



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:03 AM UTC

PDB ID : 7AOI / pdb_00007aoi
EMDB ID : EMD-11845
Title : Trypanosoma brucei mitochondrial ribosome large subunit assembly intermediate
Authors : Tobiasson, V.; Gahura, O.; Aibara, S.; Baradaran, R.; Zikova, A.; Amunts, A.
Deposited on : 2020-10-14
Resolution : 3.50 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

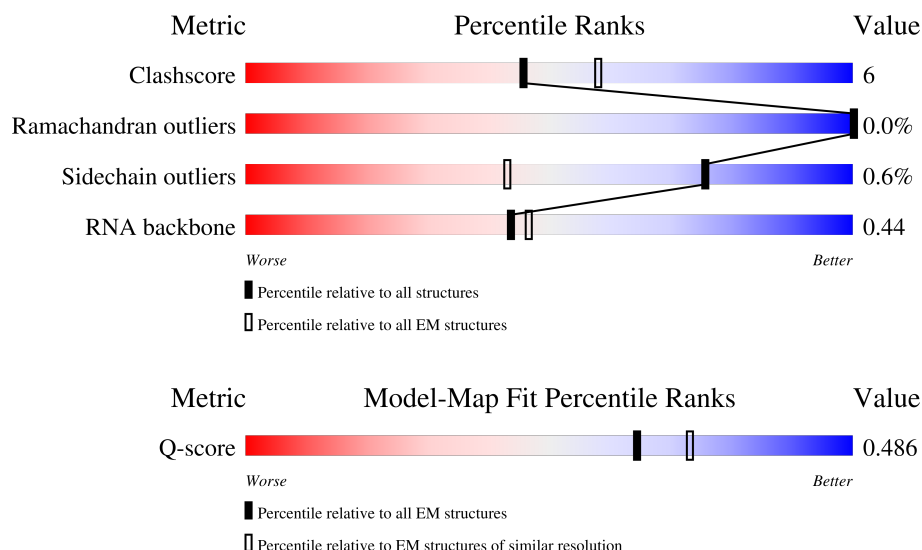
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A1	217	
2	A2	463	
3	A3	150	

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Mol	Chain	Length	Quality of chain
4	A5	55	
5	A8	142	
6	AA	758	
7	AE	367	
8	AF	442	
9	AI	212	
10	AK	278	
11	AN	171	
12	AP	354	
13	AR	256	
14	AT	138	
15	AU	196	
16	AV	180	
17	AW	277	
18	AX	165	
19	AY	340	
20	Ae	116	
21	Af	133	
22	Ag	185	
23	Al	182	
24	Ao	133	
25	Ap	288	
26	At	145	
27	Av	197	
28	BA	798	

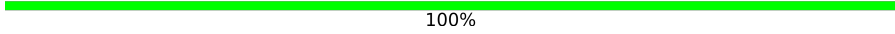
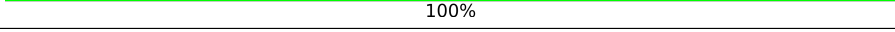
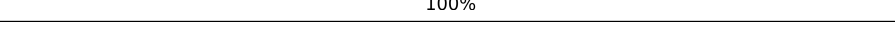
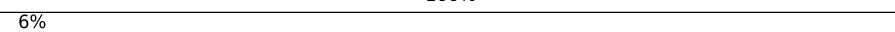
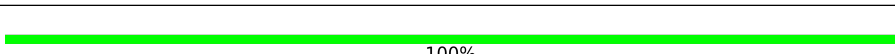
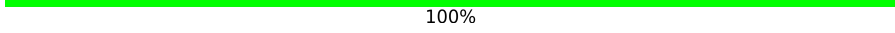
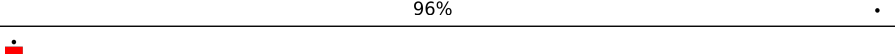
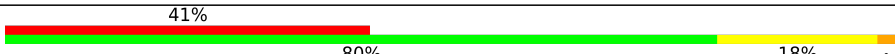
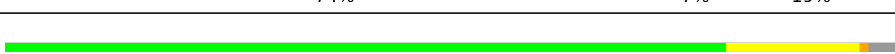
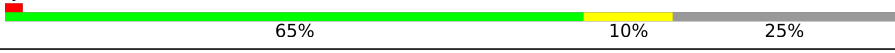
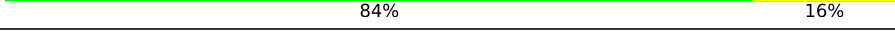
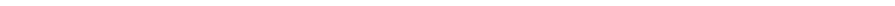
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Mol	Chain	Length	Quality of chain
29	BB	371	
30	BD	417	
31	BE	438	
32	BF	421	
33	BH	225	
34	BI	323	
35	BJ	161	
36	BK	273	
37	BL	276	
38	BN	214	
39	BO	227	
40	BQ	185	
41	BR	195	
42	BS	144	
43	BT	167	
44	BU	82	
45	BW	187	
46	BX	116	
47	BZ	189	
48	Ba	135	
49	Bb	103	
50	Bc	137	
51	Bf	86	
52	Bg	82	
53	Bh	92	

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Mol	Chain	Length	Quality of chain
54	UA	46	
55	UB	9	
56	UC	14	
57	UD	8	
58	UE	12	
59	UF	139	
60	UG	19	
61	UH	17	
62	UI	39	
63	UJ	25	
64	UK	47	
65	XA	155	
66	XB	668	
67	XC	616	
68	XD	83	
68	XE	83	
69	XF	198	
70	XG	170	
71	XH	533	
72	XI	703	
73	XJ	150	
74	XL	528	
75	XM	91	
76	XN	620	
77	XO	428	

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Mol	Chain	Length	Quality of chain
78	XP	371	81%19%
79	XQ	305	7% 78%15%7%
80	XR	161	6% 71%12%15%
81	XS	182	37% 82%17%
82	XT	97	89%11%

2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 156070 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	449	Total	C	N	O	S	0	0
			3638	2324	631	670	13		

- Molecule 3 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A3	150	Total	C	N	O	S	0	0
			1229	782	236	205	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A3	198	ASP	ALA	variant	UNP A0A3L6L456

- 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 bL33m.

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 mt-LSU rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AA	758	Total	C	N	O	P	0	0
			16041	7218	2743	5322	758		

- Molecule 7 is a protein called Ribosomal protein L3 mitochondrial, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AE	361	Total	C	N	O	S	0	0
			2955	1897	502	540	16		

- Molecule 8 is a protein called Ribosomal protein L4/L1 family.

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

- Molecule 9 is a protein called RIBOSOMAL_L9 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	212	Total	C	N	O	S	0	0
			1790	1153	316	312	9		

- Molecule 10 is a protein called Ribosomal protein L11,uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AK	272	Total	C	N	O	S	0	0
			2034	1295	372	357	10		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AN	171	Total	C	N	O	S	0	0
			1432	922	261	240	9		

- Molecule 12 is a protein called Ribosomal_L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AP	310	Total	C	N	O	S	0	0
			2565	1633	474	446	12		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AR	256	Total	C	N	O	S	0	0
			2144	1359	399	372	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AR	24	TRP	TYR	variant	UNP A0A3L6LAG5

- Molecule 14 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AT	138	Total	C	N	O	S	0	0
			1136	717	212	201	6		

- Molecule 15 is a protein called bL20m.

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

- Molecule 16 is a protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AV	180	Total	C	N	O	S	0	0
			1419	906	256	251	6		

- Molecule 17 is a protein called Ribosomal protein L22p/L17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AW	277	Total	C	N	O	S	0	0
			2243	1422	416	392	13		

- Molecule 18 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AX	165	Total	C	N	O	S	0	0
			1391	898	245	243	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AX	126	TYR	HIS	variant	UNP A0A3L6KW11

- Molecule 19 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AY	334	Total	C	N	O	S	0	0
			2741	1711	488	527	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	6	THR	ARG	variant	UNP C9ZK52

- Molecule 20 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Ae	116	Total	C	N	O	S	0	0
			927	594	170	158	5		

- Molecule 21 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Af	133	Total	C	N	O	S	0	0
			1068	670	203	190	5		

- Molecule 22 is a protein called Mitochondrial ribosomal protein L51 / S25 / CI-B8 domain containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Ag	185	Total	C	N	O	S	0	0
			1557	974	294	282	7		

- Molecule 23 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Al	170	Total	C	N	O	S	0	0
			1356	885	235	230	6		

- Molecule 24 is a protein called mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ao	133	Total	C	N	O	S	0	0
			1058	672	193	190	3		

- Molecule 25 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ap	288	Total	C	N	O	S	0	0
			2347	1519	413	403	12		

- Molecule 26 is a protein called mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	At	145	Total	C	N	O	S	0	0
			1203	752	235	212	4		

- Molecule 27 is a protein called mL64,mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Av	196	Total	C	N	O	S	0	0
			1661	1052	312	285	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Av	163	ARG	ILE	variant	UNP A0A3L6KTC7

- Molecule 28 is a protein called mL67.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BA	727	Total	C	N	O	S	0	0
			5779	3673	1022	1050	34		

- Molecule 29 is a protein called mL68,mL68,mL68.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BB	371	Total	C	N	O	S	0	0
			2862	1819	514	517	12		

- Molecule 30 is a protein called mL70.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BD	417	Total	C	N	O	S	0	0
			3339	2128	584	607	20		

- Molecule 31 is a protein called mL71.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BE	401	Total	C	N	O	S	0	0
			3178	2014	552	599	13		

- Molecule 32 is a protein called Tetratricopeptide repeat.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BF	341	Total	C	N	O	S	0	0
			2805	1778	510	504	13		

- Molecule 33 is a protein called mL74.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BH	225	Total	C	N	O	S	0	0
			1831	1171	330	327	3		

- Molecule 34 is a protein called Mitochondrial RNA binding complex 1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	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	variant	UNP A0A3L6KZH2

- Molecule 35 is a protein called mL76.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BJ	161	Total	C	N	O	S	0	0
			1329	826	257	240	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BJ	329	GLU	ALA	conflict	UNP A0A3L6KX00

- Molecule 36 is a protein called Chaperone protein DNAj, putative,mL77,Chaperone protein DNAj, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BK	242	Total	C	N	O	S	0	0
			1922	1193	367	354	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	348	THR	LEU	variant	UNP C9ZQR6

- Molecule 37 is a protein called mL78.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	234	Total	C	N	O	S	0	0
			1887	1158	370	349	10		

- Molecule 38 is a protein called mL80.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BN	214	Total	C	N	O	S	0	0
			1793	1126	331	330	6		

- Molecule 39 is a protein called mL81.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BO	211	Total	C	N	O	S	0	0
			1665	1043	293	316	13		

- Molecule 40 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BQ	185	Total	C	N	O	S	0	0
			1429	908	247	267	7		

- Molecule 41 is a protein called mL84.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BR	195	Total	C	N	O	S	0	0
			1650	1059	298	284	9		

- Molecule 42 is a protein called mL85.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BS	144	Total	C	N	O	S	0	0
			1185	732	225	221	7		

- Molecule 43 is a protein called mL86.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BT	167	Total	C	N	O	S	0	0
			1380	848	268	258	6		

- Molecule 44 is a protein called mL87.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BU	82	Total	C	N	O	S	0	0
			694	436	139	115	4		

- Molecule 45 is a protein called mL89.

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

- Molecule 46 is a protein called LIM domain containing protein,mL90.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BX	107	Total	C	N	O	S	0	0
			867	552	160	147	8		

- Molecule 47 is a protein called Peptidyl-prolyl cis-trans isomerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BZ	189	Total	C	N	O	S	0	0
			1433	903	246	278	6		

- Molecule 48 is a protein called mL93.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ba	135	Total	C	N	O	S	0	0
			1191	763	217	204	7		

- Molecule 49 is a protein called mL94.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Bb	103	Total	C	N	O	S	0	0
			805	504	152	147	2		

- Molecule 50 is a protein called mL95.

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

- Molecule 51 is a protein called mL98.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Bf	80	Total	C	N	O	S	0	0
			676	432	124	120			

- Molecule 52 is a protein called mL99.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Bg	82	Total	C	N	O	S	0	0
			656	412	126	116	2		

- Molecule 53 is a protein called mL100,mL100.

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

- Molecule 54 is a protein called UNK1.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	UA	46	Total	C	N	O	0	0
			230	138	46	46		

- Molecule 55 is a protein called UNK2.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	UB	9	Total	C	N	O	0	0
			45	27	9	9		

- Molecule 56 is a protein called UNK3.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	UC	14	Total	C	N	O	0	0
			70	42	14	14		

- Molecule 57 is a protein called UNK4.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	UD	8	Total	C	N	O	0	0
			40	24	8	8		

- Molecule 58 is a protein called UNK5.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	UE	12	Total	C	N	O	0	0
			60	36	12	12		

- Molecule 59 is a protein called UNK6/mt-LAF15_2.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	UF	139	Total	C	N	O	0	0
			695	417	139	139		

- Molecule 60 is a protein called UNK7.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	UG	19	Total	C	N	O	0	0
			95	57	19	19		

- Molecule 61 is a protein called UNK8.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	UH	17	Total	C	N	O	0	0
			85	51	17	17		

- Molecule 62 is a protein called UNK9.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	UI	39	Total	C	N	O	0	0
			195	117	39	39		

- Molecule 63 is a protein called UNK10.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	UJ	25	Total	C	N	O	0	0
			125	75	25	25		

- Molecule 64 is a protein called UNK11.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	UK	47	Total	C	N	O	0	0
			235	141	47	47		

- Molecule 65 is a protein called mt-LAF7,mt-LAF7.

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

- Molecule 66 is a protein called DEAD-box helicase, putative,mt-LAF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	XB	614	Total	C	N	O	S	0	0
			4944	3123	947	848	26		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XB	301	ALA	THR	conflict	UNP D0A9G9
XB	462	GLY	GLU	conflict	UNP D0A9G9

- Molecule 67 is a protein called mt-LAF4.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	XC	584	Total	C	N	O	S	0	0
			4652	2958	831	840	23		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XC	69	PRO	ALA	conflict	UNP D0A7A5

- Molecule 68 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	XD	83	Total	C	N	O	P	S	0	0
			685	434	107	141	1	2		
68	XE	83	Total	C	N	O	P	S	0	0
			685	434	107	141	1	2		

- Molecule 69 is a protein called mt-LAF15_1.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	XF	161	Total	C	N	O	S	0	0
			1264	801	231	227	5		

- Molecule 70 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	XG	164	Total	C	N	O	S	0	0
			1330	837	270	214	9		

- Molecule 71 is a protein called mt-LAF8.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	XH	402	Total	C	N	O	S	0	0
			3208	2029	584	581	14		

- Molecule 72 is a protein called mt-LAF14.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	XI	597	Total	C	N	O	S	0	0
			4736	2978	858	874	26		

- Molecule 73 is a protein called RNA uridylyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	XJ	150	Total	C	N	O	S	0	0
			1212	764	211	228	9		

- Molecule 74 is a protein called GTP-binding protein, putative,mt-EngA.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	XL	521	Total	C	N	O	S	0	0
			4169	2609	771	768	21		

- Molecule 75 is a protein called Complex1-LYR-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	XM	91	Total	C	N	O	S	0	0
			744	462	152	127	3		

- Molecule 76 is a protein called mt-LAF12.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	XN	541	Total	C	N	O	S	0	0
			4358	2801	757	772	28		

- Molecule 77 is a protein called SpoU rRNA Methylase family.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	XO	398	Total	C	N	O	S	0	0
			3193	1992	603	587	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XO	337	ASP	GLY	conflict	UNP A0A3L6L241

- Molecule 78 is a protein called Pseudouridylate synthase, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	XP	371	Total	C	N	O	S	0	0
			2995	1918	538	521	18		

- Molecule 79 is a protein called GTP-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	XQ	283	Total	C	N	O	S	0	0
			2206	1393	397	403	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XQ	331	ALA	PHE	conflict	UNP A0A3L6L0D5

- Molecule 80 is a protein called Lipase (Class 3).

Mol	Chain	Residues	Atoms					AltConf	Trace
80	XR	137	Total	C	N	O	S	0	0
			1135	702	220	210	3		

- Molecule 81 is a protein called mL101.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	XS	182	Total	C	N	O	S	0	0
			1532	971	282	274	5		

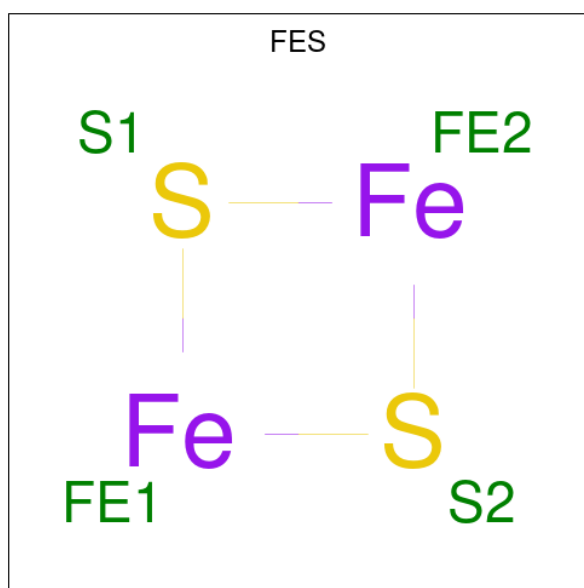
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XS	163	VAL	LEU	conflict	UNP Q4GZ80

- Molecule 82 is a protein called mt-LAF19.

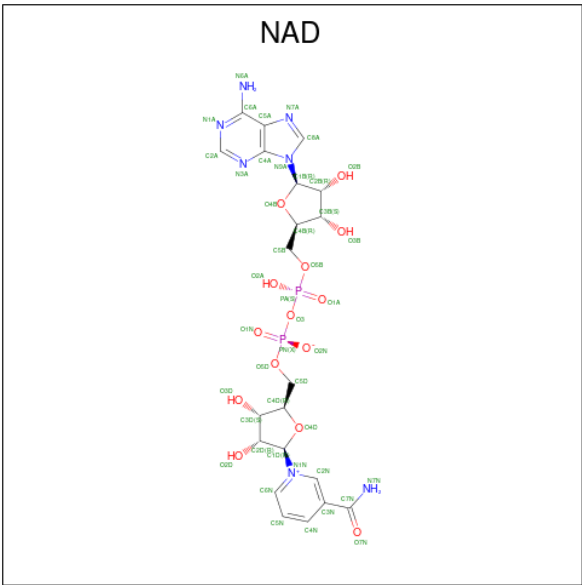
Mol	Chain	Residues	Atoms					AltConf	Trace
82	XT	97	Total	C	N	O	S	0	0
			801	505	156	136	4		

- Molecule 83 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
83	A5	1	Total	Fe	S	0
			4	2	2	

- Molecule 84 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



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

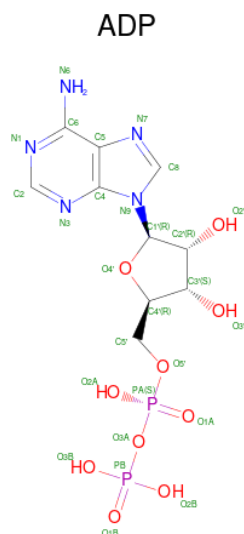
- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	BX	2	Total	Zn	0
			2	2	
85	Bh	1	Total	Zn	0
			1	1	
85	XA	1	Total	Zn	0
			1	1	

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

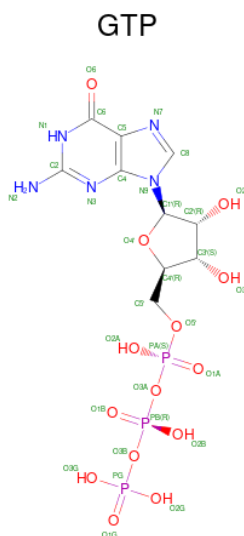
Mol	Chain	Residues	Atoms		AltConf
86	XB	1	Total	Mg	0
			1	1	

- Molecule 87 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
87	XB	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 88 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

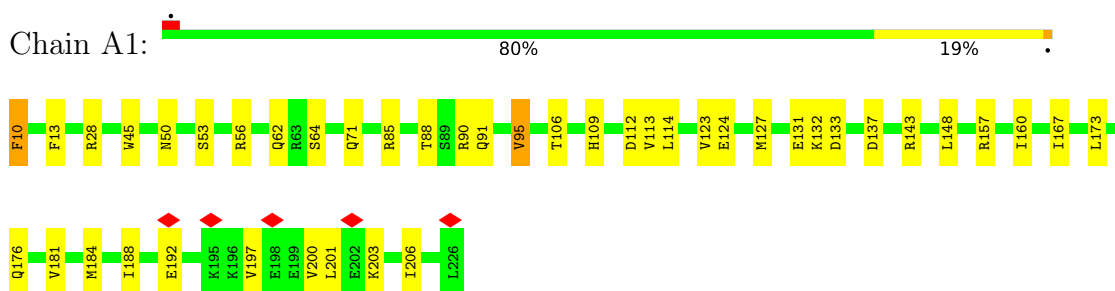


Mol	Chain	Residues	Atoms					AltConf
88	XL	1	Total 32	C 10	N 5	O 14	P 3	0
88	XL	1	Total 32	C 10	N 5	O 14	P 3	0

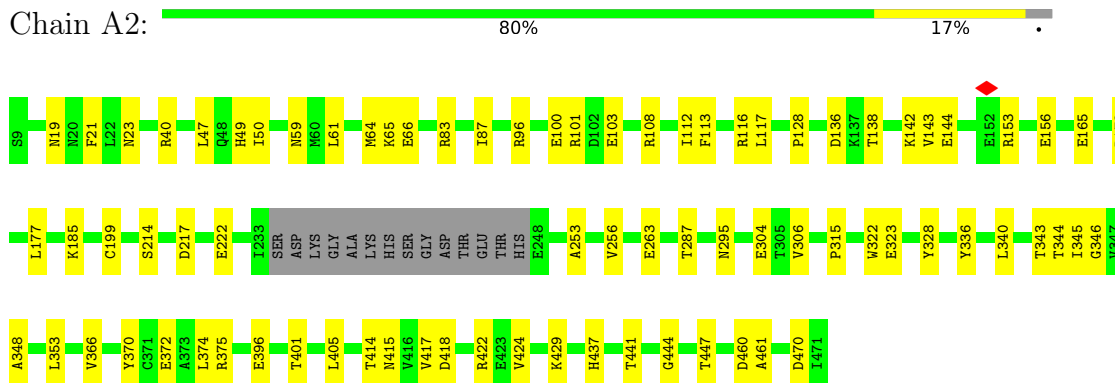
3 Residue-property plots [i](#)

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.

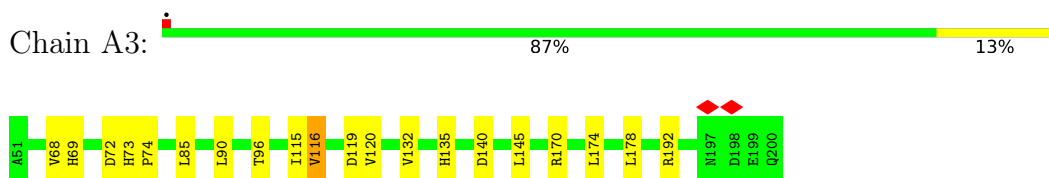
• Molecule 1: bL28m



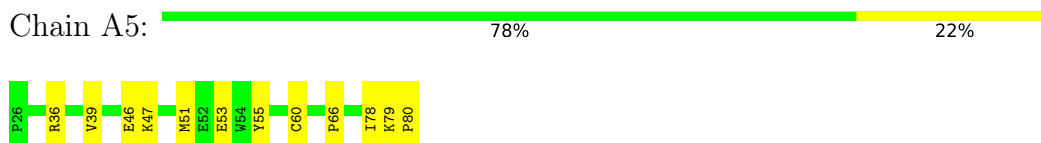
• Molecule 2: uL29m



• Molecule 3: uL30m



• Molecule 4: bL32m



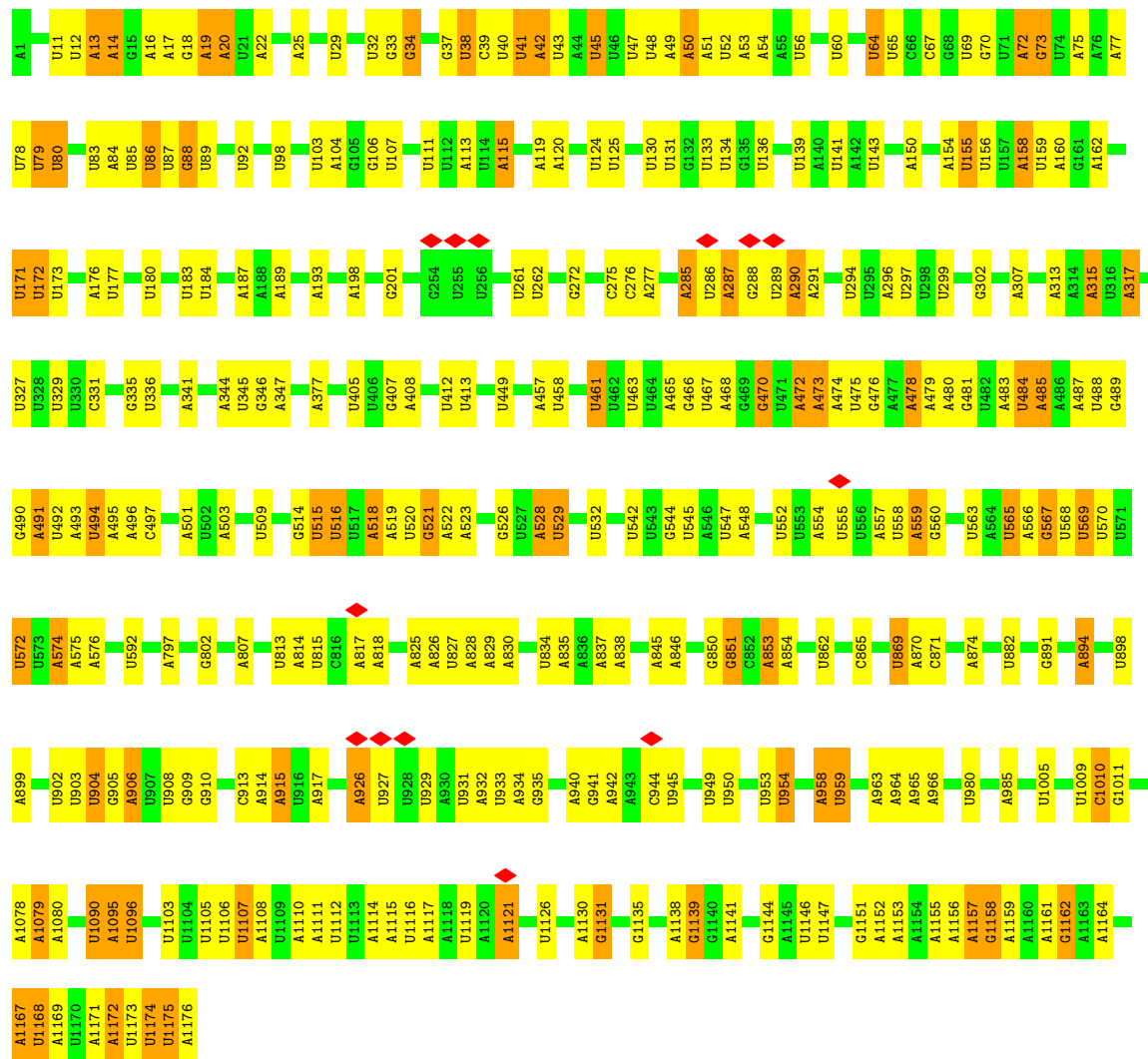
- Molecule 5: bL33m

Chain A8:  85% 15%



- Molecule 6: mt-LSU rRNA

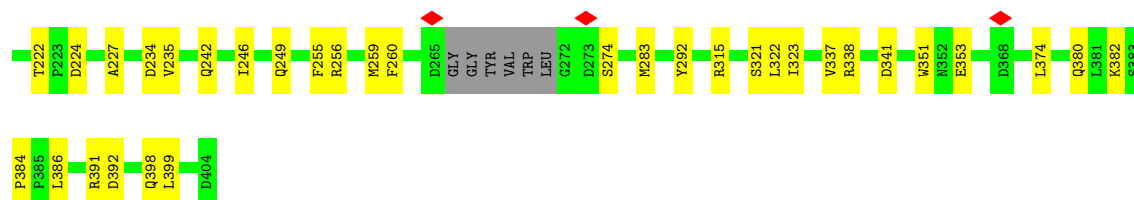
Chain AA:  56% 34% 10%



- Molecule 7: Ribosomal protein L3 mitochondrial, putative

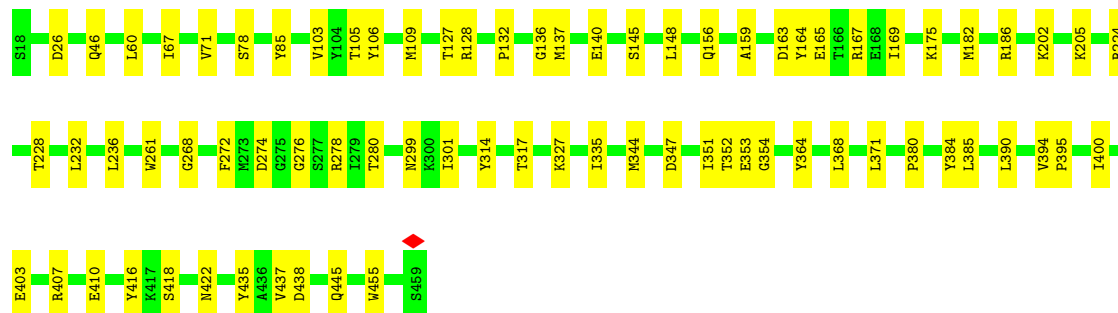
Chain AE:  80% 19%





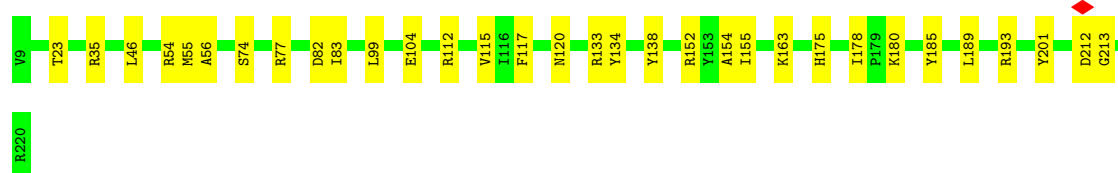
• Molecule 8: Ribosomal protein L4/L1 family

Chain AF: 83% 17%



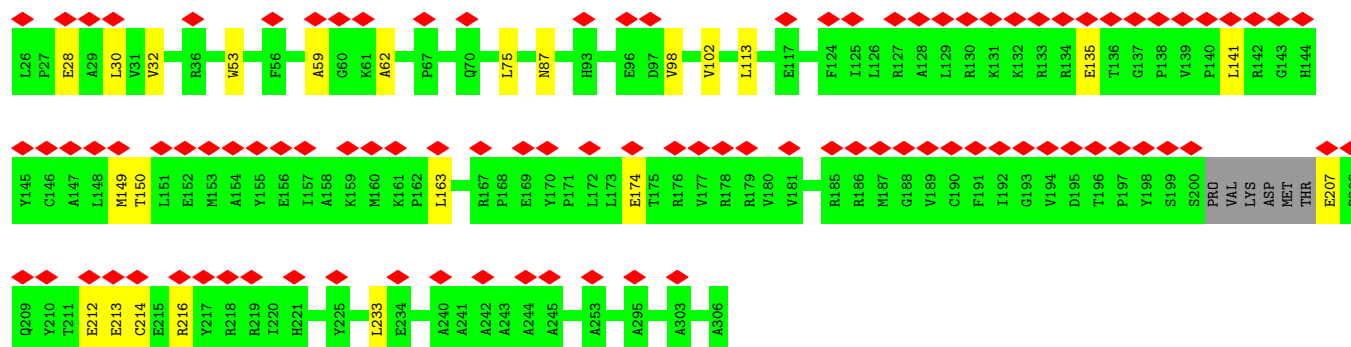
• Molecule 9: RIBOSOMAL_L9 domain-containing protein

Chain AI: 85% 15%



• Molecule 10: Ribosomal protein L11,uL11m

Chain AK: 35% 90% 8%



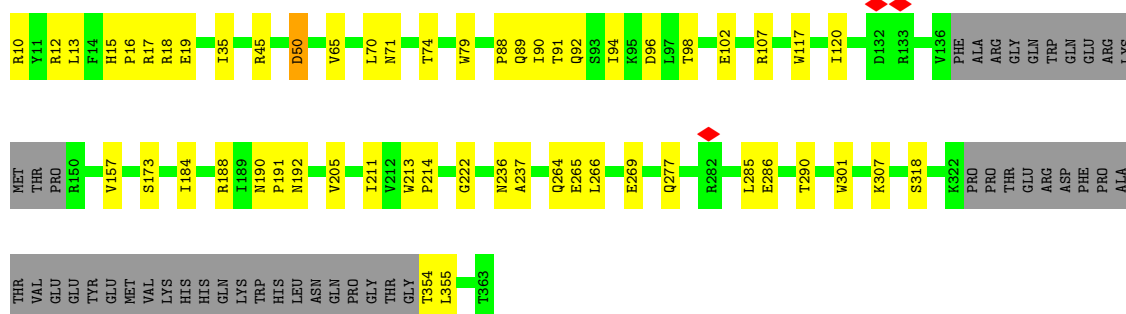
• Molecule 11: 50S ribosomal protein L13

Chain AN: 85% 15%



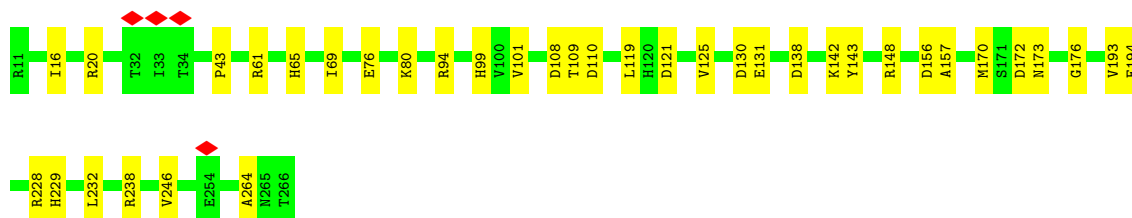
- Molecule 12: Ribosomal_L18e/L15P domain-containing protein

Chain AP: 72% 15% 12%



- Molecule 13: 50S ribosomal protein L17

Chain AR: 86% 14%



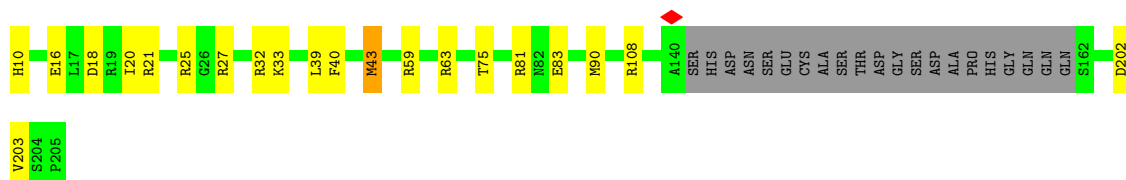
- Molecule 14: bL19m

Chain AT: 79% 20%



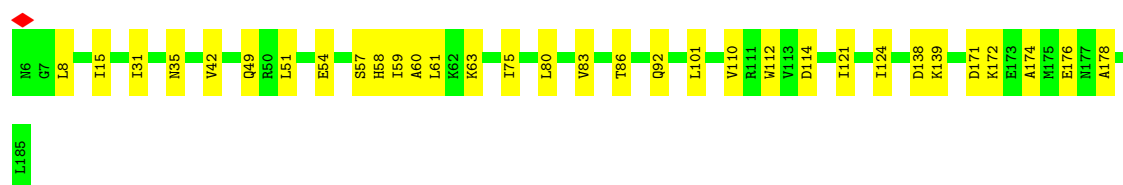
- Molecule 15: bL20m

Chain AU: 79% 10% 11%



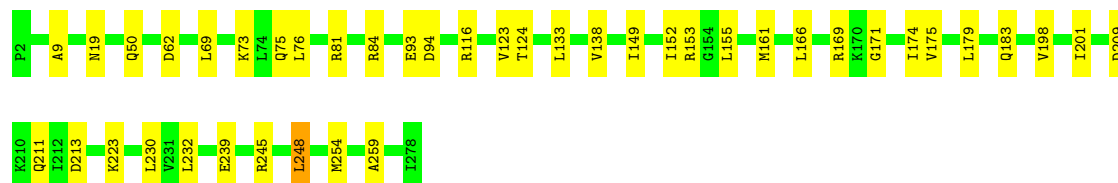
- Molecule 16: Ribosomal protein L21

Chain AV: 82% 18%



- Molecule 17: Ribosomal protein L22p/L17e

Chain AW: 85% 15%



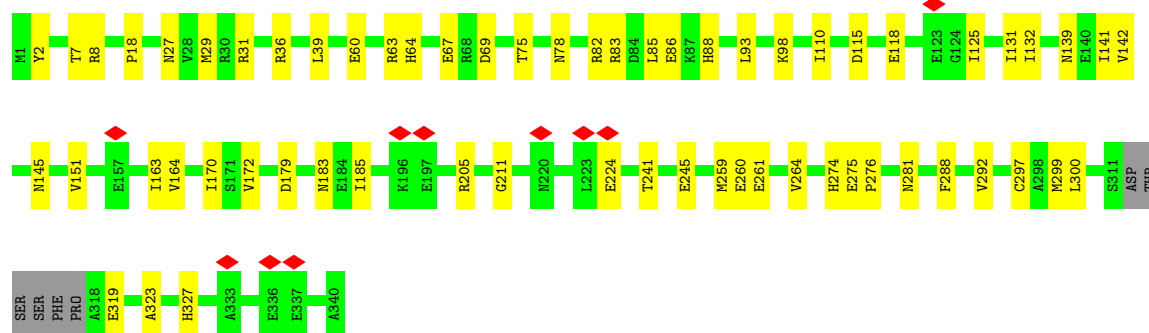
- Molecule 18: Ribosomal protein L23

Chain AX: 88% 12%



- Molecule 19: uL24m

Chain AY: 80% 18%



- Molecule 20: mL41

Chain Ae: 88% 12%

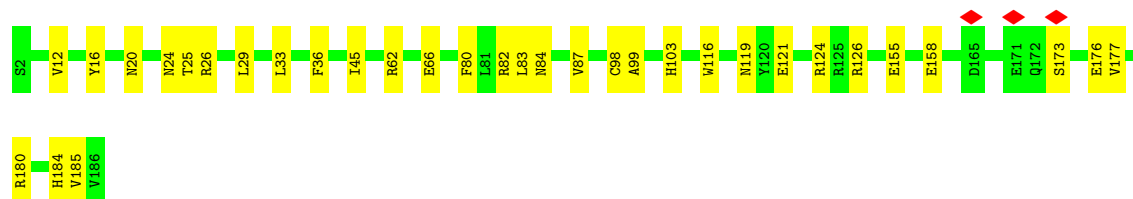
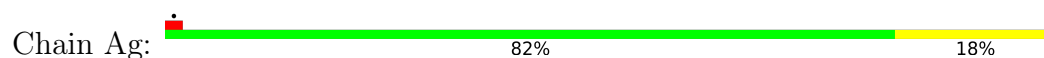


- Molecule 21: mL42

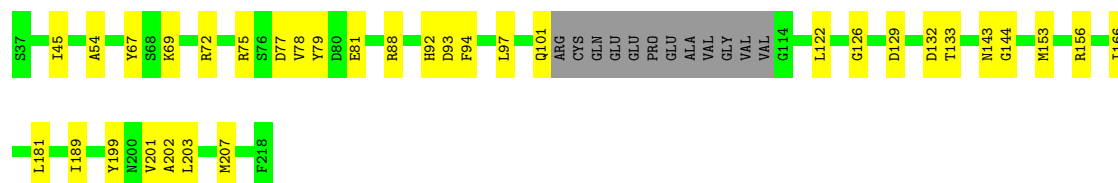
Chain Af: 84% 16%



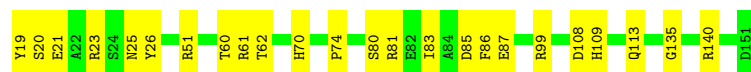
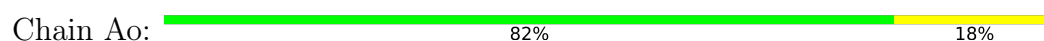
- Molecule 22: Mitochondrial ribosomal protein L51 / S25 / CI-B8 domain containing protein



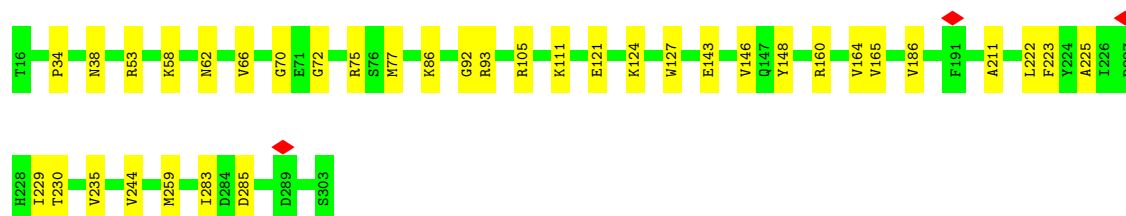
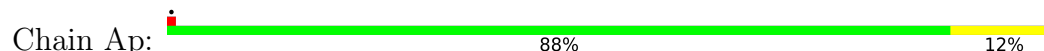
- Molecule 23: mL49



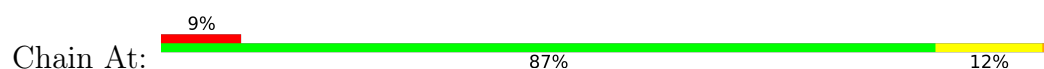
- Molecule 24: mL52



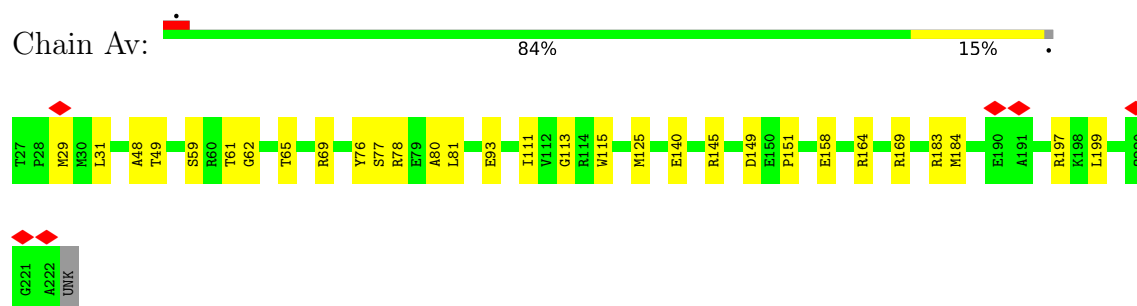
- Molecule 25: mL53



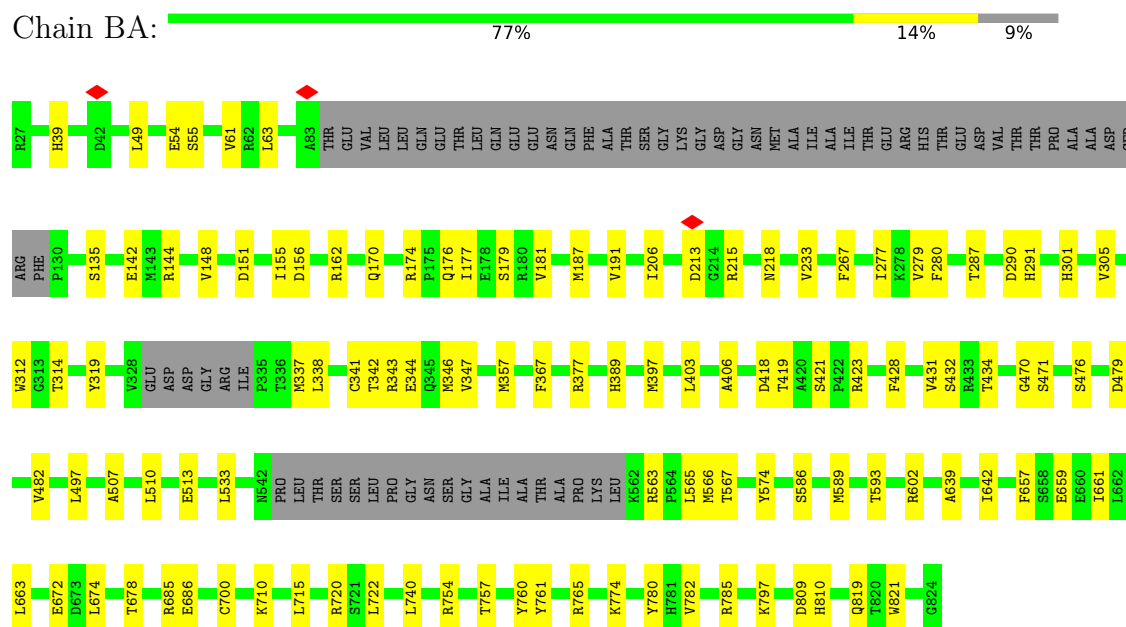
- Molecule 26: mL63



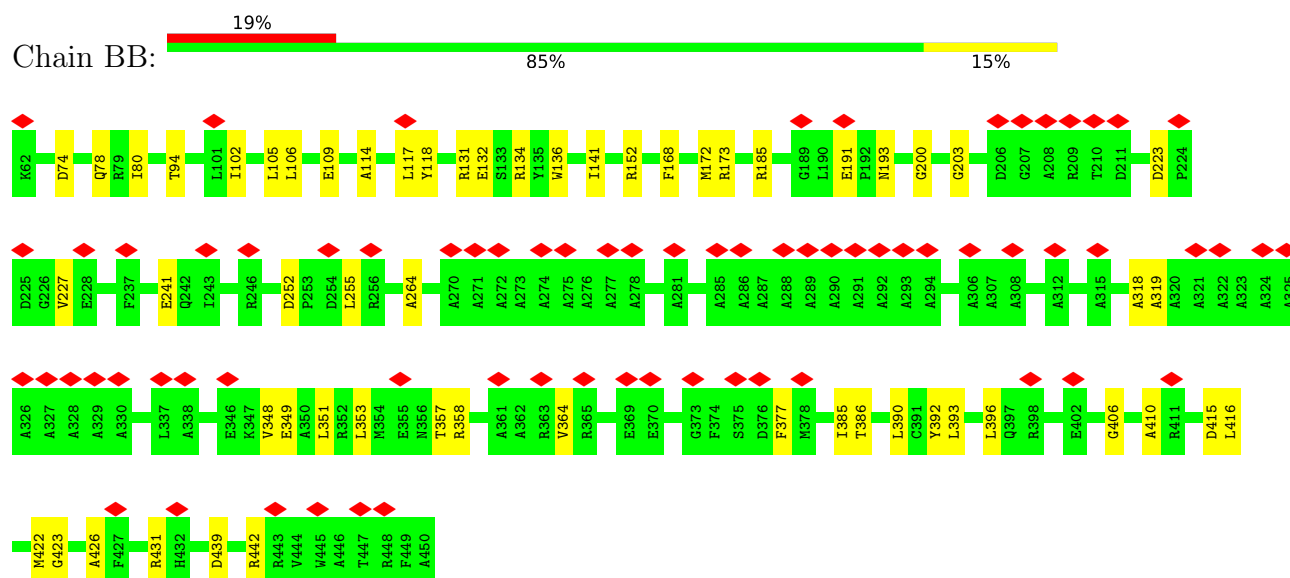
- Molecule 27: mL64,mL64



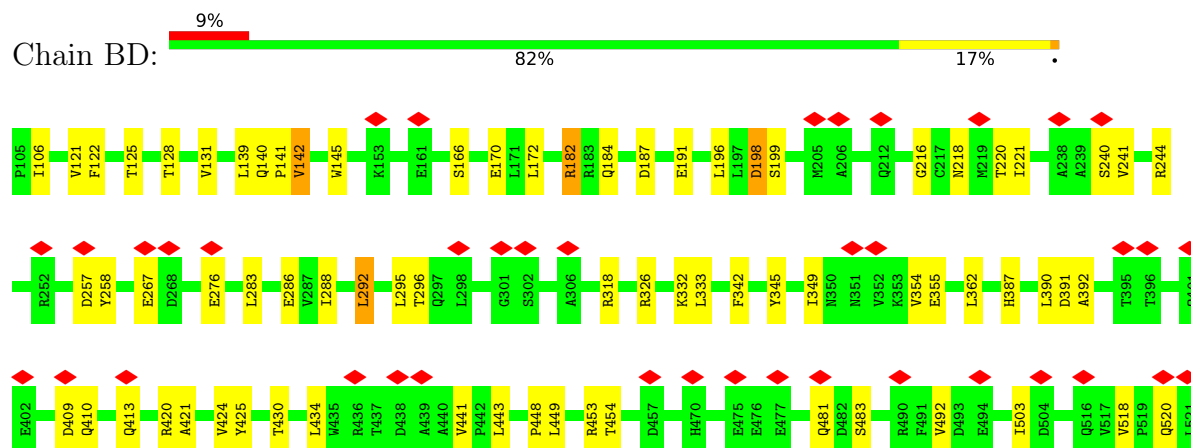
- Molecule 28: mL67



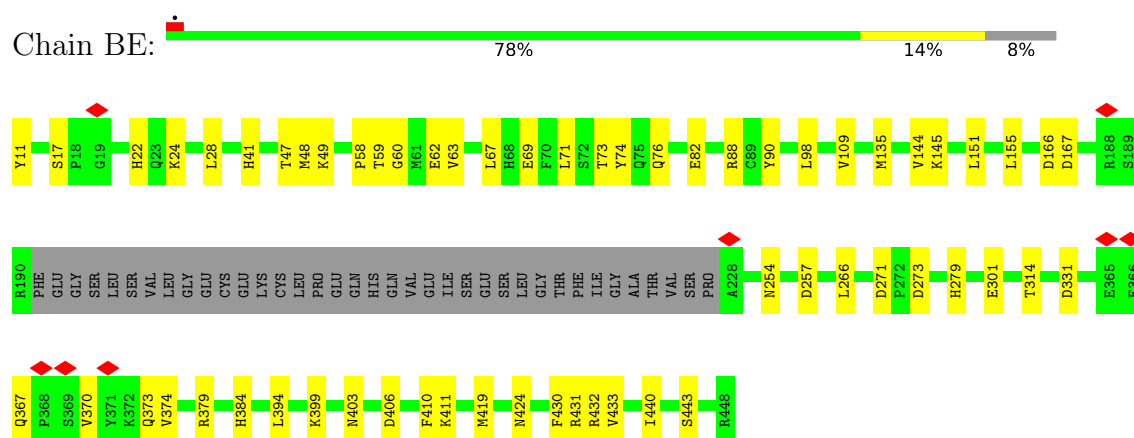
- Molecule 29: mL68,mL68,mL68



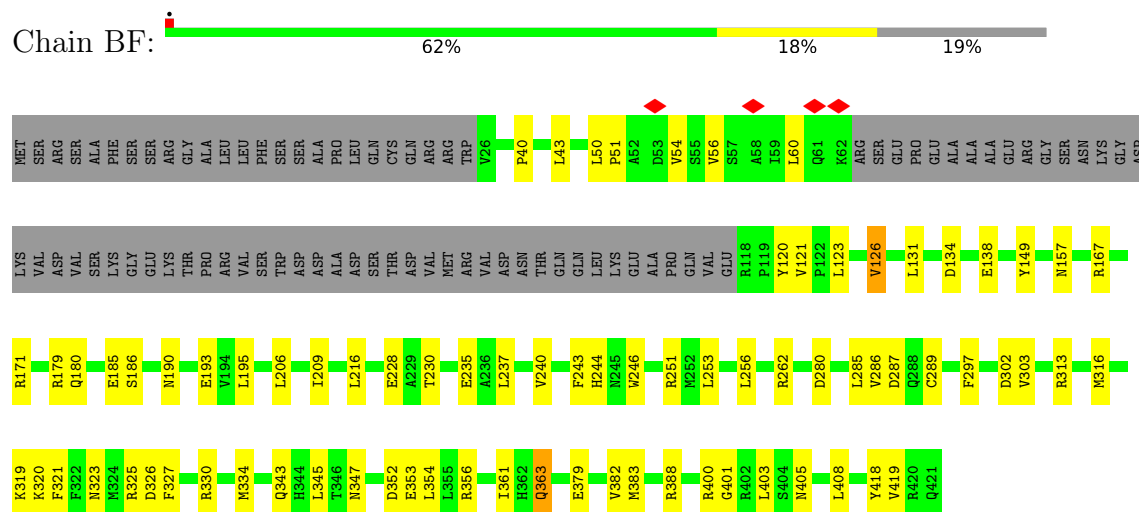
- Molecule 30: mL70



- Molecule 31: mL71

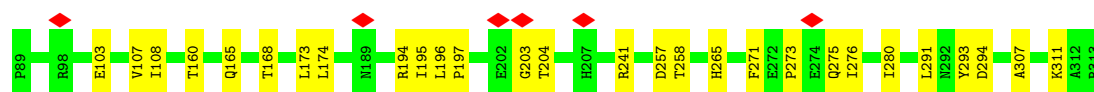


- Molecule 32: Tetratricopeptide repeat



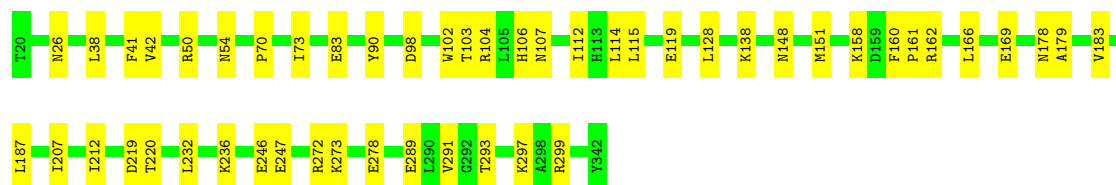
- Molecule 33: mL74





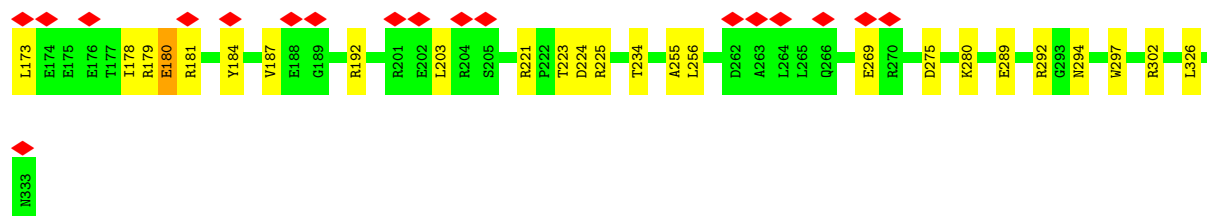
- Molecule 34: Mitochondrial RNA binding complex 1 subunit

Chain BI:



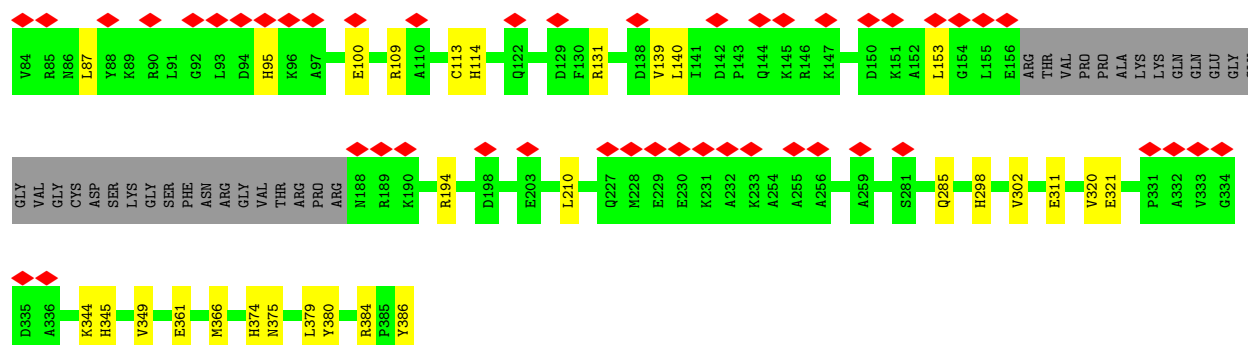
- Molecule 35: mL76

Chain BJ:



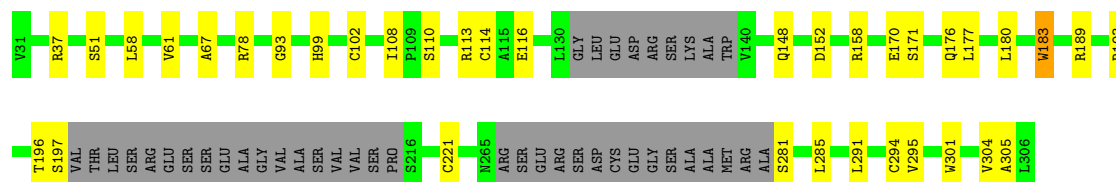
- Molecule 36: Chaperone protein DNAj, putative, mL77, Chaperone protein DNAj, putative

Chain BK:

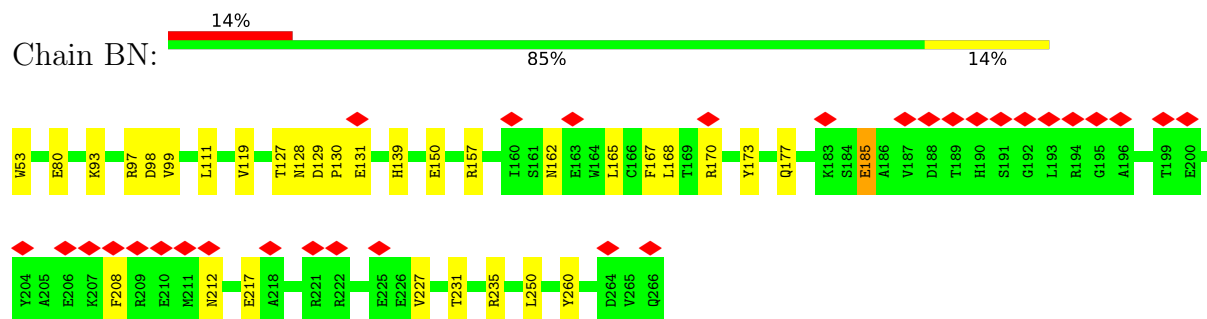


- Molecule 37: mL78

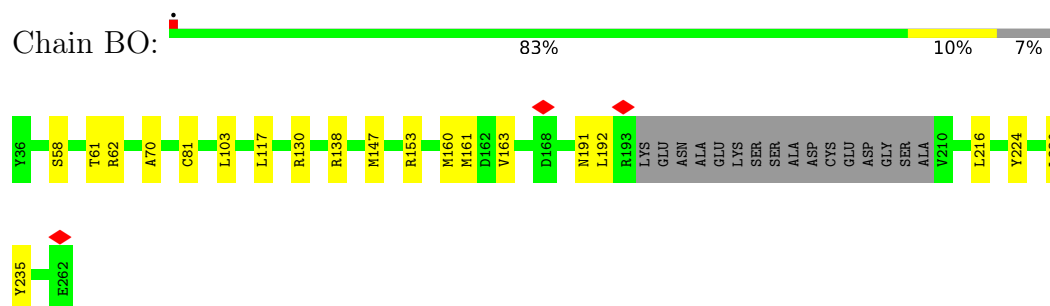
Chain BL:



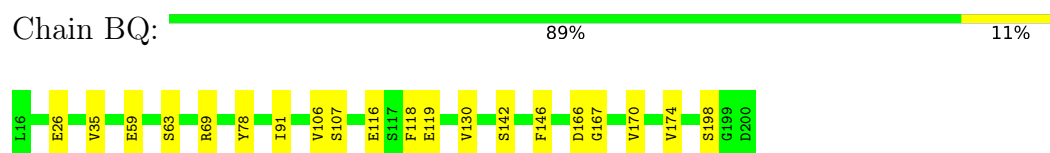
- Molecule 38: mL80



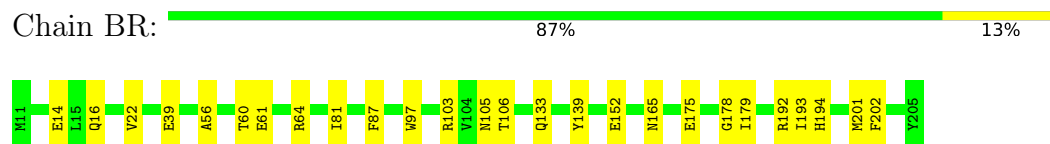
- Molecule 39: mL81



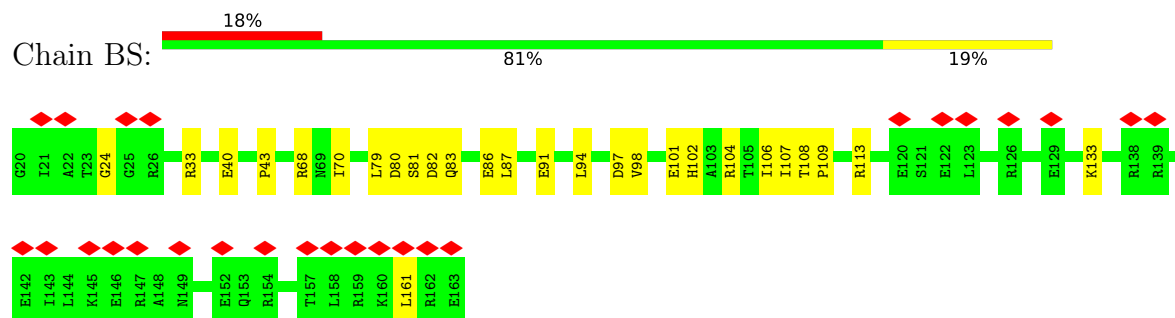
- Molecule 40: Peptidyl-prolyl cis-trans isomerase



- Molecule 41: mL84



- Molecule 42: mL85

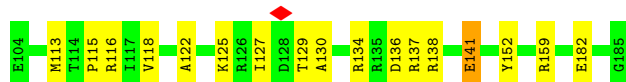
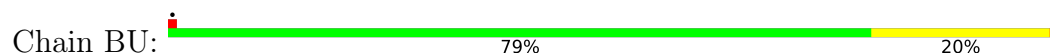


- Molecule 43: mL86

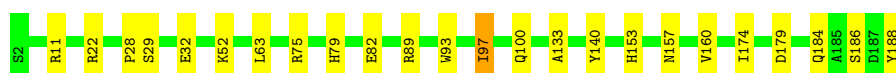




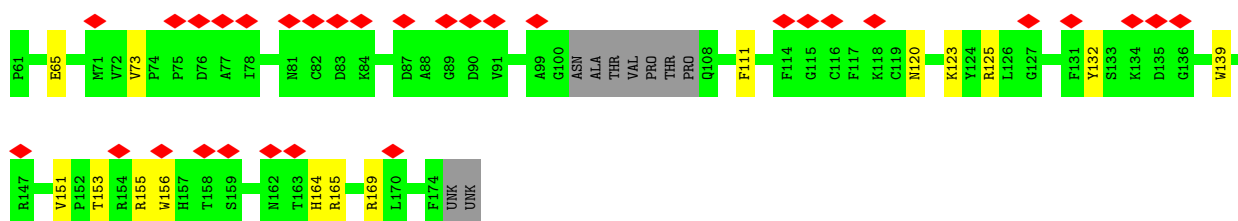
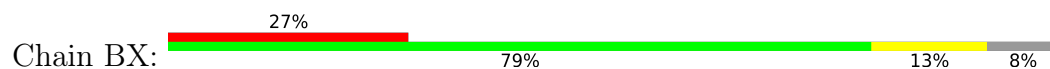
- Molecule 44: mL87



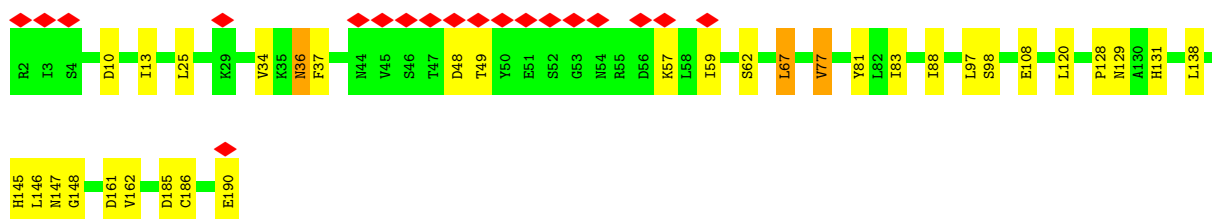
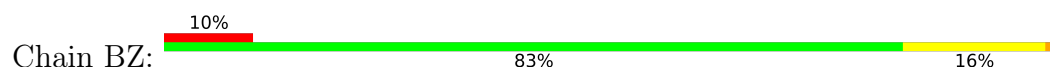
- Molecule 45: mL89



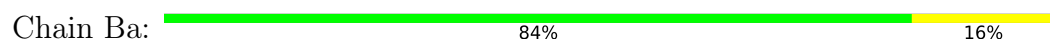
- Molecule 46: LIM domain containing protein, mL90



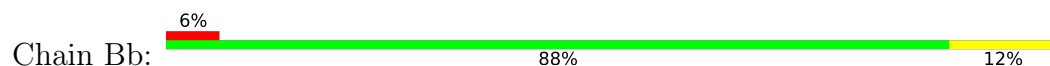
- Molecule 47: Peptidyl-prolyl cis-trans isomerase

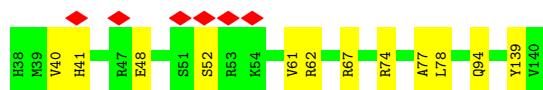


- Molecule 48: mL93



- Molecule 49: mL94

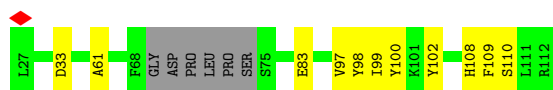
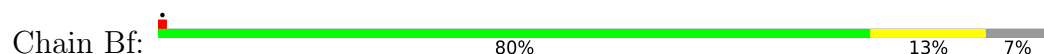




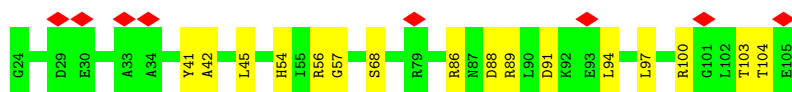
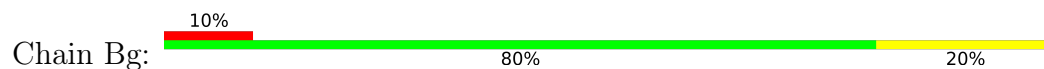
- Molecule 50: mL95



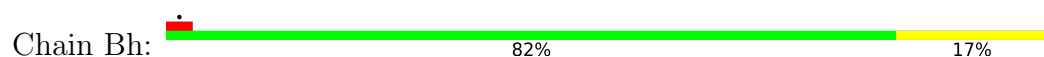
- Molecule 51: mL98



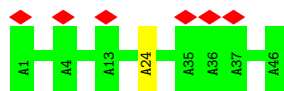
- Molecule 52: mL99



- Molecule 53: mL100,mL100



- Molecule 54: UNK1



- Molecule 55: UNK2



There are no outlier residues recorded for this chain.

- Molecule 56: UNK3



There are no outlier residues recorded for this chain.

- Molecule 57: UNK4

Chain UD:  100%

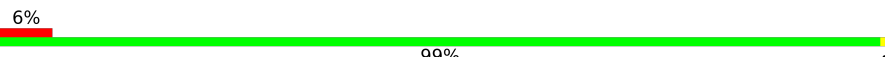
There are no outlier residues recorded for this chain.

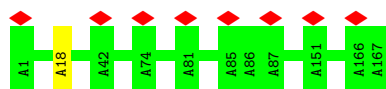
- Molecule 58: UNK5

Chain UE:  100%

There are no outlier residues recorded for this chain.

- Molecule 59: UNK6/mt-LAF15_2

Chain UF:  6% 99%



- Molecule 60: UNK7

Chain UG:  100%

There are no outlier residues recorded for this chain.

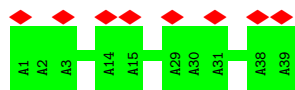
- Molecule 61: UNK8

Chain UH:  100%

There are no outlier residues recorded for this chain.

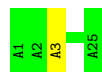
- Molecule 62: UNK9

Chain UI:  21% 100%



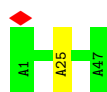
- Molecule 63: UNK10

Chain UJ:  96%



- Molecule 64: UNK11

Chain UK:  98%



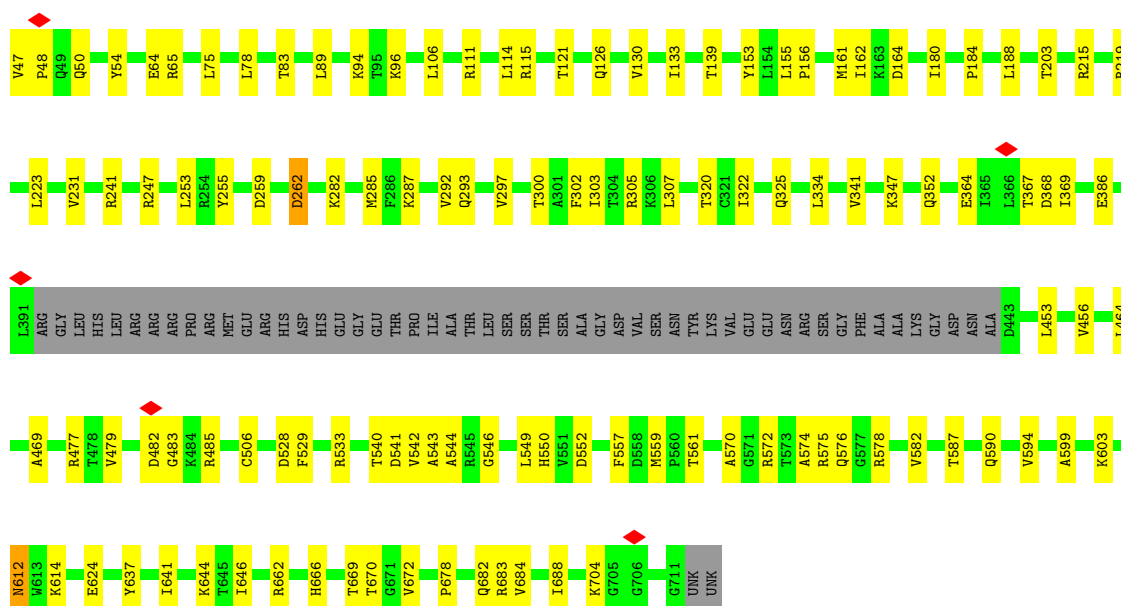
- Molecule 65: mt-LAF7,mt-LAF7

Chain XA: 83% 16%



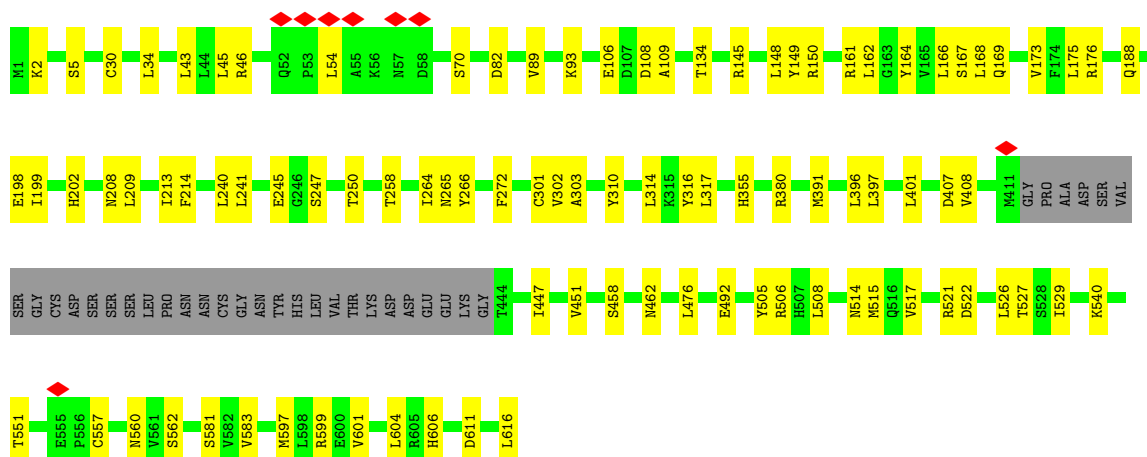
- Molecule 66: DEAD-box helicase, putative,mt-LAF2

Chain XB: 74% 18% 8%

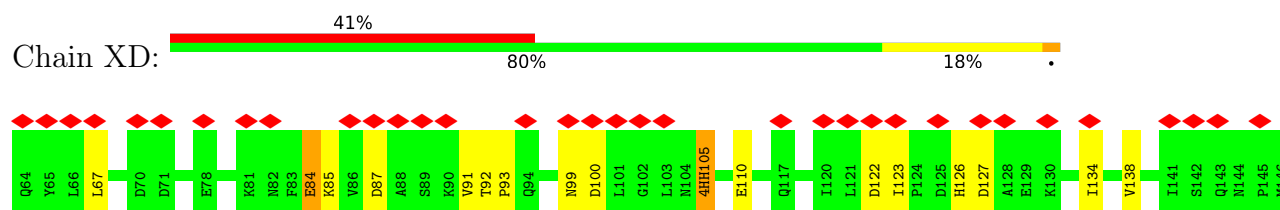


- Molecule 67: mt-LAF4

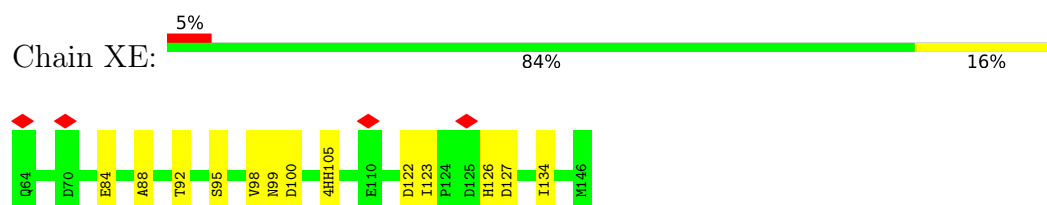
Chain XC: 80% 15% 5%



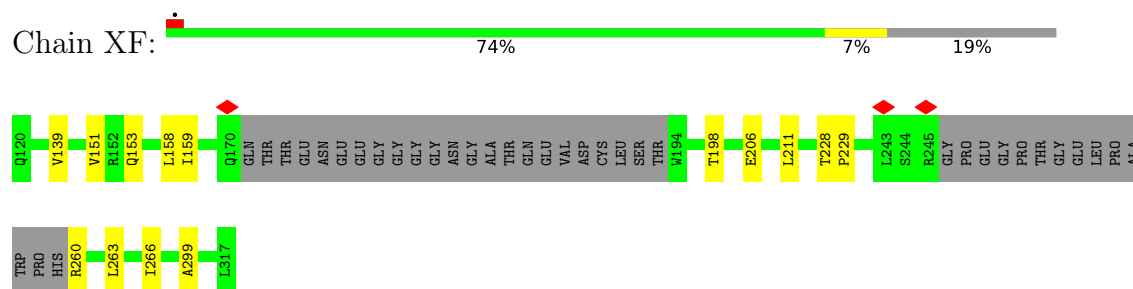
- Molecule 68: Acyl carrier protein

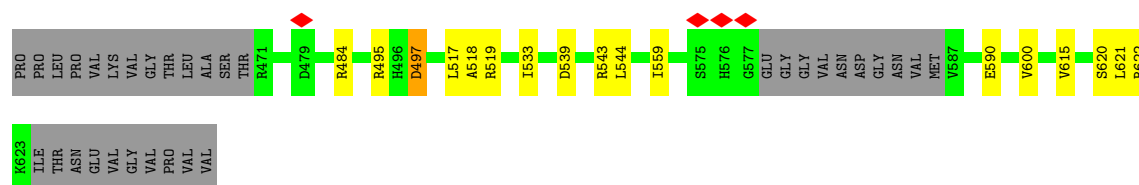


- Molecule 68: Acyl carrier protein



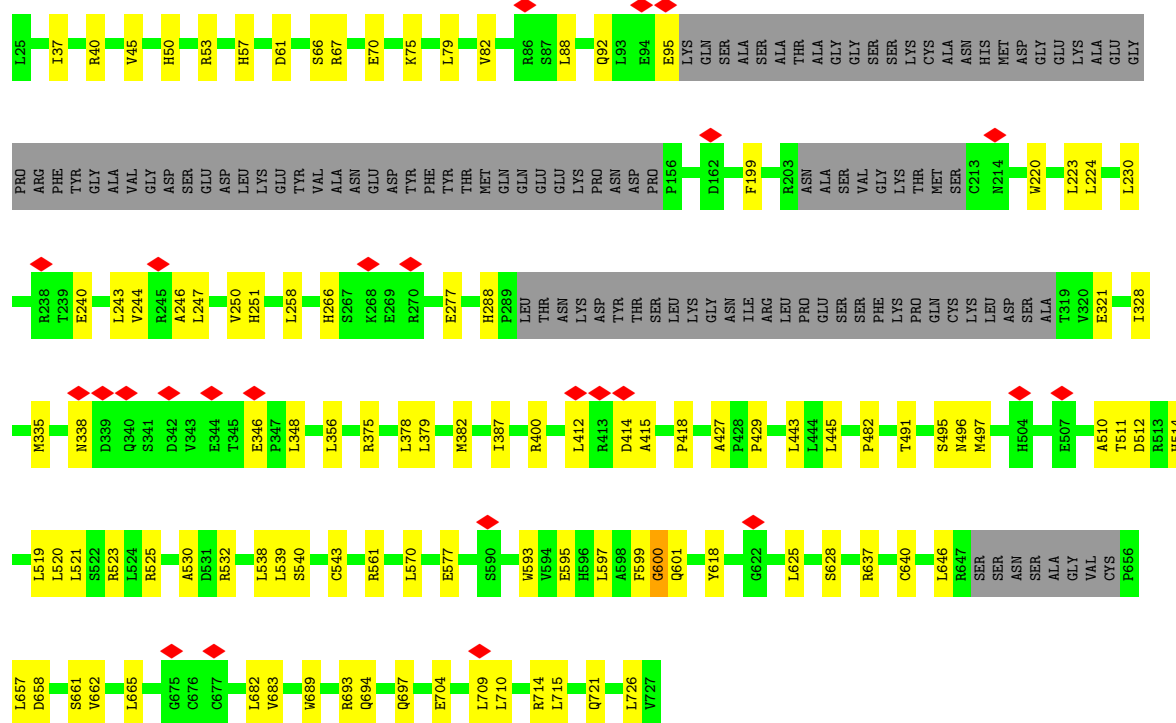
- Molecule 69: mt-LAF15_1





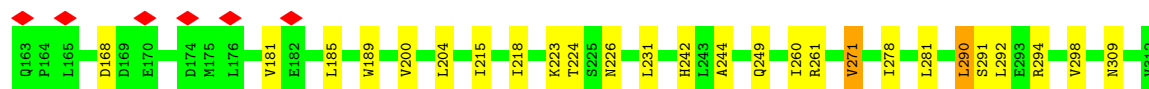
• Molecule 72: mt-LAF14

Chain XI: 70% 15% 15%



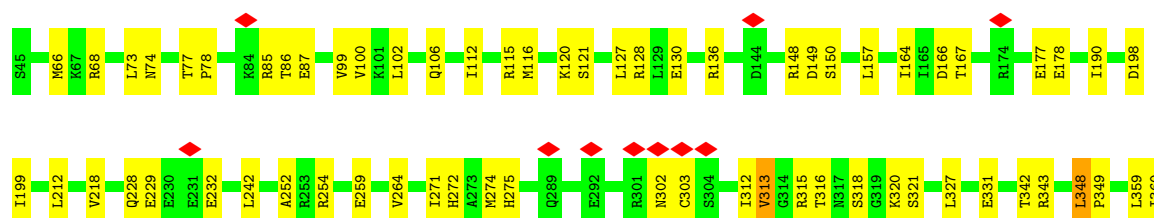
• Molecule 73: RNA uridylyltransferase

Chain XJ: 83% 16% .

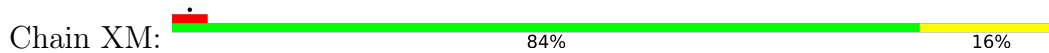


• Molecule 74: GTP-binding protein, putative,mt-EngA

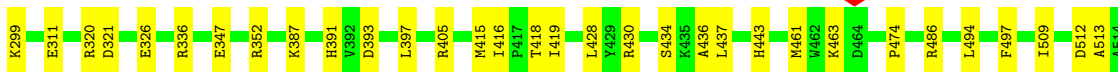
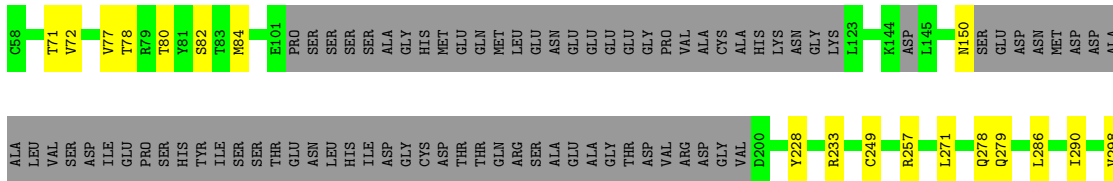
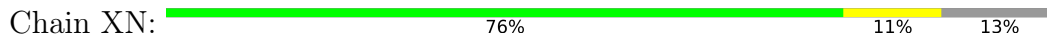
Chain XL: 78% 20% .



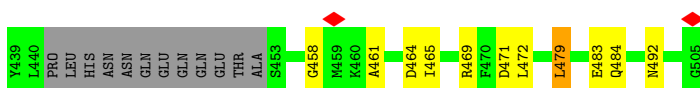
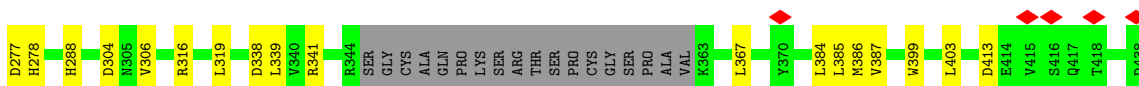
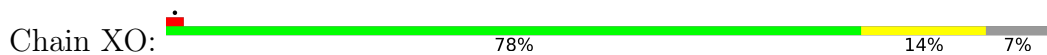
- Molecule 75: Complex1-LYR-like



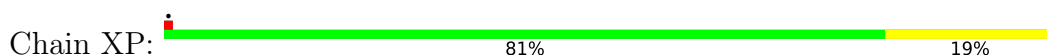
- Molecule 76: mt-LAF12

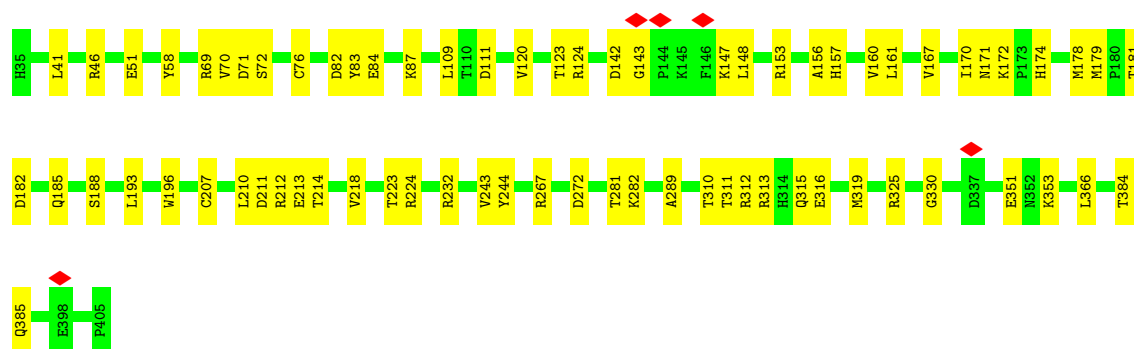


- Molecule 77: SpoU rRNA Methylase family

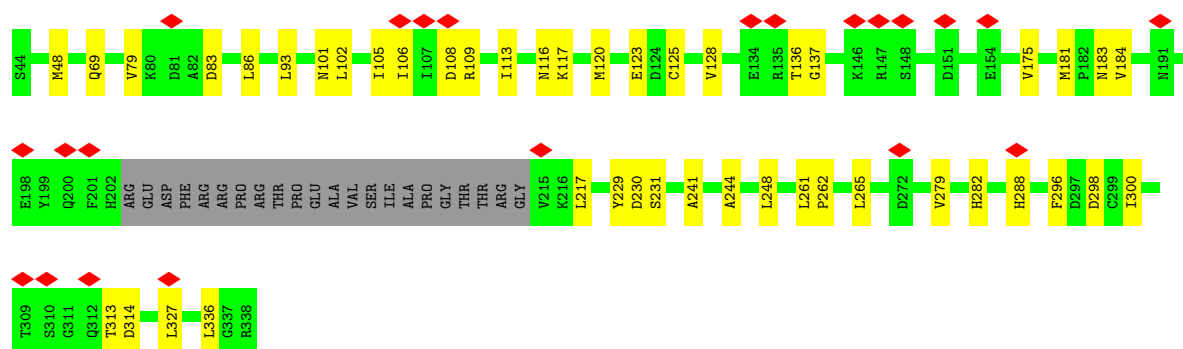
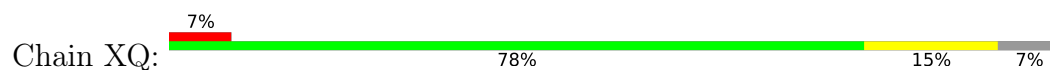


- Molecule 78: Pseudouridylate synthase, putative

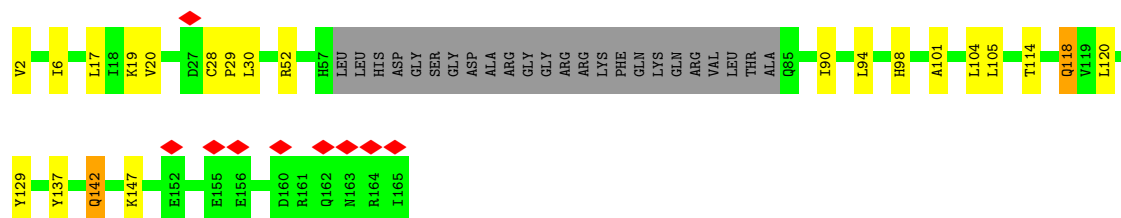
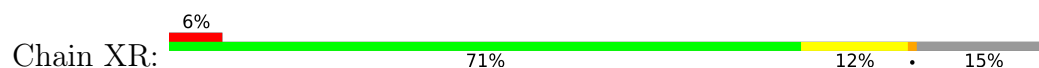




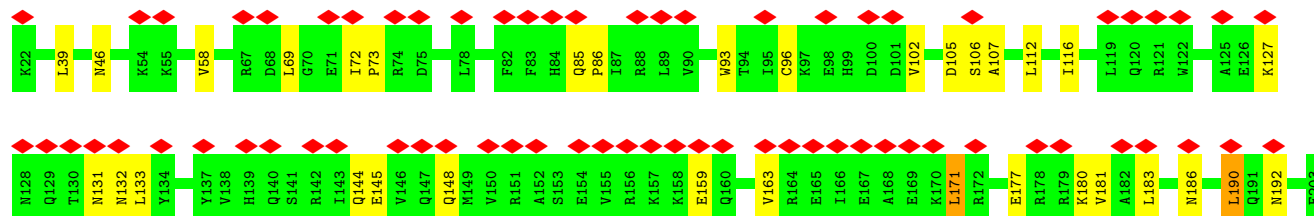
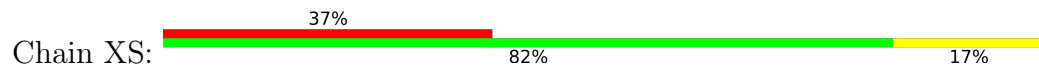
- Molecule 79: GTP-binding protein



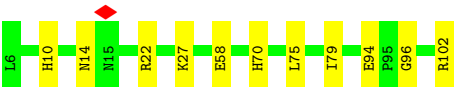
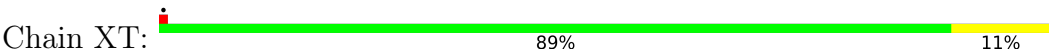
- Molecule 80: Lipase (Class 3)



- Molecule 81: mL101



- Molecule 82: mt-LAF19



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32300	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.270	Depositor
Minimum map value	-0.143	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	642.00006, 642.00006, 642.00006	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, ADP, ZN, 4HH, MG, FES, GTP

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	0.13	0/1828	0.30	0/2466
2	A2	0.12	0/3740	0.28	0/5094
3	A3	0.13	0/1255	0.32	0/1692
4	A5	0.13	0/498	0.34	0/663
5	A8	0.14	0/1231	0.34	0/1648
6	AA	0.08	0/17938	0.17	0/27870
7	AE	0.14	0/3053	0.31	0/4149
8	AF	0.13	0/3706	0.30	0/5029
9	AI	0.12	0/1850	0.29	0/2515
10	AK	0.10	0/2077	0.27	0/2815
11	AN	0.14	0/1481	0.31	0/2016
12	AP	0.13	0/2642	0.30	0/3581
13	AR	0.13	0/2210	0.29	0/2988
14	AT	0.13	0/1166	0.30	0/1576
15	AU	0.14	0/1456	0.31	0/1971
16	AV	0.14	0/1449	0.33	0/1966
17	AW	0.13	0/2299	0.29	0/3108
18	AX	0.13	0/1436	0.28	0/1952
19	AY	0.12	0/2794	0.28	0/3775
20	Ae	0.13	0/960	0.32	0/1304
21	Af	0.12	0/1095	0.26	0/1484
22	Ag	0.13	0/1600	0.29	0/2168
23	Al	0.12	0/1398	0.28	0/1901
24	Ao	0.14	0/1094	0.29	0/1489
25	Ap	0.12	0/2421	0.29	0/3289
26	At	0.14	0/1235	0.32	0/1674
27	Av	0.15	0/1706	0.31	0/2299
28	BA	0.12	0/5907	0.28	0/8009
29	BB	0.10	0/2930	0.28	0/3984
30	BD	0.12	0/3408	0.29	0/4615
31	BE	0.12	0/3259	0.28	0/4413
32	BF	0.12	0/2866	0.30	0/3863

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BH	0.12	0/1883	0.28	0/2567
34	BI	0.13	0/2717	0.31	0/3674
35	BJ	0.11	0/1356	0.28	0/1830
36	BK	0.11	0/1963	0.27	0/2647
37	BL	0.13	0/1924	0.30	0/2596
38	BN	0.12	0/1837	0.28	0/2484
39	BO	0.11	0/1693	0.29	0/2290
40	BQ	0.13	0/1466	0.31	0/1987
41	BR	0.12	0/1693	0.28	0/2284
42	BS	0.13	0/1202	0.30	0/1618
43	BT	0.14	0/1408	0.31	0/1895
44	BU	0.12	0/711	0.28	0/955
45	BW	0.13	0/1604	0.31	0/2167
46	BX	0.11	0/897	0.31	0/1215
47	BZ	0.11	0/1460	0.26	0/1975
48	Ba	0.13	0/1233	0.31	0/1667
49	Bb	0.12	0/822	0.27	0/1113
50	Bc	0.13	0/1238	0.31	0/1685
51	Bf	0.11	0/697	0.28	0/938
52	Bg	0.11	0/671	0.32	0/905
53	Bh	0.13	0/752	0.31	0/1015
54	UA	0.13	0/229	0.24	0/319
55	UB	0.27	0/44	0.20	0/60
56	UC	0.21	0/69	0.22	0/95
57	UD	0.29	0/39	0.18	0/53
58	UE	0.25	0/59	0.21	0/81
59	UF	0.08	0/688	0.14	0/952
60	UG	0.19	0/94	0.16	0/130
61	UH	0.23	0/84	0.34	0/116
62	UI	0.15	0/194	0.31	0/270
63	UJ	0.17	0/124	0.31	0/172
64	UK	0.14	0/234	0.24	0/326
65	XA	0.14	0/1331	0.34	0/1784
66	XB	0.13	0/5052	0.33	0/6829
67	XC	0.12	0/4763	0.30	0/6454
68	XD	0.09	0/667	0.23	0/906
68	XE	0.09	0/667	0.24	0/906
69	XF	0.11	0/1288	0.27	0/1747
70	XG	0.13	0/1362	0.33	0/1835
71	XH	0.12	0/3277	0.28	0/4441
72	XI	0.11	0/4820	0.29	0/6535
73	XJ	0.11	0/1234	0.27	0/1670
74	XL	0.12	0/4237	0.29	0/5715

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	XM	0.11	0/757	0.27	0/1018
76	XN	0.12	0/4487	0.28	0/6111
77	XO	0.11	0/3254	0.29	0/4400
78	XP	0.13	0/3080	0.31	0/4177
79	XQ	0.12	0/2248	0.31	0/3042
80	XR	0.12	0/1150	0.28	0/1546
81	XS	0.12	0/1557	0.28	0/2099
82	XT	0.13	0/819	0.32	0/1097
All	All	0.12	0/161123	0.28	0/221759

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	1788	0	1814	37	0
2	A2	3638	0	3601	66	0
3	A3	1229	0	1285	19	0
4	A5	483	0	493	13	0
5	A8	1203	0	1226	18	0
6	AA	16041	0	8030	196	0
7	AE	2955	0	2794	61	0
8	AF	3597	0	3509	63	0
9	AI	1790	0	1765	24	0
10	AK	2034	0	2053	17	0
11	AN	1432	0	1410	21	0
12	AP	2565	0	2518	45	0
13	AR	2144	0	2087	32	0
14	AT	1136	0	1117	26	0
15	AU	1423	0	1447	21	0
16	AV	1419	0	1452	26	0
17	AW	2243	0	2281	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	AX	1391	0	1367	19	0
19	AY	2741	0	2682	53	0
20	Ae	927	0	911	10	0
21	Af	1068	0	1050	20	0
22	Ag	1557	0	1500	31	0
23	Al	1356	0	1365	23	0
24	Ao	1058	0	1019	18	0
25	Ap	2347	0	2346	30	0
26	At	1203	0	1211	18	0
27	Av	1661	0	1635	24	0
28	BA	5779	0	5826	84	0
29	BB	2862	0	2796	38	0
30	BD	3339	0	3361	51	0
31	BE	3178	0	3101	47	0
32	BF	2805	0	2788	59	0
33	BH	1831	0	1810	24	0
34	BI	2641	0	2577	44	0
35	BJ	1329	0	1318	21	0
36	BK	1922	0	1892	28	0
37	BL	1887	0	1831	25	0
38	BN	1793	0	1729	29	0
39	BO	1665	0	1657	18	0
40	BQ	1429	0	1368	14	0
41	BR	1650	0	1632	21	0
42	BS	1185	0	1193	20	0
43	BT	1380	0	1349	16	0
44	BU	694	0	697	18	0
45	BW	1557	0	1517	21	0
46	BX	867	0	812	11	0
47	BZ	1433	0	1425	24	0
48	Ba	1191	0	1136	19	0
49	Bb	805	0	805	10	0
50	Bc	1194	0	1169	14	0
51	Bf	676	0	643	15	0
52	Bg	656	0	649	14	0
53	Bh	730	0	708	12	0
54	UA	230	0	232	1	0
55	UB	45	0	47	0	0
56	UC	70	0	72	0	0
57	UD	40	0	42	0	0
58	UE	60	0	62	0	0
59	UF	695	0	691	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	UG	95	0	97	0	0
61	UH	85	0	87	0	0
62	UI	195	0	197	0	0
63	UJ	125	0	127	1	0
64	UK	235	0	237	1	0
65	XA	1295	0	1250	21	0
66	XB	4944	0	5086	92	0
67	XC	4652	0	4670	70	0
68	XD	685	0	674	11	0
68	XE	685	0	674	8	0
69	XF	1264	0	1283	11	0
70	XG	1330	0	1350	20	0
71	XH	3208	0	3230	40	0
72	XI	4736	0	4811	88	0
73	XJ	1212	0	1211	22	0
74	XL	4169	0	4222	84	0
75	XM	744	0	765	13	0
76	XN	4358	0	4304	50	0
77	XO	3193	0	3190	47	0
78	XP	2995	0	3002	50	0
79	XQ	2206	0	2228	29	0
80	XR	1135	0	1133	10	0
81	XS	1532	0	1581	29	0
82	XT	801	0	818	9	0
83	A5	4	0	0	1	0
84	Av	44	0	25	2	0
85	BX	2	0	0	0	0
85	Bh	1	0	0	0	0
85	XA	1	0	0	0	0
86	XB	1	0	0	0	0
87	XB	27	0	11	1	0
88	XL	64	0	24	5	0
All	All	156070	0	147190	1876	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 6.

All (1876) 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)
24:Ao:19:TYR:N	32:BF:120:TYR:HH	1.65	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BF:286:VAL:HG11	32:BF:316:MET:HE1	1.53	0.89
66:XB:300:THR:OG1	66:XB:302:PHE:O	1.90	0.88
22:Ag:155:GLU:OE2	34:BI:272:ARG:NH2	2.08	0.86
72:XI:595:GLU:OE2	72:XI:628:SER:OG	1.95	0.83
6:AA:565:U:O2'	44:BU:141:GLU:OE1	1.94	0.83
7:AE:256:ARG:NH1	13:AR:20:ARG:O	2.11	0.83
66:XB:485:ARG:NH1	66:XB:529:PHE:O	2.12	0.83
9:AI:104:GLU:OE1	74:XL:68:ARG:NH2	2.10	0.83
17:AW:81:ARG:NH1	17:AW:94:ASP:OD1	2.12	0.83
66:XB:367:THR:OG1	74:XL:303:CYS:O	1.95	0.82
13:AR:194:GLU:OE2	36:BK:194:ARG:NH2	2.12	0.82
6:AA:514:G:O2'	6:AA:570:U:O2	1.95	0.82
6:AA:1147:U:OP1	7:AE:391:ARG:NH2	2.12	0.82
68:XD:99:ASN:ND2	68:XD:100:ASP:OD1	2.14	0.81
6:AA:1131:G:N2	73:XJ:260:ILE:O	2.13	0.81
12:AP:265:GLU:OE2	45:BW:11:ARG:NH1	2.14	0.81
72:XI:387:ILE:HD11	72:XI:445:LEU:HD22	1.62	0.81
4:A5:55:TYR:OH	4:A5:80:PRO:O	1.98	0.80
71:XH:255:GLU:OE2	71:XH:317:ARG:NH1	2.14	0.80
6:AA:484:U:O2'	6:AA:485:A:OP2	1.99	0.80
66:XB:106:LEU:O	66:XB:111:ARG:NH1	2.14	0.80
6:AA:1172:A:N6	28:BA:782:VAL:O	2.14	0.80
7:AE:274:SER:O	65:XA:91:ARG:NH2	2.15	0.80
23:Al:181:LEU:HD23	23:Al:189:ILE:HD12	1.64	0.80
6:AA:472:A:O2'	6:AA:473:A:OP1	1.98	0.80
34:BI:119:GLU:O	34:BI:236:LYS:NZ	2.15	0.80
13:AR:76:GLU:OE1	13:AR:80:LYS:NZ	2.13	0.80
78:XP:311:THR:O	78:XP:312:ARG:NH1	2.15	0.80
67:XC:380:ARG:NH2	67:XC:492:GLU:OE2	2.15	0.79
18:AX:204:GLU:OE2	19:AY:82:ARG:NH1	2.15	0.79
14:AT:45:PRO:O	39:BO:62:ARG:NH1	2.15	0.79
68:XE:99:ASN:ND2	68:XE:100:ASP:OD1	2.16	0.79
6:AA:834:U:OP2	21:Af:55:ARG:NH2	2.16	0.79
66:XB:121:THR:O	87:XB:902:ADP:N6	2.15	0.78
37:BL:102:CYS:O	37:BL:171:SER:OG	2.00	0.78
36:BK:109:ARG:NH1	36:BK:113:CYS:SG	2.57	0.78
2:A2:372:GLU:OE1	19:AY:274:HIS:NE2	2.17	0.78
7:AE:315:ARG:NH2	14:AT:36:GLU:OE1	2.17	0.78
7:AE:242:GLN:NE2	7:AE:341:ASP:OD1	2.17	0.78
6:AA:285:A:OP1	18:AX:66:ARG:NH1	2.16	0.78
14:AT:94:ARG:NH1	73:XJ:309:ASN:O	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AV:59:ILE:HD11	24:Ao:86:PHE:CD2	2.19	0.78
69:XF:151:VAL:HG13	69:XF:266:ILE:HD11	1.66	0.78
34:BI:247:GLU:OE1	34:BI:247:GLU:N	2.17	0.78
25:Ap:72:GLY:O	25:Ap:75:ARG:NH2	2.17	0.77
41:BR:105:ASN:O	41:BR:192:ARG:NH1	2.16	0.77
32:BF:326:ASP:OD1	32:BF:327:PHE:N	2.18	0.77
67:XC:150:ARG:NH1	67:XC:188:GLN:OE1	2.18	0.77
6:AA:187:A:O4'	6:AA:287:A:N6	2.17	0.77
30:BD:425:TYR:OH	30:BD:441:VAL:O	2.03	0.77
11:AN:35:GLN:O	28:BA:710:LYS:NZ	2.16	0.77
33:BH:160:THR:OG1	33:BH:168:THR:OG1	2.02	0.77
33:BH:160:THR:HG1	33:BH:168:THR:HG1	1.26	0.76
71:XH:495:ARG:NH1	78:XP:51:GLU:O	2.18	0.76
72:XI:95:GLU:OE1	72:XI:95:GLU:N	2.18	0.76
32:BF:171:ARG:NH2	32:BF:193:GLU:OE1	2.18	0.76
6:AA:158:A:OP2	12:AP:188:ARG:NH2	2.18	0.76
76:XN:551:GLU:OE2	76:XN:568:THR:OG1	2.02	0.76
2:A2:66:GLU:OE2	36:BK:386:TYR:OH	2.02	0.76
38:BN:98:ASP:OD2	38:BN:260:TYR:OH	2.04	0.76
66:XB:287:LYS:O	67:XC:562:SER:OG	2.03	0.76
6:AA:926:A:N6	6:AA:929:U:O2'	2.18	0.76
23:Al:79:TYR:OH	23:Al:92:HIS:O	2.04	0.76
47:BZ:57:LYS:NZ	47:BZ:59:ILE:O	2.18	0.76
6:AA:449:U:OP2	34:BI:273:LYS:NZ	2.15	0.76
71:XH:323:ARG:NH1	71:XH:325:ASN:OD1	2.18	0.76
72:XI:662:VAL:HG22	72:XI:710:LEU:HD23	1.66	0.76
8:AF:403:GLU:OE1	43:BT:113:ARG:NH1	2.18	0.76
19:AY:260:GLU:OE1	47:BZ:129:ASN:ND2	2.18	0.76
47:BZ:10:ASP:OD1	47:BZ:185:ASP:N	2.18	0.76
72:XI:70:GLU:OE2	74:XL:254:ARG:NH2	2.19	0.75
14:AT:40:GLU:OE1	14:AT:42:ARG:NH2	2.19	0.75
25:Ap:211:ALA:O	77:XO:469:ARG:NH1	2.19	0.75
74:XL:115:ARG:O	74:XL:120:LYS:NZ	2.18	0.75
6:AA:412:U:OP1	34:BI:299:ARG:NH2	2.19	0.75
12:AP:285:LEU:O	12:AP:290:THR:OG1	2.05	0.75
23:Al:75:ARG:NH1	23:Al:207:MET:SD	2.59	0.75
38:BN:157:ARG:NH2	38:BN:162:ASN:OD1	2.20	0.75
10:AK:213:GLU:OE1	10:AK:216:ARG:NH2	2.18	0.75
36:BK:361:GLU:OE1	36:BK:361:GLU:N	2.20	0.75
47:BZ:36:ASN:OD1	47:BZ:98:SER:OG	2.04	0.75
27:Av:164:ARG:O	27:Av:169:ARG:NH1	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:XL:487:ARG:NH2	74:XL:525:THR:OG1	2.19	0.75
2:A2:49:HIS:NE2	20:Ae:152:ASN:O	2.20	0.75
9:AI:163:LYS:O	35:BJ:302:ARG:NH2	2.19	0.75
70:XG:74:ASN:OD1	70:XG:103:SER:OG	2.05	0.75
17:AW:62:ASP:O	17:AW:75:GLN:NE2	2.20	0.74
77:XO:226:LYS:NZ	77:XO:304:ASP:OD2	2.20	0.74
3:A3:192:ARG:NH2	23:Al:129:ASP:OD2	2.18	0.74
6:AA:159:U:O2'	12:AP:205:VAL:O	2.04	0.74
13:AR:16:ILE:O	70:XG:47:ARG:NH2	2.20	0.74
13:AR:43:PRO:O	13:AR:99:HIS:ND1	2.20	0.74
26:At:131:SER:O	26:At:134:ARG:NH1	2.19	0.74
77:XO:269:THR:HG23	77:XO:306:VAL:HG21	1.69	0.74
6:AA:307:A:O2'	6:AA:317:A:N3	2.21	0.74
8:AF:418:SER:O	27:Av:78:ARG:NH2	2.21	0.74
1:A1:90:ARG:NH2	74:XL:373:ASP:OD1	2.20	0.73
67:XC:316:TYR:HH	67:XC:355:HIS:HE2	0.75	0.73
31:BE:279:HIS:NE2	31:BE:301:GLU:OE1	2.22	0.73
49:Bb:74:ARG:NH2	49:Bb:139:TYR:O	2.21	0.73
2:A2:117:LEU:HD12	2:A2:374:LEU:HD21	1.68	0.73
24:Ao:135:GLY:O	24:Ao:140:ARG:NH2	2.22	0.73
6:AA:913:C:O2'	66:XB:241:ARG:NH2	2.21	0.73
22:Ag:80:PHE:O	22:Ag:84:ASN:ND2	2.20	0.73
28:BA:162:ARG:NH1	28:BA:170:GLN:OE1	2.20	0.73
43:BT:61:ARG:NH1	48:Ba:138:GLU:OE2	2.21	0.73
76:XN:228:TYR:O	76:XN:233:ARG:NH1	2.21	0.73
31:BE:424:ASN:O	31:BE:431:ARG:NH2	2.21	0.73
71:XH:600:VAL:HG21	71:XH:615:VAL:HG21	1.70	0.73
5:A8:161:ASN:ND2	6:AA:72:A:O2'	2.22	0.72
66:XB:293:GLN:N	66:XB:293:GLN:OE1	2.22	0.72
4:A5:53:GLU:OE2	28:BA:765:ARG:NH1	2.21	0.72
6:AA:1126:U:OP1	73:XJ:261:ARG:NH2	2.22	0.72
22:Ag:103:HIS:O	28:BA:720:ARG:NH2	2.22	0.72
66:XB:78:LEU:HD22	66:XB:303:ILE:HD11	1.72	0.72
6:AA:518:A:N6	81:XS:39:LEU:O	2.23	0.72
27:Av:31:LEU:HD21	33:BH:307:ALA:HB3	1.72	0.72
35:BJ:269:GLU:OE1	35:BJ:280:LYS:NZ	2.22	0.72
48:Ba:102:GLN:O	48:Ba:107:GLN:NE2	2.23	0.72
67:XC:265:ASN:OD1	67:XC:506:ARG:NH2	2.23	0.71
4:A5:36:ARG:NH2	19:AY:7:THR:O	2.22	0.71
30:BD:448:PRO:O	30:BD:453:ARG:NH2	2.24	0.71
7:AE:106:ARG:NH2	25:Ap:148:TYR:OH	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BH:275:GLN:OE1	33:BH:275:GLN:N	2.24	0.71
46:BX:65:GLU:OE1	46:BX:65:GLU:N	2.22	0.71
6:AA:141:U:O2'	15:AU:27:ARG:NH2	2.23	0.71
29:BB:118:TYR:OH	29:BB:358:ARG:NH1	2.24	0.71
72:XI:658:ASP:O	72:XI:662:VAL:HG23	1.91	0.71
2:A2:40:ARG:NH2	2:A2:100:GLU:OE1	2.23	0.71
74:XL:178:GLU:OE1	74:XL:178:GLU:N	2.24	0.71
28:BA:563:ARG:NH1	28:BA:566:MET:SD	2.63	0.71
4:A5:46:GLU:OE2	19:AY:2:TYR:OH	2.07	0.71
13:AR:119:LEU:HD12	13:AR:125:VAL:HG22	1.71	0.71
5:A8:75:LYS:NZ	5:A8:77:MET:SD	2.64	0.71
47:BZ:147:ASN:OD1	47:BZ:148:GLY:N	2.23	0.71
37:BL:177:LEU:HD21	37:BL:291:LEU:HD21	1.73	0.70
74:XL:229:GLU:N	74:XL:229:GLU:OE1	2.24	0.70
76:XN:428:LEU:HD21	76:XN:437:LEU:HD22	1.72	0.70
14:AT:28:ARG:NH2	42:BS:24:GLY:O	2.24	0.70
19:AY:115:ASP:OD1	19:AY:205:ARG:NH2	2.24	0.70
26:At:143:THR:OG1	32:BF:131:LEU:HD22	1.90	0.70
1:A1:184:MET:SD	19:AY:300:LEU:HD22	2.31	0.70
40:BQ:119:GLU:OE1	40:BQ:119:GLU:N	2.23	0.70
6:AA:1095:A:O2'	6:AA:1096:U:O5'	2.09	0.70
2:A2:144:GLU:OE1	2:A2:144:GLU:N	2.25	0.70
8:AF:78:SER:HB2	32:BF:361:ILE:HD11	1.73	0.70
29:BB:102:ILE:HD12	29:BB:393:LEU:HD21	1.74	0.70
71:XH:307:GLU:OE1	71:XH:307:GLU:N	2.25	0.70
72:XI:510:ALA:O	72:XI:514:HIS:ND1	2.24	0.70
25:Ap:62:ASN:O	25:Ap:93:ARG:NH2	2.25	0.70
79:XQ:79:VAL:HG11	79:XQ:106:ILE:HG21	1.74	0.70
2:A2:214:SER:OG	8:AF:410:GLU:OE1	2.10	0.70
6:AA:478:A:OP1	32:BF:343:GLN:NE2	2.25	0.70
65:XA:113:THR:HG21	66:XB:637:TYR:OH	1.91	0.70
72:XI:530:ALA:O	72:XI:532:ARG:NH1	2.25	0.70
6:AA:1159:A:O2'	28:BA:761:TYR:O	2.07	0.70
30:BD:166:SER:OG	30:BD:318:ARG:O	2.08	0.70
74:XL:264:VAL:O	80:XR:129:TYR:OH	2.09	0.70
6:AA:515:U:O2'	6:AA:516:U:O5'	2.09	0.69
48:Ba:48:PRO:HB2	48:Ba:86:ILE:HG21	1.74	0.69
9:AI:99:LEU:O	9:AI:180:LYS:NZ	2.25	0.69
12:AP:89:GLN:O	12:AP:92:GLN:NE2	2.26	0.69
31:BE:88:ARG:NH1	36:BK:285:GLN:OE1	2.25	0.69
74:XL:394:VAL:HG11	74:XL:416:VAL:HG11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:528:A:OP1	18:AX:88:TYR:OH	2.05	0.69
7:AE:82:ARG:NH2	34:BI:83:GLU:OE2	2.25	0.69
13:AR:238:ARG:NH2	19:AY:60:GLU:O	2.25	0.69
81:XS:127:LYS:NZ	81:XS:131:ASN:O	2.25	0.69
4:A5:60:CYS:N	83:A5:101:FES:S1	2.64	0.69
6:AA:565:U:OP1	44:BU:138:ARG:NH1	2.26	0.69
38:BN:150:GLU:O	53:Bh:34:ARG:NH1	2.26	0.69
2:A2:172:ARG:NH1	48:Ba:73:GLU:OE2	2.25	0.69
38:BN:177:GLN:OE1	81:XS:180:LYS:NZ	2.24	0.69
6:AA:193:A:OP2	33:BH:311:LYS:NZ	2.25	0.69
79:XQ:69:GLN:N	79:XQ:69:GLN:OE1	2.25	0.69
79:XQ:123:GLU:OE1	79:XQ:123:GLU:N	2.25	0.69
22:Ag:12:VAL:HG21	22:Ag:83:LEU:CD1	2.23	0.69
22:Ag:66:GLU:OE2	37:BL:78:ARG:NH1	2.26	0.69
28:BA:346:MET:SD	28:BA:377:ARG:NH1	2.66	0.69
49:Bb:94:GLN:OE1	49:Bb:94:GLN:N	2.26	0.69
74:XL:121:SER:OG	88:XL:601:GTP:O2B	2.06	0.69
5:A8:104:LYS:NZ	6:AA:950:U:O2	2.25	0.69
76:XN:290:ILE:HG22	76:XN:515:MET:HG2	1.75	0.69
6:AA:480:A:O2'	6:AA:491:A:N6	2.26	0.68
14:AT:22:SER:OG	39:BO:130:ARG:NE	2.25	0.68
72:XI:662:VAL:HG22	72:XI:710:LEU:CD2	2.23	0.68
17:AW:166:LEU:O	31:BE:399:LYS:NZ	2.26	0.68
6:AA:1162:G:O2'	13:AR:148:ARG:NH2	2.26	0.68
81:XS:145:GLU:OE1	81:XS:148:GLN:NE2	2.26	0.68
6:AA:156:U:O4	8:AF:224:ARG:NH2	2.26	0.68
6:AA:131:U:O2'	6:AA:345:U:O2'	2.09	0.68
41:BR:179:ILE:HG22	41:BR:179:ILE:O	1.93	0.68
73:XJ:223:LYS:NZ	75:XM:113:GLY:O	2.22	0.68
30:BD:125:THR:OG1	30:BD:128:THR:O	2.11	0.68
41:BR:103:ARG:NH2	41:BR:139:TYR:O	2.25	0.68
76:XN:249:CYS:SG	76:XN:271:LEU:HD12	2.32	0.68
4:A5:78:ILE:HG21	17:AW:259:ALA:HB2	1.76	0.68
6:AA:290:A:N1	8:AF:186:ARG:NH2	2.42	0.68
6:AA:802:G:N2	13:AR:157:ALA:O	2.26	0.68
6:AA:933:U:O2'	72:XI:561:ARG:NH1	2.27	0.68
6:AA:1174:U:O5'	28:BA:774:LYS:NZ	2.26	0.68
38:BN:53:TRP:N	44:BU:182:GLU:OE2	2.27	0.68
66:XB:325:GLN:N	66:XB:325:GLN:OE1	2.27	0.68
6:AA:13:A:N7	19:AY:36:ARG:NH2	2.42	0.68
30:BD:191:GLU:OE1	80:XR:52:ARG:NH2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:XI:693:ARG:NE	72:XI:704:GLU:OE1	2.27	0.68
6:AA:532:U:OP2	18:AX:211:TYR:OH	2.12	0.68
6:AA:1131:G:O6	73:XJ:242:HIS:NE2	2.26	0.68
29:BB:131:ARG:NH1	29:BB:252:ASP:OD1	2.27	0.68
47:BZ:25:LEU:HD23	47:BZ:34:VAL:HG13	1.76	0.68
78:XP:142:ASP:OD1	78:XP:143:GLY:N	2.27	0.68
6:AA:576:A:O2'	7:AE:255:PHE:O	2.10	0.67
74:XL:128:ARG:NH2	74:XL:136:ARG:O	2.27	0.67
17:AW:93:GLU:OE2	32:BF:388:ARG:NH2	2.27	0.67
7:AE:341:ASP:OD2	7:AE:351:TRP:NE1	2.27	0.67
6:AA:563:U:O2'	44:BU:134:ARG:NE	2.28	0.67
68:XE:84:GLU:N	68:XE:84:GLU:OE1	2.27	0.67
66:XB:164:ASP:OD2	66:XB:255:TYR:OH	2.12	0.67
38:BN:217:GLU:OE1	38:BN:217:GLU:N	2.28	0.67
4:A5:47:LYS:O	17:AW:169:ARG:NH2	2.28	0.67
72:XI:665:LEU:HD13	72:XI:710:LEU:HD11	1.77	0.67
12:AP:286:GLU:O	27:Av:183:ARG:NH2	2.28	0.67
2:A2:263:GLU:N	2:A2:263:GLU:OE1	2.28	0.67
2:A2:142:LYS:NZ	2:A2:323:GLU:OE1	2.27	0.66
32:BF:195:LEU:HD11	32:BF:216:LEU:HD22	1.78	0.66
38:BN:208:PHE:CE1	81:XS:190:LEU:HD13	2.29	0.66
64:UK:25:ALA:O	71:XH:519:ARG:NH2	2.28	0.66
79:XQ:262:PRO:HD2	79:XQ:265:LEU:HD12	1.76	0.66
29:BB:185:ARG:NH2	29:BB:193:ASN:OD1	2.27	0.66
34:BI:102:TRP:NE1	34:BI:107:ASN:OD1	2.27	0.66
6:AA:465:A:N3	16:AV:35:ASN:ND2	2.43	0.66
38:BN:127:THR:O	38:BN:235:ARG:NH2	2.27	0.66
5:A8:175:ASP:OD1	5:A8:176:PHE:N	2.27	0.66
11:AN:65:ILE:HD13	11:AN:156:ALA:HB2	1.77	0.66
30:BD:481:GLN:OE1	30:BD:483:SER:OG	2.12	0.66
76:XN:419:ILE:HG23	76:XN:605:MET:HE2	1.76	0.66
12:AP:19:GLU:OE2	26:At:78:SER:OG	2.12	0.66
30:BD:142:VAL:HG22	30:BD:145:TRP:HD1	1.61	0.66
8:AF:335:ILE:HD11	43:BT:32:THR:HG21	1.76	0.66
12:AP:190:ASN:ND2	45:BW:100:GLN:OE1	2.29	0.66
21:Af:155:ARG:NH2	28:BA:213:ASP:OD2	2.29	0.66
72:XI:348:LEU:HD12	72:XI:379:LEU:HD21	1.78	0.66
72:XI:67:ARG:NH2	72:XI:429:PRO:O	2.29	0.66
45:BW:153:HIS:O	45:BW:157:ASN:N	2.29	0.66
8:AF:71:VAL:O	43:BT:150:ASN:ND2	2.29	0.66
40:BQ:116:GLU:OE1	40:BQ:116:GLU:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:XT:94:GLU:OE1	82:XT:96:GLY:N	2.29	0.66
2:A2:401:THR:HG22	2:A2:444:GLY:HA3	1.77	0.65
6:AA:377:A:OP2	15:AU:59:ARG:NH2	2.29	0.65
31:BE:62:GLU:OE1	31:BE:62:GLU:N	2.29	0.65
40:BQ:35:VAL:HG11	40:BQ:174:VAL:HG21	1.79	0.65
6:AA:377:A:OP1	15:AU:81:ARG:NH2	2.29	0.65
17:AW:183:GLN:OE1	31:BE:394:LEU:HD21	1.97	0.65
50:Bc:118:ASP:OD2	76:XN:617:ARG:NH1	2.29	0.65
9:AI:193:ARG:NH2	9:AI:201:TYR:OH	2.30	0.65
38:BN:129:ASP:OD1	38:BN:131:GLU:N	2.29	0.65
67:XC:258:THR:OG1	67:XC:601:VAL:HG22	1.97	0.65
72:XI:328:ILE:O	72:XI:375:ARG:NH2	2.29	0.65
29:BB:264:ALA:N	29:BB:349:GLU:OE1	2.30	0.65
49:Bb:48:GLU:O	49:Bb:52:SER:OG	2.06	0.65
59:UF:18:ALA:HA	69:XF:198:THR:HG21	1.78	0.65
76:XN:77:VAL:HG13	76:XN:78:THR:HG23	1.79	0.65
66:XB:262:ASP:OD1	66:XB:300:THR:OG1	2.14	0.65
72:XI:618:TYR:HB3	72:XI:625:LEU:HD21	1.77	0.65
2:A2:375:ARG:NH1	48:Ba:85:ASN:O	2.30	0.65
22:Ag:158:GLU:OE1	71:XH:233:LEU:HD13	1.97	0.65
34:BI:297:LYS:NZ	51:Bf:83:GLU:OE2	2.27	0.65
66:XB:549:LEU:HD23	66:XB:550:HIS:N	2.12	0.64
6:AA:479:A:N6	12:AP:96:ASP:OD1	2.29	0.64
6:AA:523:A:OP2	52:Bg:56:ARG:NH1	2.31	0.64
23:AI:92:HIS:NE2	23:AI:126:GLY:O	2.30	0.64
49:Bb:41:HIS:NE2	71:XH:620:SER:OG	2.27	0.64
18:AX:129:GLU:OE1	18:AX:129:GLU:N	2.30	0.64
3:A3:68:VAL:HG12	3:A3:90:LEU:HD11	1.78	0.64
41:BR:39:GLU:OE2	41:BR:64:ARG:NH2	2.31	0.64
76:XN:463:LYS:NZ	77:XO:483:GLU:OE2	2.31	0.64
3:A3:135:HIS:O	26:At:102:ARG:NH2	2.31	0.64
6:AA:1168:U:O4	13:AR:142:LYS:NZ	2.29	0.64
12:AP:236:ASN:OD1	12:AP:237:ALA:N	2.31	0.64
13:AR:131:GLU:OE1	13:AR:173:ASN:ND2	2.31	0.64
34:BI:119:GLU:OE2	34:BI:158:LYS:NZ	2.30	0.64
74:XL:112:ILE:HG22	74:XL:190:ILE:HD11	1.79	0.64
79:XQ:101:ASN:O	79:XQ:105:ILE:HG22	1.97	0.64
2:A2:415:ASN:HD21	36:BK:379:LEU:HD23	1.62	0.64
6:AA:1011:G:OP1	78:XP:313:ARG:NE	2.30	0.64
1:A1:181:VAL:HG11	19:AY:299:MET:HB2	1.79	0.64
75:XM:48:ASP:OD2	75:XM:97:ARG:NE	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BF:157:ASN:OD1	32:BF:167:ARG:NH2	2.31	0.64
67:XC:176:ARG:O	67:XC:188:GLN:NE2	2.29	0.64
66:XB:364:GLU:OE1	66:XB:364:GLU:N	2.31	0.63
69:XF:206:GLU:O	69:XF:260:ARG:N	2.30	0.63
6:AA:1011:G:C1'	78:XP:179:MET:HE3	2.28	0.63
7:AE:169:GLN:NE2	28:BA:156:ASP:OD2	2.31	0.63
25:Ap:121:GLU:N	25:Ap:121:GLU:OE1	2.31	0.63
74:XL:198:ASP:OD1	74:XL:199:ILE:N	2.31	0.63
13:AR:238:ARG:NH1	19:AY:64:HIS:O	2.31	0.63
22:Ag:173:SER:O	22:Ag:177:VAL:HG23	1.98	0.63
28:BA:176:GLN:N	28:BA:176:GLN:OE1	2.30	0.63
67:XC:161:ARG:NH1	67:XC:164:TYR:OH	2.31	0.63
6:AA:950:U:OP1	66:XB:247:ARG:NH2	2.30	0.63
29:BB:74:ASP:OD1	29:BB:78:GLN:NE2	2.31	0.63
31:BE:69:GLU:O	31:BE:73:THR:HG22	1.99	0.63
72:XI:657:LEU:HD23	72:XI:710:LEU:HD21	1.81	0.63
6:AA:903:U:O2'	6:AA:964:A:OP2	2.11	0.63
28:BA:657:PHE:CZ	28:BA:661:ILE:HD11	2.33	0.63
70:XG:65:VAL:CG2	70:XG:80:LEU:HD12	2.29	0.63
2:A2:304:GLU:OE1	2:A2:304:GLU:N	2.32	0.63
34:BI:178:ASN:OD1	34:BI:179:ALA:N	2.31	0.63
9:AI:54:ARG:NH2	43:BT:68:ASN:OD1	2.32	0.63
68:XD:92:THR:O	68:XD:134:ILE:HD11	1.99	0.63
7:AE:68:GLY:O	25:Ap:111:LYS:NZ	2.30	0.63
6:AA:92:U:O3'	43:BT:33:ASN:ND2	2.32	0.62
11:AN:29:TYR:N	11:AN:154:GLU:OE1	2.32	0.62
38:BN:80:GLU:OE1	38:BN:80:GLU:N	2.32	0.62
68:XE:92:THR:O	68:XE:134:ILE:HD11	1.98	0.62
6:AA:935:G:O2'	72:XI:525:ARG:NH2	2.31	0.62
8:AF:274:ASP:O	8:AF:352:THR:OG1	2.15	0.62
17:AW:239:GLU:OE1	17:AW:239:GLU:N	2.32	0.62
28:BA:135:SER:O	39:BO:153:ARG:NH1	2.32	0.62
40:BQ:166:ASP:OD1	40:BQ:167:GLY:N	2.32	0.62
71:XH:533:ILE:HD12	71:XH:559:ILE:HG22	1.79	0.62
72:XI:539:LEU:HB2	72:XI:570:LEU:HD21	1.80	0.62
53:Bh:40:LEU:HD23	53:Bh:41:PHE:N	2.14	0.62
6:AA:19:A:O2'	6:AA:20:A:O5'	2.14	0.62
6:AA:966:A:OP1	65:XA:3:ASN:N	2.32	0.62
38:BN:208:PHE:CD1	81:XS:190:LEU:HD13	2.34	0.62
2:A2:165:GLU:N	2:A2:165:GLU:OE1	2.31	0.62
5:A8:126:ARG:NH1	23:AI:156:ARG:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:315:A:OP1	66:XB:282:LYS:NZ	2.30	0.62
25:Ap:124:LYS:NZ	28:BA:54:GLU:O	2.28	0.62
71:XH:40:GLN:OE1	71:XH:40:GLN:N	2.31	0.62
3:A3:116:VAL:O	26:At:40:ASN:ND2	2.33	0.62
6:AA:180:U:O2'	8:AF:327:LYS:NZ	2.27	0.62
10:AK:174:GLU:N	10:AK:174:GLU:OE1	2.32	0.62
34:BI:112:ILE:HD11	51:Bf:98:TYR:HE1	1.64	0.62
67:XC:166:LEU:O	67:XC:167:SER:OG	2.12	0.62
72:XI:637:ARG:NH1	72:XI:640:CYS:SG	2.73	0.62
6:AA:103:U:OP1	19:AY:8:ARG:NH1	2.33	0.62
12:AP:10:ARG:NH1	12:AP:12:ARG:O	2.33	0.62
15:AU:16:GLU:OE1	15:AU:16:GLU:N	2.33	0.62
70:XG:186:ASN:O	73:XJ:226:ASN:ND2	2.32	0.62
81:XS:132:ASN:OD1	81:XS:133:LEU:N	2.32	0.62
34:BI:90:TYR:CZ	34:BI:128:LEU:HD22	2.35	0.62
72:XI:658:ASP:OD1	72:XI:661:SER:OG	2.12	0.62
1:A1:71:GLN:NE2	6:AA:48:U:O2	2.33	0.61
6:AA:457:A:N6	21:Af:64:SER:OG	2.33	0.61
7:AE:315:ARG:NH2	7:AE:380:GLN:OE1	2.33	0.61
25:Ap:164:VAL:HG23	25:Ap:165:VAL:HG23	1.81	0.61
67:XC:208:ASN:ND2	82:XT:102:ARG:O	2.33	0.61
70:XG:174:ASN:O	70:XG:174:ASN:ND2	2.33	0.61
70:XG:81:ILE:HD11	70:XG:98:VAL:HG23	1.81	0.61
8:AF:280:THR:OG1	8:AF:400:ILE:HD11	1.99	0.61
38:BN:111:LEU:HB3	38:BN:168:LEU:HD11	1.82	0.61
41:BR:16:GLN:OE1	67:XC:521:ARG:NH2	2.33	0.61
66:XB:78:LEU:CD2	66:XB:303:ILE:HD11	2.30	0.61
8:AF:416:TYR:O	8:AF:422:ASN:ND2	2.33	0.61
6:AA:37:G:O2'	6:AA:38:U:OP1	2.15	0.61
6:AA:461:U:OP1	15:AU:63:ARG:NH1	2.34	0.61
27:Av:77:SER:OG	43:BT:90:GLN:O	2.14	0.61
47:BZ:190:GLU:OE1	47:BZ:190:GLU:N	2.34	0.61
6:AA:570:U:O3'	31:BE:432:ARG:NH1	2.33	0.61
24:Ao:21:GLU:OE2	24:Ao:23:ARG:NE	2.31	0.61
72:XI:543:CYS:O	72:XI:601:GLN:NE2	2.32	0.61
13:AR:76:GLU:OE2	31:BE:431:ARG:NH1	2.32	0.61
31:BE:331:ASP:O	31:BE:379:ARG:NH1	2.34	0.61
32:BF:179:ARG:NH2	32:BF:180:GLN:OE1	2.33	0.61
38:BN:185:GLU:OE1	38:BN:185:GLU:N	2.34	0.61
2:A2:61:LEU:HD21	2:A2:83:ARG:HB3	1.83	0.61
9:AI:115:VAL:HG12	9:AI:154:ALA:HB1	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BF:352:ASP:OD1	32:BF:353:GLU:N	2.34	0.61
36:BK:311:GLU:N	36:BK:311:GLU:OE1	2.33	0.61
67:XC:240:LEU:HD13	67:XC:583:VAL:HG22	1.83	0.61
14:AT:5:ARG:NE	14:AT:7:ARG:O	2.34	0.61
24:Ao:109:HIS:NE2	24:Ao:113:GLN:OE1	2.34	0.61
29:BB:109:GLU:HB3	29:BB:117:LEU:HD21	1.81	0.61
41:BR:152:GLU:OE1	41:BR:152:GLU:N	2.33	0.61
6:AA:1009:U:O2'	78:XP:207:CYS:O	2.18	0.60
19:AY:75:THR:HG23	31:BE:58:PRO:O	2.02	0.60
22:Ag:184:HIS:ND1	69:XF:153:GLN:OE1	2.33	0.60
28:BA:513:GLU:OE1	28:BA:565:LEU:N	2.32	0.60
65:XA:109:GLY:O	65:XA:126:GLN:NE2	2.34	0.60
67:XC:517:VAL:HG12	72:XI:726:LEU:HD13	1.83	0.60
79:XQ:116:ASN:OD1	79:XQ:117:LYS:N	2.34	0.60
1:A1:203:LYS:O	35:BJ:234:THR:HG21	2.01	0.60
10:AK:207:GLU:N	10:AK:207:GLU:OE1	2.34	0.60
76:XN:257:ARG:NH1	76:XN:393:ASP:O	2.34	0.60
42:BS:68:ARG:NH2	42:BS:91:GLU:OE2	2.34	0.60
22:Ag:24:ASN:OD1	22:Ag:25:THR:N	2.34	0.60
31:BE:166:ASP:OD1	31:BE:167:ASP:N	2.34	0.60
37:BL:116:GLU:OE1	37:BL:189:ARG:NH1	2.35	0.60
72:XI:224:LEU:HD21	72:XI:288:HIS:CG	2.37	0.60
74:XL:524:ASN:OD1	74:XL:525:THR:N	2.33	0.60
6:AA:13:A:O2'	19:AY:31:ARG:NH2	2.34	0.60
11:AN:50:ARG:O	34:BI:54:ASN:ND2	2.34	0.60
23:Al:77:ASP:OD1	23:Al:78:VAL:N	2.35	0.60
8:AF:145:SER:OG	12:AP:98:THR:O	2.18	0.60
19:AY:27:ASN:ND2	37:BL:51:SER:O	2.35	0.60
19:AY:78:ASN:O	19:AY:83:ARG:NH2	2.34	0.60
32:BF:230:THR:HG21	32:BF:297:PHE:CZ	2.36	0.60
13:AR:172:ASP:OD1	13:AR:173:ASN:N	2.34	0.60
16:AV:15:ILE:HD11	21:Af:90:PHE:CD2	2.36	0.60
30:BD:296:THR:HG21	30:BD:349:ILE:HD12	1.83	0.60
66:XB:139:THR:HG23	66:XB:297:VAL:HG13	1.82	0.60
41:BR:201:MET:SD	41:BR:202:PHE:N	2.74	0.60
12:AP:269:GLU:OE1	45:BW:89:ARG:NH1	2.34	0.60
28:BA:49:LEU:O	76:XN:352:ARG:NH1	2.34	0.60
32:BF:40:PRO:O	32:BF:43:LEU:HD23	2.02	0.60
39:BO:160:MET:HE1	39:BO:224:TYR:CD1	2.37	0.60
72:XI:220:TRP:CE2	72:XI:258:LEU:HD11	2.37	0.60
8:AF:85:TYR:OH	8:AF:236:LEU:O	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:BF:379:GLU:OE1	32:BF:379:GLU:N	2.33	0.60
34:BI:112:ILE:HG23	51:Bf:100:TYR:O	2.02	0.60
38:BN:212:ASN:OD1	81:XS:183:LEU:HD13	2.02	0.60
72:XI:491:THR:HG22	72:XI:520:LEU:HD21	1.83	0.60
6:AA:466:G:N2	16:AV:49:GLN:OE1	2.32	0.59
40:BQ:78:TYR:OH	40:BQ:142:SER:O	2.20	0.59
71:XH:10:SER:O	71:XH:13:THR:OG1	2.19	0.59
72:XI:697:GLN:OE1	72:XI:697:GLN:N	2.35	0.59
80:XR:6:ILE:HG23	80:XR:90:ILE:HG21	1.82	0.59
81:XS:186:ASN:O	81:XS:190:LEU:HD12	2.02	0.59
1:A1:10:PHE:N	72:XI:66:SER:HG	1.99	0.59
5:A8:55:GLN:OE1	6:AA:56:U:N3	2.34	0.59
30:BD:390:LEU:HD21	33:BH:197:PRO:HB3	1.84	0.59
32:BF:228:GLU:OE1	32:BF:228:GLU:N	2.35	0.59
66:XB:469:ALA:O	66:XB:578:ARG:NH2	2.35	0.59
67:XC:148:LEU:HD12	67:XC:214:PHE:CE2	2.37	0.59
67:XC:458:SER:O	67:XC:462:ASN:ND2	2.34	0.59
81:XS:144:GLN:OE1	81:XS:144:GLN:N	2.36	0.59
6:AA:1173:U:C4	42:BS:94:LEU:HD21	2.36	0.59
70:XG:116:ARG:NH1	70:XG:163:THR:OG1	2.35	0.59
72:XI:335:MET:HE3	72:XI:378:LEU:HD22	1.84	0.59
74:XL:503:SER:O	79:XQ:217:LEU:HD13	2.01	0.59
74:XL:517:ILE:HG22	74:XL:534:LEU:HD23	1.85	0.59
76:XN:278:GLN:OE1	76:XN:278:GLN:N	2.34	0.59
8:AF:167:ARG:NH1	18:AX:69:GLU:OE1	2.34	0.59
42:BS:68:ARG:NH2	42:BS:86:GLU:OE1	2.35	0.59
82:XT:22:ARG:NH2	82:XT:27:LYS:O	2.35	0.59
3:A3:74:PRO:HB3	3:A3:85:LEU:HD13	1.85	0.59
29:BB:168:PHE:O	29:BB:173:ARG:NH1	2.35	0.59
47:BZ:120:LEU:HD11	47:BZ:138:LEU:HD21	1.84	0.59
71:XH:100:LEU:HD13	71:XH:102:TRP:CZ2	2.38	0.59
72:XI:538:LEU:CD2	72:XI:570:LEU:HD22	2.31	0.59
74:XL:115:ARG:NH1	74:XL:116:MET:O	2.34	0.59
1:A1:50:ASN:N	1:A1:53:SER:OG	2.30	0.59
6:AA:1175:U:O2'	13:AR:138:ASP:O	2.17	0.59
24:Ao:51:ARG:NH1	26:At:64:GLU:OE1	2.36	0.59
28:BA:421:SER:O	28:BA:423:ARG:NH1	2.36	0.59
74:XL:149:ASP:OD1	74:XL:150:SER:N	2.36	0.59
74:XL:321:SER:OG	88:XL:602:GTP:O2G	2.18	0.59
17:AW:153:ARG:NH2	17:AW:201:ILE:O	2.35	0.59
19:AY:281:ASN:HB3	48:Ba:58:MET:HE3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:BO:81:CYS:N	39:BO:163:VAL:O	2.36	0.59
71:XH:238:LEU:HD11	71:XH:252:PRO:O	2.02	0.59
72:XI:75:LYS:NZ	74:XL:228:GLN:OE1	2.29	0.59
10:AK:113:LEU:HD21	77:XO:461:ALA:HB2	1.85	0.59
17:AW:123:VAL:HG21	37:BL:113:ARG:NH1	2.18	0.59
27:Av:31:LEU:HD21	33:BH:307:ALA:CB	2.33	0.59
74:XL:252:ALA:N	88:XL:601:GTP:O6	2.35	0.59
76:XN:393:ASP:OD2	76:XN:405:ARG:NH2	2.35	0.59
29:BB:200:GLY:N	29:BB:203:GLY:O	2.36	0.59
38:BN:131:GLU:OE2	81:XS:192:ASN:ND2	2.35	0.59
66:XB:47:VAL:N	66:XB:50:GLN:OE1	2.36	0.59
72:XI:491:THR:CG2	72:XI:520:LEU:HD21	2.33	0.59
6:AA:576:A:O3'	13:AR:20:ARG:NH2	2.35	0.59
36:BK:100:GLU:N	36:BK:100:GLU:OE1	2.35	0.59
36:BK:384:ARG:NE	52:Bg:68:SER:O	2.35	0.59
71:XH:238:LEU:HD13	71:XH:247:ILE:CG2	2.32	0.59
77:XO:195:GLU:OE1	78:XP:147:LYS:NZ	2.33	0.59
28:BA:418:ASP:OD2	28:BA:423:ARG:NH2	2.36	0.58
32:BF:419:VAL:O	32:BF:419:VAL:HG12	2.02	0.58
42:BS:70:ILE:HD13	42:BS:79:LEU:HD11	1.85	0.58
43:BT:20:GLY:O	45:BW:52:LYS:NZ	2.34	0.58
47:BZ:77:VAL:HG23	47:BZ:83:ILE:HG22	1.85	0.58
67:XC:82:ASP:OD2	67:XC:145:ARG:NH2	2.36	0.58
67:XC:166:LEU:O	67:XC:166:LEU:HD23	2.02	0.58
1:A1:85:ARG:NH1	6:AA:891:G:OP1	2.36	0.58
79:XQ:296:PHE:CE2	79:XQ:300:ILE:HD11	2.38	0.58
4:A5:51:MET:HE1	17:AW:155:LEU:HD11	1.84	0.58
13:AR:108:ASP:OD1	13:AR:109:THR:N	2.36	0.58
22:Ag:12:VAL:HG21	22:Ag:83:LEU:HD13	1.84	0.58
29:BB:191:GLU:OE1	29:BB:191:GLU:N	2.34	0.58
35:BJ:224:ASP:OD1	35:BJ:225:ARG:N	2.37	0.58
12:AP:45:ARG:NH1	24:Ao:108:ASP:OD2	2.35	0.58
30:BD:391:ASP:OD1	30:BD:392:ALA:N	2.37	0.58
32:BF:280:ASP:OD2	32:BF:320:LYS:NZ	2.35	0.58
67:XC:557:CYS:N	67:XC:560:ASN:OD1	2.36	0.58
72:XI:321:GLU:OE1	72:XI:321:GLU:N	2.36	0.58
6:AA:290:A:H4'	66:XB:669:THR:HG21	1.85	0.58
48:Ba:61:GLU:OE1	48:Ba:61:GLU:N	2.37	0.58
76:XN:512:ASP:OD1	76:XN:513:ALA:N	2.36	0.58
66:XB:678:PRO:O	66:XB:682:GLN:N	2.35	0.58
67:XC:108:ASP:OD1	67:XC:109:ALA:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:XL:128:ARG:NE	74:XL:130:GLU:OE2	2.37	0.58
3:A3:68:VAL:HG13	3:A3:116:VAL:HG13	1.86	0.58
5:A8:59:THR:OG1	8:AF:317:THR:OG1	2.20	0.58
7:AE:143:VAL:N	7:AE:164:TRP:O	2.37	0.58
25:Ap:283:ILE:HD11	76:XN:556:TYR:CE1	2.39	0.58
27:Av:145:ARG:NH2	27:Av:149:ASP:O	2.37	0.58
70:XG:30:SER:O	70:XG:34:HIS:ND1	2.37	0.58
74:XL:529:THR:HG22	74:XL:567:ARG:HB2	1.86	0.58
76:XN:560:ARG:N	77:XO:304:ASP:OD1	2.37	0.58
71:XH:590:GLU:OE2	71:XH:622:ARG:NH2	2.37	0.57
74:XL:106:GLN:O	74:XL:272:HIS:NE2	2.34	0.57
32:BF:286:VAL:CG1	32:BF:316:MET:HE1	2.32	0.57
80:XR:142:GLN:OE1	80:XR:142:GLN:N	2.37	0.57
6:AA:461:U:OP1	15:AU:59:ARG:NH1	2.37	0.57
34:BI:112:ILE:HD12	51:Bf:100:TYR:O	2.04	0.57
69:XF:139:VAL:HG21	69:XF:158:LEU:HD12	1.86	0.57
6:AA:296:A:OP1	6:AA:494:U:O2'	2.16	0.57
17:AW:161:MET:HE1	17:AW:183:GLN:OE1	2.05	0.57
38:BN:227:VAL:O	38:BN:231:THR:HG23	2.04	0.57
76:XN:430:ARG:CZ	76:XN:437:LEU:HD21	2.34	0.57
65:XA:13:MET:HE2	65:XA:13:MET:HA	1.85	0.57
15:AU:75:THR:HG22	21:Af:77:VAL:HG13	1.85	0.57
65:XA:142:ARG:O	65:XA:146:ASN:ND2	2.37	0.57
76:XN:326:GLU:N	76:XN:326:GLU:OE1	2.35	0.57
6:AA:985:A:H5'	78:XP:41:LEU:HD23	1.87	0.57
7:AE:386:LEU:HD23	50:Bc:99:THR:HG21	1.86	0.57
67:XC:134:THR:HG22	67:XC:199:ILE:HD11	1.87	0.57
1:A1:88:THR:HG22	1:A1:95:VAL:HG23	1.87	0.57
6:AA:931:U:O2'	72:XI:418:PRO:O	2.22	0.57
28:BA:602:ARG:NH2	37:BL:93:GLY:O	2.37	0.57
41:BR:39:GLU:OE1	41:BR:64:ARG:NH1	2.38	0.57
74:XL:259:GLU:OE1	74:XL:259:GLU:N	2.35	0.57
6:AA:473:A:OP2	82:XT:10:HIS:ND1	2.38	0.57
30:BD:142:VAL:HG22	30:BD:145:TRP:CD1	2.40	0.57
32:BF:262:ARG:NH1	32:BF:334:MET:O	2.37	0.57
36:BK:87:LEU:HD23	36:BK:140:LEU:CD1	2.35	0.57
37:BL:108:ILE:HD12	37:BL:183:TRP:HB2	1.86	0.57
12:AP:301:TRP:O	12:AP:307:LYS:NZ	2.33	0.57
30:BD:292:LEU:HD22	30:BD:345:TYR:CD2	2.40	0.57
32:BF:356:ARG:NH1	45:BW:179:ASP:OD2	2.38	0.57
36:BK:321:GLU:OE1	36:BK:321:GLU:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:BK:349:VAL:HG23	36:BK:349:VAL:O	2.05	0.57
53:Bh:52:ASN:ND2	53:Bh:56:LYS:O	2.36	0.57
6:AA:862:U:OP1	66:XB:614:LYS:NZ	2.38	0.56
6:AA:1173:U:N3	42:BS:94:LEU:HD21	2.20	0.56
22:Ag:176:GLU:OE2	22:Ag:180:ARG:NH2	2.38	0.56
35:BJ:221:ARG:NH2	54:UA:24:ALA:O	2.38	0.56
39:BO:234:ASP:OD1	39:BO:235:TYR:N	2.38	0.56
66:XB:528:ASP:OD1	66:XB:533:ARG:NH1	2.37	0.56
67:XC:391:MET:HE2	67:XC:391:MET:HA	1.87	0.56
6:AA:184:U:OP1	8:AF:202:LYS:NZ	2.37	0.56
12:AP:102:GLU:O	32:BF:330:ARG:NH1	2.38	0.56
6:AA:1011:G:H1'	78:XP:179:MET:HE3	1.87	0.56
6:AA:1172:A:O2'	6:AA:1174:U:OP2	2.15	0.56
8:AF:148:LEU:HD21	12:AP:94:ILE:HB	1.86	0.56
12:AP:211:ILE:HG22	12:AP:211:ILE:O	2.06	0.56
13:AR:65:HIS:CE1	13:AR:69:ILE:HD11	2.40	0.56
30:BD:345:TYR:O	30:BD:349:ILE:HG23	2.04	0.56
43:BT:60:ARG:NH2	48:Ba:153:SER:O	2.38	0.56
45:BW:28:PRO:O	45:BW:29:SER:OG	2.16	0.56
65:XA:90:ASP:OD1	65:XA:92:VAL:HG22	2.05	0.56
74:XL:517:ILE:CG2	74:XL:534:LEU:HD23	2.35	0.56
6:AA:51:A:OP2	27:Av:48:ALA:N	2.37	0.56
8:AF:368:LEU:HD23	8:AF:385:LEU:HD21	1.86	0.56
14:AT:77:ASP:OD1	14:AT:78:ALA:N	2.39	0.56
28:BA:338:LEU:O	28:BA:377:ARG:NH2	2.38	0.56
75:XM:69:LEU:HD11	75:XM:74:LYS:HG2	1.86	0.56
1:A1:197:VAL:O	1:A1:201:LEU:HD23	2.05	0.56
7:AE:74:TYR:OH	7:AE:98:GLU:OE2	2.22	0.56
16:AV:60:ALA:N	24:Ao:87:GLU:O	2.36	0.56
19:AY:319:GLU:N	19:AY:319:GLU:OE1	2.35	0.56
5:A8:153:SER:O	5:A8:157:GLU:N	2.38	0.56
6:AA:49:A:OP1	9:AI:35:ARG:NH2	2.37	0.56
22:Ag:20:ASN:ND2	22:Ag:20:ASN:O	2.38	0.56
30:BD:276:GLU:OE2	30:BD:410:GLN:NE2	2.38	0.56
72:XI:496:ASN:OD1	72:XI:497:MET:N	2.38	0.56
19:AY:69:ASP:OD2	31:BE:49:LYS:NZ	2.28	0.56
41:BR:14:GLU:OE2	67:XC:526:LEU:HD12	2.06	0.56
42:BS:82:ASP:OD1	42:BS:83:GLN:N	2.39	0.56
77:XO:200:ASP:OD1	77:XO:201:ARG:N	2.39	0.56
9:AI:55:MET:HA	9:AI:55:MET:HE2	1.88	0.56
30:BD:218:ASN:OD1	30:BD:420:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:XP:71:ASP:OD1	78:XP:72:SER:N	2.38	0.56
81:XS:105:ASP:O	81:XS:106:SER:OG	2.15	0.56
6:AA:932:A:N7	66:XB:215:ARG:NH1	2.54	0.56
30:BD:332:LYS:C	30:BD:333:LEU:HD12	2.31	0.56
37:BL:37:ARG:NH1	37:BL:170:GLU:OE1	2.39	0.56
40:BQ:26:GLU:OE1	40:BQ:26:GLU:N	2.37	0.56
72:X1:538:LEU:HD23	72:X1:570:LEU:HD22	1.88	0.56
73:XJ:291:SER:OG	73:XJ:294:ARG:NH2	2.39	0.56
9:AI:152:ARG:O	35:BJ:292:ARG:NH1	2.39	0.55
21:Af:46:MET:HA	21:Af:46:MET:HE2	1.88	0.55
66:XB:184:PRO:HD2	66:XB:188:LEU:HD23	1.88	0.55
66:XB:485:ARG:N	66:XB:552:ASP:OD2	2.37	0.55
67:XC:208:ASN:OD1	67:XC:209:LEU:N	2.39	0.55
67:XC:604:LEU:HD12	67:XC:604:LEU:O	2.07	0.55
73:XJ:204:LEU:HD22	75:XM:71:VAL:HG13	1.87	0.55
6:AA:570:U:OP2	13:AR:228:ARG:NH2	2.39	0.55
7:AE:234:ASP:OD1	7:AE:235:VAL:N	2.38	0.55
10:AK:28:GLU:OE1	10:AK:30:LEU:N	2.37	0.55
15:AU:90:MET:SD	24:Ao:70:HIS:NE2	2.79	0.55
16:AV:15:ILE:HD11	21:Af:90:PHE:CE2	2.42	0.55
28:BA:312:TRP:HB3	28:BA:314:THR:HG23	1.88	0.55
40:BQ:198:SER:HG	67:XC:5:SER:HG	1.54	0.55
74:XL:302:ASN:OD1	74:XL:303:CYS:N	2.38	0.55
6:AA:515:U:HO2'	6:AA:516:U:P	2.29	0.55
26:At:116:GLN:NE2	26:At:122:THR:O	2.38	0.55
36:BK:87:LEU:HD21	36:BK:139:VAL:HB	1.89	0.55
82:XT:79:ILE:HG23	82:XT:79:ILE:O	2.05	0.55
1:A1:28:ARG:NH2	33:BH:271:PHE:O	2.40	0.55
8:AF:344:MET:HE1	12:AP:91:THR:O	2.05	0.55
47:BZ:108:GLU:OE1	47:BZ:108:GLU:N	2.34	0.55
67:XC:148:LEU:HD23	67:XC:148:LEU:C	2.31	0.55
50:Bc:51:TYR:OH	50:Bc:55:ARG:NH2	2.40	0.55
68:XE:92:THR:N	68:XE:95:SER:OG	2.40	0.55
2:A2:287:THR:O	2:A2:295:ASN:ND2	2.36	0.55
27:Av:111:ILE:O	27:Av:111:ILE:HG22	2.07	0.55
29:BB:357:THR:HG21	29:BB:392:TYR:CZ	2.42	0.55
30:BD:221:ILE:HG22	30:BD:221:ILE:O	2.06	0.55
32:BF:60:LEU:HD22	32:BF:235:GLU:OE2	2.07	0.55
35:BJ:187:VAL:O	35:BJ:192:ARG:N	2.37	0.55
71:XH:185:ILE:HG21	71:XH:326:LEU:HD12	1.86	0.55
75:XM:69:LEU:HD11	75:XM:74:LYS:CG	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:128:PRO:CB	47:BZ:146:LEU:HD21	2.37	0.55
4:A5:79:LYS:O	28:BA:785:ARG:NH2	2.40	0.55
52:Bg:54:HIS:ND1	52:Bg:91:ASP:OD2	2.39	0.55
72:XI:378:LEU:HD21	72:XI:382:MET:HE3	1.88	0.55
1:A1:188:ILE:CG2	1:A1:200:VAL:HG11	2.36	0.55
6:AA:115:A:H61	15:AU:43:MET:HE3	1.72	0.55
20:Ae:59:ASP:OD2	20:Ae:61:THR:OG1	2.13	0.55
23:Al:153:MET:HE2	23:Al:199:TYR:HD2	1.71	0.55
25:Ap:70:GLY:O	25:Ap:86:LYS:NZ	2.38	0.55
28:BA:809:ASP:OD1	28:BA:810:HIS:ND1	2.39	0.55
66:XB:669:THR:HG22	66:XB:672:VAL:HB	1.87	0.55
72:XI:577:GLU:OE1	72:XI:577:GLU:N	2.33	0.55
74:XL:458:ASN:ND2	74:XL:476:GLN:OE1	2.39	0.55
2:A2:143:VAL:HG22	2:A2:353:LEU:CD1	2.37	0.55
6:AA:466:G:OP1	24:Ao:81:ARG:NH1	2.38	0.55
6:AA:566:A:O2'	6:AA:568:U:OP1	2.09	0.55
12:AP:45:ARG:HE	26:At:144:VAL:HG23	1.71	0.55
84:Av:301:NAD:N7N	84:Av:301:NAD:O1N	2.39	0.55
28:BA:819:GLN:OE1	28:BA:821:TRP:NE1	2.38	0.55
30:BD:142:VAL:O	30:BD:142:VAL:HG13	2.07	0.55
53:Bh:3:LEU:HG	53:Bh:67:THR:HG22	1.89	0.55
68:XD:87:ASP:O	68:XD:91:VAL:HG23	2.07	0.55
71:XH:314:GLU:O	71:XH:317:ARG:NH2	2.40	0.55
74:XL:66:MET:HG3	74:XL:73:LEU:HD13	1.87	0.55
74:XL:397:VAL:HG12	74:XL:426:CYS:SG	2.47	0.55
30:BD:520:GLN:N	30:BD:520:GLN:OE1	2.37	0.55
32:BF:287:ASP:OD1	32:BF:313:ARG:NH2	2.40	0.55
74:XL:500:MET:HA	74:XL:500:MET:HE2	1.87	0.55
78:XP:172:LYS:NZ	78:XP:211:ASP:O	2.36	0.55
19:AY:323:ALA:O	19:AY:327:HIS:ND1	2.40	0.54
71:XH:394:VAL:O	71:XH:398:GLU:N	2.34	0.54
73:XJ:271:VAL:HG21	73:XJ:278:ILE:HD11	1.88	0.54
78:XP:82:ASP:OD1	78:XP:83:TYR:N	2.40	0.54
8:AF:109:MET:HE1	8:AF:232:LEU:HD21	1.90	0.54
32:BF:206:LEU:HD12	32:BF:209:ILE:HD11	1.88	0.54
47:BZ:128:PRO:O	47:BZ:131:HIS:NE2	2.39	0.54
71:XH:108:LEU:HD23	71:XH:321:GLU:OE2	2.07	0.54
74:XL:527:PRO:O	74:XL:529:THR:HG23	2.07	0.54
78:XP:210:LEU:HD13	78:XP:218:VAL:HG12	1.90	0.54
42:BS:101:GLU:OE1	42:BS:104:ARG:NH1	2.40	0.54
67:XC:70:SER:OG	67:XC:529:ILE:O	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:441:THR:HG23	36:BK:345:HIS:O	2.08	0.54
8:AF:46:GLN:OE1	8:AF:46:GLN:N	2.40	0.54
8:AF:364:TYR:OH	8:AF:384:TYR:O	2.23	0.54
15:AU:18:ASP:OD2	15:AU:32:ARG:NH1	2.40	0.54
20:Ae:100:HIS:HB2	20:Ae:106:LEU:HD23	1.88	0.54
74:XL:497:TRP:HB2	74:XL:520:ILE:HD12	1.89	0.54
76:XN:286:LEU:H	76:XN:290:ILE:HD11	1.71	0.54
7:AE:51:GLU:OE2	25:Ap:92:GLY:N	2.40	0.54
25:Ap:53:ARG:NH2	25:Ap:58:LYS:O	2.40	0.54
29:BB:134:ARG:HB2	29:BB:386:THR:HG21	1.89	0.54
30:BD:140:GLN:HB2	33:BH:174:LEU:HD23	1.88	0.54
51:Bf:109:PHE:O	51:Bf:110:SER:OG	2.25	0.54
66:XB:188:LEU:HD21	66:XB:259:ASP:OD2	2.08	0.54
5:A8:105:ASP:OD2	6:AA:913:C:O2'	2.19	0.54
74:XL:99:VAL:HG13	74:XL:100:VAL:HG13	1.89	0.54
37:BL:196:THR:O	37:BL:197:SER:OG	2.23	0.54
44:BU:122:ALA:HA	52:Bg:97:LEU:HD21	1.88	0.54
72:XI:662:VAL:HG11	72:XI:714:ARG:HD3	1.89	0.54
2:A2:19:ASN:OD1	2:A2:23:ASN:ND2	2.41	0.54
6:AA:1115:A:OP2	34:BI:26:ASN:ND2	2.36	0.54
28:BA:215:ARG:NH2	28:BA:290:ASP:OD1	2.40	0.54
47:BZ:88:ILE:HD11	47:BZ:97:LEU:HD22	1.89	0.54
74:XL:74:ASN:ND2	74:XL:74:ASN:O	2.41	0.54
2:A2:253:ALA:O	2:A2:256:VAL:HG12	2.08	0.54
6:AA:559:A:N6	81:XS:58:VAL:O	2.41	0.54
77:XO:277:ASP:OD1	77:XO:278:HIS:N	2.41	0.54
6:AA:172:U:OP2	12:AP:222:GLY:N	2.38	0.53
6:AA:853:A:O4'	66:XB:662:ARG:NH1	2.41	0.53
31:BE:48:MET:HE2	31:BE:48:MET:HA	1.89	0.53
51:Bf:99:ILE:HG23	51:Bf:100:TYR:N	2.22	0.53
70:XG:106:ARG:NH1	79:XQ:298:ASP:OD1	2.41	0.53
78:XP:289:ALA:HB2	78:XP:319:MET:HE1	1.90	0.53
82:XT:58:GLU:OE2	82:XT:70:HIS:ND1	2.39	0.53
2:A2:113:PHE:O	2:A2:117:LEU:HD23	2.08	0.53
23:Al:72:ARG:NH2	23:Al:144:GLY:O	2.41	0.53
68:XD:84:GLU:OE1	68:XD:84:GLU:N	2.41	0.53
68:XD:92:THR:HG22	68:XD:93:PRO:HD2	1.89	0.53
1:A1:106:THR:HG23	1:A1:106:THR:O	2.07	0.53
10:AK:62:ALA:N	10:AK:87:ASN:OD1	2.42	0.53
30:BD:345:TYR:CE2	30:BD:349:ILE:HG21	2.44	0.53
7:AE:153:GLU:OE1	7:AE:153:GLU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AF:232:LEU:HD13	12:AP:88:PRO:HG3	1.90	0.53
18:AX:201:GLU:OE2	36:BK:380:TYR:N	2.37	0.53
27:Av:184:MET:HA	27:Av:184:MET:HE2	1.89	0.53
31:BE:73:THR:HG23	31:BE:74:TYR:N	2.23	0.53
81:XS:69:LEU:HD11	81:XS:112:LEU:CB	2.39	0.53
8:AF:156:GLN:NE2	17:AW:9:ALA:O	2.39	0.53
30:BD:170:GLU:OE1	30:BD:170:GLU:N	2.38	0.53
66:XB:300:THR:HG21	66:XB:307:LEU:HD21	1.90	0.53
72:XI:199:PHE:CD2	72:XI:230:LEU:HD21	2.43	0.53
80:XR:29:PRO:O	80:XR:118:GLN:NE2	2.42	0.53
6:AA:1078:A:O3'	78:XP:46:ARG:NH1	2.42	0.53
14:AT:134:GLU:OE1	63:UJ:3:ALA:N	2.41	0.53
23:Al:101:GLN:OE1	23:Al:101:GLN:N	2.41	0.53
23:Al:132:ASP:OD1	23:Al:133:THR:N	2.41	0.53
46:BX:132:TYR:N	46:BX:139:TRP:O	2.39	0.53
47:BZ:185:ASP:OD1	47:BZ:186:CYS:N	2.42	0.53
78:XP:351:GLU:OE1	78:XP:351:GLU:N	2.41	0.53
6:AA:1139:G:OP2	76:XN:646:ARG:NH2	2.41	0.53
17:AW:149:ILE:HD11	17:AW:230:LEU:HD13	1.91	0.53
19:AY:86:GLU:OE1	19:AY:88:HIS:NE2	2.39	0.53
21:Af:64:SER:C	21:Af:65:LEU:HD12	2.34	0.53
29:BB:439:ASP:OD1	29:BB:442:ARG:NH1	2.38	0.53
34:BI:219:ASP:OD1	34:BI:220:THR:N	2.41	0.53
36:BK:87:LEU:HD23	36:BK:140:LEU:HD12	1.91	0.53
50:Bc:136:ARG:NH1	50:Bc:138:LYS:O	2.36	0.53
66:XB:54:TYR:O	66:XB:670:THR:OG1	2.27	0.53
67:XC:173:VAL:HG22	67:XC:175:LEU:HD13	1.91	0.53
74:XL:199:ILE:CD1	74:XL:242:LEU:HD11	2.38	0.53
6:AA:501:A:OP1	31:BE:17:SER:OG	2.25	0.53
6:AA:1146:U:O2	7:AE:398:GLN:NE2	2.40	0.53
7:AE:143:VAL:O	7:AE:164:TRP:N	2.40	0.53
7:AE:246:ILE:HG23	7:AE:337:VAL:CG1	2.39	0.53
34:BI:169:GLU:OE2	69:XF:211:LEU:N	2.41	0.53
34:BI:207:ILE:HD12	34:BI:212:ILE:O	2.09	0.53
37:BL:158:ARG:NH2	37:BL:221:CYS:O	2.38	0.53
67:XC:310:TYR:CZ	67:XC:314:LEU:HD11	2.44	0.53
76:XN:581:ALA:HB2	76:XN:610:ALA:HB1	1.91	0.53
4:A5:78:ILE:HG23	28:BA:780:TYR:CD2	2.44	0.53
6:AA:1080:A:OP1	65:XA:22:ARG:NH2	2.41	0.53
19:AY:63:ARG:NH1	19:AY:67:GLU:OE1	2.42	0.53
34:BI:289:GLU:OE1	34:BI:289:GLU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BR:179:ILE:HD12	41:BR:179:ILE:N	2.24	0.53
50:Bc:48:GLU:OE1	50:Bc:48:GLU:N	2.39	0.53
6:AA:521:G:O6	44:BU:130:ALA:N	2.42	0.53
9:AI:23:THR:O	9:AI:46:LEU:HD21	2.09	0.53
28:BA:319:TYR:OH	28:BA:357:MET:SD	2.66	0.53
30:BD:182:ARG:NH2	30:BD:257:ASP:OD1	2.41	0.53
32:BF:246:TRP:CH2	32:BF:316:MET:HE2	2.44	0.53
44:BU:125:LYS:HD3	52:Bg:97:LEU:HD23	1.90	0.53
52:Bg:42:ALA:HA	52:Bg:45:LEU:HD12	1.90	0.53
52:Bg:100:ARG:O	52:Bg:103:THR:HG22	2.09	0.53
72:XI:593:TRP:CD1	72:XI:618:TYR:HH	2.26	0.53
74:XL:429:LYS:HE3	88:XL:602:GTP:H1'	1.90	0.53
77:XO:196:ILE:N	77:XO:196:ILE:HD12	2.25	0.53
2:A2:96:ARG:NE	2:A2:100:GLU:OE2	2.39	0.52
4:A5:36:ARG:O	4:A5:39:VAL:HG22	2.09	0.52
6:AA:78:U:OP2	43:BT:63:THR:HG21	2.09	0.52
7:AE:80:ASN:ND2	34:BI:246:GLU:O	2.41	0.52
15:AU:16:GLU:O	37:BL:67:ALA:HB1	2.09	0.52
38:BN:128:ASN:O	38:BN:231:THR:HG21	2.08	0.52
74:XL:464:ALA:N	88:XL:602:GTP:O6	2.42	0.52
78:XP:84:GLU:OE1	78:XP:224:ARG:NH1	2.42	0.52
1:A1:62:GLN:OE1	1:A1:64:SER:OG	2.26	0.52
2:A2:117:LEU:HD13	2:A2:370:TYR:OH	2.09	0.52
32:BF:123:LEU:HA	32:BF:126:VAL:HG22	1.90	0.52
18:AX:225:GLU:N	18:AX:225:GLU:OE1	2.43	0.52
37:BL:177:LEU:CD2	37:BL:291:LEU:HD21	2.37	0.52
79:XQ:120:MET:HA	79:XQ:327:LEU:HD13	1.91	0.52
7:AE:164:TRP:HA	7:AE:322:LEU:HD23	1.92	0.52
8:AF:163:ASP:OD1	8:AF:164:TYR:N	2.42	0.52
28:BA:566:MET:HE1	28:BA:574:TYR:CE1	2.44	0.52
66:XB:341:VAL:CG2	66:XB:587:THR:HG22	2.38	0.52
75:XM:92:THR:O	75:XM:97:ARG:NH1	2.43	0.52
6:AA:294:U:O2'	17:AW:19:ASN:ND2	2.41	0.52
6:AA:807:A:O2'	17:AW:213:ASP:OD2	2.27	0.52
11:AN:154:GLU:O	50:Bc:23:ARG:NH2	2.42	0.52
48:Ba:149:LYS:O	48:Ba:152:ARG:NH1	2.39	0.52
67:XC:93:LYS:O	67:XC:202:HIS:NE2	2.37	0.52
67:XC:198:GLU:OE1	67:XC:198:GLU:N	2.41	0.52
70:XG:81:ILE:HD11	70:XG:98:VAL:CG2	2.39	0.52
76:XN:419:ILE:CG2	76:XN:605:MET:HE2	2.38	0.52
81:XS:177:GLU:O	81:XS:181:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:XJ:168:ASP:O	75:XM:36:ARG:NH2	2.43	0.52
7:AE:113:GLU:OE1	76:XN:352:ARG:NH2	2.41	0.52
11:AN:119:THR:HG23	25:Ap:66:VAL:HG21	1.92	0.52
32:BF:345:LEU:HD12	32:BF:345:LEU:O	2.10	0.52
44:BU:127:ILE:HD13	46:BX:155:ARG:NH2	2.25	0.52
79:XQ:296:PHE:CZ	79:XQ:300:ILE:HD11	2.45	0.52
1:A1:206:ILE:HG23	19:AY:297:CYS:SG	2.50	0.52
1:A1:56:ARG:NH1	33:BH:294:ASP:OD1	2.43	0.52
7:AE:173:HIS:NE2	7:AE:227:ALA:O	2.43	0.52
15:AU:40:PHE:CD1	16:AV:101:LEU:HD21	2.45	0.52
22:Ag:29:LEU:HD23	22:Ag:33:LEU:HD22	1.92	0.52
31:BE:266:LEU:HD11	31:BE:279:HIS:CE1	2.45	0.52
71:XH:214:ILE:HG23	71:XH:319:VAL:HG13	1.91	0.52
77:XO:109:GLN:OE1	78:XP:212:ARG:NH2	2.44	0.52
8:AF:182:MET:HE2	31:BE:28:LEU:HD21	1.91	0.51
16:AV:112:TRP:NE1	16:AV:114:ASP:OD1	2.43	0.51
19:AY:151:VAL:N	19:AY:164:VAL:O	2.42	0.51
73:XJ:244:ALA:HB3	73:XJ:281:LEU:HD13	1.91	0.51
8:AF:182:MET:HE3	31:BE:11:TYR:HD2	1.75	0.51
19:AY:75:THR:HG21	31:BE:60:GLY:HA3	1.91	0.51
20:Ae:69:ARG:NH2	20:Ae:119:HIS:O	2.42	0.51
66:XB:368:ASP:OD1	66:XB:369:ILE:N	2.44	0.51
2:A2:336:TYR:CE2	2:A2:340:LEU:HD11	2.45	0.51
6:AA:86:U:OP2	36:BK:344:LYS:N	2.37	0.51
8:AF:137:MET:SD	8:AF:224:ARG:NH1	2.77	0.51
30:BD:121:VAL:HG13	30:BD:122:PHE:N	2.25	0.51
37:BL:193:ARG:NH1	37:BL:301:TRP:O	2.42	0.51
38:BN:130:PRO:HB3	38:BN:231:THR:HG22	1.93	0.51
41:BR:22:VAL:HG22	41:BR:56:ALA:HB1	1.93	0.51
77:XO:220:ILE:HD11	77:XO:276:TYR:CD2	2.46	0.51
2:A2:185:LYS:HD2	9:AI:56:ALA:HB1	1.93	0.51
9:AI:112:ARG:NH2	9:AI:138:TYR:O	2.41	0.51
19:AY:145:ASN:OD1	36:BK:298:HIS:NE2	2.43	0.51
21:Af:80:THR:OG1	22:Ag:126:ARG:NH1	2.43	0.51
28:BA:432:SER:O	28:BA:476:SER:OG	2.26	0.51
33:BH:165:GLN:O	33:BH:241:ARG:NH1	2.43	0.51
66:XB:153:TYR:HB2	66:XB:297:VAL:HG11	1.92	0.51
19:AY:224:GLU:OE1	19:AY:224:GLU:N	2.40	0.51
28:BA:187:MET:O	28:BA:191:VAL:HG23	2.10	0.51
50:Bc:75:GLU:OE1	50:Bc:75:GLU:N	2.43	0.51
72:XI:495:SER:CB	72:XI:521:LEU:HD21	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:XL:112:ILE:HG22	74:XL:190:ILE:CD1	2.40	0.51
10:AK:59:ALA:N	10:AK:98:VAL:O	2.39	0.51
53:Bh:56:LYS:HB3	53:Bh:60:VAL:HG11	1.92	0.51
53:Bh:60:VAL:HG23	53:Bh:61:PRO:HD3	1.92	0.51
66:XB:334:LEU:HD13	66:XB:574:ALA:HB2	1.93	0.51
67:XC:2:LYS:NZ	67:XC:317:LEU:O	2.30	0.51
77:XO:479:LEU:N	77:XO:479:LEU:HD23	2.26	0.51
2:A2:113:PHE:CZ	2:A2:117:LEU:HD21	2.45	0.51
2:A2:128:PRO:HB2	47:BZ:146:LEU:HD21	1.93	0.51
6:AA:827:U:OP1	65:XA:45:ARG:NH1	2.41	0.51
24:Ao:74:PRO:O	24:Ao:80:SER:OG	2.24	0.51
30:BD:106:ILE:HD11	30:BD:443:LEU:HD11	1.93	0.51
66:XB:94:LYS:NZ	66:XB:96:LYS:O	2.42	0.51
6:AA:1107:U:OP2	7:AE:198:LYS:NZ	2.43	0.51
28:BA:674:LEU:O	28:BA:678:THR:HG23	2.11	0.51
3:A3:170:ARG:CZ	23:Al:181:LEU:HD22	2.40	0.51
26:At:66:ILE:HD12	26:At:66:ILE:H	1.74	0.51
28:BA:757:THR:O	28:BA:757:THR:HG22	2.11	0.51
71:XH:373:LEU:HD23	71:XH:374:THR:N	2.26	0.51
72:XI:220:TRP:CD2	72:XI:258:LEU:HD11	2.45	0.51
75:XM:69:LEU:HD13	75:XM:72:THR:O	2.11	0.51
6:AA:1103:U:OP1	14:AT:7:ARG:N	2.44	0.51
8:AF:435:TYR:N	12:AP:318:SER:O	2.41	0.51
28:BA:657:PHE:CE2	28:BA:661:ILE:HD11	2.46	0.51
29:BB:114:ALA:HB3	29:BB:117:LEU:HD13	1.92	0.51
30:BD:424:VAL:HG12	30:BD:434:LEU:HD12	1.93	0.51
41:BR:14:GLU:CD	67:XC:526:LEU:HD12	2.36	0.51
42:BS:80:ASP:OD1	42:BS:81:SER:N	2.38	0.51
72:XI:277:GLU:OE1	72:XI:277:GLU:N	2.42	0.51
76:XN:497:PHE:CZ	76:XN:518:LEU:HD22	2.46	0.51
6:AA:88:G:H4'	32:BF:403:LEU:HD23	1.92	0.50
6:AA:1116:U:OP2	11:AN:114:TYR:OH	2.26	0.50
6:AA:1135:G:N2	6:AA:1138:A:OP2	2.38	0.50
7:AE:203:ALA:HB1	28:BA:181:VAL:HG11	1.94	0.50
7:AE:259:MET:SD	7:AE:260:PHE:N	2.84	0.50
31:BE:59:THR:OG1	31:BE:62:GLU:OE1	2.28	0.50
34:BI:38:LEU:O	34:BI:42:VAL:HG23	2.11	0.50
68:XD:105:4HH:HO2	75:XM:89:ALA:HB1	1.93	0.50
72:XI:387:ILE:HD11	72:XI:445:LEU:CD2	2.35	0.50
72:XI:683:VAL:O	72:XI:714:ARG:NH2	2.44	0.50
77:XO:471:ASP:OD1	77:XO:472:LEU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:25:A:O2'	8:AF:159:ALA:O	2.16	0.50
9:AI:120:ASN:OD1	9:AI:133:ARG:N	2.41	0.50
10:AK:149:MET:SD	10:AK:150:THR:N	2.84	0.50
32:BF:50:LEU:HD21	32:BF:54:VAL:HB	1.93	0.50
70:XG:78:VAL:CG1	70:XG:97:ALA:HB1	2.41	0.50
25:Ap:244:VAL:HG23	25:Ap:244:VAL:O	2.12	0.50
30:BD:430:THR:HG22	30:BD:434:LEU:CD1	2.41	0.50
76:XN:71:THR:OG1	76:XN:84:MET:O	2.27	0.50
77:XO:118:GLN:O	77:XO:132:HIS:NE2	2.43	0.50
6:AA:14:A:N6	19:AY:18:PRO:O	2.45	0.50
8:AF:455:TRP:NE1	84:Av:301:NAD:O2N	2.41	0.50
17:AW:149:ILE:HG23	17:AW:201:ILE:HG22	1.94	0.50
28:BA:301:HIS:HB3	28:BA:305:VAL:HG22	1.93	0.50
66:XB:292:VAL:O	66:XB:292:VAL:HG13	2.12	0.50
78:XP:174:HIS:ND1	78:XP:213:GLU:O	2.43	0.50
79:XQ:108:ASP:OD1	79:XQ:109:ARG:N	2.45	0.50
8:AF:78:SER:CB	32:BF:361:ILE:HD11	2.39	0.50
21:Af:80:THR:O	22:Ag:124:ARG:N	2.41	0.50
21:Af:94:ASP:OD1	21:Af:95:GLY:N	2.44	0.50
32:BF:56:VAL:O	32:BF:60:LEU:HD23	2.11	0.50
37:BL:148:GLN:NE2	37:BL:152:ASP:OD1	2.44	0.50
49:Bb:61:VAL:HG23	49:Bb:61:VAL:O	2.11	0.50
59:UF:18:ALA:CA	69:XF:198:THR:HG21	2.42	0.50
67:XC:166:LEU:HD22	67:XC:168:LEU:HD23	1.94	0.50
3:A3:68:VAL:HG13	3:A3:116:VAL:CG1	2.42	0.50
3:A3:69:HIS:ND1	3:A3:96:THR:OG1	2.38	0.50
7:AE:49:MET:HE1	50:Bc:57:TRP:HB3	1.94	0.50
7:AE:170:VAL:HG13	7:AE:185:VAL:HG13	1.94	0.50
7:AE:171:VAL:N	7:AE:186:TYR:O	2.43	0.50
21:Af:143:THR:OG1	21:Af:144:VAL:N	2.45	0.50
24:Ao:60:THR:HG22	24:Ao:61:ARG:N	2.27	0.50
28:BA:301:HIS:NE2	50:Bc:14:GLU:OE1	2.38	0.50
30:BD:345:TYR:CD2	30:BD:349:ILE:HD13	2.47	0.50
47:BZ:67:LEU:HD12	47:BZ:67:LEU:O	2.11	0.50
66:XB:482:ASP:OD1	66:XB:483:GLY:N	2.43	0.50
28:BA:593:THR:HG21	28:BA:642:ILE:HD12	1.93	0.50
30:BD:449:LEU:O	30:BD:454:THR:HG23	2.12	0.50
38:BN:119:VAL:HG13	53:Bh:86:VAL:HA	1.94	0.50
42:BS:68:ARG:HG3	42:BS:87:LEU:HD21	1.94	0.50
47:BZ:25:LEU:HD21	47:BZ:37:PHE:HD2	1.75	0.50
67:XC:514:ASN:OD1	67:XC:515:MET:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:XG:53:GLU:OE1	70:XG:53:GLU:N	2.45	0.50
71:XH:539:ASP:OD1	71:XH:543:ARG:NH1	2.45	0.50
76:XN:497:PHE:HZ	76:XN:518:LEU:HD22	1.75	0.50
77:XO:97:ASP:O	79:XQ:241:ALA:HB1	2.12	0.50
10:AK:113:LEU:HD22	77:XO:458:GLY:HA2	1.92	0.50
70:XG:70:VAL:HG23	70:XG:70:VAL:O	2.10	0.50
74:XL:177:GLU:OE1	74:XL:177:GLU:N	2.43	0.50
76:XN:494:LEU:HD11	76:XN:509:ILE:O	2.12	0.50
32:BF:43:LEU:HD22	45:BW:188:TYR:CE1	2.47	0.50
38:BN:99:VAL:HG23	38:BN:99:VAL:O	2.12	0.50
74:XL:413:LEU:HD23	74:XL:454:VAL:HG13	1.94	0.50
1:A1:62:GLN:O	6:AA:50:A:O2'	2.26	0.49
6:AA:173:U:H2'	23:A1:203:LEU:HD23	1.94	0.49
17:AW:245:ARG:NH2	28:BA:754:ARG:O	2.44	0.49
28:BA:174:ARG:O	28:BA:179:SER:OG	2.26	0.49
30:BD:244:ARG:NH2	30:BD:267:GLU:OE1	2.45	0.49
48:Ba:80:ASP:OD1	48:Ba:81:GLN:N	2.45	0.49
68:XD:84:GLU:OE1	68:XD:85:LYS:N	2.44	0.49
72:XI:482:PRO:O	72:XI:523:ARG:NH2	2.45	0.49
74:XL:77:THR:OG1	74:XL:343:ARG:NH1	2.45	0.49
1:A1:133:ASP:OD2	1:A1:143:ARG:NH1	2.44	0.49
2:A2:185:LYS:NZ	2:A2:315:PRO:O	2.44	0.49
8:AF:438:ASP:OD2	8:AF:445:GLN:NE2	2.45	0.49
15:AU:108:ARG:NH1	22:Ag:121:GLU:OE2	2.45	0.49
32:BF:50:LEU:HD23	32:BF:51:PRO:O	2.13	0.49
66:XB:590:GLN:O	66:XB:594:VAL:HG13	2.12	0.49
74:XL:348:LEU:N	74:XL:348:LEU:HD12	2.27	0.49
6:AA:39:C:O3'	18:AX:107:LYS:NZ	2.46	0.49
6:AA:487:A:OP1	17:AW:84:ARG:NH2	2.45	0.49
6:AA:1108:A:OP2	7:AE:200:HIS:NE2	2.42	0.49
7:AE:246:ILE:HG23	7:AE:337:VAL:HG11	1.94	0.49
28:BA:218:ASN:ND2	28:BA:287:THR:O	2.44	0.49
31:BE:90:TYR:OH	36:BK:302:VAL:HG12	2.12	0.49
38:BN:170:ARG:NH2	81:XS:177:GLU:OE1	2.46	0.49
66:XB:219:ARG:O	66:XB:223:LEU:HD23	2.11	0.49
67:XC:89:VAL:HG13	67:XC:213:ILE:HD11	1.93	0.49
72:XI:646:LEU:HD22	72:XI:709:LEU:CD1	2.42	0.49
78:XP:58:TYR:CD2	78:XP:120:VAL:HG22	2.47	0.49
6:AA:335:G:N2	6:AA:336:U:O4	2.42	0.49
7:AE:102:ASP:OD2	25:Ap:146:VAL:HG11	2.12	0.49
7:AE:103:ALA:O	7:AE:107:LEU:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AF:390:LEU:CD1	45:BW:97:ILE:HG21	2.43	0.49
17:AW:248:LEU:N	17:AW:248:LEU:HD23	2.26	0.49
23:AI:97:LEU:O	23:AI:122:LEU:HD12	2.12	0.49
52:Bg:41:TYR:CE2	52:Bg:45:LEU:HD11	2.48	0.49
66:XB:549:LEU:HD23	66:XB:550:HIS:H	1.76	0.49
71:XH:238:LEU:HD13	71:XH:247:ILE:HG21	1.93	0.49
71:XH:260:THR:HG23	71:XH:260:THR:O	2.12	0.49
75:XM:69:LEU:C	75:XM:69:LEU:HD12	2.38	0.49
76:XN:311:GLU:OE2	76:XN:486:ARG:NH1	2.45	0.49
1:A1:132:LYS:NZ	9:AI:175:HIS:O	2.43	0.49
3:A3:140:ASP:OD2	26:At:102:ARG:NH1	2.44	0.49
13:AR:264:ALA:O	36:BK:131:ARG:NH1	2.43	0.49
29:BB:348:VAL:HG22	29:BB:426:ALA:HB1	1.93	0.49
30:BD:326:ARG:NH2	33:BH:173:LEU:HD21	2.27	0.49
49:Bb:77:ALA:C	49:Bb:78:LEU:HD22	2.37	0.49
71:XH:227:THR:HG22	71:XH:228:PRO:HD2	1.94	0.49
72:XI:223:LEU:HG	72:XI:230:LEU:HD22	1.95	0.49
76:XN:286:LEU:N	76:XN:290:ILE:HD11	2.28	0.49
34:BI:90:TYR:HB2	34:BI:114:LEU:HD21	1.93	0.49
67:XC:597:MET:O	67:XC:601:VAL:HG23	2.12	0.49
71:XH:185:ILE:HG21	71:XH:326:LEU:CD1	2.42	0.49
72:XI:520:LEU:C	72:XI:520:LEU:HD23	2.37	0.49
73:XJ:218:ILE:N	73:XJ:218:ILE:HD12	2.27	0.49
42:BS:43:PRO:O	42:BS:113:ARG:NH1	2.45	0.49
50:Bc:102:LEU:O	50:Bc:102:LEU:HD12	2.13	0.49
72:XI:356:LEU:HD23	72:XI:356:LEU:O	2.12	0.49
78:XP:181:THR:HG22	78:XP:182:ASP:H	1.78	0.49
2:A2:345:ILE:HD12	2:A2:345:ILE:N	2.27	0.49
31:BE:22:HIS:O	31:BE:24:LYS:NZ	2.44	0.49
51:Bf:99:ILE:O	51:Bf:100:TYR:C	2.55	0.49
77:XO:275:LEU:O	77:XO:288:HIS:NE2	2.42	0.49
6:AA:187:A:OP1	8:AF:175:LYS:NZ	2.33	0.49
19:AY:185:ILE:H	19:AY:185:ILE:HD12	1.77	0.49
73:XJ:298:VAL:HG13	75:XM:103:ARG:HG2	1.94	0.49
74:XL:127:LEU:CD2	74:XL:157:LEU:HD21	2.43	0.49
77:XO:105:GLN:NE2	78:XP:330:GLY:O	2.46	0.49
81:XS:69:LEU:HB3	81:XS:116:ILE:HD13	1.93	0.49
1:A1:192:GLU:N	1:A1:192:GLU:OE1	2.45	0.49
34:BI:106:HIS:NE2	69:XF:299:ALA:O	2.46	0.49
45:BW:157:ASN:O	45:BW:160:VAL:HG22	2.12	0.49
16:AV:121:ILE:HD12	16:AV:121:ILE:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BA:142:GLU:OE1	28:BA:144:ARG:NH1	2.43	0.48
33:BH:280:ILE:HG21	74:XL:66:MET:HE2	1.95	0.48
66:XB:456:VAL:HG22	66:XB:578:ARG:HG2	1.95	0.48
70:XG:65:VAL:HG21	70:XG:80:LEU:HD12	1.94	0.48
72:XI:45:VAL:HG13	72:XI:45:VAL:O	2.12	0.48
76:XN:71:THR:N	76:XN:82:SER:O	2.41	0.48
77:XO:189:ASN:OD1	77:XO:190:THR:N	2.46	0.48
78:XP:153:ARG:O	78:XP:157:HIS:ND1	2.46	0.48
6:AA:503:A:OP1	31:BE:41:HIS:NE2	2.42	0.48
19:AY:185:ILE:HD12	19:AY:185:ILE:N	2.28	0.48
38:BN:168:LEU:HD12	38:BN:168:LEU:N	2.28	0.48
76:XN:536:MET:HG3	76:XN:583:LEU:HD12	1.95	0.48
6:AA:1010:C:N4	78:XP:316:GLU:OE2	2.41	0.48
16:AV:171:ASP:OD1	16:AV:172:LYS:N	2.39	0.48
22:Ag:36:PHE:CE1	22:Ag:87:VAL:HG21	2.48	0.48
30:BD:362:LEU:HD22	30:BD:492:VAL:HG23	1.95	0.48
72:XI:414:ASP:OD1	72:XI:415:ALA:N	2.46	0.48
74:XL:410:MET:HE3	74:XL:446:LYS:HB3	1.94	0.48
2:A2:21:PHE:CD2	2:A2:64:MET:HE1	2.48	0.48
15:AU:83:GLU:OE2	21:Af:76:LEU:N	2.38	0.48
15:AU:202:ASP:OD1	15:AU:203:VAL:N	2.47	0.48
28:BA:419:THR:HG22	28:BA:419:THR:O	2.14	0.48
72:XI:346:GLU:OE1	72:XI:346:GLU:N	2.44	0.48
77:XO:386:MET:HE1	77:XO:403:LEU:HD21	1.96	0.48
9:AI:82:ASP:OD1	9:AI:83:ILE:N	2.46	0.48
13:AR:232:LEU:HD12	31:BE:419:MET:SD	2.53	0.48
30:BD:198:ASP:OD1	30:BD:199:SER:N	2.46	0.48
35:BJ:256:LEU:HD12	35:BJ:256:LEU:O	2.14	0.48
66:XB:612:ASN:O	66:XB:612:ASN:ND2	2.42	0.48
67:XC:34:LEU:HD12	67:XC:34:LEU:N	2.28	0.48
72:XI:53:ARG:HD3	72:XI:519:LEU:HD21	1.96	0.48
74:XL:570:GLN:OE1	74:XL:570:GLN:N	2.46	0.48
77:XO:124:GLY:O	78:XP:185:GLN:NE2	2.46	0.48
78:XP:310:THR:O	78:XP:315:GLN:NE2	2.41	0.48
1:A1:88:THR:HG22	1:A1:95:VAL:CG2	2.44	0.48
6:AA:143:U:OP1	15:AU:33:LYS:N	2.45	0.48
6:AA:906:A:OP1	66:XB:561:THR:OG1	2.29	0.48
19:AY:131:ILE:HG23	19:AY:141:ILE:HG23	1.95	0.48
32:BF:363:GLN:HB2	45:BW:174:ILE:HG23	1.95	0.48
41:BR:106:THR:HG22	41:BR:106:THR:O	2.14	0.48
16:AV:174:ALA:O	16:AV:178:ALA:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:XP:325:ARG:NH2	79:XQ:48:MET:O	2.43	0.48
1:A1:112:ASP:O	9:AI:152:ARG:NH2	2.47	0.48
2:A2:437:HIS:NE2	36:BK:366:MET:HE3	2.29	0.48
6:AA:485:A:N1	17:AW:50:GLN:NE2	2.59	0.48
14:AT:72:ILE:HD11	73:XJ:189:TRP:CZ2	2.49	0.48
19:AY:139:ASN:C	19:AY:172:VAL:HG23	2.38	0.48
28:BA:187:MET:SD	28:BA:206:ILE:HD11	2.54	0.48
45:BW:82:GLU:OE1	45:BW:82:GLU:N	2.46	0.48
74:XL:199:ILE:HD11	74:XL:242:LEU:HD11	1.95	0.48
6:AA:291:A:OP1	66:XB:666:HIS:ND1	2.47	0.48
38:BN:97:ARG:NH2	44:BU:182:GLU:OE2	2.47	0.48
67:XC:451:VAL:HG21	67:XC:505:TYR:HB3	1.95	0.48
71:XH:484:ARG:NH2	78:XP:76:CYS:SG	2.87	0.48
79:XQ:102:LEU:HD23	79:XQ:102:LEU:C	2.39	0.48
25:Ap:222:LEU:HD23	25:Ap:223:PHE:N	2.27	0.48
28:BA:233:VAL:O	28:BA:233:VAL:HG13	2.14	0.48
28:BA:470:GLY:O	28:BA:471:SER:C	2.57	0.48
42:BS:133:LYS:HB2	73:XJ:181:VAL:HG11	1.95	0.48
66:XB:188:LEU:HD13	66:XB:546:GLY:O	2.14	0.48
67:XC:46:ARG:NH1	67:XC:599:ARG:O	2.46	0.48
81:XS:72:ILE:HB	81:XS:73:PRO:HD3	1.95	0.48
75:XM:82:ARG:NE	75:XM:86:GLU:OE1	2.45	0.47
6:AA:458:U:OP1	12:AP:10:ARG:NE	2.42	0.47
74:XL:228:GLN:O	74:XL:232:GLU:N	2.41	0.47
2:A2:345:ILE:HG22	2:A2:346:GLY:N	2.30	0.47
6:AA:115:A:OP1	15:AU:25:ARG:NH2	2.46	0.47
6:AA:850:G:N1	6:AA:1090:U:O2'	2.47	0.47
7:AE:90:GLN:N	7:AE:90:GLN:OE1	2.47	0.47
2:A2:136:ASP:OD1	2:A2:138:THR:HG22	2.14	0.47
6:AA:33:G:N1	48:Ba:34:SER:O	2.40	0.47
6:AA:50:A:H4'	27:Av:48:ALA:HB2	1.97	0.47
6:AA:572:U:O2'	13:AR:156:ASP:OD2	2.29	0.47
11:AN:42:GLU:OE1	11:AN:82:HIS:NE2	2.45	0.47
17:AW:138:VAL:CG1	17:AW:174:ILE:HD13	2.44	0.47
20:Ae:105:LYS:C	20:Ae:106:LEU:HD22	2.39	0.47
31:BE:403:ASN:OD1	31:BE:406:ASP:N	2.48	0.47
49:Bb:62:ARG:O	49:Bb:67:ARG:NH2	2.47	0.47
3:A3:115:ILE:HG22	3:A3:115:ILE:O	2.13	0.47
6:AA:552:U:OP2	6:AA:554:A:N6	2.46	0.47
41:BR:175:GLU:HB3	71:XH:411:ILE:HD13	1.96	0.47
46:BX:165:ARG:O	46:BX:169:ARG:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:123:VAL:HG12	1:A1:124:GLU:N	2.30	0.47
6:AA:470:G:OP2	12:AP:70:LEU:N	2.48	0.47
6:AA:569:U:O2'	13:AR:228:ARG:NH2	2.47	0.47
15:AU:21:ARG:HA	15:AU:39:LEU:HD11	1.95	0.47
17:AW:116:ARG:NH2	37:BL:110:SER:O	2.48	0.47
17:AW:138:VAL:HG13	17:AW:174:ILE:HD13	1.94	0.47
28:BA:685:ARG:NE	28:BA:722:LEU:O	2.45	0.47
44:BU:116:ARG:NH2	46:BX:153:THR:O	2.48	0.47
65:XA:66:ARG:NH2	65:XA:126:GLN:OE1	2.48	0.47
3:A3:120:VAL:CG2	26:At:43:ILE:HG23	2.45	0.47
9:AI:115:VAL:HG13	9:AI:155:ILE:O	2.15	0.47
28:BA:177:ILE:O	28:BA:181:VAL:HG23	2.15	0.47
29:BB:353:LEU:HD21	29:BB:392:TYR:CE2	2.50	0.47
30:BD:196:LEU:HD13	68:XE:98:VAL:HG12	1.96	0.47
30:BD:286:GLU:OE2	30:BD:387:HIS:NE2	2.41	0.47
32:BF:134:ASP:OD1	32:BF:149:TYR:OH	2.28	0.47
32:BF:246:TRP:HH2	32:BF:316:MET:HE2	1.80	0.47
35:BJ:178:ILE:HG22	35:BJ:181:ARG:NH2	2.29	0.47
74:XL:78:PRO:O	74:XL:148:ARG:NH1	2.45	0.47
74:XL:274:MET:N	74:XL:274:MET:SD	2.87	0.47
77:XO:119:ASN:O	77:XO:133:HIS:NE2	2.45	0.47
78:XP:123:THR:HG22	78:XP:124:ARG:N	2.30	0.47
81:XS:106:SER:O	81:XS:107:ALA:HB3	2.15	0.47
2:A2:222:GLU:O	8:AF:278:ARG:NH1	2.48	0.47
6:AA:130:U:OP1	66:XB:666:HIS:NE2	2.40	0.47
11:AN:88:ILE:HA	11:AN:91:VAL:HG23	1.96	0.47
19:AY:141:ILE:O	19:AY:170:ILE:N	2.43	0.47
39:BO:103:LEU:HB2	39:BO:216:LEU:HD21	1.96	0.47
53:Bh:35:CYS:SG	53:Bh:39:THR:HG21	2.54	0.47
73:XJ:200:VAL:HG13	73:XJ:231:LEU:HD21	1.96	0.47
14:AT:72:ILE:HD12	14:AT:72:ILE:N	2.30	0.47
25:Ap:146:VAL:O	25:Ap:146:VAL:HG13	2.15	0.47
25:Ap:186:VAL:O	25:Ap:225:ALA:N	2.47	0.47
27:Av:140:GLU:OE1	27:Av:140:GLU:N	2.47	0.47
35:BJ:179:ARG:O	35:BJ:180:GLU:C	2.57	0.47
39:BO:138:ARG:HD3	39:BO:160:MET:HE3	1.97	0.47
66:XB:65:ARG:NH2	66:XB:624:GLU:OE2	2.45	0.47
2:A2:345:ILE:N	2:A2:348:ALA:O	2.42	0.47
6:AA:467:U:OP2	24:Ao:99:ARG:NH1	2.48	0.47
6:AA:954:U:O2	72:XI:40:ARG:NH2	2.46	0.47
22:Ag:29:LEU:CD2	22:Ag:33:LEU:HD22	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BA:586:SER:N	28:BA:672:GLU:OE2	2.43	0.47
66:XB:180:ILE:HD12	66:XB:253:LEU:CD1	2.45	0.47
67:XC:173:VAL:HG22	67:XC:175:LEU:CD1	2.45	0.47
71:XH:497:ASP:N	71:XH:497:ASP:OD1	2.46	0.47
74:XL:413:LEU:HD23	74:XL:454:VAL:CG1	2.45	0.47
77:XO:156:VAL:HG11	77:XO:161:LEU:HD22	1.97	0.47
2:A2:153:ARG:NH1	2:A2:156:GLU:OE2	2.48	0.46
11:AN:172:ARG:NH1	22:Ag:119:ASN:O	2.42	0.46
12:AP:354:THR:OG1	12:AP:355:LEU:N	2.47	0.46
16:AV:8:LEU:HD23	16:AV:8:LEU:C	2.40	0.46
47:BZ:97:LEU:HD23	47:BZ:98:SER:N	2.30	0.46
71:XH:214:ILE:HD12	71:XH:271:LEU:HD12	1.97	0.46
2:A2:59:ASN:ND2	18:AX:175:TYR:OH	2.47	0.46
7:AE:150:ASP:OD1	7:AE:151:TYR:N	2.42	0.46
7:AE:152:ASP:OD1	7:AE:153:GLU:N	2.46	0.46
12:AP:264:GLN:OE1	12:AP:277:GLN:NE2	2.43	0.46
15:AU:10:HIS:NE2	16:AV:110:VAL:HG23	2.30	0.46
27:Av:145:ARG:NH2	27:Av:151:PRO:O	2.42	0.46
28:BA:291:HIS:NE2	28:BA:700:CYS:O	2.48	0.46
77:XO:116:LEU:HD23	77:XO:116:LEU:O	2.15	0.46
2:A2:372:GLU:OE2	48:Ba:49:ARG:NH2	2.41	0.46
6:AA:815:U:O4	11:AN:13:LYS:N	2.42	0.46
11:AN:123:GLU:O	25:Ap:62:ASN:ND2	2.47	0.46
32:BF:302:ASP:OD1	32:BF:303:VAL:N	2.48	0.46
37:BL:176:GLN:O	37:BL:180:LEU:HD13	2.15	0.46
39:BO:191:ASN:OD1	39:BO:192:LEU:N	2.49	0.46
43:BT:61:ARG:CB	48:Ba:144:VAL:HG21	2.45	0.46
70:XG:71:ASP:OD1	70:XG:73:THR:OG1	2.29	0.46
70:XG:173:VAL:O	70:XG:173:VAL:HG12	2.14	0.46
74:XL:212:LEU:HD23	74:XL:212:LEU:O	2.15	0.46
76:XN:536:MET:HE2	76:XN:579:TYR:HB2	1.97	0.46
2:A2:405:LEU:HD21	19:AY:98:LYS:HA	1.97	0.46
4:A5:66:PRO:O	6:AA:1162:G:N2	2.45	0.46
5:A8:88:LEU:HD11	12:AP:157:VAL:HG12	1.97	0.46
6:AA:171:U:O2'	6:AA:172:U:OP1	2.24	0.46
13:AR:101:VAL:HG11	13:AR:143:TYR:CG	2.51	0.46
16:AV:138:ASP:OD1	16:AV:139:LYS:N	2.48	0.46
25:Ap:229:ILE:HG22	25:Ap:230:THR:N	2.30	0.46
29:BB:351:LEU:HD11	29:BB:422:MET:HG2	1.98	0.46
29:BB:357:THR:HG21	29:BB:392:TYR:OH	2.15	0.46
30:BD:503:ILE:HD12	30:BD:503:ILE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:BO:138:ARG:CD	39:BO:160:MET:HE3	2.46	0.46
66:XB:303:ILE:HD13	66:XB:322:ILE:HD13	1.97	0.46
66:XB:320:THR:HG22	66:XB:322:ILE:HG13	1.97	0.46
66:XB:559:MET:HE2	66:XB:594:VAL:HG12	1.97	0.46
2:A2:422:ARG:NH1	31:BE:76:GLN:O	2.44	0.46
6:AA:84:A:H2'	6:AA:84:A:N3	2.31	0.46
12:AP:211:ILE:HG21	12:AP:266:LEU:HD11	1.96	0.46
27:Av:59:SER:O	27:Av:61:THR:HG23	2.16	0.46
34:BI:70:PRO:HG2	34:BI:73:ILE:HD13	1.97	0.46
74:XL:313:VAL:O	74:XL:397:VAL:HG22	2.15	0.46
80:XR:104:LEU:HD12	80:XR:137:TYR:CE2	2.50	0.46
7:AE:382:LYS:NZ	14:AT:40:GLU:OE2	2.46	0.46
19:AY:110:ILE:H	19:AY:110:ILE:HD12	1.80	0.46
20:Ae:161:LEU:HD23	20:Ae:162:GLN:N	2.30	0.46
24:Ao:25:ASN:OD1	24:Ao:26:TYR:N	2.49	0.46
31:BE:98:LEU:HD23	31:BE:98:LEU:C	2.41	0.46
66:XB:386:GLU:OE1	66:XB:386:GLU:N	2.42	0.46
66:XB:544:ALA:O	66:XB:572:ARG:NH2	2.48	0.46
72:XI:224:LEU:HD21	72:XI:288:HIS:CB	2.46	0.46
72:XI:243:LEU:HA	72:XI:247:LEU:HD12	1.96	0.46
77:XO:464:ASP:OD1	77:XO:465:ILE:N	2.49	0.46
79:XQ:336:LEU:HD23	79:XQ:336:LEU:N	2.31	0.46
7:AE:235:VAL:HG21	7:AE:321:SER:HA	1.97	0.46
10:AK:233:LEU:O	10:AK:233:LEU:HD23	2.16	0.46
11:AN:63:GLN:NE2	21:Af:60:GLN:OE1	2.48	0.46
14:AT:96:GLU:OE1	14:AT:96:GLU:N	2.48	0.46
28:BA:301:HIS:CB	28:BA:305:VAL:HG22	2.46	0.46
29:BB:318:ALA:O	29:BB:319:ALA:HB3	2.15	0.46
34:BI:112:ILE:HD13	34:BI:115:LEU:HD11	1.97	0.46
37:BL:281:SER:O	37:BL:285:LEU:HD23	2.15	0.46
41:BR:165:ASN:O	41:BR:193:ILE:N	2.39	0.46
52:Bg:54:HIS:HA	52:Bg:86:ARG:HE	1.80	0.46
53:Bh:45:SER:OG	53:Bh:67:THR:HG23	2.15	0.46
68:XD:122:ASP:OD1	68:XD:123:ILE:N	2.49	0.46
72:XI:539:LEU:CB	72:XI:570:LEU:HD21	2.45	0.46
72:XI:682:LEU:O	72:XI:689:TRP:NE1	2.48	0.46
80:XR:28:CYS:SG	80:XR:114:THR:HG23	2.55	0.46
4:A5:51:MET:CE	17:AW:155:LEU:HD11	2.46	0.46
11:AN:136:ASP:OD2	65:XA:60:HIS:NE2	2.48	0.46
25:Ap:143:GLU:OE2	25:Ap:160:ARG:NE	2.48	0.46
29:BB:422:MET:SD	29:BB:423:GLY:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BD:430:THR:HG22	30:BD:434:LEU:HD12	1.96	0.46
31:BE:410:PHE:O	31:BE:411:LYS:C	2.59	0.46
44:BU:127:ILE:HD13	46:BX:155:ARG:CZ	2.46	0.46
46:BX:120:ASN:O	46:BX:123:LYS:NZ	2.39	0.46
74:XL:112:ILE:CG2	74:XL:190:ILE:HD11	2.46	0.46
74:XL:526:ARG:HB2	74:XL:527:PRO:CD	2.46	0.46
1:A1:109:HIS:NE2	1:A1:127:MET:SD	2.85	0.46
2:A2:143:VAL:HG22	2:A2:353:LEU:HD13	1.98	0.46
2:A2:199:CYS:HB2	2:A2:306:VAL:HG23	1.97	0.46
8:AF:276:GLY:O	8:AF:354:GLY:N	2.44	0.46
9:AI:185:TYR:CE2	9:AI:189:LEU:HD11	2.51	0.46
17:AW:171:GLY:O	17:AW:175:VAL:HG23	2.16	0.46
18:AX:143:GLU:OE1	18:AX:143:GLU:N	2.48	0.46
31:BE:67:LEU:O	31:BE:71:LEU:HD13	2.16	0.46
72:XI:597:LEU:O	72:XI:597:LEU:HD23	2.15	0.46
79:XQ:244:ALA:O	79:XQ:248:LEU:HD13	2.16	0.46
6:AA:515:U:O2'	6:AA:516:U:P	2.73	0.46
6:AA:965:A:O3'	74:XL:545:LYS:NZ	2.41	0.46
12:AP:15:HIS:O	12:AP:17:ARG:NH1	2.43	0.46
12:AP:65:VAL:HG23	12:AP:65:VAL:O	2.16	0.46
41:BR:178:GLY:C	41:BR:179:ILE:HD12	2.40	0.46
66:XB:133:ILE:HG12	66:XB:139:THR:HG21	1.96	0.46
71:XH:389:LEU:HD23	71:XH:389:LEU:C	2.41	0.46
77:XO:144:ASN:OD1	77:XO:147:TYR:N	2.40	0.46
78:XP:147:LYS:C	78:XP:148:LEU:HD12	2.41	0.46
1:A1:143:ARG:O	1:A1:157:ARG:NH1	2.50	0.45
5:A8:93:ARG:NH1	6:AA:910:G:O6	2.46	0.45
6:AA:19:A:C5	17:AW:69:LEU:HD23	2.51	0.45
6:AA:159:U:OP1	23:AI:143:ASN:ND2	2.49	0.45
17:AW:76:LEU:HD21	19:AY:29:MET:CE	2.45	0.45
18:AX:97:PRO:HB2	20:Ae:87:VAL:HG23	1.98	0.45
28:BA:39:HIS:N	76:XN:347:GLU:OE1	2.49	0.45
28:BA:566:MET:HE1	28:BA:574:TYR:CD1	2.51	0.45
30:BD:296:THR:CG2	30:BD:349:ILE:HD12	2.46	0.45
38:BN:250:LEU:H	38:BN:250:LEU:HD12	1.81	0.45
43:BT:142:TYR:CE1	43:BT:165:ILE:HG23	2.52	0.45
47:BZ:120:LEU:C	47:BZ:120:LEU:HD12	2.41	0.45
3:A3:72:ASP:OD1	3:A3:73:HIS:N	2.49	0.45
3:A3:145:LEU:HD12	3:A3:145:LEU:O	2.16	0.45
7:AE:374:LEU:N	39:BO:232:GLU:OE2	2.49	0.45
8:AF:416:TYR:OH	45:BW:79:HIS:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AT:102:LEU:N	14:AT:102:LEU:HD23	2.31	0.45
65:XA:67:PHE:HB2	65:XA:74:VAL:HG21	1.99	0.45
67:XC:522:ASP:OD2	67:XC:527:THR:OG1	2.30	0.45
74:XL:556:VAL:HG23	74:XL:566:ILE:HD12	1.98	0.45
81:XS:46:ASN:ND2	81:XS:46:ASN:O	2.49	0.45
1:A1:173:LEU:C	1:A1:173:LEU:HD23	2.41	0.45
1:A1:173:LEU:HG	19:AY:292:VAL:HG22	1.99	0.45
2:A2:138:THR:OG1	2:A2:328:TYR:O	2.30	0.45
2:A2:460:ASP:OD1	2:A2:461:ALA:N	2.46	0.45
8:AF:60:LEU:O	22:Ag:26:ARG:NH2	2.49	0.45
13:AR:121:ASP:OD1	31:BE:443:SER:OG	2.29	0.45
25:Ap:34:PRO:O	25:Ap:38:ASN:ND2	2.46	0.45
28:BA:663:LEU:C	28:BA:663:LEU:HD23	2.41	0.45
32:BF:251:ARG:NH2	32:BF:353:GLU:OE1	2.44	0.45
72:XI:665:LEU:HD22	72:XI:710:LEU:HD13	1.99	0.45
6:AA:813:U:OP1	15:AU:27:ARG:NH2	2.49	0.45
7:AE:384:PRO:HG2	50:Bc:99:THR:HG23	1.99	0.45
11:AN:163:ILE:N	11:AN:163:ILE:HD12	2.31	0.45
27:Av:76:TYR:HB3	27:Av:80:ALA:HB3	1.98	0.45
38:BN:250:LEU:HD11	44:BU:152:TYR:CG	2.52	0.45
48:Ba:48:PRO:CB	48:Ba:86:ILE:HG21	2.45	0.45
2:A2:415:ASN:ND2	36:BK:379:LEU:HD23	2.29	0.45
6:AA:1167:A:OP2	13:AR:94:ARG:NH2	2.45	0.45
7:AE:51:GLU:OE1	25:Ap:93:ARG:N	2.50	0.45
17:AW:123:VAL:HG11	37:BL:113:ARG:NH1	2.31	0.45
19:AY:245:GLU:OE1	19:AY:245:GLU:N	2.45	0.45
35:BJ:275:ASP:OD1	35:BJ:275:ASP:N	2.46	0.45
66:XB:50:GLN:HG3	66:XB:688:ILE:HD13	1.98	0.45
76:XN:72:VAL:HG13	76:XN:72:VAL:O	2.16	0.45
82:XT:14:ASN:OD1	82:XT:14:ASN:N	2.50	0.45
82:XT:75:LEU:O	82:XT:79:ILE:HG22	2.15	0.45
1:A1:50:ASN:H	1:A1:53:SER:HG	1.62	0.45
2:A2:217:ASP:O	43:BT:112:ARG:NH2	2.49	0.45
3:A3:132:VAL:HG12	12:AP:35:ILE:HD13	1.99	0.45
6:AA:544:G:OP2	18:AX:192:ASN:ND2	2.50	0.45
11:AN:107:THR:HG22	11:AN:108:ALA:N	2.31	0.45
12:AP:50:ASP:N	12:AP:50:ASP:OD1	2.48	0.45
16:AV:58:HIS:CE1	16:AV:86:THR:HG21	2.51	0.45
22:Ag:185:VAL:HG11	34:BI:98:ASP:OD2	2.17	0.45
27:Av:93:GLU:OE1	27:Av:93:GLU:N	2.49	0.45
36:BK:374:HIS:NE2	36:BK:375:ASN:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:BT:97:THR:O	45:BW:75:ARG:NH2	2.49	0.45
66:XB:477:ARG:NE	66:XB:479:VAL:O	2.47	0.45
74:XL:271:ILE:O	74:XL:275:HIS:ND1	2.48	0.45
74:XL:500:MET:SD	74:XL:554:THR:HG21	2.57	0.45
76:XN:430:ARG:NH1	76:XN:437:LEU:HD21	2.32	0.45
3:A3:68:VAL:CG1	3:A3:90:LEU:HD11	2.44	0.45
6:AA:16:A:O3'	17:AW:73:LYS:NZ	2.50	0.45
6:AA:80:U:O4	8:AF:314:TYR:OH	2.34	0.45
27:Av:81:LEU:HD23	27:Av:125:MET:HE1	1.99	0.45
28:BA:347:VAL:HG22	28:BA:397:MET:HE2	1.98	0.45
32:BF:186:SER:O	32:BF:190:ASN:ND2	2.44	0.45
32:BF:253:LEU:HA	32:BF:256:LEU:HD23	1.98	0.45
42:BS:97:ASP:OD1	42:BS:98:VAL:N	2.49	0.45
50:Bc:136:ARG:NE	51:Bf:33:ASP:O	2.49	0.45
72:XI:721:GLN:N	72:XI:721:GLN:OE1	2.49	0.45
74:XL:312:ILE:HD11	74:XL:359:LEU:HD11	1.98	0.45
79:XQ:136:THR:HG22	79:XQ:137:GLY:N	2.31	0.45
1:A1:131:GLU:OE1	9:AI:175:HIS:NE2	2.46	0.45
6:AA:865:C:H42	6:AA:966:A:H61	1.63	0.45
7:AE:222:THR:OG1	7:AE:224:ASP:OD1	2.24	0.45
8:AF:103:VAL:HG21	8:AF:371:LEU:HD11	1.98	0.45
8:AF:268:GLY:O	8:AF:347:ASP:N	2.39	0.45
8:AF:394:VAL:HG22	8:AF:395:PRO:HD2	1.99	0.45
14:AT:24:LEU:CD2	14:AT:26:ILE:HD13	2.47	0.45
17:AW:155:LEU:O	17:AW:198:VAL:HG22	2.16	0.45
21:Af:125:THR:HG22	21:Af:126:SER:N	2.32	0.45
27:Av:49:THR:HG21	48:Ba:131:LEU:HD22	1.99	0.45
31:BE:135:MET:CE	31:BE:151:LEU:HD22	2.47	0.45
32:BF:240:VAL:HG11	32:BF:286:VAL:HG21	1.99	0.45
34:BI:183:VAL:HG21	51:Bf:97:VAL:HG11	1.99	0.45
34:BI:293:THR:OG1	77:XO:484:GLN:OE1	2.35	0.45
66:XB:161:MET:HE1	66:XB:231:VAL:CG2	2.46	0.45
67:XC:45:LEU:HD13	67:XC:397:LEU:HD21	1.99	0.45
72:XI:511:THR:HG23	72:XI:512:ASP:N	2.31	0.45
5:A8:92:MET:HE1	67:XC:106:GLU:HG3	1.98	0.45
6:AA:958:A:N6	74:XL:130:GLU:O	2.50	0.45
6:AA:1110:A:N6	6:AA:1111:A:N1	2.65	0.45
8:AF:128:ARG:NH1	8:AF:353:GLU:OE1	2.50	0.45
9:AI:74:SER:OG	9:AI:77:ARG:O	2.34	0.45
13:AR:110:ASP:OD2	38:BN:93:LYS:NZ	2.28	0.45
13:AR:176:GLY:O	13:AR:193:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AY:85:LEU:HD11	31:BE:63:VAL:HG11	1.99	0.45
28:BA:497:LEU:CB	28:BA:507:ALA:HB2	2.47	0.45
32:BF:319:LYS:O	32:BF:323:ASN:ND2	2.43	0.45
37:BL:294:CYS:O	37:BL:295:VAL:C	2.60	0.45
38:BN:165:LEU:HD23	38:BN:167:PHE:CZ	2.52	0.45
40:BQ:59:GLU:OE2	40:BQ:63:SER:OG	2.34	0.45
47:BZ:48:ASP:OD1	47:BZ:49:THR:N	2.50	0.45
67:XC:245:GLU:OE1	67:XC:245:GLU:N	2.50	0.45
13:AR:119:LEU:HD12	13:AR:125:VAL:CG2	2.43	0.45
21:Af:152:TRP:CZ3	28:BA:403:LEU:HD23	2.52	0.45
44:BU:129:THR:HG23	52:Bg:94:LEU:HD22	1.99	0.45
67:XC:264:ILE:HD12	67:XC:264:ILE:N	2.32	0.45
74:XL:474:MET:O	74:XL:478:LEU:HD23	2.17	0.45
1:A1:13:PHE:CD1	72:XI:37:ILE:HG21	2.52	0.44
1:A1:91:GLN:N	1:A1:91:GLN:OE1	2.49	0.44
7:AE:218:GLY:O	7:AE:338:ARG:NH1	2.50	0.44
8:AF:67:ILE:HD12	8:AF:67:ILE:N	2.32	0.44
22:Ag:185:VAL:HG11	34:BI:98:ASP:CG	2.43	0.44
31:BE:367:GLN:O	31:BE:370:VAL:N	2.42	0.44
66:XB:162:ILE:HD11	66:XB:203:THR:HB	1.98	0.44
76:XN:387:LYS:O	76:XN:391:HIS:ND1	2.47	0.44
77:XO:104:LEU:HD13	78:XP:353:LYS:HG3	1.99	0.44
16:AV:54:GLU:O	16:AV:57:SER:OG	2.32	0.44
19:AY:163:ILE:N	19:AY:163:ILE:HD12	2.32	0.44
19:AY:179:ASP:O	19:AY:183:ASN:N	2.45	0.44
22:Ag:16:TYR:HB3	22:Ag:25:THR:HG21	1.98	0.44
28:BA:431:VAL:O	28:BA:434:THR:HG22	2.17	0.44
29:BB:241:GLU:OE1	29:BB:241:GLU:N	2.43	0.44
32:BF:206:LEU:HD22	32:BF:243:PHE:O	2.17	0.44
32:BF:401:GLY:O	32:BF:405:ASN:ND2	2.42	0.44
33:BH:195:ILE:HD12	33:BH:195:ILE:N	2.33	0.44
76:XN:279:GLN:OE1	76:XN:279:GLN:N	2.50	0.44
77:XO:237:ASP:OD1	77:XO:238:ARG:N	2.46	0.44
23:Al:45:ILE:HD11	23:Al:54:ALA:HB3	1.98	0.44
28:BA:279:VAL:HG23	28:BA:280:PHE:CD1	2.52	0.44
28:BA:344:GLU:OE2	28:BA:389:HIS:NE2	2.49	0.44
65:XA:135:TRP:O	65:XA:138:ARG:NH1	2.50	0.44
66:XB:590:GLN:OE1	66:XB:590:GLN:N	2.50	0.44
78:XP:172:LYS:NZ	78:XP:214:THR:O	2.34	0.44
6:AA:92:U:OP2	32:BF:400:ARG:NH2	2.48	0.44
6:AA:173:U:O2'	23:Al:67:TYR:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:AT:109:PRO:O	14:AT:112:ARG:NE	2.45	0.44
16:AV:63:LYS:NZ	24:Ao:83:ILE:O	2.50	0.44
22:Ag:45:ILE:N	22:Ag:45:ILE:HD12	2.32	0.44
32:BF:121:VAL:O	32:BF:123:LEU:N	2.51	0.44
49:Bb:40:VAL:HG12	49:Bb:41:HIS:H	1.82	0.44
2:A2:116:ARG:NH1	19:AY:260:GLU:OE2	2.51	0.44
2:A2:414:THR:O	2:A2:417:VAL:HG22	2.18	0.44
8:AF:261:TRP:O	32:BF:418:TYR:OH	2.35	0.44
28:BA:151:ASP:O	28:BA:155:ILE:N	2.45	0.44
35:BJ:255:ALA:HA	48:Ba:51:LEU:HD21	1.99	0.44
37:BL:58:LEU:O	37:BL:61:VAL:HG23	2.17	0.44
72:XI:400:ARG:NH2	74:XL:229:GLU:OE2	2.50	0.44
77:XO:188:THR:OG1	77:XO:189:ASN:N	2.51	0.44
77:XO:277:ASP:OD1	77:XO:278:HIS:ND1	2.49	0.44
78:XP:281:THR:HG22	78:XP:282:LYS:N	2.33	0.44
3:A3:174:LEU:O	3:A3:178:LEU:HD23	2.17	0.44
6:AA:272:G:OP1	66:XB:704:LYS:NZ	2.33	0.44
12:AP:16:PRO:HB2	12:AP:18:ARG:HG2	1.99	0.44
26:At:144:VAL:HG23	26:At:144:VAL:O	2.17	0.44
28:BA:589:MET:HG2	28:BA:639:ALA:HB2	2.00	0.44
30:BD:441:VAL:O	30:BD:441:VAL:HG23	2.17	0.44
34:BI:299:ARG:NH1	77:XO:492:ASN:OD1	2.50	0.44
39:BO:70:ALA:O	42:BS:33:ARG:NH1	2.51	0.44
47:BZ:13:ILE:HD12	47:BZ:13:ILE:N	2.33	0.44
67:XC:391:MET:HE1	67:XC:476:LEU:CD2	2.47	0.44
72:XI:378:LEU:HD23	72:XI:378:LEU:C	2.42	0.44
1:A1:167:ILE:HD13	35:BJ:289:GLU:OE1	2.18	0.44
2:A2:47:LEU:HD23	2:A2:50:ILE:HD11	2.00	0.44
7:AE:283:MET:CG	66:XB:641:ILE:HD13	2.48	0.44
8:AF:109:MET:HE3	8:AF:228:THR:CG2	2.48	0.44
8:AF:132:PRO:O	8:AF:136:GLY:CA	2.65	0.44
17:AW:179:LEU:HD23	17:AW:232:LEU:HD21	1.98	0.44
53:Bh:60:VAL:N	53:Bh:61:PRO:HD2	2.32	0.44
66:XB:334:LEU:HD21	66:XB:570:ALA:HB1	2.00	0.44
71:XH:371:ILE:HD12	71:XH:371:ILE:N	2.32	0.44
73:XJ:215:ILE:HD12	73:XJ:215:ILE:N	2.33	0.44
74:XL:384:SER:O	74:XL:388:ILE:HD13	2.18	0.44
78:XP:156:ALA:HB1	78:XP:196:TRP:CE3	2.52	0.44
79:XQ:125:CYS:HA	79:XQ:128:VAL:HG22	2.00	0.44
7:AE:91:THR:HG22	51:Bf:108:HIS:CD2	2.53	0.44
14:AT:59:THR:HG21	73:XJ:185:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:XM:38:LEU:HD23	75:XM:38:LEU:C	2.43	0.44
2:A2:401:THR:HG22	2:A2:444:GLY:CA	2.47	0.44
7:AE:178:GLY:O	25:Ap:105:ARG:NH2	2.51	0.44
12:AP:192:ASN:O	45:BW:22:ARG:NH1	2.46	0.44
17:AW:75:GLN:O	17:AW:76:LEU:HD12	2.18	0.44
25:Ap:285:ASP:OD2	77:XO:316:ARG:NH1	2.50	0.44
28:BA:148:VAL:HG21	39:BO:147:MET:HG3	1.98	0.44
43:BT:75:THR:HG22	43:BT:75:THR:O	2.18	0.44
66:XB:582:VAL:O	66:XB:582:VAL:HG13	2.18	0.44
67:XC:264:ILE:HG21	67:XC:266:TYR:CZ	2.53	0.44
67:XC:316:TYR:HH	67:XC:355:HIS:CE1	2.21	0.44
70:XG:61:PHE:HB3	70:XG:65:VAL:HG21	2.00	0.44
70:XG:85:THR:HG22	70:XG:129:LEU:HD11	2.00	0.44
71:XH:517:LEU:HD12	71:XH:518:ALA:N	2.32	0.44
6:AA:139:U:OP2	66:XB:683:ARG:NH2	2.45	0.43
16:AV:176:GLU:O	22:Ag:124:ARG:NH1	2.51	0.43
17:AW:248:LEU:HD23	17:AW:248:LEU:H	1.83	0.43
65:XA:62:ARG:NH1	65:XA:81:ASP:OD2	2.51	0.43
67:XC:241:LEU:HD12	67:XC:241:LEU:N	2.33	0.43
77:XO:220:ILE:HD11	77:XO:276:TYR:CG	2.53	0.43
78:XP:178:MET:O	78:XP:188:SER:OG	2.35	0.43
2:A2:470:ASP:N	2:A2:470:ASP:OD1	2.50	0.43
9:AI:99:LEU:HD23	9:AI:99:LEU:C	2.43	0.43
9:AI:212:ASP:OD1	9:AI:213:GLY:N	2.49	0.43
18:AX:202:VAL:O	18:AX:202:VAL:HG12	2.16	0.43
26:At:113:PRO:HG2	40:BQ:91:ILE:HD13	2.00	0.43
30:BD:140:GLN:N	30:BD:141:PRO:CD	2.81	0.43
30:BD:345:TYR:CD2	30:BD:349:ILE:HG21	2.53	0.43
31:BE:144:VAL:HG22	31:BE:145:LYS:N	2.34	0.43
31:BE:367:GLN:OE1	31:BE:373:GLN:NE2	2.48	0.43
71:XH:315:ASN:OD1	71:XH:316:VAL:N	2.49	0.43
72:XI:223:LEU:CG	72:XI:230:LEU:HD22	2.48	0.43
72:XI:443:LEU:HD23	72:XI:443:LEU:C	2.43	0.43
74:XL:86:THR:HG22	74:XL:87:GLU:N	2.32	0.43
74:XL:360:ILE:HG21	74:XL:387:GLU:HG2	1.99	0.43
1:A1:113:VAL:HG21	1:A1:160:ILE:HG23	2.00	0.43
2:A2:396:GLU:OE1	2:A2:396:GLU:N	2.51	0.43
6:AA:45:U:OP1	20:Ae:85:SER:N	2.49	0.43
6:AA:1158:G:O4'	28:BA:233:VAL:HG11	2.18	0.43
10:AK:28:GLU:O	10:AK:32:VAL:HG23	2.18	0.43
16:AV:124:ILE:HD12	16:AV:124:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BA:760:TYR:OH	28:BA:797:LYS:NZ	2.52	0.43
30:BD:240:SER:O	30:BD:241:VAL:HG23	2.19	0.43
65:XA:136:ASP:OD2	78:XP:232:ARG:NH2	2.52	0.43
72:XI:715:LEU:HD23	72:XI:715:LEU:C	2.44	0.43
74:XL:190:ILE:HG22	74:XL:218:VAL:CG1	2.48	0.43
76:XN:443:HIS:HB2	76:XN:474:PRO:HG2	2.00	0.43
77:XO:120:VAL:O	77:XO:120:VAL:HG23	2.17	0.43
5:A8:180:VAL:O	5:A8:181:VAL:HG13	2.18	0.43
10:AK:212:GLU:OE1	10:AK:216:ARG:NH2	2.51	0.43
15:AU:20:ILE:HG13	15:AU:39:LEU:HD13	2.00	0.43
19:AY:132:ILE:N	19:AY:142:VAL:O	2.51	0.43
22:Ag:12:VAL:O	22:Ag:12:VAL:HG13	2.18	0.43
31:BE:109:VAL:HG13	31:BE:155:LEU:HD21	2.01	0.43
33:BH:257:ASP:OD1	33:BH:258:THR:N	2.51	0.43
45:BW:32:GLU:HB3	45:BW:97:ILE:HD11	2.00	0.43
81:XS:69:LEU:HD11	81:XS:112:LEU:HB3	1.99	0.43
6:AA:478:A:O4'	6:AA:493:A:N6	2.52	0.43
6:AA:904:U:O4	65:XA:5:LYS:N	2.52	0.43
6:AA:915:A:N1	72:XI:50:HIS:NE2	2.63	0.43
8:AF:132:PRO:O	8:AF:136:GLY:N	2.52	0.43
13:AR:229:HIS:CG	13:AR:246:VAL:HG11	2.54	0.43
27:Av:158:GLU:O	33:BH:265:HIS:NE2	2.42	0.43
41:BR:81:ILE:HD12	41:BR:87:PHE:CZ	2.54	0.43
66:XB:347:LYS:NZ	66:XB:557:PHE:O	2.48	0.43
68:XE:126:HIS:NE2	68:XE:127:ASP:OD1	2.52	0.43
72:XI:199:PHE:HD2	72:XI:223:LEU:HD21	1.83	0.43
74:XL:451:VAL:HG23	74:XL:452:ARG:N	2.33	0.43
79:XQ:113:ILE:N	79:XQ:113:ILE:HD12	2.33	0.43
6:AA:1172:A:OP1	39:BO:130:ARG:NH2	2.43	0.43
8:AF:105:THR:HG22	8:AF:106:TYR:N	2.33	0.43
11:AN:69:HIS:NE2	11:AN:81:ASP:OD2	2.45	0.43
14:AT:127:ASP:OD1	14:AT:128:GLU:N	2.52	0.43
28:BA:510:LEU:HD23	28:BA:510:LEU:C	2.44	0.43
32:BF:185:GLU:OE1	32:BF:185:GLU:N	2.45	0.43
33:BH:103:GLU:O	33:BH:107:VAL:HG23	2.19	0.43
44:BU:113:MET:HB2	52:Bg:104:THR:HG22	1.99	0.43
66:XB:64:GLU:OE2	66:XB:305:ARG:NE	2.46	0.43
72:XI:658:ASP:OD1	72:XI:658:ASP:N	2.50	0.43
74:XL:85:ARG:NH2	74:XL:331:GLU:OE1	2.52	0.43
78:XP:267:ARG:NH1	78:XP:272:ASP:OD1	2.49	0.43
81:XS:85:GLN:HB2	81:XS:86:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A8:54:VAL:HG21	8:AF:165:GLU:OE1	2.18	0.43
5:A8:144:ASN:HD22	12:AP:173:SER:HG	1.64	0.43
7:AE:165:PHE:CE2	7:AE:323:ILE:HD12	2.53	0.43
10:AK:53:TRP:HH2	10:AK:75:LEU:HD22	1.84	0.43
28:BA:267:PHE:CE2	28:BA:337:MET:HE1	2.53	0.43
28:BA:740:LEU:O	28:BA:740:LEU:HD23	2.18	0.43
29:BB:415:ASP:OD1	29:BB:416:LEU:N	2.51	0.43
34:BI:103:THR:HG22	34:BI:104:ARG:N	2.33	0.43
35:BJ:178:ILE:HG22	35:BJ:181:ARG:HH22	1.84	0.43
66:XB:83:THR:HG23	66:XB:89:LEU:HB2	2.01	0.43
77:XO:385:LEU:HG	77:XO:387:VAL:HG13	2.01	0.43
11:AN:107:THR:HG22	11:AN:108:ALA:H	1.84	0.43
29:BB:406:GLY:O	29:BB:410:ALA:N	2.40	0.43
31:BE:430:PHE:O	31:BE:433:VAL:HG12	2.19	0.43
33:BH:108:ILE:N	33:BH:108:ILE:HD12	2.34	0.43
40:BQ:118:PHE:N	40:BQ:119:GLU:OE1	2.52	0.43
43:BT:173:LEU:C	43:BT:173:LEU:HD12	2.42	0.43
47:BZ:81:TYR:OH	47:BZ:145:HIS:NE2	2.41	0.43
67:XC:43:LEU:HD12	67:XC:43:LEU:N	2.34	0.43
68:XE:122:ASP:OD1	68:XE:123:ILE:N	2.52	0.43
78:XP:87:LYS:CB	78:XP:109:LEU:HD11	2.49	0.43
78:XP:310:THR:HG22	78:XP:311:THR:N	2.33	0.43
81:XS:69:LEU:HD11	81:XS:112:LEU:HB2	2.00	0.43
81:XS:93:TRP:CG	81:XS:107:ALA:HB2	2.54	0.43
1:A1:45:TRP:HA	6:AA:64:U:O2'	2.19	0.43
3:A3:119:ASP:OD1	3:A3:120:VAL:N	2.51	0.43
6:AA:79:U:O2'	6:AA:80:U:OP1	2.25	0.43
6:AA:516:U:OP1	13:AR:61:ARG:NH1	2.52	0.43
7:AE:292:TYR:CG	11:AN:110:PRO:HG3	2.53	0.43
8:AF:272:PHE:HB2	8:AF:301:ILE:HD12	2.01	0.43
39:BO:117:LEU:HD12	39:BO:161:MET:HE2	2.00	0.43
41:BR:179:ILE:O	41:BR:179:ILE:CG2	2.64	0.43
70:XG:33:ARG:O	70:XG:37:ILE:HG22	2.19	0.43
74:XL:102:LEU:HD12	74:XL:349:PRO:O	2.19	0.43
74:XL:315:ARG:O	74:XL:320:LYS:NZ	2.52	0.43
74:XL:547:LEU:HD23	74:XL:547:LEU:O	2.19	0.43
2:A2:424:VAL:HG13	2:A2:429:LYS:O	2.19	0.43
6:AA:466:G:O2'	16:AV:49:GLN:NE2	2.52	0.43
10:AK:141:LEU:HD22	10:AK:141:LEU:N	2.34	0.43
17:AW:124:THR:HG23	37:BL:99:HIS:CG	2.54	0.43
23:AL:81:GLU:OE1	40:BQ:69:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Al:88:ARG:NH2	23:Al:132:ASP:OD2	2.52	0.43
29:BB:377:PHE:CZ	29:BB:385:ILE:HG23	2.54	0.43
41:BR:60:THR:HG22	41:BR:61:GLU:N	2.34	0.43
46:BX:125:ARG:N	46:BX:156:TRP:O	2.52	0.43
67:XC:162:LEU:HD13	67:XC:173:VAL:HG21	2.01	0.43
67:XC:302:VAL:HG13	67:XC:616:LEU:HD22	2.00	0.43
74:XL:547:LEU:HD23	74:XL:547:LEU:C	2.44	0.43
79:XQ:217:LEU:HD21	79:XQ:229:TYR:CD2	2.53	0.43
6:AA:547:U:OP1	52:Bg:57:GLY:N	2.52	0.42
7:AE:283:MET:HE2	66:XB:644:LYS:O	2.19	0.42
8:AF:299:ASN:O	8:AF:299:ASN:ND2	2.52	0.42
12:AP:213:TRP:CG	12:AP:214:PRO:HA	2.54	0.42
16:AV:51:LEU:O	16:AV:92:GLN:NE2	2.47	0.42
17:AW:198:VAL:O	17:AW:198:VAL:HG23	2.18	0.42
28:BA:342:THR:HG22	28:BA:343:ARG:N	2.34	0.42
30:BD:354:VAL:HG22	30:BD:355:GLU:N	2.34	0.42
32:BF:321:PHE:O	32:BF:325:ARG:HG2	2.19	0.42
34:BI:112:ILE:HD13	34:BI:115:LEU:CD1	2.49	0.42
67:XC:34:LEU:HD13	67:XC:606:HIS:ND1	2.34	0.42
77:XO:104:LEU:HD23	77:XO:107:ARG:NH2	2.34	0.42
78:XP:160:VAL:HA	78:XP:170:ILE:HG22	2.01	0.42
2:A2:217:ASP:OD1	8:AF:407:ARG:NH1	2.51	0.42
6:AA:1121:A:N1	7:AE:38:ARG:NH2	2.68	0.42
8:AF:26:ASP:OD2	22:Ag:82:ARG:NH2	2.50	0.42
10:AK:163:LEU:HD23	10:AK:163:LEU:C	2.44	0.42
12:AP:120:ILE:O	12:AP:120:ILE:HG22	2.19	0.42
27:Av:197:ARG:HG3	82:XT:79:ILE:HD11	2.00	0.42
29:BB:353:LEU:HD23	29:BB:353:LEU:C	2.44	0.42
29:BB:357:THR:HA	29:BB:364:VAL:HG12	2.01	0.42
36:BK:95:HIS:NE2	36:BK:153:LEU:HD22	2.34	0.42
39:BO:58:SER:HB3	39:BO:61:THR:HG22	2.01	0.42
72:XI:495:SER:HB2	72:XI:521:LEU:HD21	2.01	0.42
79:XQ:279:VAL:HG22	79:XQ:282:HIS:HB3	2.01	0.42
2:A2:417:VAL:HG23	2:A2:418:ASP:N	2.33	0.42
6:AA:73:G:OP1	27:Av:62:GLY:N	2.42	0.42
6:AA:959:U:OP2	74:XL:389:ARG:NH2	2.52	0.42
20:Ae:56:ASN:N	20:Ae:56:ASN:OD1	2.52	0.42
21:Af:84:SER:N	21:Af:85:PRO:HD2	2.35	0.42
29:BB:431:ARG:NE	35:BJ:184:TYR:OH	2.53	0.42
42:BS:102:HIS:NE2	42:BS:106:ILE:HD12	2.34	0.42
69:XF:228:THR:N	69:XF:229:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:YN:298:VAL:HG12	76:YN:299:LYS:N	2.35	0.42
76:YN:418:THR:HG22	76:YN:419:ILE:N	2.34	0.42
76:YN:545:LEU:HD21	77:XO:339:LEU:HD13	2.01	0.42
81:XS:93:TRP:CD2	81:XS:107:ALA:HB2	2.54	0.42
16:AV:83:VAL:O	24:AO:20:SER:OG	2.23	0.42
19:AY:211:GLY:O	36:BK:320:VAL:HG23	2.20	0.42
25:AP:77:MET:SD	34:BI:50:ARG:NH1	2.91	0.42
28:BA:61:VAL:O	28:BA:61:VAL:HG13	2.19	0.42
30:BD:409:ASP:O	30:BD:413:GLN:HG2	2.19	0.42
34:BI:160:PHE:N	34:BI:161:PRO:HD2	2.33	0.42
65:XA:92:VAL:HG12	65:XA:107:MET:HG2	2.02	0.42
67:XC:149:TYR:HD2	67:XC:213:ILE:HG22	1.84	0.42
71:XH:517:LEU:HD12	71:XH:517:LEU:C	2.44	0.42
78:XP:123:THR:HG22	78:XP:124:ARG:H	1.85	0.42
6:AA:542:U:OP1	18:AX:168:SER:OG	2.37	0.42
8:AF:163:ASP:O	8:AF:205:LYS:NZ	2.50	0.42
29:BB:141:ILE:HG12	29:BB:172:MET:HE2	2.01	0.42
34:BI:162:ARG:O	34:BI:166:LEU:HD23	2.19	0.42
34:BI:232:LEU:HD23	51:Bf:99:ILE:HG12	2.01	0.42
38:BN:173:TYR:OH	81:XS:181:VAL:HG21	2.20	0.42
45:BW:63:LEU:C	45:BW:63:LEU:HD12	2.44	0.42
67:XC:247:SER:H	67:XC:250:THR:HG22	1.84	0.42
68:XD:126:HIS:NE2	68:XD:127:ASP:OD1	2.52	0.42
72:XI:240:GLU:O	72:XI:244:VAL:HG23	2.19	0.42
78:XP:161:LEU:HD11	78:XP:171:ASN:HB2	2.02	0.42
7:AE:106:ARG:NH1	28:BA:55:SER:OG	2.53	0.42
26:At:137:TYR:OH	32:BF:138:GLU:OE2	2.35	0.42
30:BD:390:LEU:HD23	30:BD:390:LEU:C	2.44	0.42
44:BU:136:ASP:OD1	52:Bg:45:LEU:HD13	2.19	0.42
49:Bb:40:VAL:HG12	49:Bb:41:HIS:N	2.34	0.42
50:Bc:125:VAL:HG21	76:YN:415:MET:HE2	2.01	0.42
74:XL:313:VAL:HG12	74:XL:365:LEU:HD13	2.01	0.42
76:YN:397:LEU:HD12	76:YN:516:ALA:HA	2.02	0.42
6:AA:13:A:H61	19:AY:39:LEU:HD13	1.84	0.42
6:AA:160:A:OP2	23:Al:69:LYS:NZ	2.43	0.42
7:AE:107:LEU:HD11	25:AP:127:TRP:HZ2	1.83	0.42
18:AX:145:ARG:NH2	18:AX:162:GLN:OE1	2.48	0.42
21:Af:129:THR:HG21	28:BA:406:ALA:HB2	2.01	0.42
26:At:137:TYR:HB2	26:At:145:PRO:HG3	2.02	0.42
48:Ba:58:MET:HE1	48:Ba:65:GLU:HG3	2.01	0.42
52:Bg:88:ASP:OD1	52:Bg:89:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:XA:92:VAL:O	65:XA:92:VAL:HG23	2.20	0.42
66:XB:83:THR:HG23	66:XB:89:LEU:CB	2.49	0.42
67:XC:168:LEU:C	67:XC:168:LEU:HD12	2.44	0.42
67:XC:407:ASP:OD1	67:XC:408:VAL:N	2.53	0.42
68:XE:88:ALA:O	72:XI:338:ASN:ND2	2.51	0.42
72:XI:61:ASP:OD2	72:XI:67:ARG:NH1	2.53	0.42
78:XP:70:VAL:HG23	78:XP:111:ASP:O	2.20	0.42
79:XQ:136:THR:HG22	79:XQ:137:GLY:H	1.83	0.42
80:XR:17:LEU:O	80:XR:17:LEU:HD23	2.20	0.42
1:A1:167:ILE:HD13	35:BJ:289:GLU:CD	2.45	0.42
6:AA:467:U:H2'	6:AA:468:A:O4'	2.20	0.42
14:AT:81:GLU:OE1	14:AT:81:GLU:N	2.51	0.42
16:AV:15:ILE:HD11	21:Af:90:PHE:HD2	1.85	0.42
26:At:126:THR:O	26:At:130:GLY:N	2.48	0.42
33:BH:194:ARG:NH1	33:BH:196:LEU:HD21	2.35	0.42
66:XB:89:LEU:HD21	66:XB:303:ILE:HD12	2.02	0.42
66:XB:285:MET:O	66:XB:287:LYS:NZ	2.48	0.42
67:XC:611:ASP:OD1	67:XC:611:ASP:N	2.52	0.42
72:XI:662:VAL:HG11	72:XI:714:ARG:CD	2.50	0.42
78:XP:223:THR:HG22	78:XP:224:ARG:N	2.33	0.42
80:XR:20:VAL:HG21	80:XR:101:ALA:HB1	2.00	0.42
1:A1:113:VAL:HG23	1:A1:114:LEU:N	2.33	0.42
8:AF:105:THR:HG22	8:AF:106:TYR:H	1.84	0.42
21:Af:131:VAL:HG13	22:Ag:116:TRP:CD1	2.55	0.42
23:Al:166:ILE:H	23:Al:166:ILE:HD12	1.84	0.42
28:BA:740:LEU:HD23	28:BA:740:LEU:C	2.45	0.42
35:BJ:173:LEU:HD12	35:BJ:173:LEU:N	2.35	0.42
72:XI:88:LEU:HD21	72:XI:92:GLN:NE2	2.35	0.42
72:XI:618:TYR:CD2	72:XI:625:LEU:HD21	2.55	0.42
73:XJ:290:LEU:CD1	73:XJ:292:LEU:HD23	2.50	0.42
74:XL:342:THR:HG23	74:XL:363:ALA:HA	2.01	0.42
76:XN:150:ASN:O	76:XN:150:ASN:ND2	2.53	0.42
78:XP:243:VAL:HG22	78:XP:244:TYR:N	2.35	0.42
79:XQ:83:ASP:H	79:XQ:175:VAL:HG23	1.84	0.42
6:AA:155:U:N3	8:AF:140:GLU:OE1	2.47	0.42
6:AA:287:A:N3	6:AA:288:G:N1	2.68	0.42
6:AA:567:G:O6	31:BE:440:ILE:HG23	2.20	0.42
6:AA:851:G:O2'	66:XB:684:VAL:HG22	2.20	0.42
12:AP:74:THR:HG23	32:BF:345:LEU:O	2.20	0.42
30:BD:172:LEU:HD23	30:BD:172:LEU:C	2.45	0.42
30:BD:216:GLY:O	30:BD:220:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:BD:283:LEU:HD13	30:BD:288:ILE:HD12	2.01	0.42
42:BS:161:LEU:HD23	42:BS:161:LEU:C	2.45	0.42
72:XI:646:LEU:HD22	72:XI:709:LEU:HD12	2.01	0.42
81:XS:159:GLU:O	81:XS:163:VAL:HG23	2.19	0.42
6:AA:1078:A:H5''	6:AA:1079:A:O5'	2.20	0.41
9:AI:178:ILE:O	9:AI:178:ILE:HG23	2.20	0.41
14:AT:72:ILE:HD11	73:XJ:189:TRP:CH2	2.55	0.41
25:Ap:235:VAL:HG23	25:Ap:235:VAL:O	2.20	0.41
28:BA:479:ASP:HB3	28:BA:482:VAL:HG12	2.02	0.41
28:BA:686:GLU:N	28:BA:686:GLU:OE1	2.53	0.41
29:BB:80:ILE:HD13	47:BZ:62:SER:OG	2.19	0.41
30:BD:106:ILE:HD12	30:BD:421:ALA:CB	2.50	0.41
31:BE:271:ASP:OD1	31:BE:273:ASP:N	2.48	0.41
35:BJ:326:LEU:HD23	35:BJ:326:LEU:O	2.20	0.41
39:BO:62:ARG:NH2	42:BS:40:GLU:OE2	2.53	0.41
66:XB:453:LEU:HD23	66:XB:453:LEU:O	2.20	0.41
67:XC:303:ALA:HB1	67:XC:310:TYR:HA	2.01	0.41
6:AA:41:U:H5''	6:AA:42:A:P	2.61	0.41
6:AA:474:A:O2'	12:AP:117:TRP:O	2.34	0.41
6:AA:869:U:O2'	6:AA:870:A:O5'	2.34	0.41
17:AW:211:GLN:O	17:AW:223:LYS:N	2.53	0.41
19:AY:275:GLU:N	19:AY:276:PRO:HD2	2.35	0.41
31:BE:314:THR:HG22	31:BE:314:THR:O	2.20	0.41
32:BF:347:ASN:ND2	45:BW:184:GLN:OE1	2.53	0.41
48:Ba:38:TYR:O	48:Ba:81:GLN:NE2	2.47	0.41
65:XA:90:ASP:OD1	65:XA:92:VAL:HG13	2.20	0.41
66:XB:540:THR:OG1	66:XB:541:ASP:N	2.53	0.41
66:XB:599:ALA:O	66:XB:603:LYS:HG2	2.21	0.41
67:XC:240:LEU:HD11	67:XC:581:SER:OG	2.20	0.41
68:XD:67:LEU:H	68:XD:67:LEU:HD22	1.85	0.41
72:XI:246:ALA:O	72:XI:250:VAL:HG23	2.20	0.41
72:XI:599:PHE:O	72:XI:600:GLY:C	2.63	0.41
73:XJ:224:THR:HG23	73:XJ:224:THR:O	2.20	0.41
79:XQ:288:HIS:ND1	79:XQ:288:HIS:O	2.52	0.41
7:AE:48:LEU:HD11	34:BI:41:PHE:CZ	2.55	0.41
7:AE:148:CYS:HB2	14:AT:85:ILE:HD12	2.03	0.41
7:AE:353:GLU:OE2	76:XN:336:ARG:NH2	2.52	0.41
7:AE:399:LEU:HD21	14:AT:65:ASN:OD1	2.20	0.41
14:AT:102:LEU:HD23	14:AT:102:LEU:H	1.86	0.41
30:BD:295:LEU:O	30:BD:295:LEU:HD23	2.20	0.41
33:BH:196:LEU:HD22	33:BH:196:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:BH:291:LEU:HD12	33:BH:293:TYR:HB3	2.02	0.41
66:XB:352:GLN:NE2	66:XB:506:CYS:SG	2.93	0.41
68:XD:134:ILE:O	68:XD:138:VAL:HG23	2.20	0.41
69:XF:263:LEU:O	69:XF:266:ILE:HG22	2.20	0.41
74:XL:166:ASP:OD1	74:XL:167:THR:N	2.53	0.41
77:XO:399:TRP:O	77:XO:403:LEU:HD23	2.19	0.41
2:A2:447:THR:HG21	6:AA:34:G:N3	2.35	0.41
5:A8:52:ARG:O	5:A8:53:ARG:NH1	2.39	0.41
5:A8:105:ASP:OD1	66:XB:241:ARG:NH2	2.49	0.41
6:AA:150:A:OP1	12:AP:107:ARG:NH2	2.53	0.41
7:AE:224:ASP:OD1	7:AE:224:ASP:N	2.52	0.41
16:AV:31:ILE:HG21	16:AV:61:LEU:HD13	2.02	0.41
17:AW:123:VAL:HG21	37:BL:113:ARG:HH12	1.85	0.41
25:Ap:164:VAL:HG23	25:Ap:165:VAL:N	2.35	0.41
41:BR:193:ILE:HG22	41:BR:194:HIS:N	2.34	0.41
45:BW:93:TRP:O	45:BW:97:ILE:HD12	2.21	0.41
46:BX:164:HIS:ND1	46:BX:164:HIS:O	2.53	0.41
53:Bh:24:LYS:O	53:Bh:28:ARG:NE	2.53	0.41
66:XB:644:LYS:HG3	66:XB:646:ILE:HG23	2.02	0.41
67:XC:396:LEU:HD11	67:XC:508:LEU:HD21	2.02	0.41
74:XL:127:LEU:HD12	74:XL:164:ILE:CD1	2.51	0.41
77:XO:192:VAL:HG22	77:XO:193:LYS:N	2.35	0.41
2:A2:108:ARG:NE	2:A2:112:ILE:HD11	2.36	0.41
6:AA:1011:G:O4'	78:XP:179:MET:HE3	2.20	0.41
12:AP:79:TRP:CE3	12:AP:90:ILE:HD12	2.55	0.41
13:AR:130:ASP:OD2	44:BU:159:ARG:NE	2.52	0.41
18:AX:202:VAL:HG13	19:AY:93:LEU:HD11	2.01	0.41
19:AY:131:ILE:HG23	19:AY:141:ILE:CG2	2.50	0.41
26:At:129:TYR:OH	32:BF:179:ARG:NH1	2.54	0.41
28:BA:428:PHE:HA	28:BA:431:VAL:HG22	2.03	0.41
31:BE:73:THR:HG23	31:BE:74:TYR:H	1.83	0.41
32:BF:382:VAL:HG12	32:BF:383:MET:N	2.34	0.41
34:BI:138:LYS:HG2	69:XF:159:ILE:HD12	2.01	0.41
45:BW:133:ALA:HB2	45:BW:140:TYR:CD2	2.56	0.41
53:Bh:40:LEU:HD23	53:Bh:41:PHE:H	1.85	0.41
67:XC:401:LEU:O	67:XC:447:ILE:HD12	2.20	0.41
72:XI:88:LEU:HD23	72:XI:88:LEU:C	2.46	0.41
79:XQ:230:ASP:OD1	79:XQ:231:SER:N	2.54	0.41
7:AE:392:ASP:OD2	70:XG:140:SER:OG	2.35	0.41
27:Av:113:GLY:O	27:Av:115:TRP:N	2.53	0.41
29:BB:102:ILE:O	29:BB:106:LEU:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:BB:152:ARG:CZ	29:BB:172:MET:HE1	2.51	0.41
29:BB:396:LEU:HD23	29:BB:396:LEU:C	2.46	0.41
30:BD:122:PHE:HB2	30:BD:131:VAL:HG11	2.03	0.41
35:BJ:294:ASN:OD1	35:BJ:297:TRP:N	2.44	0.41
42:BS:107:ILE:HG23	42:BS:108:THR:N	2.34	0.41
67:XC:161:ARG:HA	67:XC:164:TYR:CE2	2.55	0.41
77:XO:152:GLN:HB3	77:XO:220:ILE:HG22	2.02	0.41
80:XR:94:LEU:O	80:XR:98:HIS:ND1	2.49	0.41
2:A2:65:LYS:NZ	36:BK:374:HIS:O	2.50	0.41
2:A2:177:LEU:HD21	2:A2:322:TRP:CE2	2.56	0.41
6:AA:1157:A:O2'	6:AA:1158:G:N2	2.45	0.41
9:AI:117:PHE:O	9:AI:134:TYR:N	2.50	0.41
18:AX:121:PRO:HG3	19:AY:259:MET:HE3	2.02	0.41
42:BS:161:LEU:HD23	42:BS:161:LEU:O	2.20	0.41
44:BU:115:PRO:HA	44:BU:118:VAL:HG12	2.02	0.41
66:XB:47:VAL:N	66:XB:48:PRO:HD2	2.36	0.41
67:XC:54:LEU:HD12	67:XC:54:LEU:N	2.36	0.41
67:XC:148:LEU:HD21	67:XC:150:ARG:HB3	2.02	0.41
72:XI:57:HIS:NE2	72:XI:427:ALA:O	2.49	0.41
72:XI:335:MET:CE	72:XI:378:LEU:HD22	2.49	0.41
78:XP:167:VAL:HG11	78:XP:366:LEU:HD13	2.02	0.41
6:AA:529:U:N3	18:AX:197:ARG:O	2.48	0.41
6:AA:894:A:N1	74:XL:316:THR:HG21	2.36	0.41
12:AP:184:ILE:HG23	12:AP:191:PRO:HG3	2.02	0.41
16:AV:42:VAL:O	16:AV:42:VAL:HG12	2.21	0.41
19:AY:261:GLU:O	19:AY:264:VAL:HG12	2.20	0.41
19:AY:288:PHE:O	19:AY:292:VAL:HG23	2.21	0.41
24:Ao:85:ASP:OD1	24:Ao:85:ASP:N	2.53	0.41
31:BE:254:ASN:ND2	31:BE:257:ASP:OD2	2.53	0.41
33:BH:194:ARG:C	33:BH:195:ILE:HD12	2.46	0.41
34:BI:148:ASN:HA	34:BI:151:MET:HG2	2.03	0.41
34:BI:187:LEU:HD22	51:Bf:99:ILE:HD11	2.03	0.41
40:BQ:106:VAL:HG12	40:BQ:107:SER:N	2.36	0.41
51:Bf:99:ILE:HG22	51:Bf:102:TYR:O	2.21	0.41
65:XA:59:THR:O	65:XA:59:THR:HG22	2.21	0.41
73:XJ:271:VAL:CG2	73:XJ:278:ILE:HD11	2.51	0.41
74:XL:377:ILE:O	74:XL:380:ILE:HG12	2.21	0.41
76:XN:434:SER:O	76:XN:436:ALA:N	2.51	0.41
77:XO:250:LEU:HD23	77:XO:250:LEU:C	2.45	0.41
77:XO:384:LEU:CD1	77:XO:386:MET:HE3	2.50	0.41
78:XP:384:THR:HG23	78:XP:385:GLN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:100:GLU:O	2:A2:103:GLU:HG3	2.21	0.41
6:AA:834:U:H2'	6:AA:835:A:O4'	2.21	0.41
8:AF:380:PRO:HD3	8:AF:385:LEU:HD12	2.02	0.41
10:AK:102:VAL:O	10:AK:102:VAL:HG13	2.21	0.41
11:AN:111:GLY:O	11:AN:113:LYS:N	2.51	0.41
16:AV:75:ILE:O	16:AV:80:LEU:HD21	2.21	0.41
17:AW:116:ARG:HE	37:BL:114:CYS:HB2	1.86	0.41
17:AW:152:ILE:O	17:AW:152:ILE:HG22	2.20	0.41
19:AY:118:GLU:OE1	19:AY:185:ILE:HD11	2.21	0.41
19:AY:241:THR:HG22	19:AY:241:THR:O	2.20	0.41
20:Ae:87:VAL:N	20:Ae:88:PRO:CD	2.84	0.41
23:Al:201:VAL:HG12	23:Al:202:ALA:N	2.36	0.41
27:Av:199:LEU:HD21	67:XC:134:THR:OG1	2.20	0.41
29:BB:114:ALA:CB	29:BB:117:LEU:HD13	2.50	0.41
29:BB:223:ASP:OD2	29:BB:227:VAL:N	2.54	0.41
29:BB:386:THR:O	29:BB:390:LEU:HD23	2.20	0.41
31:BE:73:THR:HG21	36:BK:380:TYR:CE1	2.56	0.41
32:BF:408:LEU:C	32:BF:408:LEU:HD12	2.46	0.41
34:BI:273:LYS:NZ	71:XH:232:GLU:OE2	2.52	0.41
36:BK:114:HIS:CD2	36:BK:210:LEU:HD13	2.56	0.41
41:BR:97:TRP:CZ3	41:BR:179:ILE:HG21	2.56	0.41
44:BU:136:ASP:OD1	44:BU:137:ARG:N	2.53	0.41
66:XB:75:LEU:HD12	66:XB:302:PHE:HB3	2.03	0.41
66:XB:106:LEU:HD22	66:XB:155:LEU:HD21	2.03	0.41
66:XB:542:VAL:HG13	66:XB:543:ALA:N	2.35	0.41
66:XB:637:TYR:CE1	66:XB:641:ILE:HD11	2.55	0.41
67:XC:164:TYR:CD1	67:XC:164:TYR:C	2.99	0.41
72:XI:79:LEU:HB2	72:XI:82:VAL:HG22	2.02	0.41
72:XI:199:PHE:HZ	72:XI:250:VAL:HG12	1.86	0.41
77:XO:338:ASP:OD1	77:XO:341:ARG:NH2	2.54	0.41
81:XS:96:CYS:HB3	81:XS:102:VAL:HG21	2.02	0.41
5:A8:123:SER:HB3	6:AA:341:A:OP1	2.20	0.41
12:AP:13:LEU:HD21	24:Ao:62:THR:HB	2.03	0.41
17:AW:209:ASP:OD2	31:BE:47:THR:HG23	2.21	0.41
33:BH:273:PRO:HA	33:BH:276:ILE:HG12	2.03	0.41
34:BI:112:ILE:HD11	51:Bf:98:TYR:CE1	2.48	0.41
40:BQ:170:VAL:O	40:BQ:174:VAL:HG23	2.21	0.41
46:BX:73:VAL:HG13	46:BX:111:PHE:CE2	2.56	0.41
46:BX:151:VAL:HG22	46:BX:156:TRP:HE1	1.85	0.41
51:Bf:61:ALA:HB1	76:XN:416:ILE:HD13	2.03	0.41
66:XB:464:LEU:HD23	66:XB:464:LEU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:XB:572:ARG:NE	66:XB:572:ARG:HA	2.36	0.41
67:XC:89:VAL:HG22	67:XC:213:ILE:CD1	2.51	0.41
67:XC:540:LYS:NZ	67:XC:551:THR:HG23	2.36	0.41
76:XN:320:ARG:NH1	76:XN:321:ASP:OD1	2.53	0.41
79:XQ:86:LEU:HD23	79:XQ:86:LEU:C	2.46	0.41
81:XS:171:LEU:C	81:XS:171:LEU:HD12	2.46	0.41
17:AW:254:MET:SD	28:BA:785:ARG:HA	2.61	0.40
23:Al:93:ASP:OD1	23:Al:94:PHE:N	2.53	0.40
28:BA:367:PHE:CZ	28:BA:406:ALA:HB3	2.56	0.40
33:BH:203:GLY:O	33:BH:204:THR:HG23	2.21	0.40
35:BJ:223:THR:HG22	35:BJ:224:ASP:N	2.36	0.40
35:BJ:326:LEU:HD23	35:BJ:326:LEU:C	2.47	0.40
37:BL:304:VAL:HG12	37:BL:305:ALA:N	2.37	0.40
42:BS:108:THR:HB	42:BS:109:PRO:HD3	2.04	0.40
47:BZ:161:ASP:OD1	47:BZ:162:VAL:N	2.54	0.40
49:Bb:48:GLU:O	49:Bb:52:SER:CB	2.69	0.40
50:Bc:79:ALA:O	50:Bc:83:THR:HG22	2.21	0.40
66:XB:126:GLN:O	66:XB:130:VAL:HG23	2.21	0.40
66:XB:155:LEU:HB3	66:XB:156:PRO:HD3	2.03	0.40
74:XL:99:VAL:HG12	74:XL:327:LEU:HA	2.03	0.40
77:XO:367:LEU:HD11	77:XO:413:ASP:OD1	2.20	0.40
78:XP:69:ARG:NH1	78:XP:71:ASP:OD2	2.49	0.40
2:A2:366:VAL:HG11	48:Ba:67:PRO:HB3	2.03	0.40
7:AE:249:GLN:OE1	14:AT:16:ARG:NH1	2.54	0.40
28:BA:341:CYS:O	28:BA:377:ARG:NH1	2.54	0.40
29:BB:136:TRP:HB2	29:BB:141:ILE:HD12	2.04	0.40
29:BB:255:LEU:C	29:BB:255:LEU:HD12	2.46	0.40
31:BE:374:VAL:O	31:BE:379:ARG:NH2	2.55	0.40
66:XB:575:ARG:O	66:XB:576:GLN:C	2.64	0.40
74:XL:318:SER:CB	74:XL:397:VAL:HG23	2.52	0.40
76:XN:461:MET:HE2	76:XN:461:MET:HA	2.02	0.40
2:A2:40:ARG:O	2:A2:101:ARG:NH2	2.55	0.40
10:AK:30:LEU:C	10:AK:30:LEU:HD23	2.47	0.40
11:AN:72:ASP:HB2	28:BA:715:LEU:HD21	2.04	0.40
12:AP:71:ASN:ND2	45:BW:186:SER:O	2.42	0.40
28:BA:277:ILE:HG13	28:BA:277:ILE:O	2.21	0.40
28:BA:567:THR:OG1	28:BA:659:GLU:OE1	2.38	0.40
32:BF:237:LEU:O	32:BF:240:VAL:HG12	2.21	0.40
66:XB:114:LEU:HD12	66:XB:115:ARG:N	2.36	0.40
2:A2:343:THR:HG23	2:A2:344:THR:HG22	2.02	0.40
3:A3:145:LEU:HD12	3:A3:145:LEU:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AA:574:A:H61	6:AA:1167:A:N6	2.20	0.40
8:AF:169:ILE:O	8:AF:169:ILE:HG22	2.21	0.40
8:AF:437:VAL:O	8:AF:437:VAL:HG23	2.21	0.40
14:AT:13:PHE:O	14:AT:16:ARG:NH2	2.54	0.40
22:Ag:12:VAL:HG21	22:Ag:83:LEU:HD11	2.01	0.40
22:Ag:98:CYS:SG	22:Ag:99:ALA:N	2.94	0.40
25:Ap:259:MET:CG	34:BI:291:VAL:HG12	2.51	0.40
26:At:133:LEU:HD21	32:BF:285:LEU:HD23	2.03	0.40
28:BA:177:ILE:HD12	28:BA:177:ILE:N	2.36	0.40
29:BB:94:THR:HG21	29:BB:105:LEU:HD22	2.03	0.40
39:BO:230:LEU:N	39:BO:230:LEU:HD12	2.36	0.40
71:XH:234:ARG:O	71:XH:238:LEU:HG	2.22	0.40
71:XH:238:LEU:HD13	71:XH:247:ILE:HG22	2.03	0.40
71:XH:621:LEU:O	71:XH:621:LEU:HD23	2.21	0.40
79:XQ:181:MET:HB3	79:XQ:184:VAL:HG23	2.03	0.40
79:XQ:313:THR:HG23	79:XQ:314:ASP:N	2.37	0.40
1:A1:113:VAL:HG22	1:A1:137:ASP:OD2	2.22	0.40
2:A2:366:VAL:O	2:A2:366:VAL:HG12	2.22	0.40
6:AA:1010:C:OP2	78:XP:311:THR:HB	2.22	0.40
8:AF:236:LEU:HD11	8:AF:351:ILE:HD12	2.04	0.40
22:Ag:62:ARG:O	28:BA:533:LEU:HD22	2.21	0.40
27:Av:65:THR:O	27:Av:69:ARG:NH2	2.55	0.40
31:BE:82:GLU:OE1	31:BE:82:GLU:N	2.43	0.40
32:BF:206:LEU:HD21	32:BF:244:HIS:HB2	2.03	0.40
38:BN:98:ASP:O	38:BN:139:HIS:NE2	2.52	0.40
40:BQ:130:VAL:HG22	40:BQ:146:PHE:CD2	2.56	0.40
65:XA:21:ILE:HD12	65:XA:21:ILE:N	2.37	0.40
71:XH:375:LEU:HD12	71:XH:375:LEU:N	2.36	0.40
76:XN:80:THR:HG23	76:XN:80:THR:O	2.22	0.40
77:XO:116:LEU:HD23	77:XO:116:LEU:C	2.47	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	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
2	A2	445/463 (96%)	438 (98%)	7 (2%)	0	100	100
3	A3	148/150 (99%)	140 (95%)	8 (5%)	0	100	100
4	A5	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
5	A8	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
7	AE	357/367 (97%)	344 (96%)	13 (4%)	0	100	100
8	AF	440/442 (100%)	421 (96%)	19 (4%)	0	100	100
9	AI	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
10	AK	266/278 (96%)	259 (97%)	7 (3%)	0	100	100
11	AN	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
12	AP	304/354 (86%)	298 (98%)	6 (2%)	0	100	100
13	AR	254/256 (99%)	246 (97%)	8 (3%)	0	100	100
14	AT	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
15	AU	171/196 (87%)	162 (95%)	9 (5%)	0	100	100
16	AV	178/180 (99%)	172 (97%)	6 (3%)	0	100	100
17	AW	275/277 (99%)	272 (99%)	3 (1%)	0	100	100
18	AX	163/165 (99%)	159 (98%)	4 (2%)	0	100	100
19	AY	330/340 (97%)	322 (98%)	8 (2%)	0	100	100
20	Ae	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
21	Af	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
22	Ag	183/185 (99%)	181 (99%)	2 (1%)	0	100	100
23	Al	166/182 (91%)	161 (97%)	5 (3%)	0	100	100
24	Ao	131/133 (98%)	126 (96%)	5 (4%)	0	100	100
25	Ap	286/288 (99%)	272 (95%)	14 (5%)	0	100	100
26	At	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
27	Av	194/197 (98%)	186 (96%)	8 (4%)	0	100	100
28	BA	719/798 (90%)	692 (96%)	27 (4%)	0	100	100
29	BB	363/371 (98%)	354 (98%)	9 (2%)	0	100	100
30	BD	415/417 (100%)	403 (97%)	12 (3%)	0	100	100
31	BE	397/438 (91%)	374 (94%)	23 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BF	337/421 (80%)	329 (98%)	8 (2%)	0	100	100
33	BH	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
34	BI	321/323 (99%)	312 (97%)	9 (3%)	0	100	100
35	BJ	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
36	BK	234/273 (86%)	228 (97%)	6 (3%)	0	100	100
37	BL	226/276 (82%)	217 (96%)	9 (4%)	0	100	100
38	BN	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
39	BO	207/227 (91%)	203 (98%)	4 (2%)	0	100	100
40	BQ	183/185 (99%)	176 (96%)	7 (4%)	0	100	100
41	BR	193/195 (99%)	188 (97%)	5 (3%)	0	100	100
42	BS	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
43	BT	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
44	BU	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
45	BW	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
46	BX	103/116 (89%)	96 (93%)	7 (7%)	0	100	100
47	BZ	187/189 (99%)	182 (97%)	5 (3%)	0	100	100
48	Ba	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
49	Bb	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
50	Bc	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
51	Bf	76/86 (88%)	72 (95%)	4 (5%)	0	100	100
52	Bg	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
53	Bh	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
54	UA	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
55	UB	7/9 (78%)	7 (100%)	0	0	100	100
56	UC	12/14 (86%)	12 (100%)	0	0	100	100
57	UD	6/8 (75%)	6 (100%)	0	0	100	100
58	UE	10/12 (83%)	10 (100%)	0	0	100	100
59	UF	125/139 (90%)	125 (100%)	0	0	100	100
60	UG	17/19 (90%)	16 (94%)	1 (6%)	0	100	100
61	UH	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
62	UI	37/39 (95%)	36 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	UJ	23/25 (92%)	23 (100%)	0	0	100	100
64	UK	45/47 (96%)	43 (96%)	2 (4%)	0	100	100
65	XA	152/155 (98%)	145 (95%)	7 (5%)	0	100	100
66	XB	610/668 (91%)	584 (96%)	26 (4%)	0	100	100
67	XC	580/616 (94%)	556 (96%)	24 (4%)	0	100	100
68	XD	80/83 (96%)	77 (96%)	3 (4%)	0	100	100
68	XE	80/83 (96%)	77 (96%)	3 (4%)	0	100	100
69	XF	155/198 (78%)	154 (99%)	1 (1%)	0	100	100
70	XG	160/170 (94%)	156 (98%)	4 (2%)	0	100	100
71	XH	388/533 (73%)	374 (96%)	14 (4%)	0	100	100
72	XI	587/703 (84%)	568 (97%)	18 (3%)	1 (0%)	43	74
73	XJ	148/150 (99%)	138 (93%)	10 (7%)	0	100	100
74	XL	517/528 (98%)	507 (98%)	10 (2%)	0	100	100
75	XM	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
76	XN	535/620 (86%)	507 (95%)	28 (5%)	0	100	100
77	XO	392/428 (92%)	379 (97%)	13 (3%)	0	100	100
78	XP	369/371 (100%)	351 (95%)	18 (5%)	0	100	100
79	XQ	279/305 (92%)	265 (95%)	14 (5%)	0	100	100
80	XR	133/161 (83%)	132 (99%)	1 (1%)	0	100	100
81	XS	180/182 (99%)	173 (96%)	7 (4%)	0	100	100
82	XT	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
All	All	17137/18343 (93%)	16559 (97%)	577 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
72	XI	600	GLY

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	195/195 (100%)	191 (98%)	4 (2%)	47	66
2	A2	394/405 (97%)	393 (100%)	1 (0%)	86	83
3	A3	135/135 (100%)	134 (99%)	1 (1%)	76	78
4	A5	52/52 (100%)	52 (100%)	0	100	100
5	A8	126/126 (100%)	126 (100%)	0	100	100
7	AE	312/316 (99%)	310 (99%)	2 (1%)	78	79
8	AF	394/394 (100%)	393 (100%)	1 (0%)	86	83
9	AI	192/192 (100%)	192 (100%)	0	100	100
10	AK	179/185 (97%)	177 (99%)	2 (1%)	65	74
11	AN	152/152 (100%)	152 (100%)	0	100	100
12	AP	275/314 (88%)	274 (100%)	1 (0%)	84	81
13	AR	222/222 (100%)	221 (100%)	1 (0%)	81	80
14	AT	119/119 (100%)	116 (98%)	3 (2%)	42	63
15	AU	151/168 (90%)	150 (99%)	1 (1%)	76	78
16	AV	153/153 (100%)	153 (100%)	0	100	100
17	AW	245/245 (100%)	243 (99%)	2 (1%)	73	77
18	AX	153/153 (100%)	152 (99%)	1 (1%)	76	78
19	AY	299/305 (98%)	298 (100%)	1 (0%)	86	83
20	Ae	100/100 (100%)	100 (100%)	0	100	100
21	Af	116/116 (100%)	116 (100%)	0	100	100
22	Ag	169/169 (100%)	169 (100%)	0	100	100
23	Al	146/156 (94%)	146 (100%)	0	100	100
24	Ao	107/107 (100%)	107 (100%)	0	100	100
25	Ap	249/249 (100%)	249 (100%)	0	100	100
26	At	132/132 (100%)	131 (99%)	1 (1%)	73	77
27	Av	172/172 (100%)	171 (99%)	1 (1%)	78	79
28	BA	641/698 (92%)	640 (100%)	1 (0%)	87	85
29	BB	266/266 (100%)	265 (100%)	1 (0%)	84	81
30	BD	356/356 (100%)	346 (97%)	10 (3%)	38	61
31	BE	343/375 (92%)	342 (100%)	1 (0%)	86	83
32	BF	295/363 (81%)	291 (99%)	4 (1%)	59	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	BH	194/194 (100%)	194 (100%)	0	100	100
34	BI	271/271 (100%)	270 (100%)	1 (0%)	84	81
35	BJ	140/140 (100%)	138 (99%)	2 (1%)	59	71
36	BK	198/223 (89%)	198 (100%)	0	100	100
37	BL	201/234 (86%)	200 (100%)	1 (0%)	81	80
38	BN	189/189 (100%)	188 (100%)	1 (0%)	81	80
39	BO	181/193 (94%)	181 (100%)	0	100	100
40	BQ	155/155 (100%)	155 (100%)	0	100	100
41	BR	171/171 (100%)	170 (99%)	1 (1%)	78	79
42	BS	128/128 (100%)	128 (100%)	0	100	100
43	BT	146/146 (100%)	146 (100%)	0	100	100
44	BU	71/71 (100%)	70 (99%)	1 (1%)	59	71
45	BW	163/163 (100%)	162 (99%)	1 (1%)	78	79
46	BX	92/98 (94%)	92 (100%)	0	100	100
47	BZ	159/159 (100%)	156 (98%)	3 (2%)	50	68
48	Ba	128/128 (100%)	128 (100%)	0	100	100
49	Bb	88/88 (100%)	88 (100%)	0	100	100
50	Bc	127/127 (100%)	127 (100%)	0	100	100
51	Bf	71/76 (93%)	71 (100%)	0	100	100
52	Bg	65/65 (100%)	65 (100%)	0	100	100
53	Bh	79/79 (100%)	78 (99%)	1 (1%)	61	72
65	XA	134/134 (100%)	134 (100%)	0	100	100
66	XB	535/577 (93%)	533 (100%)	2 (0%)	84	81
67	XC	517/544 (95%)	513 (99%)	4 (1%)	73	77
68	XD	77/77 (100%)	75 (97%)	2 (3%)	40	62
68	XE	77/77 (100%)	77 (100%)	0	100	100
69	XF	134/161 (83%)	134 (100%)	0	100	100
70	XG	142/146 (97%)	141 (99%)	1 (1%)	76	78
71	XH	352/454 (78%)	350 (99%)	2 (1%)	78	79
72	XI	531/618 (86%)	526 (99%)	5 (1%)	70	76
73	XJ	134/134 (100%)	131 (98%)	3 (2%)	45	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	XL	452/457 (99%)	450 (100%)	2 (0%)	84	81
75	XM	76/76 (100%)	75 (99%)	1 (1%)	61	72
76	XN	472/538 (88%)	470 (100%)	2 (0%)	84	81
77	XO	348/373 (93%)	346 (99%)	2 (1%)	78	79
78	XP	326/326 (100%)	325 (100%)	1 (0%)	86	83
79	XQ	239/257 (93%)	236 (99%)	3 (1%)	61	72
80	XR	120/138 (87%)	112 (93%)	8 (7%)	15	41
81	XS	169/169 (100%)	167 (99%)	2 (1%)	63	73
82	XT	84/84 (100%)	84 (100%)	0	100	100
All	All	14776/15528 (95%)	14684 (99%)	92 (1%)	76	79

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	10	PHE
1	A1	95	VAL
1	A1	148	LEU
1	A1	176	GLN
2	A2	87	ILE
3	A3	116	VAL
7	AE	107	LEU
7	AE	215	VAL
8	AF	127	THR
10	AK	135	GLU
10	AK	214	CYS
12	AP	50	ASP
13	AR	170	MET
14	AT	21	PHE
14	AT	96	GLU
14	AT	113	HIS
15	AU	43	MET
17	AW	133	LEU
17	AW	248	LEU
18	AX	190	VAL
19	AY	125	ILE
26	At	143	THR
27	Av	29	MET
28	BA	63	LEU
29	BB	132	GLU

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Mol	Chain	Res	Type
30	BD	139	LEU
30	BD	142	VAL
30	BD	182	ARG
30	BD	184	GLN
30	BD	187	ASP
30	BD	198	ASP
30	BD	258	TYR
30	BD	292	LEU
30	BD	342	PHE
30	BD	518	VAL
31	BE	384	HIS
32	BF	126	VAL
32	BF	289	CYS
32	BF	354	LEU
32	BF	363	GLN
34	BI	278	GLU
35	BJ	180	GLU
35	BJ	203	LEU
37	BL	183	TRP
38	BN	185	GLU
41	BR	133	GLN
44	BU	141	GLU
45	BW	97	ILE
47	BZ	36	ASN
47	BZ	67	LEU
47	BZ	77	VAL
53	Bh	7	PHE
66	XB	262	ASP
66	XB	612	ASN
67	XC	30	CYS
67	XC	169	GLN
67	XC	272	PHE
67	XC	301	CYS
68	XD	84	GLU
68	XD	110	GLU
70	XG	174	ASN
71	XH	497	ASP
71	XH	544	LEU
72	XI	251	HIS
72	XI	266	HIS
72	XI	412	LEU
72	XI	540	SER

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Mol	Chain	Res	Type
72	XI	694	GLN
73	XJ	249	GLN
73	XJ	271	VAL
73	XJ	290	LEU
74	XL	313	VAL
74	XL	348	LEU
75	XM	67	GLN
76	XN	598	VAL
76	XN	612	LEU
77	XO	319	LEU
77	XO	479	LEU
78	XP	193	LEU
79	XQ	93	LEU
79	XQ	183	ASN
79	XQ	261	LEU
80	XR	2	VAL
80	XR	19	LYS
80	XR	30	LEU
80	XR	105	LEU
80	XR	118	GLN
80	XR	120	LEU
80	XR	142	GLN
80	XR	147	LYS
81	XS	171	LEU
81	XS	190	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	138	ASN
5	A8	161	ASN
7	AE	116	GLN
7	AE	262	HIS
7	AE	277	GLN
8	AF	80	GLN
8	AF	95	HIS
8	AF	299	ASN
8	AF	445	GLN
11	AN	63	GLN
13	AR	113	GLN
15	AU	65	ASN
15	AU	82	ASN

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Mol	Chain	Res	Type
17	AW	19	ASN
17	AW	75	GLN
22	Ag	73	ASN
22	Ag	151	GLN
22	Ag	170	GLN
23	Al	167	GLN
25	Ap	133	HIS
28	BA	269	GLN
28	BA	453	ASN
30	BD	231	GLN
30	BD	350	ASN
32	BF	166	GLN
32	BF	337	HIS
32	BF	365	HIS
33	BH	191	GLN
34	BI	120	GLN
34	BI	279	GLN
34	BI	301	GLN
35	BJ	185	GLN
37	BL	88	ASN
37	BL	112	HIS
38	BN	115	GLN
39	BO	112	GLN
40	BQ	51	HIS
40	BQ	60	ASN
40	BQ	196	GLN
41	BR	32	GLN
42	BS	38	HIS
42	BS	153	GLN
47	BZ	44	ASN
47	BZ	96	GLN
52	Bg	63	GLN
53	Bh	29	ASN
53	Bh	31	HIS
66	XB	50	GLN
66	XB	360	ASN
66	XB	474	HIS
67	XC	318	ASN
70	XG	35	ASN
70	XG	105	GLN
72	XI	92	GLN
72	XI	158	GLN

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Mol	Chain	Res	Type
72	XI	581	GLN
73	XJ	264	GLN
74	XL	450	GLN
76	XN	341	GLN
77	XO	290	GLN
78	XP	227	HIS
78	XP	262	HIS
79	XQ	183	ASN
81	XS	42	HIS
82	XT	92	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	AA	744/758 (98%)	219 (29%)	8 (1%)

All (219) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	AA	11	U
6	AA	12	U
6	AA	13	A
6	AA	14	A
6	AA	17	A
6	AA	18	G
6	AA	20	A
6	AA	22	A
6	AA	29	U
6	AA	32	U
6	AA	34	G
6	AA	38	U
6	AA	40	U
6	AA	41	U
6	AA	42	A
6	AA	43	U
6	AA	45	U
6	AA	47	U
6	AA	50	A
6	AA	52	U
6	AA	53	A
6	AA	54	A

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Mol	Chain	Res	Type
6	AA	60	U
6	AA	64	U
6	AA	65	U
6	AA	67	C
6	AA	70	G
6	AA	72	A
6	AA	73	G
6	AA	75	A
6	AA	77	A
6	AA	79	U
6	AA	80	U
6	AA	83	U
6	AA	85	U
6	AA	86	U
6	AA	87	U
6	AA	88	G
6	AA	89	U
6	AA	98	U
6	AA	104	A
6	AA	106	G
6	AA	107	U
6	AA	111	U
6	AA	113	A
6	AA	115	A
6	AA	119	A
6	AA	120	A
6	AA	124	U
6	AA	125	U
6	AA	133	U
6	AA	134	U
6	AA	136	U
6	AA	154	A
6	AA	155	U
6	AA	158	A
6	AA	162	A
6	AA	171	U
6	AA	172	U
6	AA	176	A
6	AA	177	U
6	AA	183	U
6	AA	189	A
6	AA	198	A

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Mol	Chain	Res	Type
6	AA	201	G
6	AA	261	U
6	AA	262	U
6	AA	275	C
6	AA	276	C
6	AA	277	A
6	AA	285	A
6	AA	286	U
6	AA	287	A
6	AA	289	U
6	AA	290	A
6	AA	297	U
6	AA	299	U
6	AA	302	G
6	AA	313	A
6	AA	315	A
6	AA	317	A
6	AA	327	U
6	AA	329	U
6	AA	331	C
6	AA	344	A
6	AA	346	G
6	AA	347	A
6	AA	405	U
6	AA	407	G
6	AA	408	A
6	AA	413	U
6	AA	461	U
6	AA	463	U
6	AA	470	G
6	AA	472	A
6	AA	473	A
6	AA	475	U
6	AA	476	G
6	AA	478	A
6	AA	481	G
6	AA	483	A
6	AA	485	A
6	AA	488	U
6	AA	489	G
6	AA	490	G
6	AA	491	A

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Mol	Chain	Res	Type
6	AA	492	U
6	AA	494	U
6	AA	495	A
6	AA	496	A
6	AA	497	C
6	AA	509	U
6	AA	515	U
6	AA	516	U
6	AA	518	A
6	AA	519	A
6	AA	520	U
6	AA	521	G
6	AA	522	A
6	AA	526	G
6	AA	528	A
6	AA	529	U
6	AA	545	U
6	AA	548	A
6	AA	555	U
6	AA	557	A
6	AA	558	U
6	AA	559	A
6	AA	560	G
6	AA	565	U
6	AA	567	G
6	AA	569	U
6	AA	572	U
6	AA	574	A
6	AA	575	A
6	AA	592	U
6	AA	797	A
6	AA	814	A
6	AA	817	A
6	AA	818	A
6	AA	825	A
6	AA	826	A
6	AA	828	A
6	AA	829	A
6	AA	830	A
6	AA	837	A
6	AA	838	A
6	AA	845	A

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Mol	Chain	Res	Type
6	AA	846	A
6	AA	851	G
6	AA	853	A
6	AA	854	A
6	AA	869	U
6	AA	871	C
6	AA	874	A
6	AA	882	U
6	AA	894	A
6	AA	898	U
6	AA	899	A
6	AA	902	U
6	AA	904	U
6	AA	905	G
6	AA	906	A
6	AA	908	U
6	AA	909	G
6	AA	914	A
6	AA	915	A
6	AA	917	A
6	AA	926	A
6	AA	927	U
6	AA	934	A
6	AA	940	A
6	AA	941	G
6	AA	942	A
6	AA	944	C
6	AA	945	U
6	AA	949	U
6	AA	953	U
6	AA	954	U
6	AA	958	A
6	AA	959	U
6	AA	963	A
6	AA	980	U
6	AA	1005	U
6	AA	1010	C
6	AA	1079	A
6	AA	1090	U
6	AA	1096	U
6	AA	1105	U
6	AA	1106	U

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Mol	Chain	Res	Type
6	AA	1107	U
6	AA	1112	U
6	AA	1114	A
6	AA	1117	A
6	AA	1119	U
6	AA	1121	A
6	AA	1130	A
6	AA	1131	G
6	AA	1139	G
6	AA	1141	A
6	AA	1144	G
6	AA	1151	G
6	AA	1152	A
6	AA	1153	A
6	AA	1155	A
6	AA	1156	A
6	AA	1157	A
6	AA	1158	G
6	AA	1161	A
6	AA	1162	G
6	AA	1164	A
6	AA	1167	A
6	AA	1168	U
6	AA	1169	A
6	AA	1171	A
6	AA	1172	A
6	AA	1174	U
6	AA	1175	U
6	AA	1176	A

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	AA	19	A
6	AA	41	U
6	AA	69	U
6	AA	171	U
6	AA	484	U
6	AA	490	G
6	AA	515	U
6	AA	1095	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
68	4HH	XE	105	68	22,26,27	1.87	4 (18%)	27,35,37	1.10	2 (7%)
68	4HH	XD	105	68	22,26,27	1.86	4 (18%)	27,35,37	1.04	0

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
68	4HH	XE	105	68	-	5/33/35/37	-
68	4HH	XD	105	68	-	12/33/35/37	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	XE	105	4HH	CQ-NR	5.18	1.45	1.33
68	XD	105	4HH	CQ-NR	5.18	1.45	1.33
68	XE	105	4HH	CL3-NN	5.09	1.45	1.33
68	XD	105	4HH	CL3-NN	5.06	1.45	1.33
68	XD	105	4HH	ON-CL3	-2.33	1.18	1.23
68	XE	105	4HH	ON-CL3	-2.31	1.19	1.23
68	XE	105	4HH	OR-CQ	-2.22	1.18	1.23
68	XD	105	4HH	OR-CQ	-2.16	1.19	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	XE	105	4HH	OG-CB-CA	2.40	110.48	108.14
68	XE	105	4HH	CM-CL3-NN	2.02	120.33	116.48

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
68	XD	105	4HH	C-CA-CB-OG
68	XD	105	4HH	N-CA-CB-OG
68	XD	105	4HH	CJ-CK-CM-CL3
68	XD	105	4HH	CJ-CK-CM-OM
68	XD	105	4HH	CL1-CK-CM-CL3
68	XD	105	4HH	CL1-CK-CM-OM
68	XD	105	4HH	CL2-CK-CM-CL3
68	XD	105	4HH	CL2-CK-CM-OM
68	XD	105	4HH	CJ-O3P-P-OG
68	XD	105	4HH	NR-CS-CT-SU
68	XE	105	4HH	CB-OG-P-O2P
68	XE	105	4HH	CB-OG-P-O3P
68	XD	105	4HH	NN-CO-CP-CQ
68	XE	105	4HH	CJ-CK-CM-CL3
68	XE	105	4HH	NR-CS-CT-SU
68	XE	105	4HH	CL2-CK-CM-OM
68	XD	105	4HH	CK-CJ-O3P-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
68	XD	105	4HH	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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
88	GTP	XL	601	-	33,34,34	0.94	1 (3%)	50,54,54	1.59	9 (18%)
83	FES	A5	101	4	0,4,4	-	-	-	-	-
84	NAD	Av	301	-	46,48,48	3.75	19 (41%)	64,73,73	1.93	13 (20%)
87	ADP	XB	902	86	28,29,29	3.41	15 (53%)	43,45,45	2.96	12 (27%)
88	GTP	XL	602	-	33,34,34	0.93	1 (3%)	50,54,54	1.59	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	GTP	XL	601	-	-	3/22/38/38	0/3/3/3
83	FES	A5	101	4	-	-	0/1/1/1
84	NAD	Av	301	-	-	4/30/62/62	0/5/5/5
87	ADP	XB	902	86	-	2/16/32/32	0/3/3/3
88	GTP	XL	602	-	-	5/22/38/38	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	Av	301	NAD	O4D-C1D	15.96	1.61	1.40
84	Av	301	NAD	O4B-C1B	8.59	1.61	1.42
87	XB	902	ADP	C3'-C4'	-8.43	1.31	1.53
87	XB	902	ADP	O4'-C4'	7.79	1.62	1.45
84	Av	301	NAD	O4B-C4B	-7.35	1.28	1.45
87	XB	902	ADP	PA-O3A	7.21	1.67	1.59
84	Av	301	NAD	C2B-C1B	-6.84	1.32	1.53
87	XB	902	ADP	C6-N6	5.81	1.49	1.34
84	Av	301	NAD	O4D-C4D	-5.62	1.32	1.45
87	XB	902	ADP	O4'-C1'	-5.01	1.30	1.42
84	Av	301	NAD	PA-O3	4.97	1.64	1.59
84	Av	301	NAD	C6A-N6A	4.80	1.46	1.34
84	Av	301	NAD	C7N-N7N	4.65	1.41	1.33
84	Av	301	NAD	PN-O3	4.19	1.64	1.59
84	Av	301	NAD	O3D-C3D	-3.49	1.34	1.43
84	Av	301	NAD	O2B-C2B	3.41	1.51	1.43
87	XB	902	ADP	O2'-C2'	-3.39	1.34	1.43
87	XB	902	ADP	C5-N7	-3.31	1.33	1.39
84	Av	301	NAD	C5A-C4A	-3.28	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	XB	902	ADP	C8-N9	-3.12	1.32	1.37
87	XB	902	ADP	C8-N7	2.88	1.37	1.31
87	XB	902	ADP	O3'-C3'	2.87	1.50	1.43
84	Av	301	NAD	C5A-N7A	-2.73	1.34	1.39
87	XB	902	ADP	PB-O2B	-2.70	1.44	1.54
84	Av	301	NAD	O2D-C2D	2.60	1.49	1.43
84	Av	301	NAD	C5B-C4B	2.53	1.59	1.51
87	XB	902	ADP	C5-C4	-2.32	1.35	1.39
84	Av	301	NAD	PA-O5B	2.31	1.68	1.59
87	XB	902	ADP	C1'-N9	2.26	1.52	1.46
84	Av	301	NAD	C5N-C4N	-2.24	1.35	1.38
88	XL	601	GTP	C2-N3	2.20	1.38	1.33
88	XL	602	GTP	C2-N3	2.19	1.38	1.33
87	XB	902	ADP	C2-N1	2.18	1.37	1.33
84	Av	301	NAD	C4A-N9A	-2.14	1.33	1.37
84	Av	301	NAD	C2A-N1A	2.11	1.37	1.33
87	XB	902	ADP	C6-N1	-2.02	1.30	1.35

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	XB	902	ADP	C4-N9-C1'	-8.66	106.37	126.63
87	XB	902	ADP	C1'-N9-C8	8.50	145.96	127.09
87	XB	902	ADP	N6-C6-N1	-7.09	102.59	118.38
84	Av	301	NAD	N6A-C6A-N1A	-6.98	102.83	118.38
84	Av	301	NAD	N3A-C2A-N1A	-5.65	120.03	128.58
84	Av	301	NAD	C5A-C6A-N6A	5.65	137.27	123.29
87	XB	902	ADP	C5-C4-N3	-5.64	118.94	126.72
87	XB	902	ADP	N3-C2-N1	-5.64	120.04	128.58
87	XB	902	ADP	C5-C6-N6	5.46	136.81	123.29
88	XL	602	GTP	C5-C4-N3	-5.16	120.17	128.39
88	XL	601	GTP	C5-C4-N3	-5.05	120.35	128.39
84	Av	301	NAD	C5A-C4A-N3A	-4.78	120.14	126.72
88	XL	602	GTP	C2-N3-C4	4.71	120.42	112.30
88	XL	601	GTP	C2-N3-C4	4.63	120.28	112.30
84	Av	301	NAD	N9A-C8A-N7A	-4.11	108.11	113.94
87	XB	902	ADP	N9-C8-N7	-3.94	108.35	113.94
87	XB	902	ADP	C2-N3-C4	3.64	120.72	111.83
87	XB	902	ADP	N3-C4-N9	3.63	133.34	127.17
88	XL	602	GTP	N9-C4-N3	3.38	132.71	125.95
84	Av	301	NAD	C2A-N3A-C4A	3.32	119.94	111.83
88	XL	601	GTP	N9-C4-N3	3.26	132.47	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	XL	601	GTP	C2-N1-C6	-2.93	119.80	125.11
88	XL	602	GTP	C2-N1-C6	-2.92	119.82	125.11
87	XB	902	ADP	C5-N7-C8	2.90	108.01	103.45
84	Av	301	NAD	C5A-N7A-C8A	2.85	107.94	103.45
84	Av	301	NAD	N3A-C4A-N9A	2.84	131.99	127.17
88	XL	602	GTP	N9-C8-N7	-2.74	108.31	113.40
88	XL	601	GTP	N9-C8-N7	-2.70	108.39	113.40
88	XL	601	GTP	C8-N7-C5	2.63	108.95	104.26
88	XL	602	GTP	C8-N7-C5	2.61	108.90	104.26
88	XL	601	GTP	C5-C6-N1	2.52	119.66	113.25
88	XL	602	GTP	C5-C6-N1	2.51	119.64	113.25
88	XL	602	GTP	O6-C6-C5	-2.42	120.14	126.53
88	XL	601	GTP	O6-C6-C5	-2.38	120.25	126.53
87	XB	902	ADP	C6-C5-C4	2.18	120.16	117.18
84	Av	301	NAD	C4A-C5A-N7A	-2.16	108.12	110.58
84	Av	301	NAD	C4A-N9A-C8A	2.12	107.97	105.74
88	XL	601	GTP	C3'-C2'-C1'	2.12	105.47	101.46
88	XL	602	GTP	C3'-C2'-C1'	2.09	105.41	101.46
84	Av	301	NAD	C6N-N1N-C2N	-2.09	120.10	121.88
87	XB	902	ADP	C4-C5-N7	-2.04	108.25	110.58
84	Av	301	NAD	C3N-C7N-N7N	2.02	120.22	117.74
84	Av	301	NAD	O7N-C7N-N7N	-2.00	119.73	122.62

There are no chirality outliers.

All (14) torsion outliers are listed below:

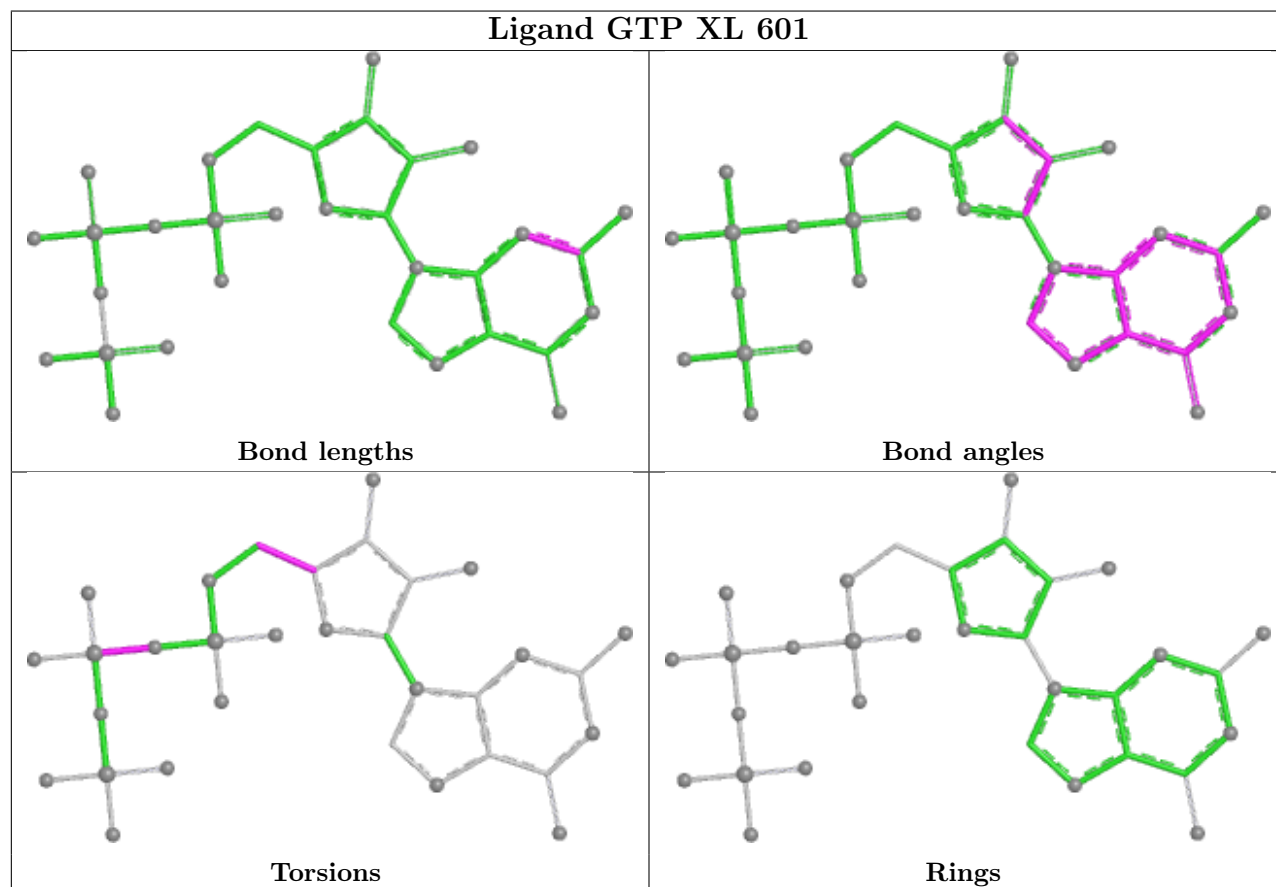
Mol	Chain	Res	Type	Atoms
87	XB	902	ADP	C5'-O5'-PA-O1A
88	XL	602	GTP	C5'-O5'-PA-O3A
88	XL	602	GTP	C5'-O5'-PA-O2A
84	Av	301	NAD	O4B-C4B-C5B-O5B
88	XL	601	GTP	C3'-C4'-C5'-O5'
88	XL	601	GTP	O4'-C4'-C5'-O5'
84	Av	301	NAD	C3B-C4B-C5B-O5B
84	Av	301	NAD	C5B-O5B-PA-O1A
88	XL	602	GTP	C5'-O5'-PA-O1A
88	XL	602	GTP	PG-O3B-PB-O2B
84	Av	301	NAD	O4D-C4D-C5D-O5D
87	XB	902	ADP	C2'-C1'-N9-C8
88	XL	601	GTP	PA-O3A-PB-O2B
88	XL	602	GTP	PG-O3B-PB-O1B

There are no ring outliers.

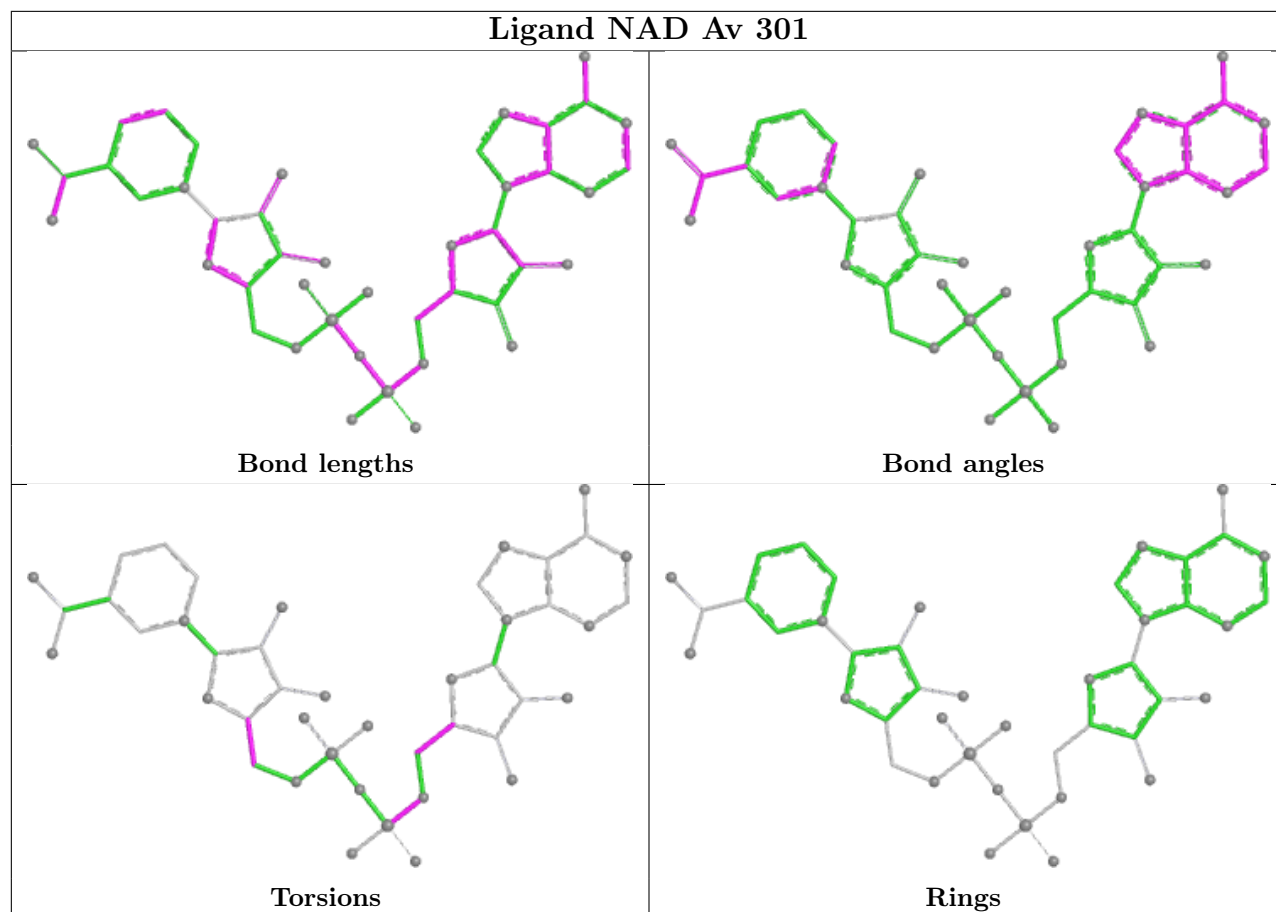
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	XL	601	GTP	2	0
83	A5	101	FES	1	0
84	Av	301	NAD	2	0
87	XB	902	ADP	1	0
88	XL	602	GTP	3	0

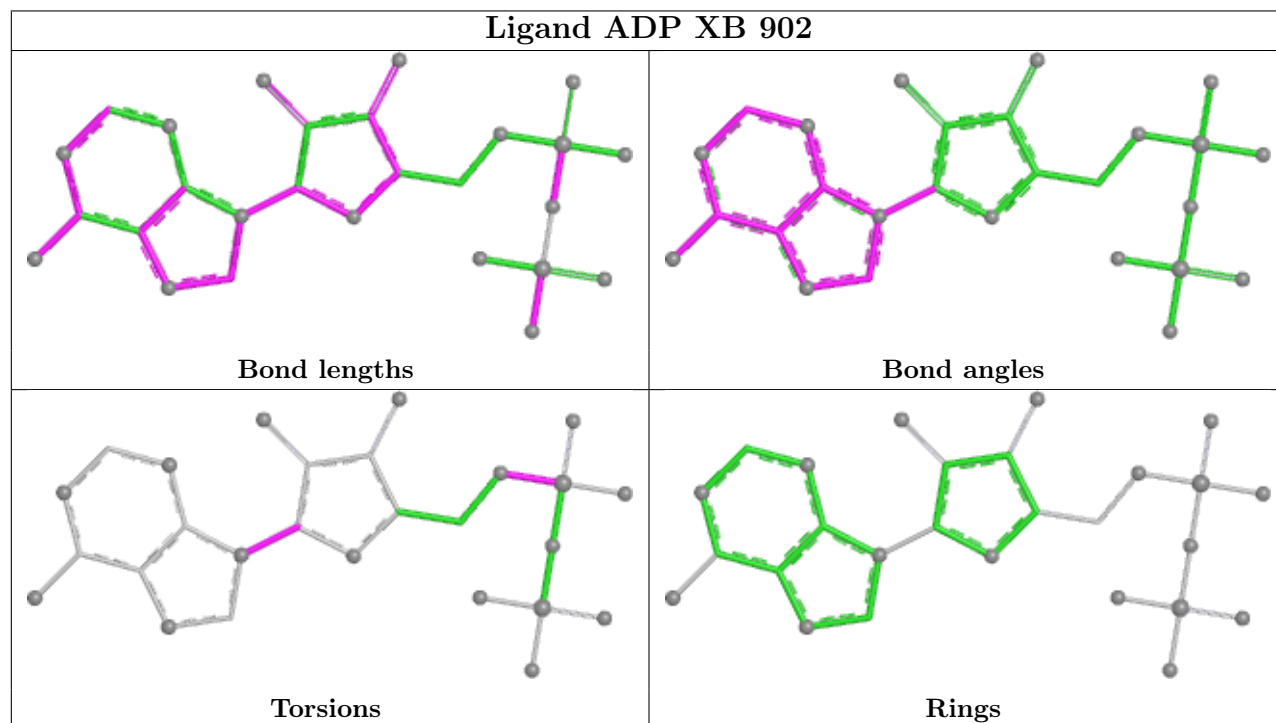
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

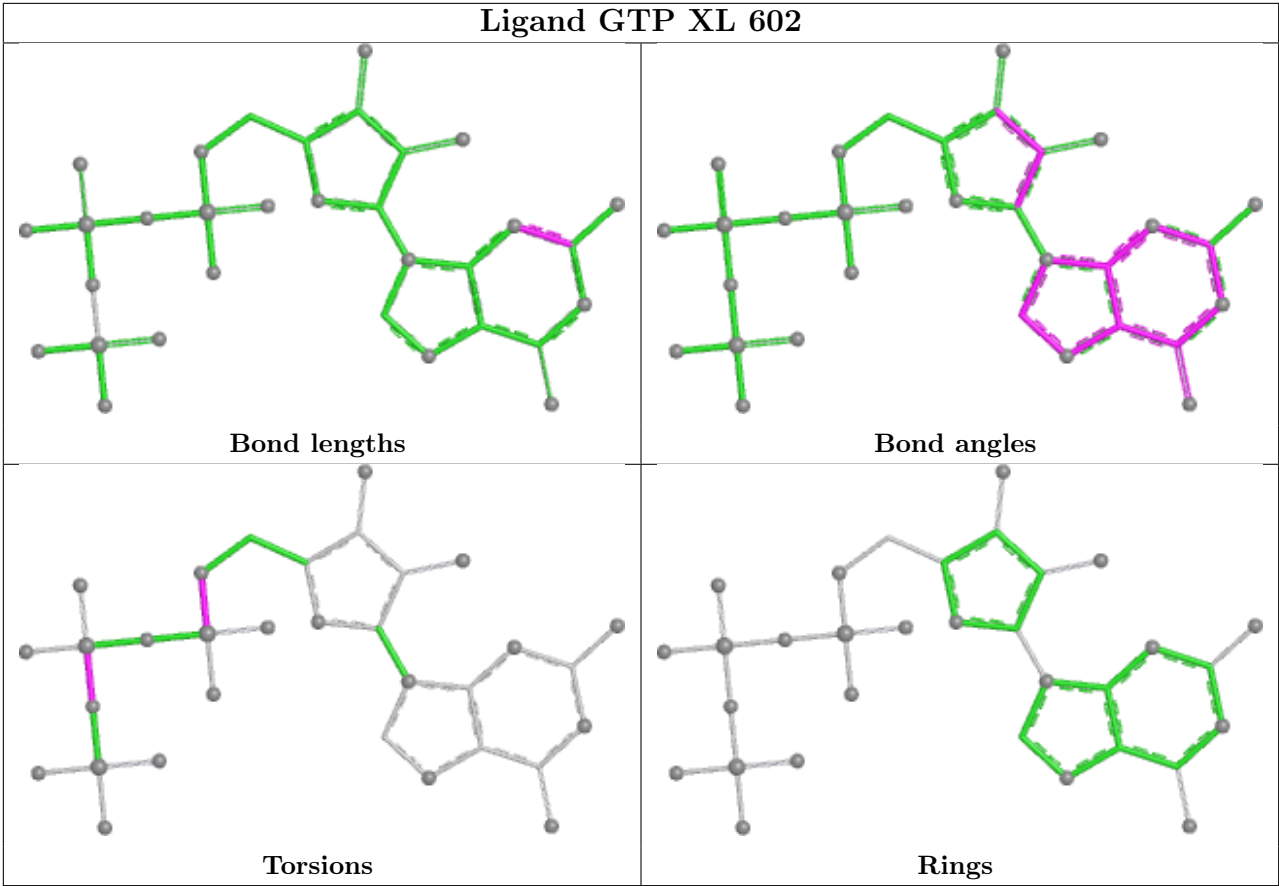


Ligand NAD Av 301



Ligand ADP XB 902





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
6	AA	14
59	UF	6
29	BB	3
36	BK	2
71	XH	2
10	AK	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	356:A	O3'	369:U	P	34.53

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	594:A	O3'	796:A	P	31.20
1	UF	105:ALA	C	122:ALA	N	30.57
1	BK	233:LYS	C	254:ALA	N	28.37
1	UF	34:ALA	C	37:ALA	N	22.56
1	AA	380:G	O3'	404:U	P	20.97
1	AA	534:U	O3'	541:A	P	19.51
1	BK	269:ALA	C	280:LEU	N	19.38
1	UF	135:ALA	C	140:ALA	N	18.98
1	AA	989:U	O3'	1001:G	P	17.71
1	AA	582:A	O3'	591:G	P	16.56
1	AA	264:U	O3'	270:A	P	16.48
1	AA	1090:U	O3'	1095:A	P	16.18
1	AA	205:U	O3'	254:G	P	15.15
1	AA	1013:C	O3'	1071:U	P	15.08
1	AA	450:U	O3'	456:U	P	14.15
1	AA	413:U	O3'	445:U	P	12.66
1	XH	113:LEU	C	184:ILE	N	12.09
1	BB	258:PHE	C	264:ALA	N	11.96
1	AA	967:G	O3'	972:G	P	11.71
1	BB	294:ALA	C	304:ALA	N	11.57
1	UF	87:ALA	C	92:ALA	N	10.93
1	AA	883:U	O3'	887:A	P	10.10
1	AK	235:GLU	C	239:ALA	N	8.23
1	BB	341:ALA	C	346:GLU	N	7.64
1	XH	55:PRO	C	86:SER	N	7.57
1	UF	27:ALA	C	29:ALA	N	6.13
1	UF	63:ALA	C	65:ALA	N	5.33

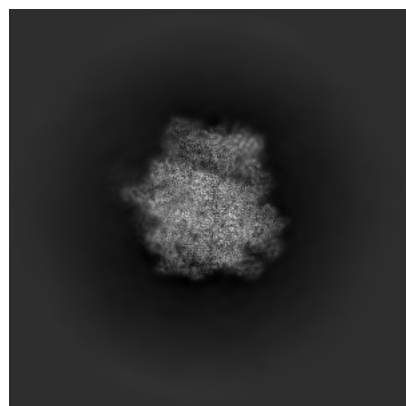
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11845. These allow visual inspection of the internal detail of the map and identification of artifacts.

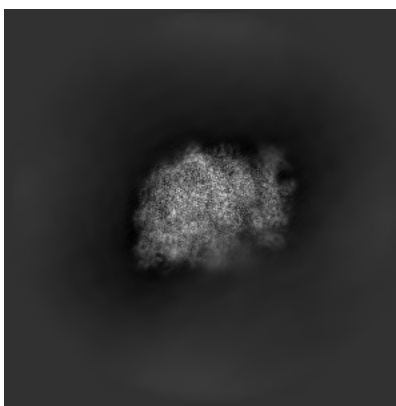
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

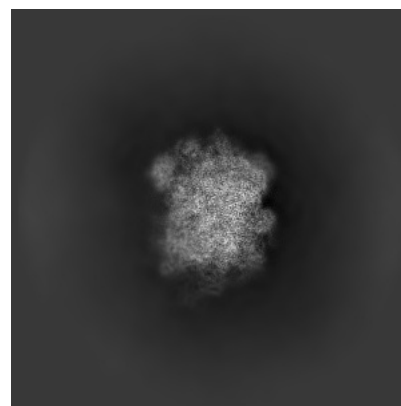
6.1.1 Primary map



X

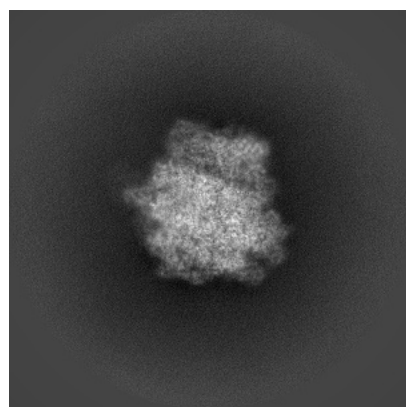


Y

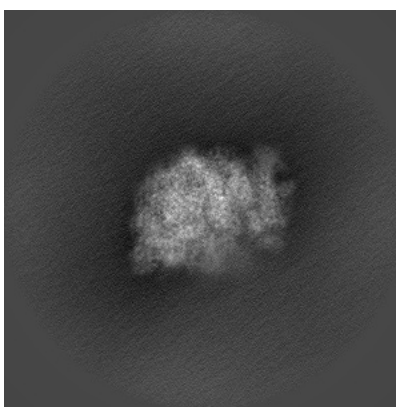


Z

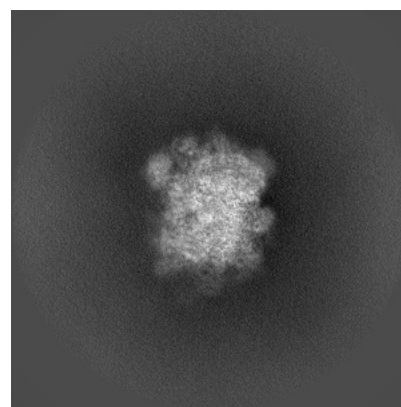
6.1.2 Raw map



X



Y

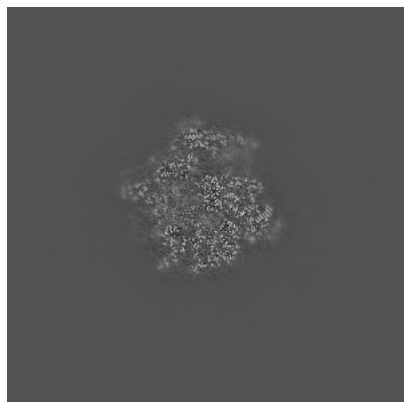


Z

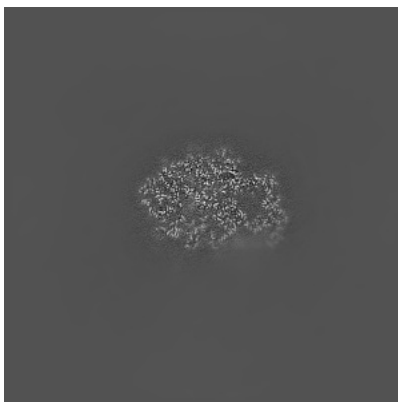
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

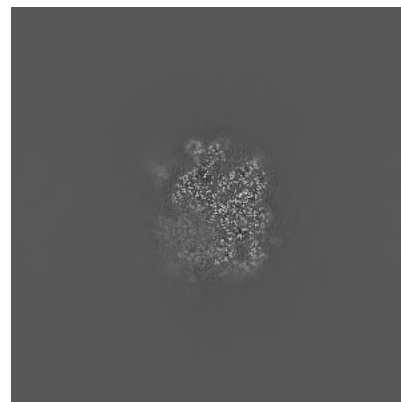
6.2.1 Primary map



X Index: 300

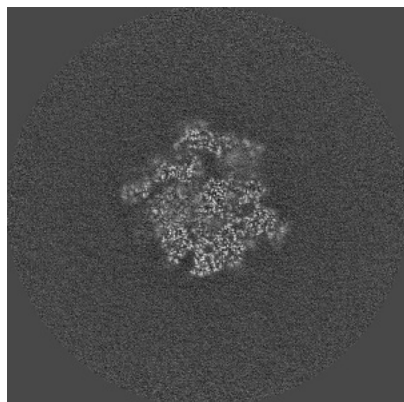


Y Index: 300

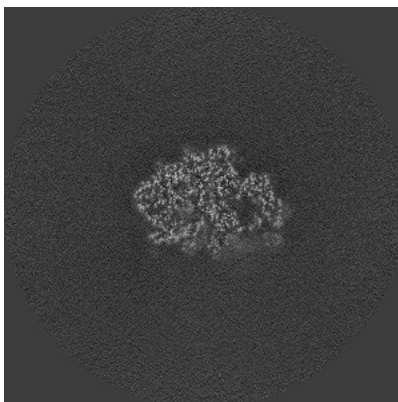


Z Index: 300

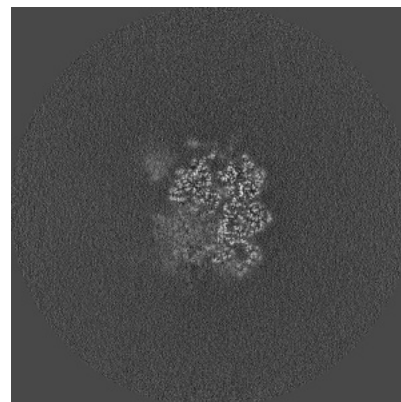
6.2.2 Raw map



X Index: 300



Y Index: 300

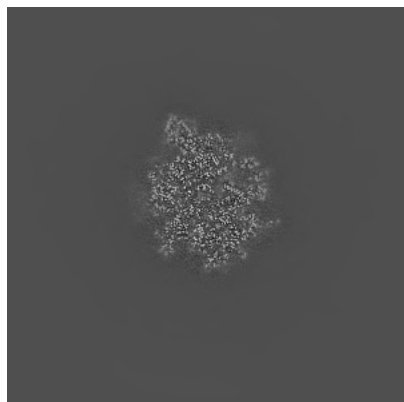


Z Index: 300

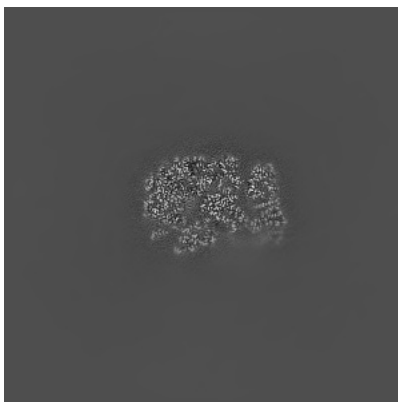
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

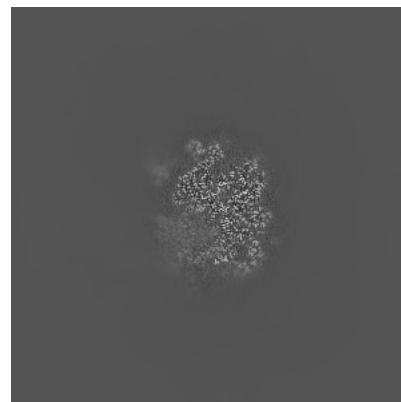
6.3.1 Primary map



X Index: 331

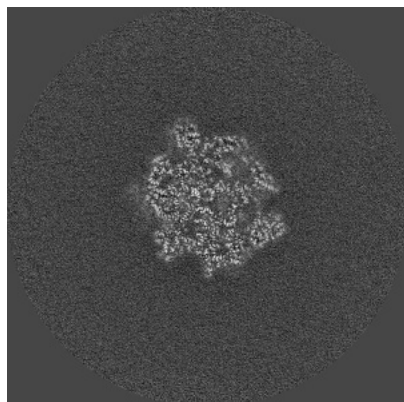


Y Index: 309

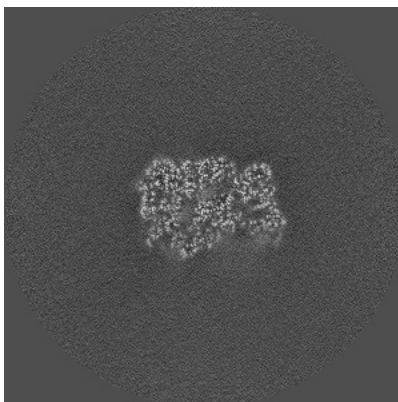


Z Index: 301

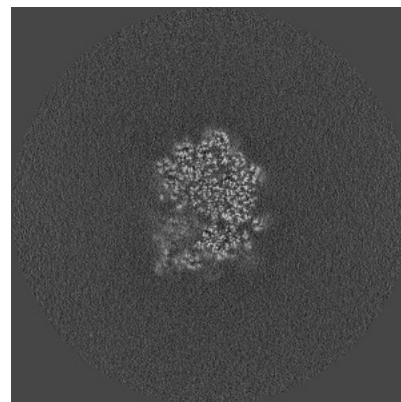
6.3.2 Raw map



X Index: 318



Y Index: 319

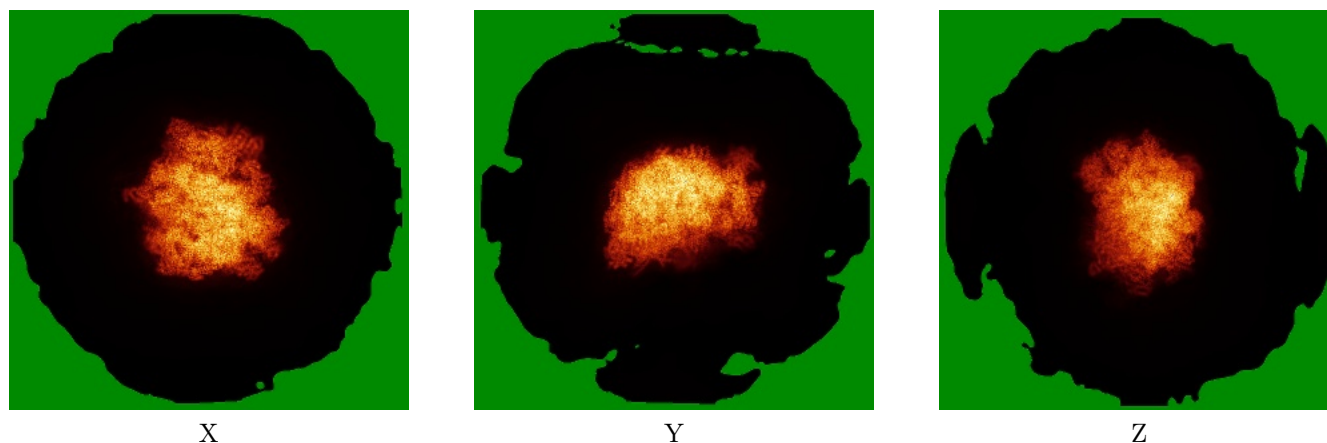


Z Index: 259

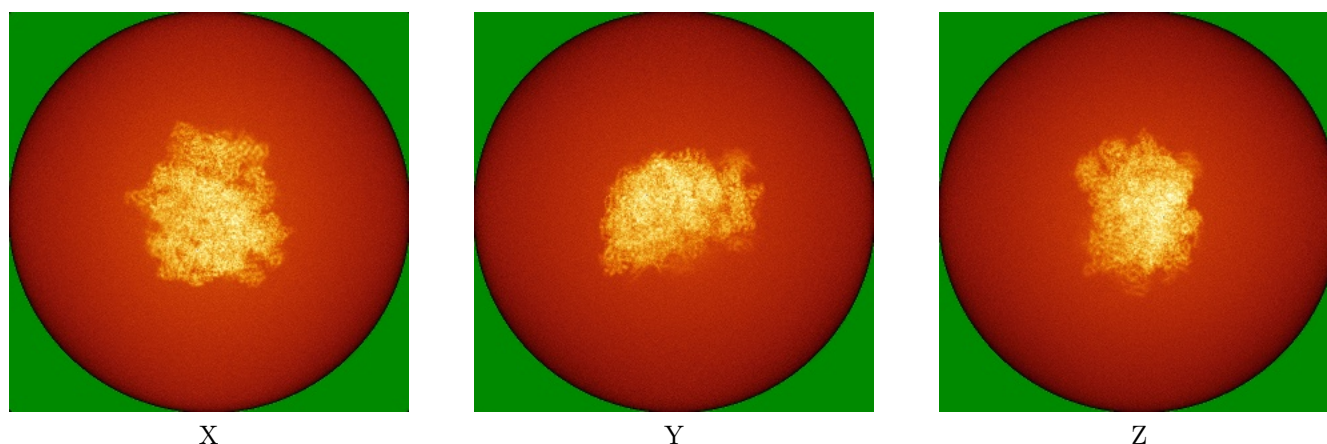
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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.

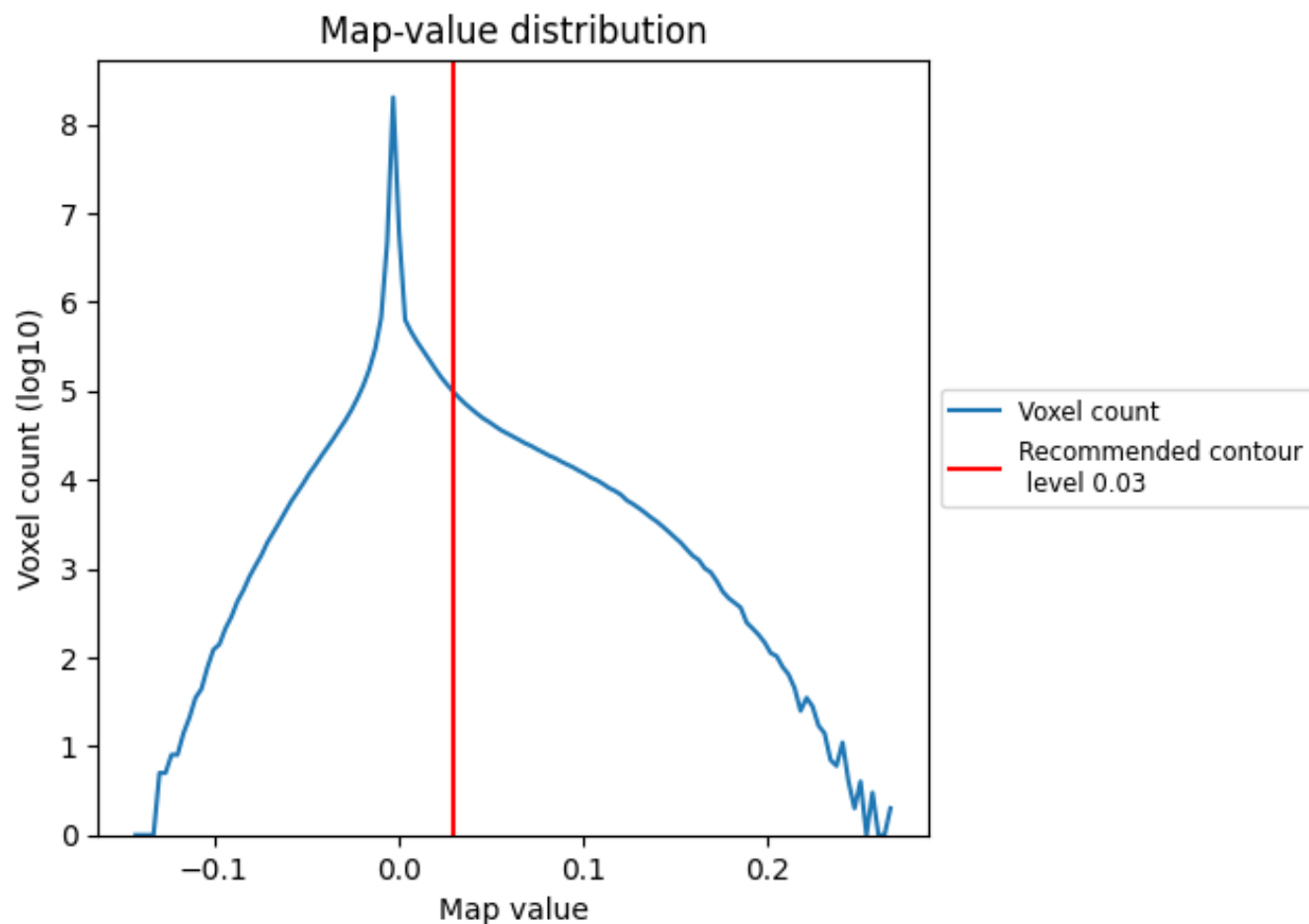
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

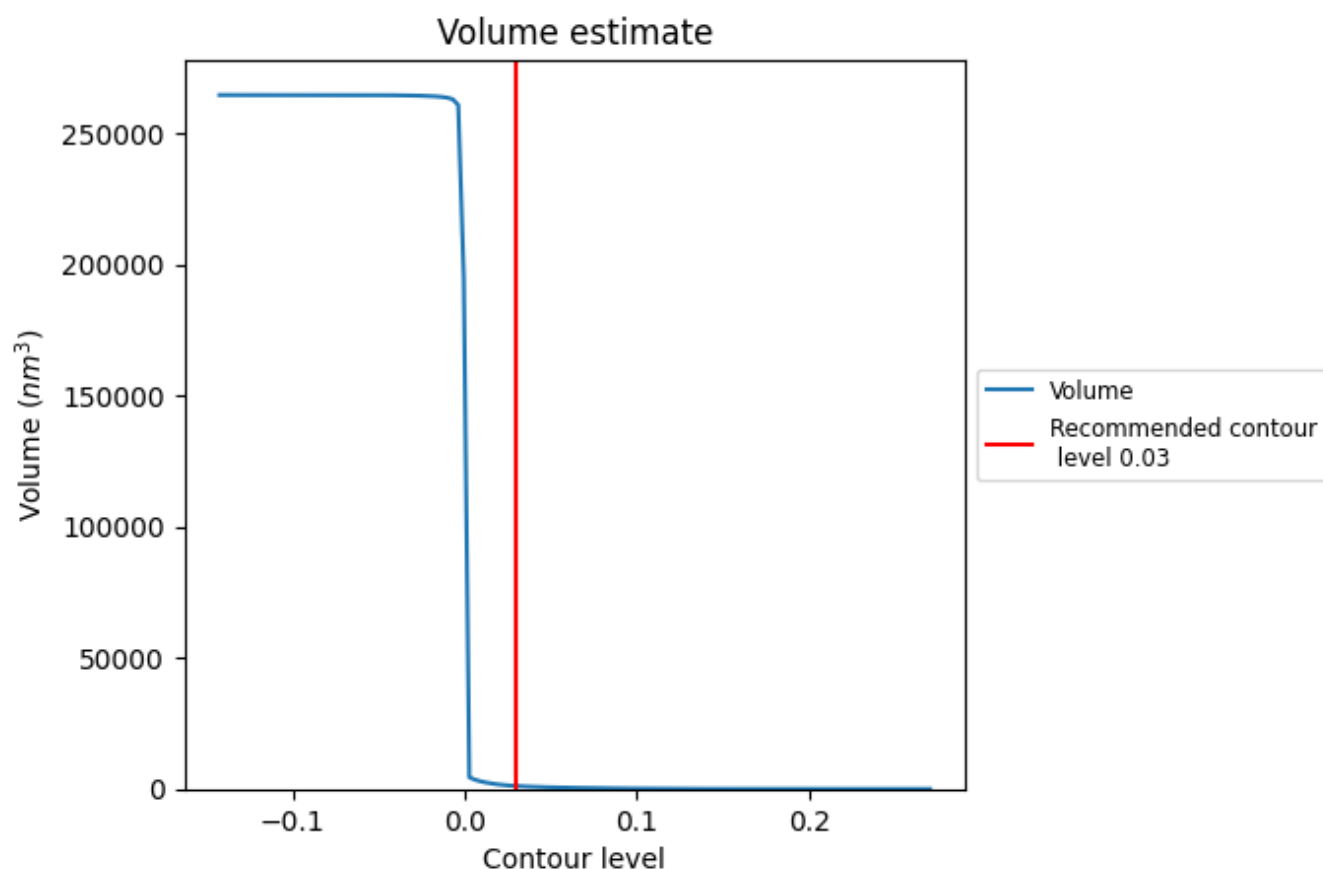
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

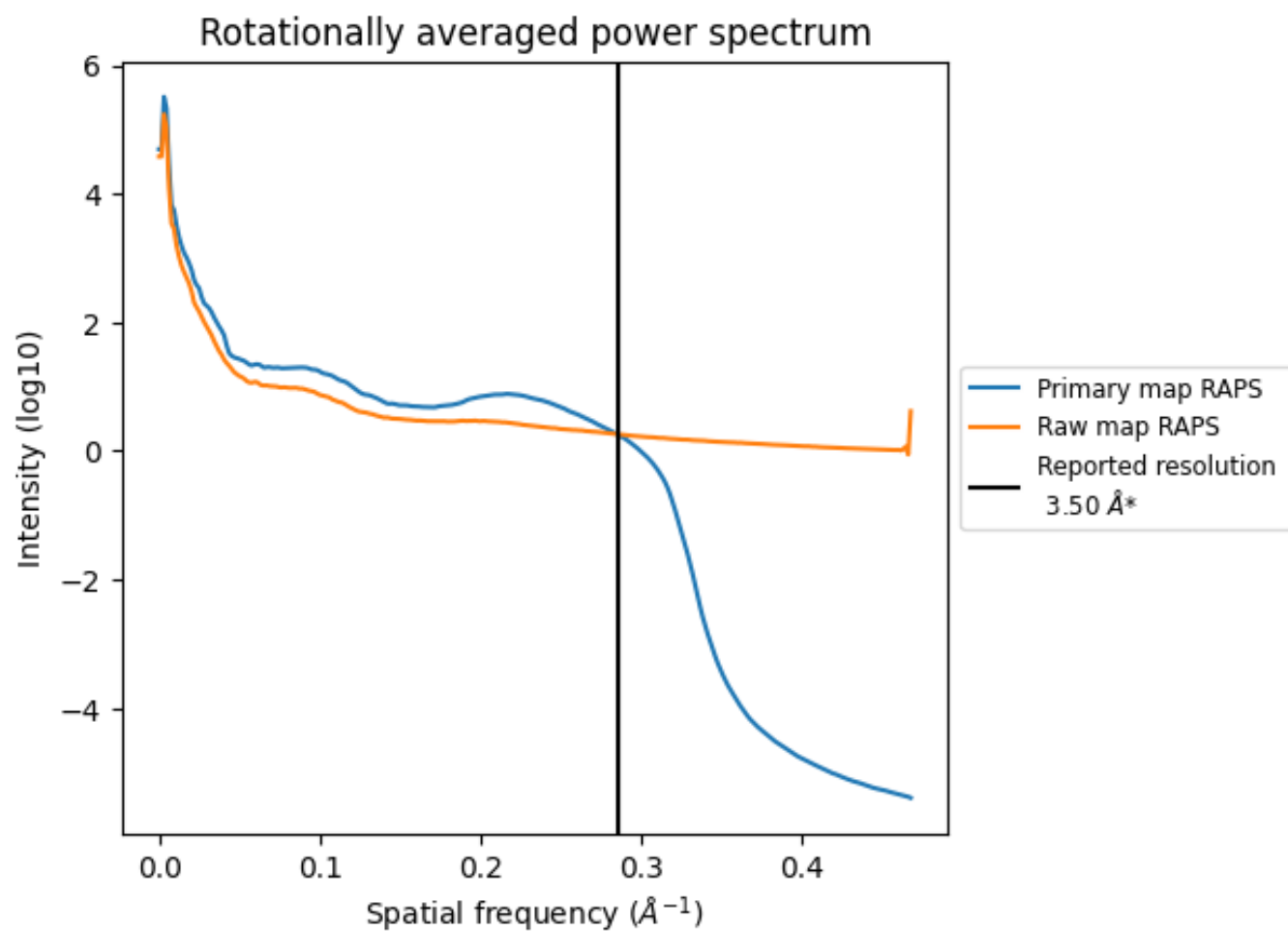
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1128 nm^3 ; this corresponds to an approximate mass of 1019 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

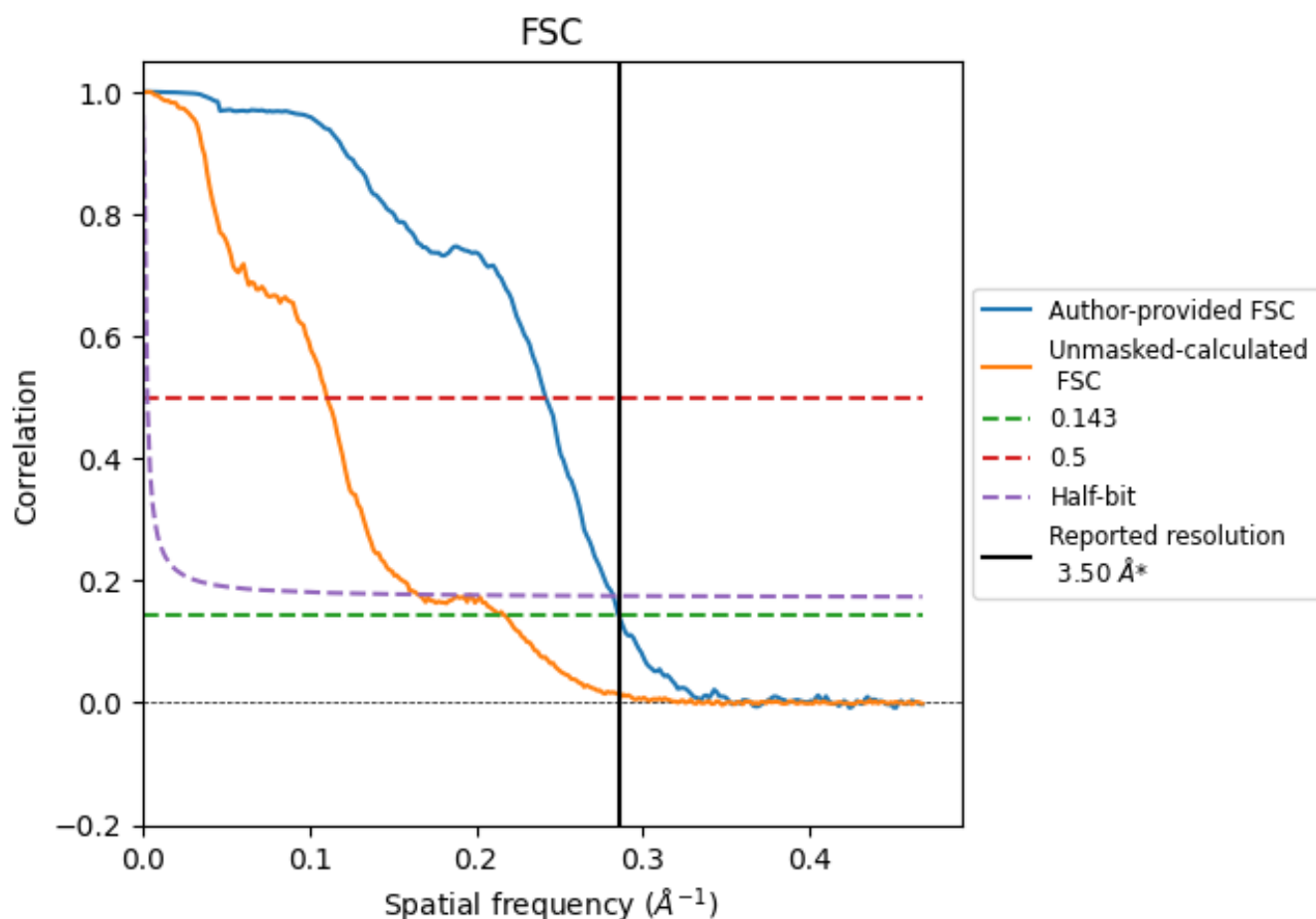


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

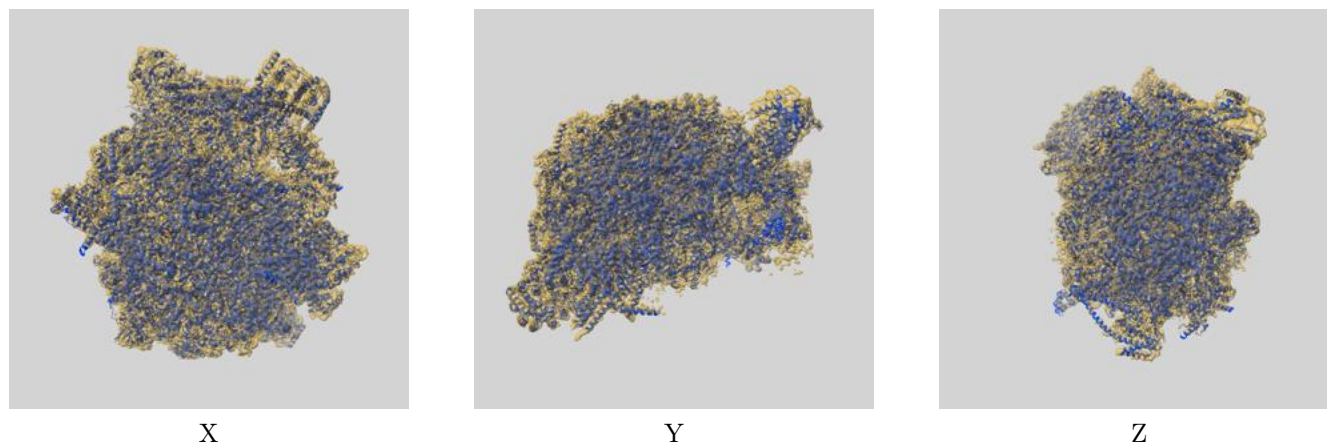
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.50	4.14	3.54
Unmasked-calculated*	4.69	9.04	6.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.69 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

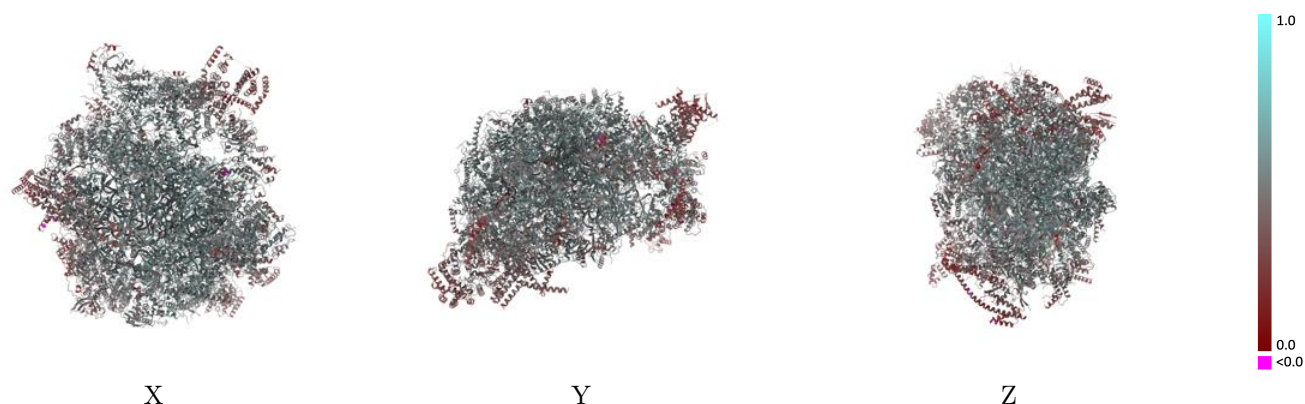
This section contains information regarding the fit between EMDB map EMD-11845 and PDB model 7AOI. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.03 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](#)

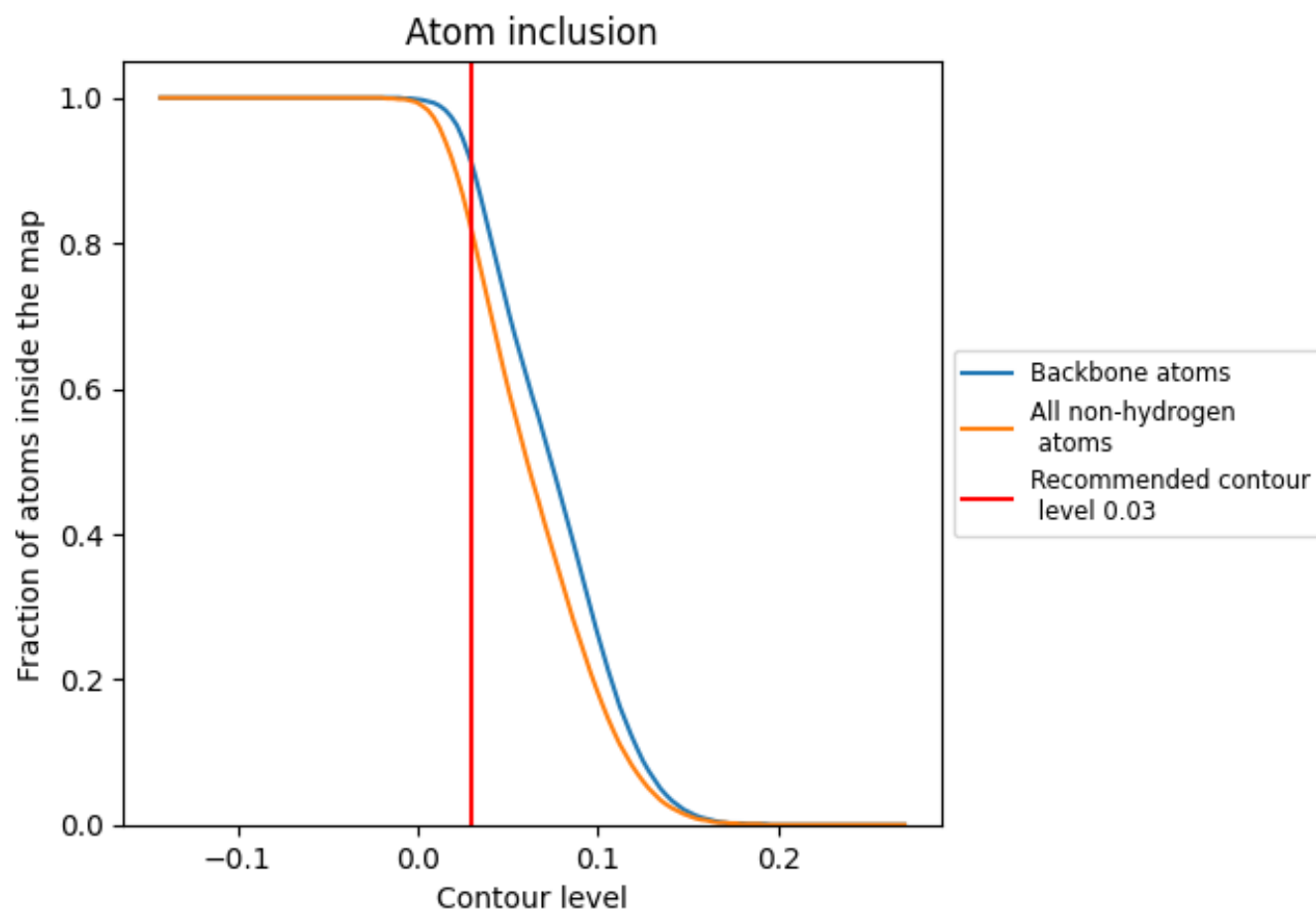


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 91% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.4860
A1	 0.8050	 0.4690
A2	 0.8680	 0.5070
A3	 0.8760	 0.5420
A5	 0.8950	 0.5460
A8	 0.8730	 0.5340
AA	 0.8980	 0.5140
AE	 0.8990	 0.5550
AF	 0.8950	 0.5460
AI	 0.8390	 0.4910
AK	 0.4990	 0.3180
AN	 0.9030	 0.5550
AP	 0.8790	 0.5410
AR	 0.8400	 0.5100
AT	 0.8590	 0.5180
AU	 0.8810	 0.5360
AV	 0.8950	 0.5440
AW	 0.8730	 0.5450
AX	 0.8740	 0.5290
AY	 0.8130	 0.4830
Ae	 0.8540	 0.5080
Af	 0.8570	 0.5210
Ag	 0.8770	 0.5300
Al	 0.9000	 0.5500
Ao	 0.8860	 0.5460
Ap	 0.8630	 0.5130
At	 0.7900	 0.4790
Av	 0.8360	 0.5000
BA	 0.8740	 0.5220
BB	 0.6320	 0.3210
BD	 0.6630	 0.3580
BE	 0.8010	 0.4630
BF	 0.8670	 0.5240
BH	 0.8030	 0.4960
BI	 0.8750	 0.5200



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Chain	Atom inclusion	Q-score
BJ	 0.7250	 0.3880
BK	 0.6480	 0.4040
BL	 0.8450	 0.4880
BN	 0.6630	 0.3740
BO	 0.8210	 0.4880
BQ	 0.8800	 0.5270
BR	 0.8320	 0.5050
BS	 0.7030	 0.4240
BT	 0.8780	 0.5200
BU	 0.8040	 0.4630
BW	 0.9140	 0.5380
BX	 0.5320	 0.4160
BZ	 0.7170	 0.4080
Ba	 0.8860	 0.5290
Bb	 0.7720	 0.4310
Bc	 0.8500	 0.5250
Bf	 0.8330	 0.5090
Bg	 0.7450	 0.4620
Bh	 0.7680	 0.4550
UA	 0.8040	 0.3060
UB	 0.9560	 0.5380
UC	 0.8710	 0.5040
UD	 0.8500	 0.5170
UE	 0.9170	 0.5460
UF	 0.8560	 0.3150
UG	 0.7890	 0.4900
UH	 0.8710	 0.4510
UI	 0.7540	 0.4190
UJ	 0.9440	 0.5420
UK	 0.9110	 0.5410
XA	 0.9150	 0.5670
XB	 0.8690	 0.5360
XC	 0.8510	 0.5050
XD	 0.4570	 0.2780
XE	 0.6980	 0.3850
XF	 0.7590	 0.3950
XG	 0.8380	 0.5300
XH	 0.8010	 0.4550
XI	 0.7490	 0.4340
XJ	 0.7560	 0.4880
XL	 0.7800	 0.4760
XM	 0.7150	 0.4440

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Chain	Atom inclusion	Q-score
XN	 0.8470	 0.4930
XO	 0.7620	 0.4510
XP	 0.8510	 0.5360
XQ	 0.6680	 0.4360
XR	 0.6980	 0.3790
XS	 0.4720	 0.3340
XT	 0.8570	 0.5340