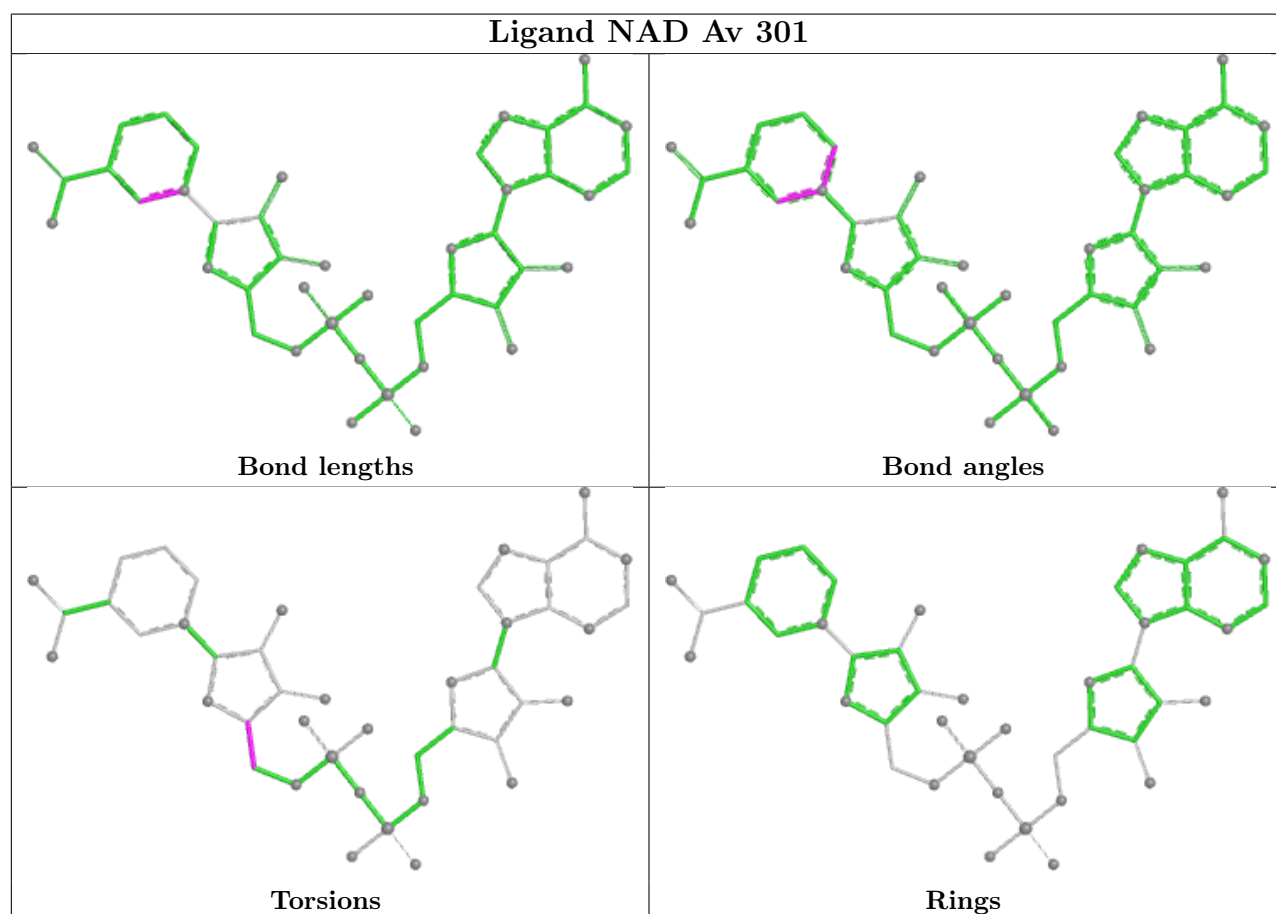
Mol	Chain	Res	Type	Atoms
88	ER	200	PM8	C7-C8-C9-C10
88	ER	200	PM8	C31-C29-C32-C34
88	ER	200	PM8	C5-C6-C7-C8
84	AA	1250	SPD	C2-C3-C4-C5
88	EK	200	PM8	O33-C32-C34-O35
88	ER	200	PM8	O33-C32-C34-O35
88	ER	200	PM8	O27-C28-C29-C31
88	ER	200	PM8	C28-C29-C32-C34
85	EQ	1000	GTP	C3'-C4'-C5'-O5'
88	EK	200	PM8	C43-C42-N41-C39
89	Av	301	NAD	C3D-C4D-C5D-O5D
88	EK	200	PM8	C5-C6-C7-C8
85	EA	2001	GTP	C3'-C4'-C5'-O5'
88	ER	200	PM8	C6-C7-C8-C9
88	ER	200	PM8	C3-C4-C5-C6
88	EK	200	PM8	C37-C38-C39-O40
88	EK	200	PM8	C37-C38-C39-N41
88	EK	200	PM8	C2-C3-C4-C5
85	EA	1001	GTP	PA-O3A-PB-O1B
85	EQ	1000	GTP	O4'-C4'-C5'-O5'
88	ER	200	PM8	C2-C3-C4-C5
88	ER	200	PM8	C30-C29-C32-C34
84	AA	1250	SPD	C4-C5-N6-C7
88	ER	200	PM8	C30-C29-C32-O33
85	EA	2001	GTP	PA-O3A-PB-O2B
88	EK	200	PM8	O33-C32-C34-N36
88	ER	200	PM8	O33-C32-C34-N36
85	EA	1001	GTP	PA-O3A-PB-O2B
87	EB	1001	ATP	PA-O3A-PB-O1B
87	EB	1001	ATP	PA-O3A-PB-O2B

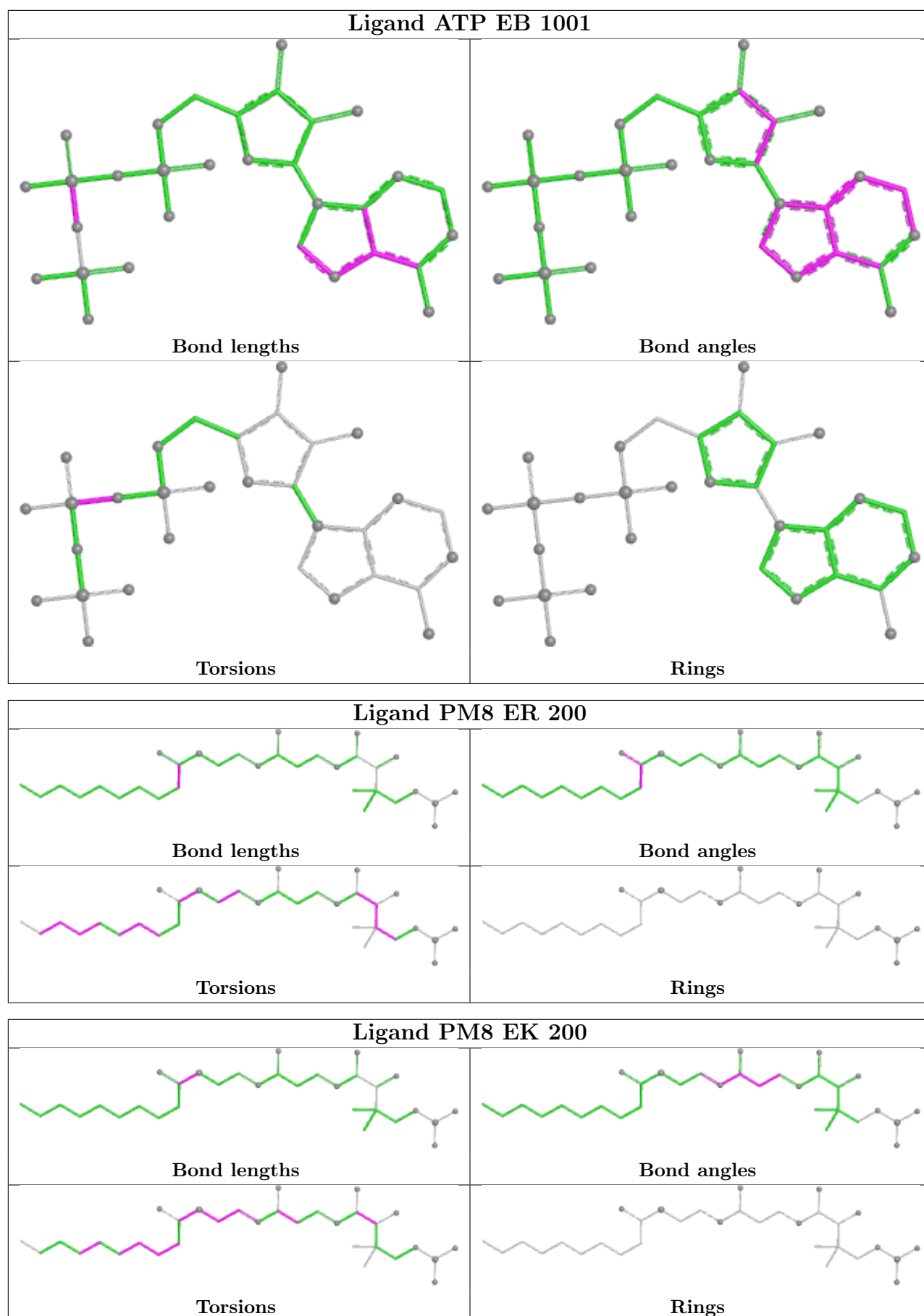
There are no ring outliers.

7 monomers are involved in 15 short contacts:

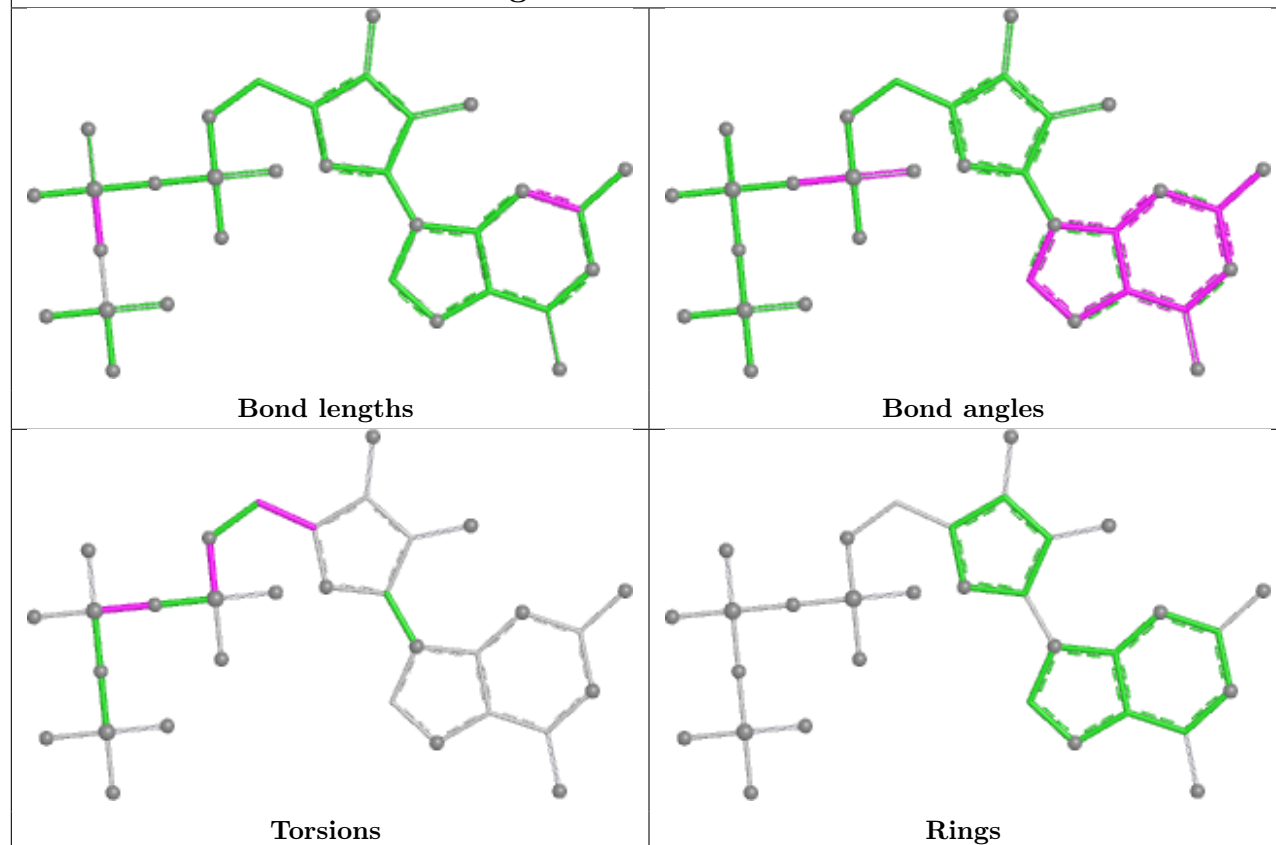
Mol	Chain	Res	Type	Clashes	Symm-Clashes
84	AA	1250	SPD	2	0
87	EB	1001	ATP	1	0
88	ER	200	PM8	4	0
88	EK	200	PM8	2	0
85	EA	2001	GTP	4	0
85	EQ	1000	GTP	1	0
85	EA	1001	GTP	1	0

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.

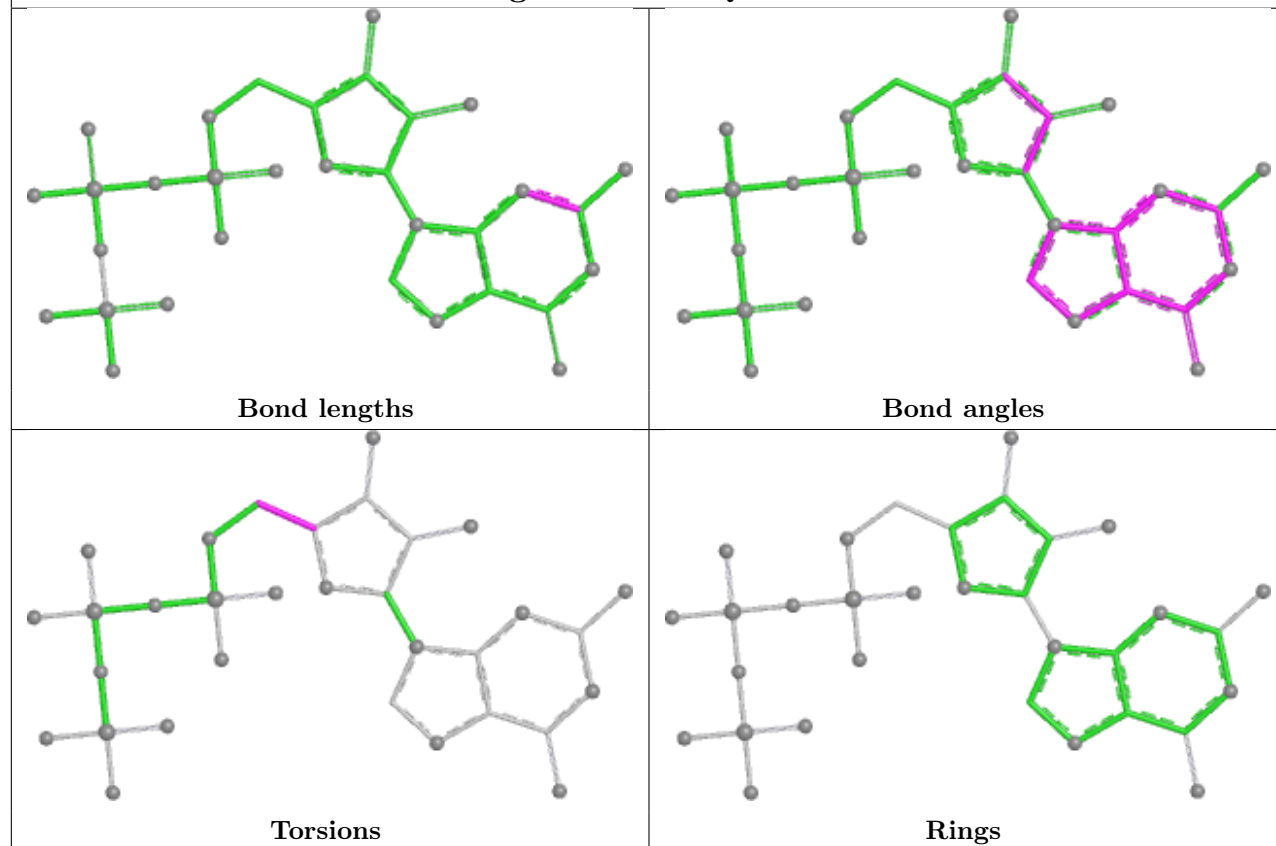


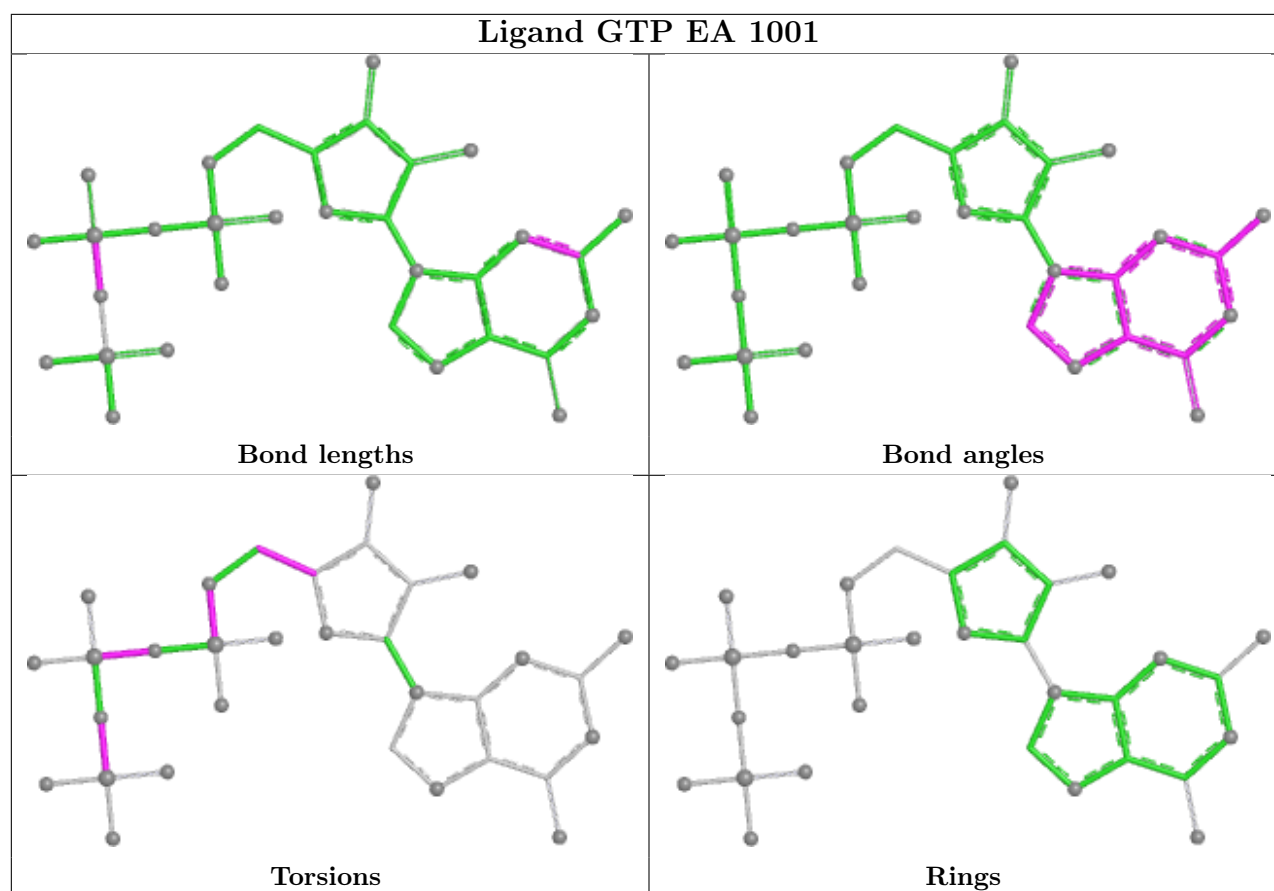


Ligand GTP EA 2001



Ligand GTP EQ 1000





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
64	UX	13
36	UL	3
17	UE	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	UX	66:UNK	C	117:UNK	N	41.11
1	UX	341:UNK	C	402:UNK	N	39.28
1	UX	233:UNK	C	264:UNK	N	29.49
1	UX	35:UNK	C	56:UNK	N	28.81

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	UX	15:UNK	C	26:UNK	N	26.47
1	UX	433:UNK	C	474:UNK	N	24.55
1	UX	310:UNK	C	331:UNK	N	20.01
1	UX	278:UNK	C	299:UNK	N	17.76
1	UL	13:UNK	C	19:UNK	N	15.09
1	UX	161:UNK	C	172:UNK	N	10.77
1	UX	213:UNK	C	224:UNK	N	10.56
1	UX	416:UNK	C	422:UNK	N	8.69
1	UX	133:UNK	C	144:UNK	N	7.85
1	UL	54:UNK	C	106:UNK	N	7.22
1	UL	35:UNK	C	40:UNK	N	6.54
1	UX	182:UNK	C	203:UNK	N	5.92
1	UE	28:UNK	C	56:UNK	N	4.72

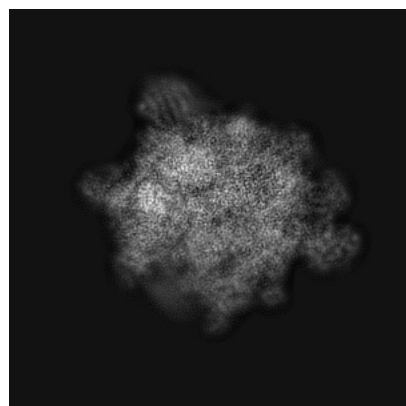
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11000. These allow visual inspection of the internal detail of the map and identification of artifacts.

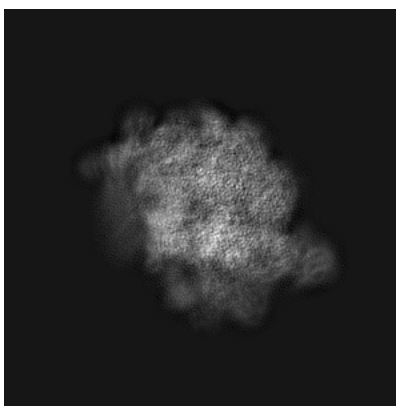
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

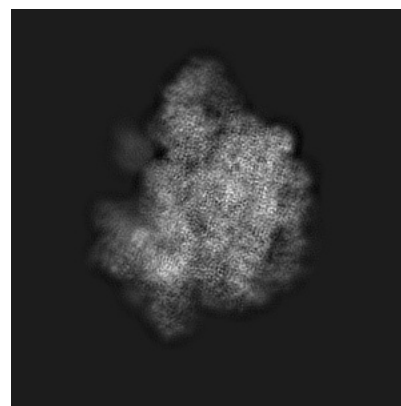
6.1.1 Primary map



X

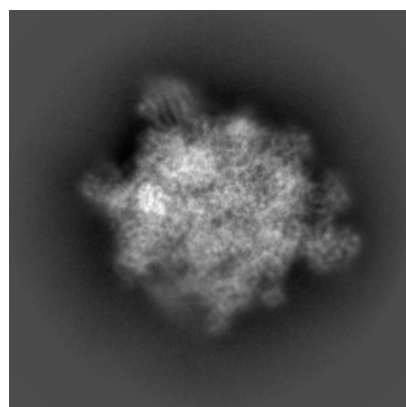


Y

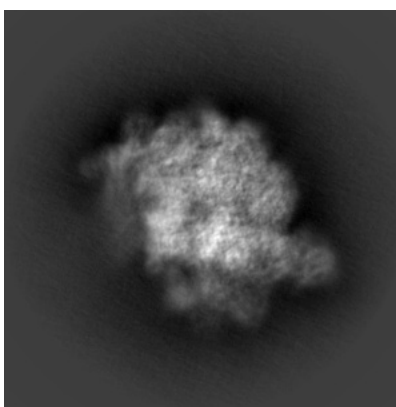


Z

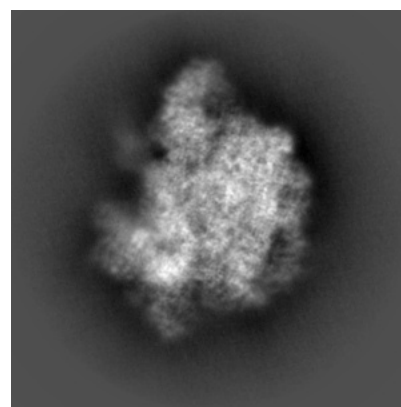
6.1.2 Raw map



X



Y

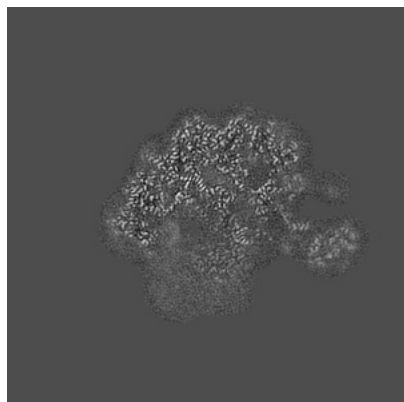


Z

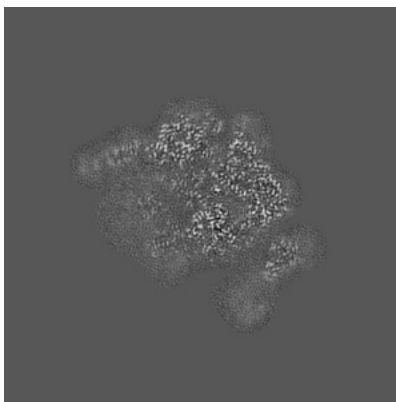
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

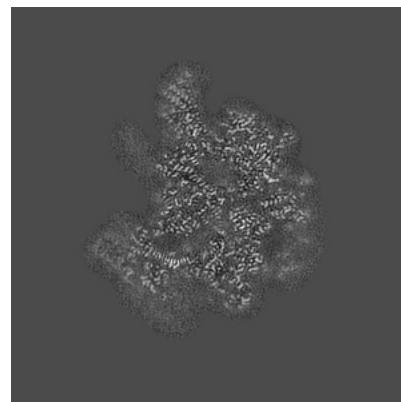
6.2.1 Primary map



X Index: 200

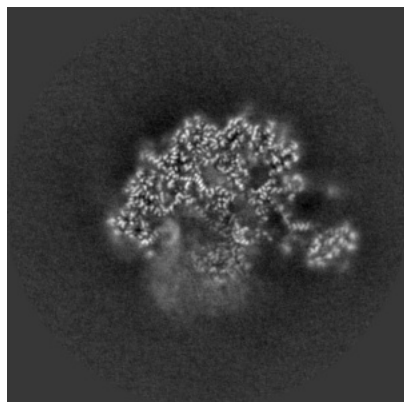


Y Index: 200

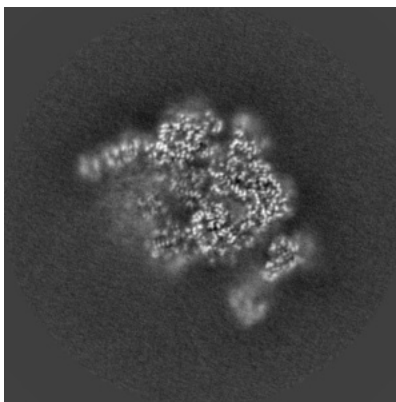


Z Index: 200

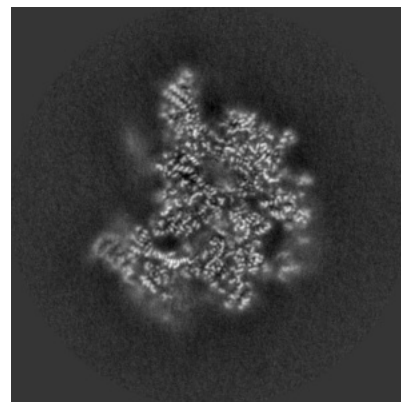
6.2.2 Raw map



X Index: 200



Y Index: 200

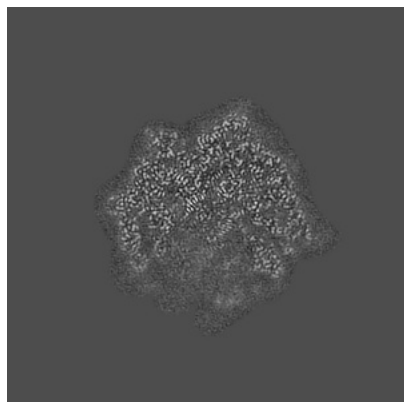


Z Index: 200

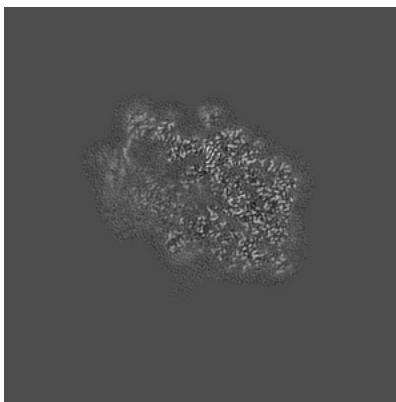
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

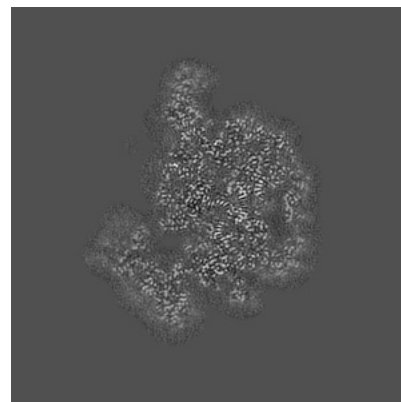
6.3.1 Primary map



X Index: 226

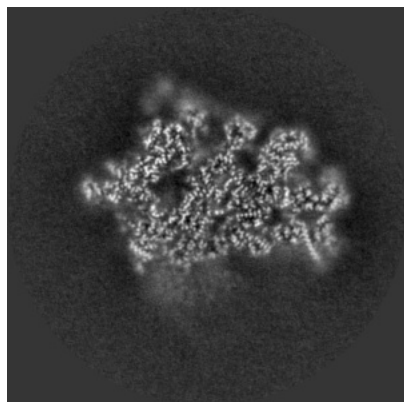


Y Index: 227

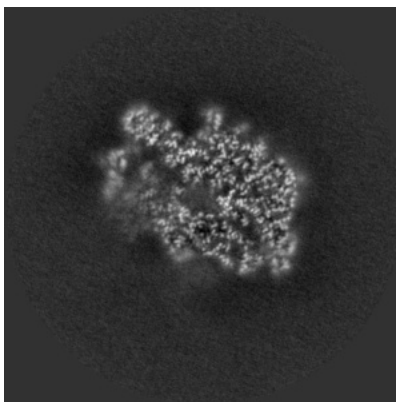


Z Index: 210

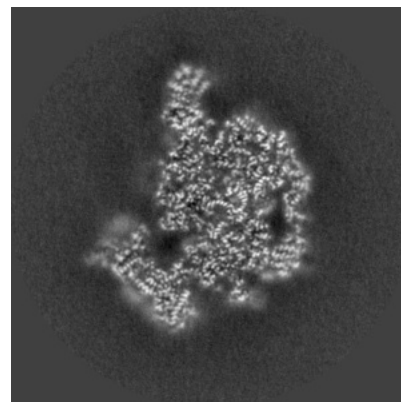
6.3.2 Raw map



X Index: 170



Y Index: 232

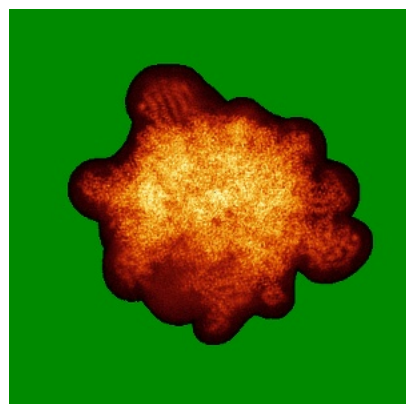


Z Index: 211

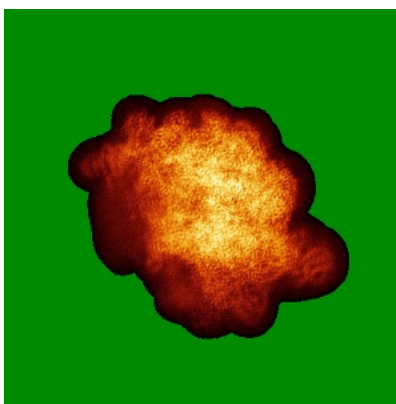
The images above show the largest variance slices of the map in three orthogonal directions.

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

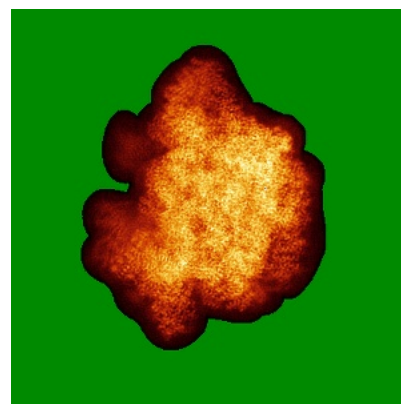
6.4.1 Primary map



X

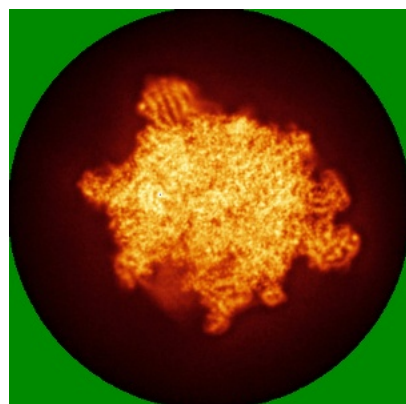


Y

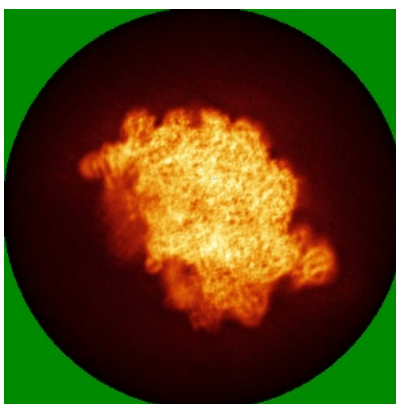


Z

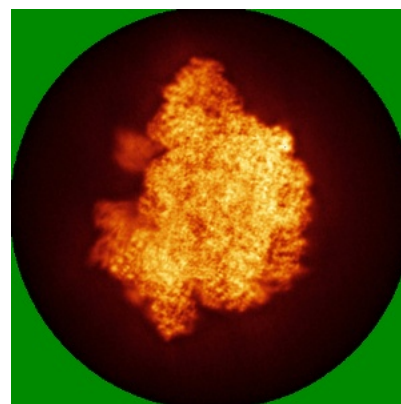
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

This section was not generated.

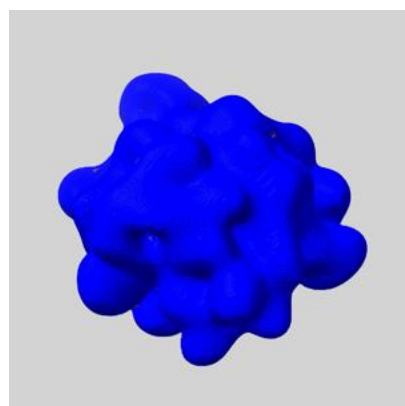
6.6 Mask visualisation [i](#)

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

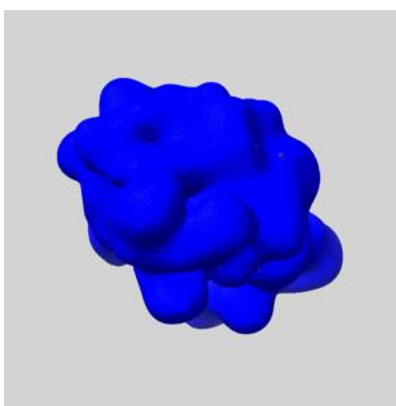
A mask typically either:

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

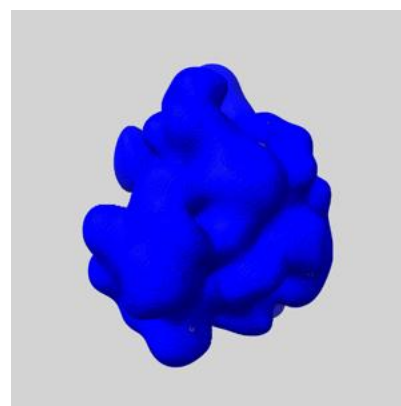
6.6.1 emd_11000_msk_1.map [i](#)



X



Y

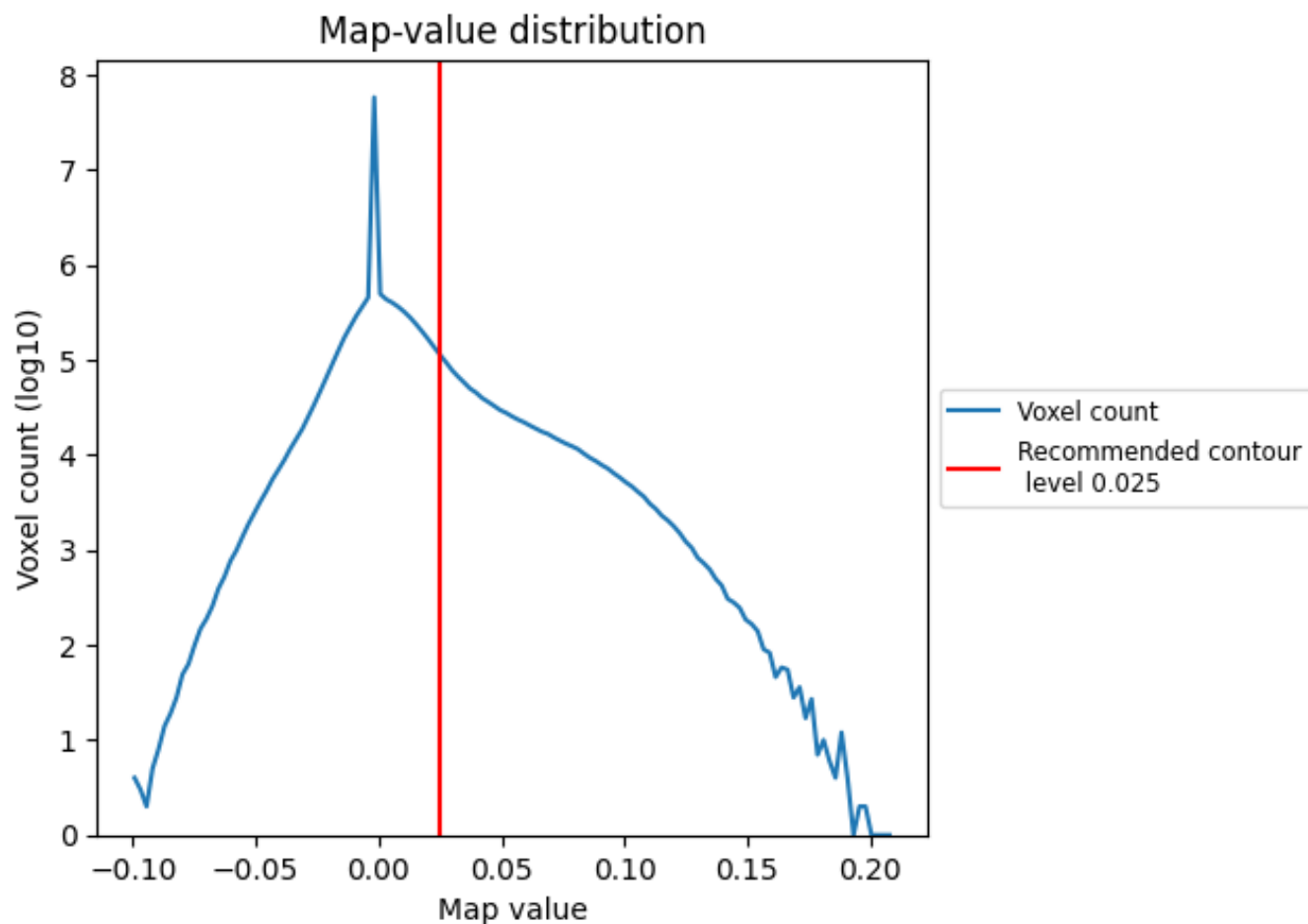


Z

7 Map analysis [i](#)

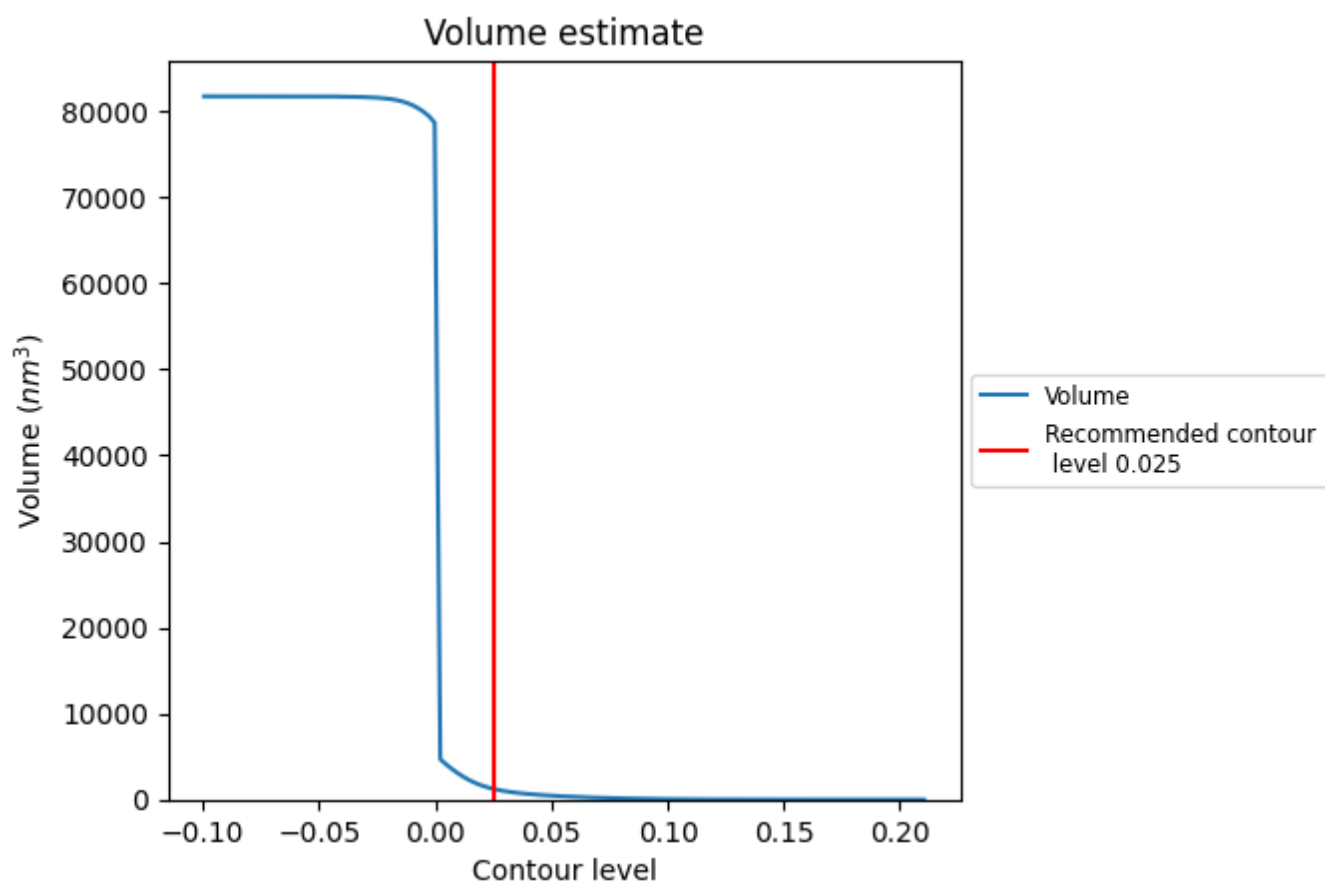
This section contains the results of statistical analysis of the map.

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.

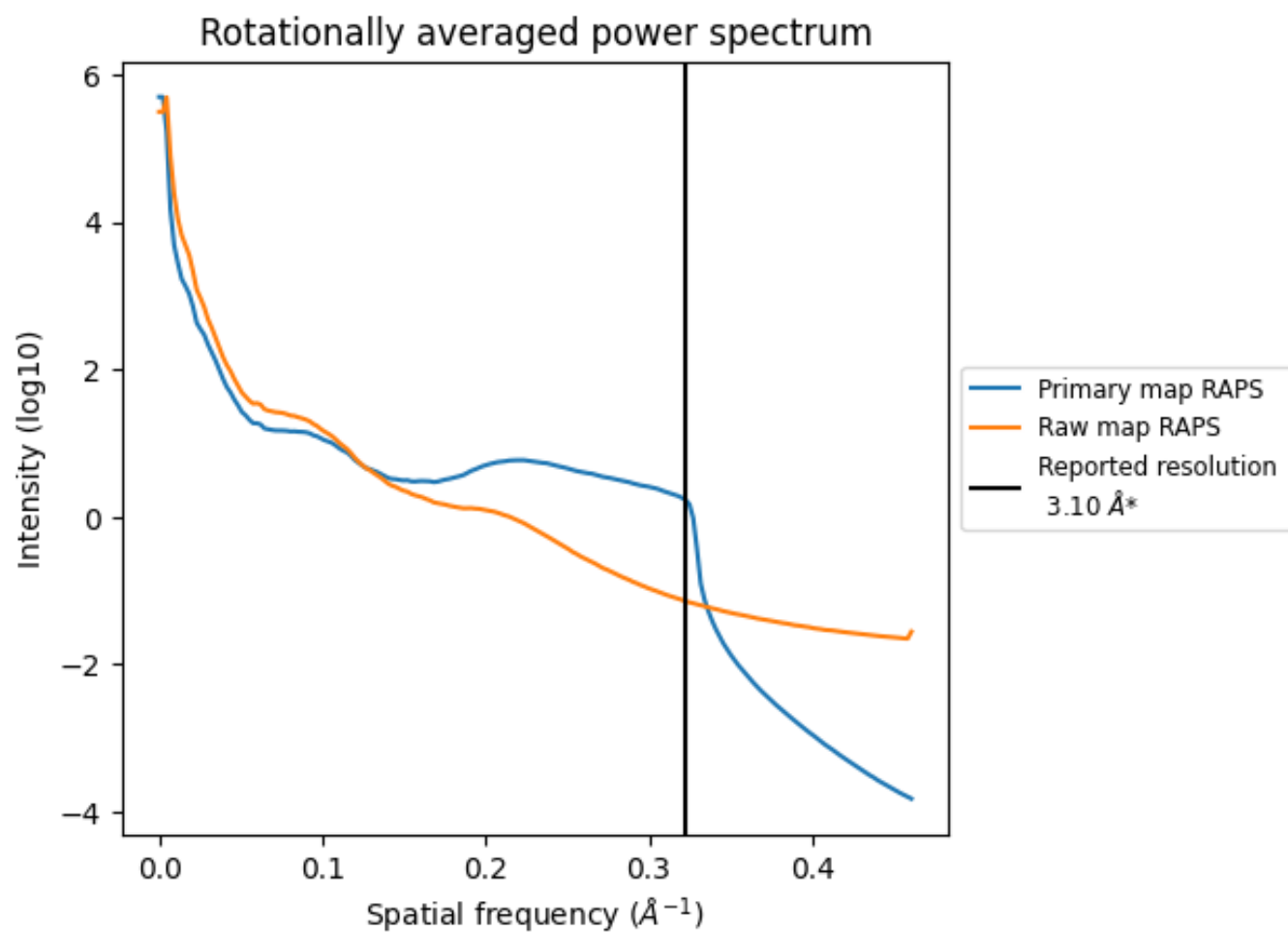
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1249 nm^3 ; this corresponds to an approximate mass of 1128 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 ⓘ

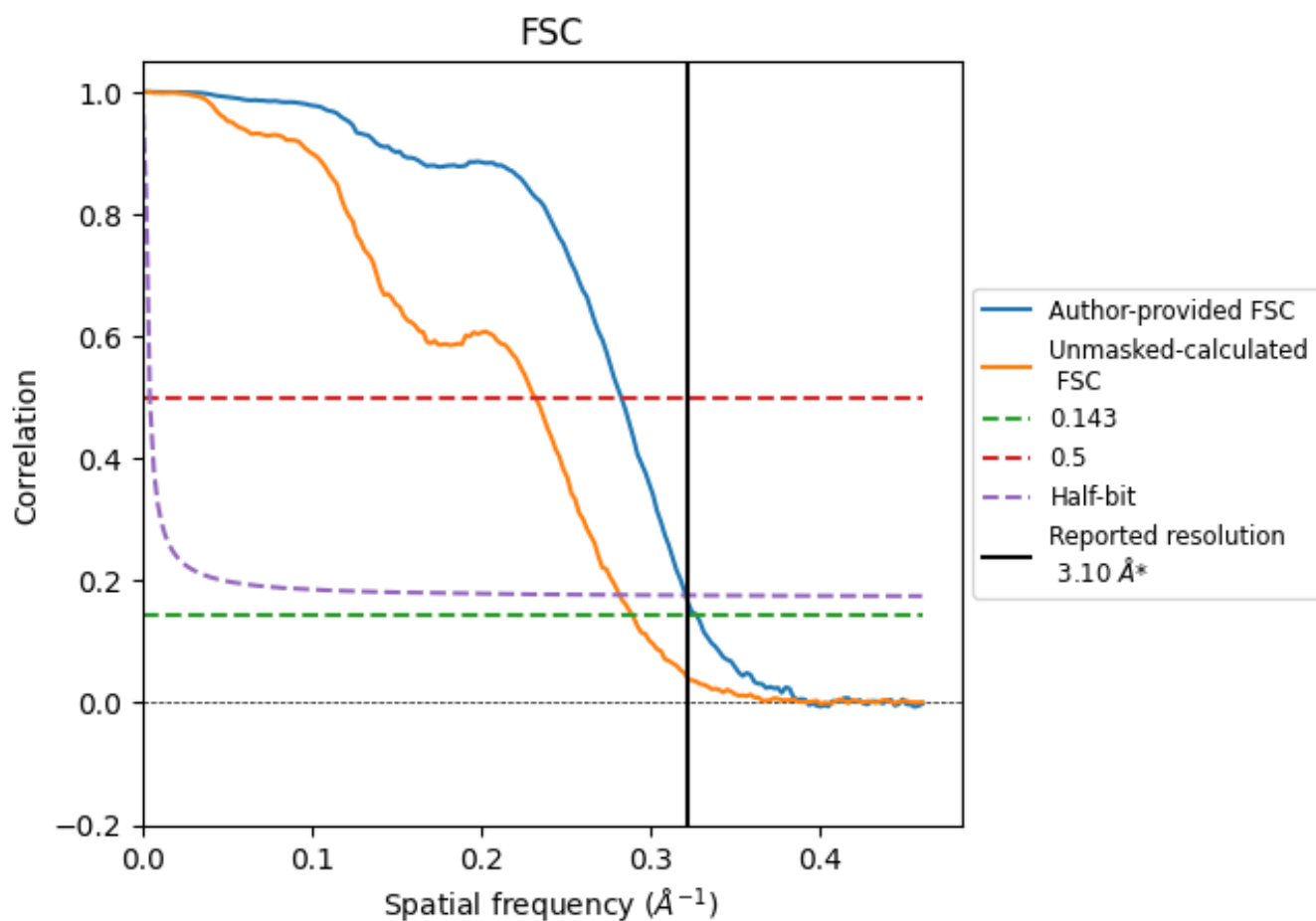


*Reported resolution corresponds to spatial frequency of $0.323 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

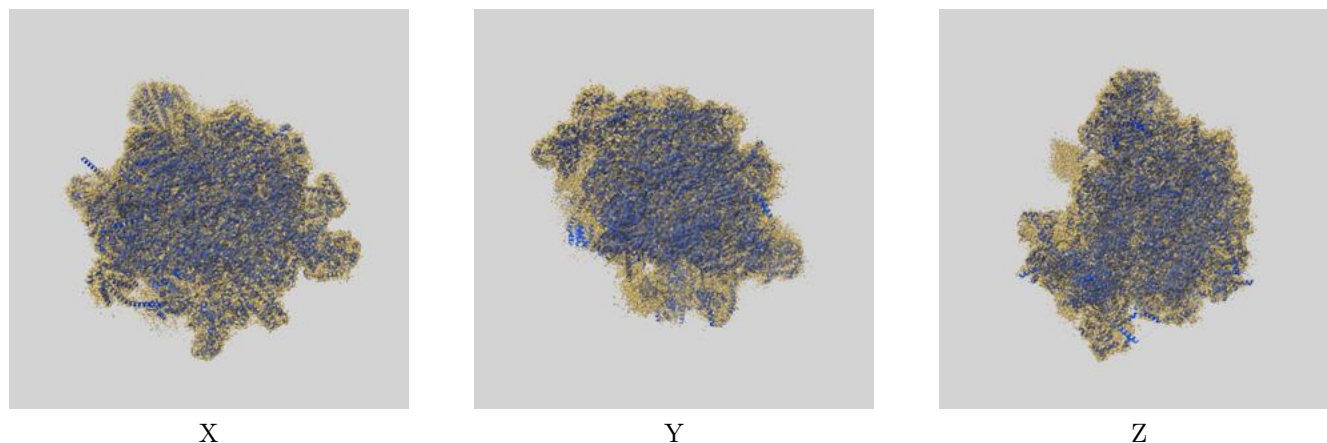
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.05	3.53	3.11
Unmasked-calculated*	3.45	4.31	3.55

*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 3.45 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

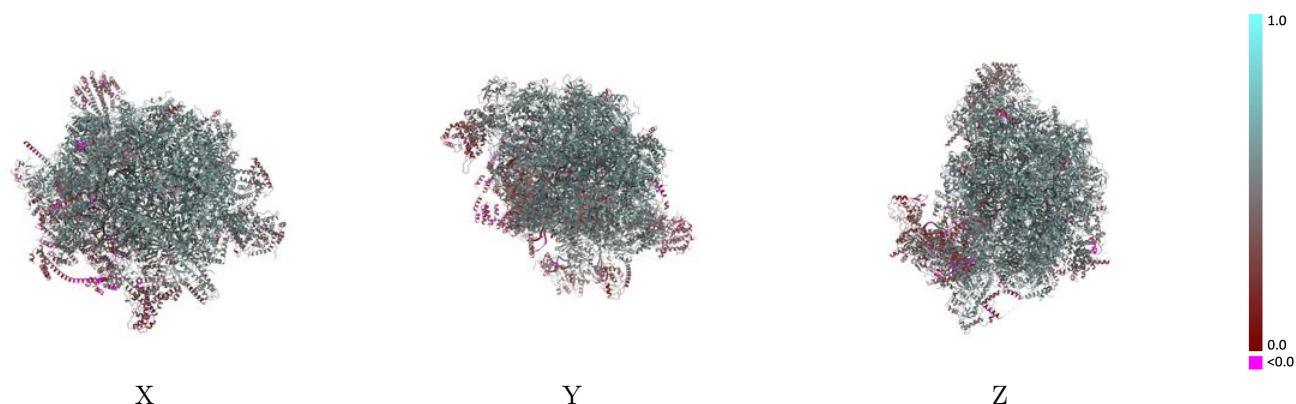
This section contains information regarding the fit between EMDB map EMD-11000 and PDB model 6YXY. Per-residue inclusion information can be found in section [3](#) on page [29](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.025 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](#)

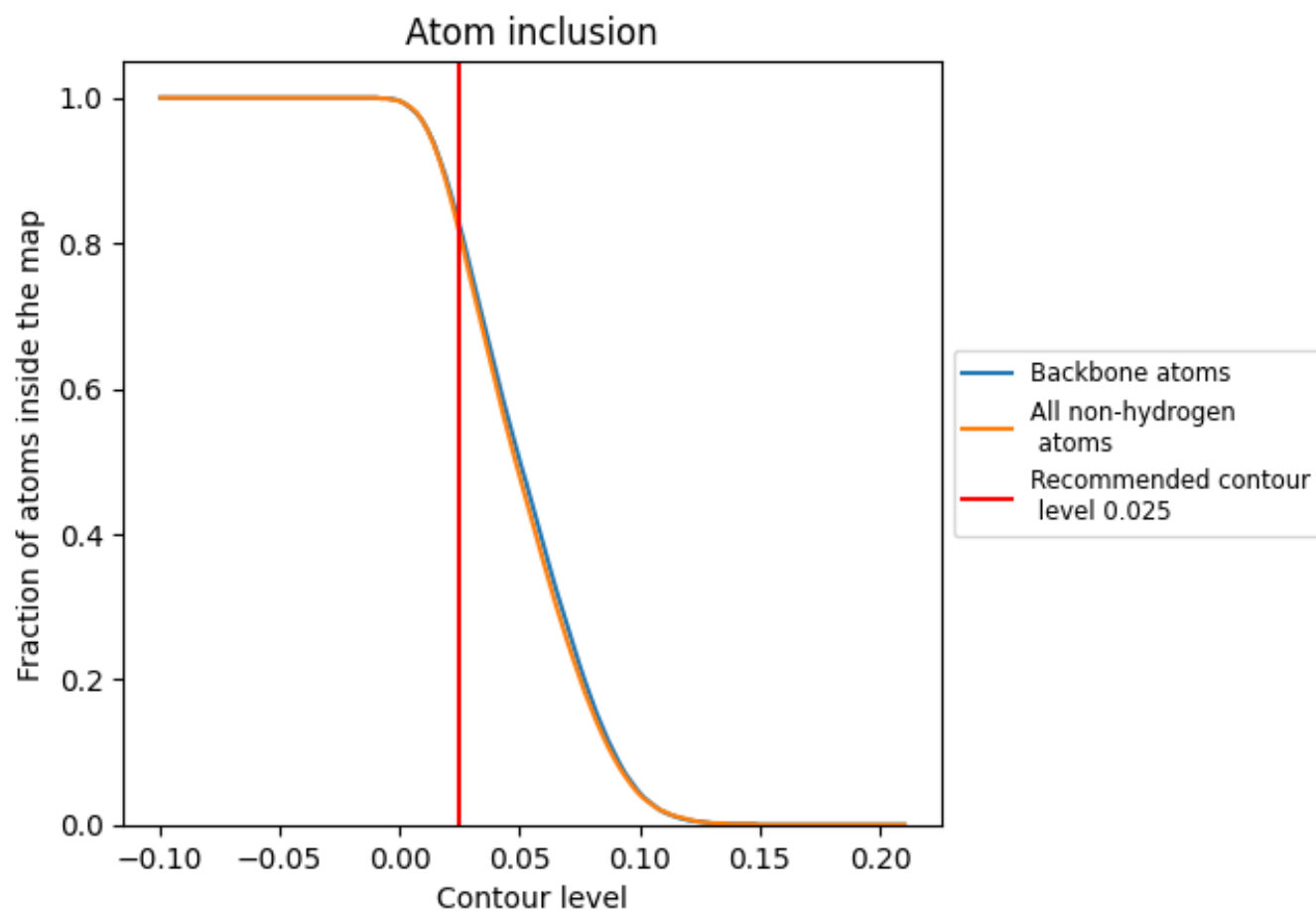


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8150	 0.5080
A1	 0.8650	 0.5280
A2	 0.9140	 0.5520
A3	 0.9050	 0.5720
A5	 0.8990	 0.5690
A8	 0.8800	 0.5770
AA	 0.8200	 0.4900
AE	 0.8100	 0.5410
AF	 0.9320	 0.5840
AI	 0.8560	 0.5300
AK	 0.6790	 0.3790
AN	 0.8830	 0.5680
AO	 0.8990	 0.5800
AP	 0.8980	 0.5620
AR	 0.8890	 0.5660
AT	 0.9230	 0.5710
AU	 0.9200	 0.5710
AV	 0.9320	 0.5810
AW	 0.9200	 0.5780
AX	 0.9140	 0.5660
AY	 0.8550	 0.5220
Ae	 0.8900	 0.5510
Af	 0.8890	 0.5580
Ag	 0.8770	 0.5550
Al	 0.8890	 0.5650
Ao	 0.8800	 0.5720
Ap	 0.9110	 0.5670
At	 0.8510	 0.5380
Av	 0.8960	 0.5640
BA	 0.8840	 0.5420
BB	 0.7290	 0.3580
BD	 0.7850	 0.4450
BE	 0.8520	 0.5200
BF	 0.9020	 0.5570
BH	 0.7520	 0.5010



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Chain	Atom inclusion	Q-score
BI	 0.9190	 0.5640
BJ	 0.6700	 0.3940
BK	 0.6680	 0.4270
BL	 0.8590	 0.5030
BN	 0.8450	 0.4590
BO	 0.9000	 0.5500
BQ	 0.8730	 0.5360
BR	 0.8600	 0.5520
BS	 0.8010	 0.4910
BT	 0.9190	 0.5610
BU	 0.8390	 0.5070
BV	 0.4710	 0.2670
BW	 0.9310	 0.5660
BX	 0.3200	 0.4020
BZ	 0.8240	 0.4810
Ba	 0.9180	 0.5690
Bb	 0.8330	 0.4870
Bc	 0.8700	 0.5560
Bf	 0.8040	 0.5340
Bg	 0.8380	 0.5130
Bh	 0.8390	 0.5270
Bi	 0.4560	 0.3450
EA	 0.8580	 0.5460
EB	 0.8820	 0.5740
EC	 0.8910	 0.5780
ED	 0.8930	 0.5520
EE	 0.8070	 0.4970
EF	 0.4010	 0.3220
EG	 0.9270	 0.6010
EH	 0.8520	 0.5160
EI	 0.7070	 0.4690
EJ	 0.8130	 0.4580
EK	 0.6790	 0.3430
EL	 0.9130	 0.5460
EM	 0.7490	 0.5070
EN	 0.7960	 0.4840
EO	 0.7500	 0.3810
EP	 0.6310	 0.2550
EQ	 0.6780	 0.4960
ER	 0.8050	 0.4740
ES	 0.7940	 0.4480
ET	 0.8460	 0.5650

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Chain	Atom inclusion	Q-score
EU	 0.6320	 0.4880
UE	 0.7640	 0.4010
UI	 0.2960	 0.2930
UK	 0.3600	 0.1900
UL	 0.0810	 0.2040
UM	 0.8750	 0.5240
UX	 0.0310	 0.0710