



## Full wwPDB EM Validation Report ⓘ

Nov 13, 2025 – 03:18 PM EST

PDB ID : 9N9J / pdb\_00009n9j  
EMDB ID : EMD-49171  
Title : Structure of a GRP94 folding intermediate engaged with a CCDC134- and FKBP11-bound secretory translocon  
Authors : Yamsek, M.; Jha, R.; Keenan, R.J.  
Deposited on : 2025-02-10  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

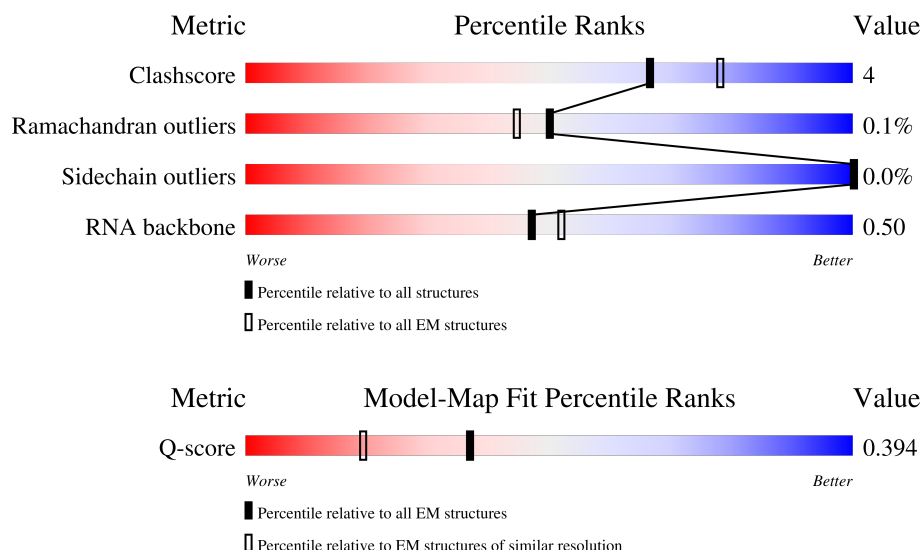
EMDB validation analysis : 0.0.1.dev129  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB 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) : 2.46

# 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 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	15020 ( 2.70 - 3.70 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	5	286	<div> <div>28%</div> <div>43%</div> <div>6%</div> <div>51%</div> </div>
2	6	183	<div> <div>40%</div> <div>69%</div> <div>19%</div> <div>11%</div> </div>
3	7	185	<div> <div>19%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>






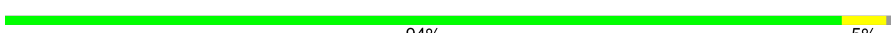



















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Mol	Chain	Length	Quality of chain
4	8	173	
5	A	201	
6	B	229	
7	D	476	
8	E	96	
9	F	68	
10	G	66	
11	I	705	
12	J	149	
13	K2	37	
14	L2	79	
15	L5	5066	
16	L7	121	
17	L8	157	
18	LA	257	
19	LB	403	
20	LC	427	
21	LD	297	
22	LE	288	
23	LF	248	
24	LG	266	
25	LH	192	
26	LI	214	
27	LL	211	
28	LM	215	


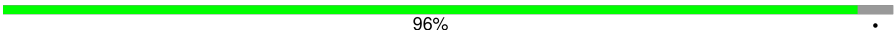






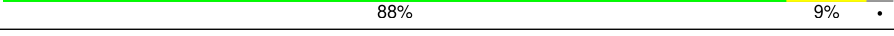
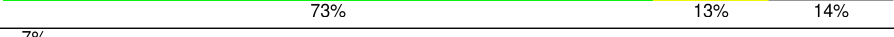
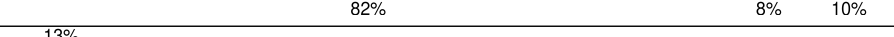

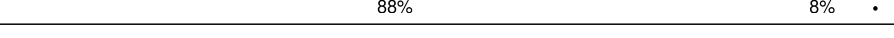
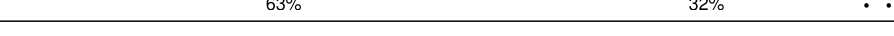
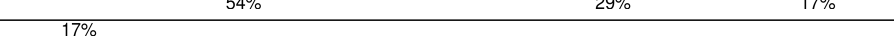






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Mol	Chain	Length	Quality of chain
29	LN	204	
30	LO	203	
31	LP	184	
32	LQ	188	
33	LR	196	
34	LS	176	
35	LT	160	
36	LU	128	
37	LV	140	
38	LW	157	
39	LX	156	
40	LY	145	
41	LZ	136	
42	La	148	
43	Lb	159	
44	Lc	115	
45	Ld	125	
46	Le	135	
47	Lf	110	
48	Lg	117	
49	Lh	123	
50	Li	105	
51	Lj	97	
52	Lk	70	
53	Ll	51	

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Mol	Chain	Length	Quality of chain
54	Lm	128	
55	Ln	25	
56	Lo	106	
57	Lp	92	
58	Lr	137	
59	Ls	317	
60	Lt	165	
61	Lz	217	
62	M2	113	
63	N	136	
64	N2	456	
65	O2	607	
66	P2	631	
67	u3	76	
68	v3	76	
69	y3	846	
70	LJ	178	
71	K	8	
72	C	2	
73	H	8	
74	L	2	

## 2 Entry composition [i](#)

There are 78 unique types of molecules in this entry. The entry contains 326107 atoms, of which 142818 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 Translocon-associated protein subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	5	140	Total	C	H	N	O	S	0	0
			2192	723	1071	179	217	2		

- Molecule 2 is a protein called Translocon-associated protein subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	6	162	Total	C	H	N	O	S	0	0
			2500	808	1241	212	237	2		

- Molecule 3 is a protein called Translocon-associated protein subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	7	179	Total	C	H	N	O	S	0	0
			2938	946	1487	239	263	3		

- Molecule 4 is a protein called Translocon-associated protein subunit delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	8	150	Total	C	H	N	O	S	0	0
			2333	755	1148	199	228	3		

- Molecule 5 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP11.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	A	167	Total	C	H	N	O	S	0	0
			2695	842	1390	230	228	5		

- Molecule 6 is a protein called Coiled-coil domain-containing protein 134.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	B	197	Total	C	H	N	O	S	0	0
			3279	1046	1646	289	294	4		

- Molecule 7 is a protein called Protein transport protein Sec61 subunit alpha isoform 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	D	454	Total	C	H	N	O	S	0	0
			7189	2324	3661	564	616	24		

- Molecule 8 is a protein called Protein transport protein Sec61 subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	E	32	Total	C	H	N	O	S	0	0
			523	171	273	40	37	2		

- Molecule 9 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	F	67	Total	C	H	N	O	S	0	0
			1112	353	574	93	87	5		

- Molecule 10 is a protein called Stress-associated endoplasmic reticulum protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	G	56	Total	C	H	N	O	S	0	0
			904	280	467	82	71	4		

- Molecule 11 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3A.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	I	701	Total	C	H	N	O	S	0	0
			11261	3701	5612	913	998	37		

- Molecule 12 is a protein called Oligosaccharyltransferase complex subunit OSTC.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	J	149	Total	C	H	N	O	S	0	0
			2409	789	1227	189	192	12		

- Molecule 13 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	K2	37	Total	C	H	N	O	S	0	0
			607	196	312	46	51	2		

- Molecule 14 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit TMEM258.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	L2	79	Total	C	H	N	O	S	0	0
			1302	440	659	92	107	4		

- Molecule 15 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	L5	3718	Total	C	H	N	O	P	0	0
			119751	35431	40176	14552	25875	3717		

- Molecule 16 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	L7	120	Total	C	H	N	O	P	0	0
			3855	1141	1294	456	844	120		

- Molecule 17 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	L8	156	Total	C	H	N	O	P	0	0
			4996	1480	1682	585	1094	155		

- Molecule 18 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	LA	248	Total	C	H	N	O	S	0	0
			3891	1189	1993	389	314	6		

- Molecule 19 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	LB	400	Total	C	H	N	O	S	0	0
			6598	2055	3369	606	554	14		

- Molecule 20 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	LC	368	Total	C	H	N	O	S	0	0
			6031	1840	3104	583	489	15		

- Molecule 21 is a protein called Large ribosomal subunit protein uL18.



Mol	Chain	Residues	Atoms						AltConf	Trace
21	LD	293	Total	C	H	N	O	S	0	0
			4792	1507	2410	434	427	14		

- Molecule 22 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	LE	236	Total	C	H	N	O	S	0	0
			3959	1222	2055	361	317	4		

- Molecule 23 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	LF	225	Total	C	H	N	O	S	0	0
			3866	1202	1996	358	301	9		

- Molecule 24 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	LG	241	Total	C	H	N	O	S	0	0
			4001	1228	2074	371	324	4		

- Molecule 25 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	LH	190	Total	C	H	N	O	S	0	0
			3119	956	1601	284	272	6		

- Molecule 26 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	LI	202	Total	C	H	N	O	S	0	0
			3305	1037	1671	314	269	14		

- Molecule 27 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	LL	210	Total	C	H	N	O	S	0	0
			3519	1064	1818	352	281	4		

- Molecule 28 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	LM	136	Total	C	H	N	O	S	0	0
			2307	719	1187	215	179	7		

- Molecule 29 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	LN	203	Total	C	H	N	O	S	0	0
			3450	1072	1749	359	266	4		

- Molecule 30 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	LO	201	Total	C	H	N	O	S	0	0
			3444	1063	1794	321	261	5		

- Molecule 31 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	LP	181	Total	C	H	N	O	S	0	0
			3006	923	1536	282	255	10		

- Molecule 32 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	LQ	187	Total	C	H	N	O	S	0	0
			3141	944	1628	314	250	5		

- Molecule 33 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	LR	177	Total	C	H	N	O	S	0	0
			3118	918	1633	323	235	9		

- Molecule 34 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	LS	175	Total	C	H	N	O	S	0	0
			2943	925	1490	283	235	10		

- Molecule 35 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	LT	159	Total	C	H	N	O	S	0	0
			2664	823	1366	252	217	6		

- Molecule 36 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	LU	101	Total	C	H	N	O	S	0	0
			1675	529	850	144	150	2		

- Molecule 37 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	LV	131	Total	C	H	N	O	S	0	0
			2018	618	1039	184	172	5		

- Molecule 38 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	LW	63	Total	C	H	N	O	S	0	0
			1069	337	541	103	85	3		

- Molecule 39 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	LX	119	Total	C	H	N	O	S	0	0
			2029	624	1053	183	168	1		

- Molecule 40 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	LY	134	Total	C	H	N	O	S	0	0
			2320	700	1205	226	186	3		

- Molecule 41 is a protein called Large ribosomal subunit protein eL27.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	LZ	135	Total	C	H	N	O	S	0	0
			2289	714	1182	208	182	3		

- Molecule 42 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	La	147	Total	C	H	N	O	S	0	0
			2376	736	1214	237	186	3		

- Molecule 43 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	Lb	109	Total	C	H	N	O	S	0	0
			1824	546	948	189	137	4		

- Molecule 44 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	Lc	98	Total	C	H	N	O	S	0	0
			1568	485	804	135	138	6		

- Molecule 45 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	Ld	107	Total	C	H	N	O	S	0	0
			1818	560	930	171	155	2		

- Molecule 46 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	Le	129	Total	C	H	N	O	S	0	0
			2224	673	1160	220	166	5		

- Molecule 47 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	Lf	109	Total	C	H	N	O	S	0	0
			1788	555	912	174	144	3		

- Molecule 48 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	Lg	114	Total	C	H	N	O	S	0	0
			1904	566	998	187	147	6		

- Molecule 49 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	Lh	122	Total	C	H	N	O	S	0	0
			2163	641	1148	205	168	1		

- Molecule 50 is a protein called Large ribosomal subunit protein eL36.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	Li	102	Total	C	H	N	O	S	0	0
			1749	521	917	177	129	5		

- Molecule 51 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	Lj	86	Total	C	H	N	O	S	0	0
			1441	434	736	155	111	5		

- Molecule 52 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	Lk	69	Total	C	H	N	O	S	0	0
			1206	366	637	103	99	1		

- Molecule 53 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	Ll	50	Total	C	H	N	O	S	0	0
			927	281	483	98	64	1		

- Molecule 54 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	Lm	52	Total	C	H	N	O	S	0	0
			894	266	465	90	67	6		

- Molecule 55 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	Ln	24	Total	C	H	N	O	S	0	0
			506	139	276	62	26	3		

- Molecule 56 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	Lo	105	Total	C	H	N	O	S	0	0
			1791	542	929	175	139	6		

- Molecule 57 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	Lp	91	Total	C	H	N	O	S	0	0
			1464	445	756	136	120	7		

- Molecule 58 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	Lr	125	Total	C	H	N	O	S	0	0
			2070	622	1068	207	168	5		

- Molecule 59 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	Ls	196	Total	C	H	N	O	S	0	0
			3036	952	1540	259	276	9		

- Molecule 60 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	Lt	141	Total	C	H	N	O	S	0	0
			2122	652	1076	191	199	4		

- Molecule 61 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	Lz	217	Total	C	H	N	O	S	0	0
			3595	1113	1854	312	307	9		

- Molecule 62 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit DAD1.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	M2	110	Total	C	H	N	O	S	0	0
			1743	573	880	135	151	4		

- Molecule 63 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit KCP2.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	N	117	Total	C	H	N	O	S	0	0
			1816	591	925	138	156	6		

- Molecule 64 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase 48 kDa subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	N2	410	Total	C	H	N	O	S	0	0
			6385	2079	3161	531	608	6		

- Molecule 65 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	O2	580	Total	C	H	N	O	S	0	0
			9342	2978	4687	785	883	9		

- Molecule 66 is a protein called Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	P2	607	Total	C	H	N	O	S	0	0
			9445	3020	4724	783	909	9		

- Molecule 67 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	u3	75	Total	C	H	N	O	P	0	0
			2402	710	809	278	530	75		

- Molecule 68 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	v3	76	Total	C	H	N	O	P	0	0
			2440	721	822	287	534	76		

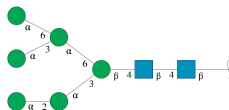
- Molecule 69 is a protein called Endoplasmin.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	y3	275	Total	C	H	N	O	S	0	0
			4069	1284	2011	355	415	4		

- Molecule 70 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	LJ	176	Total	C	H	N	O	S	0	0
			2851	888	1441	263	253	6		

- Molecule 71 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



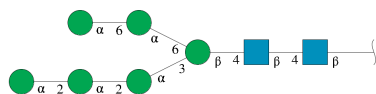
Mol	Chain	Residues	Atoms						AltConf	Trace
71	K	8	Total	C	H	N	O		0	0
			173	52	79	2	40			

- Molecule 72 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms						AltConf	Trace
72	C	2	Total	C	H	N	O		0	0
			53	16	25	2	10			

- Molecule 73 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms						AltConf	Trace
73	H	8	Total	C	H	N	O		0	0
			173	52	79	2	40			

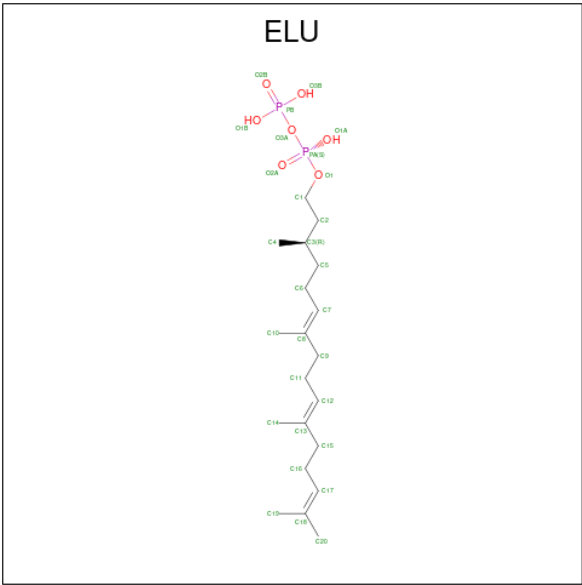
- Molecule 74 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose.





Mol	Chain	Residues	Atoms					AltConf	Trace
74	L	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 75 is phosphono [(3 {R},6 {E},10 {E})-3,7,11,15-tetramethylhexadeca-6,10,14-trienyl] hydrogen phosphate (CCD ID: ELU) (formula: C<sub>20</sub>H<sub>38</sub>O<sub>7</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
75	I	1	Total	C	H	O	P	0
			64	20	35	7	2	

- Molecule 76 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
76	L5	213	Total	Mg	0
			213	213	
76	L7	3	Total	Mg	0
			3	3	
76	L8	3	Total	Mg	0
			3	3	
76	LA	1	Total	Mg	0
			1	1	

Continued on next page...

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Mol	Chain	Residues	Atoms		AltConf
76	LI	1	Total 1	Mg 1	0
76	LP	1	Total 1	Mg 1	0
76	LV	1	Total 1	Mg 1	0
76	Le	1	Total 1	Mg 1	0
76	Lg	1	Total 1	Mg 1	0
76	Lj	1	Total 1	Mg 1	0

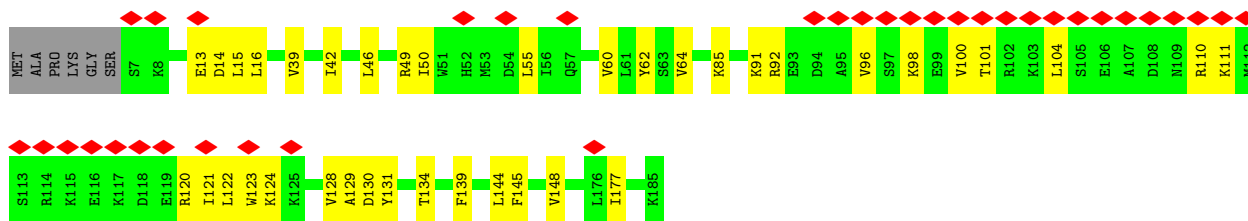
- Molecule 77 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
77	Lg	1	Total 1	Zn 1	0
77	Lj	1	Total 1	Zn 1	0
77	Lm	1	Total 1	Zn 1	0
77	Lo	1	Total 1	Zn 1	0
77	Lp	1	Total 1	Zn 1	0

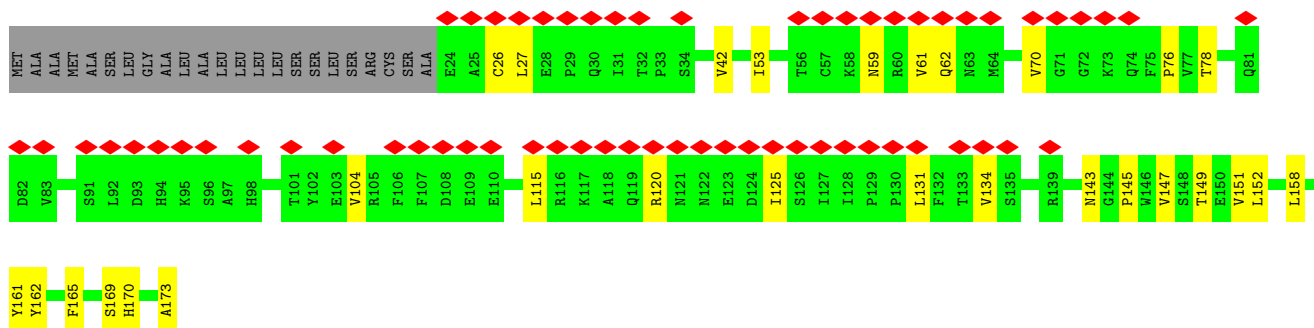
- Molecule 78 is water.

Mol	Chain	Residues	Atoms		AltConf
78	u3	1	Total 1	O 1	0

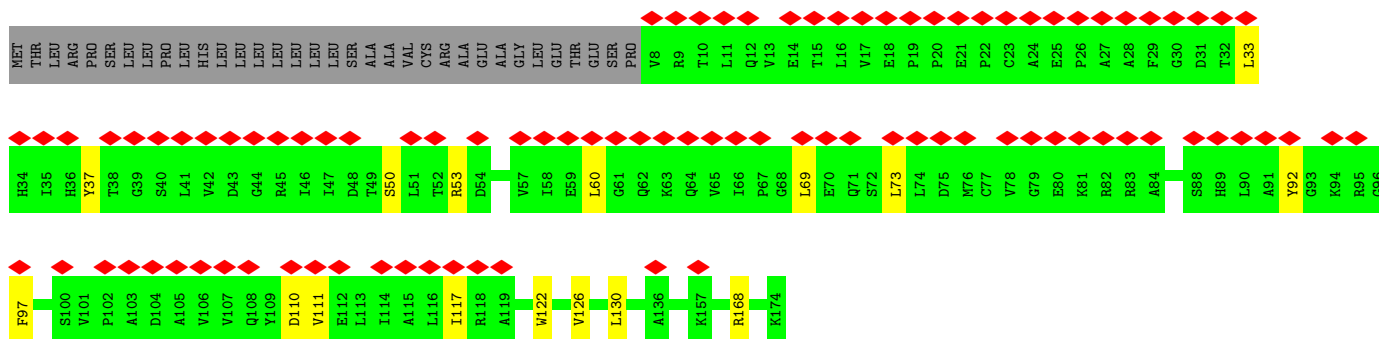




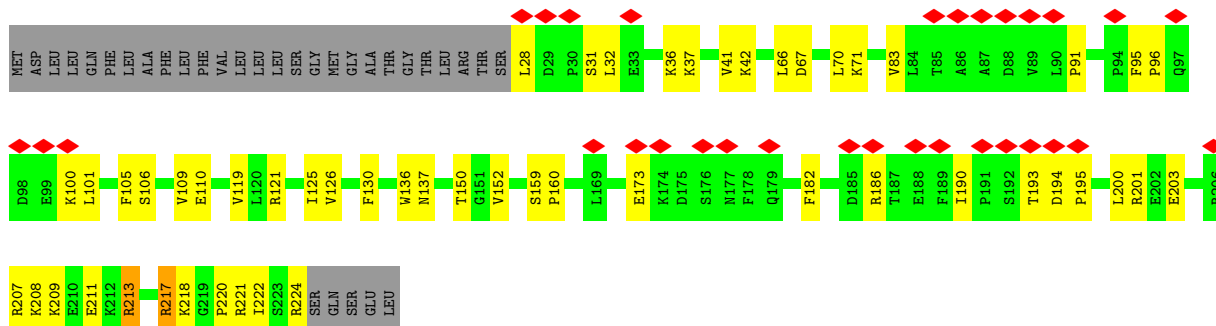
• Molecule 4: Translocon-associated protein subunit delta



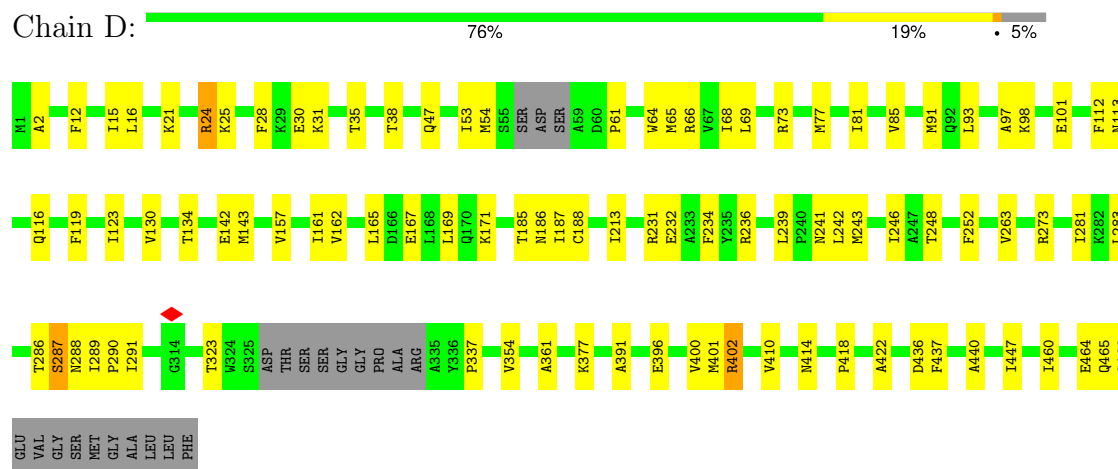
• Molecule 5: Peptidyl-prolyl cis-trans isomerase FKBP11



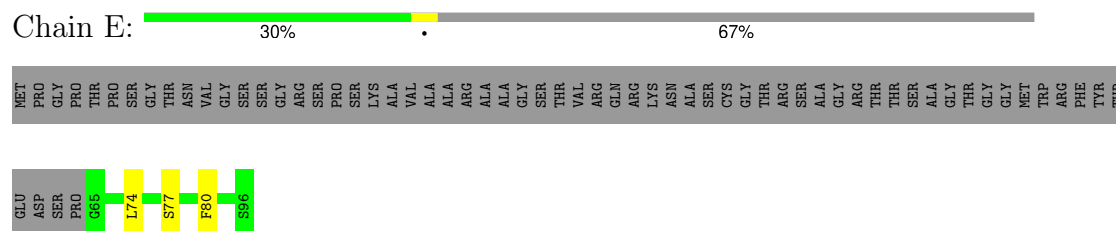
• Molecule 6: Coiled-coil domain-containing protein 134



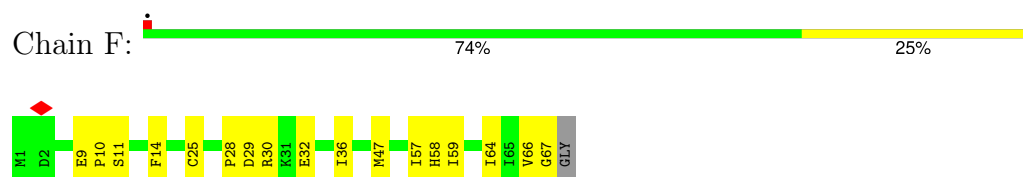
- Molecule 7: Protein transport protein Sec61 subunit alpha isoform 1



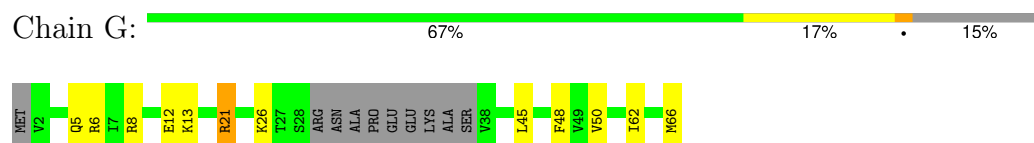
- Molecule 8: Protein transport protein Sec61 subunit beta



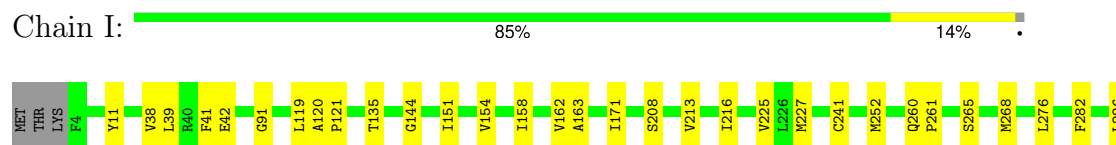
- Molecule 9: Protein transport protein Sec61 subunit gamma

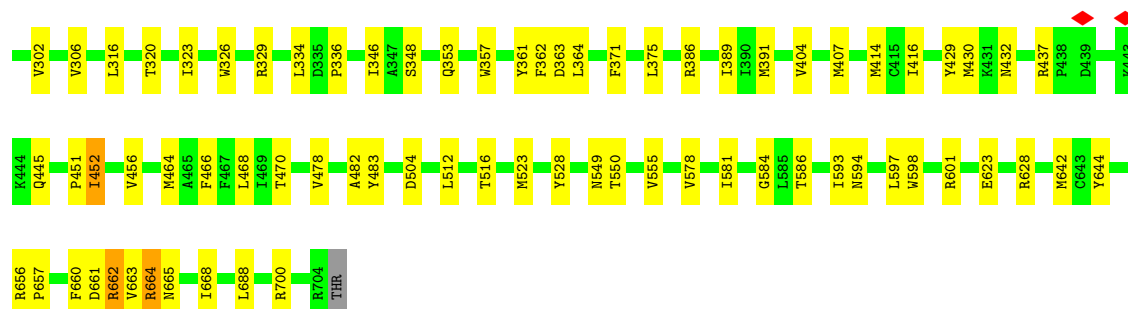


- Molecule 10: Stress-associated endoplasmic reticulum protein 1

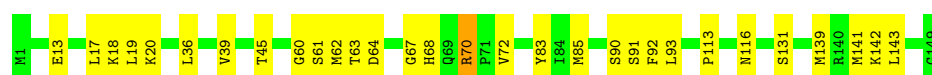
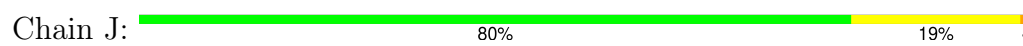


- Molecule 11: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit STT3A





- Molecule 12: Oligosaccharyltransferase complex subunit OSTC



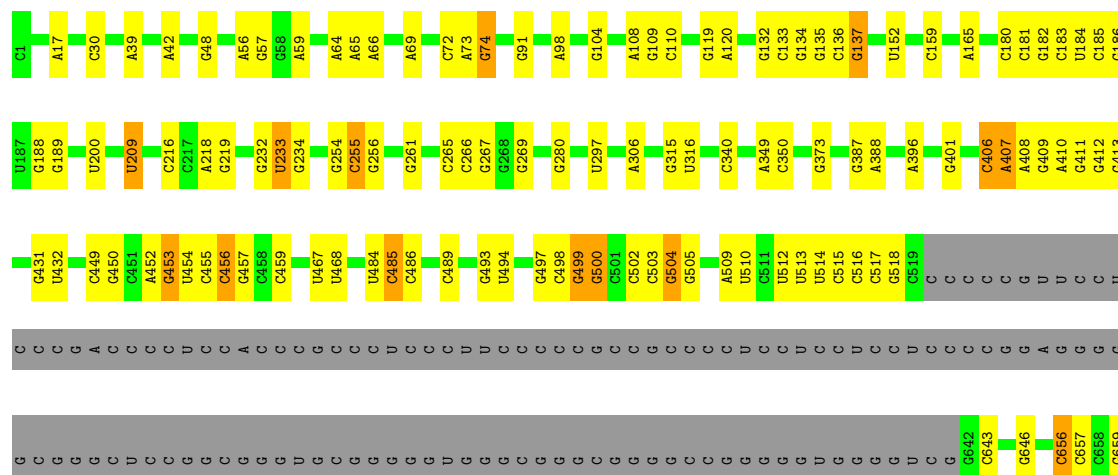
- Molecule 13: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 4



- Molecule 14: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit TMEM258



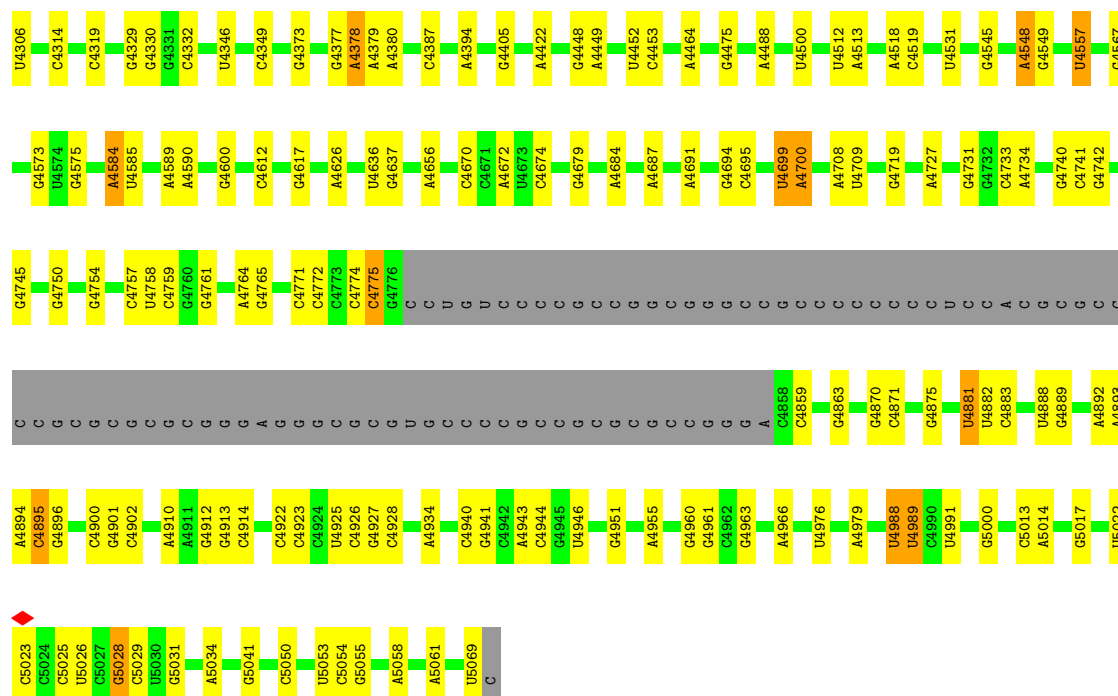
- Molecule 15: 28S ribosomal RNA





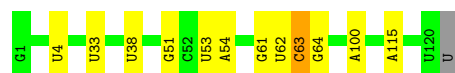






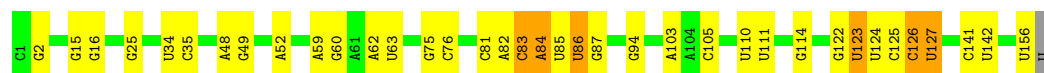
• Molecule 16: 5S ribosomal RNA

Chain L7: 89% 9% ..



• Molecule 17: 5.8S ribosomal RNA

Chain L8: 76% 20% . .



• Molecule 18: 60S ribosomal protein L8

Chain LA: 86% 11% .



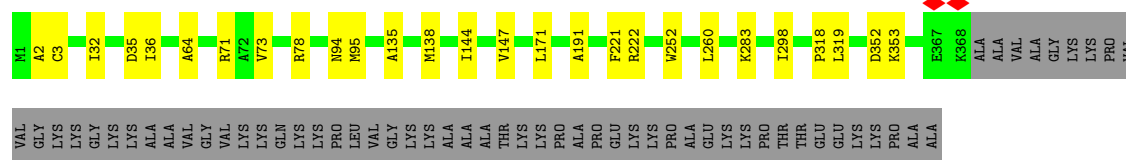
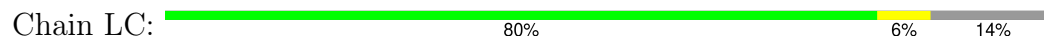
• Molecule 19: 60S ribosomal protein L3

Chain LB: 90% 10% .





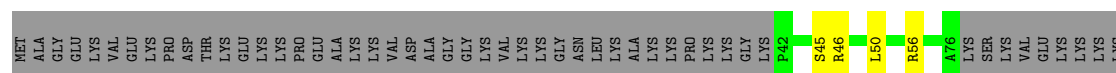
- Molecule 20: Large ribosomal subunit protein uL4



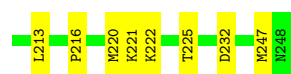
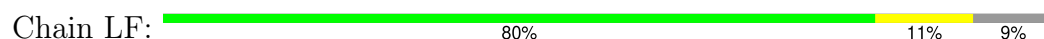
- Molecule 21: Large ribosomal subunit protein uL18



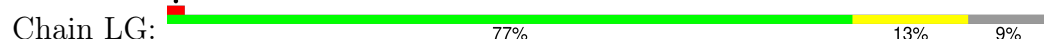
- Molecule 22: Large ribosomal subunit protein eL6



- Molecule 23: 60S ribosomal protein L7



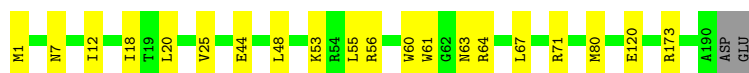
- Molecule 24: Large ribosomal subunit protein eL8





- Molecule 25: Large ribosomal subunit protein uL6

Chain LH: 89% 10%



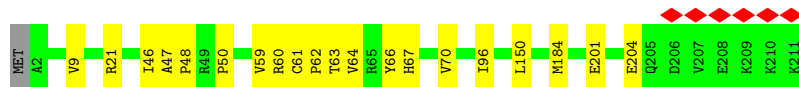
- Molecule 26: Ribosomal protein uL16-like

Chain LI: 80% 14% 6%



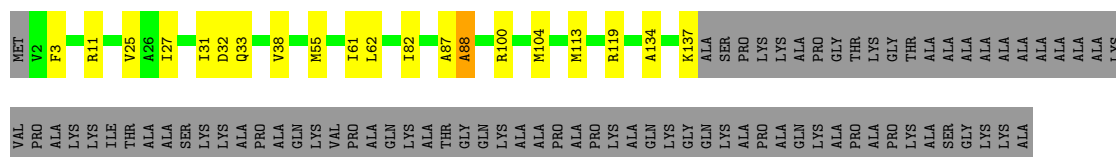
- Molecule 27: Large ribosomal subunit protein eL13

Chain LL: 90% 9%



- Molecule 28: Large ribosomal subunit protein eL14

Chain LM: 54% 9% 37%



- Molecule 29: Large ribosomal subunit protein eL15

Chain LN: 90% 8%

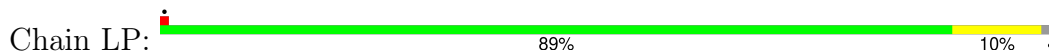


- Molecule 30: Large ribosomal subunit protein uL13

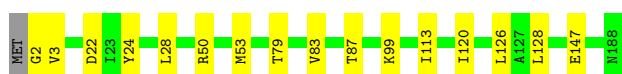
Chain LO: 86% 13%



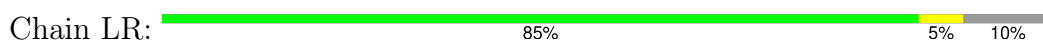
- Molecule 31: Large ribosomal subunit protein uL22



- Molecule 32: Large ribosomal subunit protein eL18



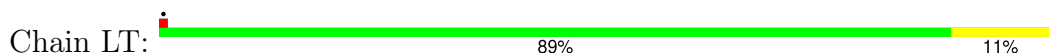
- Molecule 33: Large ribosomal subunit protein eL19



- Molecule 34: Large ribosomal subunit protein eL20



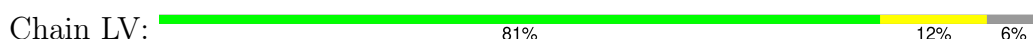
- Molecule 35: Large ribosomal subunit protein eL21



- Molecule 36: Large ribosomal subunit protein eL22

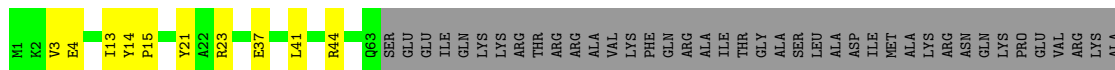


- Molecule 37: Large ribosomal subunit protein uL14

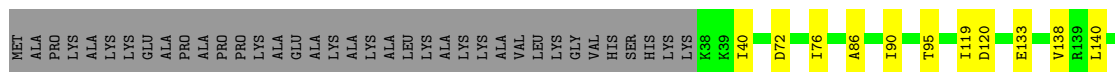




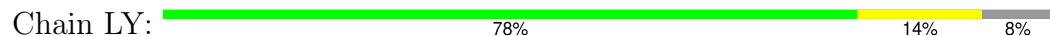
- Molecule 38: Large ribosomal subunit protein eL24



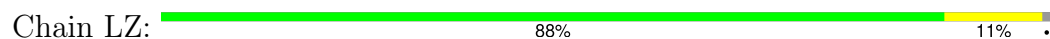
- Molecule 39: Large ribosomal subunit protein uL23



- Molecule 40: Large ribosomal subunit protein uL24



- Molecule 41: Large ribosomal subunit protein eL27

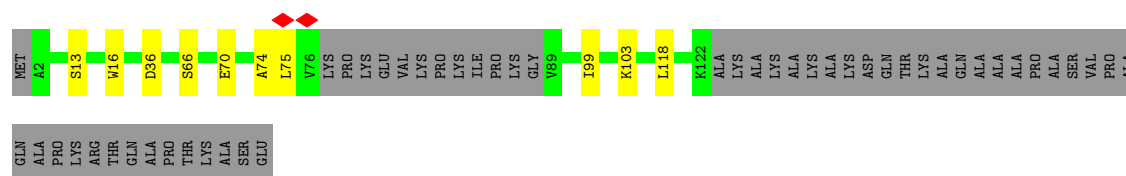


- Molecule 42: 60S ribosomal protein L27a



- Molecule 43: 60S ribosomal protein L29





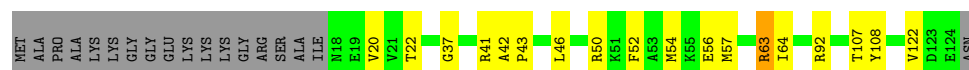
- Molecule 44: Large ribosomal subunit protein eL30

Chain Lc: 75% 10% 15%



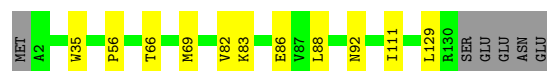
- Molecule 45: Large ribosomal subunit protein eL31

Chain Ld: 71% 14% 14%



- Molecule 46: Large ribosomal subunit protein eL32

Chain Le: 87% 8% 5%



- Molecule 47: Large ribosomal subunit protein eL33

Chain Lf: 80% 18% 2%



- Molecule 48: Large ribosomal subunit protein eL34

Chain Lg: 89% 9% 2%



- Molecule 49: Large ribosomal subunit protein uL29

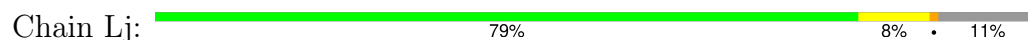
Chain Lh: 88% 11% 1%



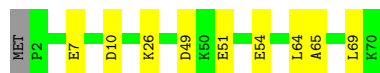
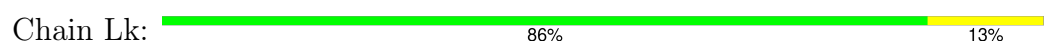
- Molecule 50: Large ribosomal subunit protein eL36



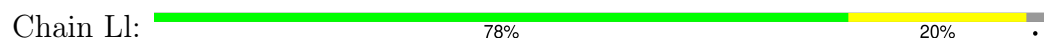
- Molecule 51: Large ribosomal subunit protein eL37



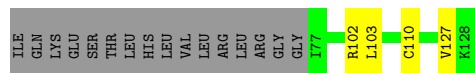
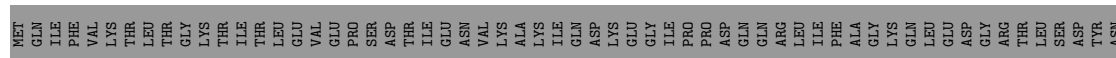
- Molecule 52: Large ribosomal subunit protein eL38



- Molecule 53: Large ribosomal subunit protein eL39



- Molecule 54: Ubiquitin-60S ribosomal protein L40



- Molecule 55: Small ribosomal subunit protein eS32

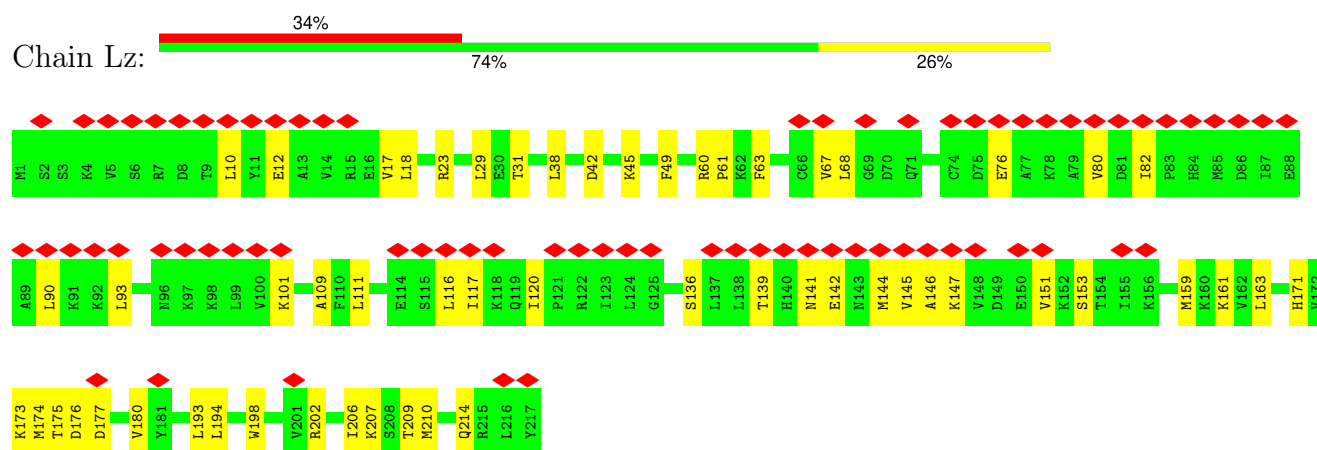


- Molecule 56: Large ribosomal subunit protein eL42

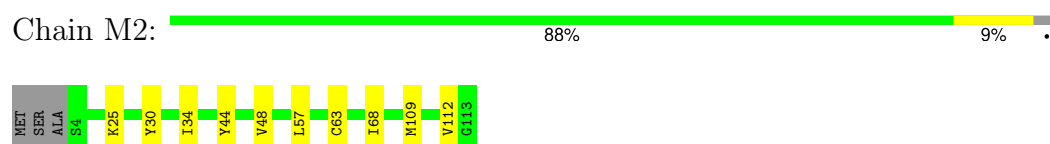




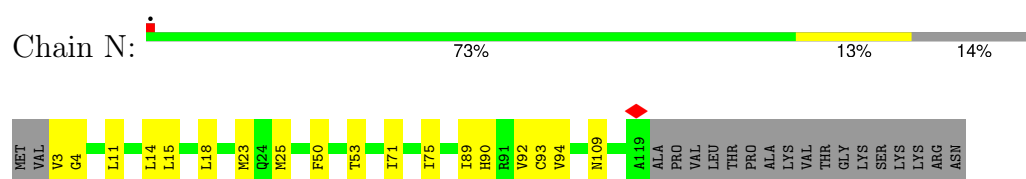




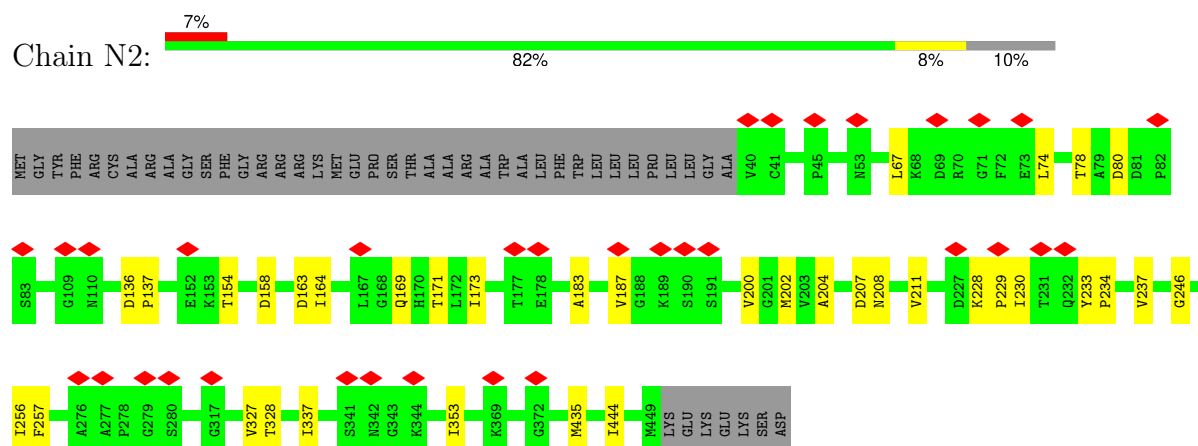
- Molecule 62: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit DAD1



- Molecule 63: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit KCP2

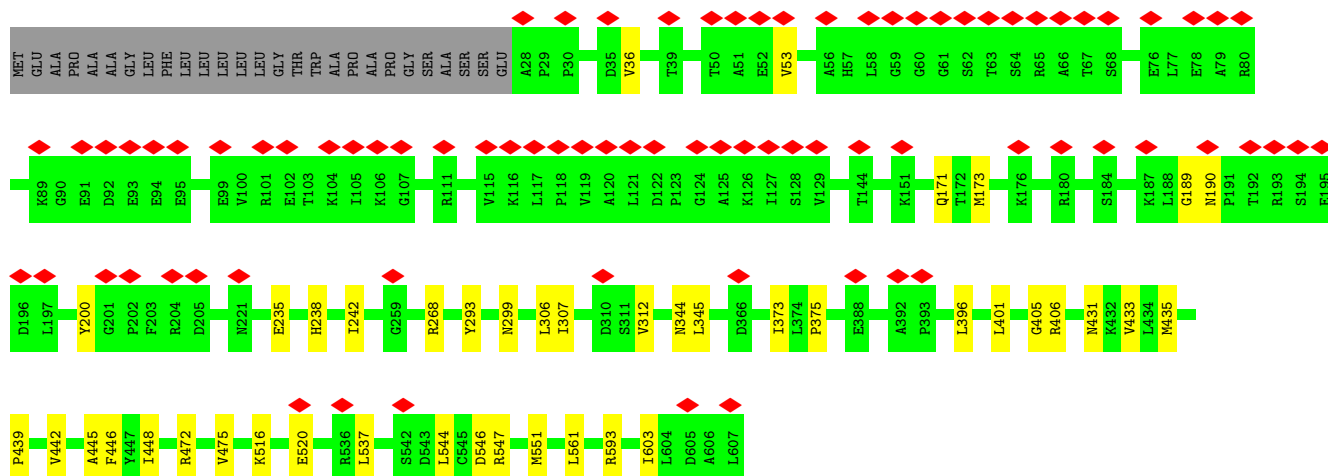


- Molecule 64: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase 48 kDa subunit

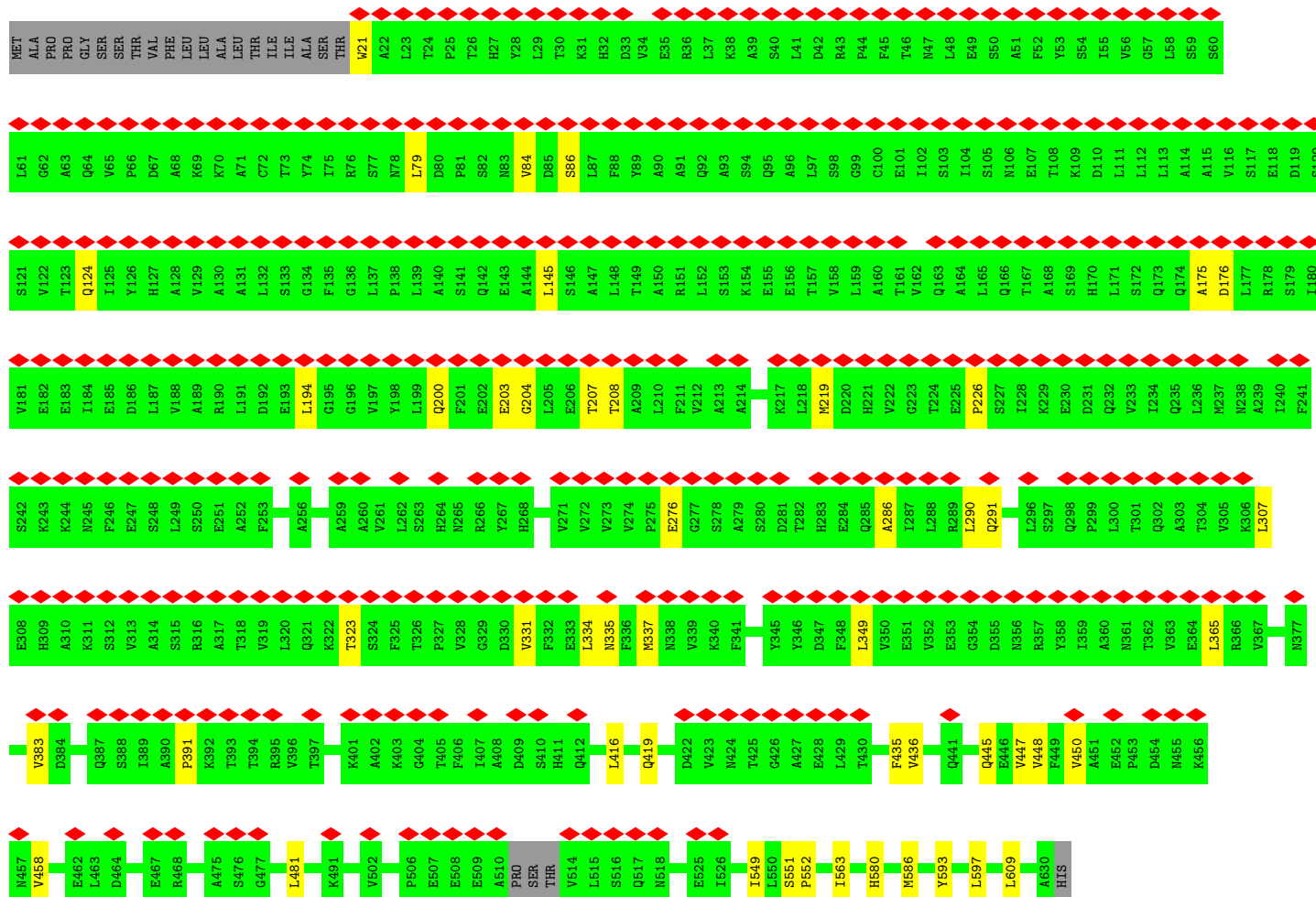


- Molecule 65: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 1





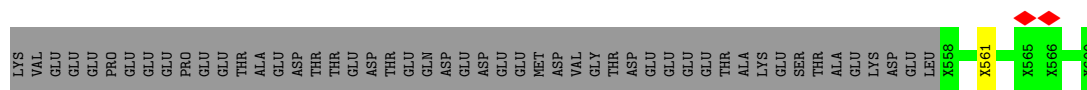
• Molecule 66: Dolichyl-diphosphooligosaccharide--protein glycosyltransferase subunit 2



• Molecule 67: tRNA

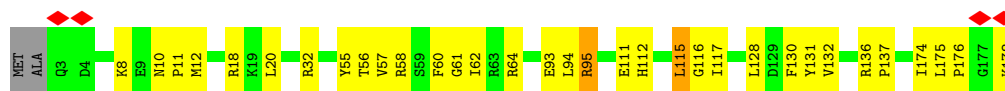






- Molecule 70: Large ribosomal subunit protein uL5

Chain LJ: 80% 17%



- Molecule 71: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 12% 25% 62% 12%



- Molecule 72: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 50% 50% 50%



- Molecule 73: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 25% 50% 75%



- Molecule 74: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose

Chain L: 100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55750	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	53000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.114	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.019	Depositor
Map size ( $\text{\AA}$ )	673.1687, 673.1687, 673.1687	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.4024348, 1.4024348, 1.4024348	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NDG, MAN, BMA, ELU, MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	5	0.13	0/1150	0.36	0/1569
2	6	0.15	0/1291	0.51	1/1757 (0.1%)
3	7	0.14	0/1481	0.37	0/2000
4	8	0.13	0/1214	0.39	0/1654
5	A	0.13	0/1331	0.41	0/1801
6	B	0.16	0/1670	0.42	0/2248
7	D	0.14	0/3604	0.37	0/4884
8	E	0.11	0/257	0.31	0/348
9	F	0.13	0/548	0.34	0/733
10	G	0.16	0/442	0.42	0/590
11	I	0.12	0/5806	0.34	1/7884 (0.0%)
12	J	0.13	0/1216	0.41	0/1649
13	K2	0.12	0/300	0.35	0/406
14	L2	0.10	0/663	0.28	0/903
15	L5	0.15	0/89009	0.29	0/138839
16	L7	0.15	0/2861	0.28	0/4459
17	L8	0.15	0/3701	0.27	0/5766
18	LA	0.14	0/1936	0.40	0/2596
19	LB	0.14	0/3297	0.41	0/4412
20	LC	0.15	0/2981	0.40	0/4002
21	LD	0.13	0/2428	0.37	0/3252
22	LE	0.14	0/1942	0.39	0/2606
23	LF	0.15	0/1905	0.36	0/2539
24	LG	0.14	0/1960	0.39	0/2637
25	LH	0.13	0/1537	0.36	0/2066
26	LI	0.16	0/1673	0.42	0/2233
27	LL	0.14	0/1732	0.37	0/2315
28	LM	0.15	0/1142	0.37	0/1527
29	LN	0.15	0/1746	0.39	0/2338
30	LO	0.14	0/1682	0.36	0/2250
31	LP	0.13	0/1498	0.42	0/2004
32	LQ	0.14	0/1537	0.34	0/2052

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	LR	0.13	0/1501	0.32	0/1984
34	LS	0.14	0/1493	0.35	0/2003
35	LT	0.14	0/1326	0.33	0/1770
36	LU	0.13	0/839	0.41	0/1126
37	LV	0.14	0/993	0.36	0/1332
38	LW	0.13	0/541	0.35	0/720
39	LX	0.14	0/993	0.36	0/1334
40	LY	0.16	0/1132	0.35	0/1504
41	LZ	0.12	0/1130	0.33	0/1507
42	La	0.13	0/1191	0.34	0/1591
43	Lb	0.13	0/889	0.39	0/1175
44	Lc	0.13	0/774	0.32	0/1038
45	Ld	0.15	0/903	0.38	0/1216
46	Le	0.13	0/1082	0.37	0/1443
47	Lf	0.22	0/895	0.50	1/1198 (0.1%)
48	Lg	0.12	0/916	0.34	0/1220
49	Lh	0.13	0/1023	0.35	0/1351
50	Li	0.13	0/843	0.36	0/1115
51	Lj	0.15	0/720	0.43	0/952
52	Lk	0.14	0/575	0.36	0/761
53	Ll	0.17	0/454	0.40	0/599
54	Lm	0.13	0/435	0.36	0/575
55	Ln	0.10	0/231	0.27	0/294
56	Lo	0.14	0/876	0.36	0/1156
57	Lp	0.14	0/718	0.37	0/953
58	Lr	0.17	0/1017	0.38	0/1364
59	Ls	0.12	0/1519	0.34	0/2052
60	Lt	0.15	0/1058	0.51	0/1430
61	Lz	0.16	0/1769	0.49	0/2371
62	M2	0.10	0/883	0.27	0/1197
63	N	0.12	0/908	0.31	0/1229
64	N2	0.09	0/3306	0.29	0/4493
65	O2	0.11	0/4752	0.31	0/6444
66	P2	0.09	0/4814	0.29	0/6553
67	u3	0.10	0/1777	0.28	0/2767
68	v3	0.12	0/1806	0.32	0/2813
69	y3	0.15	0/1864	0.45	0/2511
70	LJ	0.83	0/1433	0.86	0/1915
All	All	0.16	0/194919	0.34	3/283375 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	6	0	2
3	7	0	2
4	8	0	1
5	A	0	2
6	B	0	6
7	D	0	5
10	G	0	3
11	I	0	4
12	J	0	1
29	LN	0	1
30	LO	0	1
31	LP	0	1
33	LR	0	1
40	LY	0	1
45	Ld	0	3
69	y3	0	6
70	LJ	0	3
All	All	0	43

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
47	Lf	107	PRO	CA-N-CD	-5.62	104.12	112.00
2	6	32	ARG	CB-CA-C	-5.49	101.51	110.85
11	I	452	ILE	N-CA-C	5.02	119.78	109.34

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	6	137	ARG	Sidechain
2	6	142	ARG	Sidechain
3	7	110	ARG	Sidechain
3	7	92	ARG	Sidechain
4	8	120	ARG	Sidechain
5	A	117	ILE	Peptide
5	A	168	ARG	Sidechain
6	B	186	ARG	Sidechain
6	B	201	ARG	Sidechain

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Mol	Chain	Res	Type	Group
6	B	207	ARG	Sidechain
6	B	213	ARG	Sidechain
6	B	221	ARG	Sidechain
6	B	224	ARG	Sidechain
7	D	231	ARG	Sidechain
7	D	24	ARG	Sidechain
7	D	402	ARG	Sidechain
7	D	66	ARG	Sidechain
7	D	73	ARG	Sidechain
10	G	21	ARG	Sidechain
10	G	6	ARG	Sidechain
10	G	8	ARG	Sidechain
11	I	628	ARG	Sidechain
11	I	662	ARG	Sidechain
11	I	664	ARG	Sidechain
11	I	700	ARG	Sidechain
12	J	70	ARG	Sidechain
70	LJ	115	LEU	Peptide
70	LJ	18	ARG	Sidechain
70	LJ	32	ARG	Sidechain
29	LN	24	ARG	Sidechain
30	LO	94	ARG	Sidechain
31	LP	18	ARG	Sidechain
33	LR	16	ARG	Sidechain
40	LY	11	ARG	Sidechain
45	Ld	50	ARG	Sidechain
45	Ld	63	ARG	Sidechain
45	Ld	92	ARG	Sidechain
69	y3	39	ARG	Sidechain
69	y3	43	ARG	Sidechain
69	y3	51	ARG	Sidechain
69	y3	67	ARG	Sidechain
69	y3	70	ARG	Sidechain
69	y3	84	ARG	Sidechain

## 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	5	1121	1071	1071	9	0
2	6	1259	1241	1241	32	0
3	7	1451	1487	1487	29	0
4	8	1185	1148	1148	29	0
5	A	1305	1390	1390	9	0
6	B	1633	1646	1646	38	0
7	D	3528	3661	3661	71	0
8	E	250	273	272	3	0
9	F	538	574	574	15	0
10	G	437	467	467	8	0
11	I	5649	5612	5612	77	0
12	J	1182	1227	1227	29	0
13	K2	295	312	312	7	0
14	L2	643	659	659	6	0
15	L5	79575	40176	40187	196	0
16	L7	2561	1294	1295	7	0
17	L8	3314	1682	1683	13	0
18	LA	1898	1993	1993	20	0
19	LB	3229	3369	3368	23	0
20	LC	2927	3104	3104	25	0
21	LD	2382	2410	2410	21	0
22	LE	1904	2055	2055	22	0
23	LF	1870	1996	1996	22	0
24	LG	1927	2074	2074	28	0
25	LH	1518	1601	1601	17	0
26	LI	1634	1671	1671	22	0
27	LL	1701	1818	1818	18	0
28	LM	1120	1187	1187	15	0
29	LN	1701	1749	1749	16	0
30	LO	1650	1794	1794	20	0
31	LP	1470	1536	1536	10	0
32	LQ	1513	1628	1628	19	0
33	LR	1485	1633	1633	10	0
34	LS	1453	1490	1490	7	0
35	LT	1298	1366	1366	12	0
36	LU	825	850	850	10	0
37	LV	979	1039	1039	13	0
38	LW	528	541	541	8	0
39	LX	976	1053	1053	11	0
40	LY	1115	1205	1205	16	0
41	LZ	1107	1182	1182	9	0
42	La	1162	1214	1213	7	0
43	Lb	876	948	948	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Lc	764	804	804	6	0
45	Ld	888	930	930	15	0
46	Le	1064	1160	1160	6	0
47	Lf	876	912	912	15	0
48	Lg	906	998	998	7	0
49	Lh	1015	1148	1148	10	0
50	Li	832	917	917	9	0
51	Lj	705	736	736	6	0
52	Lk	569	637	637	6	0
53	Ll	444	483	483	9	0
54	Lm	429	465	465	3	0
55	Ln	230	276	276	0	0
56	Lo	862	929	929	5	0
57	Lp	708	756	756	10	0
58	Lr	1002	1068	1068	7	0
59	Ls	1496	1540	1540	33	0
60	Lt	1046	1076	1076	36	0
61	Lz	1741	1854	1854	43	0
62	M2	863	880	880	9	0
63	N	891	925	925	20	0
64	N2	3224	3161	3161	25	0
65	O2	4655	4687	4687	31	0
66	P2	4721	4724	4724	34	0
67	u3	1593	809	809	4	0
68	v3	1618	822	822	12	0
69	y3	2058	2011	1897	42	0
70	LJ	1410	1441	1441	26	0
71	K	94	79	79	1	0
72	C	28	25	25	0	0
73	H	94	79	79	0	0
74	L	28	25	24	0	0
75	I	29	35	0	0	0
76	L5	213	0	0	0	0
76	L7	3	0	0	0	0
76	L8	3	0	0	0	0
76	LA	1	0	0	0	0
76	LI	1	0	0	0	0
76	LP	1	0	0	0	0
76	LV	1	0	0	0	0
76	Le	1	0	0	0	0
76	Lg	1	0	0	0	0
76	Lj	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
77	Lg	1	0	0	0	0
77	Lj	1	0	0	0	0
77	Lm	1	0	0	0	0
77	Lo	1	0	0	0	0
77	Lp	1	0	0	0	0
78	u3	1	0	0	0	0
All	All	183289	142818	142678	1200	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (1200) 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)
15:L5:2373:C:H5'	45:Ld:46:LEU:HD21	1.59	0.85
66:P2:416:LEU:HD11	66:P2:481:LEU:HD21	1.59	0.82
11:I:241:CYS:HB3	62:M2:68:ILE:HD11	1.60	0.81
7:D:85:VAL:HG11	69:y3:561:UNK:CB	2.11	0.80
37:LV:112:MET:HE1	37:LV:117:ILE:HD11	1.64	0.78
3:7:15:LEU:HD22	3:7:123:TRP:CD1	2.20	0.76
11:I:430:MET:HE1	13:K2:27:TYR:HB2	1.65	0.76
66:P2:84:VAL:HG11	66:P2:124:GLN:OE1	1.86	0.75
61:Lz:17:VAL:HG13	61:Lz:18:LEU:H	1.52	0.74
4:8:158:LEU:HD13	63:N:18:LEU:HD22	1.68	0.74
28:LM:25:VAL:HG22	28:LM:38:VAL:HG22	1.70	0.73
3:7:16:LEU:HD11	3:7:122:LEU:HD21	1.71	0.72
3:7:144:LEU:O	3:7:148:VAL:HG23	1.89	0.72
69:y3:145:LEU:HD11	69:y3:251:LEU:HD11	1.71	0.72
62:M2:34:ILE:HD12	64:N2:435:MET:HE1	1.71	0.72
46:Le:88:LEU:HD23	46:Le:88:LEU:O	1.90	0.72
66:P2:286:ALA:HB3	66:P2:337:MET:HE1	1.72	0.71
47:Lf:39:THR:HG21	47:Lf:77:ALA:HB2	1.71	0.71
2:6:146:HIS:CD2	4:8:42:VAL:HG22	2.26	0.70
69:y3:62:ASN:O	69:y3:66:ILE:HD12	1.90	0.70
61:Lz:117:ILE:HD11	61:Lz:136:SER:HA	1.73	0.70
64:N2:327:VAL:O	64:N2:328:THR:HG22	1.92	0.70
6:B:119:VAL:HG22	6:B:126:VAL:HG11	1.74	0.69
26:LI:149:ILE:HD12	26:LI:165:ILE:HG21	1.73	0.69
47:Lf:106:TYR:HB3	47:Lf:107:PRO:HD2	1.74	0.69
61:Lz:80:VAL:HG23	61:Lz:82:ILE:HG13	1.74	0.69
4:8:173:ALA:HB2	63:N:3:VAL:HG13	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:Ls:40:MET:HE1	59:Ls:44:ARG:NH1	2.08	0.68
28:LM:27:ILE:HD11	28:LM:55:MET:HE1	1.73	0.68
15:L5:3756:A:H61	15:L5:3768:U:H3	1.41	0.68
15:L5:4946:U:HO2'	47:Lf:2:SER:N	1.92	0.68
11:I:482:ALA:HB2	69:y3:35:LEU:HD11	1.75	0.67
61:Lz:209:THR:O	61:Lz:210:MET:HE2	1.93	0.67
32:LQ:50:ARG:HB3	32:LQ:83:VAL:HG21	1.77	0.67
1:5:95:PHE:O	1:5:196:VAL:HG13	1.95	0.67
11:I:252:MET:HE1	62:M2:57:LEU:HD21	1.76	0.66
47:Lf:36:ARG:O	47:Lf:39:THR:HG22	1.95	0.66
19:LB:303:ALA:HB1	19:LB:368:ILE:HG21	1.76	0.66
17:L8:49:G:H5'	49:Lh:47:ILE:HD11	1.77	0.66
20:LC:138:MET:HE1	20:LC:144:ILE:O	1.96	0.66
61:Lz:145:VAL:HG23	61:Lz:146:ALA:H	1.59	0.66
7:D:54:MET:HE3	7:D:143:MET:SD	2.35	0.66
23:LF:169:LEU:HB3	23:LF:187:MET:HE1	1.77	0.66
7:D:12:PHE:O	7:D:15:ILE:HG22	1.96	0.66
36:LU:19:LEU:HD23	36:LU:74:SER:O	1.95	0.66
39:LX:119:ILE:HG21	39:LX:140:LEU:HD22	1.78	0.65
12:J:61:SER:HA	12:J:70:ARG:O	1.95	0.65
14:L2:69:LEU:HD11	65:O2:439:PRO:HA	1.79	0.65
25:LH:12:ILE:HD12	25:LH:53:LYS:O	1.97	0.65
2:6:167:LEU:HD21	3:7:131:TYR:OH	1.97	0.64
15:L5:3751:G:H21	15:L5:3775:A:H8	1.44	0.64
66:P2:383:VAL:HG22	66:P2:391:PRO:HB3	1.79	0.64
15:L5:2373:C:C5'	45:Ld:46:LEU:HD21	2.28	0.64
36:LU:18:VAL:HG21	36:LU:76:VAL:O	1.97	0.64
5:A:50:SER:HA	5:A:53:ARG:HE	1.61	0.64
29:LN:135:ILE:HD11	29:LN:142:ILE:HD12	1.79	0.64
42:La:75:LEU:HD13	42:La:117:LEU:HD11	1.79	0.64
3:7:39:VAL:HA	3:7:42:ILE:HD12	1.80	0.64
15:L5:74:G:H5'	27:LL:59:VAL:HG13	1.79	0.64
6:B:66:LEU:HD22	6:B:125:ILE:HG22	1.80	0.63
27:LL:184:MET:N	27:LL:184:MET:HE2	2.13	0.63
51:Lj:84:PRO:O	51:Lj:85:LYS:HB3	1.98	0.63
6:B:91:PRO:O	6:B:150:THR:HG22	1.98	0.63
66:P2:276:GLU:OE1	66:P2:331:VAL:HG11	1.98	0.63
18:LA:180:LEU:HD11	57:Lp:18:TYR:HB3	1.81	0.63
50:Li:2:ALA:N	50:Li:5:TYR:HH	1.97	0.63
52:Lk:26:LYS:HB2	52:Lk:69:LEU:HD12	1.81	0.62
4:8:53:ILE:HD11	4:8:134:VAL:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L5:4037:C:H2'	15:L5:4039:G:H22	1.64	0.62
11:I:512:LEU:HD23	11:I:516:THR:HG21	1.81	0.62
12:J:63:THR:HG22	12:J:64:ASP:H	1.63	0.62
47:Lf:106:TYR:CB	47:Lf:107:PRO:HD2	2.30	0.62
68:v3:17:A:H1'	68:v3:18:G:O5'	1.99	0.62
7:D:24:ARG:HG3	7:D:25:LYS:N	2.14	0.62
59:Ls:93:GLU:OE2	59:Ls:98:ILE:HD11	2.00	0.62
11:I:265:SER:HG	11:I:326:TRP:CD1	2.18	0.62
70:LJ:56:THR:HG23	70:LJ:62:ILE:O	1.99	0.62
41:LZ:92:ASP:O	41:LZ:96:VAL:HG22	2.00	0.61
4:8:151:VAL:HG21	63:N:25:MET:HE2	1.82	0.61
59:Ls:160:LEU:HG	59:Ls:161:ILE:HG23	1.81	0.61
37:LV:92:ASP:OD1	37:LV:94:VAL:HG12	2.00	0.61
33:LR:3:MET:HE2	33:LR:5:ARG:HG3	1.81	0.61
65:O2:401:LEU:O	65:O2:401:LEU:HD23	2.00	0.61
61:Lz:68:LEU:HB3	61:Lz:116:LEU:HD11	1.82	0.61
50:Li:102:ALA:O	50:Li:103:LYS:HE2	1.99	0.61
11:I:656:ARG:HG2	11:I:660:PHE:CG	2.36	0.60
18:LA:101:VAL:HG22	18:LA:165:VAL:HG22	1.81	0.60
44:Lc:38:ILE:HD11	44:Lc:64:ALA:HA	1.83	0.60
15:L5:180:C:H42	15:L5:255:C:H42	1.50	0.60
17:L8:75:G:O2'	53:Ll:29:MET:HE1	2.02	0.60
30:LO:186:GLU:HA	30:LO:189:ILE:HG22	1.82	0.60
2:6:89:VAL:HG13	4:8:76:PRO:HG2	1.82	0.60
3:7:96:VAL:O	3:7:100:VAL:HG23	2.02	0.60
12:J:70:ARG:NH1	12:J:72:VAL:HG12	2.16	0.60
41:LZ:100:VAL:HG23	41:LZ:106:LEU:HB3	1.83	0.60
29:LN:123:GLU:O	29:LN:124:ASP:HB2	2.00	0.60
34:LS:27:LEU:H	34:LS:27:LEU:HD23	1.67	0.60
47:Lf:30:ILE:HD11	47:Lf:84:VAL:HG22	1.83	0.60
11:I:357:TRP:CG	12:J:90:SER:HG	2.20	0.59
4:8:165:PHE:CD2	63:N:11:LEU:HD23	2.37	0.59
20:LC:138:MET:HB3	58:Lr:43:LEU:HD11	1.84	0.59
60:Lt:123:ARG:CB	60:Lt:129:ILE:HD11	2.32	0.59
7:D:77:MET:HE1	7:D:162:VAL:CG2	2.33	0.59
44:Lc:11:LEU:HD13	44:Lc:75:SER:OG	2.03	0.59
25:LH:48:LEU:HD11	25:LH:56:ARG:HE	1.67	0.59
30:LO:37:ARG:HD2	30:LO:108:ILE:HD11	1.85	0.59
36:LU:72:VAL:HG12	36:LU:72:VAL:O	2.03	0.58
53:Ll:24:PRO:O	53:Ll:27:ILE:HG22	2.03	0.58
2:6:146:HIS:HD2	4:8:42:VAL:HG22	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:158:ILE:O	11:I:162:VAL:HG23	2.02	0.58
12:J:60:GLY:C	12:J:72:VAL:HG22	2.28	0.58
15:L5:2464:C:HO2'	15:L5:2465:C:H6	1.52	0.58
24:LG:173:LEU:HD23	50:Li:43:MET:HE3	1.86	0.58
15:L5:3946:G:H21	15:L5:3947:A:H62	1.50	0.58
24:LG:129:PRO:O	24:LG:130:THR:HG22	2.03	0.58
4:8:70:VAL:CG1	4:8:104:VAL:HG22	2.34	0.58
26:LI:36:LEU:HD22	26:LI:69:ARG:HD3	1.84	0.58
28:LM:11:ARG:CZ	28:LM:61:ILE:HD11	2.33	0.58
36:LU:24:ASP:OD1	36:LU:26:THR:HG23	2.03	0.58
2:6:145:PRO:HA	2:6:148:LEU:HB3	1.86	0.58
18:LA:5:ILE:HG22	18:LA:208:GLU:O	2.03	0.58
15:L5:5000:G:O3'	19:LB:382:MET:HE1	2.04	0.57
41:LZ:96:VAL:HG23	41:LZ:96:VAL:O	2.02	0.57
61:Lz:29:LEU:HD23	61:Lz:173:LYS:NZ	2.19	0.57
20:LC:298:ILE:HD11	32:LQ:128:LEU:HD23	1.87	0.57
15:L5:3970:G:H4'	15:L5:4052:C:H41	1.68	0.57
30:LO:31:ARG:O	30:LO:33:VAL:HG13	2.04	0.57
65:O2:396:LEU:HD11	65:O2:405:GLY:HA3	1.87	0.57
4:8:169:SER:CB	63:N:11:LEU:HD11	2.35	0.57
7:D:119:PHE:CE2	7:D:123:ILE:HD11	2.39	0.57
15:L5:4346:U:O4'	56:Lo:82:MET:HE1	2.04	0.57
17:L8:49:G:C5'	49:Lh:47:ILE:HD11	2.35	0.57
66:P2:194:LEU:HD11	66:P2:200:GLN:HE22	1.70	0.57
9:F:57:ILE:HD11	12:J:92:PHE:CD2	2.38	0.57
26:LI:76:MET:HE1	26:LI:148:VAL:HA	1.86	0.57
13:K2:17:SER:O	13:K2:21:LEU:HD23	2.05	0.57
15:L5:3971:G:O6	15:L5:4050:A:H2'	2.03	0.57
65:O2:36:VAL:HG22	65:O2:53:VAL:HG12	1.87	0.57
69:y3:133:THR:HG22	69:y3:278:PRO:HG2	1.85	0.57
5:A:73:LEU:HD21	5:A:111:VAL:HG11	1.86	0.57
38:LW:3:VAL:HG23	38:LW:13:ILE:O	2.04	0.57
50:Li:98:ARG:O	50:Li:102:ALA:HB2	2.04	0.57
9:F:59:ILE:HD13	12:J:85:MET:HE3	1.87	0.56
64:N2:233:TYR:OH	64:N2:237:VAL:HG11	2.05	0.56
7:D:134:THR:HG21	10:G:62:ILE:HG12	1.87	0.56
18:LA:2:GLY:HA2	18:LA:207:VAL:HG13	1.88	0.56
27:LL:21:ARG:HB3	29:LN:197:THR:HG22	1.87	0.56
61:Lz:29:LEU:HD22	61:Lz:60:ARG:HD3	1.86	0.56
28:LM:62:LEU:HD21	28:LM:82:ILE:HD11	1.88	0.56
30:LO:16:LEU:HA	30:LO:41:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Lf:78:HIS:HB3	47:Lf:83:MET:O	2.06	0.56
64:N2:230:ILE:HG23	64:N2:230:ILE:O	2.05	0.56
30:LO:185:VAL:O	30:LO:185:VAL:HG13	2.05	0.56
32:LQ:24:TYR:O	32:LQ:28:LEU:HD12	2.06	0.56
54:Lm:103:LEU:HD21	54:Lm:110:CYS:HA	1.87	0.56
5:A:53:ARG:NH1	6:B:137:ASN:HB2	2.20	0.56
26:LI:131:ILE:HD12	26:LI:131:ILE:H	1.71	0.56
39:LX:119:ILE:HG22	39:LX:120:ASP:N	2.20	0.56
65:O2:537:LEU:HD13	65:O2:544:LEU:CD1	2.36	0.56
3:7:85:LYS:HG3	3:7:129:ALA:HB1	1.86	0.55
5:A:126:VAL:O	5:A:130:LEU:HB2	2.06	0.55
15:L5:1633:G:H5'	15:L5:1634:A:OP1	2.06	0.55
15:L5:4257:A:C4	70:LJ:60:PHE:CZ	2.94	0.55
69:y3:103:GLU:HB3	69:y3:198:GLY:HA2	1.88	0.55
70:LJ:10:ASN:N	70:LJ:11:PRO:HD2	2.22	0.55
69:y3:92:SER:O	69:y3:94:TYR:N	2.39	0.55
7:D:77:MET:HE1	7:D:162:VAL:HG21	1.89	0.55
11:I:663:VAL:HG13	11:I:664:ARG:HD2	1.88	0.55
15:L5:1179:U:H3'	15:L5:1180:C:H5''	1.88	0.55
3:7:100:VAL:HG22	3:7:124:LYS:CG	2.37	0.55
15:L5:2675:G:H1'	15:L5:2676:A:OP2	2.06	0.55
65:O2:293:TYR:O	65:O2:299:ASN:ND2	2.39	0.55
34:LS:127:MET:HE1	35:LT:155:PRO:HG3	1.88	0.55
60:Lt:9:GLU:O	60:Lt:10:ILE:HG13	2.07	0.55
3:7:96:VAL:HG21	3:7:128:VAL:HG21	1.88	0.55
29:LN:193:ARG:O	29:LN:197:THR:HG23	2.07	0.55
3:7:111:LYS:HZ3	15:L5:2488:C:H4'	1.72	0.55
7:D:130:VAL:O	7:D:134:THR:HG23	2.07	0.55
12:J:63:THR:HG22	12:J:64:ASP:N	2.21	0.55
19:LB:223:THR:HG22	19:LB:275:HIS:H	1.71	0.55
21:LD:44:TYR:O	35:LT:33:ILE:HG12	2.07	0.55
39:LX:86:ALA:O	39:LX:90:ILE:HD12	2.07	0.55
61:Lz:10:LEU:HD12	61:Lz:12:GLU:N	2.22	0.54
12:J:60:GLY:CA	12:J:72:VAL:HG22	2.37	0.54
22:LE:95:PRO:HA	22:LE:104:THR:HG22	1.89	0.54
27:LL:63:THR:HG23	27:LL:66:TYR:H	1.72	0.54
18:LA:171:GLY:O	57:Lp:68:ALA:HB2	2.08	0.54
21:LD:38:ILE:HD12	35:LT:30:TYR:HB3	1.88	0.54
53:Ll:34:LYS:HD2	53:Ll:34:LYS:O	2.07	0.54
59:Ls:141:LEU:HD22	59:Ls:143:ILE:HG13	1.89	0.54
60:Lt:34:PRO:O	60:Lt:37:LEU:HD22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:Lt:121:LEU:HD23	60:Lt:129:ILE:CD1	2.38	0.54
6:B:36:LYS:HE3	6:B:152:VAL:HG22	1.89	0.54
11:I:353:GLN:O	11:I:404:VAL:HG23	2.06	0.54
62:M2:34:ILE:HG23	64:N2:435:MET:HE1	1.89	0.54
70:LJ:57:VAL:HG22	70:LJ:62:ILE:CG1	2.37	0.54
11:I:363:ASP:HB2	11:I:407:MET:HE2	1.89	0.54
15:L5:1631:A:N1	18:LA:204:MET:HE2	2.23	0.54
61:Lz:10:LEU:HD11	61:Lz:12:GLU:OE1	2.07	0.54
15:L5:4108:G:H2'	15:L5:4109:G:C8	2.42	0.54
46:Le:66:THR:HA	46:Le:69:MET:HE2	1.90	0.54
15:L5:1631:A:C6	18:LA:204:MET:HE2	2.43	0.54
23:LF:133:LEU:HD23	23:LF:142:TRP:CE2	2.42	0.54
61:Lz:198:TRP:HE1	61:Lz:202:ARG:HB2	1.73	0.54
68:v3:15:G:H22	68:v3:48:C:H42	1.56	0.54
10:G:12:GLU:OE2	10:G:13:LYS:HG3	2.08	0.54
59:Ls:51:ALA:HB1	59:Ls:90:PHE:O	2.08	0.53
24:LG:58:PRO:HD2	24:LG:61:ILE:HD12	1.90	0.53
36:LU:19:LEU:HD22	36:LU:73:THR:OG1	2.08	0.53
60:Lt:85:LEU:HD11	60:Lt:110:VAL:HG12	1.89	0.53
70:LJ:20:LEU:HD12	70:LJ:132:VAL:HG12	1.89	0.53
6:B:83:VAL:HG13	6:B:100:LYS:HD3	1.90	0.53
2:6:149:ASP:OD2	3:7:49:ARG:HB3	2.09	0.53
23:LF:86:GLU:OE2	35:LT:136:ARG:N	2.42	0.53
28:LM:25:VAL:CG2	28:LM:38:VAL:HG22	2.38	0.53
50:Li:63:VAL:O	50:Li:63:VAL:HG22	2.07	0.53
7:D:15:ILE:HG23	7:D:16:LEU:HD22	1.92	0.52
11:I:593:ILE:HB	11:I:664:ARG:HH21	1.73	0.52
22:LE:224:LYS:N	22:LE:225:PRO:HD3	2.23	0.52
27:LL:64:VAL:HA	27:LL:67:HIS:HD2	1.75	0.52
64:N2:230:ILE:HD11	64:N2:234:PRO:HG3	1.91	0.52
68:v3:61:C:H2'	68:v3:61:C:O2	2.09	0.52
15:L5:3748:A:H5''	18:LA:243:THR:HG21	1.92	0.52
60:Lt:160:VAL:HG12	60:Lt:160:VAL:O	2.09	0.52
7:D:236:ARG:N	7:D:241:ASN:OD1	2.43	0.52
68:v3:55:U:H2'	68:v3:56:C:H2'	1.90	0.52
69:y3:66:ILE:HG22	69:y3:70:ARG:CZ	2.39	0.52
11:I:482:ALA:CB	69:y3:35:LEU:HD11	2.40	0.52
12:J:67:GLY:O	12:J:68:HIS:HB2	2.08	0.52
37:LV:99:GLU:CD	38:LW:23:ARG:HA	2.34	0.52
60:Lt:123:ARG:HB2	60:Lt:129:ILE:HD11	1.92	0.52
7:D:65:MET:O	7:D:68:ILE:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:302:VAL:O	11:I:306:VAL:HG22	2.09	0.52
11:I:329:ARG:NH1	11:I:346:ILE:HG23	2.25	0.52
15:L5:2112:G:H4'	15:L5:2250:C:H42	1.75	0.52
15:L5:3946:G:H21	15:L5:3947:A:N6	2.08	0.52
61:Lz:194:LEU:HD23	61:Lz:194:LEU:O	2.10	0.52
12:J:63:THR:HG21	69:y3:72:LYS:NZ	2.25	0.52
15:L5:1912:G:N2	30:LO:87:MET:HE3	2.25	0.52
15:L5:3765:G:H21	15:L5:3766:A:N6	2.08	0.52
15:L5:3946:G:H22	15:L5:4067:U:H3	1.56	0.52
65:O2:431:ASN:OD1	65:O2:433:VAL:HG12	2.09	0.52
69:y3:256:SER:HA	69:y3:259:LEU:HD12	1.91	0.52
15:L5:1660:U:O2'	42:La:12:ARG:HG3	2.10	0.52
20:LC:283:LYS:HD3	32:LQ:24:TYR:CB	2.40	0.52
35:LT:48:VAL:HG11	35:LT:94:GLU:OE2	2.10	0.52
44:Lc:34:THR:HG23	44:Lc:95:ALA:HB2	1.92	0.52
4:8:27:LEU:HD12	4:8:59:ASN:HD21	1.75	0.52
7:D:24:ARG:NE	40:LY:91:ASN:O	2.41	0.52
7:D:93:LEU:O	7:D:93:LEU:HD23	2.10	0.52
23:LF:216:PRO:HD3	23:LF:247:MET:HE2	1.92	0.52
29:LN:17:ASP:OD1	29:LN:18:VAL:N	2.43	0.52
61:Lz:109:ALA:HB1	61:Lz:139:THR:HG23	1.92	0.52
66:P2:435:PHE:CE1	66:P2:450:VAL:HG22	2.45	0.52
7:D:185:THR:HA	9:F:47:MET:SD	2.50	0.52
12:J:20:LYS:O	63:N:71:ILE:HD12	2.10	0.52
24:LG:176:LYS:HD3	50:Li:43:MET:HE1	1.92	0.52
51:Lj:21:ARG:O	51:Lj:22:CYS:SG	2.68	0.52
57:Lp:29:ILE:HD11	57:Lp:69:TRP:CE2	2.44	0.52
12:J:72:VAL:HG23	12:J:83:TYR:CE2	2.45	0.51
57:Lp:29:ILE:HD11	57:Lp:69:TRP:CD1	2.44	0.51
66:P2:436:VAL:CG1	66:P2:481:LEU:HD11	2.41	0.51
3:7:130:ASP:O	3:7:134:THR:OG1	2.25	0.51
11:I:464:MET:O	11:I:468:LEU:HD23	2.10	0.51
20:LC:32:ILE:HD11	58:Lr:5:LEU:HD21	1.92	0.51
20:LC:71:ARG:HG3	20:LC:73:VAL:HG22	1.90	0.51
32:LQ:113:ILE:HG21	32:LQ:120:ILE:HD11	1.92	0.51
62:M2:109:MET:O	62:M2:112:VAL:HG12	2.10	0.51
15:L5:4881:U:C4	28:LM:113:MET:HE2	2.45	0.51
60:Lt:57:ARG:HD2	60:Lt:83:LYS:HG3	1.91	0.51
64:N2:246:GLY:CA	64:N2:256:ILE:HD13	2.39	0.51
68:v3:12:C:H42	68:v3:23:A:N6	2.08	0.51
2:6:33:TYR:HB3	2:6:134:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:188:CYS:HB3	9:F:47:MET:HE1	1.91	0.51
26:LI:14:ASN:O	26:LI:15:LYS:HB3	2.08	0.51
64:N2:207:ASP:OD1	64:N2:208:ASN:N	2.44	0.51
13:K2:32:ASN:OD1	13:K2:34:LYS:HG2	2.11	0.51
16:L7:115:A:H1'	21:LD:74:ILE:HD11	1.93	0.51
5:A:122:TRP:O	5:A:126:VAL:HG23	2.10	0.51
15:L5:137:G:H4'	49:Lh:98:HIS:CD2	2.45	0.51
15:L5:186:G:H1'	15:L5:1366:G:H21	1.76	0.51
17:L8:75:G:OP2	40:LY:74:TYR:OH	2.29	0.51
26:LI:52:MET:HE3	26:LI:136:MET:HG2	1.92	0.51
66:P2:203:GLU:HB2	66:P2:207:THR:HG21	1.93	0.51
70:LJ:10:ASN:OD1	70:LJ:11:PRO:CD	2.59	0.51
20:LC:283:LYS:HD3	32:LQ:24:TYR:CG	2.46	0.51
20:LC:318:PRO:O	20:LC:319:LEU:HB2	2.11	0.51
66:P2:549:ILE:O	66:P2:552:PRO:HD2	2.11	0.51
3:7:100:VAL:HG11	3:7:121:ILE:N	2.26	0.51
6:B:220:PRO:CG	66:P2:447:VAL:HG13	2.41	0.51
7:D:286:THR:HG21	7:D:290:PRO:HG3	1.93	0.51
7:D:436:ASP:OD1	7:D:437:PHE:N	2.44	0.51
15:L5:2045:G:N1	30:LO:62:MET:HE1	2.25	0.51
64:N2:202:MET:HE1	64:N2:257:PHE:O	2.10	0.51
65:O2:537:LEU:HD13	65:O2:544:LEU:HD11	1.93	0.51
2:6:135:ALA:HB3	2:6:138:GLU:OE1	2.11	0.51
19:LB:248:LEU:HD23	19:LB:248:LEU:H	1.76	0.51
20:LC:135:ALA:HA	58:Lr:43:LEU:HD21	1.92	0.51
45:Ld:64:ILE:HG13	45:Ld:64:ILE:O	2.10	0.51
50:Li:98:ARG:O	50:Li:102:ALA:N	2.43	0.51
60:Lt:38:SER:OG	60:Lt:39:PRO:HD3	2.11	0.51
66:P2:307:LEU:HD12	66:P2:349:LEU:O	2.11	0.51
6:B:41:VAL:HG21	69:y3:197:VAL:HG21	1.92	0.50
7:D:30:GLU:OE2	12:J:116:ASN:HB2	2.10	0.50
26:LI:25:GLY:HA2	67:u3:64:A:OP1	2.11	0.50
45:Ld:107:THR:HG22	45:Ld:108:TYR:N	2.27	0.50
52:Lk:64:LEU:HD23	52:Lk:65:ALA:O	2.10	0.50
12:J:45:THR:HG23	12:J:91:SER:CB	2.41	0.50
40:LY:85:VAL:HG23	40:LY:85:VAL:O	2.12	0.50
3:7:104:LEU:HD21	3:7:120:ARG:HG2	1.93	0.50
15:L5:1999:A:N6	59:Ls:40:MET:HE3	2.27	0.50
61:Lz:145:VAL:HG23	61:Lz:146:ALA:N	2.25	0.50
62:M2:63:CYS:HA	64:N2:435:MET:HE2	1.92	0.50
15:L5:1565:A:C5	15:L5:1566:C:H1'	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LE:176:THR:HG23	22:LE:176:THR:O	2.11	0.50
70:LJ:57:VAL:HG22	70:LJ:62:ILE:HG12	1.94	0.50
7:D:69:LEU:HD13	9:F:59:ILE:HG23	1.93	0.50
7:D:243:MET:O	7:D:246:ILE:HG22	2.12	0.50
11:I:119:LEU:HD21	11:I:171:ILE:HD11	1.92	0.50
32:LQ:113:ILE:CG2	32:LQ:120:ILE:HD11	2.42	0.50
33:LR:3:MET:HE3	33:LR:3:MET:HA	1.92	0.50
49:Lh:91:MET:O	49:Lh:94:ARG:HG2	2.11	0.50
64:N2:204:ALA:HB1	64:N2:211:VAL:HG11	1.94	0.50
6:B:37:LYS:O	6:B:41:VAL:HG23	2.12	0.50
23:LF:116:GLN:OE1	32:LQ:3:VAL:HG22	2.12	0.50
36:LU:56:LEU:HD12	36:LU:61:VAL:HB	1.93	0.50
57:Lp:29:ILE:HD11	57:Lp:69:TRP:CD2	2.47	0.50
7:D:354:VAL:HG13	7:D:361:ALA:CB	2.42	0.50
11:I:389:ILE:HD11	11:I:416:ILE:HD11	1.94	0.50
40:LY:47:MET:HE2	40:LY:118:ILE:HD12	1.94	0.50
19:LB:47:LEU:HD23	19:LB:166:THR:HG23	1.94	0.50
33:LR:40:GLN:OE1	33:LR:40:GLN:N	2.45	0.50
59:Ls:123:VAL:HG13	59:Ls:160:LEU:HB2	1.94	0.50
64:N2:444:ILE:HD13	66:P2:580:HIS:CD2	2.47	0.50
23:LF:107:LYS:O	23:LF:111:LEU:HD23	2.13	0.49
26:LI:138:ILE:HD13	26:LI:152:LEU:HD21	1.92	0.49
40:LY:79:VAL:HG11	40:LY:98:GLY:HA3	1.94	0.49
59:Ls:91:THR:HG21	59:Ls:98:ILE:HG13	1.92	0.49
60:Lt:58:ILE:HG23	60:Lt:58:ILE:O	2.12	0.49
2:6:141:ARG:O	2:6:141:ARG:HG2	2.10	0.49
15:L5:406:C:O2'	15:L5:407:A:OP1	2.28	0.49
15:L5:1976:G:H21	60:Lt:138:SER:HB3	1.77	0.49
19:LB:215:GLU:O	19:LB:284:ILE:HD12	2.12	0.49
22:LE:281:ILE:HD12	22:LE:286:LEU:HD21	1.93	0.49
23:LF:116:GLN:OE1	32:LQ:2:GLY:O	2.30	0.49
15:L5:180:C:N4	15:L5:255:C:H42	2.10	0.49
21:LD:83:LEU:N	21:LD:84:PRO:HD2	2.27	0.49
35:LT:64:VAL:HG13	35:LT:72:VAL:CG2	2.42	0.49
69:y3:118:ILE:HG22	69:y3:125:ALA:HB2	1.94	0.49
11:I:389:ILE:HD11	11:I:416:ILE:CD1	2.42	0.49
15:L5:1705:G:H2'	15:L5:1706:A:O4'	2.12	0.49
15:L5:3964:U:O2'	15:L5:3966:A:O4'	2.30	0.49
15:L5:4098:A:H8	15:L5:4099:G:HO2'	1.61	0.49
65:O2:344:ASN:OD1	65:O2:345:LEU:N	2.44	0.49
70:LJ:61:GLY:O	70:LJ:62:ILE:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:83:VAL:HG13	6:B:100:LYS:CD	2.42	0.49
15:L5:4626:A:C5'	19:LB:53:MET:HE2	2.42	0.49
22:LE:50:LEU:HD23	22:LE:50:LEU:H	1.77	0.49
29:LN:148:THR:O	29:LN:151:ILE:HG22	2.13	0.49
59:Ls:44:ARG:HE	59:Ls:53:VAL:HG23	1.77	0.49
19:LB:235:TRP:CD1	19:LB:267:ALA:HB1	2.47	0.49
22:LE:99:ASP:O	22:LE:100:LYS:HG2	2.13	0.49
31:LP:35:ALA:O	31:LP:39:MET:HE3	2.12	0.49
37:LV:85:ARG:O	37:LV:97:TYR:HB2	2.13	0.49
13:K2:18:LEU:O	13:K2:22:VAL:HG23	2.12	0.49
22:LE:154:THR:HG21	22:LE:193:PHE:CD1	2.47	0.49
26:LI:120:GLY:O	26:LI:121:LYS:HE2	2.13	0.49
40:LY:82:ILE:HB	40:LY:85:VAL:HG22	1.93	0.49
59:Ls:102:LEU:O	59:Ls:105:ASN:O	2.31	0.49
68:v3:71:G:H2'	68:v3:71:G:N3	2.28	0.49
11:I:268:MET:HE3	11:I:323:ILE:HD12	1.95	0.49
15:L5:3949:A:H62	15:L5:4064:C:N4	2.11	0.49
49:Lh:57:VAL:O	49:Lh:60:VAL:HG12	2.13	0.49
11:I:598:TRP:NE1	69:y3:48:VAL:HG21	2.28	0.49
15:L5:1176:C:H42	15:L5:1184:A:H61	1.60	0.49
15:L5:4346:U:C1'	56:Lo:82:MET:HE1	2.42	0.49
19:LB:141:ASP:OD1	19:LB:142:GLY:N	2.46	0.49
24:LG:162:ASP:HB3	24:LG:163:PRO:HD3	1.95	0.49
39:LX:148:ASP:OD1	39:LX:149:VAL:N	2.46	0.49
47:Lf:47:CYS:HA	47:Lf:102:ARG:O	2.13	0.49
3:7:100:VAL:HG11	3:7:121:ILE:HA	1.93	0.49
15:L5:4041:C:OP2	15:L5:4042:G:H5''	2.13	0.49
28:LM:31:ILE:O	28:LM:32:ASP:OD1	2.30	0.49
29:LN:59:TYR:CE1	29:LN:135:ILE:HD13	2.48	0.49
61:Lz:176:ASP:O	61:Lz:180:VAL:HG23	2.13	0.49
70:LJ:10:ASN:OD1	70:LJ:11:PRO:HD3	2.13	0.49
15:L5:1387:A:C6	42:La:112:LEU:HD23	2.48	0.48
22:LE:223:ARG:O	22:LE:224:LYS:CG	2.61	0.48
31:LP:29:THR:HG21	31:LP:146:ILE:HD11	1.95	0.48
4:8:147:VAL:O	4:8:147:VAL:HG22	2.12	0.48
64:N2:337:ILE:HD12	64:N2:353:ILE:HD13	1.95	0.48
1:5:107:PHE:CD1	1:5:175:LEU:HD21	2.48	0.48
2:6:158:LEU:HD12	2:6:162:GLY:HA3	1.95	0.48
11:I:528:TYR:CZ	11:I:581:ILE:HD12	2.48	0.48
15:L5:1912:G:H21	30:LO:87:MET:HE3	1.77	0.48
22:LE:178:PRO:HG2	22:LE:181:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:LP:148:MET:HE2	31:LP:150:LEU:HD21	1.95	0.48
2:6:78:VAL:HB	4:8:78:THR:OG1	2.13	0.48
15:L5:1266:G:H5'	43:Lb:99:ILE:HD11	1.94	0.48
39:LX:95:THR:HG23	39:LX:138:VAL:O	2.12	0.48
61:Lz:17:VAL:HG13	61:Lz:18:LEU:N	2.23	0.48
66:P2:323:THR:HG22	66:P2:334:LEU:HD11	1.95	0.48
67:u3:55:U:H2'	67:u3:55:U:O2	2.12	0.48
7:D:30:GLU:OE2	12:J:113:PRO:HB2	2.13	0.48
7:D:288:ASN:O	7:D:291:ILE:HG22	2.12	0.48
11:I:594:ASN:OD1	11:I:664:ARG:NH2	2.47	0.48
15:L5:3937:C:H1'	29:LN:125:SER:HB2	1.94	0.48
24:LG:69:ILE:O	24:LG:72:LYS:HG2	2.14	0.48
39:LX:133:GLU:N	39:LX:133:GLU:OE1	2.47	0.48
57:Lp:29:ILE:HD11	57:Lp:69:TRP:CG	2.48	0.48
3:7:100:VAL:HG21	3:7:121:ILE:HA	1.95	0.48
15:L5:3614:G:O2'	15:L5:3615:G:OP1	2.26	0.48
15:L5:3946:G:N2	15:L5:3947:A:H62	2.10	0.48
25:LH:55:LEU:HD23	25:LH:56:ARG:N	2.28	0.48
11:I:362:PHE:CZ	11:I:478:VAL:HG23	2.48	0.48
12:J:63:THR:CG2	12:J:67:GLY:HA2	2.44	0.48
21:LD:62:CYS:HB3	21:LD:105:LEU:HD22	1.95	0.48
53:Ll:33:ASN:O	53:Ll:34:LYS:HG3	2.13	0.48
65:O2:561:LEU:HD13	65:O2:593:ARG:HG3	1.94	0.48
2:6:42:LEU:HD11	2:6:64:PHE:CZ	2.48	0.48
2:6:148:LEU:HD12	2:6:151:ALA:HB3	1.95	0.48
4:8:149:THR:HB	4:8:152:LEU:HB3	1.96	0.48
11:I:334:LEU:O	11:I:336:PRO:HD3	2.14	0.48
11:I:364:LEU:HD13	11:I:414:MET:HE3	1.96	0.48
15:L5:453:G:N3	15:L5:453:G:H2'	2.28	0.48
15:L5:1534:A:C4	51:Lj:13:ASN:O	2.67	0.48
40:LY:133:GLY:O	40:LY:134:LYS:C	2.57	0.48
61:Lz:49:PHE:HD2	61:Lz:193:LEU:HD13	1.79	0.48
9:F:32:GLU:OE1	9:F:36:ILE:HD11	2.14	0.48
11:I:213:VAL:O	11:I:216:ILE:HG22	2.14	0.48
11:I:584:GLY:HA2	11:I:663:VAL:HG12	1.94	0.48
21:LD:65:ALA:HB2	21:LD:74:ILE:HG22	1.95	0.48
28:LM:33:GLN:O	28:LM:33:GLN:HG2	2.14	0.48
49:Lh:59:THR:HG22	49:Lh:63:GLN:OE1	2.14	0.48
56:Lo:85:ILE:HG22	56:Lo:86:LYS:N	2.29	0.48
65:O2:442:VAL:HG12	65:O2:446:PHE:HE2	1.77	0.48
15:L5:4036:G:H3'	15:L5:4037:C:H5''	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Lf:30:ILE:CD1	47:Lf:84:VAL:HG22	2.43	0.48
60:Lt:147:HIS:O	60:Lt:151:ILE:HG22	2.14	0.48
7:D:93:LEU:HD23	7:D:93:LEU:C	2.39	0.47
11:I:135:THR:HB	11:I:144:GLY:HA2	1.95	0.47
20:LC:2:ALA:HA	20:LC:3:CYS:HB3	1.94	0.47
3:7:104:LEU:HD21	3:7:120:ARG:CG	2.45	0.47
15:L5:2760:G:H1'	15:L5:2761:U:OP2	2.14	0.47
19:LB:359:ALA:O	19:LB:360:LEU:HG	2.13	0.47
52:Lk:49:ASP:HB2	52:Lk:51:GLU:OE1	2.14	0.47
65:O2:307:ILE:HD13	65:O2:312:VAL:HG13	1.95	0.47
69:y3:107:ASN:OD1	69:y3:198:GLY:HA3	2.14	0.47
69:y3:145:LEU:CD1	69:y3:251:LEU:HD11	2.40	0.47
3:7:100:VAL:HG22	3:7:124:LYS:HG3	1.95	0.47
15:L5:3949:A:H62	15:L5:4064:C:H42	1.62	0.47
25:LH:12:ILE:HD13	25:LH:18:ILE:HG21	1.97	0.47
45:Ld:107:THR:HG22	45:Ld:108:TYR:H	1.79	0.47
49:Lh:23:ASP:O	49:Lh:27:GLU:OE1	2.33	0.47
49:Lh:44:LEU:O	49:Lh:47:ILE:HG12	2.14	0.47
53:Ll:29:MET:O	53:Ll:29:MET:SD	2.71	0.47
61:Lz:38:LEU:O	61:Lz:163:LEU:HD21	2.14	0.47
6:B:194:ASP:N	6:B:195:PRO:HD3	2.30	0.47
9:F:29:ASP:OD1	9:F:30:ARG:N	2.47	0.47
11:I:660:PHE:CZ	11:I:665:ASN:HA	2.50	0.47
15:L5:3764:U:C4	15:L5:3765:G:C6	3.02	0.47
30:LO:202:LEU:O	30:LO:203:VAL:C	2.58	0.47
48:Lg:23:SER:HB2	48:Lg:33:LEU:HD12	1.95	0.47
60:Lt:52:ASP:O	60:Lt:55:GLY:N	2.48	0.47
2:6:147:PHE:HB3	4:8:143:ASN:O	2.14	0.47
8:E:74:LEU:HD23	8:E:74:LEU:C	2.39	0.47
15:L5:3658:C:O4'	18:LA:237:LEU:HD12	2.14	0.47
15:L5:4098:A:H2'	15:L5:4099:G:H4'	1.97	0.47
15:L5:4548:A:H1'	67:u3:75:C:OP1	2.15	0.47
36:LU:43:LEU:O	36:LU:47:ILE:HG12	2.14	0.47
40:LY:49:ILE:CD1	40:LY:80:ILE:HD13	2.44	0.47
51:Lj:19:CYS:SG	51:Lj:21:ARG:O	2.73	0.47
70:LJ:95:ARG:HA	70:LJ:176:PRO:HG3	1.96	0.47
2:6:34:ALA:O	2:6:133:ILE:HA	2.14	0.47
2:6:34:ALA:O	2:6:133:ILE:HG23	2.14	0.47
15:L5:934:C:H5''	15:L5:935:A:OP1	2.15	0.47
15:L5:2563:C:H2'	15:L5:2564:G:O4'	2.14	0.47
48:Lg:5:LEU:HD22	48:Lg:32:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:P2:291:GLN:CD	66:P2:331:VAL:HG12	2.40	0.47
69:y3:119:SER:HA	69:y3:125:ALA:HB3	1.97	0.47
5:A:69:LEU:HD11	5:A:111:VAL:HG21	1.96	0.47
6:B:159:SER:N	6:B:160:PRO:HD2	2.30	0.47
7:D:236:ARG:NE	7:D:239:LEU:HB2	2.29	0.47
11:I:363:ASP:CB	11:I:407:MET:HE2	2.44	0.47
11:I:466:PHE:O	11:I:470:THR:HG23	2.15	0.47
11:I:523:MET:HE3	11:I:555:VAL:HG13	1.96	0.47
12:J:17:LEU:HD22	63:N:75:ILE:HD11	1.97	0.47
12:J:18:LYS:O	12:J:18:LYS:HG3	2.15	0.47
14:L2:17:VAL:HG12	14:L2:21:LEU:HG	1.97	0.47
15:L5:2017:A:O2'	15:L5:2018:C:O5'	2.32	0.47
15:L5:2101:C:H2'	15:L5:2102:G:C8	2.50	0.47
16:L7:115:A:C1'	21:LD:74:ILE:HD11	2.44	0.47
23:LF:116:GLN:HB2	23:LF:119:ASN:OD1	2.14	0.47
30:LO:191:LYS:O	30:LO:194:GLU:OE1	2.33	0.47
34:LS:161:ARG:HE	34:LS:164:LYS:HB2	1.79	0.47
41:LZ:25:ILE:HD13	41:LZ:43:VAL:HG12	1.97	0.47
45:Ld:42:ALA:HB3	45:Ld:43:PRO:HD3	1.96	0.47
59:Ls:82:ILE:HD11	59:Ls:86:VAL:CG1	2.44	0.47
64:N2:246:GLY:HA2	64:N2:256:ILE:HD13	1.96	0.47
4:8:165:PHE:HD2	63:N:11:LEU:HD23	1.78	0.47
15:L5:406:C:HO2'	15:L5:407:A:P	2.38	0.47
15:L5:2334:C:C5	20:LC:191:ALA:HB2	2.49	0.47
45:Ld:20:VAL:HG12	45:Ld:20:VAL:O	2.14	0.47
64:N2:158:ASP:HB3	64:N2:173:ILE:HG22	1.97	0.47
66:P2:145:LEU:HD21	66:P2:176:ASP:O	2.14	0.47
9:F:57:ILE:HD11	12:J:92:PHE:CE2	2.50	0.47
11:I:227:MET:HE1	11:I:276:LEU:HG	1.97	0.47
11:I:329:ARG:HH12	11:I:346:ILE:HG23	1.80	0.47
21:LD:40:ASP:OD1	21:LD:41:LYS:N	2.47	0.47
47:Lf:104:MET:O	47:Lf:105:LEU:HB2	2.15	0.47
60:Lt:29:ALA:N	60:Lt:30:PRO:HD2	2.30	0.47
66:P2:219:MET:HE3	66:P2:226:PRO:HA	1.96	0.47
70:LJ:57:VAL:HG23	70:LJ:58:ARG:N	2.30	0.47
6:B:66:LEU:HD22	6:B:125:ILE:CG2	2.44	0.47
7:D:252:PHE:CE1	7:D:447:ILE:HG23	2.50	0.47
11:I:151:ILE:O	11:I:154:VAL:HG12	2.15	0.47
15:L5:4042:G:H2'	15:L5:4042:G:N3	2.30	0.47
15:L5:4162:C:C4	24:LG:72:LYS:HE2	2.50	0.47
15:L5:4926:C:O2	15:L5:4926:C:O4'	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LB:291:TYR:CE1	19:LB:299:ILE:HG22	2.50	0.47
23:LF:105:VAL:HG13	23:LF:136:VAL:HG12	1.96	0.47
32:LQ:83:VAL:HG23	32:LQ:83:VAL:O	2.14	0.47
61:Lz:60:ARG:HB2	61:Lz:173:LYS:HZ1	1.80	0.47
7:D:97:ALA:O	7:D:98:LYS:HB2	2.15	0.46
14:L2:47:THR:HG22	14:L2:47:THR:O	2.14	0.46
15:L5:485:C:H2'	15:L5:485:C:O2	2.14	0.46
44:Lc:22:MET:O	44:Lc:23:LYS:HB3	2.15	0.46
59:Ls:23:ASP:OD1	59:Ls:24:TYR:N	2.48	0.46
59:Ls:82:ILE:HG23	59:Ls:82:ILE:O	2.15	0.46
60:Lt:54:LYS:N	60:Lt:55:GLY:HA2	2.30	0.46
62:M2:30:TYR:CZ	62:M2:34:ILE:HD11	2.51	0.46
64:N2:78:THR:HG22	64:N2:80:ASP:H	1.80	0.46
64:N2:136:ASP:OD1	64:N2:137:PRO:HD3	2.15	0.46
66:P2:200:GLN:HB2	66:P2:208:THR:HG21	1.97	0.46
2:6:53:ALA:CB	2:6:82:ARG:HE	2.28	0.46
6:B:190:ILE:HD11	65:O2:268:ARG:CB	2.46	0.46
7:D:21:LYS:HZ3	7:D:171:LYS:HD3	1.80	0.46
7:D:186:ASN:OD1	7:D:187:ILE:N	2.49	0.46
7:D:400:VAL:HG12	7:D:401:MET:N	2.30	0.46
15:L5:1487:G:C4'	27:LL:184:MET:HE1	2.45	0.46
15:L5:1973:G:H1'	60:Lt:121:LEU:HD11	1.97	0.46
23:LF:222:LYS:HD3	23:LF:225:THR:HG23	1.98	0.46
26:LI:61:SER:HA	26:LI:126:VAL:HG12	1.97	0.46
45:Ld:54:MET:O	45:Ld:57:MET:O	2.34	0.46
7:D:232:GLU:O	7:D:236:ARG:HB2	2.16	0.46
11:I:483:TYR:HE1	69:y3:39:ARG:HG3	1.80	0.46
31:LP:115:GLU:OE2	31:LP:149:ILE:HG22	2.15	0.46
6:B:32:LEU:HB2	6:B:95:PHE:HB2	1.98	0.46
7:D:2:ALA:HB3	7:D:101:GLU:H	1.81	0.46
23:LF:59:LYS:O	23:LF:62:ARG:HG2	2.15	0.46
29:LN:13:LYS:HZ3	50:Li:44:ILE:HG23	1.80	0.46
42:La:117:LEU:N	42:La:117:LEU:HD12	2.29	0.46
61:Lz:38:LEU:HD13	61:Lz:159:MET:HE1	1.97	0.46
69:y3:199:PHE:CZ	69:y3:209:VAL:HG11	2.50	0.46
7:D:35:THR:HG22	7:D:169:LEU:HD11	1.97	0.46
15:L5:1913:C:H1'	30:LO:87:MET:HE2	1.97	0.46
26:LI:15:LYS:HG2	26:LI:16:PRO:HD2	1.96	0.46
69:y3:37:LYS:HG3	69:y3:38:SER:N	2.31	0.46
69:y3:103:GLU:HB2	69:y3:201:SER:OG	2.15	0.46
69:y3:251:LEU:HD12	69:y3:259:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:33:LEU:HD11	5:A:60:LEU:HD11	1.97	0.46
15:L5:1564:A:C6	15:L5:1565:A:C6	3.04	0.46
15:L5:3764:U:H2'	15:L5:3765:G:O4'	2.16	0.46
18:LA:115:CYS:O	18:LA:164:ALA:HA	2.14	0.46
20:LC:221:PHE:O	20:LC:222:ARG:HB3	2.16	0.46
21:LD:191:ASN:O	21:LD:192:ALA:HB3	2.15	0.46
48:Lg:5:LEU:HD12	48:Lg:5:LEU:N	2.31	0.46
54:Lm:102:ARG:C	54:Lm:103:LEU:HD12	2.41	0.46
60:Lt:121:LEU:HD23	60:Lt:129:ILE:HD13	1.97	0.46
61:Lz:116:LEU:O	61:Lz:120:ILE:HG12	2.16	0.46
11:I:38:VAL:O	11:I:41:PHE:O	2.34	0.46
15:L5:4162:C:C5	24:LG:244:PRO:HD3	2.50	0.46
15:L5:4894:A:H3'	15:L5:4895:C:H5'	1.97	0.46
18:LA:29:LEU:O	18:LA:123:ARG:HD3	2.15	0.46
23:LF:133:LEU:HD23	23:LF:142:TRP:CD2	2.50	0.46
60:Lt:125:LEU:HD12	60:Lt:127:GLY:N	2.31	0.46
66:P2:204:GLY:O	66:P2:207:THR:HG22	2.15	0.46
69:y3:49:VAL:HG23	69:y3:50:GLN:N	2.31	0.46
7:D:24:ARG:CG	7:D:25:LYS:N	2.78	0.46
15:L5:1387:A:N6	42:La:112:LEU:HD23	2.31	0.46
15:L5:2786:C:O2'	15:L5:2787:A:OP2	2.27	0.46
21:LD:69:ILE:HD12	21:LD:69:ILE:H	1.80	0.46
35:LT:57:TYR:CE2	35:LT:89:ILE:HG21	2.50	0.46
1:5:171:LEU:HD21	1:5:173:ILE:HD11	1.98	0.46
6:B:208:LYS:O	6:B:211:GLU:HG3	2.16	0.46
15:L5:1949:U:H5'	25:LH:64:ARG:HH11	1.81	0.46
40:LY:79:VAL:CG1	40:LY:98:GLY:HA3	2.46	0.46
2:6:158:LEU:HB3	2:6:159:PRO:HD3	1.98	0.46
4:8:161:TYR:CE2	63:N:14:LEU:HD11	2.51	0.46
9:F:11:SER:HA	9:F:14:PHE:CE2	2.50	0.46
14:L2:69:LEU:HD21	65:O2:442:VAL:HG21	1.96	0.46
15:L5:4041:C:H2'	61:Lz:101:LYS:HG3	1.98	0.46
24:LG:69:ILE:HA	24:LG:72:LYS:NZ	2.31	0.46
49:Lh:33:VAL:O	49:Lh:37:THR:HG23	2.15	0.46
6:B:126:VAL:O	6:B:130:PHE:HB3	2.16	0.45
10:G:5:GLN:OE1	15:L5:2623:A:H5'	2.15	0.45
28:LM:82:ILE:HD12	28:LM:82:ILE:H	1.81	0.45
2:6:141:ARG:O	2:6:141:ARG:CG	2.64	0.45
7:D:28:PHE:HA	7:D:31:LYS:HB2	1.98	0.45
7:D:289:ILE:N	7:D:290:PRO:HD2	2.30	0.45
11:I:11:TYR:CE2	13:K2:33:PRO:HD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L5:1565:A:N6	15:L5:1566:C:O2	2.49	0.45
15:L5:2373:C:H4'	45:Ld:64:ILE:HD11	1.99	0.45
16:L7:61:G:H5''	21:LD:271:MET:CE	2.46	0.45
21:LD:92:LEU:O	21:LD:93:THR:HG22	2.16	0.45
24:LG:51:LEU:O	24:LG:55:VAL:HG23	2.17	0.45
25:LH:173:ARG:HB3	54:Lm:127:VAL:HG13	1.97	0.45
29:LN:124:ASP:HB3	29:LN:127:TYR:H	1.79	0.45
48:Lg:99:GLU:O	48:Lg:102:ILE:HG22	2.17	0.45
70:LJ:57:VAL:HG21	70:LJ:60:PHE:CZ	2.51	0.45
3:7:46:LEU:HD22	3:7:50:ILE:HD12	1.98	0.45
15:L5:686:A:H4'	22:LE:97:GLY:O	2.16	0.45
15:L5:2468:U:O2'	15:L5:2506:G:N2	2.49	0.45
18:LA:142:GLU:O	18:LA:143:THR:OG1	2.33	0.45
28:LM:87:ALA:O	28:LM:88:ALA:HB2	2.17	0.45
45:Ld:22:THR:HG23	45:Ld:122:VAL:HG23	1.97	0.45
3:7:91:LYS:NZ	4:8:170:HIS:O	2.49	0.45
3:7:100:VAL:HG11	3:7:121:ILE:CA	2.46	0.45
6:B:217:ARG:O	6:B:218:LYS:C	2.59	0.45
11:I:623:GLU:CD	69:y3:67:ARG:HE	2.24	0.45
29:LN:17:ASP:OD1	29:LN:18:VAL:HG23	2.15	0.45
42:La:46:ASP:OD1	42:La:47:LYS:N	2.48	0.45
57:Lp:5:THR:OG1	57:Lp:8:VAL:HG22	2.15	0.45
60:Lt:76:SER:HB3	60:Lt:116:MET:SD	2.57	0.45
65:O2:189:GLY:O	65:O2:190:ASN:OD1	2.34	0.45
66:P2:290:LEU:HD21	66:P2:365:LEU:HD22	1.98	0.45
4:8:169:SER:HB2	63:N:11:LEU:HD11	1.97	0.45
7:D:28:PHE:CD1	7:D:464:GLU:CD	2.94	0.45
11:I:361:TYR:CD1	12:J:139:MET:HE2	2.51	0.45
15:L5:182:G:H22	15:L5:254:G:H1	1.64	0.45
15:L5:1487:G:O4'	27:LL:184:MET:HE1	2.17	0.45
26:LI:152:LEU:HB3	26:LI:165:ILE:HD12	1.98	0.45
61:Lz:38:LEU:HD11	61:Lz:194:LEU:HD11	1.98	0.45
14:L2:16:ALA:O	14:L2:19:PRO:HD2	2.16	0.45
16:L7:63:C:O4'	26:LI:206:LEU:HD12	2.17	0.45
20:LC:32:ILE:HG13	20:LC:32:ILE:O	2.17	0.45
20:LC:35:ASP:OD1	20:LC:36:ILE:N	2.49	0.45
31:LP:113:VAL:HG21	31:LP:154:GLU:OE2	2.17	0.45
44:Lc:31:TYR:O	44:Lc:35:LEU:HD23	2.16	0.45
2:6:148:LEU:CD1	4:8:145:PRO:HD2	2.47	0.45
16:L7:61:G:C5'	21:LD:271:MET:HE1	2.46	0.45
16:L7:63:C:P	26:LI:206:LEU:HD13	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LB:280:ILE:HG22	19:LB:281:ASN:N	2.31	0.45
19:LB:326:VAL:HG23	19:LB:326:VAL:O	2.17	0.45
24:LG:260:GLU:O	24:LG:263:THR:HG22	2.17	0.45
26:LI:35:ASP:O	26:LI:36:LEU:HD12	2.16	0.45
30:LO:141:LEU:C	30:LO:141:LEU:HD23	2.42	0.45
40:LY:58:VAL:HG22	40:LY:103:LYS:O	2.16	0.45
40:LY:88:GLU:OE2	40:LY:94:THR:HG22	2.17	0.45
60:Lt:80:LEU:HD12	60:Lt:81:ILE:HG23	1.98	0.45
70:LJ:128:LEU:HD11	70:LJ:130:PHE:CE1	2.52	0.45
15:L5:74:G:H1'	27:LL:62:PRO:HG2	1.98	0.45
15:L5:4378:A:O2'	15:L5:4379:A:H2'	2.17	0.45
30:LO:110:PRO:N	30:LO:111:PRO:HD2	2.31	0.45
4:8:162:TYR:CZ	63:N:15:LEU:HD21	2.52	0.45
15:L5:3971:G:H8	15:L5:3971:G:O5'	1.99	0.45
32:LQ:126:LEU:C	32:LQ:126:LEU:HD23	2.42	0.45
37:LV:112:MET:CE	37:LV:117:ILE:HD11	2.42	0.45
60:Lt:10:ILE:HD13	60:Lt:67:ARG:HA	1.97	0.45
63:N:15:LEU:HD13	63:N:50:PHE:CE1	2.52	0.45
6:B:220:PRO:HB3	66:P2:448:VAL:H	1.82	0.45
7:D:234:PHE:CE1	7:D:242:LEU:HD23	2.52	0.45
15:L5:1977:C:O2'	15:L5:1978:C:OP1	2.32	0.45
18:LA:47:ASP:OD1	18:LA:48:ILE:N	2.49	0.45
59:Ls:44:ARG:HE	59:Ls:53:VAL:CG2	2.30	0.45
60:Lt:10:ILE:HG21	60:Lt:67:ARG:HA	1.98	0.45
2:6:138:GLU:O	2:6:142:ARG:HD3	2.18	0.44
3:7:145:PHE:HA	3:7:177:ILE:HD11	1.98	0.44
15:L5:499:G:H2'	15:L5:504:G:H22	1.83	0.44
15:L5:1241:C:C5	43:Lb:118:LEU:HD23	2.53	0.44
20:LC:171:LEU:HD23	20:LC:171:LEU:O	2.16	0.44
27:LL:50:PRO:O	27:LL:150:LEU:O	2.35	0.44
45:Ld:37:GLY:O	45:Ld:41:ARG:HG3	2.17	0.44
53:Ll:30:LYS:HG2	53:Ll:31:THR:N	2.33	0.44
64:N2:169:GLN:HG3	64:N2:171:THR:HG23	1.98	0.44
6:B:70:LEU:HB3	6:B:136:TRP:CZ3	2.51	0.44
15:L5:1503:A:N6	32:LQ:87:THR:HG21	2.32	0.44
15:L5:3784:A:O2'	15:L5:3785:A:H3'	2.16	0.44
22:LE:45:SER:O	22:LE:46:ARG:HB2	2.18	0.44
23:LF:213:LEU:HD23	23:LF:247:MET:HG2	2.00	0.44
61:Lz:10:LEU:HD12	61:Lz:12:GLU:H	1.81	0.44
61:Lz:161:LYS:HD2	68:v3:54:U:O2'	2.17	0.44
68:v3:48:C:H2'	68:v3:59:U:H1'	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:y3:144:LEU:HA	69:y3:249:LEU:O	2.17	0.44
6:B:200:LEU:O	6:B:203:GLU:HG3	2.18	0.44
7:D:377:LYS:HD2	7:D:422:ALA:HB2	1.99	0.44
12:J:13:GLU:O	63:N:53:THR:HG23	2.18	0.44
15:L5:1600:A:OP2	31:LP:132:ALA:O	2.35	0.44
15:L5:1707:C:C2	43:Lb:103:LYS:HB2	2.52	0.44
15:L5:3971:G:O6	15:L5:4051:C:H1'	2.17	0.44
18:LA:96:LEU:HD21	57:Lp:83:ILE:HD11	1.98	0.44
19:LB:39:LYS:O	19:LB:187:GLY:O	2.35	0.44
24:LG:194:VAL:HG22	24:LG:194:VAL:O	2.16	0.44
37:LV:30:ASP:OD2	37:LV:32:THR:HG23	2.17	0.44
43:Lb:36:ASP:C	43:Lb:36:ASP:OD1	2.61	0.44
60:Lt:152:ILE:O	60:Lt:155:ILE:HG12	2.17	0.44
61:Lz:63:PHE:O	61:Lz:153:SER:OG	2.27	0.44
61:Lz:90:LEU:HD13	61:Lz:93:LEU:HD21	1.99	0.44
4:8:26:CYS:HB3	4:8:131:LEU:HD21	1.99	0.44
11:I:598:TRP:NE1	69:y3:48:VAL:CG2	2.80	0.44
27:LL:96:ILE:HG22	27:LL:96:ILE:O	2.17	0.44
29:LN:120:TRP:HE1	29:LN:123:GLU:CG	2.30	0.44
31:LP:161:GLU:O	31:LP:164:VAL:HG22	2.17	0.44
38:LW:4:GLU:N	38:LW:4:GLU:OE1	2.51	0.44
39:LX:95:THR:HG23	39:LX:138:VAL:C	2.43	0.44
61:Lz:206:ILE:HG21	61:Lz:214:GLN:HB2	1.99	0.44
66:P2:419:GLN:HG2	66:P2:458:VAL:HG23	2.00	0.44
7:D:81:ILE:HG22	7:D:85:VAL:HG23	2.00	0.44
66:P2:145:LEU:HD22	66:P2:175:ALA:HB1	2.00	0.44
6:B:190:ILE:HD11	65:O2:268:ARG:HG3	1.99	0.44
11:I:578:VAL:HG12	11:I:642:MET:HE1	2.00	0.44
12:J:93:LEU:HD22	12:J:131:SER:HA	2.00	0.44
20:LC:135:ALA:CA	58:Lr:43:LEU:HD21	2.47	0.44
30:LO:121:PRO:HA	30:LO:124:LEU:HD12	1.99	0.44
70:LJ:20:LEU:O	70:LJ:131:TYR:O	2.35	0.44
3:7:100:VAL:HG11	3:7:120:ARG:C	2.43	0.44
15:L5:2017:A:O2'	15:L5:2018:C:C6	2.68	0.44
15:L5:2262:G:N3	15:L5:2262:G:H2'	2.32	0.44
25:LH:63:ASN:O	25:LH:67:LEU:HG	2.18	0.44
27:LL:184:MET:HE2	27:LL:184:MET:CA	2.48	0.44
60:Lt:114:ARG:HE	60:Lt:133:LEU:HB2	1.83	0.44
60:Lt:124:GLU:HB3	60:Lt:128:THR:HG21	1.99	0.44
5:A:92:TYR:CD1	5:A:97:PHE:HB2	2.53	0.44
11:I:316:LEU:O	11:I:320:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L5:4674:C:O3'	19:LB:334:LYS:HE3	2.18	0.44
20:LC:352:ASP:OD1	20:LC:353:LYS:N	2.51	0.44
24:LG:99:ALA:HB1	24:LG:193:LEU:HD21	2.00	0.44
32:LQ:79:THR:HG23	32:LQ:99:LYS:HG2	2.00	0.44
41:LZ:76:ASN:OD1	41:LZ:77:TYR:N	2.51	0.44
44:Lc:20:LEU:HD23	44:Lc:101:ASP:HB2	2.00	0.44
59:Ls:94:ASP:HB3	59:Ls:97:GLU:OE1	2.18	0.44
59:Ls:141:LEU:HD22	59:Ls:143:ILE:CG1	2.48	0.44
60:Lt:141:CYS:O	60:Lt:142:ASN:HB2	2.18	0.44
7:D:61:PRO:HD2	12:J:68:HIS:ND1	2.33	0.44
10:G:21:ARG:HB2	45:Ld:63:ARG:NH1	2.32	0.44
15:L5:1339:U:H2'	15:L5:1340:C:C6	2.52	0.44
15:L5:1431:C:H2'	15:L5:1432:G:O4'	2.18	0.44
17:L8:15:G:C6	17:L8:16:G:N1	2.86	0.44
17:L8:84:A:H5'	17:L8:86:U:O4'	2.18	0.44
22:LE:56:ARG:O	22:LE:56:ARG:NH1	2.51	0.44
25:LH:44:GLU:OE2	28:LM:3:PHE:CE2	2.71	0.44
25:LH:60:TRP:O	25:LH:61:TRP:HB2	2.18	0.44
26:LI:30:LYS:HG3	26:LI:63:GLU:HG3	1.99	0.44
39:LX:119:ILE:CG2	39:LX:140:LEU:HD22	2.46	0.44
63:N:93:CYS:O	63:N:94:VAL:C	2.57	0.44
9:F:9:GLU:HB2	9:F:10:PRO:HD3	1.99	0.43
11:I:42:GLU:CD	65:O2:299:ASN:HB3	2.43	0.43
11:I:437:ARG:HG2	11:I:437:ARG:HH11	1.83	0.43
11:I:661:ASP:OD2	11:I:664:ARG:HD3	2.17	0.43
11:I:662:ARG:HH22	69:y3:30:THR:HG23	1.83	0.43
15:L5:1367:C:O4'	15:L5:1367:C:O2	2.35	0.43
15:L5:1787:A:N3	15:L5:4210:U:O2'	2.50	0.43
19:LB:86:VAL:HG12	19:LB:201:LEU:HD12	2.00	0.43
21:LD:84:PRO:HA	21:LD:87:GLY:O	2.18	0.43
23:LF:213:LEU:HD12	23:LF:213:LEU:N	2.33	0.43
59:Ls:144:THR:OG1	59:Ls:156:SER:HB3	2.18	0.43
61:Lz:17:VAL:CG1	61:Lz:18:LEU:H	2.28	0.43
61:Lz:42:ASP:HB3	61:Lz:45:LYS:HG2	2.00	0.43
62:M2:44:TYR:CE1	62:M2:48:VAL:HG21	2.52	0.43
15:L5:1975:G:H22	15:L5:1983:A:P	2.41	0.43
15:L5:2373:C:H5''	45:Ld:64:ILE:HD11	1.99	0.43
23:LF:116:GLN:CD	32:LQ:3:VAL:HG22	2.41	0.43
36:LU:56:LEU:HD11	36:LU:63:ILE:HD11	2.00	0.43
39:LX:119:ILE:HG22	39:LX:120:ASP:H	1.83	0.43
47:Lf:30:ILE:HD11	47:Lf:84:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:O2:306:LEU:HD13	71:K:6:MAN:H62	2.00	0.43
65:O2:472:ARG:O	65:O2:475:VAL:HG22	2.19	0.43
2:6:143:PHE:N	2:6:143:PHE:CD1	2.86	0.43
7:D:93:LEU:HD13	10:G:50:VAL:HG11	2.00	0.43
12:J:62:MET:HG3	12:J:72:VAL:HG11	2.00	0.43
15:L5:3615:G:H21	38:LW:44:ARG:HH12	1.67	0.43
15:L5:4040:C:O2'	15:L5:4049:U:OP2	2.31	0.43
18:LA:3:ARG:HG2	18:LA:207:VAL:HG12	2.00	0.43
23:LF:220:MET:O	23:LF:221:LYS:HB2	2.18	0.43
24:LG:27:VAL:O	24:LG:27:VAL:HG22	2.17	0.43
27:LL:47:ALA:HB3	27:LL:48:PRO:HD3	2.00	0.43
56:Lo:104:ILE:HA	56:Lo:105:GLN:HA	1.77	0.43
7:D:167:GLU:O	7:D:171:LYS:HG2	2.19	0.43
15:L5:4139:G:N2	15:L5:4140:C:H41	2.16	0.43
61:Lz:76:GLU:O	61:Lz:80:VAL:HG22	2.18	0.43
69:y3:109:SER:HB2	69:y3:275:ILE:HD12	2.00	0.43
70:LJ:111:GLU:N	70:LJ:111:GLU:OE1	2.51	0.43
2:6:143:PHE:O	2:6:143:PHE:CD2	2.71	0.43
7:D:35:THR:HG22	7:D:169:LEU:CD1	2.48	0.43
7:D:113:ASN:O	7:D:116:GLN:HG3	2.19	0.43
11:I:348:SER:HA	11:I:598:TRP:CE2	2.54	0.43
11:I:362:PHE:CE2	11:I:478:VAL:HG23	2.53	0.43
15:L5:57:G:H4'	29:LN:155:VAL:HG12	2.01	0.43
19:LB:53:MET:HB3	19:LB:76:VAL:O	2.18	0.43
36:LU:75:GLU:N	36:LU:75:GLU:OE1	2.52	0.43
52:Lk:51:GLU:OE1	52:Lk:51:GLU:N	2.51	0.43
69:y3:86:MET:O	69:y3:90:ILE:HG22	2.18	0.43
70:LJ:112:HIS:ND1	70:LJ:117:ILE:HD11	2.34	0.43
6:B:220:PRO:HB3	66:P2:448:VAL:O	2.19	0.43
12:J:142:LYS:C	12:J:143:LEU:HD22	2.43	0.43
15:L5:1968:G:O2'	59:Ls:34:ASN:HA	2.19	0.43
15:L5:4038:C:N4	15:L5:4050:A:OP2	2.51	0.43
15:L5:4133:C:H42	15:L5:4151:G:H1	1.67	0.43
20:LC:298:ILE:CD1	32:LQ:128:LEU:HD23	2.47	0.43
22:LE:258:LEU:N	22:LE:259:PRO:HD2	2.33	0.43
24:LG:221:ALA:O	24:LG:224:THR:HG22	2.18	0.43
25:LH:20:LEU:CD2	25:LH:25:VAL:HG12	2.49	0.43
37:LV:99:GLU:OE2	38:LW:21:TYR:CZ	2.72	0.43
40:LY:82:ILE:HG22	40:LY:83:GLU:N	2.33	0.43
60:Lt:149:HIS:O	60:Lt:152:ILE:HG22	2.18	0.43
1:5:107:PHE:O	1:5:151:GLN:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L5:1445:U:C2	15:L5:2102:G:O6	2.72	0.43
21:LD:215:ASP:OD1	21:LD:216:GLU:N	2.51	0.43
33:LR:173:ARG:O	33:LR:177:LEU:HD23	2.18	0.43
45:Ld:52:PHE:O	45:Ld:56:GLU:OE1	2.37	0.43
56:Lo:57:ARG:O	56:Lo:57:ARG:HG3	2.18	0.43
59:Ls:174:LEU:O	59:Ls:177:MET:HG3	2.19	0.43
63:N:23:MET:HB3	63:N:89:ILE:HD11	2.00	0.43
70:LJ:55:TYR:HA	70:LJ:64:ARG:HB3	2.00	0.43
4:8:27:LEU:HD12	4:8:59:ASN:ND2	2.34	0.43
6:B:42:LYS:HD2	69:y3:93:LEU:HD12	2.01	0.43
11:I:445:GLN:OE1	40:LY:61:HIS:HB3	2.18	0.43
15:L5:500:G:N3	15:L5:504:G:H2'	2.33	0.43
15:L5:2490:U:O2'	15:L5:2491:C:O4'	2.32	0.43
15:L5:3661:G:N2	18:LA:126:LEU:HD13	2.34	0.43
17:L8:81:C:H2'	17:L8:83:C:OP2	2.19	0.43
24:LG:104:PRO:HG2	24:LG:194:VAL:HG23	2.00	0.43
31:LP:24:VAL:HG12	31:LP:25:HIS:N	2.33	0.43
58:Lr:97:ILE:HG23	58:Lr:98:ARG:N	2.33	0.43
59:Ls:186:GLY:C	59:Ls:187:LEU:HD12	2.44	0.43
61:Lz:60:ARG:HB3	61:Lz:61:PRO:HD3	2.01	0.43
62:M2:25:LYS:HB3	66:P2:563:ILE:HD11	2.01	0.43
21:LD:90:VAL:HG22	21:LD:91:GLY:N	2.34	0.43
23:LF:220:MET:HB3	23:LF:232:ASP:OD2	2.18	0.43
26:LI:208:LYS:O	26:LI:211:VAL:HG22	2.19	0.43
59:Ls:95:LEU:HD12	59:Ls:192:VAL:HG11	2.00	0.43
6:B:67:ASP:OD1	6:B:71:LYS:HD3	2.19	0.43
9:F:28:PRO:HB2	9:F:32:GLU:OE2	2.19	0.43
15:L5:1676:C:H5'	15:L5:1677:U:OP1	2.19	0.43
15:L5:4612:C:C2	25:LH:120:GLU:OE1	2.72	0.43
23:LF:216:PRO:HB3	23:LF:247:MET:HE3	2.01	0.43
42:La:23:GLY:HA3	42:La:24:LYS:HA	1.76	0.43
6:B:173:GLU:N	6:B:173:GLU:OE1	2.52	0.42
7:D:54:MET:HE1	7:D:142:GLU:CB	2.49	0.42
9:F:64:ILE:HD12	12:J:141:MET:HG3	2.00	0.42
11:I:482:ALA:HB2	69:y3:35:LEU:CD1	2.48	0.42
11:I:656:ARG:HG2	11:I:660:PHE:CD2	2.54	0.42
11:I:656:ARG:CD	11:I:657:PRO:HD2	2.49	0.42
15:L5:504:G:O6	15:L5:656:C:H1'	2.19	0.42
15:L5:1975:G:C4	15:L5:1984:A:C4	3.07	0.42
15:L5:2667:C:C1'	33:LR:96:MET:HE1	2.48	0.42
15:L5:3873:G:C6	15:L5:3874:G:C6	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LB:29:VAL:O	19:LB:30:LYS:HB2	2.18	0.42
19:LB:337:VAL:HG12	19:LB:338:VAL:N	2.34	0.42
20:LC:283:LYS:NZ	32:LQ:22:ASP:OD2	2.52	0.42
21:LD:205:ALA:HB2	21:LD:236:MET:HE3	2.00	0.42
38:LW:14:TYR:HB3	38:LW:15:PRO:HD2	2.01	0.42
45:Ld:22:THR:HG23	45:Ld:122:VAL:CG2	2.49	0.42
60:Lt:17:CYS:HA	60:Lt:60:VAL:HA	2.01	0.42
70:LJ:175:LEU:O	70:LJ:175:LEU:HD23	2.19	0.42
2:6:148:LEU:HD12	4:8:145:PRO:HD2	2.01	0.42
3:7:55:LEU:HD12	3:7:62:TYR:CD2	2.54	0.42
6:B:121:ARG:HA	6:B:182:PHE:CG	2.54	0.42
11:I:452:ILE:HG13	11:I:456:VAL:HG23	2.01	0.42
15:L5:3771:C:H3'	15:L5:3772:U:O2	2.20	0.42
33:LR:130:ASN:OD1	33:LR:130:ASN:O	2.37	0.42
37:LV:39:ILE:CD1	37:LV:61:VAL:HG21	2.48	0.42
59:Ls:25:PRO:HD2	59:Ls:92:LYS:HB3	2.02	0.42
4:8:151:VAL:HG21	63:N:25:MET:CE	2.48	0.42
6:B:106:SER:O	6:B:110:GLU:HB2	2.19	0.42
6:B:193:THR:HG23	6:B:193:THR:O	2.20	0.42
11:I:225:VAL:HG11	11:I:391:MET:HE3	2.01	0.42
11:I:371:PHE:O	11:I:375:LEU:HD23	2.18	0.42
11:I:598:TRP:HE1	69:y3:45:ASP:HB3	1.85	0.42
15:L5:1692:C:H5''	32:LQ:53:MET:CE	2.49	0.42
15:L5:3950:U:H3	15:L5:4062:A:H61	1.68	0.42
15:L5:4076:G:C8	24:LG:73:ARG:HD2	2.55	0.42
22:LE:96:VAL:HG12	22:LE:103:GLY:O	2.19	0.42
24:LG:155:VAL:CG1	24:LG:157:ILE:HD11	2.49	0.42
28:LM:100:ARG:O	28:LM:104:MET:HE2	2.19	0.42
28:LM:134:ALA:O	28:LM:137:LYS:HG2	2.20	0.42
37:LV:99:GLU:OE2	38:LW:23:ARG:HA	2.19	0.42
59:Ls:20:LEU:HD11	59:Ls:24:TYR:CE2	2.54	0.42
59:Ls:93:GLU:O	59:Ls:94:ASP:HB2	2.18	0.42
68:v3:16:A:O4'	68:v3:17:A:C8	2.72	0.42
70:LJ:95:ARG:HB3	70:LJ:178:LYS:HZ2	1.82	0.42
70:LJ:115:LEU:HD12	70:LJ:116:GLY:CA	2.49	0.42
11:I:282:PHE:CE2	11:I:286:LEU:HD11	2.54	0.42
15:L5:4037:C:H2'	15:L5:4039:G:N2	2.33	0.42
24:LG:66:GLN:O	24:LG:69:ILE:HG12	2.20	0.42
25:LH:25:VAL:HG23	25:LH:80:MET:HE1	2.02	0.42
27:LL:60:ARG:HD2	27:LL:67:HIS:O	2.19	0.42
40:LY:30:MET:HE2	40:LY:101:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:47:GLN:HB3	9:F:58:HIS:CD2	2.55	0.42
11:I:39:LEU:HD11	13:K2:2:ILE:O	2.20	0.42
11:I:91:GLY:HA3	11:I:208:SER:HA	2.01	0.42
15:L5:2033:A:O2'	15:L5:2034:G:O5'	2.36	0.42
15:L5:2805:C:N4	15:L5:2806:A:N6	2.67	0.42
15:L5:3756:A:N6	15:L5:3768:U:H3	2.14	0.42
20:LC:147:VAL:O	58:Lr:73:PRO:HG2	2.19	0.42
33:LR:96:MET:HE2	33:LR:96:MET:HA	2.02	0.42
40:LY:49:ILE:HD13	40:LY:80:ILE:HD13	2.01	0.42
46:Le:35:TRP:CZ2	46:Le:56:PRO:HD2	2.54	0.42
46:Le:83:LYS:O	46:Le:86:GLU:HG3	2.19	0.42
46:Le:129:LEU:HD23	46:Le:129:LEU:H	1.84	0.42
48:Lg:85:LYS:HA	48:Lg:88:ARG:HD2	2.02	0.42
61:Lz:175:THR:HG23	61:Lz:177:ASP:H	1.84	0.42
63:N:90:HIS:CE1	63:N:92:VAL:HG23	2.55	0.42
69:y3:101:LEU:HD23	69:y3:267:LEU:CB	2.49	0.42
3:7:98:LYS:O	3:7:101:THR:HG22	2.20	0.42
11:I:578:VAL:CG1	11:I:642:MET:HE1	2.49	0.42
15:L5:453:G:H5''	22:LE:228:GLN:HG2	2.02	0.42
15:L5:4557:U:O2	15:L5:4557:U:O4'	2.36	0.42
26:LI:177:ASN:OD1	26:LI:178:ALA:N	2.53	0.42
31:LP:153:LYS:O	31:LP:153:LYS:HG3	2.20	0.42
59:Ls:64:ALA:O	59:Ls:68:HIS:HB2	2.20	0.42
64:N2:154:THR:O	64:N2:200:VAL:HG22	2.20	0.42
65:O2:36:VAL:O	65:O2:171:GLN:HA	2.19	0.42
69:y3:166:ILE:HG23	69:y3:200:TYR:CE2	2.55	0.42
11:I:549:ASN:OD1	11:I:550:THR:N	2.53	0.42
12:J:36:LEU:O	12:J:39:VAL:HG12	2.19	0.42
15:L5:4139:G:H21	15:L5:4140:C:N4	2.18	0.42
24:LG:50:ASP:CG	24:LG:52:THR:HG1	2.28	0.42
25:LH:7:ASN:OD1	25:LH:7:ASN:C	2.63	0.42
61:Lz:67:VAL:HA	61:Lz:68:LEU:HA	1.73	0.42
64:N2:228:LYS:HD3	64:N2:229:PRO:O	2.19	0.42
6:B:96:PRO:HG2	6:B:105:PHE:CG	2.55	0.42
7:D:396:GLU:O	31:LP:180:LEU:HD13	2.20	0.42
11:I:268:MET:HE3	11:I:323:ILE:HG23	2.01	0.42
11:I:386:ARG:O	11:I:389:ILE:HG22	2.20	0.42
15:L5:2045:G:H1	30:LO:62:MET:HE1	1.82	0.42
15:L5:3773:U:O2	15:L5:3775:A:C2	2.72	0.42
15:L5:4093:G:H2'	15:L5:4094:G:O4'	2.19	0.42
15:L5:4548:A:N7	67:u3:74:C:H4'	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LL:46:ILE:O	27:LL:46:ILE:HG13	2.19	0.42
65:O2:173:MET:HB2	65:O2:200:TYR:HB2	2.01	0.42
2:6:143:PHE:CD2	4:8:42:VAL:HG12	2.55	0.42
7:D:28:PHE:HA	7:D:31:LYS:HE2	2.01	0.42
7:D:273:ARG:NH2	15:L5:2432:U:P	2.93	0.42
7:D:465:GLN:O	7:D:466:SER:C	2.63	0.42
15:L5:1504:G:OP1	32:LQ:147:GLU:OE1	2.37	0.42
15:L5:1564:A:H2'	15:L5:1565:A:C8	2.55	0.42
15:L5:1821:G:H2'	15:L5:1821:G:N3	2.34	0.42
15:L5:4162:C:C5	24:LG:72:LYS:HD2	2.54	0.42
19:LB:103:LYS:HG2	19:LB:149:ASP:OD1	2.18	0.42
24:LG:50:ASP:HA	39:LX:40:ILE:HD11	2.01	0.42
60:Lt:114:ARG:HE	60:Lt:133:LEU:CB	2.32	0.42
61:Lz:147:LYS:HE2	61:Lz:151:VAL:H	1.84	0.42
69:y3:110:ASP:O	69:y3:114:LYS:HG2	2.20	0.42
11:I:597:LEU:HB3	11:I:601:ARG:NH1	2.35	0.42
15:L5:455:C:N4	15:L5:456:C:H41	2.18	0.42
15:L5:1774:C:H2'	15:L5:1775:A:O4'	2.19	0.42
15:L5:2096:G:H3'	15:L5:2096:G:N3	2.35	0.42
18:LA:116:LEU:HD21	18:LA:158:ILE:HD13	2.02	0.42
21:LD:217:ASP:OD1	21:LD:218:ALA:N	2.53	0.42
30:LO:21:ALA:HA	30:LO:87:MET:HE1	2.01	0.42
37:LV:109:LYS:HB2	37:LV:111:GLU:OE1	2.19	0.42
41:LZ:11:VAL:HG21	41:LZ:80:LEU:HB3	2.02	0.42
65:O2:445:ALA:O	65:O2:448:ILE:HG22	2.20	0.42
2:6:144:SER:HB3	2:6:145:PRO:HD3	2.00	0.41
6:B:96:PRO:HB3	6:B:101:LEU:CD1	2.50	0.41
6:B:209:LYS:O	6:B:213:ARG:CD	2.68	0.41
7:D:53:ILE:HG12	7:D:64:TRP:CG	2.55	0.41
7:D:101:GLU:OE1	7:D:101:GLU:N	2.52	0.41
7:D:248:THR:HA	7:D:440:ALA:HB1	2.02	0.41
7:D:281:ILE:HG13	7:D:281:ILE:O	2.20	0.41
15:L5:1281:G:OP2	22:LE:128:HIS:HE1	2.02	0.41
15:L5:4054:C:H1'	61:Lz:207:LYS:HD3	2.01	0.41
24:LG:115:LEU:HD12	24:LG:116:ALA:N	2.35	0.41
24:LG:200:THR:HG22	24:LG:201:THR:HG23	2.01	0.41
52:Lk:51:GLU:O	52:Lk:54:GLU:OE1	2.38	0.41
59:Ls:175:LEU:HD22	59:Ls:180:ILE:HD12	2.01	0.41
65:O2:238:HIS:CB	65:O2:435:MET:HE3	2.50	0.41
7:D:213:ILE:H	7:D:213:ILE:HD12	1.86	0.41
7:D:263:VAL:HG22	9:F:25:CYS:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:66:VAL:O	9:F:67:GLY:C	2.63	0.41
15:L5:2671:C:OP1	57:Lp:46:LYS:HE3	2.20	0.41
15:L5:4189:U:H2'	15:L5:4190:U:O4'	2.19	0.41
15:L5:4727:A:H5'	19:LB:130:PHE:H	1.86	0.41
20:LC:252:TRP:CZ3	20:LC:260:LEU:HD11	2.55	0.41
21:LD:37:VAL:CG2	21:LD:67:ALA:HB2	2.50	0.41
24:LG:72:LYS:O	24:LG:240:ASN:N	2.53	0.41
24:LG:129:PRO:C	24:LG:130:THR:HG22	2.45	0.41
28:LM:119:ARG:CG	30:LO:189:ILE:HD11	2.50	0.41
61:Lz:29:LEU:HD23	61:Lz:173:LYS:HZ1	1.85	0.41
64:N2:67:LEU:HD23	64:N2:74:LEU:HD21	2.02	0.41
65:O2:551:MET:HE2	65:O2:603:ILE:HG22	2.02	0.41
69:y3:102:ARG:CG	69:y3:271:TYR:HB3	2.50	0.41
70:LJ:136:ARG:CG	70:LJ:137:PRO:HD2	2.50	0.41
6:B:37:LYS:HZ1	69:y3:166:ILE:HB	1.85	0.41
7:D:283:LEU:HD23	7:D:283:LEU:C	2.46	0.41
12:J:19:LEU:HD12	63:N:109:ASN:ND2	2.35	0.41
15:L5:4584:A:H2'	15:L5:4585:U:O4'	2.20	0.41
26:LI:36:LEU:HD23	26:LI:73:ASN:OD1	2.19	0.41
43:Lb:74:ALA:C	43:Lb:75:LEU:HD12	2.46	0.41
61:Lz:31:THR:HB	61:Lz:171:HIS:CD2	2.54	0.41
61:Lz:142:GLU:O	61:Lz:144:MET:HG2	2.20	0.41
70:LJ:93:GLU:C	70:LJ:94:LEU:HD22	2.45	0.41
1:5:130:TYR:OH	1:5:193:THR:HG23	2.21	0.41
1:5:162:GLU:N	1:5:163:PRO:HD2	2.36	0.41
3:7:111:LYS:NZ	15:L5:2488:C:H4'	2.35	0.41
6:B:222:ILE:HD12	66:P2:445:GLN:HG2	2.01	0.41
7:D:91:MET:HE3	7:D:112:PHE:CE1	2.56	0.41
15:L5:4774:C:O2'	15:L5:4775:C:O2	2.36	0.41
15:L5:4988:U:H4'	15:L5:4989:U:H5	1.86	0.41
17:L8:75:G:H2'	17:L8:76:C:C6	2.56	0.41
18:LA:180:LEU:HD11	57:Lp:18:TYR:CB	2.48	0.41
27:LL:59:VAL:O	27:LL:70:VAL:HG23	2.21	0.41
27:LL:61:CYS:HA	27:LL:62:PRO:HD3	1.90	0.41
27:LL:201:GLU:O	27:LL:204:GLU:HG3	2.19	0.41
34:LS:45:TRP:HA	34:LS:48:VAL:HG12	2.03	0.41
47:Lf:59:THR:OG1	47:Lf:65:ASN:OD1	2.38	0.41
53:LI:27:ILE:HD12	53:LI:30:LYS:HE3	2.02	0.41
60:Lt:143:VAL:HB	60:Lt:146:ARG:HB3	2.02	0.41
65:O2:373:ILE:HG22	65:O2:406:ARG:HE	1.85	0.41
68:v3:53:G:C2	68:v3:62:C:C2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:y3:206:ALA:CB	69:y3:249:LEU:HD11	2.50	0.41
7:D:28:PHE:CD1	7:D:464:GLU:OE1	2.73	0.41
19:LB:305:THR:HG21	19:LB:367:PHE:HA	2.02	0.41
20:LC:64:ALA:HB1	20:LC:78:ARG:O	2.20	0.41
22:LE:237:LYS:O	22:LE:237:LYS:HG2	2.20	0.41
35:LT:131:GLN:CD	35:LT:134:PRO:HD3	2.46	0.41
38:LW:37:GLU:O	38:LW:41:LEU:HD23	2.19	0.41
59:Ls:61:MET:CE	59:Ls:86:VAL:HG21	2.50	0.41
60:Lt:120:SER:O	60:Lt:123:ARG:HG2	2.20	0.41
60:Lt:127:GLY:HA2	60:Lt:130:LYS:HE3	2.03	0.41
61:Lz:193:LEU:H	61:Lz:193:LEU:HD23	1.85	0.41
63:N:71:ILE:HA	63:N:75:ILE:HD12	2.03	0.41
64:N2:136:ASP:N	64:N2:137:PRO:HD2	2.35	0.41
65:O2:238:HIS:CD2	65:O2:375:PRO:HG2	2.56	0.41
2:6:100:ALA:HA	2:6:133:ILE:HB	2.02	0.41
7:D:402:ARG:HH12	15:L5:2434:G:P	2.44	0.41
15:L5:1891:A:N6	15:L5:1892:A:H61	2.19	0.41
15:L5:2615:C:H5''	33:LR:60:ARG:HH12	1.85	0.41
15:L5:4881:U:C4	28:LM:113:MET:CE	3.03	0.41
29:LN:135:ILE:HD11	29:LN:142:ILE:CD1	2.48	0.41
41:LZ:29:ILE:HG13	41:LZ:40:HIS:NE2	2.35	0.41
46:Le:82:VAL:HG12	46:Le:111:ILE:HD13	2.03	0.41
65:O2:546:ASP:OD1	65:O2:547:ARG:N	2.53	0.41
69:y3:241:LEU:HD21	69:y3:246:THR:OG1	2.21	0.41
1:5:82:SER:O	1:5:110:LYS:HB2	2.21	0.41
6:B:96:PRO:HB3	6:B:101:LEU:HD12	2.02	0.41
15:L5:209:U:C4	15:L5:233:U:O4	2.73	0.41
15:L5:459:C:C5'	22:LE:110:ARG:HH21	2.33	0.41
15:L5:1977:C:HO2'	15:L5:1978:C:P	2.43	0.41
15:L5:4106:G:O2'	15:L5:4107:G:OP1	2.39	0.41
15:L5:4220:A:OP2	35:LT:2:THR:OG1	2.36	0.41
15:L5:4691:A:O3'	25:LH:71:ARG:HD3	2.20	0.41
17:L8:126:C:H1'	17:L8:127:U:O4'	2.21	0.41
19:LB:351:LEU:H	19:LB:351:LEU:HD23	1.84	0.41
35:LT:147:GLU:HG2	35:LT:148:PRO:HD2	2.01	0.41
39:LX:72:ASP:O	39:LX:76:ILE:HG12	2.20	0.41
43:Lb:13:SER:HA	43:Lb:16:TRP:CZ2	2.56	0.41
47:Lf:50:VAL:HG22	47:Lf:69:VAL:HG22	2.03	0.41
66:P2:323:THR:CG2	66:P2:334:LEU:HD11	2.49	0.41
70:LJ:174:ILE:HG22	70:LJ:175:LEU:H	1.85	0.41
7:D:38:THR:HG23	7:D:165:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:53:ILE:O	7:D:54:MET:C	2.64	0.41
10:G:26:LYS:HG2	33:LR:30:ASN:OD1	2.21	0.41
11:I:656:ARG:HG3	11:I:657:PRO:HD2	2.03	0.41
15:L5:914:U:H1'	15:L5:915:A:OP2	2.20	0.41
15:L5:1272:C:H5''	23:LF:34:ARG:HG2	2.02	0.41
20:LC:94:ASN:OD1	20:LC:95:MET:N	2.54	0.41
21:LD:92:LEU:C	21:LD:93:THR:HG22	2.46	0.41
60:Lt:125:LEU:HD12	60:Lt:127:GLY:H	1.85	0.41
64:N2:183:ALA:O	64:N2:187:VAL:HG22	2.21	0.41
3:7:13:GLU:O	3:7:14:ASP:C	2.64	0.41
4:8:61:VAL:HG12	4:8:62:GLN:N	2.36	0.41
5:A:37:TYR:HA	5:A:110:ASP:O	2.21	0.41
6:B:28:LEU:HD11	6:B:150:THR:O	2.21	0.41
7:D:157:VAL:HG11	8:E:80:PHE:CD1	2.56	0.41
7:D:460:ILE:HG22	7:D:464:GLU:OE2	2.20	0.41
11:I:429:TYR:O	11:I:432:ASN:HB3	2.21	0.41
15:L5:914:U:O2'	15:L5:915:A:OP2	2.33	0.41
15:L5:1444:G:C2	15:L5:1445:U:O2	2.73	0.41
15:L5:2710:C:O2	15:L5:2710:C:C2'	2.69	0.41
15:L5:4892:A:H2'	15:L5:4893:A:O4'	2.21	0.41
18:LA:150:LEU:HB3	18:LA:151:PRO:HD2	2.02	0.41
22:LE:155:GLY:O	22:LE:158:ARG:HG3	2.21	0.41
23:LF:30:ILE:HD13	23:LF:33:LEU:HD21	2.03	0.41
24:LG:131:LYS:O	24:LG:132:ARG:C	2.63	0.41
27:LL:9:VAL:HG23	27:LL:9:VAL:O	2.19	0.41
30:LO:183:LYS:O	30:LO:186:GLU:OE1	2.39	0.41
34:LS:27:LEU:HG	35:LT:148:PRO:HB3	2.03	0.41
37:LV:106:VAL:HG12	37:LV:112:MET:HA	2.03	0.41
47:Lf:35:ALA:HA	47:Lf:81:SER:HA	2.02	0.41
52:Lk:7:GLU:O	52:Lk:10:ASP:OD1	2.39	0.41
59:Ls:24:TYR:CD2	59:Ls:90:PHE:HB3	2.56	0.41
59:Ls:55:MET:SD	59:Ls:55:MET:C	3.04	0.41
61:Lz:111:LEU:HG	61:Lz:141:ASN:OD1	2.21	0.41
65:O2:235:GLU:O	65:O2:242:ILE:HG23	2.21	0.41
66:P2:79:LEU:HD12	66:P2:86:SER:OG	2.21	0.41
66:P2:335:ASN:OD1	66:P2:337:MET:HG2	2.21	0.41
70:LJ:58:ARG:NH1	70:LJ:58:ARG:O	2.53	0.41
15:L5:934:C:H4'	15:L5:935:A:H5''	2.03	0.41
15:L5:3965:A:N6	15:L5:4043:G:H22	2.18	0.41
15:L5:4139:G:H1'	15:L5:4146:G:N1	2.36	0.41
15:L5:4758:U:O2	15:L5:4758:U:O4'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LD:234:ASP:O	21:LD:235:MET:HB3	2.20	0.41
22:LE:214:ASP:OD1	22:LE:215:ALA:N	2.54	0.41
36:LU:27:HIS:N	36:LU:28:PRO:HD2	2.36	0.41
49:Lh:24:LEU:HA	49:Lh:27:GLU:OE1	2.22	0.41
59:Ls:51:ALA:HB2	59:Ls:91:THR:HG22	2.03	0.41
59:Ls:130:LEU:O	59:Ls:151:THR:HG23	2.21	0.41
60:Lt:77:ALA:HB3	60:Lt:80:LEU:CD2	2.51	0.41
68:v3:12:C:H42	68:v3:23:A:H61	1.68	0.41
69:y3:154:MET:SD	69:y3:159:LEU:HD23	2.61	0.41
1:5:114:ASP:OD1	1:5:114:ASP:C	2.64	0.40
6:B:31:SER:HB2	6:B:95:PHE:CD2	2.56	0.40
7:D:286:THR:O	7:D:287:SER:CB	2.69	0.40
7:D:323:THR:O	7:D:337:PRO:HA	2.21	0.40
7:D:391:ALA:CB	7:D:410:VAL:HG22	2.51	0.40
11:I:504:ASP:HB2	11:I:688:LEU:HD12	2.03	0.40
11:I:644:TYR:CD1	11:I:668:ILE:HG21	2.55	0.40
15:L5:1270:A:H1'	15:L5:1440:U:O4'	2.20	0.40
15:L5:2667:C:H1'	33:LR:96:MET:HE1	2.03	0.40
20:LC:2:ALA:HA	20:LC:3:CYS:C	2.46	0.40
20:LC:283:LYS:HD3	32:LQ:24:TYR:HB2	2.02	0.40
22:LE:89:LEU:H	22:LE:89:LEU:HD23	1.86	0.40
23:LF:64:MET:O	23:LF:68:GLU:OE1	2.38	0.40
26:LI:146:GLU:O	26:LI:149:ILE:HG22	2.21	0.40
30:LO:27:VAL:CG1	30:LO:98:ALA:O	2.69	0.40
30:LO:63:ASN:OD1	30:LO:64:THR:N	2.54	0.40
37:LV:112:MET:HE3	37:LV:132:ILE:HD13	2.03	0.40
40:LY:49:ILE:HD13	40:LY:80:ILE:HG21	2.03	0.40
53:Ll:12:PHE:CE2	53:Ll:51:LEU:HD23	2.56	0.40
60:Lt:80:LEU:HD12	60:Lt:81:ILE:N	2.36	0.40
64:N2:230:ILE:HD13	66:P2:435:PHE:HZ	1.86	0.40
65:O2:516:LYS:O	65:O2:520:GLU:OE1	2.39	0.40
66:P2:21:TRP:CZ3	66:P2:349:LEU:HD13	2.56	0.40
68:v3:19:G:N3	68:v3:57:G:N2	2.69	0.40
2:6:21:ALA:HB3	2:6:114:ALA:HA	2.03	0.40
2:6:71:ILE:HG12	2:6:95:LEU:HD22	2.03	0.40
2:6:164:PRO:HB2	3:7:139:PHE:HB2	2.04	0.40
3:7:60:VAL:O	3:7:64:VAL:HG23	2.21	0.40
7:D:161:ILE:HD11	8:E:77:SER:HB2	2.04	0.40
7:D:414:ASN:O	7:D:418:PRO:HD2	2.20	0.40
15:L5:2901:G:H1	15:L5:3598:C:H42	1.69	0.40
15:L5:4699:U:H4'	15:L5:4700:A:OP1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L5:5028:G:N3	15:L5:5028:G:H2'	2.36	0.40
17:L8:122:G:C6	17:L8:123:U:H1'	2.56	0.40
18:LA:243:THR:HG22	18:LA:244:GLY:N	2.36	0.40
51:Lj:64:MET:HE1	51:Lj:67:LEU:HD12	2.03	0.40
60:Lt:16:ARG:HD2	60:Lt:28:LEU:HD21	2.02	0.40
64:N2:163:ASP:OD1	64:N2:164:ILE:N	2.54	0.40
65:O2:396:LEU:HD11	65:O2:405:GLY:C	2.46	0.40
70:LJ:115:LEU:HA	70:LJ:116:GLY:HA2	1.87	0.40
1:5:261:LEU:O	1:5:264:ILE:HG22	2.21	0.40
6:B:109:VAL:HG11	6:B:152:VAL:HG11	2.03	0.40
10:G:62:ILE:HG22	10:G:66:MET:HE2	2.03	0.40
11:I:504:ASP:CG	11:I:688:LEU:HD12	2.46	0.40
11:I:586:THR:OG1	11:I:688:LEU:HD21	2.22	0.40
15:L5:661:C:H2'	15:L5:662:C:O4'	2.22	0.40
15:L5:1444:G:H2'	15:L5:1445:U:O4'	2.21	0.40
15:L5:2439:G:C6	15:L5:2440:U:C4	3.09	0.40
15:L5:3938:G:H5'	29:LN:24:ARG:HH12	1.87	0.40
17:L8:52:A:C6	53:Ll:23:ILE:HD11	2.56	0.40
17:L8:141:C:H2'	17:L8:142:U:C6	2.56	0.40
22:LE:96:VAL:HG23	22:LE:97:GLY:N	2.36	0.40
25:LH:120:GLU:OE1	25:LH:120:GLU:HA	2.21	0.40
34:LS:17:LEU:HD21	34:LS:60:GLU:HG3	2.04	0.40
34:LS:173:ASN:OD1	34:LS:173:ASN:C	2.64	0.40
37:LV:16:ILE:CD1	37:LV:57:VAL:HG22	2.51	0.40
41:LZ:14:LEU:CD1	48:Lg:88:ARG:NH1	2.84	0.40
41:LZ:123:LYS:O	41:LZ:124:THR:OG1	2.36	0.40
59:Ls:28:PHE:CD1	59:Ls:192:VAL:HG22	2.55	0.40
66:P2:593:TYR:HA	66:P2:597:LEU:HB2	2.03	0.40
69:y3:148:THR:HG23	69:y3:246:THR:OG1	2.21	0.40
2:6:110:ILE:HD12	2:6:125:THR:HG22	2.03	0.40
4:8:70:VAL:HG12	4:8:104:VAL:HG22	2.02	0.40
11:I:260:GLN:N	11:I:261:PRO:CD	2.85	0.40
11:I:437:ARG:HD2	13:K2:31:ASN:HA	2.04	0.40
14:L2:60:ALA:O	14:L2:64:MET:HG3	2.22	0.40
15:L5:1951:G:P	25:LH:1:MET:HE1	2.61	0.40
15:L5:2528:G:N3	15:L5:2528:G:H3'	2.36	0.40
15:L5:4037:C:H4'	15:L5:4037:C:OP1	2.21	0.40
16:L7:51:G:H21	70:LJ:12:MET:CE	2.35	0.40
29:LN:6:TYR:CZ	50:Li:40:VAL:HG22	2.56	0.40
43:Lb:66:SER:O	43:Lb:70:GLU:OE1	2.40	0.40
47:Lf:35:ALA:HB3	47:Lf:37:ASP:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Lg:100:GLN:O	48:Lg:103:VAL:HG22	2.21	0.40
63:N:3:VAL:HG12	63:N:4:GLY:N	2.36	0.40
69:y3:109:SER:CB	69:y3:275:ILE:HD12	2.52	0.40
2:6:159:PRO:O	2:6:164:PRO:HD3	2.21	0.40
4:8:115:LEU:CD1	4:8:125:ILE:HG23	2.51	0.40
10:G:45:LEU:HA	10:G:48:PHE:CE2	2.57	0.40
11:I:120:ALA:HB3	11:I:121:PRO:HD3	2.04	0.40
11:I:162:VAL:HG12	11:I:163:ALA:N	2.37	0.40
15:L5:924:C:H2'	15:L5:925:C:O4'	2.21	0.40
15:L5:964:A:H2'	15:L5:965:G:H4'	2.03	0.40
15:L5:1565:A:C4	15:L5:1566:C:H1'	2.57	0.40
15:L5:1726:U:O4'	23:LF:132:MET:HE1	2.22	0.40
15:L5:4076:G:OP1	24:LG:73:ARG:NE	2.55	0.40
15:L5:4764:A:N3	25:LH:44:GLU:OE2	2.55	0.40
17:L8:94:G:H21	51:Lj:82:THR:HB	1.85	0.40
26:LI:31:ILE:O	26:LI:31:ILE:HG23	2.21	0.40
26:LI:207:ASP:OD1	26:LI:208:LYS:N	2.55	0.40
35:LT:126:VAL:HG22	35:LT:127:GLN:N	2.37	0.40
58:Lr:97:ILE:HG13	58:Lr:102:TYR:O	2.22	0.40
59:Ls:12:ASN:OD1	59:Ls:13:TYR:N	2.55	0.40
61:Lz:23:ARG:NH1	61:Lz:174:MET:O	2.55	0.40
61:Lz:29:LEU:HD12	61:Lz:29:LEU:N	2.36	0.40
65:O2:190:ASN:OD1	65:O2:190:ASN:O	2.40	0.40
66:P2:551:SER:OG	66:P2:552:PRO:HD3	2.21	0.40
66:P2:586:MET:HA	66:P2:609:LEU:HD23	2.03	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	5	136/286 (48%)	133 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	6	160/183 (87%)	153 (96%)	7 (4%)	0	100	100
3	7	177/185 (96%)	173 (98%)	4 (2%)	0	100	100
4	8	148/173 (86%)	145 (98%)	3 (2%)	0	100	100
5	A	165/201 (82%)	161 (98%)	4 (2%)	0	100	100
6	B	195/229 (85%)	190 (97%)	4 (2%)	1 (0%)	25	60
7	D	448/476 (94%)	441 (98%)	6 (1%)	1 (0%)	44	75
8	E	30/96 (31%)	30 (100%)	0	0	100	100
9	F	65/68 (96%)	65 (100%)	0	0	100	100
10	G	52/66 (79%)	51 (98%)	1 (2%)	0	100	100
11	I	699/705 (99%)	689 (99%)	9 (1%)	1 (0%)	48	80
12	J	147/149 (99%)	146 (99%)	1 (1%)	0	100	100
13	K2	35/37 (95%)	35 (100%)	0	0	100	100
14	L2	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
18	LA	246/257 (96%)	239 (97%)	7 (3%)	0	100	100
19	LB	398/403 (99%)	390 (98%)	7 (2%)	1 (0%)	37	69
20	LC	366/427 (86%)	350 (96%)	16 (4%)	0	100	100
21	LD	291/297 (98%)	283 (97%)	8 (3%)	0	100	100
22	LE	232/288 (81%)	230 (99%)	2 (1%)	0	100	100
23	LF	223/248 (90%)	221 (99%)	2 (1%)	0	100	100
24	LG	239/266 (90%)	231 (97%)	8 (3%)	0	100	100
25	LH	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
26	LI	198/214 (92%)	192 (97%)	6 (3%)	0	100	100
27	LL	208/211 (99%)	200 (96%)	8 (4%)	0	100	100
28	LM	134/215 (62%)	131 (98%)	2 (2%)	1 (1%)	19	54
29	LN	201/204 (98%)	195 (97%)	4 (2%)	2 (1%)	13	47
30	LO	199/203 (98%)	197 (99%)	2 (1%)	0	100	100
31	LP	179/184 (97%)	174 (97%)	5 (3%)	0	100	100
32	LQ	185/188 (98%)	183 (99%)	2 (1%)	0	100	100
33	LR	175/196 (89%)	172 (98%)	3 (2%)	0	100	100
34	LS	173/176 (98%)	167 (96%)	6 (4%)	0	100	100
35	LT	157/160 (98%)	153 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	LU	99/128 (77%)	94 (95%)	5 (5%)	0	100	100
37	LV	129/140 (92%)	128 (99%)	1 (1%)	0	100	100
38	LW	61/157 (39%)	61 (100%)	0	0	100	100
39	LX	117/156 (75%)	116 (99%)	1 (1%)	0	100	100
40	LY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
41	LZ	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
42	La	145/148 (98%)	143 (99%)	2 (1%)	0	100	100
43	Lb	105/159 (66%)	101 (96%)	4 (4%)	0	100	100
44	Lc	96/115 (84%)	94 (98%)	2 (2%)	0	100	100
45	Ld	105/125 (84%)	103 (98%)	2 (2%)	0	100	100
46	Le	127/135 (94%)	125 (98%)	1 (1%)	1 (1%)	16	51
47	Lf	107/110 (97%)	102 (95%)	4 (4%)	1 (1%)	14	49
48	Lg	112/117 (96%)	112 (100%)	0	0	100	100
49	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
50	Li	100/105 (95%)	100 (100%)	0	0	100	100
51	Lj	84/97 (87%)	81 (96%)	2 (2%)	1 (1%)	11	43
52	Lk	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
53	Ll	48/51 (94%)	48 (100%)	0	0	100	100
54	Lm	50/128 (39%)	50 (100%)	0	0	100	100
55	Ln	22/25 (88%)	22 (100%)	0	0	100	100
56	Lo	103/106 (97%)	102 (99%)	1 (1%)	0	100	100
57	Lp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
58	Lr	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
59	Ls	194/317 (61%)	187 (96%)	7 (4%)	0	100	100
60	Lt	137/165 (83%)	122 (89%)	14 (10%)	1 (1%)	19	54
61	Lz	215/217 (99%)	198 (92%)	17 (8%)	0	100	100
62	M2	108/113 (96%)	108 (100%)	0	0	100	100
63	N	115/136 (85%)	115 (100%)	0	0	100	100
64	N2	408/456 (90%)	401 (98%)	7 (2%)	0	100	100
65	O2	578/607 (95%)	572 (99%)	6 (1%)	0	100	100
66	P2	603/631 (96%)	594 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	y3	228/846 (27%)	222 (97%)	5 (2%)	1 (0%)	30	64
70	LJ	174/178 (98%)	167 (96%)	6 (3%)	1 (1%)	22	57
All	All	11560/13633 (85%)	11296 (98%)	251 (2%)	13 (0%)	50	80

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	LM	88	ALA
29	LN	124	ASP
47	Lf	107	PRO
51	Lj	85	LYS
69	y3	93	LEU
70	LJ	95	ARG
6	B	217	ARG
7	D	287	SER
46	Le	92	ASN
60	Lt	142	ASN
29	LN	83	LYS
19	LB	302	ASN
11	I	451	PRO

### 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	5	125/253 (49%)	125 (100%)	0	100	100
2	6	135/153 (88%)	134 (99%)	1 (1%)	81	92
3	7	161/165 (98%)	161 (100%)	0	100	100
4	8	129/145 (89%)	129 (100%)	0	100	100
5	A	143/172 (83%)	143 (100%)	0	100	100
6	B	181/208 (87%)	181 (100%)	0	100	100
7	D	382/398 (96%)	382 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	E	28/74 (38%)	28 (100%)	0	100	100
9	F	59/59 (100%)	59 (100%)	0	100	100
10	G	47/55 (86%)	47 (100%)	0	100	100
11	I	611/615 (99%)	611 (100%)	0	100	100
12	J	130/130 (100%)	130 (100%)	0	100	100
13	K2	33/33 (100%)	33 (100%)	0	100	100
14	L2	70/70 (100%)	70 (100%)	0	100	100
18	LA	190/199 (96%)	190 (100%)	0	100	100
19	LB	348/349 (100%)	348 (100%)	0	100	100
20	LC	306/348 (88%)	306 (100%)	0	100	100
21	LD	246/250 (98%)	246 (100%)	0	100	100
22	LE	209/252 (83%)	209 (100%)	0	100	100
23	LF	194/215 (90%)	194 (100%)	0	100	100
24	LG	203/223 (91%)	203 (100%)	0	100	100
25	LH	169/171 (99%)	169 (100%)	0	100	100
26	LI	172/181 (95%)	172 (100%)	0	100	100
27	LL	176/177 (99%)	176 (100%)	0	100	100
28	LM	116/161 (72%)	116 (100%)	0	100	100
29	LN	171/172 (99%)	171 (100%)	0	100	100
30	LO	173/174 (99%)	173 (100%)	0	100	100
31	LP	160/163 (98%)	160 (100%)	0	100	100
32	LQ	164/165 (99%)	164 (100%)	0	100	100
33	LR	157/175 (90%)	157 (100%)	0	100	100
34	LS	156/157 (99%)	156 (100%)	0	100	100
35	LT	139/140 (99%)	139 (100%)	0	100	100
36	LU	91/115 (79%)	91 (100%)	0	100	100
37	LV	101/107 (94%)	101 (100%)	0	100	100
38	LW	55/126 (44%)	55 (100%)	0	100	100
39	LX	107/133 (80%)	107 (100%)	0	100	100
40	LY	124/135 (92%)	124 (100%)	0	100	100
41	LZ	117/118 (99%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	La	120/121 (99%)	120 (100%)	0	100	100
43	Lb	88/126 (70%)	88 (100%)	0	100	100
44	Lc	83/97 (86%)	83 (100%)	0	100	100
45	Ld	98/110 (89%)	98 (100%)	0	100	100
46	Le	115/121 (95%)	115 (100%)	0	100	100
47	Lf	88/89 (99%)	87 (99%)	1 (1%)	70	86
48	Lg	98/100 (98%)	98 (100%)	0	100	100
49	Lh	109/110 (99%)	109 (100%)	0	100	100
50	Li	86/89 (97%)	86 (100%)	0	100	100
51	Lj	73/80 (91%)	73 (100%)	0	100	100
52	Lk	64/65 (98%)	64 (100%)	0	100	100
53	Ll	47/48 (98%)	47 (100%)	0	100	100
54	Lm	48/116 (41%)	48 (100%)	0	100	100
55	Ln	23/24 (96%)	23 (100%)	0	100	100
56	Lo	93/94 (99%)	93 (100%)	0	100	100
57	Lp	74/75 (99%)	74 (100%)	0	100	100
58	Lr	109/121 (90%)	109 (100%)	0	100	100
59	Ls	162/258 (63%)	162 (100%)	0	100	100
60	Lt	112/137 (82%)	112 (100%)	0	100	100
61	Lz	195/196 (100%)	195 (100%)	0	100	100
62	M2	96/98 (98%)	96 (100%)	0	100	100
63	N	97/113 (86%)	97 (100%)	0	100	100
64	N2	356/391 (91%)	356 (100%)	0	100	100
65	O2	519/537 (97%)	519 (100%)	0	100	100
66	P2	521/541 (96%)	521 (100%)	0	100	100
69	y3	207/725 (29%)	207 (100%)	0	100	100
70	LJ	148/149 (99%)	147 (99%)	1 (1%)	81	92
All	All	10107/11667 (87%)	10104 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	6	134	LEU

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Mol	Chain	Res	Type
47	Lf	107	PRO
70	LJ	8	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	5	258	GLN
2	6	146	HIS
3	7	141	ASN
4	8	59	ASN
4	8	98	HIS
4	8	143	ASN
6	B	137	ASN
7	D	360	HIS
7	D	397	GLN
9	F	58	HIS
9	F	62	ASN
9	F	63	ASN
10	G	23	ASN
11	I	114	ASN
11	I	168	ASN
11	I	234	HIS
11	I	446	GLN
12	J	68	HIS
12	J	116	ASN
18	LA	97	ASN
18	LA	140	ASN
18	LA	205	ASN
19	LB	167	GLN
19	LB	204	GLN
19	LB	275	HIS
19	LB	301	ASN
20	LC	21	ASN
20	LC	38	ASN
20	LC	60	HIS
20	LC	245	HIS
21	LD	111	ASN
21	LD	131	ASN
21	LD	202	GLN
21	LD	275	GLN
22	LE	47	ASN
24	LG	141	ASN

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Mol	Chain	Res	Type
24	LG	195	HIS
25	LH	98	HIS
25	LH	140	GLN
25	LH	156	ASN
26	LI	59	GLN
26	LI	144	ASN
28	LM	20	HIS
28	LM	48	GLN
29	LN	32	GLN
29	LN	37	HIS
29	LN	158	HIS
30	LO	180	GLN
30	LO	184	ASN
31	LP	21	ASN
31	LP	34	GLN
31	LP	56	GLN
31	LP	133	HIS
32	LQ	7	HIS
33	LR	118	HIS
35	LT	144	ASN
38	LW	59	HIS
39	LX	107	HIS
40	LY	96	HIS
42	La	34	ASN
42	La	44	ASN
42	La	74	ASN
43	Lb	6	ASN
43	Lb	60	ASN
45	Ld	79	ASN
45	Ld	121	ASN
46	Le	23	HIS
47	Lf	56	ASN
48	Lg	112	GLN
49	Lh	68	ASN
50	Li	26	HIS
52	Lk	31	ASN
53	Ll	19	GLN
58	Lr	100	ASN
60	Lt	149	HIS
61	Lz	19	HIS
61	Lz	44	GLN
61	Lz	171	HIS

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Mol	Chain	Res	Type
62	M2	81	ASN
63	N	57	ASN
66	P2	232	GLN
66	P2	543	ASN
66	P2	601	GLN
69	y3	57	GLN
69	y3	129	ASN
70	LJ	46	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	L5	3697/5066 (72%)	795 (21%)	17 (0%)
16	L7	119/121 (98%)	9 (7%)	0
17	L8	155/157 (98%)	26 (16%)	0
67	u3	74/76 (97%)	26 (35%)	0
68	v3	75/76 (98%)	31 (41%)	0
All	All	4120/5496 (74%)	887 (21%)	17 (0%)

All (887) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	L5	17	A
15	L5	30	C
15	L5	39	A
15	L5	42	A
15	L5	48	G
15	L5	56	A
15	L5	59	A
15	L5	64	A
15	L5	65	A
15	L5	66	A
15	L5	69	A
15	L5	72	C
15	L5	73	A
15	L5	74	G
15	L5	91	G
15	L5	98	A
15	L5	104	G
15	L5	108	A
15	L5	109	G

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Mol	Chain	Res	Type
15	L5	110	C
15	L5	119	G
15	L5	120	A
15	L5	132	G
15	L5	133	C
15	L5	134	G
15	L5	135	G
15	L5	136	C
15	L5	137	G
15	L5	152	U
15	L5	159	C
15	L5	165	A
15	L5	181	C
15	L5	183	C
15	L5	184	U
15	L5	185	C
15	L5	188	G
15	L5	189	G
15	L5	200	U
15	L5	209	U
15	L5	216	C
15	L5	218	A
15	L5	219	G
15	L5	232	G
15	L5	233	U
15	L5	234	G
15	L5	255	C
15	L5	256	G
15	L5	261	G
15	L5	265	C
15	L5	266	C
15	L5	267	G
15	L5	269	G
15	L5	280	G
15	L5	297	U
15	L5	306	A
15	L5	315	G
15	L5	316	U
15	L5	340	C
15	L5	349	A
15	L5	350	C
15	L5	373	G

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Mol	Chain	Res	Type
15	L5	387	G
15	L5	388	A
15	L5	396	A
15	L5	401	G
15	L5	407	A
15	L5	408	A
15	L5	409	G
15	L5	410	A
15	L5	411	G
15	L5	412	G
15	L5	413	G
15	L5	431	G
15	L5	432	U
15	L5	449	C
15	L5	450	G
15	L5	452	A
15	L5	453	G
15	L5	454	U
15	L5	456	C
15	L5	457	G
15	L5	467	U
15	L5	468	U
15	L5	484	U
15	L5	485	C
15	L5	486	C
15	L5	489	C
15	L5	493	G
15	L5	494	U
15	L5	497	G
15	L5	498	C
15	L5	499	G
15	L5	500	G
15	L5	502	C
15	L5	503	C
15	L5	504	G
15	L5	505	G
15	L5	509	A
15	L5	510	U
15	L5	512	U
15	L5	513	U
15	L5	514	U
15	L5	515	C

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Mol	Chain	Res	Type
15	L5	516	C
15	L5	517	C
15	L5	518	G
15	L5	643	C
15	L5	646	G
15	L5	656	C
15	L5	657	C
15	L5	659	G
15	L5	665	C
15	L5	666	G
15	L5	667	A
15	L5	668	C
15	L5	669	C
15	L5	673	C
15	L5	685	C
15	L5	686	A
15	L5	687	U
15	L5	688	U
15	L5	696	C
15	L5	703	G
15	L5	704	C
15	L5	730	G
15	L5	731	G
15	L5	738	C
15	L5	739	G
15	L5	740	G
15	L5	742	G
15	L5	744	G
15	L5	746	A
15	L5	753	C
15	L5	758	G
15	L5	759	G
15	L5	760	G
15	L5	904	C
15	L5	913	U
15	L5	914	U
15	L5	915	A
15	L5	917	A
15	L5	918	G
15	L5	923	C
15	L5	924	C
15	L5	926	G

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Mol	Chain	Res	Type
15	L5	932	A
15	L5	933	G
15	L5	934	C
15	L5	935	A
15	L5	936	C
15	L5	937	U
15	L5	944	A
15	L5	945	U
15	L5	956	A
15	L5	959	G
15	L5	960	A
15	L5	961	G
15	L5	962	C
15	L5	965	G
15	L5	967	C
15	L5	970	G
15	L5	977	C
15	L5	982	U
15	L5	984	C
15	L5	985	C
15	L5	989	U
15	L5	990	C
15	L5	992	C
15	L5	1070	G
15	L5	1072	C
15	L5	1074	G
15	L5	1075	G
15	L5	1082	C
15	L5	1083	U
15	L5	1095	A
15	L5	1168	G
15	L5	1171	G
15	L5	1173	G
15	L5	1178	G
15	L5	1179	U
15	L5	1180	C
15	L5	1181	C
15	L5	1182	C
15	L5	1183	C
15	L5	1202	C
15	L5	1203	G
15	L5	1204	C

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Mol	Chain	Res	Type
15	L5	1210	C
15	L5	1211	G
15	L5	1214	C
15	L5	1215	C
15	L5	1217	G
15	L5	1218	G
15	L5	1219	G
15	L5	1222	A
15	L5	1235	G
15	L5	1241	C
15	L5	1246	G
15	L5	1253	G
15	L5	1254	A
15	L5	1257	A
15	L5	1258	G
15	L5	1266	G
15	L5	1267	C
15	L5	1269	G
15	L5	1270	A
15	L5	1271	G
15	L5	1272	C
15	L5	1273	G
15	L5	1274	A
15	L5	1275	G
15	L5	1277	G
15	L5	1280	C
15	L5	1284	G
15	L5	1285	U
15	L5	1287	G
15	L5	1294	A
15	L5	1295	C
15	L5	1301	C
15	L5	1324	A
15	L5	1326	A
15	L5	1330	A
15	L5	1337	A
15	L5	1344	C
15	L5	1354	A
15	L5	1358	G
15	L5	1359	G
15	L5	1365	C
15	L5	1367	C

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Mol	Chain	Res	Type
15	L5	1378	C
15	L5	1387	A
15	L5	1393	G
15	L5	1394	G
15	L5	1397	A
15	L5	1404	G
15	L5	1405	C
15	L5	1407	C
15	L5	1409	C
15	L5	1410	U
15	L5	1411	C
15	L5	1414	C
15	L5	1420	A
15	L5	1435	G
15	L5	1437	C
15	L5	1439	C
15	L5	1440	U
15	L5	1441	C
15	L5	1443	A
15	L5	1446	C
15	L5	1447	C
15	L5	1482	G
15	L5	1483	C
15	L5	1493	G
15	L5	1497	A
15	L5	1498	G
15	L5	1502	G
15	L5	1514	U
15	L5	1517	G
15	L5	1534	A
15	L5	1547	A
15	L5	1562	G
15	L5	1566	C
15	L5	1578	U
15	L5	1591	U
15	L5	1596	U
15	L5	1624	G
15	L5	1625	G
15	L5	1631	A
15	L5	1633	G
15	L5	1634	A
15	L5	1638	A

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Mol	Chain	Res	Type
15	L5	1640	C
15	L5	1654	G
15	L5	1661	C
15	L5	1676	C
15	L5	1677	U
15	L5	1678	C
15	L5	1694	C
15	L5	1697	G
15	L5	1699	A
15	L5	1700	G
15	L5	1703	C
15	L5	1704	C
15	L5	1705	G
15	L5	1707	C
15	L5	1715	C
15	L5	1716	G
15	L5	1717	C
15	L5	1718	C
15	L5	1726	U
15	L5	1734	G
15	L5	1735	U
15	L5	1741	G
15	L5	1742	A
15	L5	1745	G
15	L5	1750	G
15	L5	1755	C
15	L5	1757	U
15	L5	1758	G
15	L5	1760	G
15	L5	1761	G
15	L5	1762	C
15	L5	1763	C
15	L5	1764	G
15	L5	1765	A
15	L5	1766	A
15	L5	1768	C
15	L5	1770	A
15	L5	1775	A
15	L5	1785	C
15	L5	1787	A
15	L5	1804	A
15	L5	1810	G

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Mol	Chain	Res	Type
15	L5	1820	C
15	L5	1821	G
15	L5	1822	U
15	L5	1834	U
15	L5	1836	G
15	L5	1837	A
15	L5	1842	G
15	L5	1843	A
15	L5	1855	G
15	L5	1869	G
15	L5	1882	U
15	L5	1897	A
15	L5	1918	U
15	L5	1919	G
15	L5	1920	C
15	L5	1921	C
15	L5	1922	G
15	L5	1925	G
15	L5	1931	C
15	L5	1932	A
15	L5	1936	C
15	L5	1940	G
15	L5	1947	U
15	L5	1948	G
15	L5	1951	G
15	L5	1959	U
15	L5	1960	A
15	L5	1961	G
15	L5	1962	A
15	L5	1974	U
15	L5	1975	G
15	L5	1978	C
15	L5	1980	U
15	L5	1983	A
15	L5	1984	A
15	L5	1985	G
15	L5	1987	C
15	L5	1988	G
15	L5	1991	A
15	L5	1992	U
15	L5	1993	C
15	L5	1997	U

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Mol	Chain	Res	Type
15	L5	1998	A
15	L5	2001	G
15	L5	2002	A
15	L5	2014	C
15	L5	2017	A
15	L5	2018	C
15	L5	2024	G
15	L5	2026	A
15	L5	2034	G
15	L5	2044	U
15	L5	2046	G
15	L5	2048	U
15	L5	2055	G
15	L5	2056	G
15	L5	2062	C
15	L5	2069	A
15	L5	2084	C
15	L5	2085	G
15	L5	2089	G
15	L5	2092	G
15	L5	2093	A
15	L5	2095	A
15	L5	2096	G
15	L5	2097	U
15	L5	2098	G
15	L5	2101	C
15	L5	2102	G
15	L5	2108	G
15	L5	2112	G
15	L5	2113	G
15	L5	2250	C
15	L5	2252	G
15	L5	2253	A
15	L5	2256	C
15	L5	2257	C
15	L5	2258	C
15	L5	2260	C
15	L5	2289	C
15	L5	2300	A
15	L5	2301	G
15	L5	2306	G
15	L5	2313	A

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Mol	Chain	Res	Type
15	L5	2332	A
15	L5	2333	G
15	L5	2346	C
15	L5	2348	G
15	L5	2351	C
15	L5	2369	U
15	L5	2395	A
15	L5	2397	G
15	L5	2417	A
15	L5	2418	A
15	L5	2421	G
15	L5	2425	U
15	L5	2437	C
15	L5	2441	C
15	L5	2445	C
15	L5	2447	U
15	L5	2450	G
15	L5	2453	A
15	L5	2464	C
15	L5	2465	C
15	L5	2474	G
15	L5	2475	G
15	L5	2478	C
15	L5	2479	G
15	L5	2483	G
15	L5	2484	A
15	L5	2485	U
15	L5	2487	G
15	L5	2488	C
15	L5	2489	C
15	L5	2490	U
15	L5	2494	U
15	L5	2503	G
15	L5	2504	C
15	L5	2505	C
15	L5	2506	G
15	L5	2513	A
15	L5	2519	U
15	L5	2537	A
15	L5	2544	G
15	L5	2546	G
15	L5	2547	G

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Mol	Chain	Res	Type
15	L5	2554	U
15	L5	2560	C
15	L5	2565	A
15	L5	2573	A
15	L5	2583	C
15	L5	2587	A
15	L5	2589	C
15	L5	2601	A
15	L5	2611	A
15	L5	2618	G
15	L5	2638	G
15	L5	2652	G
15	L5	2653	C
15	L5	2662	G
15	L5	2669	C
15	L5	2676	A
15	L5	2687	U
15	L5	2694	G
15	L5	2695	A
15	L5	2696	A
15	L5	2703	G
15	L5	2707	U
15	L5	2708	U
15	L5	2709	C
15	L5	2710	C
15	L5	2711	G
15	L5	2721	G
15	L5	2724	G
15	L5	2726	G
15	L5	2739	C
15	L5	2742	G
15	L5	2743	A
15	L5	2756	G
15	L5	2761	U
15	L5	2763	U
15	L5	2764	A
15	L5	2769	U
15	L5	2770	C
15	L5	2787	A
15	L5	2788	U
15	L5	2790	U
15	L5	2815	A

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Mol	Chain	Res	Type
15	L5	2826	U
15	L5	2827	G
15	L5	2838	G
15	L5	2848	G
15	L5	2855	G
15	L5	2867	C
15	L5	2877	G
15	L5	2892	C
15	L5	2902	G
15	L5	2903	G
15	L5	2904	U
15	L5	2905	C
15	L5	2906	G
15	L5	2907	G
15	L5	2908	U
15	L5	3585	G
15	L5	3586	G
15	L5	3587	C
15	L5	3590	G
15	L5	3591	C
15	L5	3594	C
15	L5	3595	U
15	L5	3596	A
15	L5	3597	G
15	L5	3604	A
15	L5	3606	U
15	L5	3615	G
15	L5	3616	U
15	L5	3618	C
15	L5	3626	G
15	L5	3630	A
15	L5	3635	A
15	L5	3644	U
15	L5	3646	A
15	L5	3653	A
15	L5	3662	A
15	L5	3673	C
15	L5	3674	G
15	L5	3711	A
15	L5	3713	U
15	L5	3714	G
15	L5	3727	A

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Mol	Chain	Res	Type
15	L5	3748	A
15	L5	3750	G
15	L5	3753	G
15	L5	3754	G
15	L5	3757	G
15	L5	3758	U
15	L5	3759	A
15	L5	3760	A
15	L5	3771	C
15	L5	3776	G
15	L5	3777	G
15	L5	3784	A
15	L5	3786	U
15	L5	3802	U
15	L5	3811	G
15	L5	3814	U
15	L5	3817	A
15	L5	3818	U
15	L5	3819	G
15	L5	3823	G
15	L5	3838	U
15	L5	3839	G
15	L5	3840	U
15	L5	3851	U
15	L5	3865	A
15	L5	3867	A
15	L5	3877	A
15	L5	3878	C
15	L5	3879	G
15	L5	3885	G
15	L5	3887	C
15	L5	3897	G
15	L5	3898	G
15	L5	3901	A
15	L5	3906	A
15	L5	3907	G
15	L5	3908	A
15	L5	3915	U
15	L5	3938	G
15	L5	3942	A
15	L5	3943	A
15	L5	3944	G

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Mol	Chain	Res	Type
15	L5	3947	A
15	L5	3948	C
15	L5	3950	U
15	L5	3953	G
15	L5	3955	G
15	L5	3956	G
15	L5	3957	U
15	L5	3958	G
15	L5	3959	U
15	L5	3961	G
15	L5	3962	A
15	L5	3963	A
15	L5	3964	U
15	L5	3965	A
15	L5	3966	A
15	L5	3968	U
15	L5	3969	G
15	L5	3970	G
15	L5	3971	G
15	L5	3974	G
15	L5	3977	C
15	L5	4035	G
15	L5	4036	G
15	L5	4037	C
15	L5	4040	C
15	L5	4041	C
15	L5	4042	G
15	L5	4043	G
15	L5	4044	U
15	L5	4046	A
15	L5	4048	A
15	L5	4049	U
15	L5	4050	A
15	L5	4051	C
15	L5	4052	C
15	L5	4053	A
15	L5	4054	C
15	L5	4055	U
15	L5	4056	A
15	L5	4057	C
15	L5	4058	U
15	L5	4059	C

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Mol	Chain	Res	Type
15	L5	4062	A
15	L5	4063	U
15	L5	4064	C
15	L5	4065	G
15	L5	4076	G
15	L5	4084	G
15	L5	4086	G
15	L5	4094	G
15	L5	4095	G
15	L5	4096	C
15	L5	4097	G
15	L5	4098	A
15	L5	4099	G
15	L5	4101	C
15	L5	4102	C
15	L5	4103	C
15	L5	4104	G
15	L5	4107	G
15	L5	4108	G
15	L5	4111	U
15	L5	4113	U
15	L5	4114	C
15	L5	4115	G
15	L5	4116	C
15	L5	4117	U
15	L5	4119	C
15	L5	4122	G
15	L5	4127	A
15	L5	4140	C
15	L5	4141	G
15	L5	4142	C
15	L5	4143	G
15	L5	4144	C
15	L5	4146	G
15	L5	4162	C
15	L5	4163	U
15	L5	4168	G
15	L5	4170	A
15	L5	4177	C
15	L5	4183	G
15	L5	4184	G
15	L5	4191	G

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Mol	Chain	Res	Type
15	L5	4196	G
15	L5	4203	A
15	L5	4222	G
15	L5	4228	G
15	L5	4229	U
15	L5	4233	A
15	L5	4237	C
15	L5	4251	A
15	L5	4254	G
15	L5	4256	A
15	L5	4257	A
15	L5	4258	C
15	L5	4265	U
15	L5	4268	A
15	L5	4273	A
15	L5	4281	A
15	L5	4291	G
15	L5	4305	G
15	L5	4306	U
15	L5	4314	C
15	L5	4319	C
15	L5	4329	G
15	L5	4330	G
15	L5	4332	C
15	L5	4349	C
15	L5	4373	G
15	L5	4377	G
15	L5	4378	A
15	L5	4380	A
15	L5	4387	C
15	L5	4394	A
15	L5	4405	G
15	L5	4422	A
15	L5	4448	G
15	L5	4449	A
15	L5	4452	U
15	L5	4453	C
15	L5	4464	A
15	L5	4475	G
15	L5	4488	A
15	L5	4500	U
15	L5	4512	U

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Mol	Chain	Res	Type
15	L5	4513	A
15	L5	4518	A
15	L5	4519	C
15	L5	4531	U
15	L5	4545	G
15	L5	4548	A
15	L5	4549	G
15	L5	4557	U
15	L5	4567	G
15	L5	4573	G
15	L5	4575	G
15	L5	4584	A
15	L5	4589	A
15	L5	4590	A
15	L5	4600	G
15	L5	4617	G
15	L5	4636	U
15	L5	4637	G
15	L5	4656	A
15	L5	4670	C
15	L5	4672	A
15	L5	4679	G
15	L5	4684	A
15	L5	4687	A
15	L5	4694	G
15	L5	4695	C
15	L5	4700	A
15	L5	4708	A
15	L5	4709	U
15	L5	4719	G
15	L5	4731	G
15	L5	4733	C
15	L5	4734	A
15	L5	4740	G
15	L5	4741	C
15	L5	4742	G
15	L5	4745	G
15	L5	4750	G
15	L5	4754	G
15	L5	4757	C
15	L5	4759	C
15	L5	4761	G

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Mol	Chain	Res	Type
15	L5	4765	G
15	L5	4771	C
15	L5	4772	C
15	L5	4775	C
15	L5	4859	C
15	L5	4863	G
15	L5	4870	G
15	L5	4871	C
15	L5	4875	G
15	L5	4881	U
15	L5	4882	U
15	L5	4883	C
15	L5	4888	U
15	L5	4889	G
15	L5	4895	C
15	L5	4896	G
15	L5	4900	C
15	L5	4901	G
15	L5	4902	C
15	L5	4910	A
15	L5	4912	G
15	L5	4914	C
15	L5	4922	C
15	L5	4923	C
15	L5	4925	U
15	L5	4927	G
15	L5	4928	C
15	L5	4934	A
15	L5	4940	C
15	L5	4941	G
15	L5	4943	A
15	L5	4944	C
15	L5	4951	G
15	L5	4955	A
15	L5	4960	G
15	L5	4961	G
15	L5	4963	G
15	L5	4966	A
15	L5	4976	U
15	L5	4979	A
15	L5	4988	U
15	L5	4989	U

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Mol	Chain	Res	Type
15	L5	4991	U
15	L5	5013	C
15	L5	5014	A
15	L5	5017	G
15	L5	5022	U
15	L5	5023	C
15	L5	5025	C
15	L5	5026	U
15	L5	5028	G
15	L5	5029	C
15	L5	5031	G
15	L5	5034	A
15	L5	5041	G
15	L5	5050	C
15	L5	5053	U
15	L5	5054	C
15	L5	5055	G
15	L5	5058	A
15	L5	5061	A
15	L5	5069	U
16	L7	4	U
16	L7	33	U
16	L7	38	U
16	L7	53	U
16	L7	54	A
16	L7	62	U
16	L7	63	C
16	L7	64	G
16	L7	100	A
17	L8	2	G
17	L8	25	G
17	L8	34	U
17	L8	35	C
17	L8	48	A
17	L8	59	A
17	L8	60	G
17	L8	62	A
17	L8	63	U
17	L8	82	A
17	L8	83	C
17	L8	84	A
17	L8	85	U

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Mol	Chain	Res	Type
17	L8	86	U
17	L8	87	G
17	L8	103	A
17	L8	105	C
17	L8	110	U
17	L8	111	U
17	L8	114	G
17	L8	123	U
17	L8	124	U
17	L8	125	C
17	L8	126	C
17	L8	127	U
17	L8	156	U
67	u3	4	C
67	u3	8	U
67	u3	15	G
67	u3	17	C
67	u3	18	G
67	u3	19	G
67	u3	20	U
67	u3	21	A
67	u3	24	G
67	u3	44	G
67	u3	46	G
67	u3	48	C
67	u3	50	U
67	u3	52	G
67	u3	55	U
67	u3	56	C
67	u3	57	G
67	u3	59	U
67	u3	60	U
67	u3	61	C
67	u3	64	A
67	u3	69	G
67	u3	71	G
67	u3	72	C
67	u3	74	C
67	u3	76	A
68	v3	8	U
68	v3	11	C
68	v3	12	C

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Mol	Chain	Res	Type
68	v3	13	C
68	v3	16	A
68	v3	17	A
68	v3	18	G
68	v3	19	G
68	v3	20	U
68	v3	21	A
68	v3	22	G
68	v3	23	A
68	v3	30	G
68	v3	44	G
68	v3	47	U
68	v3	48	C
68	v3	49	C
68	v3	51	U
68	v3	54	U
68	v3	55	U
68	v3	56	C
68	v3	58	A
68	v3	61	C
68	v3	62	C
68	v3	68	C
68	v3	69	G
68	v3	71	G
68	v3	72	C
68	v3	73	A
68	v3	75	C
68	v3	76	A

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	L5	406	C
15	L5	493	G
15	L5	914	U
15	L5	1082	C
15	L5	1633	G
15	L5	1977	C
15	L5	2033	A
15	L5	2416	G
15	L5	2675	G
15	L5	2760	G

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Mol	Chain	Res	Type
15	L5	2786	C
15	L5	3614	G
15	L5	3673	C
15	L5	4054	C
15	L5	4106	G
15	L5	4699	U
15	L5	4913	G

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

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

## 5.5 Carbohydrates [i](#)

20 monosaccharides 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	$\# Z  > 2$
72	NAG	C	1	72	14,14,15	0.72	0	17,19,21	1.07	1 (5%)
72	NAG	C	2	72	14,14,15	0.72	0	17,19,21	0.85	0
73	NAG	H	1	11,73	14,14,15	0.70	0	17,19,21	0.74	0
73	NAG	H	2	73	14,14,15	0.73	0	17,19,21	0.79	0
73	BMA	H	3	73	11,11,12	0.83	0	15,15,17	0.97	1 (6%)
73	MAN	H	4	73	11,11,12	0.76	0	15,15,17	1.14	1 (6%)
73	MAN	H	5	73	11,11,12	0.76	0	15,15,17	1.03	1 (6%)
73	MAN	H	6	73	11,11,12	0.77	0	15,15,17	1.01	1 (6%)
73	MAN	H	7	73	11,11,12	0.69	0	15,15,17	1.21	1 (6%)
73	MAN	H	8	73	11,11,12	0.72	0	15,15,17	1.00	1 (6%)
71	NAG	K	1	71	14,14,15	0.66	0	17,19,21	1.30	3 (17%)
71	NAG	K	2	71	14,14,15	0.75	0	17,19,21	0.76	0
71	BMA	K	3	71	11,11,12	0.84	0	15,15,17	1.39	1 (6%)
71	MAN	K	4	71	11,11,12	0.80	1 (9%)	15,15,17	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
71	MAN	K	5	71	11,11,12	0.85	1 (9%)	15,15,17	0.94	0
71	MAN	K	6	71	11,11,12	0.82	1 (9%)	15,15,17	0.93	0
71	MAN	K	7	71	11,11,12	0.76	0	15,15,17	0.97	1 (6%)
71	MAN	K	8	71	11,11,12	0.76	0	15,15,17	0.90	0
74	NDG	L	1	74,75	14,14,15	0.83	0	17,19,21	1.70	3 (17%)
74	NAG	L	2	74	14,14,15	0.75	0	17,19,21	0.92	1 (5%)

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
72	NAG	C	1	72	-	4/6/23/26	0/1/1/1
72	NAG	C	2	72	-	0/6/23/26	0/1/1/1
73	NAG	H	1	11,73	-	2/6/23/26	0/1/1/1
73	NAG	H	2	73	-	0/6/23/26	0/1/1/1
73	BMA	H	3	73	-	0/2/19/22	0/1/1/1
73	MAN	H	4	73	-	0/2/19/22	0/1/1/1
73	MAN	H	5	73	-	2/2/19/22	0/1/1/1
73	MAN	H	6	73	-	1/2/19/22	0/1/1/1
73	MAN	H	7	73	-	2/2/19/22	1/1/1/1
73	MAN	H	8	73	-	1/2/19/22	1/1/1/1
71	NAG	K	1	71	-	2/6/23/26	0/1/1/1
71	NAG	K	2	71	-	1/6/23/26	0/1/1/1
71	BMA	K	3	71	-	0/2/19/22	0/1/1/1
71	MAN	K	4	71	-	0/2/19/22	0/1/1/1
71	MAN	K	5	71	-	0/2/19/22	0/1/1/1
71	MAN	K	6	71	-	2/2/19/22	0/1/1/1
71	MAN	K	7	71	-	0/2/19/22	0/1/1/1
71	MAN	K	8	71	-	0/2/19/22	0/1/1/1
74	NDG	L	1	74,75	-	2/6/23/26	0/1/1/1
74	NAG	L	2	74	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	K	5	MAN	O5-C1	-2.27	1.39	1.43
71	K	4	MAN	O5-C1	-2.09	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
71	K	6	MAN	O5-C1	-2.09	1.40	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
74	L	1	NDG	C1-O5-C5	4.73	118.52	112.19
71	K	3	BMA	C1-O5-C5	4.62	118.38	112.19
73	H	7	MAN	C1-O5-C5	3.67	117.10	112.19
72	C	1	NAG	C2-N2-C7	3.36	127.41	122.90
71	K	1	NAG	C2-N2-C7	3.21	127.20	122.90
74	L	1	NDG	O5-C1-C2	3.21	116.25	111.29
73	H	4	MAN	C1-O5-C5	3.04	116.25	112.19
73	H	3	BMA	C1-O5-C5	2.90	116.07	112.19
73	H	5	MAN	C1-O5-C5	2.80	115.94	112.19
73	H	8	MAN	C1-O5-C5	2.69	115.80	112.19
74	L	1	NDG	C3-C4-C5	-2.61	105.50	110.23
73	H	6	MAN	C1-O5-C5	2.54	115.59	112.19
74	L	2	NAG	O5-C1-C2	-2.47	107.48	111.29
71	K	7	MAN	C1-O5-C5	2.38	115.37	112.19
71	K	1	NAG	C4-C3-C2	-2.09	107.95	111.02
71	K	1	NAG	O5-C1-C2	-2.03	108.14	111.29

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
71	K	6	MAN	C4-C5-C6-O6
72	C	1	NAG	C4-C5-C6-O6
71	K	6	MAN	O5-C5-C6-O6
74	L	2	NAG	O5-C5-C6-O6
73	H	7	MAN	O5-C5-C6-O6
73	H	1	NAG	C4-C5-C6-O6
74	L	2	NAG	C4-C5-C6-O6
71	K	1	NAG	C8-C7-N2-C2
71	K	1	NAG	O7-C7-N2-C2
72	C	1	NAG	C8-C7-N2-C2
72	C	1	NAG	O7-C7-N2-C2
72	C	1	NAG	O5-C5-C6-O6
73	H	5	MAN	O5-C5-C6-O6
73	H	1	NAG	O5-C5-C6-O6
73	H	7	MAN	C4-C5-C6-O6
71	K	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
73	H	8	MAN	O5-C5-C6-O6
73	H	6	MAN	O5-C5-C6-O6
74	L	1	NDG	C4-C5-C6-O6
73	H	5	MAN	C4-C5-C6-O6
74	L	1	NDG	O5-C5-C6-O6

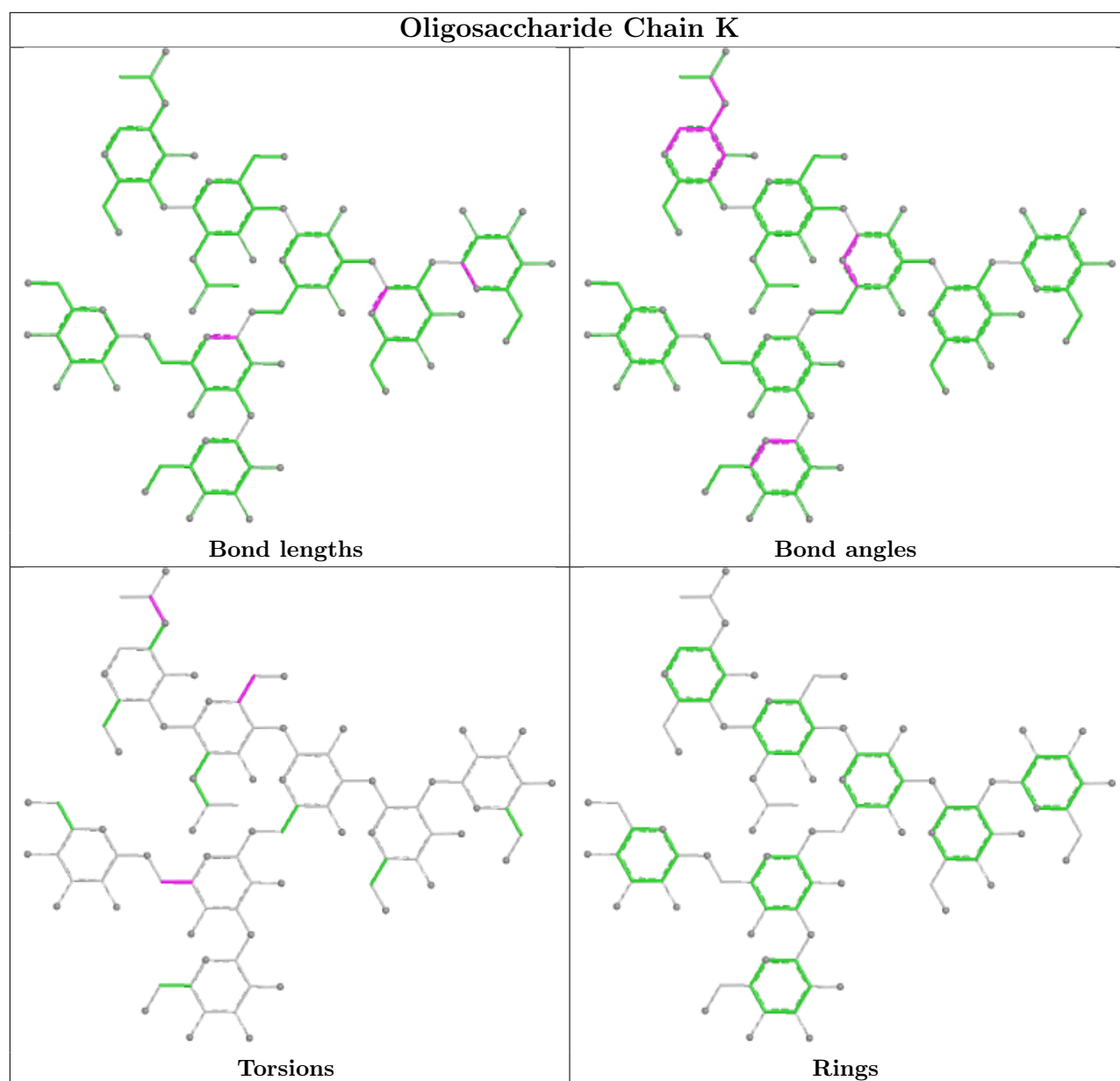
All (2) ring outliers are listed below:

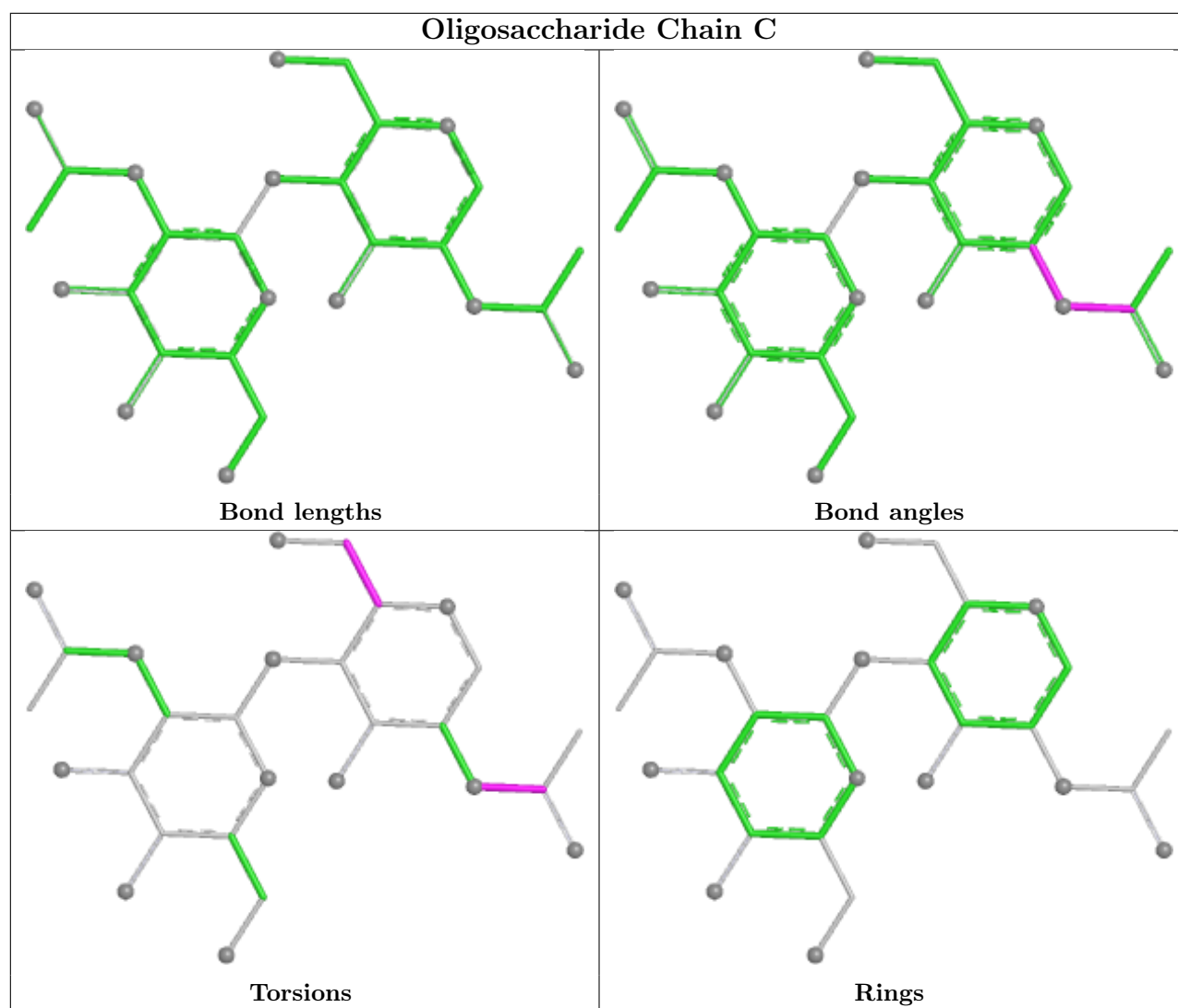
Mol	Chain	Res	Type	Atoms
73	H	7	MAN	C1-C2-C3-C4-C5-O5
73	H	8	MAN	C1-C2-C3-C4-C5-O5

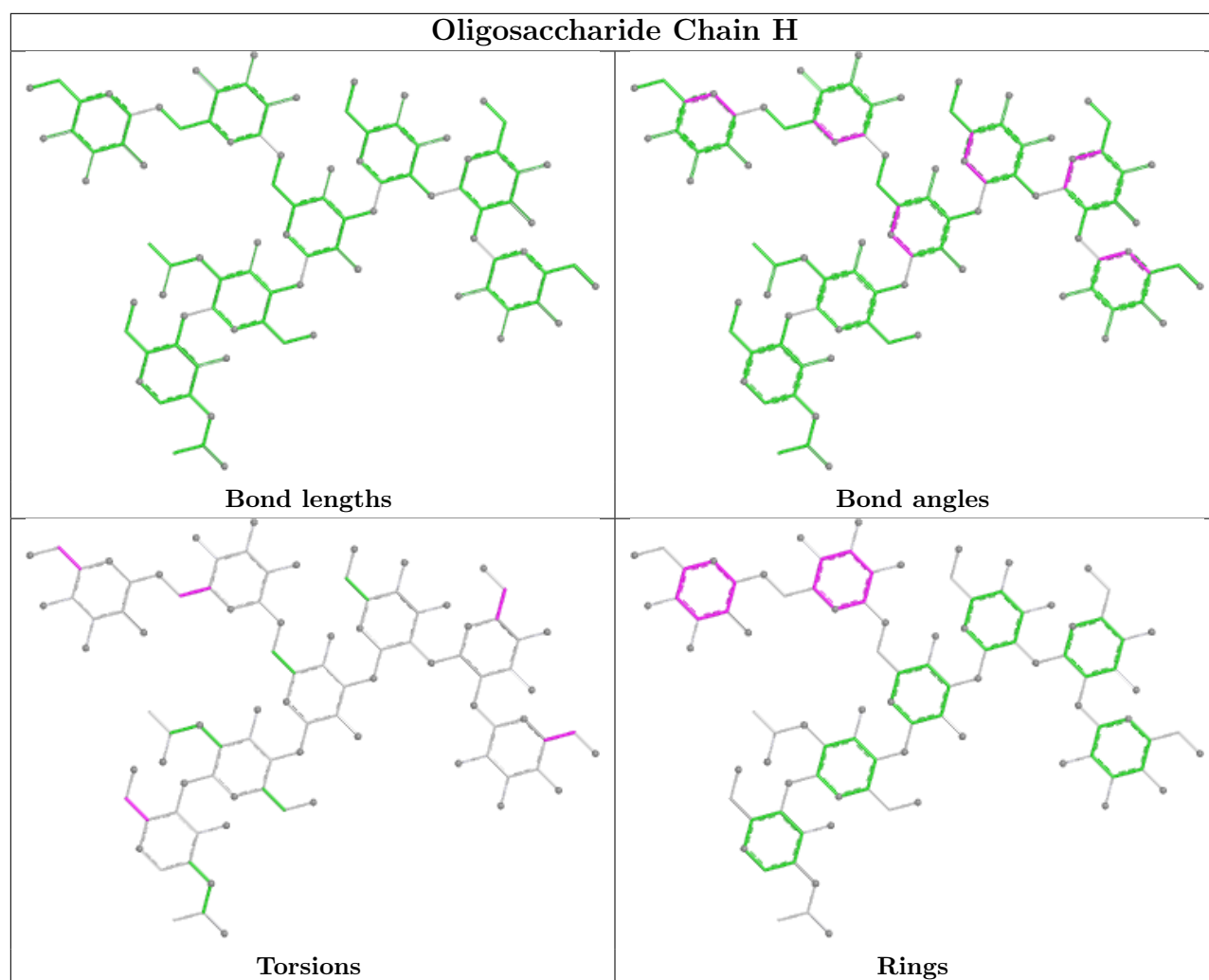
1 monomer is involved in 1 short contact:

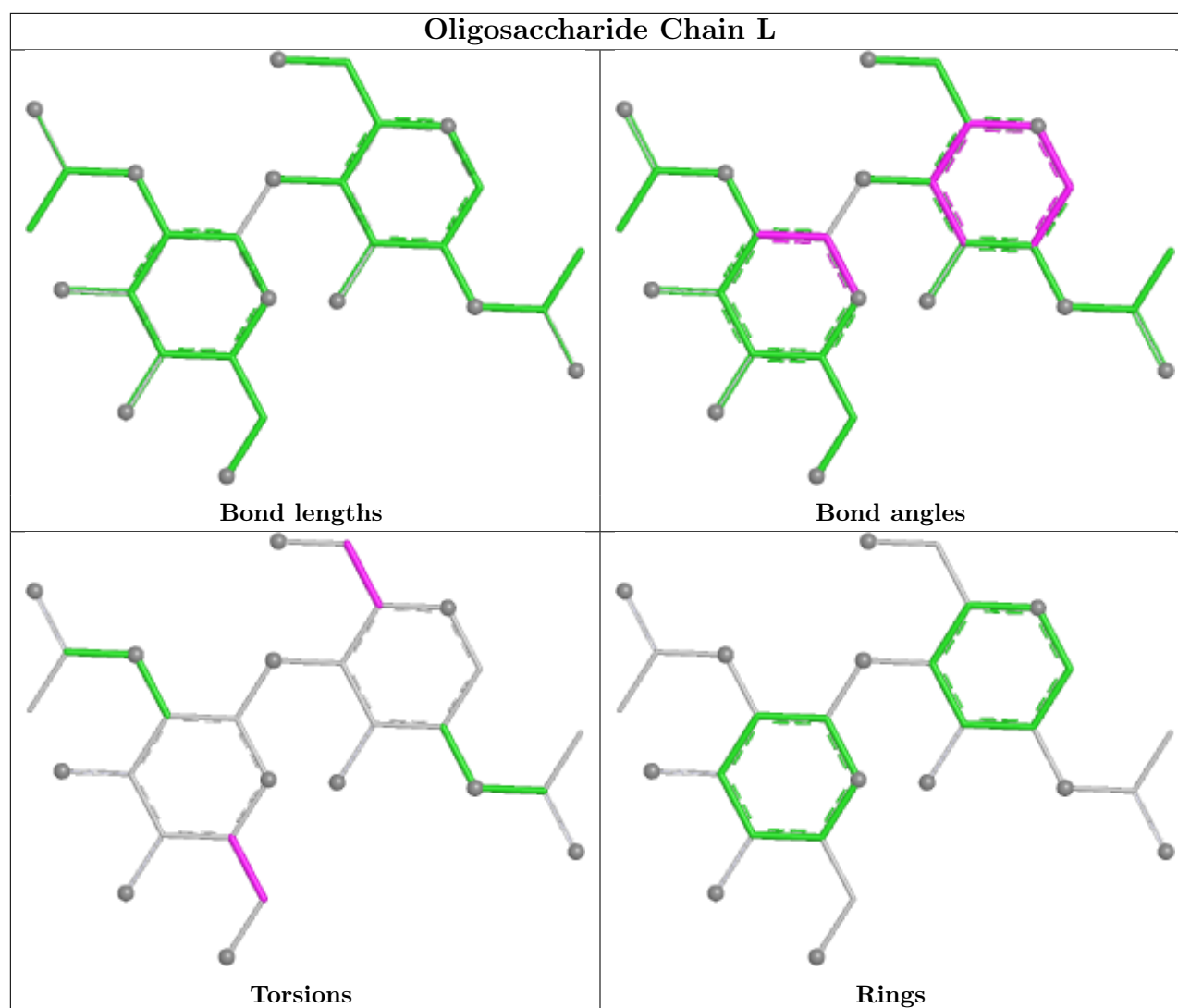
Mol	Chain	Res	Type	Clashes	Symm-Clashes
71	K	6	MAN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









## 5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 231 are monoatomic - leaving 1 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	$\# Z  > 2$
75	ELU	I	801	74	27,28,28	0.92	2 (7%)	33,37,37	1.21	5 (15%)

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
75	ELU	I	801	74	-	12/31/31/31	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	I	801	ELU	PA-O3A	2.79	1.62	1.59
75	I	801	ELU	PB-O2B	2.65	1.58	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	I	801	ELU	O1B-PB-O3A	3.12	115.08	104.64
75	I	801	ELU	O3B-PB-O1B	2.49	117.14	107.80
75	I	801	ELU	O1-PA-O2A	2.36	118.27	108.94
75	I	801	ELU	O3A-PB-O2B	-2.31	98.90	111.04
75	I	801	ELU	O1B-PB-O2B	2.06	118.88	110.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

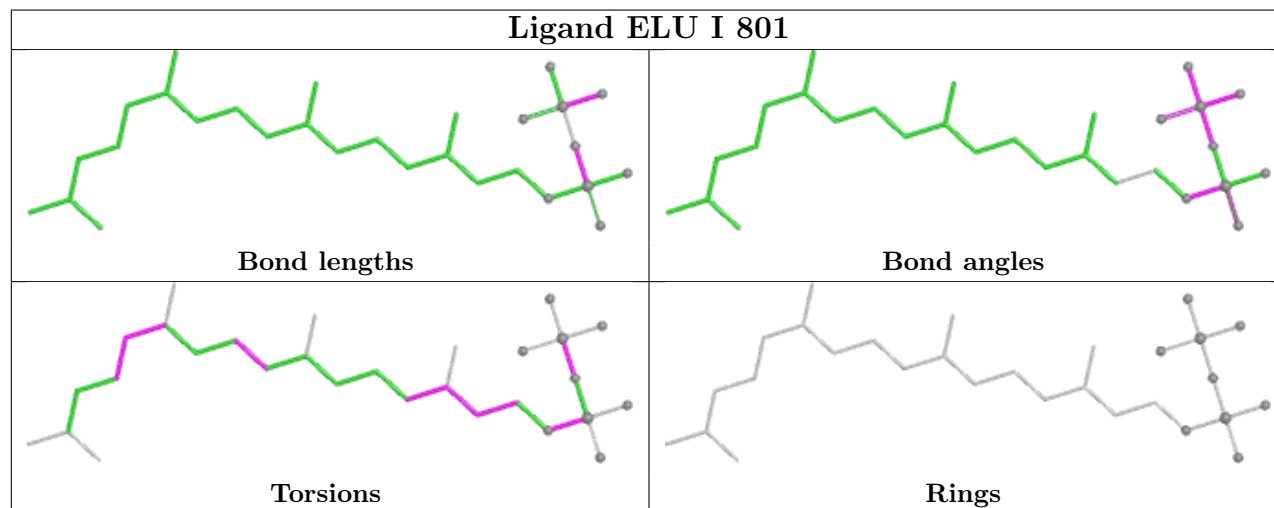
Mol	Chain	Res	Type	Atoms
75	I	801	ELU	C1-O1-PA-O2A
75	I	801	ELU	C1-O1-PA-O3A
75	I	801	ELU	PA-O3A-PB-O1B
75	I	801	ELU	C1-C2-C3-C4
75	I	801	ELU	C14-C13-C15-C16
75	I	801	ELU	C12-C11-C9-C8
75	I	801	ELU	C12-C13-C15-C16
75	I	801	ELU	C13-C15-C16-C17
75	I	801	ELU	C2-C3-C5-C6
75	I	801	ELU	O1-C1-C2-C3
75	I	801	ELU	C1-O1-PA-O1A
75	I	801	ELU	C4-C3-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

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.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



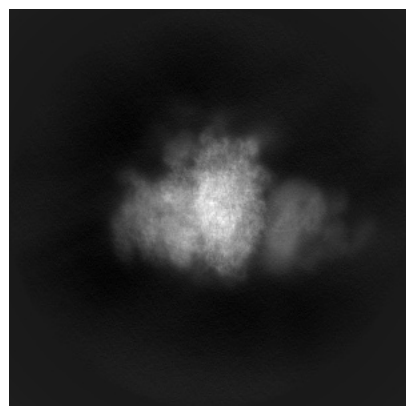
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49171. These allow visual inspection of the internal detail of the map and identification of artifacts.

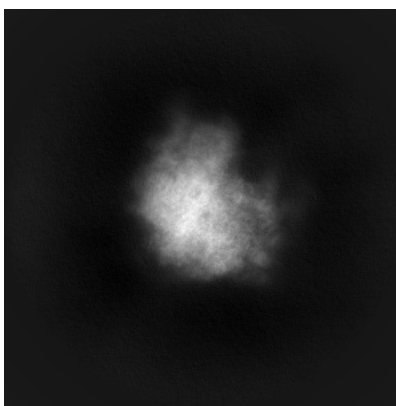
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

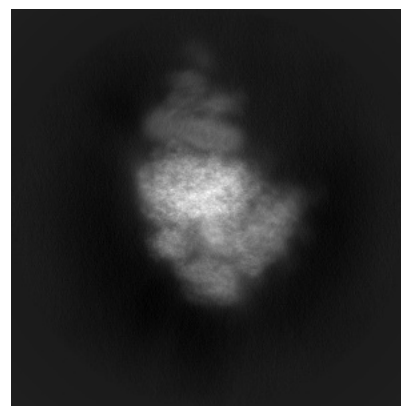
#### 6.1.1 Primary map



X

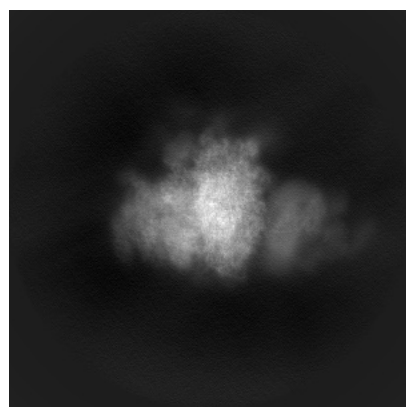


Y

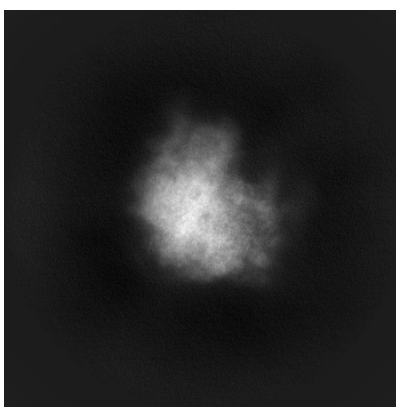


Z

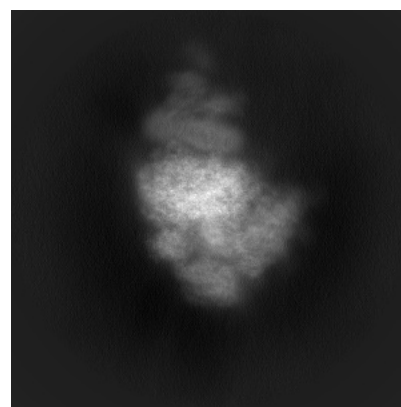
#### 6.1.2 Raw map



X



Y

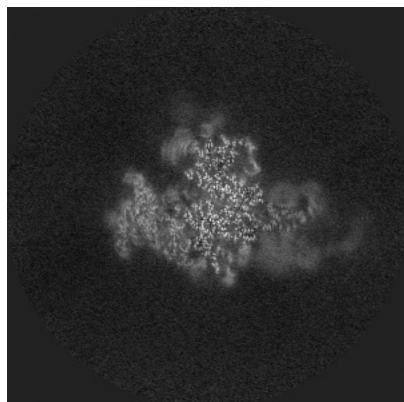


Z

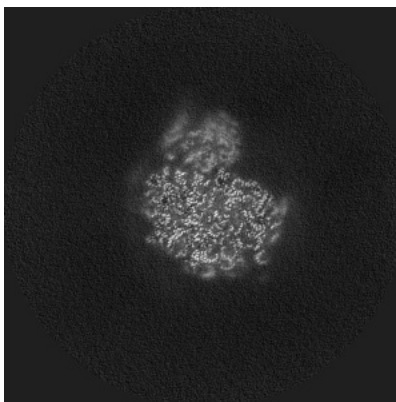
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

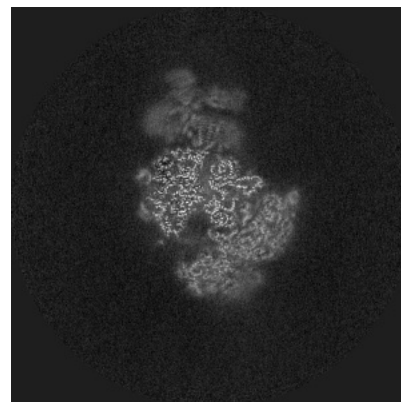
### 6.2.1 Primary map



X Index: 240

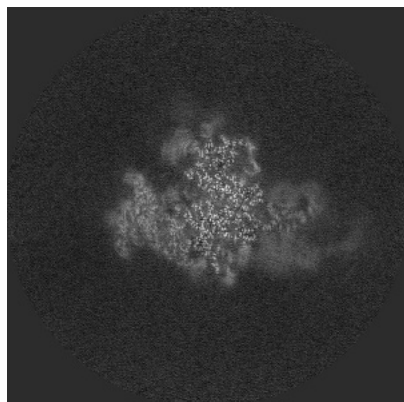


Y Index: 240

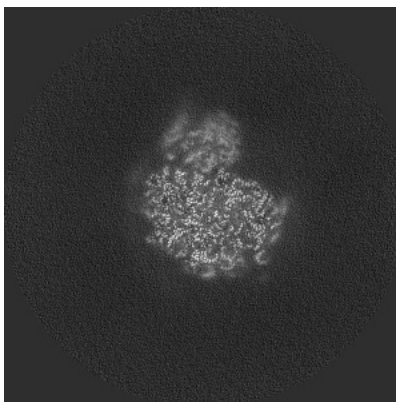


Z Index: 240

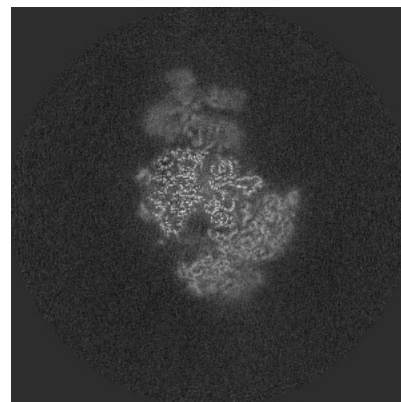
### 6.2.2 Raw map



X Index: 240



Y Index: 240

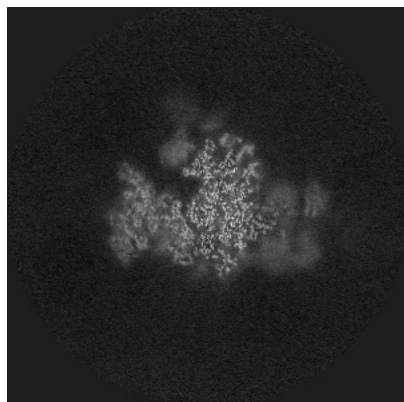


Z Index: 240

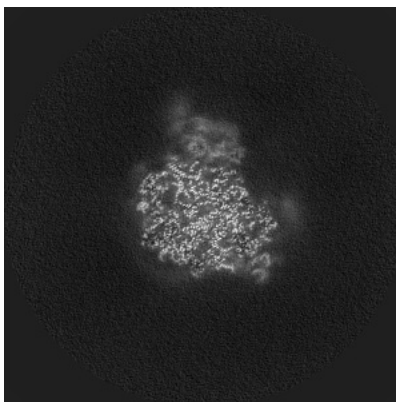
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

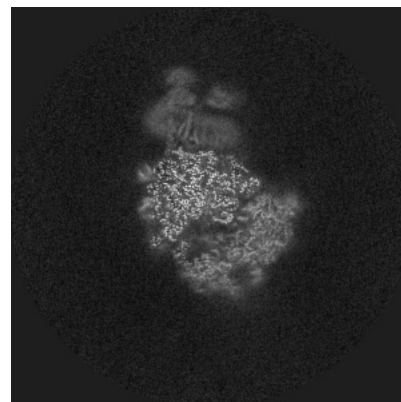
### 6.3.1 Primary map



X Index: 249

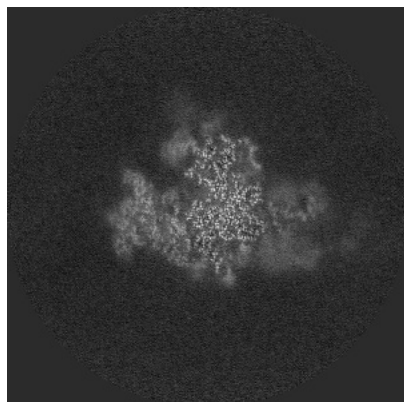


Y Index: 252

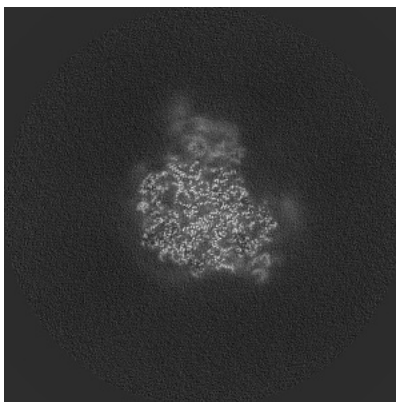


Z Index: 247

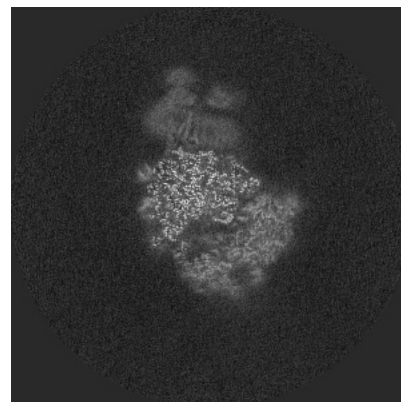
### 6.3.2 Raw map



X Index: 242



Y Index: 252

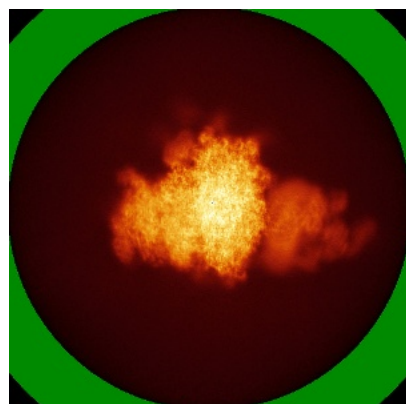


Z Index: 247

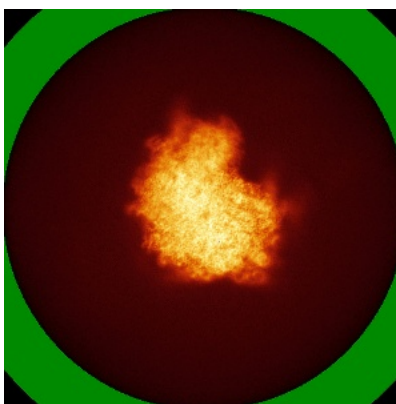
The images above show the largest variance slices of the map in three orthogonal directions.

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

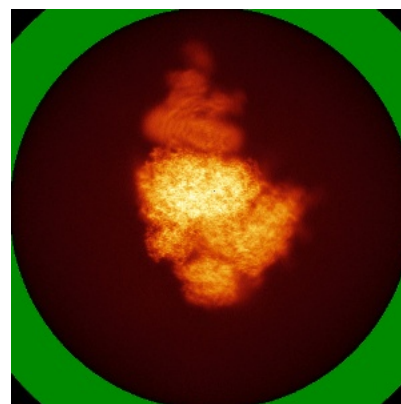
### 6.4.1 Primary map



X

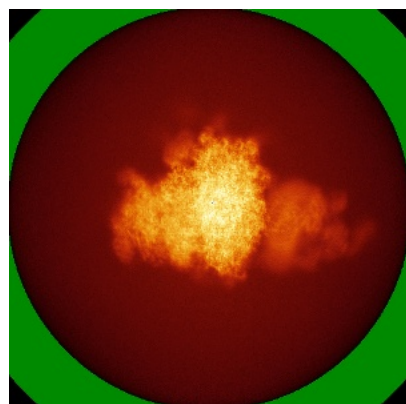


Y

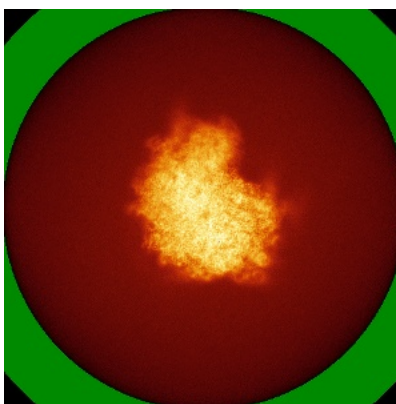


Z

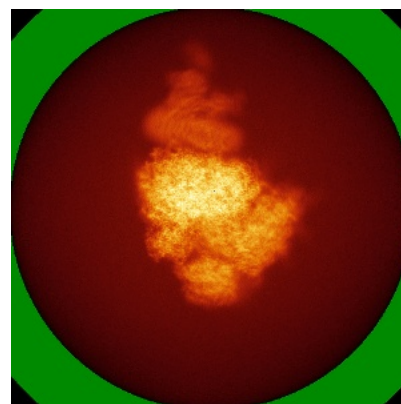
### 6.4.2 Raw map



X



Y



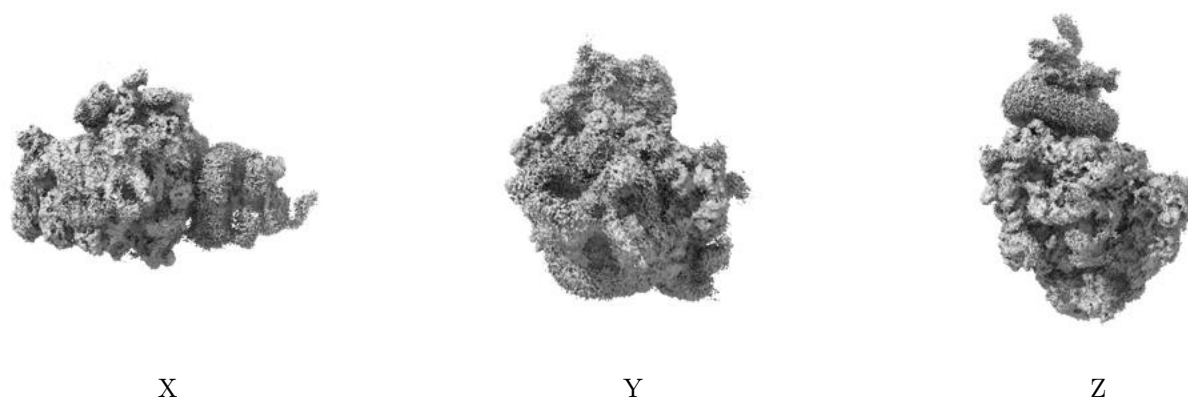
Z

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



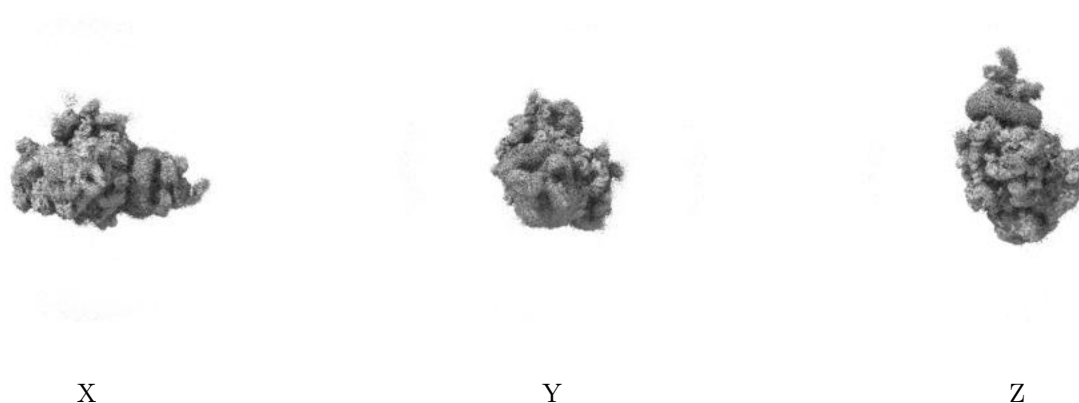
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

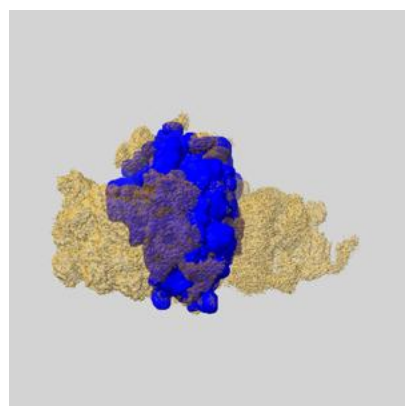
## 6.6 Mask visualisation [i](#)

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

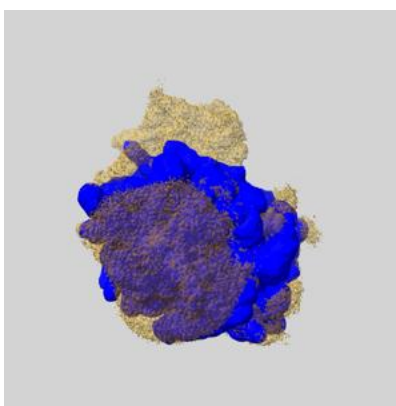
A mask typically either:

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

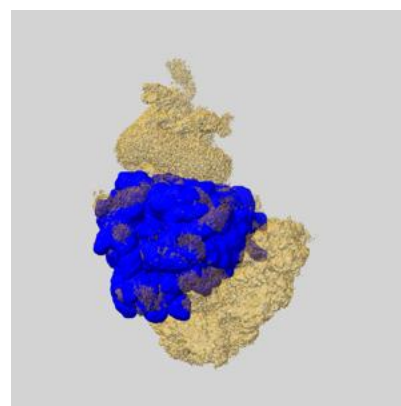
### 6.6.1 emd\_49171\_msk\_1.map [i](#)



X



Y

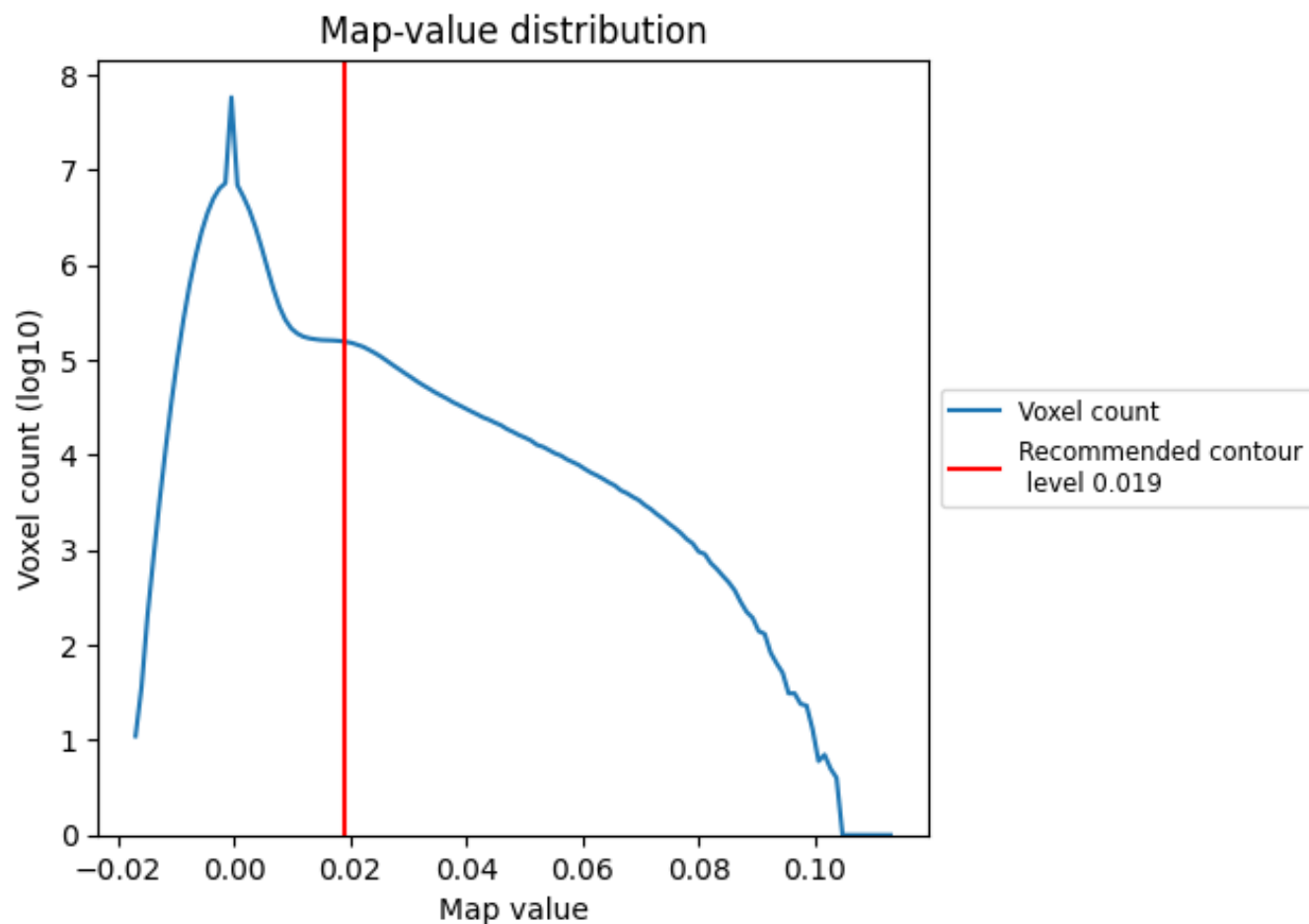


Z

## 7 Map analysis [i](#)

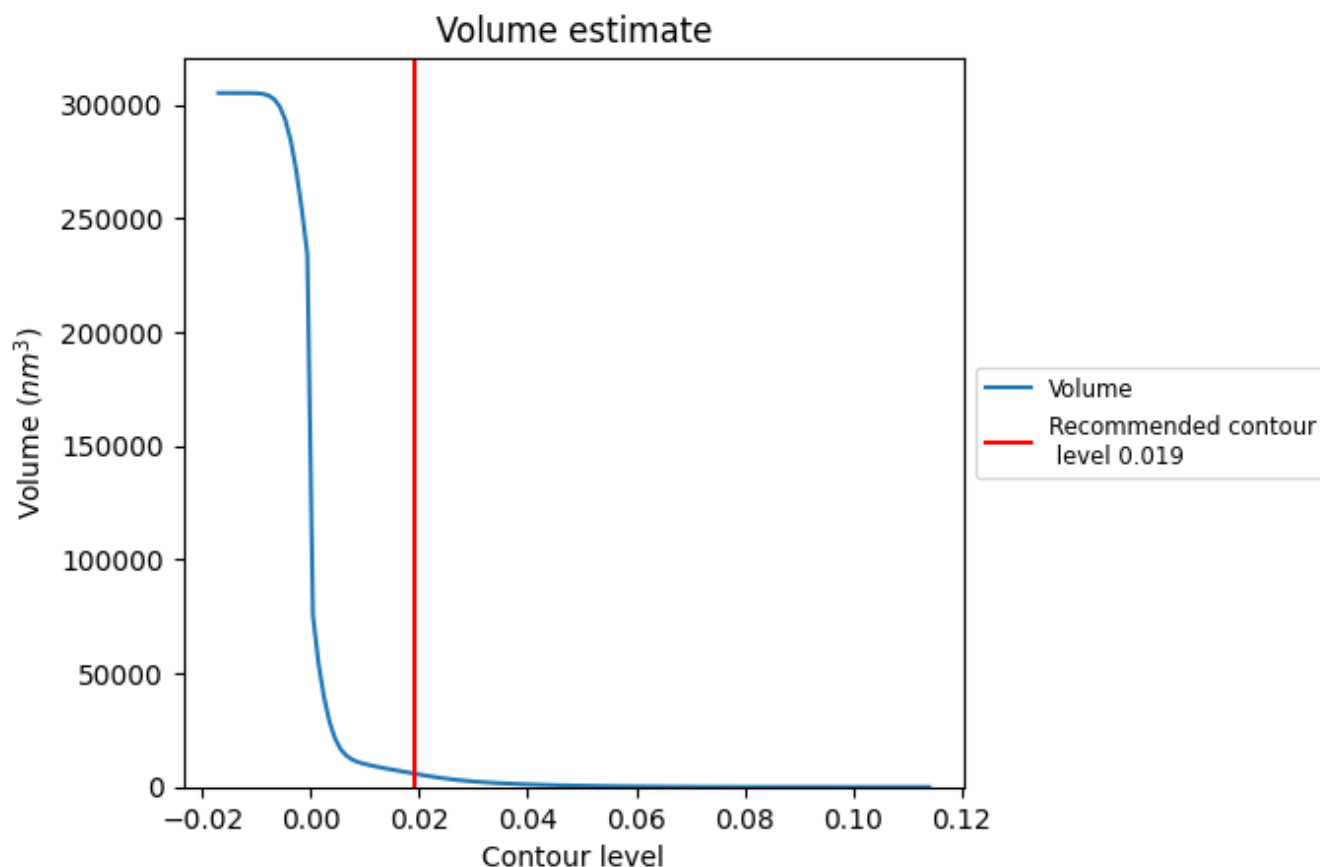
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

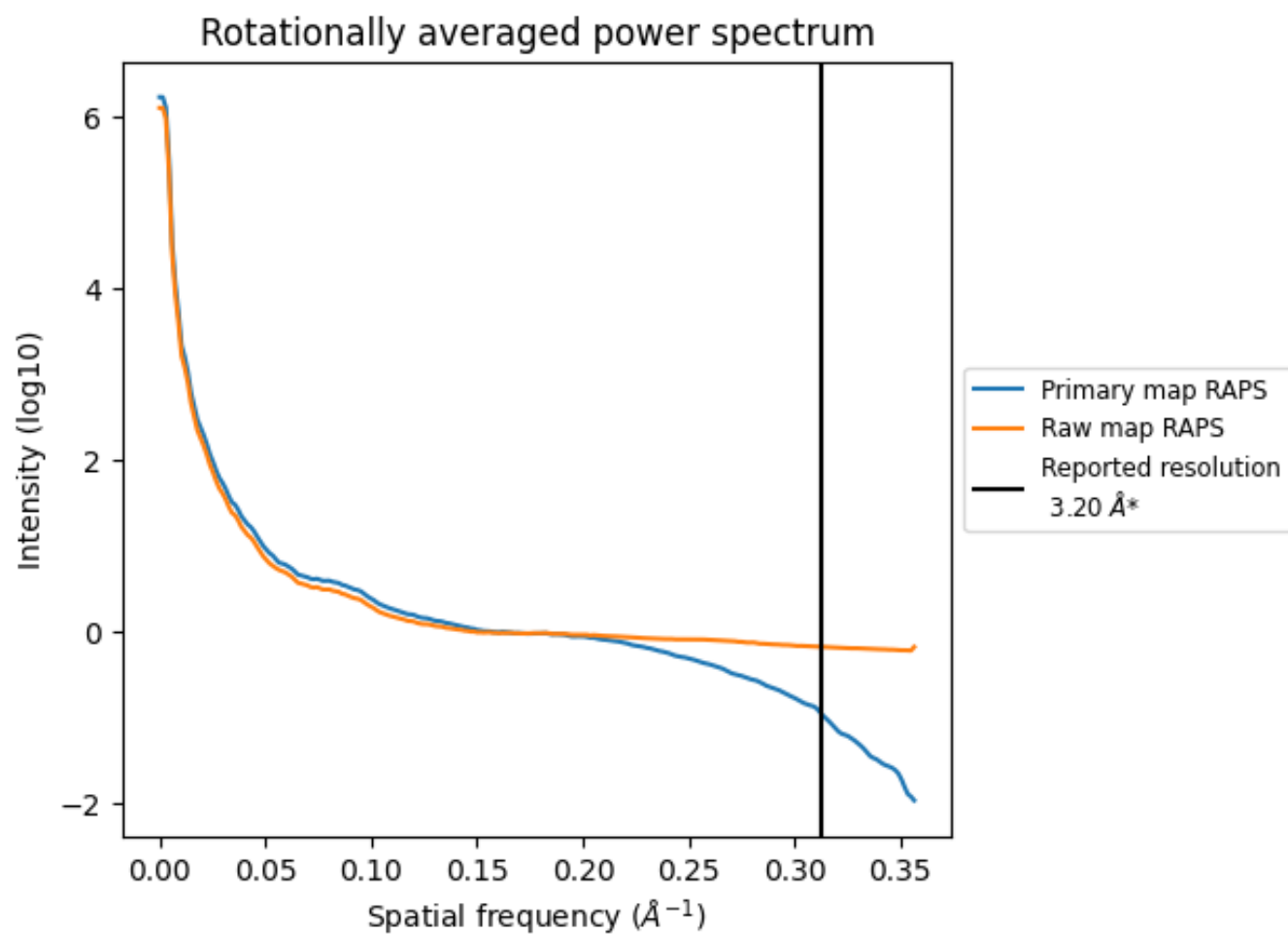


The volume at the recommended contour level is 5887  $\text{nm}^3$ ; this corresponds to an approximate mass of 5318 kDa.

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



### 7.3 Rotationally averaged power spectrum ⓘ

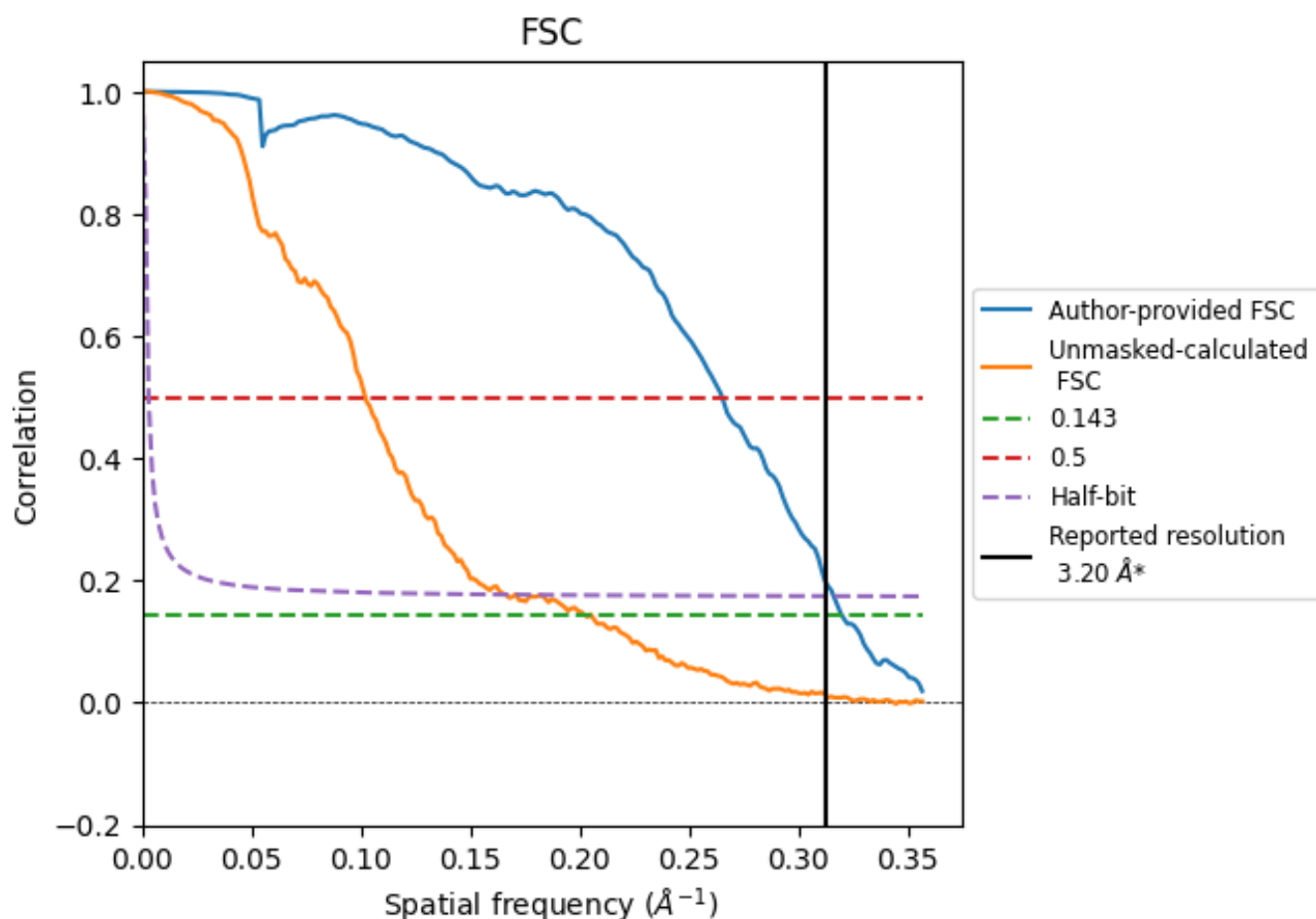


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

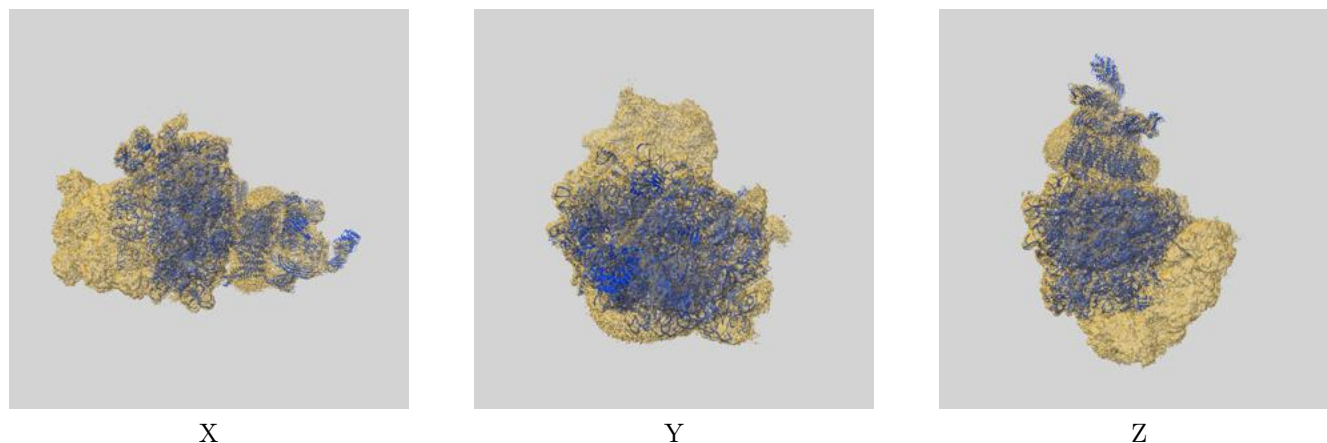
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.13	3.77	3.16
Unmasked-calculated*	4.94	9.80	6.02

\*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 4.94 differs from the reported value 3.2 by more than 10 %

## 9 Map-model fit [i](#)

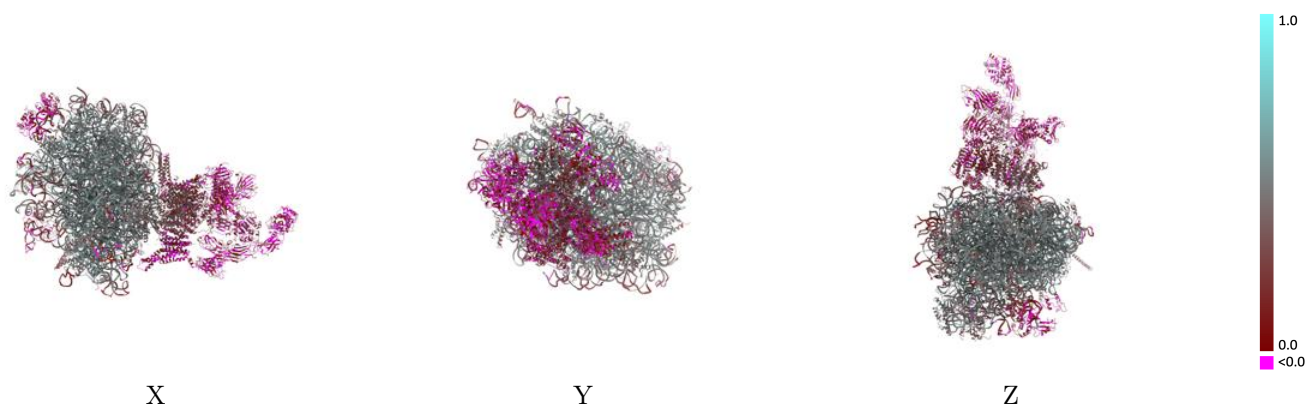
This section contains information regarding the fit between EMDB map EMD-49171 and PDB model 9N9J. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

### 9.1 Map-model overlay [i](#)



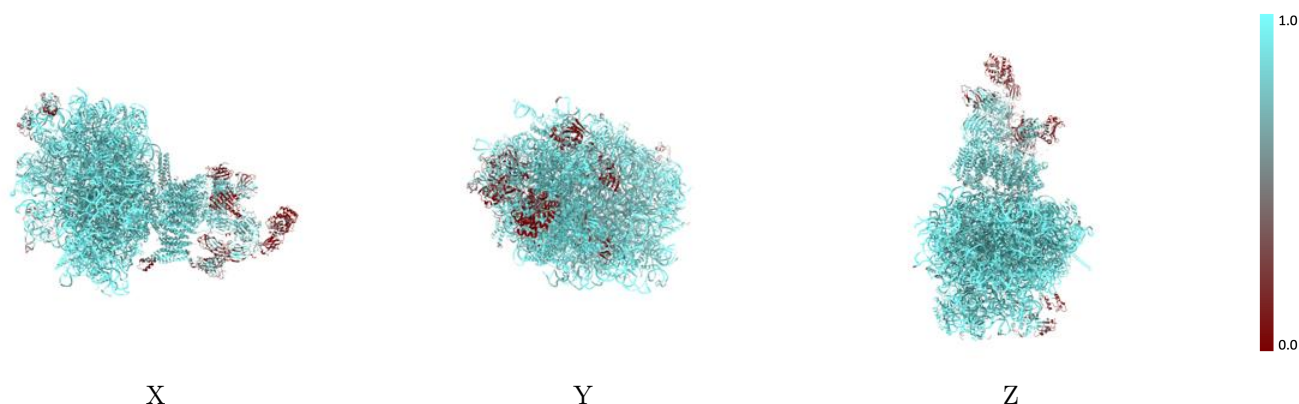
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



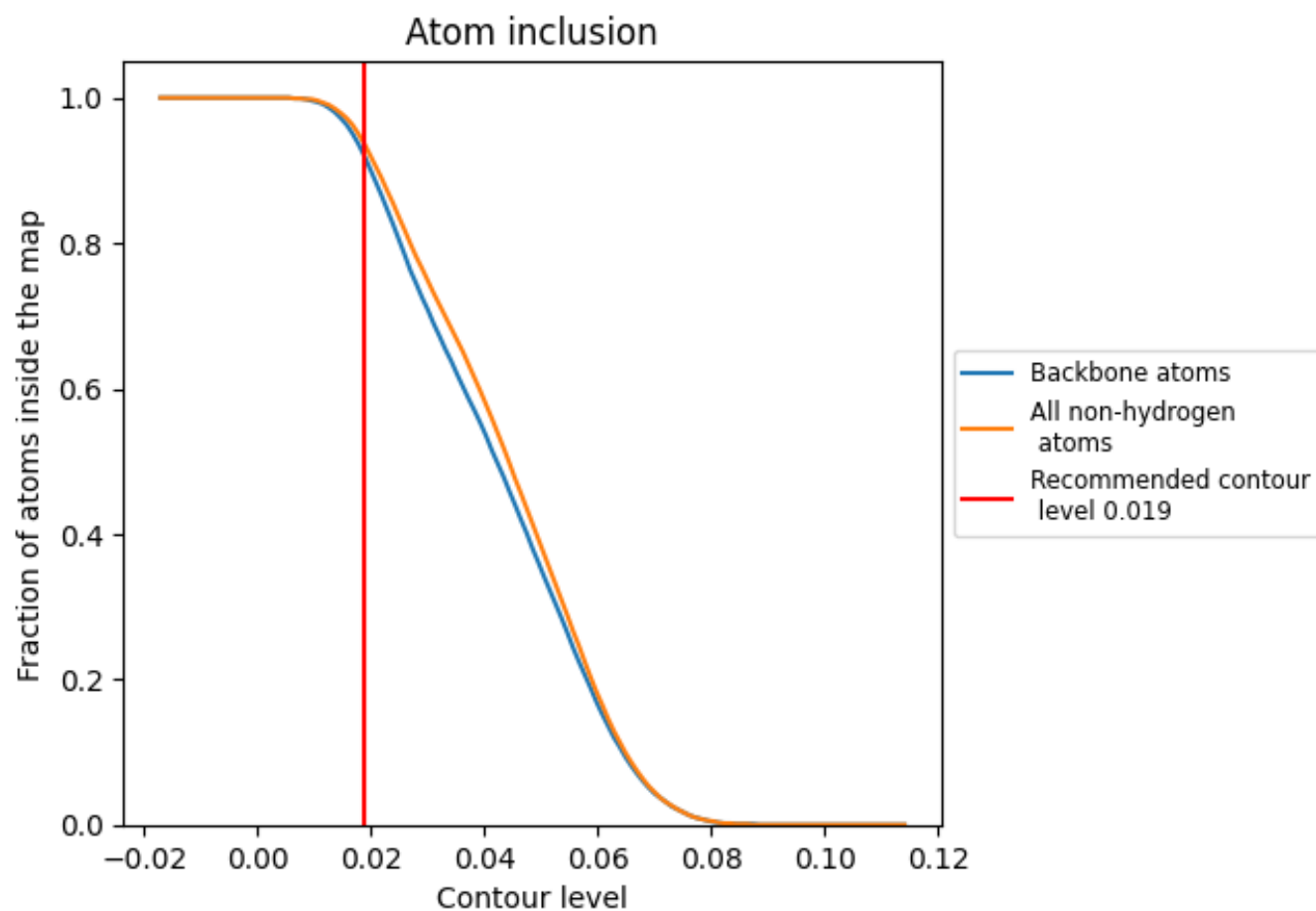
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.019).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 94% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9350	 0.3940
5	 0.3950	 0.0740
6	 0.5040	 0.0300
7	 0.7320	 0.0430
8	 0.4880	 0.0410
A	 0.4230	 0.0690
B	 0.7570	 0.1050
C	 0.6430	 0.0610
D	 0.9400	 0.3100
E	 0.9190	 0.2680
F	 0.9280	 0.2870
G	 0.9440	 0.3280
H	 0.5750	 0.0950
I	 0.9370	 0.1550
J	 0.9200	 0.2310
K	 0.7870	 0.1830
K2	 0.8050	 0.1640
L	 1.0000	 0.1520
L2	 0.9080	 0.0780
L5	 0.9930	 0.4690
L7	 0.9980	 0.5280
L8	 0.9980	 0.4850
LA	 0.9970	 0.5290
LB	 0.9810	 0.5030
LC	 0.9890	 0.5070
LD	 0.9840	 0.4770
LE	 0.9850	 0.4510
LF	 0.9960	 0.5020
LG	 0.9460	 0.4420
LH	 0.9900	 0.4880
LI	 0.9860	 0.4920
LJ	 0.9450	 0.4150
LL	 0.9620	 0.4840
LM	 0.9950	 0.4900
LN	 0.9990	 0.5220



*Continued on next page...*

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Chain	Atom inclusion	Q-score
LO	 0.9910	 0.4990
LP	 0.9630	 0.4710
LQ	 1.0000	 0.5260
LR	 0.9960	 0.4670
LS	 0.9980	 0.5140
LT	 0.9900	 0.4940
LU	 0.9730	 0.4010
LV	 0.9940	 0.5150
LW	 0.9980	 0.4900
LX	 0.9870	 0.4860
LY	 0.9810	 0.4890
LZ	 0.9880	 0.4930
La	 0.9960	 0.5320
Lb	 0.9620	 0.4280
Lc	 0.9840	 0.4650
Ld	 0.9880	 0.4810
Le	 0.9960	 0.5170
Lf	 1.0000	 0.5330
Lg	 0.9920	 0.4830
Lh	 0.9860	 0.4680
Li	 0.9850	 0.4710
Lj	 0.9990	 0.5240
Lk	 0.9460	 0.4540
Ll	 0.9980	 0.5010
Lm	 0.9710	 0.4880
Ln	 1.0000	 0.4640
Lo	 0.9930	 0.4940
Lp	 0.9960	 0.4980
Lr	 0.9900	 0.5080
Ls	 0.5770	 0.0880
Lt	 0.5610	 0.0900
Lz	 0.5990	 0.0760
M2	 0.9450	 0.1010
N	 0.9620	 0.0870
N2	 0.8440	 0.0910
O2	 0.7740	 0.0990
P2	 0.3680	 0.0500
u3	 0.9810	 0.2950
v3	 0.9980	 0.3160
y3	 0.4390	 0.1250