



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 10:55 AM UTC

PDB ID : 9H3G / pdb_00009h3g
EMDB ID : EMD-51820
Title : Structure of the Arabidopsis thaliana 80S ribosome in complex with P- and E-site tRNAs and mRNA
Authors : Faille, A.; Warren, A.J.
Deposited on : 2024-10-16
Resolution : 1.82 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

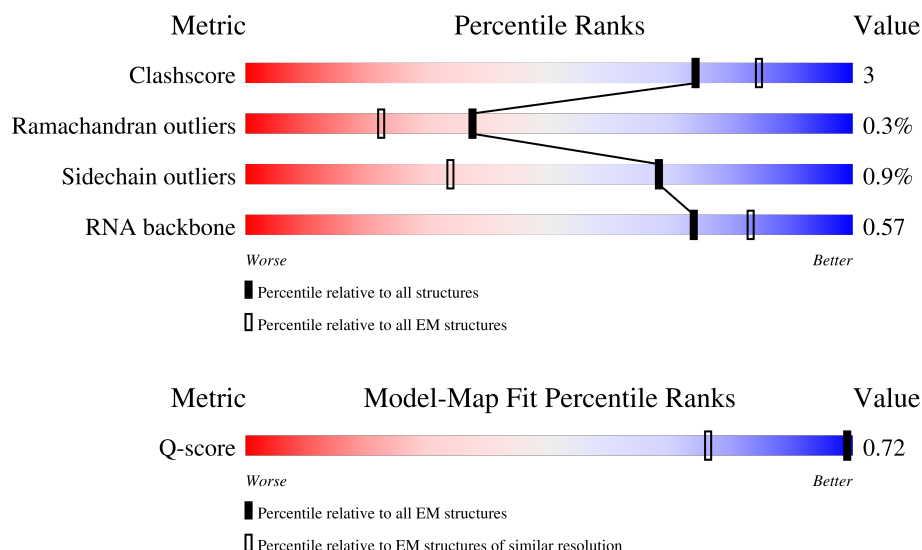
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 1.82 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	882 (1.33 - 2.32)

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

Mol	Chain	Length	Quality of chain
1	3	164	<div> <div>6%</div> <div>71%</div> <div>25%</div> <div>...</div> </div>
2	A	3385	<div> <div>6%</div> <div>67%</div> <div>22%</div> <div>7%</div> </div>
3	W2	76	<div> <div>30%</div> <div>74%</div> <div>22%</div> <div>...</div> </div>



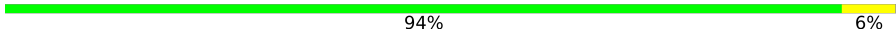

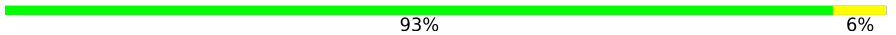




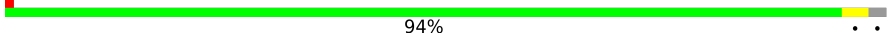















Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	i2	76	
4	C3	121	
5	BC	25	
6	BM	176	
7	BO	146	
8	AR	83	
9	AU	119	
10	Ma	131	
11	Ia	194	
12	AE	130	
13	AX	112	
14	AP	135	
15	Ja	262	
16	Ea	204	
17	AL	217	
18	Va	142	
19	Ka	133	
20	AW	112	
21	BD	105	
22	BS	389	
23	AM	164	
24	AC	284	
25	BI	140	
26	AH	134	
27	BT	406	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	AV	133	
29	AD	207	
30	AJ	187	
31	BQ	258	
32	BH	206	
33	Da	151	
34	BK	301	
35	AT	112	
36	Pa	62	
37	BP	123	
38	BN	154	
39	BG	256	
40	Fa	120	
41	Ha	146	
42	BU	182	
43	BR	247	
44	Xa	160	
45	BV	262	
46	BJ	221	
47	AO	164	
48	BW	82	
49	AK	214	
50	Na	86	
51	AB	197	
52	BF	233	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	AA	250	
54	AG	206	
55	Ga	128	
56	BA	51	
57	AF	146	
58	Wa	152	
59	Ta	249	
60	AZ	69	
61	BE	92	
62	Za	298	
63	AQ	143	
64	Oa	64	
65	Ua	150	
66	Ya	150	
67	BB	141	
68	AN	124	
69	Ra	190	
70	BL	143	
71	La	108	
72	Aa	222	
73	AY	95	
74	Ca	56	
75	h1	1805	
76	B1	12	
77	Ba	122	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
78	AI	177	<div><div><div>14%</div><div>46%</div><div>6%</div><div>48%</div></div></div>
79	L3	23	<div><div><div>83%</div><div>96%</div><div></div></div></div>

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 209234 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called Ribosomal RNA 5.8S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	162	Total	C	N	O	P	0	0
			3453	1544	617	1130	162		

- Molecule 2 is a RNA chain called Ribosomal RNA 25S.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	3149	Total	C	N	O	P	1	0
			67525	30162	12266	21947	3150		

- Molecule 3 is a RNA chain called Transfer RNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	i2	76	Total	C	N	O	P	0	0
			1630	726	298	530	76		
3	W2	76	Total	C	N	O	P	0	0
			1629	726	298	529	76		

- Molecule 4 is a RNA chain called Ribosomal RNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C3	119	Total	C	N	O	P	0	0
			2536	1132	454	831	119		

- Molecule 5 is a protein called Small ribosomal subunit protein eS32 eS32z/eS32y/eS32x/eS32w/eS32v.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BC	25	Total	C	N	O	S	0	0
			237	145	62	27	3		

- Molecule 6 is a protein called Large ribosomal subunit protein uL22z.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BM	155	Total	C	N	O	S	0	0
			1246	774	247	221	4		

- Molecule 7 is a protein called Large ribosomal subunit protein uL24z.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BO	125	Total	C	N	O	S	0	0
			1030	637	211	179	3		

- Molecule 8 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AR	51	Total	C	N	O	S	0	0
			425	258	100	66	1		

- Molecule 9 is a protein called Large ribosomal subunit protein eL31y.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AU	109	Total	C	N	O	S	0	0
			888	558	168	160	2		

- Molecule 10 is a protein called Small ribosomal subunit protein eS26y.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Ma	98	Total	C	N	O	S	0	0
			789	485	166	132	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6z/uL6y.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Ia	190	Total	C	N	O	S	0	0
			1512	961	270	275	6		

- Molecule 12 is a protein called Small ribosomal subunit protein uS8z/uS8w.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AE	129	Total	C	N	O	S	0	0
			1033	660	188	180	5		

- Molecule 13 is a protein called Large ribosomal subunit protein eL36y.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AX	97	Total	C	N	O	S	0	0
			786	492	166	126	2		

- Molecule 14 is a protein called Large ribosomal subunit protein eL27x.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AP	134	Total	C	N	O	S	0	0
			1092	706	200	183	3		

- Molecule 15 is a protein called Small ribosomal subunit protein eS4x.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ja	258	Total	C	N	O	S	0	0
			2074	1325	386	357	6		

- Molecule 16 is a protein called Large ribosomal subunit protein eL15z.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ea	203	Total	C	N	O	S	1	0
			1713	1070	361	279	3		

- Molecule 17 is a protein called Ribosomal protein L18ae/LX family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AL	175	Total	C	N	O	S	0	0
			1485	960	273	244	8		

- Molecule 18 is a protein called Small ribosomal subunit protein uS12y.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Va	139	Total	C	N	O	S	0	0
			1082	689	207	183	3		

- Molecule 19 is a protein called Small ribosomal subunit protein eS24y.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Ka	120	Total	C	N	O	S	0	0
			986	627	191	165	3		

- Molecule 20 is a protein called Large ribosomal subunit protein eL33y.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AW	111	Total	C	N	O	S	0	0
			901	568	174	155	4		

- Molecule 21 is a protein called Large ribosomal subunit protein eL42z/eL42y.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BD	97	Total	C	N	O	S	0	0
			792	497	158	132	5		

- Molecule 22 is a protein called Large ribosomal subunit protein uL3z.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BS	386	Total	C	N	O	S	0	0
			3111	1981	581	532	17		

- Molecule 23 is a protein called Large ribosomal subunit protein eL21z/eL21y.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AM	163	Total	C	N	O	S	0	0
			1307	827	254	222	4		

- Molecule 24 is a protein called Small ribosomal subunit protein uS5y/uS5u/uS5v.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AC	215	Total	C	N	O	S	0	0
			1672	1075	300	290	7		

- Molecule 25 is a protein called Large ribosomal subunit protein uL14x/uL14z/uL14y.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BI	131	Total	C	N	O	S	0	0
			986	624	183	171	8		

- Molecule 26 is a protein called Large ribosomal subunit protein eL14y.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AH	128	Total	C	N	O	S	0	0
			1042	665	194	179	4		

- Molecule 27 is a protein called Large ribosomal subunit protein uL4z.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BT	393	Total	C	N	O	S	0	0
			3056	1934	573	535	14		

- Molecule 28 is a protein called Large ribosomal subunit protein eL32z.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AV	126	Total	C	N	O	S	0	0
			1028	649	204	171	4		

- Molecule 29 is a protein called Small ribosomal subunit protein uS7y.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AD	184	Total	C	N	O	S	0	0
			1454	912	275	261	6		

- Molecule 30 is a protein called Large ribosomal subunit protein eL18x.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AJ	186	Total	C	N	O	S	0	0
			1468	932	283	249	4		

- Molecule 31 is a protein called Large ribosomal subunit protein uL2z.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BQ	245	Total	C	N	O	S	1	0
			1881	1179	379	316	7		

- Molecule 32 is a protein called Large ribosomal subunit protein uL13y.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BH	205	Total	C	N	O	S	0	0
			1636	1038	314	273	11		

- Molecule 33 is a protein called Small ribosomal subunit protein uS15y.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Da	149	Total	C	N	O	S	0	0
			1190	759	223	206	2		

- Molecule 34 is a protein called Large ribosomal subunit protein uL18z.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BK	281	Total	C	N	O	S	0	0
			2277	1441	418	414	4		

- Molecule 35 is a protein called Large ribosomal subunit protein eL30y.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AT	94	Total	C	N	O	S	0	0
			720	457	127	131	5		

- Molecule 36 is a protein called Small ribosomal subunit protein eS30z/eS30y/eS30x.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	Pa	49	Total	C	N	O	0	0
			389	236	92	61		

- Molecule 37 is a protein called Large ribosomal subunit protein uL29x.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BP	120	Total	C	N	O	S	0	0
			975	617	191	166	1		

- Molecule 38 is a protein called Large ribosomal subunit protein uL23y.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BN	117	Total	C	N	O	S	0	0
			955	615	170	168	2		

- Molecule 39 is a protein called Large ribosomal subunit protein eL8y.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BG	234	Total	C	N	O	S	0	0
			1874	1207	339	323	5		

- Molecule 40 is a protein called Large ribosomal subunit protein eL34z.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Fa	111	Total	C	N	O	S	0	0
			896	560	187	148	1		

- Molecule 41 is a protein called Large ribosomal subunit protein uL15x.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ha	145	Total	C	N	O	S	0	0
			1156	744	225	184	3		

- Molecule 42 is a protein called Large ribosomal subunit protein uL5z.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BU	169	Total	C	N	O	S	0	0
			1366	863	254	242	7		

- Molecule 43 is a protein called Ribosomal protein L30/L7 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BR	232	Total	C	N	O	S	0	0
			1898	1221	348	325	4		

- Molecule 44 is a protein called Small ribosomal subunit protein uS17z.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Xa	146	Total	C	N	O	S	0	0
			1163	742	224	192	5		

- Molecule 45 is a protein called Small ribosomal subunit protein eS1y.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BV	212	Total	C	N	O	S	0	0
			1718	1087	313	310	8		

- Molecule 46 is a protein called Large ribosomal subunit protein uL16y.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BJ	207	Total	C	N	O	S	0	0
			1653	1047	327	268	11		

- Molecule 47 is a protein called Large ribosomal subunit protein eL24z.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AO	62	Total	C	N	O	S	0	0
			528	343	100	81	4		

- Molecule 48 is a protein called Small ribosomal subunit protein eS21y.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BW	73	Total	C	N	O	S	0	0
			568	355	104	107	2		

- Molecule 49 is a protein called Large ribosomal subunit protein eL19x.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AK	178	Total	C	N	O	S	0	0
			1480	920	308	241	11		

- Molecule 50 is a protein called Small ribosomal subunit protein eS27y.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Na	83	Total	C	N	O	S	0	0
			647	405	118	117	7		

- Molecule 51 is a protein called Small ribosomal subunit protein uS4y.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AB	180	Total	C	N	O	S	0	0
			1514	953	303	254	4		

- Molecule 52 is a protein called Large ribosomal subunit protein eL6y.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BF	190	Total	C	N	O	S	0	0
			1491	966	273	250	2		

- Molecule 53 is a protein called Small ribosomal subunit protein uS3z.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AA	208	Total	C	N	O	S	0	0
			1625	1031	296	290	8		

- Molecule 54 is a protein called Large ribosomal subunit protein eL13z.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AG	203	Total	C	N	O	S	0	0
			1648	1041	326	277	4		

- Molecule 55 is a protein called Ubiquitin-ribosomal protein eL40z fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Ga	52	Total	C	N	O	S	0	0
			433	271	89	66	7		

- Molecule 56 is a protein called Large ribosomal subunit protein eL39z/eL39x.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BA	50	Total	C	N	O	S	0	0
			444	282	97	63	2		

- Molecule 57 is a protein called Small ribosomal subunit protein uS9z.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AF	138	Total	C	N	O	S	0	0
			1113	708	213	187	5		

- Molecule 58 is a protein called Small ribosomal subunit protein uS13z/uS13y/uS13x.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Wa	139	Total	C	N	O	S	0	0
			1136	709	224	198	5		

- Molecule 59 is a protein called Small ribosomal subunit protein eS6y.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Ta	225	Total	C	N	O	S	0	0
			1795	1123	354	310	8		

- Molecule 60 is a protein called Large ribosomal subunit protein eL38z/eL38y.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AZ	68	Total	C	N	O	S	0	0
			562	359	103	98	2		

- Molecule 61 is a protein called Large ribosomal subunit protein eL43y.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BE	90	Total	C	N	O	S	0	0
			702	441	135	120	6		

- Molecule 62 is a protein called Small ribosomal subunit protein uS2z.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Za	198	Total	C	N	O	S	0	0
			1575	1000	283	279	13		

- Molecule 63 is a protein called Large ribosomal subunit protein eL28z.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AQ	136	Total	C	N	O	S	0	0
			1056	667	197	190	2		

- Molecule 64 is a protein called Small ribosomal subunit protein eS28x.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Oa	59	Total	C	N	O	S	0	0
			471	289	96	84	2		

- Molecule 65 is a protein called Small ribosomal subunit protein uS11y.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Ua	127	Total	C	N	O	S	0	0
			962	591	189	177	5		

- Molecule 66 is a protein called Small ribosomal subunit protein uS19y.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Ya	129	Total	C	N	O	S	0	0
			1024	657	190	172	5		

- Molecule 67 is a protein called Small ribosomal subunit protein eS17w.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BB	119	Total	C	N	O	S	0	0
			955	597	175	178	5		

- Molecule 68 is a protein called Large ribosomal subunit protein eL22z.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AN	99	Total	C	N	O	S	0	0
			808	517	143	146	2		

- Molecule 69 is a protein called Small ribosomal subunit protein eS7x.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ra	184	Total	C	N	O	S	0	0
			1506	955	275	270	6		

- Molecule 70 is a protein called Small ribosomal subunit protein eS19x.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	BL	136	Total	C	N	O	S	0	0
			1064	673	202	186	3		

- Molecule 71 is a protein called Small ribosomal subunit protein eS25w.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	La	71	Total	C	N	O	S	0	0
			562	354	105	99	4		

- Molecule 72 is a protein called Small ribosomal subunit protein eS8z.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Aa	185	Total	C	N	O	S	0	0
			1494	928	296	266	4		

- Molecule 73 is a protein called Large ribosomal subunit protein eL37z.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AY	87	Total	C	N	O	S	0	0
			705	429	157	113	6		

- Molecule 74 is a protein called Small ribosomal subunit protein uS14z/uS14y/uS14x.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Ca	55	Total	C	N	O	S	0	0
			440	273	91	71	5		

- Molecule 75 is a RNA chain called Ribosomal RNA 18S.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	h1	1612	Total	C	N	O	P	0	0
			34449	15422	6154	11261	1612		

- Molecule 76 is a RNA chain called Messenger RNA (poly-U).

Mol	Chain	Residues	Atoms					AltConf	Trace
76	B1	12	Total	C	N	O	P	0	0
			240	108	24	96	12		

- Molecule 77 is a protein called Small ribosomal subunit protein uS10y.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ba	101	Total	C	N	O	S	0	0
			799	505	149	142	3		

- Molecule 78 is a protein called Small ribosomal subunit protein eS10z.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AI	92	Total	C	N	O	S	0	0
			779	514	127	133	5		

- Molecule 79 is a protein called Nascent polypeptide (poly-A).

Mol	Chain	Residues	Atoms				AltConf	Trace
79	L3	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 80 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
80	3	5	Total	Mg	0
			5	5	
80	A	197	Total	Mg	0
			197	197	
80	i2	1	Total	Mg	0
			1	1	
80	C3	4	Total	Mg	0
			4	4	
80	BM	1	Total	Mg	0
			1	1	
80	BS	4	Total	Mg	0
			4	4	
80	AM	1	Total	Mg	0
			1	1	
80	AC	1	Total	Mg	0
			1	1	
80	BI	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
80	BR	1	Total 1	Mg 1	0
80	AG	1	Total 1	Mg 1	0
80	Wa	1	Total 1	Mg 1	0
80	Ta	1	Total 1	Mg 1	0
80	AY	2	Total 2	Mg 2	0
80	h1	78	Total 78	Mg 78	0

- Molecule 81 is POTASSIUM ION (CCD ID: K) (formula: K).

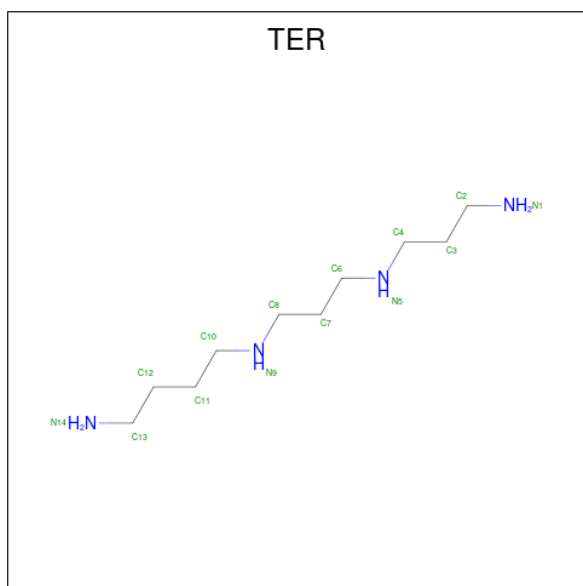
Mol	Chain	Residues	Atoms		AltConf
81	3	4	Total 4	K 4	0
81	A	127	Total 127	K 127	0
81	C3	1	Total 1	K 1	0
81	BM	1	Total 1	K 1	0
81	AR	1	Total 1	K 1	0
81	Ea	1	Total 1	K 1	0
81	Va	1	Total 1	K 1	0
81	BD	1	Total 1	K 1	0
81	BS	2	Total 2	K 2	0
81	AV	1	Total 1	K 1	0
81	AD	1	Total 1	K 1	0
81	AJ	1	Total 1	K 1	0
81	BQ	2	Total 2	K 2	0

Continued on next page...

Continued from previous page...

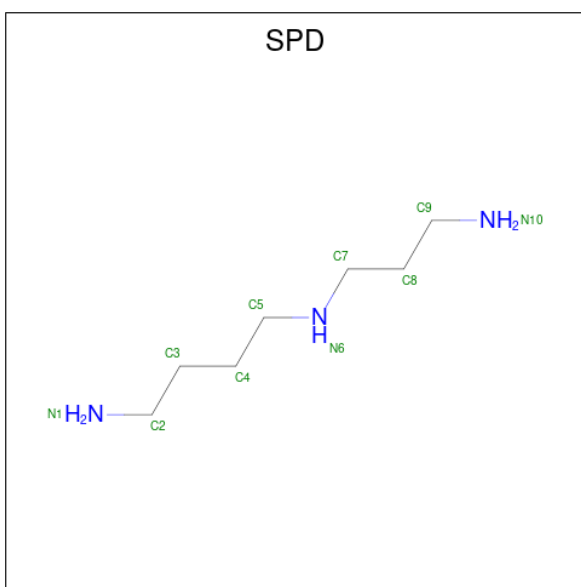
Mol	Chain	Residues	Atoms		AltConf
81	Fa	1	Total	K	0
			1	1	
81	BJ	1	Total	K	0
			1	1	
81	Wa	1	Total	K	0
			1	1	
81	Ua	1	Total	K	0
			1	1	
81	Ca	1	Total	K	0
			1	1	
81	h1	40	Total	K	0
			40	40	

- Molecule 82 is N-(3-AMINO-PROPYL)-N-(5-AMINOPROPYL)-1,4-DIAMINOBUTANE (CCD ID: TER) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of Interest" by depositor).



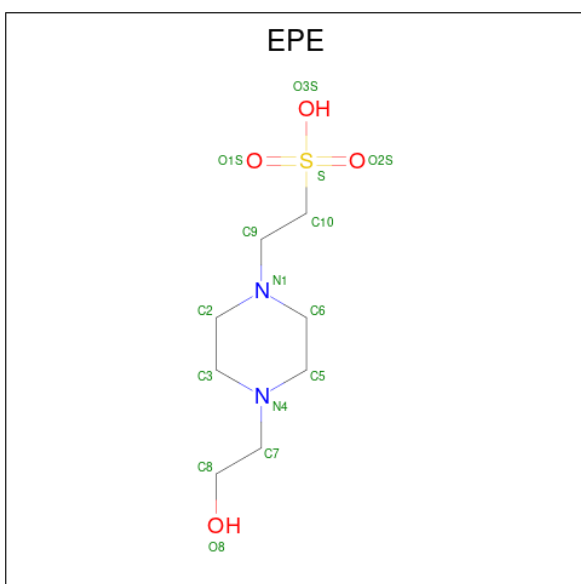
Mol	Chain	Residues	Atoms			AltConf
82	A	1	Total	C	N	0
			14	10	4	

- Molecule 83 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms			AltConf
83	A	1	Total	C	N	0
			10	7	3	
83	A	1	Total	C	N	0
			10	7	3	
83	A	1	Total	C	N	0
			10	7	3	
83	A	1	Total	C	N	0
			10	7	3	

- Molecule 84 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					AltConf
84	A	1	Total	C	N	O	S	0
			15	8	2	4	1	

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

Mol	Chain	Residues	Atoms		AltConf
85	Ma	1	Total	Zn	0
			1	1	
85	BD	1	Total	Zn	0
			1	1	
85	Ga	1	Total	Zn	0
			1	1	
85	BE	1	Total	Zn	0
			1	1	
85	AY	1	Total	Zn	0
			1	1	
85	Ca	1	Total	Zn	0
			1	1	

- Molecule 86 is water.

Mol	Chain	Residues	Atoms		AltConf
86	3	341	Total	O	0
			341	341	
86	A	7528	Total	O	0
			7528	7528	
86	i2	7	Total	O	0
			7	7	
86	C3	178	Total	O	0
			178	178	
86	BC	10	Total	O	0
			10	10	
86	BM	66	Total	O	0
			66	66	
86	BO	31	Total	O	0
			31	31	
86	AR	38	Total	O	0
			38	38	
86	AU	28	Total	O	0
			28	28	
86	Ma	26	Total	O	0
			26	26	
86	Ia	24	Total	O	0
			24	24	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
86	AE	22	Total 22	O 22	0
86	AX	28	Total 28	O 28	0
86	AP	16	Total 16	O 16	0
86	Ja	16	Total 16	O 16	0
86	Ea	133	Total 133	O 133	0
86	AL	65	Total 65	O 65	0
86	Va	30	Total 30	O 30	0
86	Ka	2	Total 2	O 2	0
86	AW	58	Total 58	O 58	0
86	BD	65	Total 65	O 65	0
86	BS	170	Total 170	O 170	0
86	AM	79	Total 79	O 79	0
86	AC	23	Total 23	O 23	0
86	BI	41	Total 41	O 41	0
86	AH	24	Total 24	O 24	0
86	BT	138	Total 138	O 138	0
86	AV	69	Total 69	O 69	0
86	AD	8	Total 8	O 8	0
86	AJ	117	Total 117	O 117	0
86	BQ	131	Total 131	O 131	0
86	BH	90	Total 90	O 90	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
86	Da	23	Total 23	O 23	0
86	BK	70	Total 70	O 70	0
86	AT	16	Total 16	O 16	0
86	Pa	3	Total 3	O 3	0
86	BP	22	Total 22	O 22	0
86	BN	34	Total 34	O 34	0
86	BG	40	Total 40	O 40	0
86	Fa	51	Total 51	O 51	0
86	Ha	87	Total 87	O 87	0
86	BU	11	Total 11	O 11	0
86	BR	77	Total 77	O 77	0
86	Xa	17	Total 17	O 17	0
86	BV	16	Total 16	O 16	0
86	BJ	36	Total 36	O 36	0
86	AO	22	Total 22	O 22	0
86	BW	1	Total 1	O 1	0
86	AK	46	Total 46	O 46	0
86	Na	3	Total 3	O 3	0
86	AB	7	Total 7	O 7	0
86	BF	17	Total 17	O 17	0
86	AA	3	Total 3	O 3	0

Continued on next page...

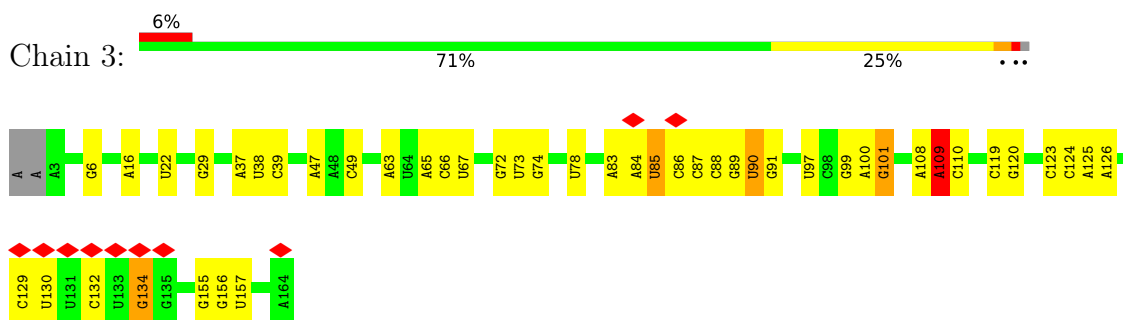
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
86	AG	91	Total 91	O 91	0
86	Ga	18	Total 18	O 18	0
86	BA	22	Total 22	O 22	0
86	AF	9	Total 9	O 9	0
86	Wa	1	Total 1	O 1	0
86	Ta	7	Total 7	O 7	0
86	AZ	4	Total 4	O 4	0
86	BE	34	Total 34	O 34	0
86	Za	3	Total 3	O 3	0
86	AQ	3	Total 3	O 3	0
86	Oa	2	Total 2	O 2	0
86	Ua	29	Total 29	O 29	0
86	Ya	1	Total 1	O 1	0
86	BL	3	Total 3	O 3	0
86	Aa	6	Total 6	O 6	0
86	AY	71	Total 71	O 71	0
86	h1	1709	Total 1709	O 1709	0
86	B1	22	Total 22	O 22	0
86	W2	22	Total 22	O 22	0
86	Ba	4	Total 4	O 4	0
86	L3	1	Total 1	O 1	0

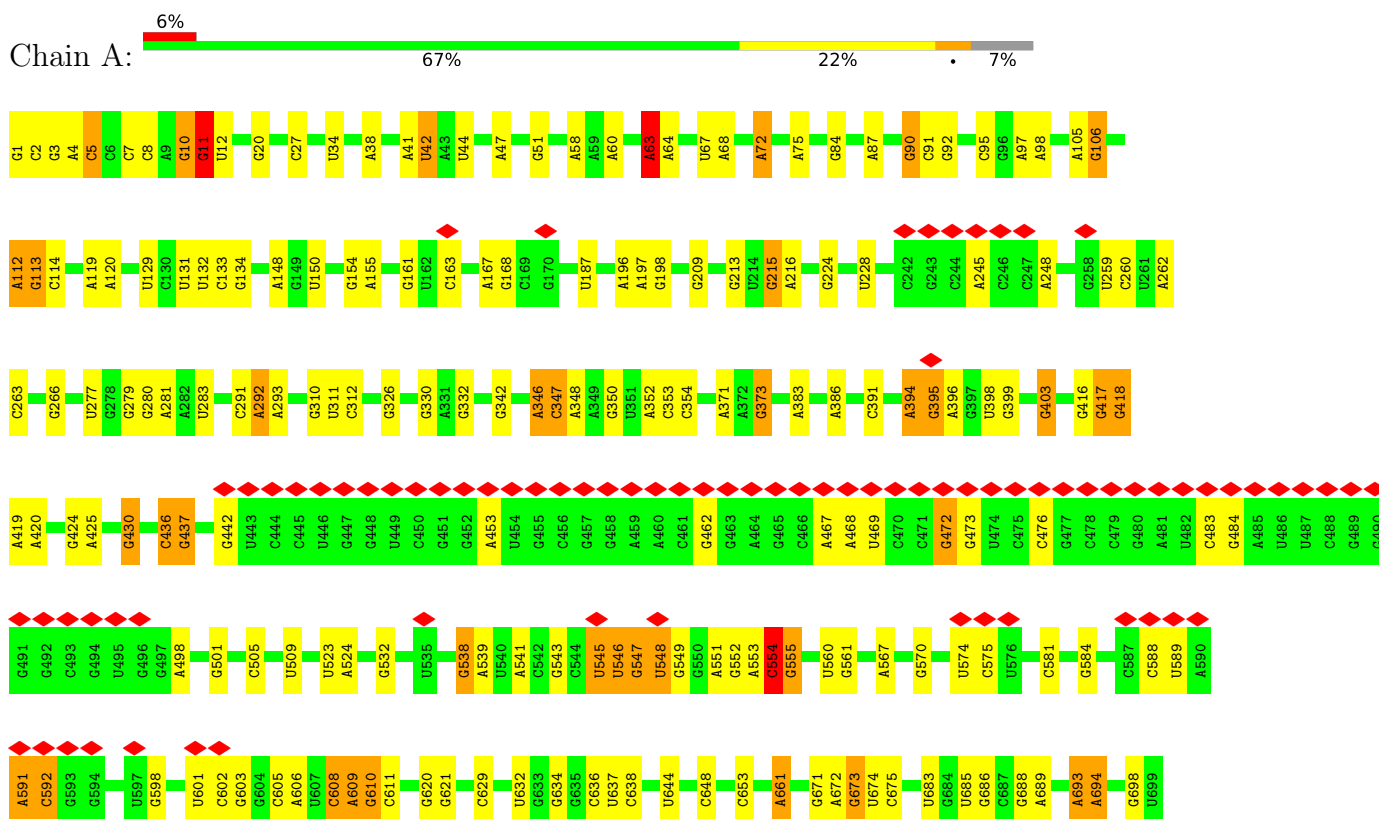
3 Residue-property plots

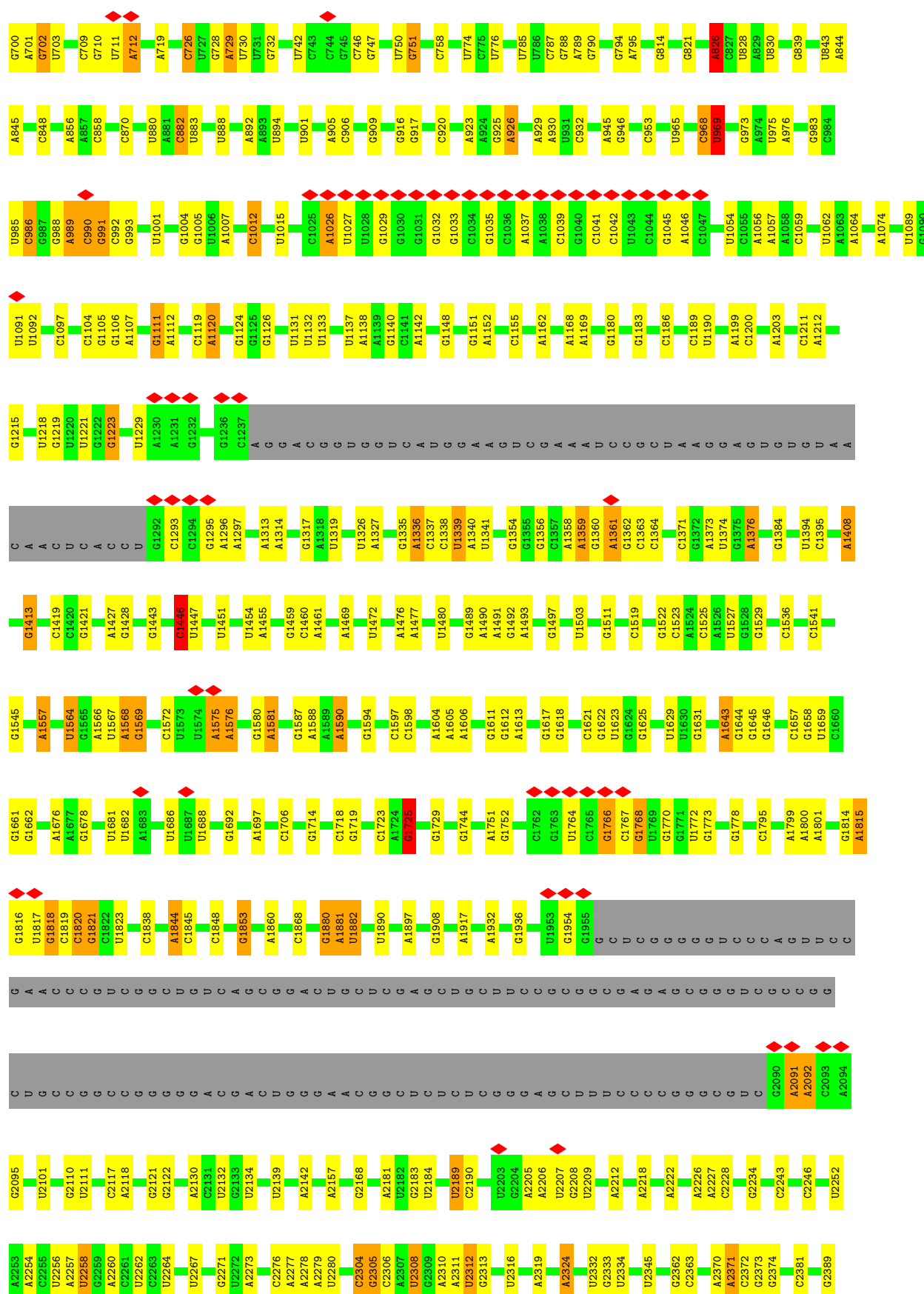
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

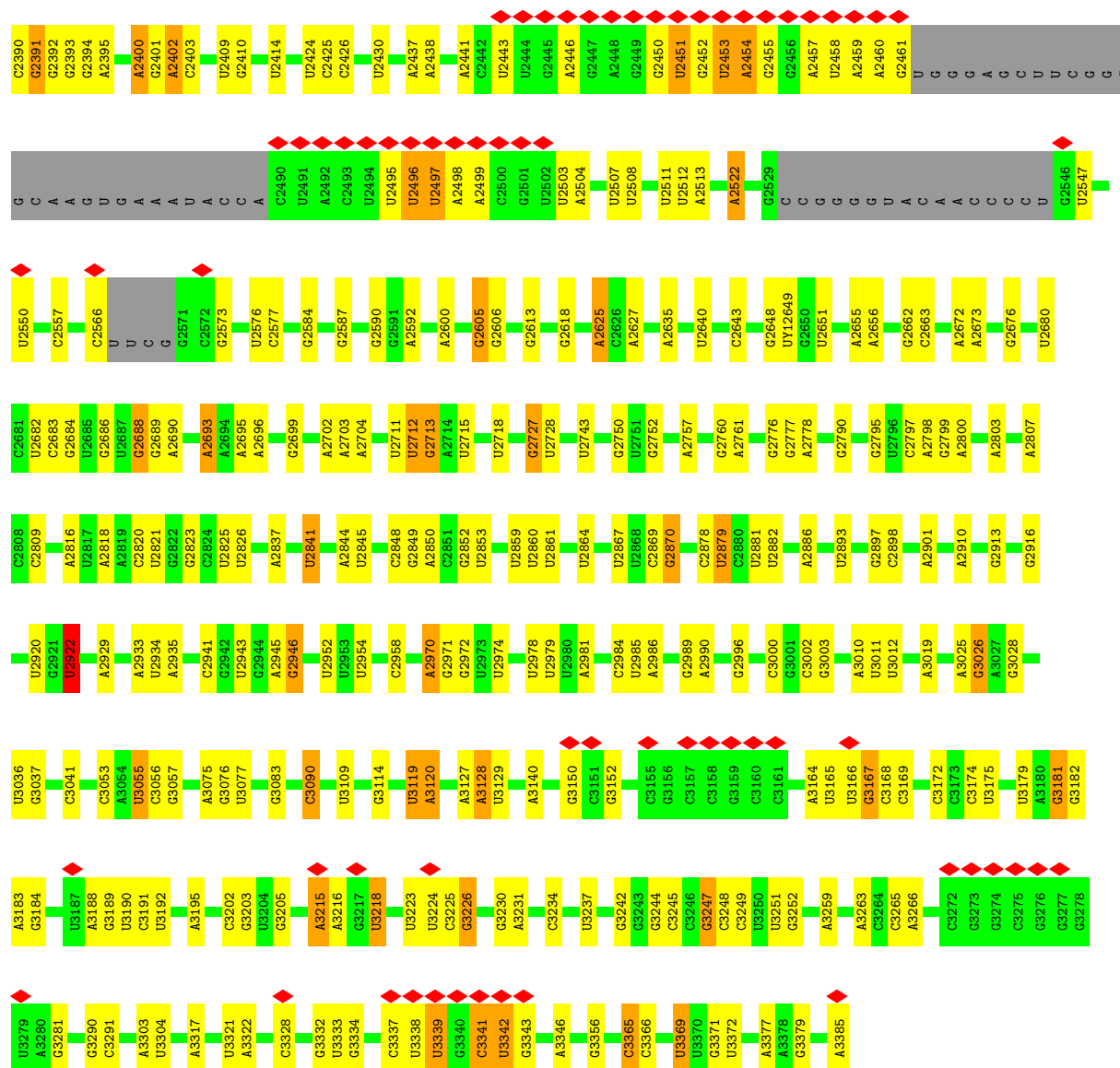
• Molecule 1: Ribosomal RNA 5.8S



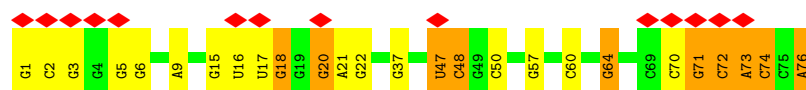
• Molecule 2: Ribosomal RNA 25S



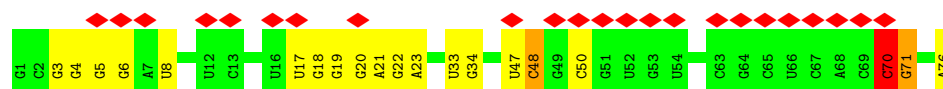
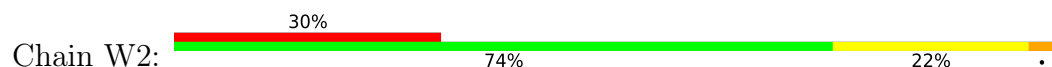





• Molecule 3: Transfer RNA Phe

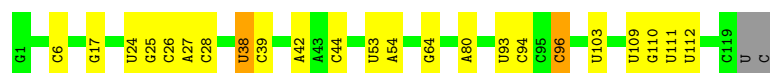


• Molecule 3: Transfer RNA Phe



• Molecule 4: Ribosomal RNA 5S

Chain C3:  79% 17% ..




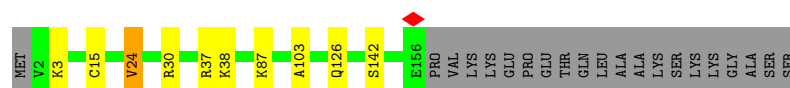
- Molecule 5: Small ribosomal subunit protein eS32 eS32z/eS32y/eS32x/eS32w/eS32v

Chain BC:  100%


There are no outlier residues recorded for this chain.

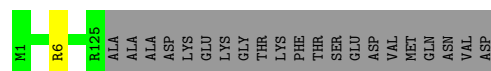
- Molecule 6: Large ribosomal subunit protein uL22z

Chain BM:  82% 5% • 12%



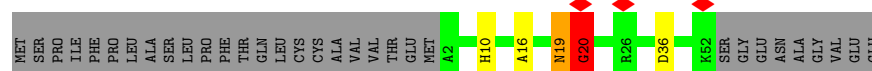
- Molecule 7: Large ribosomal subunit protein uL24z

Chain BO:  85% • 14%




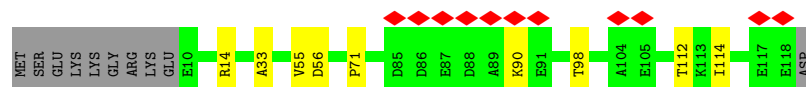
- Molecule 8: 60S ribosomal protein L29

Chain AR:  55% • • 39%



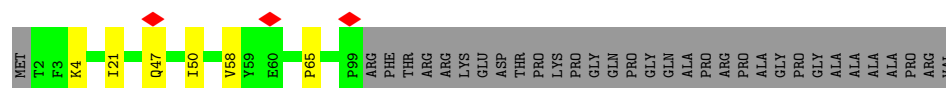
- Molecule 9: Large ribosomal subunit protein eL31y

Chain AU:  9% 84% 8% 8%




- Molecule 10: Small ribosomal subunit protein eS26y

Chain Ma:  70% 5% 25%



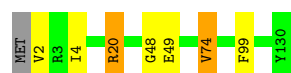
- Molecule 11: Large ribosomal subunit protein uL6z/uL6y

Chain Ia:  89% 9%




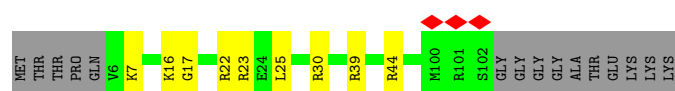
- Molecule 12: Small ribosomal subunit protein uS8z/uS8w

Chain AE:  94%



- Molecule 13: Large ribosomal subunit protein eL36y

Chain AX:  79% 8% 13%




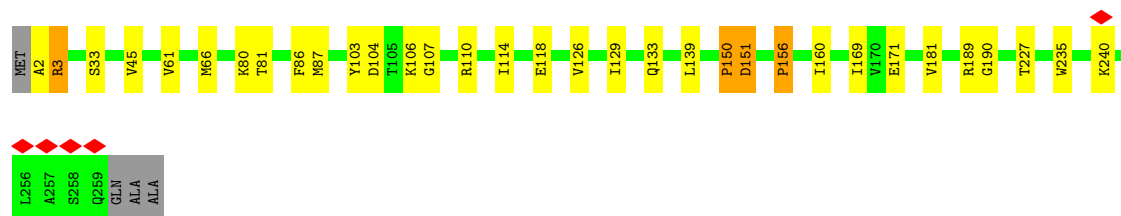
- Molecule 14: Large ribosomal subunit protein eL27x

Chain AP:  90% 9%



- Molecule 15: Small ribosomal subunit protein eS4x

Chain Ja:  86% 11%



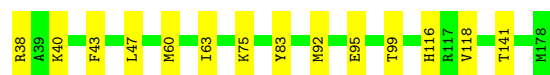
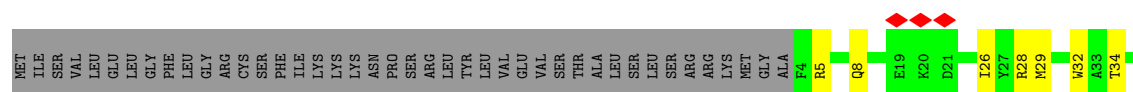
- Molecule 16: Large ribosomal subunit protein eL15z

Chain Ea:  93% 7%



- Molecule 17: Ribosomal protein L18ae/LX family protein

Chain AL:  71% 10% 19%



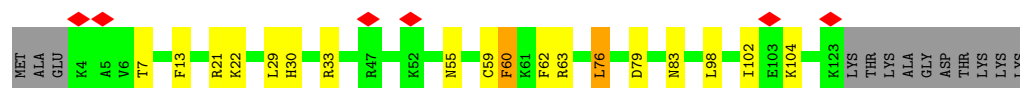
- Molecule 18: Small ribosomal subunit protein uS12y

Chain Va: 94%



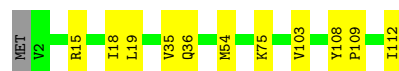
- Molecule 19: Small ribosomal subunit protein eS24y

Chain Ka: 5% 77% 12% 10%



- Molecule 20: Large ribosomal subunit protein eL33y

Chain AW: 89% 10%



- Molecule 21: Large ribosomal subunit protein eL42z/eL42y

Chain BD: 89% 8%



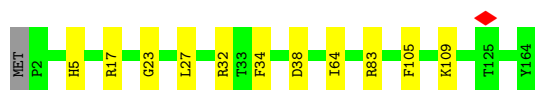
- Molecule 22: Large ribosomal subunit protein uL3z

Chain BS: 90% 9%



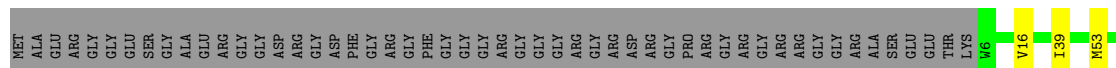
- Molecule 23: Large ribosomal subunit protein eL21z/eL21y

Chain AM: 93% 7%



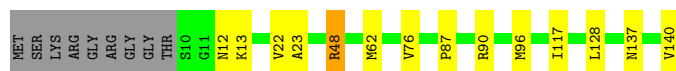
- Molecule 24: Small ribosomal subunit protein uS5y/uS5u/uS5v

Chain AC: 68% 7% 24%



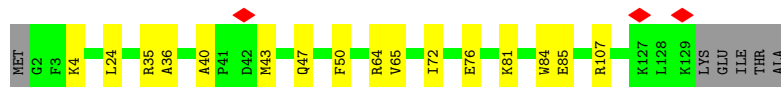
- Molecule 25: Large ribosomal subunit protein uL14x/uL14z/uL14y

Chain BI: 84% 9% 6%



- Molecule 26: Large ribosomal subunit protein eL14y

Chain AH: 84% 12% 4%



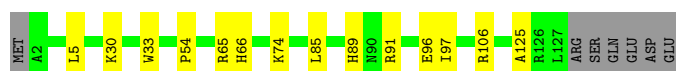
- Molecule 27: Large ribosomal subunit protein uL4z

Chain BT: 85% 12% 3%



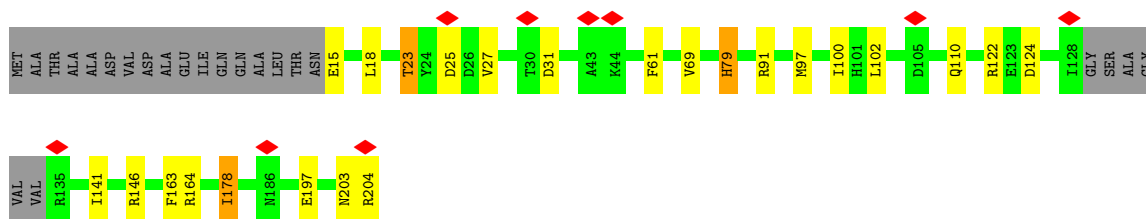
- Molecule 28: Large ribosomal subunit protein eL32z

Chain AV: 84% 11% 5%



- Molecule 29: Small ribosomal subunit protein uS7y

Chain AD: 77% 10% 11%



- Molecule 30: Large ribosomal subunit protein eL18x

Chain AJ: 94% 6%



- Molecule 31: Large ribosomal subunit protein uL2z

Chain BQ: 89% 6% 5%



- Molecule 32: Large ribosomal subunit protein uL13y

Chain BH: 93% 6%



- Molecule 33: Small ribosomal subunit protein uS15y

Chain Da: 91% 8%



- Molecule 34: Large ribosomal subunit protein uL18z

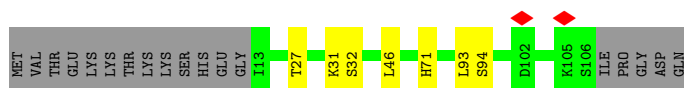
Chain BK: 88% 5% 7%



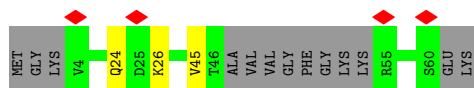
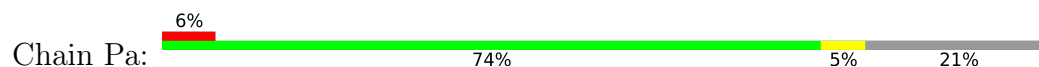
- Molecule 35: Large ribosomal subunit protein eL30y

Chain AT: 78% 6% 16%





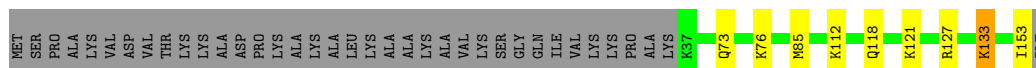
- Molecule 36: Small ribosomal subunit protein eS30z/eS30y/eS30x



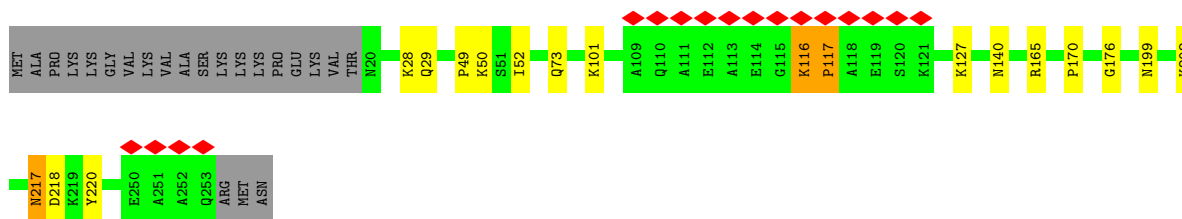
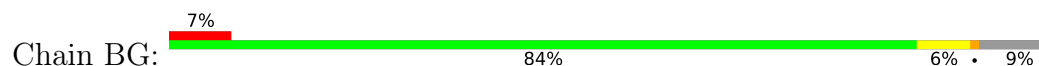
- Molecule 37: Large ribosomal subunit protein uL29x



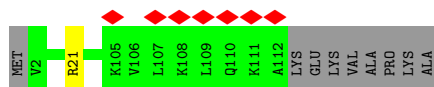
- Molecule 38: Large ribosomal subunit protein uL23y



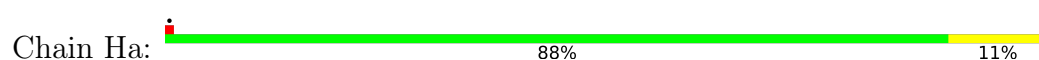
- Molecule 39: Large ribosomal subunit protein eL8y



- Molecule 40: Large ribosomal subunit protein eL34z

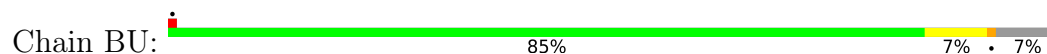


- Molecule 41: Large ribosomal subunit protein uL15x





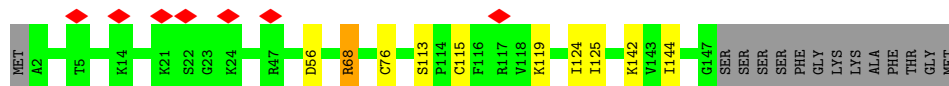
- Molecule 42: Large ribosomal subunit protein uL5z



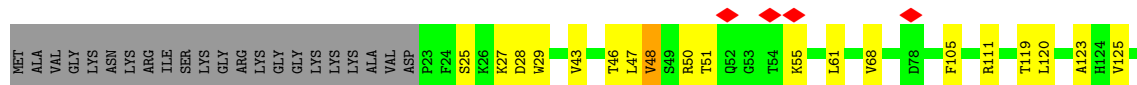
- Molecule 43: Ribosomal protein L30/L7 family protein



- Molecule 44: Small ribosomal subunit protein uS17z



- Molecule 45: Small ribosomal subunit protein eS1y

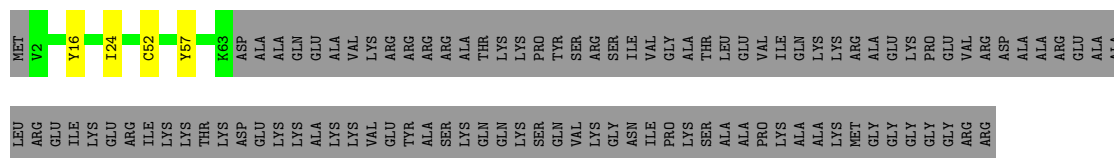


- Molecule 46: Large ribosomal subunit protein uL16y




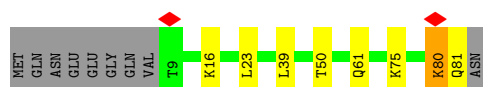
- Molecule 47: Large ribosomal subunit protein eL24z

Chain AO:  35% 62%




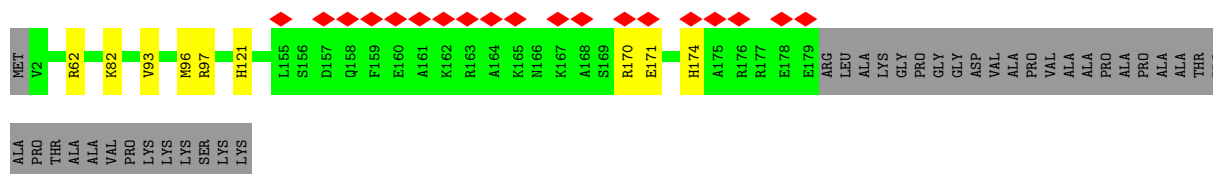
- Molecule 48: Small ribosomal subunit protein eS21y

Chain BW:  79% 9% 11%




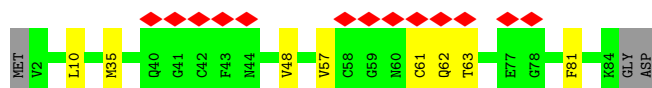
- Molecule 49: Large ribosomal subunit protein eL19x

Chain AK:  9% 79% 17%




- Molecule 50: Small ribosomal subunit protein eS27y

Chain Na:  15% 87% 9%




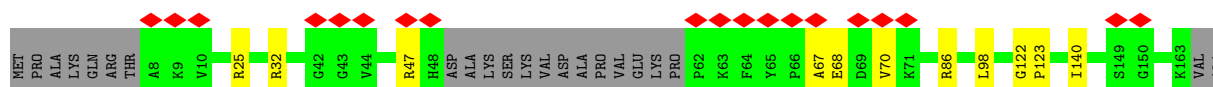
- Molecule 51: Small ribosomal subunit protein uS4y

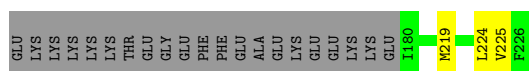
Chain AB:  80% 12% 9%



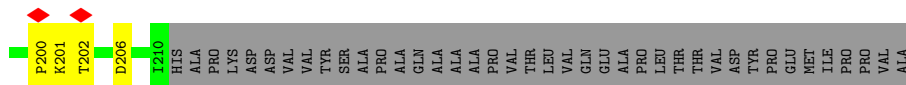
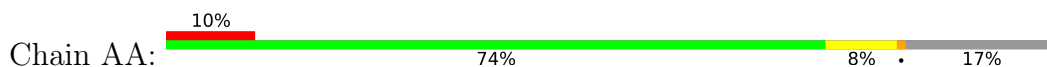
- Molecule 52: Large ribosomal subunit protein eL6y

Chain BF:  8% 76% 6% 18%

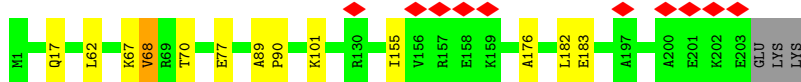




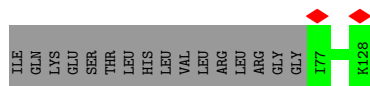
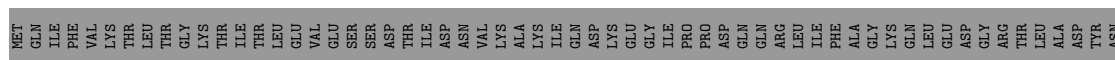
- Molecule 53: Small ribosomal subunit protein uS3z



- Molecule 54: Large ribosomal subunit protein eL13z



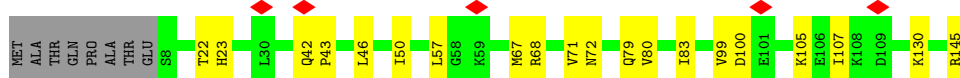
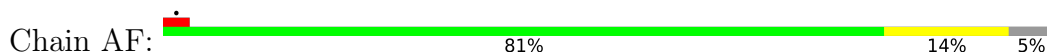
- Molecule 55: Ubiquitin-ribosomal protein eL40z fusion protein



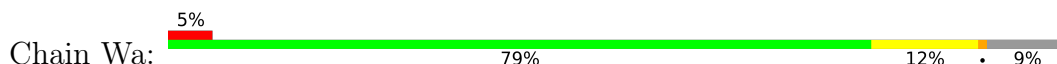
- Molecule 56: Large ribosomal subunit protein eL39z/eL39x



- Molecule 57: Small ribosomal subunit protein uS9z

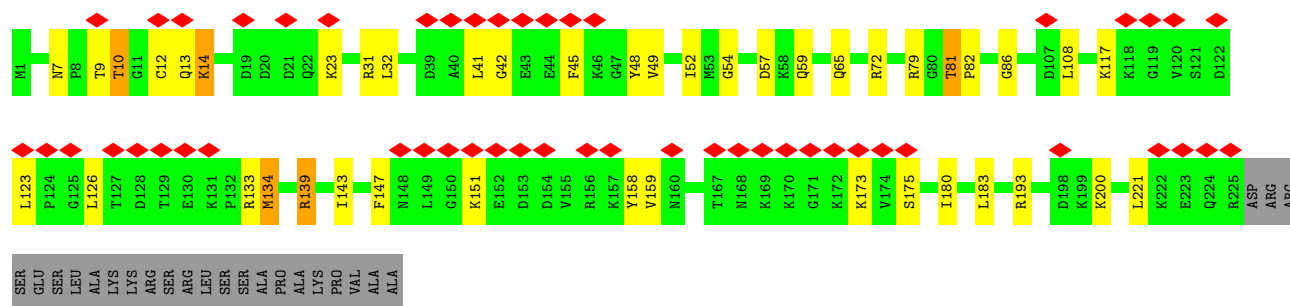
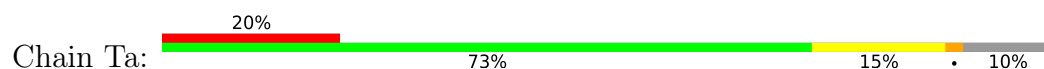


- Molecule 58: Small ribosomal subunit protein uS13z/uS13y/uS13x

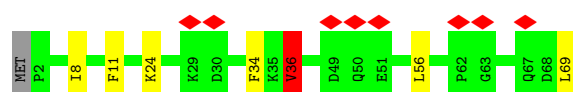
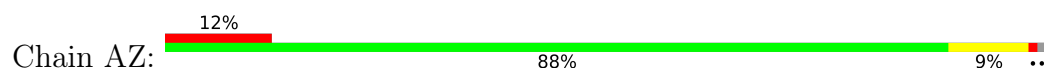




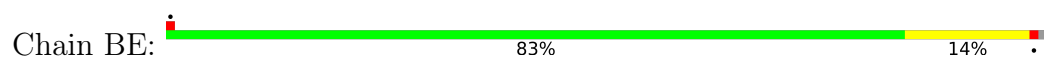
- Molecule 59: Small ribosomal subunit protein eS6y



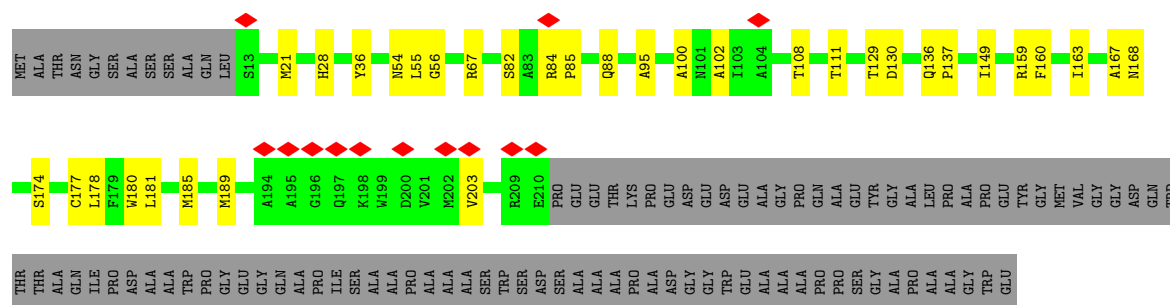
- Molecule 60: Large ribosomal subunit protein eL38z/eL38y



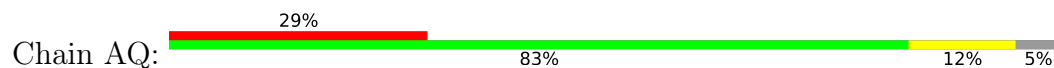
- Molecule 61: Large ribosomal subunit protein eL43y

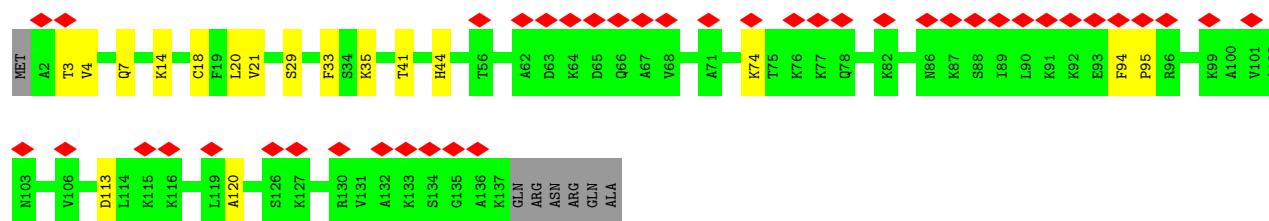


- Molecule 62: Small ribosomal subunit protein uS2z

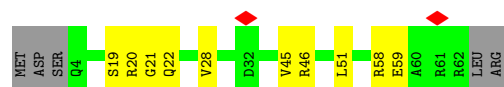
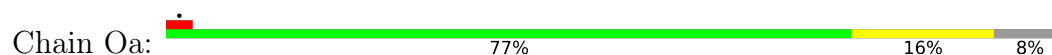


- Molecule 63: Large ribosomal subunit protein eL28z

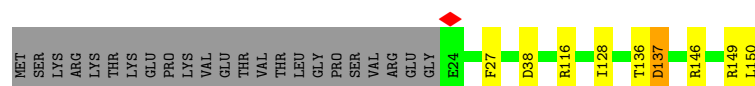
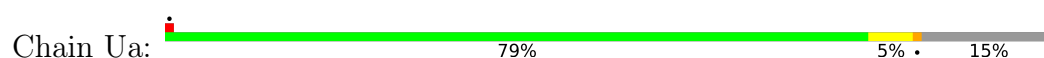




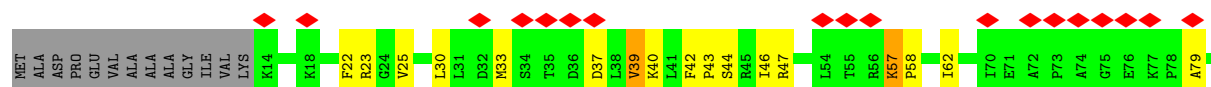
- Molecule 64: Small ribosomal subunit protein eS28x



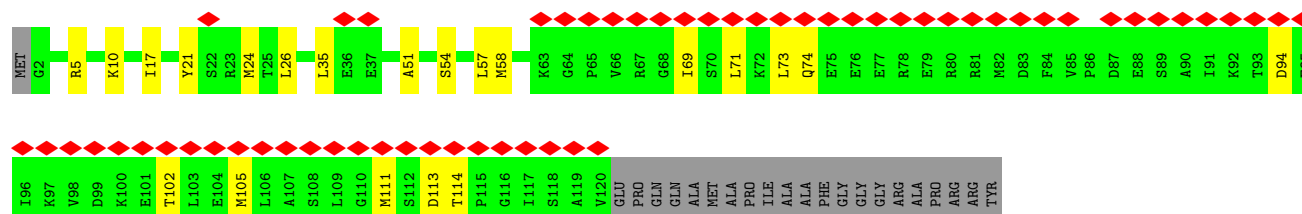
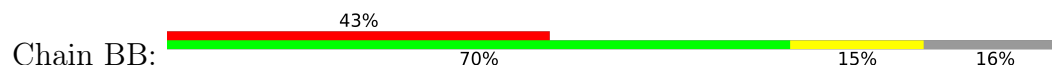
- Molecule 65: Small ribosomal subunit protein uS11y



- Molecule 66: Small ribosomal subunit protein uS19y



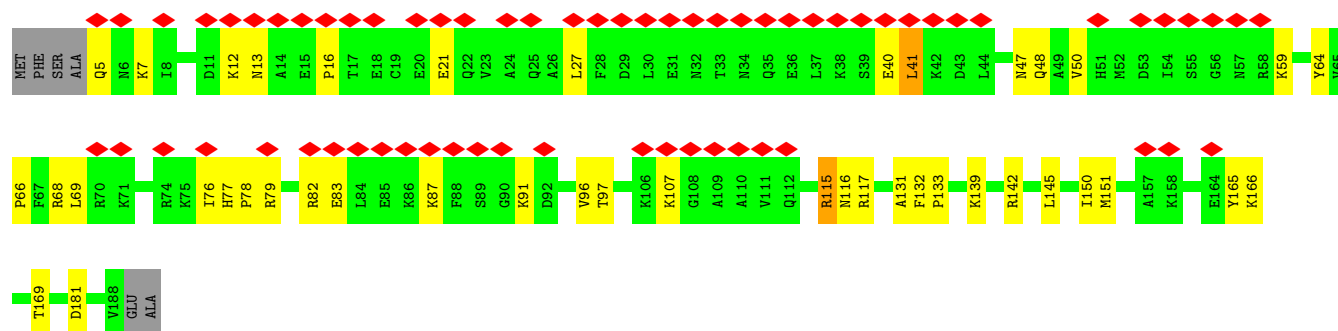
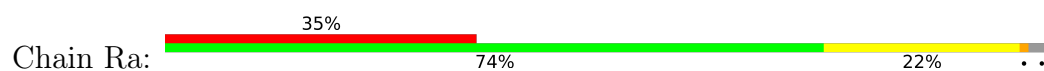
- Molecule 67: Small ribosomal subunit protein eS17w



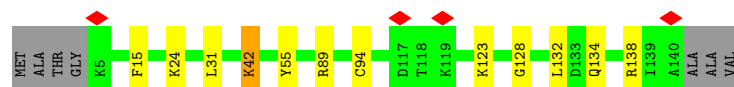
- Molecule 68: Large ribosomal subunit protein eL22z



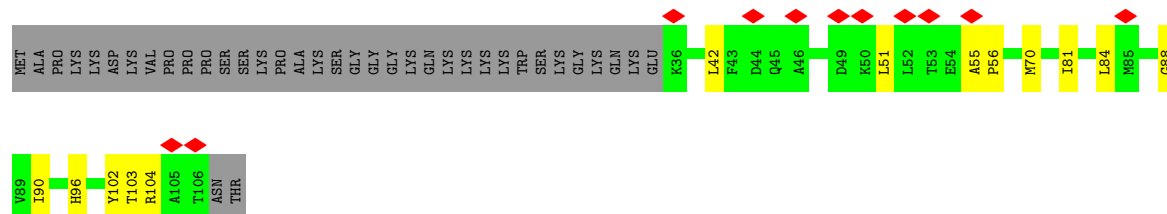
- Molecule 69: Small ribosomal subunit protein eS7x



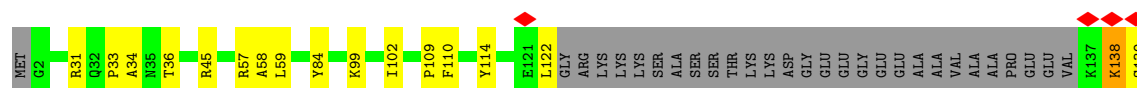
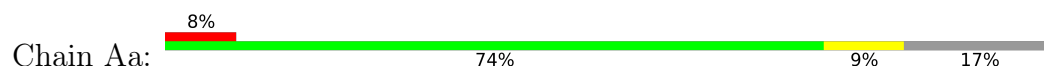
- Molecule 70: Small ribosomal subunit protein eS19x

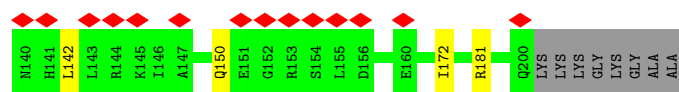


- Molecule 71: Small ribosomal subunit protein eS25w

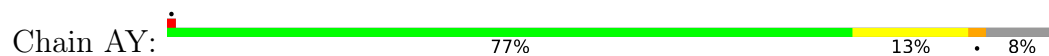


- Molecule 72: Small ribosomal subunit protein eS8z

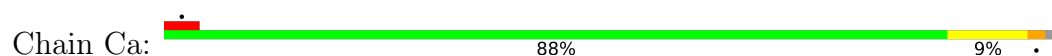




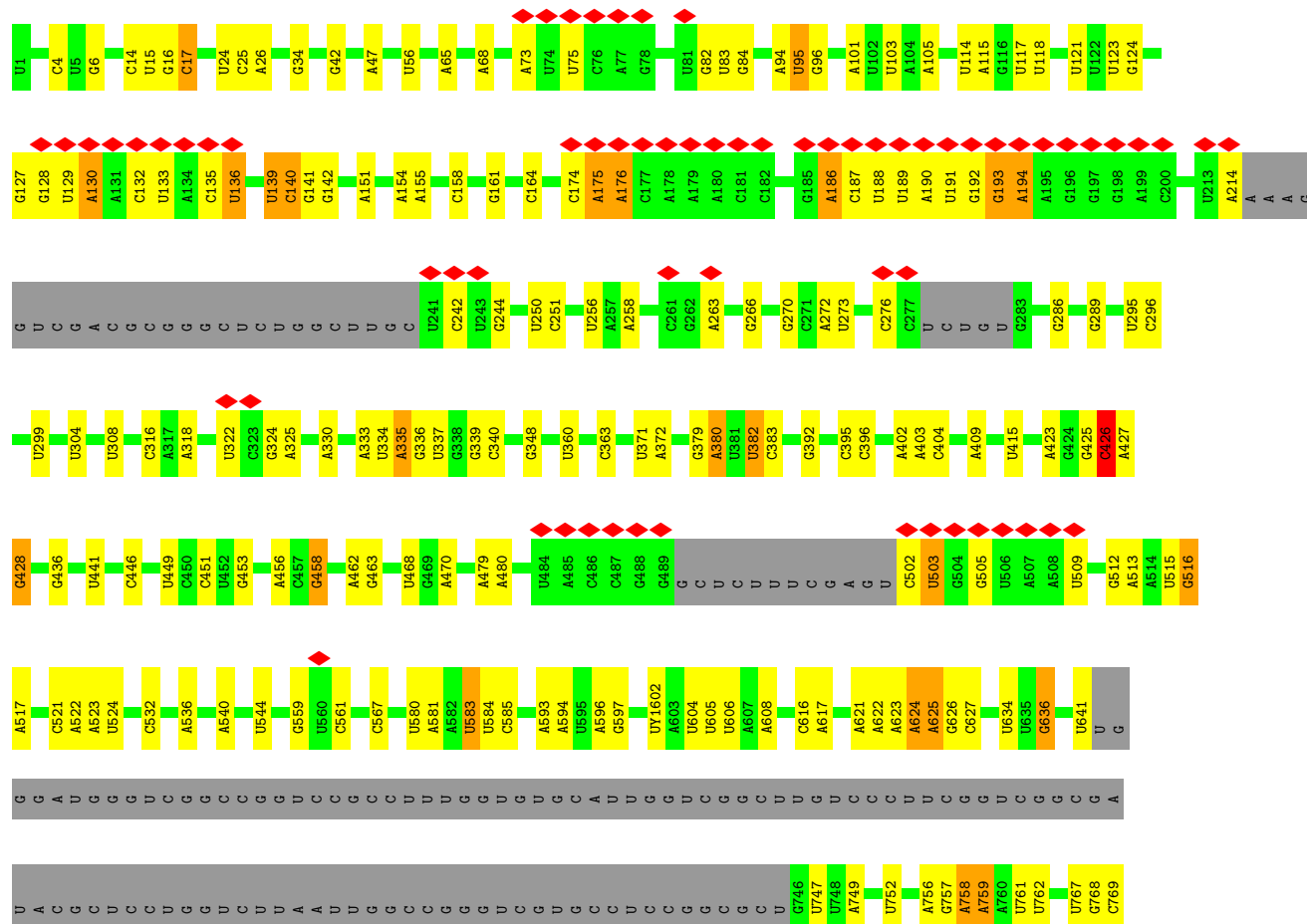
- Molecule 73: Large ribosomal subunit protein eL37z

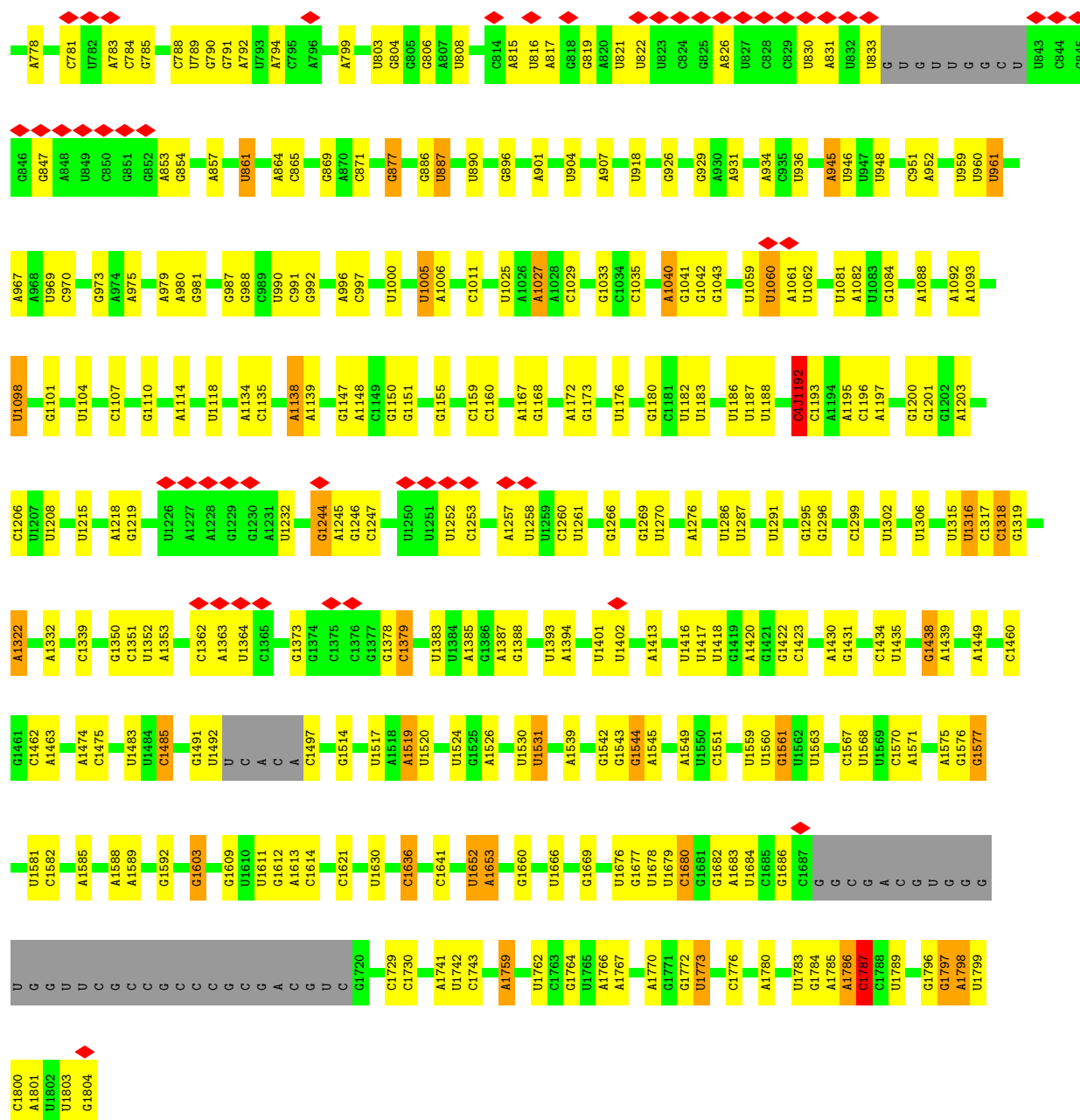


- Molecule 74: Small ribosomal subunit protein uS14z/uS14y/uS14x

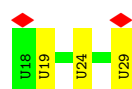
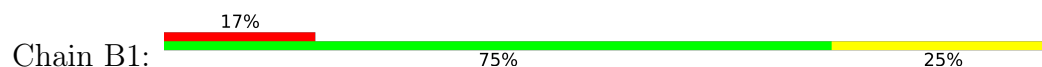


- Molecule 75: Ribosomal RNA 18S



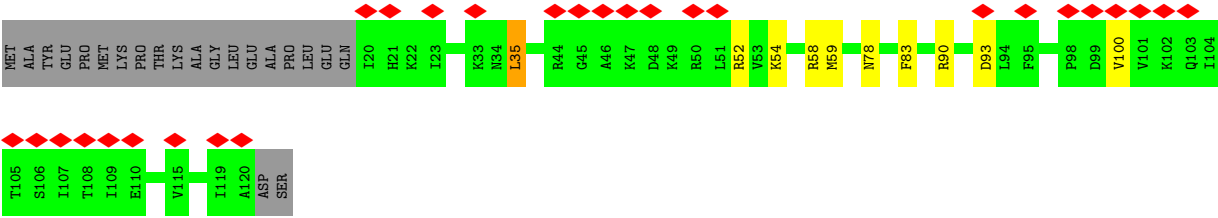


• Molecule 76: Messenger RNA (poly-U)

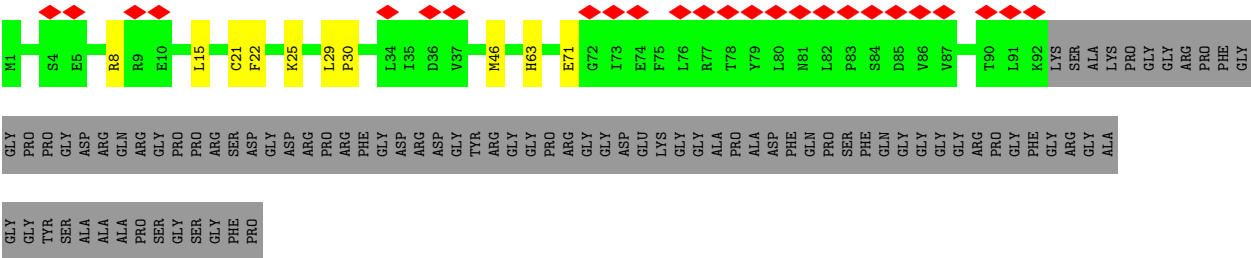


• Molecule 77: Small ribosomal subunit protein uS10y

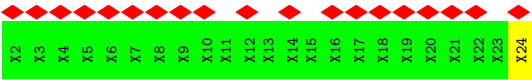
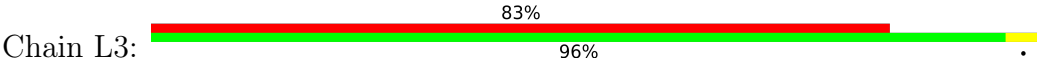




• Molecule 78: Small ribosomal subunit protein eS10z



• Molecule 79: Nascent polypeptide (poly-A)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	243821	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	11.827	Depositor
Minimum map value	-3.649	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.245	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	495.978, 495.978, 495.978	wwPDB
Map dimensions	686, 686, 686	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.723, 0.723, 0.723	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MLY, SPD, 4AC, C4J, K, G7M, PSU, 5MC, 1MG, TER, UR3, OMC, EPE, 1MA, HIC, OMG, 6MZ, MA6, OMU, A2M, ZN, UY1, MG

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	3	0.47	0/3713	0.95	8/5784 (0.1%)
2	A	0.49	1/72590 (0.0%)	0.97	137/113222 (0.1%)
3	W2	0.53	0/1822	0.85	2/2840 (0.1%)
3	i2	0.52	0/1823	0.85	4/2840 (0.1%)
4	C3	0.46	0/2834	0.93	4/4415 (0.1%)
5	BC	0.53	0/238	0.95	0/302
6	BM	0.53	0/1269	0.89	0/1705
7	BO	0.51	0/1042	0.86	0/1390
8	AR	0.55	0/435	0.94	0/577
9	AU	0.49	0/900	0.85	0/1202
10	Ma	0.51	0/804	0.76	0/1081
11	Ia	0.47	0/1533	0.79	0/2050
12	AE	0.47	0/1051	0.83	0/1406
13	AX	0.50	0/793	0.93	0/1047
14	AP	0.47	0/1110	0.82	0/1477
15	Ja	0.46	0/2116	0.81	0/2841
16	Ea	0.53	0/1754	0.86	0/2349
17	AL	0.49	0/1523	0.85	1/2042 (0.0%)
18	Va	0.49	0/1100	0.83	0/1465
19	Ka	0.45	0/1001	0.81	0/1329
20	AW	0.51	0/921	0.81	0/1234
21	BD	0.51	0/806	0.85	0/1065
22	BS	0.50	0/3165	0.83	0/4238
23	AM	0.49	0/1335	0.86	0/1789
24	AC	0.49	0/1709	0.84	1/2310 (0.0%)
25	BI	0.52	0/1002	0.86	0/1347
26	AH	0.46	0/1054	0.81	0/1408
27	BT	0.51	0/3112	0.84	1/4187 (0.0%)
28	AV	0.51	0/1045	0.82	0/1399
29	AD	0.45	0/1473	0.87	1/1985 (0.1%)
30	AJ	0.53	0/1492	0.87	0/1995

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	BQ	0.54	0/1928	0.86	1/2594 (0.0%)
32	BH	0.52	0/1664	0.85	1/2224 (0.0%)
33	Da	0.50	0/1214	0.86	0/1630
34	BK	0.47	0/2321	0.83	0/3119
35	AT	0.50	0/731	0.83	0/982
36	Pa	0.50	0/394	0.88	0/519
37	BP	0.49	0/984	0.83	0/1306
38	BN	0.49	0/972	0.83	0/1309
39	BG	0.48	0/1908	0.87	1/2561 (0.0%)
40	Fa	0.52	0/909	0.91	0/1214
41	Ha	0.55	0/1187	0.91	0/1584
42	BU	0.44	0/1388	0.81	0/1858
43	BR	0.48	0/1931	0.87	0/2584
44	Xa	0.48	0/1189	0.73	0/1590
45	BV	0.45	0/1746	0.81	0/2341
46	BJ	0.48	0/1691	0.82	0/2263
47	AO	0.48	0/541	0.76	0/718
48	BW	0.46	0/577	0.83	0/777
49	AK	0.50	0/1499	0.86	0/1975
50	Na	0.46	0/657	0.80	0/883
51	AB	0.44	0/1540	0.83	0/2061
52	BF	0.48	0/1521	0.83	0/2040
53	AA	0.45	0/1647	0.82	0/2212
54	AG	0.49	0/1680	0.87	0/2251
55	Ga	0.49	0/428	0.80	0/564
56	BA	0.56	0/456	0.81	0/603
57	AF	0.46	0/1133	0.82	0/1513
58	Wa	0.44	0/1152	0.84	0/1541
59	Ta	0.45	0/1819	0.87	0/2422
60	AZ	0.49	0/570	0.84	1/758 (0.1%)
61	BE	0.51	0/711	0.92	1/942 (0.1%)
62	Za	0.45	0/1609	0.83	0/2173
63	AQ	0.46	0/1070	0.85	0/1436
64	Oa	0.44	0/474	0.75	0/632
65	Ua	0.49	0/974	0.87	0/1305
66	Ya	0.48	0/1044	0.85	0/1398
67	BB	0.45	0/965	0.90	0/1287
68	AN	0.45	0/820	0.83	0/1097
69	Ra	0.44	0/1530	0.87	0/2052
70	BL	0.47	0/1086	0.90	1/1459 (0.1%)
71	La	0.45	0/568	0.85	0/762
72	Aa	0.45	0/1517	0.81	0/2027
73	AY	1.45	1/718 (0.1%)	1.04	1/954 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	Ca	1.98	1/451 (0.2%)	0.94	3/601 (0.5%)
75	h1	0.50	0/36567	0.91	49/56975 (0.1%)
76	B1	0.52	0/263	0.87	0/404
77	Ba	0.45	0/809	0.82	0/1090
78	AI	0.44	0/801	0.82	0/1082
All	All	0.50	3/205919 (0.0%)	0.91	218/301993 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	7
8	AR	0	2
14	AP	0	1
22	BS	0	1
23	AM	0	2
25	BI	0	1
27	BT	0	1
34	BK	0	1
37	BP	0	1
41	Ha	0	1
42	BU	0	1
44	Xa	0	1
46	BJ	0	1
49	AK	0	1
69	Ra	0	1
73	AY	0	2
All	All	0	25

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
74	Ca	53	ILE	C-N	40.62	1.90	1.33
73	AY	76	THR	C-N	35.88	1.85	1.33
2	A	2279	A2M	O3'-P	5.24	1.61	1.56

All (218) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
73	AY	76	THR	O-C-N	-14.09	101.86	122.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	426	C	O3'-P-O5'	-11.10	87.36	104.00
2	A	3127	A	O3'-P-O5'	-10.99	87.51	104.00
75	h1	1422	G	O3'-P-O5'	-10.38	88.44	104.00
2	A	1111	G	O3'-P-O5'	-9.96	89.06	104.00
75	h1	1196	C	O3'-P-O5'	-9.47	89.79	104.00
2	A	728	G	O3'-P-O5'	9.36	118.05	104.00
75	h1	992	G	O3'-P-O5'	-8.96	90.56	104.00
2	A	2672	A	O3'-P-O5'	-8.93	90.61	104.00
2	A	291	C	O3'-P-O5'	8.88	117.31	104.00
1	3	156	G	O3'-P-O5'	-8.69	90.97	104.00
2	A	1111	G	C2'-C3'-O3'	-8.63	100.75	113.70
2	A	2511	U	O3'-P-O5'	-8.62	91.07	104.00
75	h1	996	A	O3'-P-O5'	-8.49	91.27	104.00
2	A	332	G	O3'-P-O5'	-8.48	91.27	104.00
75	h1	1114	A	O3'-P-O5'	-8.33	91.51	104.00
2	A	1339	U	O3'-P-O5'	-8.13	91.81	104.00
74	Ca	53	ILE	CA-C-N	-8.13	109.88	121.50
74	Ca	53	ILE	C-N-CA	-8.13	109.88	121.50
2	A	945	A2M	O3'-P-O5'	-8.00	88.80	104.00
2	A	72	A	O3'-P-O5'	-7.96	92.07	104.00
2	A	10	G	O3'-P-O5'	-7.93	92.11	104.00
2	A	1001	PSU	O3'-P-O5'	-7.89	92.17	104.00
2	A	729	A	O5'-P-OP2	-7.78	84.67	108.00
2	A	1644	G	O3'-P-O5'	-7.37	92.94	104.00
2	A	1882	U	O3'-P-O5'	-7.29	93.06	104.00
1	3	65	A	O3'-P-O5'	-7.29	93.07	104.00
75	h1	1797	G	O3'-P-O5'	-7.13	93.31	104.00
2	A	2587	G	O3'-P-O5'	-7.12	93.31	104.00
2	A	1661	G	O3'-P-O5'	-7.01	93.48	104.00
75	h1	926	G	O3'-P-O5'	-7.01	93.48	104.00
75	h1	1787	C	O5'-P-OP2	-6.94	87.19	108.00
1	3	37	A	O3'-P-O5'	-6.90	93.64	104.00
4	C3	17	G	O3'-P-O5'	-6.87	93.70	104.00
75	h1	371	U	O3'-P-O5'	-6.84	93.73	104.00
2	A	789	A	O3'-P-O5'	-6.84	93.75	104.00
2	A	1054	PSU	O3'-P-O5'	-6.80	93.79	104.00
75	h1	1092	A	O3'-P-O5'	-6.80	93.80	104.00
2	A	505	C	O3'-P-O5'	-6.78	93.82	104.00
75	h1	808	PSU	O3'-P-O5'	-6.78	93.84	104.00
2	A	2727	G	C1'-O4'-C4'	-6.77	102.93	109.70
2	A	1725	G	O3'-P-O5'	-6.76	93.86	104.00
2	A	425	A	O3'-P-O5'	-6.74	93.89	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	882	C	C2'-C3'-O3'	-6.72	103.62	113.70
2	A	1489	G	O3'-P-O5'	-6.67	94.00	104.00
75	h1	624	A	O3'-P-O5'	-6.64	94.04	104.00
75	h1	325	A	O3'-P-O5'	-6.63	94.05	104.00
2	A	1451	U	O3'-P-O5'	-6.62	94.06	104.00
2	A	3333	U	O3'-P-O5'	-6.59	94.12	104.00
2	A	266	G	O3'-P-O5'	-6.56	94.16	104.00
75	h1	951	C	O3'-P-O5'	-6.54	94.19	104.00
29	AD	79	HIS	CB-CA-C	6.54	123.43	110.42
2	A	698	G	O3'-P-O5'	-6.53	94.21	104.00
2	A	417	G	O3'-P-O5'	-6.52	94.22	104.00
2	A	1180	G	O3'-P-O5'	-6.50	94.25	104.00
2	A	386	A	O3'-P-O5'	-6.41	94.38	104.00
2	A	1890	OMU	O3'-P-O5'	-6.41	91.82	104.00
2	A	2142	A	O3'-P-O5'	-6.38	94.42	104.00
2	A	2267	U	O3'-P-O5'	-6.31	94.54	104.00
75	h1	1269	G	C4'-C3'-O3'	-6.30	103.54	113.00
2	A	1221	U	O3'-P-O5'	-6.29	94.57	104.00
2	A	2760	G	O3'-P-O5'	-6.25	94.63	104.00
74	Ca	53	ILE	O-C-N	6.23	129.90	123.18
75	h1	1138	A	O3'-P-O5'	6.17	113.26	104.00
1	3	119	C	O3'-P-O5'	-6.16	94.77	104.00
2	A	2168	G	O3'-P-O5'	-6.15	94.77	104.00
2	A	2391	G	O5'-P-OP2	-6.15	89.55	108.00
75	h1	1005	U	O3'-P-O5'	-6.15	94.78	104.00
75	h1	1423	C	C4'-C3'-O3'	-6.14	103.79	113.00
3	W2	23	A	O3'-P-O5'	-6.13	94.81	104.00
2	A	1336	A	O3'-P-O5'	-6.12	94.82	104.00
2	A	845	A	O3'-P-O5'	-6.12	94.83	104.00
2	A	1413	G	C1'-C2'-O2'	6.11	117.56	108.40
75	h1	1155	G	O3'-P-O5'	-6.10	94.84	104.00
75	h1	616	C	O3'-P-O5'	-6.09	94.87	104.00
24	AC	58	VAL	N-CA-CB	-6.07	100.58	111.92
2	A	2990	A	O3'-P-O5'	-6.06	94.91	104.00
2	A	1897	A	O3'-P-O5'	-6.05	94.93	104.00
75	h1	330	A	O3'-P-O5'	-6.04	94.94	104.00
3	i2	3	G	O3'-P-O5'	-6.03	94.96	104.00
2	A	2400	A	O3'-P-O5'	-6.03	94.96	104.00
2	A	882	C	C4'-C3'-O3'	6.01	122.02	113.00
75	h1	1150	G	O3'-P-O5'	-5.98	95.03	104.00
2	A	1199	A	C4'-C3'-O3'	-5.97	104.05	113.00
2	A	1503	U	O3'-P-O5'	-5.96	95.07	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	11	G	P-O5'-C5'	-5.95	111.97	120.90
2	A	1527	U	O3'-P-O5'	-5.94	95.09	104.00
2	A	1427	A	O3'-P-O5'	-5.94	95.09	104.00
75	h1	382	U	O3'-P-O5'	-5.92	95.12	104.00
2	A	215	G	O5'-P-OP2	-5.91	90.26	108.00
3	i2	71	G	O3'-P-O5'	-5.91	95.13	104.00
2	A	383	A	O3'-P-O5'	-5.91	95.14	104.00
2	A	2402	A	O3'-P-O5'	-5.88	95.17	104.00
2	A	1376	A2M	O3'-P-O5'	-5.86	92.87	104.00
2	A	2712	U	O3'-P-O5'	-5.85	95.23	104.00
75	h1	1081	U	O3'-P-O5'	-5.83	95.26	104.00
2	A	3090	C	O3'-P-O5'	-5.80	95.31	104.00
75	h1	1787	C	O5'-C5'-C4'	-5.80	102.81	111.50
2	A	2181	A	O3'-P-O5'	-5.77	95.35	104.00
2	A	1340	A	O3'-P-O5'	-5.76	95.35	104.00
2	A	67	U	O3'-P-O5'	-5.75	95.37	104.00
2	A	1936	G	O3'-P-O5'	-5.74	95.39	104.00
2	A	1097	C	O3'-P-O5'	-5.74	95.39	104.00
2	A	2640	U	C2'-C3'-O3'	-5.74	105.09	113.70
2	A	3128	A	C4'-C3'-O3'	-5.74	104.39	113.00
75	h1	1318	C	O3'-P-O5'	-5.72	95.42	104.00
2	A	279	G	C2'-C3'-O3'	-5.71	105.13	113.70
2	A	2803	A	O3'-P-O5'	-5.70	95.44	104.00
32	BH	66	ARG	N-CA-CB	-5.70	100.90	110.99
2	A	553	A	O3'-P-O5'	-5.70	95.45	104.00
2	A	1215	G	O3'-P-O5'	-5.70	95.45	104.00
2	A	538	G	O3'-P-O5'	-5.68	95.47	104.00
75	h1	458	G	O3'-P-O5'	-5.68	95.48	104.00
2	A	1820	C	O3'-P-O5'	-5.67	95.50	104.00
75	h1	423	A	O3'-P-O5'	-5.66	95.51	104.00
75	h1	124	G	O3'-P-O5'	-5.65	95.52	104.00
2	A	2310	A	O3'-P-O5'	-5.65	95.53	104.00
2	A	968	C	C2'-C3'-O3'	-5.65	105.23	113.70
2	A	3083	G	O3'-P-O5'	-5.64	95.54	104.00
75	h1	1485	C	O3'-P-O5'	-5.63	95.56	104.00
2	A	3019	A	O3'-P-O5'	-5.60	95.60	104.00
2	A	1454	U	C2'-C3'-O3'	-5.59	105.32	113.70
39	BG	73	GLN	CB-CA-C	-5.57	99.33	110.42
75	h1	1291	PSU	O3'-P-O5'	-5.56	95.67	104.00
2	A	554	C	C2'-C3'-O3'	5.56	122.03	113.70
2	A	1218	U	O3'-P-O5'	-5.55	95.67	104.00
2	A	347	C	C2'-C3'-O3'	5.53	117.79	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	113	G	O4'-C1'-N9	5.52	116.47	108.20
2	A	703	U	C4'-C3'-O3'	-5.51	104.73	113.00
2	A	1384	G	O3'-P-O5'	-5.51	95.73	104.00
2	A	348	A	O3'-P-O5'	-5.51	95.73	104.00
2	A	1536	C	O3'-P-O5'	-5.50	95.75	104.00
3	i2	1	G	O3'-P-O5'	-5.50	95.75	104.00
75	h1	451	C	O3'-P-O5'	-5.50	95.75	104.00
27	BT	89	THR	OG1-CB-CG2	-5.48	98.34	109.30
75	h1	1759	A	O3'-P-O5'	-5.48	95.78	104.00
61	BE	52	VAL	N-CA-CB	5.46	120.24	111.23
2	A	726	C	O5'-P-OP2	-5.46	91.63	108.00
2	A	702	G	C2'-C3'-O3'	-5.42	105.57	113.70
2	A	1587	G	O3'-P-O5'	-5.41	95.88	104.00
2	A	1152	A	O3'-P-O5'	-5.40	95.91	104.00
2	A	2859	U	O3'-P-O5'	-5.39	95.91	104.00
2	A	63	A	O3'-P-O5'	-5.38	95.92	104.00
2	A	605	C	O3'-P-O5'	-5.38	95.92	104.00
2	A	2702	A	O3'-P-O5'	-5.38	95.93	104.00
75	h1	1544	G	O3'-P-O5'	-5.37	95.94	104.00
3	W2	70	C	C2'-C3'-O3'	5.37	121.75	113.70
2	A	1151	G	C4'-C3'-O3'	-5.36	104.97	113.00
31	BQ	226	ARG	CB-CA-C	-5.35	100.04	109.62
2	A	1395	C	O3'-P-O5'	-5.35	95.97	104.00
75	h1	516	G	O3'-P-O5'	-5.34	95.99	104.00
2	A	215	G	O5'-P-OP1	5.33	124.00	108.00
60	AZ	36	VAL	N-CA-CB	5.33	117.39	110.99
2	A	1459	OMG	O3'-P-O5'	-5.31	96.03	104.00
2	A	2978	U	O3'-P-O5'	-5.31	96.04	104.00
2	A	3000	C	O3'-P-O5'	-5.30	96.05	104.00
2	A	620	G	O3'-P-O5'	-5.30	96.06	104.00
2	A	2246	C	C4'-C3'-O3'	-5.29	105.06	113.00
75	h1	861	U	O3'-P-O5'	-5.27	96.09	104.00
2	A	751	G	O3'-P-O5'	-5.27	96.10	104.00
75	h1	625	A	O3'-P-O5'	-5.27	96.10	104.00
1	3	109	A	O3'-P-O5'	-5.26	96.12	104.00
2	A	1541	C	O3'-P-O5'	5.25	111.87	104.00
2	A	292	A	C2'-C3'-O3'	-5.24	105.84	113.70
2	A	346	A	O3'-P-O5'	-5.24	96.14	104.00
1	3	90	U	O3'-P-O5'	-5.24	96.14	104.00
2	A	2845	U	O3'-P-O5'	-5.23	96.15	104.00
2	A	1519	C	O3'-P-O5'	-5.23	96.16	104.00
2	A	2243	C	O3'-P-O5'	-5.22	96.17	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	h1	348	G	O3'-P-O5'	-5.21	96.18	104.00
2	A	2981	A	O3'-P-O5'	-5.21	96.18	104.00
2	A	554	C	C4'-C3'-O3'	-5.21	105.19	113.00
2	A	701	A	O3'-P-O5'	5.20	111.81	104.00
75	h1	1276	A	O3'-P-O5'	-5.20	96.20	104.00
4	C3	96	C	O3'-P-O5'	-5.20	96.20	104.00
2	A	671	G	C2'-C3'-O3'	-5.19	105.91	113.70
2	A	2625	A	C4'-C3'-O3'	-5.19	105.21	113.00
2	A	2273	A	O3'-P-O5'	-5.19	96.21	104.00
1	3	49	C	O3'-P-O5'	-5.19	96.22	104.00
2	A	106	G	O3'-P-O5'	-5.18	96.22	104.00
2	A	700	G	C4'-C3'-O3'	-5.18	105.22	113.00
2	A	1613	A	O3'-P-O5'	-5.18	96.23	104.00
2	A	1557	A	O3'-P-O5'	-5.17	96.25	104.00
2	A	1120	A	C4'-C3'-C2'	-5.16	97.44	102.60
75	h1	1011	C	O3'-P-O5'	-5.16	96.26	104.00
75	h1	1652	U	O3'-P-O5'	-5.16	96.27	104.00
75	h1	997	C	C4'-C3'-O3'	-5.15	105.27	113.00
75	h1	1612	G	O3'-P-O5'	5.14	111.71	104.00
2	A	1497	G	C4'-C3'-C2'	-5.14	97.46	102.60
2	A	3247	G	C2'-C3'-O3'	5.14	121.41	113.70
2	A	2916	OMG	O3'-P-O5'	-5.14	96.29	104.00
2	A	892	A	O3'-P-O5'	-5.12	96.32	104.00
2	A	2222	A	C2'-C3'-O3'	-5.12	106.02	113.70
2	A	636	C	O3'-P-O5'	-5.12	96.33	104.00
2	A	1706	C	O3'-P-O5'	-5.11	96.34	104.00
2	A	1337	C	C4'-C3'-O3'	-5.10	105.35	113.00
2	A	2226	A	O3'-P-O5'	-5.10	96.35	104.00
17	AL	28	ARG	N-CA-CB	-5.10	102.00	111.13
75	h1	877	G	O3'-P-O5'	-5.10	96.35	104.00
75	h1	1460	C	O3'-P-O5'	-5.09	96.36	104.00
2	A	420	A	C2'-C3'-O3'	-5.08	106.07	113.70
2	A	788	G	O3'-P-O5'	-5.08	96.38	104.00
2	A	2363	OMC	O3'-P-O5'	-5.07	96.39	104.00
2	A	112	A	O3'-P-O5'	-5.07	96.40	104.00
4	C3	38	U	O3'-P-O5'	-5.07	96.40	104.00
70	BL	42	LYS	CB-CA-C	-5.07	102.07	110.68
2	A	1124	G	C4'-C3'-O3'	-5.06	105.40	113.00
75	h1	871	C	O3'-P-O5'	-5.06	96.41	104.00
1	3	101	G	C4'-C3'-C2'	-5.06	97.54	102.60
4	C3	6	C	O3'-P-O5'	-5.04	96.44	104.00
2	A	758	C	O3'-P-O5'	-5.03	96.45	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1186	C	O3'-P-O5'	-5.03	96.45	104.00
3	i2	64	G	O3'-P-O5'	-5.03	96.45	104.00
75	h1	270	G	O3'-P-O5'	-5.03	96.45	104.00
2	A	703	U	O3'-P-O5'	-5.03	96.46	104.00
2	A	2750	G	C1'-C2'-O2'	5.03	115.94	108.40
75	h1	1801	A	O3'-P-O5'	-5.01	96.48	104.00
2	A	3075	A	C4'-C3'-O3'	-5.01	105.49	113.00

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	113	G	Sidechain
2	A	1413	G	Sidechain
2	A	1860	A	Sidechain
2	A	2374	G	Sidechain
2	A	403	G	Sidechain
2	A	653	C	Sidechain
2	A	92	G	Sidechain
49	AK	62	ARG	Sidechain
23	AM	32	ARG	Sidechain
23	AM	83	ARG	Sidechain
14	AP	36	ARG	Sidechain
8	AR	19	ASN	Peptide
8	AR	20	GLY	Peptide
73	AY	12	ARG	Sidechain
73	AY	33	ARG	Sidechain
25	BI	48	ARG	Sidechain
46	BJ	128	ARG	Sidechain
34	BK	24	ARG	Sidechain
37	BP	93	ARG	Sidechain
22	BS	287	ARG	Sidechain
27	BT	145	ARG	Sidechain
42	BU	139	ARG	Sidechain
41	Ha	26	ARG	Sidechain
69	Ra	115	ARG	Sidechain
44	Xa	68	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	3	3453	0	1754	17	0
2	A	67525	0	34103	294	0
3	W2	1629	0	823	6	0
3	i2	1630	0	823	16	0
4	C3	2536	0	1284	9	0
5	BC	237	0	289	0	0
6	BM	1246	0	1264	6	0
7	BO	1030	0	1110	1	0
8	AR	425	0	440	4	0
9	AU	888	0	933	5	0
10	Ma	789	0	810	5	0
11	Ia	1512	0	1598	10	0
12	AE	1033	0	1070	7	0
13	AX	786	0	888	6	0
14	AP	1092	0	1182	10	0
15	Ja	2074	0	2180	28	0
16	Ea	1713	0	1777	12	0
17	AL	1485	0	1547	12	0
18	Va	1082	0	1153	3	0
19	Ka	986	0	1053	13	0
20	AW	901	0	926	10	0
21	BD	792	0	843	2	0
22	BS	3111	0	3221	33	0
23	AM	1307	0	1359	7	0
24	AC	1672	0	1748	15	0
25	BI	986	0	1048	13	0
26	AH	1042	0	1119	9	0
27	BT	3056	0	3214	37	0
28	AV	1028	0	1105	13	0
29	AD	1454	0	1512	15	0
30	AJ	1468	0	1577	8	0
31	BQ	1881	0	1931	11	0
32	BH	1636	0	1752	11	0
33	Da	1190	0	1273	6	0
34	BK	2277	0	2311	9	0
35	AT	720	0	754	6	0
36	Pa	389	0	419	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	BP	975	0	1100	2	0
38	BN	955	0	1037	5	0
39	BG	1874	0	2015	16	0
40	Fa	896	0	975	1	0
41	Ha	1156	0	1207	12	0
42	BU	1366	0	1407	11	0
43	BR	1898	0	2005	10	0
44	Xa	1163	0	1222	6	0
45	BV	1718	0	1774	26	0
46	BJ	1653	0	1707	15	0
47	AO	528	0	557	4	0
48	BW	568	0	566	5	0
49	AK	1480	0	1610	5	0
50	Na	647	0	663	4	0
51	AB	1514	0	1576	15	0
52	BF	1491	0	1596	12	0
53	AA	1625	0	1718	14	0
54	AG	1648	0	1755	15	0
55	Ga	433	0	475	0	0
56	BA	444	0	477	3	0
57	AF	1113	0	1169	11	0
58	Wa	1136	0	1177	10	0
59	Ta	1795	0	1920	29	0
60	AZ	562	0	606	7	0
61	BE	702	0	741	11	0
62	Za	1575	0	1578	25	0
63	AQ	1056	0	1128	13	0
64	Oa	471	0	497	9	0
65	Ua	962	0	994	21	0
66	Ya	1024	0	1090	21	0
67	BB	955	0	1012	12	0
68	AN	808	0	845	6	0
69	Ra	1506	0	1571	25	0
70	BL	1064	0	1097	6	0
71	La	562	0	599	9	0
72	Aa	1494	0	1538	17	0
73	AY	705	0	724	10	0
74	Ca	440	0	431	6	0
75	h1	34449	0	17384	167	0
76	B1	240	0	120	1	0
77	Ba	799	0	868	6	0
78	AI	779	0	790	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
79	L3	115	0	36	1	0
80	3	5	0	0	0	0
80	A	197	0	0	0	0
80	AC	1	0	0	0	0
80	AG	1	0	0	0	0
80	AM	1	0	0	0	0
80	AY	2	0	0	0	0
80	BI	1	0	0	0	0
80	BM	1	0	0	0	0
80	BR	1	0	0	0	0
80	BS	4	0	0	0	0
80	C3	4	0	0	0	0
80	Ta	1	0	0	0	0
80	Wa	1	0	0	0	0
80	h1	78	0	0	0	0
80	i2	1	0	0	0	0
81	3	4	0	0	0	0
81	A	127	0	0	1	0
81	AD	1	0	0	0	0
81	AJ	1	0	0	0	0
81	AR	1	0	0	0	0
81	AV	1	0	0	0	0
81	BD	1	0	0	0	0
81	BJ	1	0	0	0	0
81	BM	1	0	0	0	0
81	BQ	2	0	0	0	0
81	BS	2	0	0	0	0
81	C3	1	0	0	0	0
81	Ca	1	0	0	0	0
81	Ea	1	0	0	0	0
81	Fa	1	0	0	0	0
81	Ua	1	0	0	0	0
81	Va	1	0	0	0	0
81	Wa	1	0	0	0	0
81	h1	40	0	0	0	0
82	A	14	0	26	1	0
83	A	40	0	76	2	0
84	A	15	0	18	0	0
85	AY	1	0	0	0	0
85	BD	1	0	0	0	0
85	BE	1	0	0	0	0
85	Ca	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	Ga	1	0	0	0	0
85	Ma	1	0	0	0	0
86	3	341	0	0	1	0
86	A	7528	0	0	45	0
86	AA	3	0	0	0	0
86	AB	7	0	0	0	0
86	AC	23	0	0	2	0
86	AD	8	0	0	0	0
86	AE	22	0	0	1	0
86	AF	9	0	0	0	0
86	AG	91	0	0	3	0
86	AH	24	0	0	0	0
86	AJ	117	0	0	1	0
86	AK	46	0	0	1	0
86	AL	65	0	0	2	0
86	AM	79	0	0	4	0
86	AO	22	0	0	0	0
86	AP	16	0	0	1	0
86	AQ	3	0	0	0	0
86	AR	38	0	0	1	0
86	AT	16	0	0	2	0
86	AU	28	0	0	0	0
86	AV	69	0	0	1	0
86	AW	58	0	0	0	0
86	AX	28	0	0	1	0
86	AY	71	0	0	3	0
86	AZ	4	0	0	0	0
86	Aa	6	0	0	1	0
86	B1	22	0	0	0	0
86	BA	22	0	0	1	0
86	BC	10	0	0	0	0
86	BD	65	0	0	0	0
86	BE	34	0	0	0	0
86	BF	17	0	0	0	0
86	BG	40	0	0	3	0
86	BH	90	0	0	0	0
86	BI	41	0	0	0	0
86	BJ	36	0	0	2	0
86	BK	70	0	0	1	0
86	BL	3	0	0	0	0
86	BM	66	0	0	0	0
86	BN	34	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	BO	31	0	0	1	0
86	BP	22	0	0	0	0
86	BQ	131	0	0	3	0
86	BR	77	0	0	3	0
86	BS	170	0	0	9	0
86	BT	138	0	0	2	0
86	BU	11	0	0	0	0
86	BV	16	0	0	2	0
86	BW	1	0	0	0	0
86	Ba	4	0	0	1	0
86	C3	178	0	0	0	0
86	Da	23	0	0	0	0
86	Ea	133	0	0	3	0
86	Fa	51	0	0	0	0
86	Ga	18	0	0	0	0
86	Ha	87	0	0	4	0
86	Ia	24	0	0	0	0
86	Ja	16	0	0	1	0
86	Ka	2	0	0	0	0
86	L3	1	0	0	0	0
86	Ma	26	0	0	0	0
86	Na	3	0	0	0	0
86	Oa	2	0	0	2	0
86	Pa	3	0	0	0	0
86	Ta	7	0	0	2	0
86	Ua	29	0	0	2	0
86	Va	30	0	0	1	0
86	W2	22	0	0	0	0
86	Wa	1	0	0	0	0
86	Xa	17	0	0	0	0
86	Ya	1	0	0	0	0
86	Za	3	0	0	0	0
86	h1	1709	0	0	6	0
86	i2	7	0	0	0	0
All	All	209234	0	145670	1072	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 3.

All (1072) 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)
73:AY:76:THR:C	73:AY:77:CYS:N	1.85	1.35
74:Ca:53:ILE:C	74:Ca:54:LYS:N	1.90	1.30
43:BR:201:LYS:NZ	86:BR:401:HOH:O	1.66	1.26
14:AP:43:VAL:HB	86:AP:215:HOH:O	1.38	1.23
22:BS:182:MET:SD	86:BS:662:HOH:O	2.02	1.13
17:AL:29:MET:SD	86:AM:371:HOH:O	2.04	1.12
3:i2:76:A:O3'	79:L3:24:UNK:C	1.98	1.12
17:AL:60:MET:SD	86:AL:261:HOH:O	2.14	1.04
59:Ta:10:THR:OG1	59:Ta:12:CYS:SG	2.16	0.98
75:h1:1492:U:O3'	86:h1:2101:HOH:O	1.84	0.95
2:A:1557:A:N6	86:A:3801:HOH:O	1.77	0.94
25:BI:90:ARG:CZ	25:BI:96:MET:HE1	1.98	0.94
54:AG:17:GLN:CD	86:AG:402:HOH:O	2.11	0.93
64:Oa:59:GLU:HG3	65:Ua:116:ARG:HH12	1.35	0.92
24:AC:178:THR:HG21	75:h1:14:C:OP2	1.71	0.91
41:Ha:69:PHE:O	86:Ha:201:HOH:O	1.89	0.91
45:BV:143:THR:HG23	45:BV:205:TYR:CE1	2.10	0.87
15:Ja:2:ALA:N	86:Ja:301:HOH:O	2.07	0.87
66:Ya:86:ARG:NH2	66:Ya:125:SER:O	2.06	0.87
64:Oa:22:GLN:OE1	86:Oa:101:HOH:O	1.92	0.86
35:AT:32:SER:OG	86:AT:201:HOH:O	1.94	0.85
3:i2:18:G:H2'	3:i2:57:G:N2	1.91	0.85
2:A:710:G:N7	86:A:3805:HOH:O	2.11	0.84
65:Ua:137:ASP:OD2	75:h1:929:G:H1'	1.77	0.83
22:BS:168:ILE:O	86:BS:501:HOH:O	1.98	0.82
65:Ua:136:THR:O	65:Ua:137:ASP:CG	2.24	0.81
2:A:1880:G:N7	86:A:3807:HOH:O	2.14	0.80
2:A:554:C:O3'	86:A:3802:HOH:O	2.00	0.80
2:A:3174:C:C4	32:BH:172:LEU:HD22	2.17	0.79
29:AD:163:PHE:O	75:h1:1475:C:OP2	2.00	0.79
46:BJ:53:VAL:HB	86:BJ:414:HOH:O	1.81	0.79
14:AP:23:ALA:HB1	14:AP:43:VAL:HG12	1.65	0.79
24:AC:178:THR:HB	86:AC:411:HOH:O	1.82	0.79
75:h1:193:G:HO2'	75:h1:194:A:H8	1.29	0.79
76:B1:24:U:H3	3:W2:34:G:H1	1.31	0.78
2:A:3184:G:H1	2:A:3190:U:H3	1.32	0.78
2:A:1142:A2M:OP1	86:A:3803:HOH:O	2.02	0.78
27:BT:129:ILE:HD11	27:BT:246:LEU:HD12	1.67	0.77
2:A:712:A:O2'	54:AG:67:LYS:HD2	1.85	0.77
25:BI:13:LYS:HD2	25:BI:128:LEU:HD11	1.66	0.76
45:BV:28:ASP:OD1	45:BV:50:ARG:NH1	2.18	0.76
2:A:2807:A:H5''	86:A:7435:HOH:O	1.84	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:Za:67:ARG:HA	62:Za:189:MET:HE1	1.66	0.76
75:h1:869:G:H1	75:h1:961:U:H3	1.32	0.76
2:A:1605:A:N7	86:A:3816:HOH:O	2.18	0.75
2:A:3182:G:H1	2:A:3192:U:H3	1.33	0.75
2:A:742:U:H3	2:A:747:G:H1	1.34	0.74
1:3:120:G:N7	86:3:301:HOH:O	2.21	0.74
2:A:424:G:H22	2:A:644:U:H3	1.36	0.74
49:AK:121:HIS:ND1	86:AK:301:HOH:O	2.20	0.73
57:AF:72:ASN:O	57:AF:79:GLN:NE2	2.20	0.73
57:AF:145:ARG:NH2	3:W2:33:U:OP2	2.19	0.73
75:h1:979:A:OP2	86:h1:2102:HOH:O	2.06	0.73
2:A:3174:C:N4	32:BH:172:LEU:HD22	2.04	0.73
72:Aa:34:ALA:HB2	72:Aa:57:ARG:HD2	1.69	0.73
45:BV:48:VAL:HG21	45:BV:61:LEU:HG	1.72	0.72
2:A:1491:A:N7	86:A:3827:HOH:O	2.23	0.72
2:A:1525:C:OP2	86:A:3804:HOH:O	2.05	0.72
2:A:112:A:N3	16:Ea:50[B]:ARG:NH2	2.36	0.72
81:A:3636:K:K	86:A:4229:HOH:O	2.00	0.72
63:AQ:3:THR:O	63:AQ:4:VAL:HG22	1.89	0.72
2:A:2304:C:O2'	2:A:2305:G:OP2	2.07	0.71
27:BT:12:ILE:HD11	27:BT:27:VAL:HG13	1.70	0.71
61:BE:37:TYR:HB3	61:BE:71:MET:HE2	1.71	0.71
65:Ua:136:THR:O	65:Ua:137:ASP:OD2	2.07	0.71
73:AY:8:PHE:CD1	86:AY:351:HOH:O	2.43	0.71
22:BS:225:LYS:HE2	86:BS:510:HOH:O	1.90	0.71
2:A:2841:U:H2'	2:A:2841:U:O2	1.91	0.70
2:A:1354:G:N7	86:A:3829:HOH:O	2.25	0.70
31:BQ:89:TYR:O	86:BQ:401:HOH:O	2.09	0.70
3:i2:18:G:H2'	3:i2:57:G:H22	1.56	0.69
73:AY:11:ARG:NH1	86:AY:301:HOH:O	2.05	0.69
2:A:2324:A2M:N7	86:A:3832:HOH:O	2.26	0.69
23:AM:27:LEU:HB2	86:AM:372:HOH:O	1.92	0.69
20:AW:18:ILE:HD11	20:AW:103:VAL:CG1	2.23	0.69
2:A:1778:G:N7	86:A:3831:HOH:O	2.25	0.69
8:AR:16:ALA:O	8:AR:20:GLY:HA2	1.93	0.69
3:W2:70:C:H2'	3:W2:71:G:C8	2.28	0.69
2:A:560:U:OP2	43:BR:147:LYS:HE2	1.93	0.68
45:BV:25:SER:O	45:BV:50:ARG:NH2	2.26	0.68
27:BT:12:ILE:HD13	27:BT:260:LYS:HD2	1.75	0.68
49:AK:170:ARG:NH2	75:h1:819:G:N7	2.42	0.68
43:BR:183:ILE:HD11	43:BR:192:GLU:HG3	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BS:86:VAL:HG13	22:BS:162:VAL:HG13	1.75	0.68
2:A:1419:C:OP2	86:A:3806:HOH:O	2.11	0.68
2:A:1012:C:N4	4:C3:103:U:O2'	2.26	0.67
43:BR:91:ILE:HD13	43:BR:132:LEU:HD21	1.75	0.67
51:AB:178:ASN:ND2	75:h1:513:A:OP2	2.28	0.67
22:BS:225:LYS:CE	86:BS:510:HOH:O	2.41	0.67
24:AC:177:LYS:HE2	75:h1:6:G:N7	2.10	0.67
2:A:991:G:N1	2:A:1111:G:H2'	2.09	0.66
12:AE:2:VAL:N	75:h1:1035:C:HO2'	1.94	0.66
45:BV:27:LYS:HB3	45:BV:47:LEU:HD22	1.77	0.66
20:AW:18:ILE:HD11	20:AW:103:VAL:HG11	1.77	0.66
41:Ha:106:PHE:CE2	86:Ha:201:HOH:O	2.48	0.66
2:A:693:A:N3	86:A:3849:HOH:O	2.29	0.66
2:A:609:A:N6	52:BF:25:ARG:O	2.27	0.66
59:Ta:193:ARG:NH2	75:h1:286:G:N7	2.43	0.66
75:h1:896:G:H1	75:h1:918:U:H3	1.44	0.66
2:A:1575:A:H2'	2:A:1576:A:O4'	1.95	0.66
75:h1:1636:C:O3'	86:h1:2103:HOH:O	2.13	0.66
2:A:584:G:N7	52:BF:32:ARG:NH2	2.44	0.65
2:A:3167:G:O2'	86:A:3808:HOH:O	2.15	0.65
16:Ea:10:LEU:HD22	86:Ea:531:HOH:O	1.95	0.65
22:BS:86:VAL:HG22	22:BS:162:VAL:HG11	1.76	0.65
24:AC:177:LYS:HB2	86:AC:422:HOH:O	1.95	0.65
19:Ka:60:PHE:HZ	19:Ka:76:LEU:HD22	1.60	0.65
2:A:3226:G:H1	2:A:3237:U:H3	1.44	0.65
28:AV:89:HIS:NE2	63:AQ:41:THR:O	2.27	0.65
65:Ua:150:LEU:HB2	75:h1:1773:U:O2	1.97	0.65
45:BV:143:THR:HG21	45:BV:154:CYS:O	1.97	0.65
86:A:5307:HOH:O	16:Ea:170:LYS:HE3	1.96	0.64
29:AD:61:PHE:CE2	64:Oa:46:ARG:HG3	2.32	0.64
4:C3:44:C:OP2	42:BU:139:ARG:NH2	2.28	0.64
2:A:830:U:OP1	86:A:3809:HOH:O	2.15	0.64
36:Pa:24:GLN:OE1	36:Pa:26:LYS:NZ	2.30	0.64
2:A:2205:A:H2'	2:A:2206:A:O4'	1.98	0.63
45:BV:166:ARG:NH1	86:BV:302:HOH:O	2.30	0.63
69:Ra:68:ARG:HG3	69:Ra:69:LEU:HD22	1.79	0.63
2:A:712:A:OP2	2:A:712:A:H3'	1.98	0.63
2:A:1567:U:O4	2:A:1580:G:O2'	2.14	0.63
42:BU:42:LEU:HD11	42:BU:127:MET:HE1	1.81	0.63
29:AD:91:ARG:NH2	75:h1:1530:U:OP1	2.32	0.62
17:AL:29:MET:HE3	17:AL:43:PHE:CD1	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:588:C:H2'	2:A:589:U:H2'	1.82	0.62
2:A:2686:G:OP2	42:BU:149:ARG:NH2	2.32	0.62
25:BI:90:ARG:NE	25:BI:96:MET:HE1	2.15	0.62
44:XA:76:CYS:HB2	44:XA:124:ILE:HD11	1.82	0.62
13:AX:25:LEU:HD11	54:AG:101:LYS:HD3	1.80	0.61
69:RA:150:ILE:HD12	69:RA:181:ASP:HB3	1.81	0.61
15:JA:110:ARG:NH2	75:h1:790:G:OP2	2.33	0.61
24:AC:175:SER:OG	24:AC:178:THR:HG23	2.01	0.61
2:A:1821:G:H8	2:A:1821:G:H5''	1.66	0.61
13:AX:23:ARG:NH2	54:AG:77:GLU:OE1	2.33	0.61
45:BV:105:PHE:HZ	45:BV:211:PHE:CG	2.19	0.61
72:Aa:34:ALA:HB2	72:Aa:57:ARG:CD	2.30	0.61
65:Ua:137:ASP:HB3	75:h1:929:G:O4'	2.01	0.61
2:A:3183:A:H61	2:A:3191:C:H42	1.47	0.61
2:A:1932:A:OP1	86:A:3810:HOH:O	2.16	0.60
27:BT:126:ARG:O	27:BT:129:ILE:HG22	2.01	0.60
71:La:88:GLY:O	71:La:90:ILE:N	2.34	0.60
19:Ka:21:ARG:NH1	19:Ka:76:LEU:HD21	2.16	0.60
58:Wa:121:ARG:NH2	75:h1:1549:A:OP2	2.35	0.60
2:A:224:G:OP1	86:A:3811:HOH:O	2.16	0.60
59:Ta:59:GLN:NE2	86:Ta:401:HOH:O	2.27	0.60
59:Ta:139:ARG:O	59:Ta:180:ILE:HG23	2.02	0.60
27:BT:129:ILE:CD1	27:BT:246:LEU:HD12	2.31	0.59
35:AT:46:LEU:HD22	35:AT:71:HIS:HB3	1.83	0.59
44:XA:142:LYS:HE2	44:XA:144:ILE:HD11	1.83	0.59
2:A:2627:A:OP1	86:A:3812:HOH:O	2.17	0.59
39:BG:165:ARG:HG3	39:BG:220:TYR:CG	2.37	0.59
2:A:608:C:H5'	2:A:609:A:H2'	1.85	0.58
2:A:2280:U:O2	2:A:2308:U:H4'	2.03	0.58
32:BH:90:ARG:HG3	32:BH:104:LEU:HD11	1.84	0.58
38:BN:85:MET:HE1	38:BN:153:ILE:HG22	1.86	0.58
2:A:567:A:OP1	20:AW:75:LYS:HE2	2.03	0.58
37:BP:73:TYR:HB3	37:BP:79:LEU:HD22	1.86	0.58
41:Ha:44:LEU:C	41:Ha:44:LEU:HD23	2.28	0.58
2:A:3174:C:C4	32:BH:172:LEU:CD2	2.87	0.58
78:AI:21:CYS:HB3	78:AI:46:MET:HE3	1.85	0.58
2:A:2970:A:H1'	3:i2:74:C:H5'	1.85	0.58
20:AW:35:VAL:HG21	20:AW:54:MET:HE1	1.85	0.58
22:BS:182:MET:HE3	22:BS:184:ILE:HD11	1.86	0.58
2:A:1815:A:O2'	2:A:1818:G:N3	2.37	0.58
23:AM:38:ASP:HB2	23:AM:64:ILE:HD12	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Ea:27:CYS:SG	16:Ea:122:ASN:CG	2.86	0.57
74:Ca:52:PHE:HB3	77:Ba:83:PHE:HB3	1.84	0.57
11:Ia:36:ARG:HG2	11:Ia:38:PHE:CZ	2.39	0.57
1:3:155:OMG:HM22	39:BG:52:ILE:CD1	2.34	0.57
2:A:2790:OMG:N7	86:A:3866:HOH:O	2.33	0.57
3:i2:72:C:H2'	3:i2:73:A:C5	2.40	0.57
51:AB:29:GLU:HB2	51:AB:44:LEU:CD2	2.35	0.57
66:Ya:114:PRO:O	66:Ya:117:ILE:HG12	2.03	0.57
75:h1:1172:A:H2'	75:h1:1173:G:C8	2.39	0.57
25:BI:140:VAL:HG11	47:AO:24:ILE:HD12	1.86	0.57
2:A:403:G:OP2	86:A:3815:HOH:O	2.17	0.57
12:AE:49:GLU:OE2	69:Ra:142:ARG:NE	2.38	0.57
75:h1:1378:G:H2'	75:h1:1379:C:O4'	2.05	0.57
2:A:3012:U:OP1	86:A:3813:HOH:O	2.17	0.57
2:A:694:A:N6	86:A:3940:HOH:O	2.38	0.57
48:BW:80:LYS:O	48:BW:81:GLN:C	2.47	0.57
66:Ya:90:ILE:O	66:Ya:117:ILE:O	2.23	0.57
2:A:2778:A:OP2	86:A:3814:HOH:O	2.17	0.57
61:BE:37:TYR:CB	61:BE:71:MET:HE2	2.35	0.56
4:C3:39:C:H4'	42:BU:46:THR:HG23	1.87	0.56
6:BM:24:VAL:HG13	6:BM:87:LYS:HG2	1.87	0.56
28:AV:30:LYS:NZ	86:AV:301:HOH:O	2.26	0.56
59:Ta:45:PHE:HB2	59:Ta:48:TYR:CD1	2.40	0.56
75:h1:161:G:H5''	75:h1:161:G:N3	2.20	0.56
75:h1:379:G:O2'	75:h1:380:A:OP2	2.14	0.56
2:A:3037:G:N7	86:A:3864:HOH:O	2.32	0.56
57:AF:71:VAL:HG11	57:AF:83:ILE:HD11	1.87	0.56
2:A:1446:OMC:HM23	27:BT:100:MET:HG3	1.87	0.56
27:BT:36:PRO:HB3	27:BT:288:ALA:HB2	1.87	0.56
45:BV:111:ARG:NH2	75:h1:931:A:N3	2.53	0.55
3:i2:18:G:C2'	3:i2:57:G:N2	2.66	0.55
75:h1:1059:U:H3'	75:h1:1060:U:C5'	2.36	0.55
2:A:3041:C:OP1	25:BI:48:ARG:HD2	2.07	0.55
19:Ka:59:CYS:HB3	19:Ka:62:PHE:HE1	1.70	0.55
43:BR:45:ALA:HB2	86:BR:474:HOH:O	2.06	0.55
75:h1:96:G:O2'	75:h1:462:A:O2'	2.24	0.55
2:A:312:C:OP2	13:AX:30:ARG:NH2	2.30	0.55
2:A:547:G:H4'	2:A:548:U:OP2	2.06	0.55
65:Ua:136:THR:C	65:Ua:137:ASP:CG	2.72	0.55
70:BL:128:GLY:O	70:BL:132:LEU:HD12	2.06	0.55
2:A:3036:U:O2	25:BI:12:ASN:ND2	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:A:7630:HOH:O	27:BT:67:THR:HG22	2.06	0.55
22:BS:87:VAL:HB	22:BS:110:LEU:HD22	1.89	0.55
53:AA:42:THR:O	53:AA:43:PRO:C	2.49	0.55
59:Ta:57:ASP:HA	59:Ta:108:LEU:HA	1.89	0.55
22:BS:348:THR:HG22	22:BS:350:THR:HG23	1.89	0.55
69:Ra:165:TYR:CE2	69:Ra:166:LYS:HG3	2.42	0.55
2:A:990:C:H3'	2:A:991:G:H5''	1.87	0.54
43:BR:154:TYR:CE1	43:BR:186:VAL:HG11	2.41	0.54
46:BJ:139:ARG:HB2	46:BJ:173:PHE:CE1	2.42	0.54
2:A:1818:G:H2'	2:A:1819:C:C6	2.43	0.54
11:Ia:97:PHE:HB2	11:Ia:145:ASP:HB3	1.88	0.54
14:AP:23:ALA:HB1	14:AP:43:VAL:CG1	2.34	0.54
22:BS:21:ARG:NH2	86:BS:502:HOH:O	2.39	0.54
39:BG:217:ASN:ND2	86:BG:302:HOH:O	2.40	0.54
45:BV:169:SER:OG	86:BV:301:HOH:O	2.18	0.54
53:AA:200:PRO:O	53:AA:202:THR:N	2.40	0.54
75:h1:1383:U:O2'	75:h1:1519:A:N1	2.34	0.54
17:AL:75:LYS:NZ	17:AL:99:THR:O	2.40	0.54
63:AQ:14:LYS:O	63:AQ:44:HIS:NE2	2.39	0.54
75:h1:1339:C:H1'	75:h1:1413:A:C4	2.42	0.54
50:Na:61:CYS:SG	50:Na:63:THR:OG1	2.64	0.54
65:Ua:150:LEU:O	86:Ua:301:HOH:O	2.18	0.54
2:A:352:A:N1	27:BT:89:THR:HG22	2.23	0.54
2:A:2878:OMC:HM21	22:BS:242:PRO:HD3	1.90	0.54
11:Ia:12:ILE:HD13	11:Ia:18:ILE:HG21	1.90	0.54
39:BG:176:GLY:HA3	86:BG:301:HOH:O	2.07	0.54
75:h1:756:A:H2'	75:h1:757:G:O4'	2.08	0.54
2:A:2547:U:C2	39:BG:29:GLN:NE2	2.76	0.54
34:BK:142:ARG:NH2	86:BK:401:HOH:O	2.37	0.54
61:BE:37:TYR:HB3	61:BE:71:MET:CE	2.38	0.54
66:Ya:42:PHE:O	66:Ya:47:ARG:NH1	2.41	0.54
11:Ia:128:LYS:NZ	11:Ia:130:GLU:OE2	2.41	0.53
75:h1:1258:U:O2'	78:AI:8:ARG:NH2	2.41	0.53
2:A:11:G:H5''	2:A:11:G:H8	1.73	0.53
2:A:437:G:C2	2:A:498:A:H2	2.26	0.53
2:A:591:A:O2'	2:A:592:C:O4'	2.24	0.53
20:AW:112:ILE:OXT	52:BF:86:ARG:NH2	2.42	0.53
75:h1:139:U:H4'	75:h1:140:C:O5'	2.08	0.53
2:A:683:U:O2'	30:AJ:20:LYS:HE3	2.08	0.53
2:A:2970:A:N3	3:i2:74:C:H4'	2.23	0.53
24:AC:62:THR:OG1	24:AC:65:GLY:O	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AD:31:ASP:OD2	29:AD:146:ARG:NH2	2.41	0.53
29:AD:124:ASP:HB2	29:AD:141:ILE:HD11	1.88	0.53
51:AB:3:ASN:HD21	51:AB:5:ARG:HD3	1.73	0.53
46:BJ:132:GLY:HA2	86:BJ:414:HOH:O	2.09	0.53
2:A:437:G:O6	2:A:634:G:H1'	2.09	0.53
29:AD:100:ILE:HG12	29:AD:178:ILE:CD1	2.38	0.53
2:A:468:A:H2'	2:A:469:U:O4'	2.09	0.53
2:A:2682:U:H2'	2:A:2683:C:C6	2.43	0.53
52:BF:67:ALA:HA	63:AQ:120:ALA:HB1	1.90	0.53
70:BL:24:LYS:HG3	70:BL:55:TYR:CE2	2.44	0.53
74:Ca:53:ILE:C	74:Ca:54:LYS:CA	2.78	0.53
3:i2:18:G:H2'	3:i2:57:G:C2	2.42	0.53
23:AM:34:PHE:HB3	23:AM:64:ILE:HD13	1.89	0.53
31:BQ:101:VAL:N	86:BQ:401:HOH:O	2.41	0.53
2:A:3011:U:H2'	2:A:3012:U:C6	2.43	0.53
16:Ea:27:CYS:SG	16:Ea:122:ASN:ND2	2.82	0.53
75:h1:154:A:H2'	75:h1:155:A:O4'	2.09	0.53
62:Za:159:ARG:HG2	62:Za:160:PHE:CD2	2.44	0.53
2:A:394:A:H4'	2:A:395:G:H3'	1.91	0.52
43:BR:147:LYS:NZ	43:BR:151:GLU:OE2	2.38	0.52
25:BI:62:MET:HE3	25:BI:76:VAL:HG12	1.90	0.52
68:AN:65:GLU:HB2	68:AN:68:LYS:HB3	1.91	0.52
69:Ra:139:LYS:HD3	69:Ra:151:MET:HE3	1.91	0.52
16:Ea:155:VAL:HG23	86:Ea:502:HOH:O	2.08	0.52
18:Va:54:ILE:HD12	18:Va:56:ILE:HD11	1.91	0.52
27:BT:12:ILE:HD13	27:BT:260:LYS:CD	2.39	0.52
27:BT:298:ILE:HD13	30:AJ:123:ASP:HB2	1.90	0.52
75:h1:803:U:H2'	75:h1:804:G:C8	2.44	0.52
54:AG:68:VAL:CG1	54:AG:155:ILE:HG21	2.40	0.52
58:Wa:133:GLY:HA3	75:h1:1561:G:H5''	1.92	0.52
24:AC:16:VAL:HG21	24:AC:39:ILE:HG23	1.91	0.52
75:h1:480:A:C2	75:h1:513:A:C2	2.97	0.52
2:A:63:A:O4'	2:A:75:A:H1'	2.09	0.52
71:La:81:ILE:HG21	71:La:102:TYR:CE1	2.44	0.52
2:A:661:A2M:OP2	2:A:2867:U:O2'	2.27	0.52
61:BE:32:SER:HB2	61:BE:70:THR:HG22	1.92	0.52
75:h1:193:G:O2'	75:h1:194:A:H8	1.89	0.52
75:h1:1652:U:H2'	75:h1:1653:A:C8	2.44	0.52
2:A:2684:G:OP1	42:BU:142:ARG:NH2	2.43	0.52
17:AL:60:MET:HE1	17:AL:63:ILE:HB	1.91	0.52
62:Za:84:ARG:HG2	62:Za:85:PRO:HD2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:Oa:59:GLU:HG3	65:Ua:116:ARG:NH1	2.16	0.52
1:3:108:A:N3	2:A:20:G:H1'	2.24	0.51
59:Ta:200:LYS:NZ	75:h1:176:A:N1	2.56	0.51
2:A:991:G:H1	2:A:1111:G:H2'	1.73	0.51
58:Wa:6:ASN:HB2	71:La:42:LEU:HD13	1.90	0.51
75:h1:1729:C:H2'	75:h1:1730:C:C6	2.45	0.51
2:A:1954:G:H2'	2:A:2091:A:H61	1.75	0.51
4:C3:93:U:H2'	4:C3:94:C:C6	2.45	0.51
54:AG:17:GLN:CG	86:AG:402:HOH:O	2.52	0.51
66:Ya:46:ILE:HG23	66:Ya:89:ILE:HD13	1.92	0.51
2:A:3369:U:O2'	2:A:3371:G:N7	2.40	0.51
31:BQ:102:LEU:HD12	86:BQ:401:HOH:O	2.11	0.51
62:Za:28:HIS:HE2	67:BB:102:THR:HG21	1.75	0.51
62:Za:36:TYR:CD1	75:h1:1041:G:H4'	2.46	0.51
2:A:973:G:H5'	41:Ha:29:PRO:HB2	1.93	0.51
2:A:2345:OMU:H5	86:A:7276:HOH:O	2.09	0.51
17:AL:95:GLU:HB3	17:AL:141:THR:HG21	1.93	0.51
23:AM:17:ARG:NH2	23:AM:23:GLY:O	2.44	0.51
27:BT:298:ILE:O	27:BT:304:ILE:HD12	2.10	0.51
59:Ta:143:ILE:HD13	59:Ta:159:VAL:HG22	1.93	0.51
69:Ra:12:LYS:O	69:Ra:13:ASN:C	2.53	0.51
2:A:1714:G:O6	35:AT:31:LYS:HE3	2.11	0.51
22:BS:86:VAL:HG13	22:BS:162:VAL:CG1	2.41	0.51
34:BK:51:PHE:CD2	34:BK:172:ILE:HD13	2.44	0.51
2:A:2920:OMU:HM23	2:A:2922:PSU:C6	2.46	0.51
2:A:3341:C:H4'	2:A:3342:U:H3'	1.93	0.51
13:AX:39:ARG:NH2	16:Ea:2:GLY:O	2.44	0.51
45:BV:29:TRP:CE2	45:BV:47:LEU:HD21	2.46	0.51
48:BW:39:LEU:HD21	62:Za:189:MET:HE3	1.92	0.51
29:AD:203:ASN:O	29:AD:204:ARG:HB2	2.10	0.51
72:Aa:36:THR:OG1	72:Aa:58:ALA:O	2.24	0.51
22:BS:220:ILE:CD1	22:BS:328:ILE:HD13	2.41	0.51
72:Aa:99:LYS:O	72:Aa:172:ILE:O	2.28	0.51
6:BM:15:CYS:SG	6:BM:103:ALA:HB2	2.51	0.51
45:BV:120:LEU:HD13	45:BV:142:PHE:CE2	2.46	0.51
53:AA:162:GLN:N	53:AA:163:PRO:CD	2.74	0.51
69:Ra:59:LYS:HB2	69:Ra:91:LYS:HG2	1.93	0.51
2:A:10:G:H2'	2:A:11:G:H5''	1.91	0.50
2:A:1723:C:H1'	49:AK:96:MET:HE2	1.92	0.50
11:Ia:7:SER:OG	11:Ia:61:ASP:OD1	2.21	0.50
15:Ja:150:PRO:O	15:Ja:151:ASP:HB2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:AH:36:ALA:HB2	26:AH:50:PHE:CE1	2.46	0.50
2:A:1522:G:OP2	86:A:3820:HOH:O	2.19	0.50
27:BT:42:VAL:HG21	27:BT:252:LEU:HD21	1.93	0.50
46:BJ:184:LEU:HB3	46:BJ:190:ILE:HG12	1.93	0.50
75:h1:1544:G:N2	75:h1:1570:C:H1'	2.26	0.50
2:A:1359:A:O4'	27:BT:305:GLN:HG3	2.10	0.50
15:Ja:126:VAL:O	15:Ja:156:PRO:O	2.28	0.50
22:BS:158:THR:HG23	86:BS:536:HOH:O	2.12	0.50
34:BK:118:GLU:OE2	34:BK:137:SER:OG	2.25	0.50
38:BN:73:GLN:OE1	38:BN:76:LYS:NZ	2.45	0.50
64:Oa:19:SER:HB3	75:h1:1621:C:O4'	2.12	0.50
75:h1:117:U:H2'	75:h1:118:U:C6	2.46	0.50
75:h1:295:U:H2'	75:h1:296:C:C6	2.47	0.50
3:i2:20:G:N3	3:i2:20:G:H3'	2.27	0.50
61:BE:51:ALA:O	61:BE:52:VAL:C	2.55	0.50
2:A:3182:G:O6	86:A:3817:HOH:O	2.18	0.50
64:Oa:21:GLY:N	86:Oa:101:HOH:O	2.43	0.50
15:Ja:2:ALA:O	75:h1:95:PSU:OP1	2.30	0.50
44:Xa:76:CYS:HB2	44:Xa:124:ILE:CD1	2.41	0.50
45:BV:48:VAL:HG21	45:BV:61:LEU:CG	2.40	0.50
51:AB:112:GLN:HE22	51:AB:128:ARG:HH11	1.60	0.50
2:A:119:A:O2'	39:BG:101:LYS:NZ	2.44	0.50
16:Ea:50[B]:ARG:HH21	16:Ea:50[B]:ARG:HB3	1.75	0.50
66:Ya:43:PRO:HG2	66:Ya:46:ILE:HG12	1.93	0.50
69:Ra:132:PHE:CD1	69:Ra:132:PHE:C	2.88	0.50
75:h1:617:A:N1	75:h1:1107:C:O2	2.45	0.50
2:A:213:G:N7	83:A:3405:SPD:H91	2.26	0.50
2:A:551:A:OP1	27:BT:359:LYS:NZ	2.44	0.50
2:A:3337:C:O2'	2:A:3339:U:OP2	2.29	0.50
15:Ja:45:VAL:HG23	15:Ja:80:LYS:O	2.11	0.50
15:Ja:45:VAL:HG22	15:Ja:80:LYS:HB2	1.92	0.50
34:BK:83:LEU:N	34:BK:84:PRO:CD	2.74	0.50
46:BJ:38:MET:HE2	46:BJ:38:MET:HA	1.93	0.50
46:BJ:201:SER:O	46:BJ:209:ARG:NH2	2.45	0.50
75:h1:1192:C4J:C6	75:h1:1192:C4J:C4'	2.90	0.50
2:A:2879:PSU:H1'	22:BS:253:ALA:HB3	1.94	0.50
14:AP:53:VAL:HG13	14:AP:62:THR:HG23	1.93	0.50
15:Ja:86:PHE:O	15:Ja:87:MET:HB2	2.12	0.50
25:BI:13:LYS:HD2	25:BI:128:LEU:CD1	2.40	0.50
52:BF:98:LEU:HD11	52:BF:140:ILE:HG13	1.94	0.50
53:AA:59:LEU:HA	53:AA:66:ILE:HG12	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:Ta:7:ASN:ND2	59:Ta:9:THR:OG1	2.44	0.50
17:AL:34:THR:OG1	17:AL:38:ARG:HD2	2.12	0.49
22:BS:174:LEU:HB2	86:BS:501:HOH:O	2.10	0.49
31:BQ:137:ILE:HD11	31:BQ:149:LYS:HB2	1.94	0.49
65:Ua:150:LEU:HD12	75:h1:1789:U:OP1	2.12	0.49
69:Ra:27:LEU:HD22	69:Ra:41:LEU:HD11	1.94	0.49
2:A:90:G:N7	83:A:3403:SPD:N6	2.56	0.49
2:A:712:A:O2'	54:AG:67:LYS:CD	2.59	0.49
2:A:1881:A:N3	86:A:3895:HOH:O	2.35	0.49
22:BS:174:LEU:HD12	86:BS:501:HOH:O	2.11	0.49
54:AG:17:GLN:HG3	86:AG:402:HOH:O	2.11	0.49
2:A:555:G:H5''	86:A:3802:HOH:O	2.12	0.49
2:A:2454:A:H2'	2:A:2454:A:N3	2.26	0.49
2:A:2688:G:N3	2:A:2688:G:H2'	2.27	0.49
44:Xa:113:SER:HG	44:Xa:115:CYS:HG	1.54	0.49
36:Pa:45:VAL:HG11	75:h1:505:G:H5'	1.94	0.49
60:AZ:11:PHE:CZ	60:AZ:36:VAL:HG22	2.48	0.49
62:Za:67:ARG:CA	62:Za:189:MET:HE1	2.39	0.49
1:3:155:OMG:HM22	39:BG:52:ILE:HD13	1.93	0.49
22:BS:259:HIS:HA	22:BS:260:PRO:C	2.37	0.49
67:BB:21:TYR:CE1	67:BB:58:MET:HE1	2.48	0.49
2:A:674:U:H2'	2:A:675:OMC:C6	2.47	0.49
15:Ja:33:SER:OG	75:h1:299:U:O2	2.26	0.49
22:BS:220:ILE:HD11	22:BS:328:ILE:HD13	1.93	0.49
48:BW:50:THR:HG21	48:BW:75:LYS:HG2	1.95	0.49
69:Ra:64:TYR:HA	69:Ra:96:VAL:O	2.12	0.49
71:La:96:HIS:HE2	75:h1:1531:PSU:P	2.35	0.49
75:h1:1101:G:N3	75:h1:1101:G:H5'	2.27	0.49
27:BT:74:THR:HG22	27:BT:80:ARG:HD3	1.95	0.49
1:3:130:U:O2'	1:3:134:G:N2	2.46	0.49
38:BN:112:LYS:HE3	38:BN:118:GLN:OE1	2.13	0.49
2:A:609:A:H4'	2:A:610:G:O5'	2.12	0.49
2:A:1814:G:N7	14:AP:64:LYS:HE2	2.27	0.49
62:Za:177:CYS:HA	62:Za:203:VAL:HG21	1.95	0.49
67:BB:24:MET:HE1	67:BB:54:SER:HB3	1.93	0.49
75:h1:877:G:H1'	75:h1:945:A:O4'	2.12	0.49
2:A:1012:C:O2	2:A:1012:C:O4'	2.29	0.49
2:A:1338:C:H2'	2:A:1339:U:O4'	2.13	0.49
2:A:1795:C:H5'	61:BE:52:VAL:HG13	1.95	0.49
2:A:2557:C:OP1	39:BG:28:LYS:NZ	2.45	0.49
2:A:3002:C:H2'	2:A:3003:G:O4'	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AW:18:ILE:HD11	20:AW:103:VAL:HG13	1.92	0.49
32:BH:204:ILE:HD12	32:BH:204:ILE:C	2.37	0.49
59:Ta:65:GLN:HE21	75:h1:1683:A:H2'	1.78	0.49
69:Ra:47:ASN:O	69:Ra:64:TYR:HB2	2.13	0.49
2:A:1523:C:O2	56:BA:45:ARG:NH1	2.44	0.48
69:Ra:115:ARG:HG3	75:h1:861:U:O4'	2.13	0.48
75:h1:987:G:H2'	75:h1:988:G:O4'	2.13	0.48
8:AR:19:ASN:O	8:AR:20:GLY:O	2.30	0.48
33:Da:70:LYS:HE3	86:h1:2111:HOH:O	2.13	0.48
65:Ua:137:ASP:CB	75:h1:929:G:O4'	2.60	0.48
68:AN:38:SER:OG	68:AN:89:TYR:OH	2.28	0.48
70:BL:134:GLN:HB3	70:BL:138:ARG:HH21	1.79	0.48
2:A:2117:C:H2'	2:A:2118:A:O4'	2.13	0.48
22:BS:224:THR:HG22	22:BS:333:VAL:HG23	1.95	0.48
2:A:1597:C:H2'	2:A:1598:C:C6	2.49	0.48
2:A:2389:OMG:HM21	22:BS:270:ALA:HB3	1.95	0.48
17:AL:5:ARG:NE	86:AL:202:HOH:O	2.46	0.48
45:BV:125:VAL:HG21	45:BV:173:VAL:CG2	2.43	0.48
53:AA:192:TRP:NE1	53:AA:201:LYS:O	2.41	0.48
75:h1:15:U:H2'	75:h1:16:G:O4'	2.13	0.48
2:A:787:C:H4'	30:AJ:186:LYS:HE2	1.94	0.48
2:A:1169:A:O2'	2:A:1376:A2M:H5'	2.13	0.48
29:AD:61:PHE:CZ	64:Oa:46:ARG:HG3	2.48	0.48
35:AT:27:THR:HG22	35:AT:94:SER:HB3	1.95	0.48
75:h1:175:A:H4'	75:h1:176:A:H5''	1.95	0.48
27:BT:295:LEU:HD21	30:AJ:31:LYS:HG2	1.95	0.48
59:Ta:49:VAL:HB	59:Ta:117:LYS:HB3	1.95	0.48
2:A:1229:U:O2'	2:A:1296:A:N1	2.45	0.48
15:Ja:3:ARG:HG3	15:Ja:3:ARG:HH11	1.78	0.48
29:AD:23:THR:OG1	29:AD:25:ASP:OD1	2.31	0.48
65:Ua:136:THR:O	65:Ua:137:ASP:CB	2.62	0.48
2:A:2693:A:OP1	86:A:3821:HOH:O	2.20	0.48
2:A:2820:C:C4	2:A:2821:U:C5	3.01	0.48
12:AE:20:ARG:NH1	75:h1:1040:A:OP1	2.44	0.48
25:BI:140:VAL:HG11	47:AO:24:ILE:CD1	2.43	0.48
62:Za:21:MET:HE1	62:Za:180:TRP:CZ3	2.48	0.48
2:A:2280:U:OP1	2:A:2972:G:O2'	2.20	0.48
45:BV:123:ALA:CB	45:BV:168:MET:HE2	2.44	0.48
58:Wa:51:ASP:HB3	58:Wa:54:LYS:HG3	1.96	0.48
2:A:105:A:H2'	2:A:106:G:O4'	2.14	0.48
2:A:3365:C:O2'	22:BS:316:PRO:HA	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:AO:52:CYS:HA	47:AO:57:TYR:CG	2.49	0.48
60:AZ:24:LYS:HB3	60:AZ:69:LEU:HD21	1.94	0.48
75:h1:758:A:O2'	75:h1:759:A:O4'	2.30	0.48
3:W2:47:U:O2'	3:W2:50:C:OP1	2.28	0.48
2:A:430:G:O2'	2:A:1408:A:N1	2.44	0.47
2:A:988:G:H4'	2:A:989:A:C4	2.49	0.47
2:A:1477:A:OP1	86:A:3818:HOH:O	2.19	0.47
2:A:2227:A:H2'	2:A:2228:C:O4'	2.14	0.47
2:A:2699:G:O2'	2:A:2704:A:N1	2.47	0.47
15:Ja:106:LYS:NZ	75:h1:791:G:OP1	2.41	0.47
65:Ua:146:ARG:HB2	65:Ua:150:LEU:HD22	1.95	0.47
71:La:55:ALA:N	71:La:56:PRO:HD2	2.28	0.47
72:Aa:138:LYS:H	72:Aa:138:LYS:HD3	1.79	0.47
2:A:437:G:N2	2:A:629:C:H1'	2.28	0.47
2:A:2837:A:OP1	46:BJ:154:ARG:NH1	2.47	0.47
4:C3:24:U:H2'	4:C3:25:G:O4'	2.14	0.47
27:BT:74:THR:CG2	27:BT:80:ARG:HD3	2.44	0.47
69:Ra:132:PHE:O	69:Ra:133:PRO:C	2.57	0.47
1:3:73:U:C4	1:3:74:G:C6	3.02	0.47
2:A:3372:U:O2'	9:AU:112:THR:O	2.32	0.47
31:BQ:226:ARG:NH1	31:BQ:228:ASP:OD1	2.46	0.47
72:Aa:57:ARG:HH22	75:h1:334:U:P	2.38	0.47
75:h1:1350:G:H2'	75:h1:1351:C:C6	2.50	0.47
2:A:2713:G:H5''	2:A:2715:U:C6	2.48	0.47
9:AU:14:ARG:HG2	9:AU:114:ILE:HD13	1.96	0.47
53:AA:59:LEU:HD23	53:AA:66:ILE:HG13	1.96	0.47
59:Ta:173:LYS:HD3	59:Ta:175:SER:HB2	1.96	0.47
66:Ya:42:PHE:HB3	66:Ya:46:ILE:HB	1.96	0.47
27:BT:33:MET:HE1	27:BT:258:TRP:CZ2	2.49	0.47
39:BG:170:PRO:HA	39:BG:217:ASN:HD21	1.80	0.47
66:Ya:39:VAL:HG13	66:Ya:47:ARG:HG2	1.96	0.47
75:h1:981:G:H4'	75:h1:1780:A:H4'	1.97	0.47
75:h1:1542:G:C6	75:h1:1543:G:C4	3.02	0.47
26:AH:107:ARG:NH2	52:BF:225:VAL:O	2.48	0.47
51:AB:29:GLU:HB2	51:AB:44:LEU:HD23	1.97	0.47
2:A:1335:G:H2'	2:A:1336:A:O4'	2.15	0.47
11:Ia:116:GLU:HG2	11:Ia:128:LYS:HD3	1.97	0.47
12:AE:74:VAL:HG22	86:AE:202:HOH:O	2.15	0.47
17:AL:40:LYS:HD3	17:AL:60:MET:HE2	1.97	0.47
30:AJ:67:LEU:HD21	30:AJ:99:VAL:HG21	1.96	0.47
33:Da:119:GLU:O	33:Da:123:HIS:ND1	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:AA:109:LEU:HD12	53:AA:184:ILE:HD11	1.96	0.47
62:Za:55:LEU:HD12	67:BB:105:MET:HE1	1.97	0.47
66:Ya:91:VAL:HG23	66:Ya:93:GLU:HG2	1.97	0.47
69:Ra:79:ARG:O	69:Ra:82:ARG:HG2	2.15	0.47
75:h1:523:A:H2'	75:h1:524:U:O4'	2.14	0.47
75:h1:1438:G:N7	78:AI:25:LYS:HE2	2.30	0.47
2:A:259:U:H2'	2:A:260:C:O4'	2.14	0.47
27:BT:31:ASP:OD2	27:BT:272:SER:HB2	2.14	0.47
57:AF:130:LYS:HE2	75:h1:1420:A:O2'	2.15	0.47
60:AZ:11:PHE:CE2	60:AZ:36:VAL:HG22	2.50	0.47
75:h1:1385:A:H1'	77:Ba:58:ARG:HD2	1.96	0.47
2:A:1566:A:C8	39:BG:49:PRO:HB3	2.50	0.47
8:AR:36:ASP:OD2	86:AR:201:HOH:O	2.20	0.47
15:Ja:240:LYS:HB2	75:h1:788:C:C2	2.50	0.47
19:Ka:13:PHE:HZ	19:Ka:22:LYS:HD2	1.80	0.47
58:Wa:74:PRO:HB2	58:Wa:79:ILE:HB	1.96	0.47
15:Ja:114:ILE:HG23	15:Ja:118:GLU:HB3	1.97	0.47
24:AC:177:LYS:HD3	75:h1:6:G:OP2	2.14	0.47
25:BI:90:ARG:NH1	25:BI:96:MET:HE1	2.29	0.47
28:AV:85:LEU:HD21	63:AQ:35:LYS:HG2	1.96	0.47
50:Na:35:MET:HE3	50:Na:81:PHE:CG	2.50	0.47
61:BE:2:ALA:O	61:BE:4:ARG:N	2.47	0.47
75:h1:1641:OMC:O2	75:h1:1767:6MZ:N1	2.48	0.47
1:3:16:A:OP1	6:BM:3:LYS:HD3	2.15	0.46
2:A:2091:A:H4'	2:A:2092:A:O5'	2.15	0.46
41:Ha:79:TRP:CZ2	41:Ha:118:LYS:HB3	2.49	0.46
51:AB:16:LYS:HB3	51:AB:17:PRO:HD2	1.97	0.46
65:Ua:137:ASP:HA	86:Ua:320:HOH:O	2.14	0.46
75:h1:141:G:H2'	75:h1:142:G:C8	2.51	0.46
75:h1:1296:G:N7	86:h1:2119:HOH:O	2.35	0.46
77:Ba:54:LYS:HB3	77:Ba:93:ASP:HB2	1.97	0.46
2:A:1354:G:O6	86:A:3823:HOH:O	2.21	0.46
2:A:1625:G:O2'	2:A:1643:A:N1	2.46	0.46
4:C3:80:A:N1	4:C3:96:C:O2	2.49	0.46
15:Ja:129:ILE:CD1	15:Ja:139:LEU:HD22	2.46	0.46
15:Ja:139:LEU:HG	15:Ja:150:PRO:HG3	1.97	0.46
19:Ka:102:ILE:HG22	19:Ka:104:LYS:HG3	1.97	0.46
41:Ha:99:ASP:HA	41:Ha:123:LYS:HB3	1.97	0.46
57:AF:99:VAL:HG12	57:AF:100:ASP:H	1.81	0.46
69:Ra:41:LEU:HD22	69:Ra:76:ILE:HD13	1.97	0.46
72:Aa:114:TYR:CD2	72:Aa:122:LEU:HD21	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BS:46:PHE:C	22:BS:182:MET:HE1	2.40	0.46
32:BH:5:SER:OG	32:BH:31:GLU:OE1	2.30	0.46
56:BA:44:TRP:CZ3	56:BA:45:ARG:HG3	2.51	0.46
74:Ca:16:PRO:HD2	75:h1:1206:C:N3	2.29	0.46
75:h1:593:A:H2'	75:h1:594:A:C8	2.50	0.46
75:h1:617:A:O2'	75:h1:623:A:N1	2.44	0.46
1:3:85:U:O3'	1:3:87:C:OP2	2.32	0.46
2:A:1056:A:H2'	2:A:1059:C:C5	2.51	0.46
3:i2:15:G:H2'	3:i2:16:U:C2	2.50	0.46
24:AC:173:ARG:HD2	75:h1:1098:U:O4	2.14	0.46
72:Aa:59:LEU:HD21	75:h1:1678:U:OP1	2.16	0.46
75:h1:515:U:H2'	75:h1:516:G:C8	2.50	0.46
2:A:2390:C:O2	2:A:2986:A:N1	2.49	0.46
15:Ja:104:ASP:O	15:Ja:190:GLY:HA3	2.16	0.46
51:AB:104:GLU:O	51:AB:108:GLU:HG2	2.16	0.46
69:Ra:107:LYS:NZ	75:h1:747:U:OP2	2.41	0.46
72:Aa:84:TYR:HB3	72:Aa:102:ILE:HB	1.98	0.46
75:h1:886:G:H2'	75:h1:887:U:C6	2.51	0.46
2:A:1853:OMG:HM22	73:AY:6:GLY:HA2	1.98	0.46
17:AL:92:MET:HE1	17:AL:116:HIS:CE1	2.50	0.46
26:AH:64:ARG:HG2	26:AH:65:VAL:HG23	1.98	0.46
38:BN:127:ARG:HD3	38:BN:133:LYS:HE2	1.97	0.46
2:A:330:G:N7	86:A:3905:HOH:O	2.36	0.46
2:A:2426:C:N3	2:A:2600:A:N1	2.64	0.46
20:AW:18:ILE:HD13	20:AW:35:VAL:HG22	1.97	0.46
24:AC:71:LYS:HD3	24:AC:73:PHE:CZ	2.51	0.46
28:AV:85:LEU:HD21	63:AQ:35:LYS:HA	1.97	0.46
69:Ra:166:LYS:O	69:Ra:169:THR:HG22	2.16	0.46
2:A:3119:U:H1'	2:A:3120:A:H5''	1.97	0.46
27:BT:150:GLU:CD	27:BT:150:GLU:H	2.24	0.46
48:BW:16:LYS:HG3	48:BW:23:LEU:HD23	1.98	0.46
71:La:56:PRO:O	71:La:104:ARG:HB3	2.14	0.46
2:A:1373:A:H2'	2:A:1374:U:O4'	2.16	0.46
2:A:2913:G:N3	2:A:2933:A2M:H2	2.31	0.46
22:BS:86:VAL:CG2	22:BS:206:ILE:HD11	2.45	0.46
57:AF:22:THR:CG2	57:AF:67:MET:HG3	2.46	0.46
75:h1:1042:G:H2'	75:h1:1043:G:C8	2.51	0.46
2:A:27:C:H4'	2:A:60:A:H4'	1.98	0.46
2:A:1697:A:OP1	40:Fa:21:ARG:NH2	2.48	0.46
2:A:2234:OMG:H4'	3:W2:71:G:OP1	2.16	0.46
28:AV:97:ILE:HG21	28:AV:106:ARG:HG2	1.99	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:909:G:H1'	2:A:1590:A:N6	2.31	0.45
2:A:2507:U:H2'	2:A:2508:U:O4'	2.16	0.45
45:BV:43:VAL:HG13	45:BV:68:VAL:HG11	1.97	0.45
45:BV:143:THR:CG2	45:BV:154:CYS:O	2.64	0.45
54:AG:62:LEU:C	54:AG:62:LEU:HD12	2.40	0.45
61:BE:47:VAL:HG11	61:BE:71:MET:SD	2.56	0.45
65:Ua:137:ASP:CG	75:h1:929:G:H1'	2.40	0.45
2:A:2497:U:O2	2:A:2497:U:O4'	2.33	0.45
2:A:2662:G:H2'	2:A:2663:C:O4'	2.16	0.45
22:BS:249:LEU:HD12	22:BS:249:LEU:C	2.41	0.45
25:BI:117:ILE:O	25:BI:137:ASN:ND2	2.42	0.45
45:BV:47:LEU:HD23	45:BV:47:LEU:HA	1.83	0.45
69:Ra:77:HIS:N	69:Ra:78:PRO:HD2	2.32	0.45
78:AI:29:LEU:HD12	78:AI:30:PRO:HD2	1.99	0.45
2:A:11:G:H8	2:A:11:G:C5'	2.29	0.45
2:A:437:G:N2	2:A:629:C:C1'	2.79	0.45
17:AL:8:GLN:HB2	17:AL:32:TRP:CH2	2.51	0.45
22:BS:379:GLU:OE2	47:AO:16:TYR:OH	2.25	0.45
62:Za:149:ILE:HG12	62:Za:163:ILE:HB	1.98	0.45
67:BB:17:ILE:HD12	67:BB:58:MET:SD	2.56	0.45
74:Ca:53:ILE:CA	74:Ca:54:LYS:N	2.77	0.45
75:h1:426:C:H4'	75:h1:428:G:OP1	2.15	0.45
2:A:2362:G:H22	2:A:2394:G:H1'	1.80	0.45
2:A:2547:U:O2	39:BG:29:GLN:NE2	2.49	0.45
2:A:2826:U:H2'	2:A:2826:U:O2	2.15	0.45
2:A:3169:C:OP1	20:AW:15:ARG:NH1	2.43	0.45
12:AE:4:ILE:HG23	75:h1:636:G:H5'	1.97	0.45
69:Ra:131:ALA:O	69:Ra:132:PHE:C	2.59	0.45
75:h1:1318:C:H2'	75:h1:1319:G:O4'	2.17	0.45
75:h1:1588:A:H2'	75:h1:1589:A:O4'	2.17	0.45
2:A:1032:G:C6	2:A:1033:G:C6	3.05	0.45
2:A:1766:G:H2'	2:A:1768:G:O4'	2.15	0.45
2:A:2183:G:O2'	2:A:2312:PSU:OP2	2.34	0.45
11:Ia:26:GLU:HG2	11:Ia:35:VAL:HG22	1.97	0.45
14:AP:68:VAL:HG22	14:AP:118:GLU:HG3	1.99	0.45
27:BT:155:MET:HE3	86:BT:586:HOH:O	2.16	0.45
30:AJ:177:ARG:HA	30:AJ:183:ARG:O	2.17	0.45
45:BV:143:THR:HG22	45:BV:154:CYS:SG	2.56	0.45
57:AF:23:HIS:O	57:AF:67:MET:O	2.33	0.45
2:A:4:A:H2'	2:A:5:C:O4'	2.16	0.45
15:Ja:45:VAL:HA	15:Ja:61:VAL:HG11	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Va:101:ILE:CG2	18:Va:119:PHE:HB3	2.47	0.45
27:BT:164:GLU:OE2	27:BT:261:SER:OG	2.30	0.45
32:BH:74:GLY:HA2	32:BH:75:PRO:C	2.42	0.45
46:BJ:46:PHE:CB	46:BJ:139:ARG:HG2	2.47	0.45
49:AK:93:VAL:O	49:AK:97:ARG:HG3	2.17	0.45
59:Ta:13:GLN:O	59:Ta:14:LYS:HB3	2.16	0.45
75:h1:425:G:H4'	75:h1:426:C:OP1	2.14	0.45
2:A:1359:A:N7	27:BT:302:ASP:HA	2.32	0.45
13:AX:7:LYS:HD3	13:AX:17:GLY:HA3	1.99	0.45
23:AM:27:LEU:HD13	86:AM:372:HOH:O	2.16	0.45
27:BT:295:LEU:HB3	63:AQ:7:GLN:HG2	1.99	0.45
33:Da:41:ALA:HB3	33:Da:80:LEU:HD23	1.98	0.45
48:BW:81:GLN:OE1	62:Za:67:ARG:NH2	2.49	0.45
62:Za:21:MET:HE1	62:Za:180:TRP:HZ3	1.81	0.45
62:Za:54:ASN:O	62:Za:56:GLY:N	2.43	0.45
62:Za:167:ALA:HB1	62:Za:178:LEU:HD11	1.98	0.45
66:Ya:25:VAL:HG11	66:Ya:33:MET:HE1	1.98	0.45
2:A:1678:G:O6	68:AN:80:ARG:NH2	2.50	0.45
2:A:1821:G:H5''	2:A:1821:G:C8	2.50	0.45
3:i2:47:U:C2	3:i2:50:C:OP1	2.70	0.45
35:AT:93:LEU:C	35:AT:93:LEU:HD12	2.41	0.45
43:BR:91:ILE:O	43:BR:119:GLY:HA2	2.17	0.45
45:BV:51:THR:HA	45:BV:55:LYS:O	2.16	0.45
72:Aa:142:LEU:HD11	75:h1:186:A:OP2	2.16	0.45
2:A:750:U:O4	2:A:751:G:C6	2.69	0.45
2:A:2841:U:O2	2:A:2841:U:C2'	2.60	0.45
20:AW:19:LEU:HD11	20:AW:36:GLN:HB2	1.99	0.45
41:Ha:132:GLU:OE2	54:AG:176:ALA:N	2.41	0.45
67:BB:73:LEU:HD12	67:BB:74:GLN:N	2.32	0.45
71:La:51:LEU:HD13	71:La:70:MET:HE1	1.99	0.45
75:h1:130:A:O2'	75:h1:175:A:N7	2.40	0.45
1:3:72:G:OP2	73:AY:87:ARG:HG2	2.17	0.45
2:A:1838:C:O2'	2:A:1844:A:N1	2.47	0.45
19:Ka:30:HIS:HB2	19:Ka:33:ARG:HB2	1.98	0.45
29:AD:102:LEU:HD21	71:La:103:THR:HB	1.99	0.45
51:AB:2:VAL:N	75:h1:463:G:OP1	2.50	0.45
59:Ta:13:GLN:O	59:Ta:14:LYS:CB	2.65	0.45
59:Ta:81:THR:OG1	59:Ta:82:PRO:HD2	2.17	0.45
62:Za:181:LEU:O	62:Za:185:MET:HG3	2.17	0.45
66:Ya:22:PHE:HB3	66:Ya:30:LEU:HD11	1.99	0.45
69:Ra:16:PRO:HB2	69:Ra:21:GLU:HG2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:Aa:139:SER:HB2	75:h1:188:U:O4	2.17	0.45
2:A:2946:G:N3	22:BS:253:ALA:HB1	2.32	0.44
2:A:1686:U:H2'	2:A:1688:U:H1'	1.99	0.44
2:A:2850:A:OP2	86:A:3822:HOH:O	2.20	0.44
19:Ka:79:ASP:OD1	19:Ka:83:ASN:ND2	2.50	0.44
28:AV:5:LEU:HD11	52:BF:68:GLU:HB3	1.98	0.44
41:Ha:2:THR:HG21	41:Ha:5:PHE:CD2	2.53	0.44
65:Ua:38:ASP:OD2	75:h1:901:A:OP1	2.35	0.44
73:AY:25:ARG:HD2	73:AY:25:ARG:O	2.18	0.44
75:h1:890:U:H4'	75:h1:990:U:OP1	2.18	0.44
75:h1:1059:U:H3'	75:h1:1060:U:H5''	1.99	0.44
1:3:123:C:H2'	1:3:124:C:O4'	2.18	0.44
2:A:416:G:N7	86:A:3908:HOH:O	2.36	0.44
2:A:3265:C:H2'	2:A:3266:A:O4'	2.17	0.44
45:BV:179:CYS:HB3	45:BV:183:GLU:HB2	1.98	0.44
69:Ra:83:GLU:O	69:Ra:87:LYS:HG3	2.18	0.44
70:BL:42:LYS:HE3	70:BL:94:CYS:SG	2.57	0.44
1:3:29:G:N3	2:A:342:G:O2'	2.50	0.44
1:3:101:G:H5''	37:BP:66:LYS:HG3	1.99	0.44
2:A:353:C:O2	27:BT:89:THR:CG2	2.65	0.44
2:A:391:C:N3	2:A:394:A:OP2	2.50	0.44
2:A:501:G:O2'	2:A:3259:A:N1	2.43	0.44
2:A:920:C:O2	2:A:926:A:N1	2.51	0.44
2:A:1446:OMC:HM22	2:A:1447:U:H5'	1.98	0.44
75:h1:1387:A:H2'	75:h1:1388:G:O4'	2.18	0.44
26:AH:81:LYS:O	26:AH:85:GLU:HG3	2.17	0.44
27:BT:155:MET:HA	27:BT:156:PRO:C	2.43	0.44
29:AD:18:LEU:HD23	29:AD:97:MET:HE1	1.99	0.44
52:BF:122:GLY:HA3	52:BF:123:PRO:C	2.42	0.44
57:AF:50:ILE:HG13	57:AF:80:VAL:HG13	1.99	0.44
59:Ta:221:LEU:HD11	75:h1:242:C:H5''	1.98	0.44
60:AZ:8:ILE:HG23	60:AZ:56:LEU:HD23	1.98	0.44
66:Ya:86:ARG:HB3	66:Ya:122:ALA:HB2	1.99	0.44
69:Ra:66:PRO:HG2	69:Ra:69:LEU:HB2	1.99	0.44
2:A:371:A:N3	2:A:373:G:H5''	2.33	0.44
2:A:856:A:N1	75:h1:973:G:O2'	2.48	0.44
2:A:2576:U:H2'	2:A:2577:C:C6	2.52	0.44
2:A:2901:A:OP1	11:Ia:173:LYS:NZ	2.51	0.44
3:i2:70:C:H2'	3:i2:71:G:C8	2.52	0.44
65:Ua:137:ASP:CG	75:h1:929:G:C4'	2.90	0.44
73:AY:38:ALA:HB2	73:AY:45:ARG:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:904:U:H1'	75:h1:907:A:N7	2.32	0.44
75:h1:1614:C:N4	86:h1:2279:HOH:O	2.50	0.44
2:A:2184:U:OP2	31:BQ:200:ARG:HD2	2.17	0.44
2:A:3366:C:H4'	22:BS:319:GLY:HA2	1.99	0.44
4:C3:26:C:H2'	4:C3:27:A:O4'	2.17	0.44
14:AP:70:CYS:SG	14:AP:117:LEU:HD12	2.58	0.44
17:AL:83:TYR:CD2	17:AL:118:VAL:HG21	2.53	0.44
39:BG:116:LYS:HB2	39:BG:117:PRO:HD2	2.00	0.44
59:Ta:32:LEU:HD12	59:Ta:52:ILE:HG22	1.99	0.44
75:h1:749:A:H62	75:h1:806:G:H21	1.64	0.44
75:h1:1679:U:H2'	75:h1:1680:C:O4'	2.18	0.44
11:Ia:27:VAL:HG12	11:Ia:87:VAL:HG21	1.99	0.44
19:Ka:60:PHE:CZ	19:Ka:76:LEU:HD22	2.48	0.44
51:AB:12:LYS:HE2	75:h1:24:U:OP1	2.17	0.44
62:Za:85:PRO:HA	62:Za:88:GLN:HG2	1.99	0.44
62:Za:108:THR:HG23	62:Za:111:THR:OG1	2.17	0.44
75:h1:1295:G:O2'	75:h1:1322:A:N1	2.44	0.44
2:A:2451:U:N3	2:A:2453:U:OP1	2.50	0.44
24:AC:184:LYS:NZ	75:h1:1299:C:O3'	2.51	0.44
29:AD:163:PHE:CE2	29:AD:164:ARG:HD3	2.53	0.44
58:Wa:15:VAL:HG13	58:Wa:68:MET:HE2	1.99	0.44
75:h1:990:U:H2'	75:h1:991:C:O4'	2.17	0.44
2:A:196:A:O2'	2:A:198:G:N7	2.48	0.43
2:A:354:C:O4'	27:BT:88:GLY:HA3	2.18	0.43
2:A:2648:G:O2'	2:A:2757:A:N1	2.51	0.43
22:BS:299:MET:HE2	22:BS:304:ARG:CZ	2.47	0.43
27:BT:99:ASN:HA	27:BT:105:ARG:O	2.18	0.43
28:AV:66:HIS:CE1	63:AQ:29:SER:HB3	2.53	0.43
59:Ta:133:ARG:O	59:Ta:134:MET:HB2	2.17	0.43
72:Aa:99:LYS:O	72:Aa:172:ILE:C	2.61	0.43
75:h1:1134:A:H2'	75:h1:1135:C:O4'	2.18	0.43
78:AI:15:LEU:HD13	78:AI:46:MET:HE1	2.00	0.43
1:3:83:A:H2'	1:3:84:A:O4'	2.18	0.43
2:A:11:G:H5''	2:A:11:G:C8	2.51	0.43
2:A:545:U:HO2'	2:A:546:U:H6	1.65	0.43
2:A:1617:G:H2'	2:A:1618:G:O4'	2.18	0.43
2:A:2371:A:N3	2:A:2823:G:O2'	2.49	0.43
2:A:2403:C:O2	2:A:2818:A:N1	2.51	0.43
2:A:3025:A:H2'	2:A:3026:G:O4'	2.18	0.43
86:A:5019:HOH:O	27:BT:74:THR:HG21	2.17	0.43
3:i2:16:U:H2'	3:i2:60:C:O2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:AH:24:LEU:HD11	26:AH:84:TRP:CG	2.53	0.43
33:Da:110:ASP:O	33:Da:114:ARG:HG2	2.16	0.43
2:A:1361:A:H4'	63:AQ:113:ASP:HB3	2.01	0.43
2:A:1371:C:H5''	27:BT:318:ALA:HB2	2.00	0.43
2:A:3053:C:O2'	2:A:3055:U:OP2	2.36	0.43
7:BO:6:ARG:NE	86:BO:204:HOH:O	2.51	0.43
54:AG:89:ALA:HB3	54:AG:90:PRO:HD3	2.00	0.43
72:Aa:181:ARG:HD3	86:Aa:301:HOH:O	2.18	0.43
75:h1:136:U:O2'	75:h1:139:U:OP1	2.36	0.43
75:h1:1581:U:H2'	75:h1:1582:C:C6	2.54	0.43
2:A:51:G:H4'	2:A:821:G:H4'	2.01	0.43
2:A:1148:G:O6	8:AR:10:HIS:CE1	2.71	0.43
2:A:1718:C:H2'	2:A:1719:G:O4'	2.19	0.43
2:A:2627:A:H1'	2:A:2797:C:C2	2.54	0.43
2:A:2946:G:C2	22:BS:253:ALA:HB1	2.53	0.43
2:A:3181:G:O6	26:AH:4:LYS:NZ	2.49	0.43
70:BL:89:ARG:HD2	75:h1:1603:G:C5	2.54	0.43
2:A:1:G:H2'	2:A:2:C:C6	2.53	0.43
2:A:581:C:OP1	52:BF:25:ARG:HD3	2.18	0.43
2:A:712:A:H1'	54:AG:67:LYS:HE2	1.99	0.43
2:A:2496:U:O2'	2:A:2497:U:OP1	2.35	0.43
2:A:3164:A:H2'	2:A:3165:U:O4'	2.18	0.43
28:AV:91:ARG:HH12	52:BF:70:VAL:HG22	1.84	0.43
46:BJ:190:ILE:HD13	46:BJ:199:PHE:HA	2.00	0.43
51:AB:80:ARG:HH22	75:h1:767:U:P	2.41	0.43
62:Za:82:SER:HB2	62:Za:129:THR:HG21	2.00	0.43
75:h1:453:G:N2	75:h1:458:G:C4	2.87	0.43
12:AE:99:PHE:CZ	24:AC:198:THR:HG22	2.53	0.43
20:AW:108:TYR:HA	20:AW:109:PRO:C	2.44	0.43
53:AA:133:GLY:HA3	53:AA:156:TYR:O	2.19	0.43
56:BA:16:LYS:NZ	86:BA:101:HOH:O	2.52	0.43
63:AQ:20:LEU:O	63:AQ:33:PHE:O	2.37	0.43
73:AY:55:ARG:CB	73:AY:55:ARG:HH11	2.31	0.43
75:h1:1339:C:H1'	75:h1:1413:A:C5	2.54	0.43
3:i2:64:G:OP1	46:BJ:25:GLY:HA2	2.17	0.43
75:h1:379:G:HO2'	75:h1:380:A:P	2.35	0.43
77:Ba:35:LEU:HD21	77:Ba:90:ARG:CG	2.48	0.43
2:A:2254:A2M:N1	3:i2:37:G:O2'	2.41	0.43
2:A:2870:G:OP2	86:A:3824:HOH:O	2.22	0.43
31:BQ:226:ARG:NH2	31:BQ:233:GLN:OE1	2.52	0.43
33:Da:40:PHE:CZ	33:Da:53:ILE:HG21	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:BK:260:PRO:O	34:BK:261:LYS:C	2.61	0.43
51:AB:29:GLU:HG3	51:AB:41:LYS:HD3	2.01	0.43
52:BF:219:MET:HE2	52:BF:224:LEU:HD11	2.00	0.43
59:Ta:23:LYS:HD2	59:Ta:41:LEU:HA	2.01	0.43
59:Ta:48:TYR:CE2	59:Ta:123:LEU:HD12	2.54	0.43
75:h1:395:C:H2'	75:h1:396:C:C6	2.54	0.43
75:h1:1519:A:H8	77:Ba:59:MET:HE1	1.83	0.43
1:3:84:A:C2'	1:3:85:U:H5'	2.49	0.43
2:A:1529:G:O2'	2:A:1604:A:N1	2.49	0.43
2:A:1662:G:H5''	2:A:1662:G:N3	2.34	0.43
2:A:1800:A:H2'	2:A:1801:A:C8	2.54	0.43
15:Ja:80:LYS:HG2	15:Ja:81:THR:HG23	2.01	0.43
33:Da:19:LYS:HZ2	33:Da:21:SER:HG	1.63	0.43
34:BK:65:VAL:CG1	34:BK:72:ASP:HB3	2.48	0.43
59:Ta:180:ILE:HG22	59:Ta:183:LEU:HB2	1.99	0.43
75:h1:790:G:H2'	75:h1:791:G:O4'	2.19	0.43
2:A:848:C:O2'	2:A:1725:G:OP1	2.34	0.43
2:A:2848:C:N4	2:A:2849:G:C6	2.87	0.43
19:Ka:59:CYS:HB3	19:Ka:62:PHE:CE1	2.53	0.43
24:AC:70:PHE:O	24:AC:89:CYS:HA	2.18	0.43
25:BI:22:VAL:O	25:BI:23:ALA:HB3	2.19	0.43
45:BV:119:THR:HG21	45:BV:161:ILE:HD11	2.01	0.43
59:Ta:147:PHE:CD2	59:Ta:158:TYR:HB3	2.54	0.43
66:Ya:42:PHE:HE1	66:Ya:117:ILE:HG22	1.84	0.43
73:AY:8:PHE:CE1	86:AY:351:HOH:O	2.69	0.43
1:3:155:OMG:CM2	39:BG:52:ILE:CD1	2.97	0.42
2:A:209:G:O6	27:BT:189:LYS:NZ	2.52	0.42
2:A:1631:G:N7	14:AP:48:LYS:NZ	2.59	0.42
42:BU:95:ARG:HH12	42:BU:162:MET:HE1	1.84	0.42
64:Oa:20:ARG:HG2	75:h1:1621:C:C2	2.54	0.42
2:A:1568:A:H3'	2:A:1569:G:O4'	2.18	0.42
2:A:1772:U:H2'	2:A:1773:G:O4'	2.19	0.42
15:Ja:103:TYR:CE1	15:Ja:189:ARG:HD3	2.55	0.42
18:Va:75:LYS:HE3	86:Va:311:HOH:O	2.19	0.42
21:BD:28:TYR:HB3	21:BD:69:VAL:HB	2.00	0.42
45:BV:214:LYS:NZ	75:h1:887:U:OP1	2.40	0.42
50:Na:35:MET:HE3	50:Na:81:PHE:CD1	2.53	0.42
66:Ya:44:SER:OG	75:h1:1551:C:H3'	2.19	0.42
72:Aa:109:PRO:O	72:Aa:110:PHE:HB2	2.19	0.42
75:h1:853:A:H2'	75:h1:854:G:O4'	2.19	0.42
75:h1:1244:G:H5''	75:h1:1244:G:N3	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:611:C:O2'	52:BF:47:ARG:O	2.26	0.42
2:A:774:U:C4	54:AG:182:LEU:HD21	2.54	0.42
2:A:2522:A:C5	31:BQ:67:PHE:CE1	3.08	0.42
2:A:3218:U:O4	2:A:3245:C:N3	2.52	0.42
6:BM:30:ARG:HD3	6:BM:30:ARG:C	2.45	0.42
19:Ka:63:ARG:NH2	75:h1:532:C:O2	2.53	0.42
29:AD:15:GLU:N	29:AD:15:GLU:OE1	2.52	0.42
41:Ha:69:PHE:HB3	86:Ha:201:HOH:O	2.19	0.42
44:Xa:125:ILE:N	44:Xa:125:ILE:HD12	2.34	0.42
54:AG:183:GLU:OE1	54:AG:183:GLU:HA	2.17	0.42
59:Ta:12:CYS:SG	59:Ta:126:LEU:O	2.77	0.42
65:Ua:137:ASP:CG	75:h1:929:G:C1'	2.92	0.42
75:h1:17:C:O2'	75:h1:1138:A:N1	2.50	0.42
75:h1:1167:A:O2'	75:h1:1589:A:H4'	2.19	0.42
2:A:87:A:N1	2:A:95:C:O2	2.52	0.42
2:A:436:C:O2'	2:A:437:G:H2'	2.19	0.42
2:A:472:G:H2'	2:A:473:G:C8	2.53	0.42
2:A:1007:A:C2	2:A:1064:A:C4	3.07	0.42
2:A:2605:G:N3	2:A:2605:G:H2'	2.35	0.42
12:AE:48:GLY:HA2	69:Ra:145:LEU:HD21	2.00	0.42
15:Ja:129:ILE:HG22	75:h1:244:OMG:HM21	2.00	0.42
34:BK:119:TYR:OH	34:BK:138:ARG:O	2.38	0.42
62:Za:85:PRO:O	62:Za:88:GLN:HG2	2.19	0.42
72:Aa:33:PRO:HA	75:h1:333:A:H5'	2.01	0.42
2:A:688:G:O2'	2:A:795:A:N1	2.52	0.42
2:A:1564:U:O2	39:BG:50:LYS:NZ	2.47	0.42
15:Ja:3:ARG:HB3	75:h1:94:A:H1'	2.01	0.42
26:AH:72:ILE:O	26:AH:76:GLU:HG3	2.20	0.42
27:BT:367:VAL:HG13	27:BT:371:GLU:HB2	2.01	0.42
29:AD:27:VAL:HG12	29:AD:110:GLN:HB2	2.01	0.42
31:BQ:206:PRO:HG3	31:BQ:213:GLY:HA3	2.02	0.42
41:Ha:69:PHE:C	86:Ha:201:HOH:O	2.49	0.42
67:BB:35:LEU:HD12	67:BB:51:ALA:HB2	2.02	0.42
72:Aa:34:ALA:HB2	72:Aa:57:ARG:HG3	2.00	0.42
74:Ca:21:CYS:HB2	74:Ca:39:CYS:HB3	2.00	0.42
3:W2:47:U:O2'	3:W2:48:C:H5''	2.20	0.42
14:AP:24:VAL:O	14:AP:43:VAL:HG13	2.20	0.42
16:Ea:64:VAL:HG21	16:Ea:106:ALA:HB2	2.00	0.42
34:BK:83:LEU:HD13	34:BK:88:LEU:HD23	2.02	0.42
39:BG:199:ASN:HA	39:BG:202:LYS:HG3	2.01	0.42
46:BJ:89:ILE:HD12	46:BJ:136:LEU:CD2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:Ra:5:GLN:C	69:Ra:7:LYS:H	2.27	0.42
75:h1:979:A:H2'	75:h1:980:A:O4'	2.20	0.42
2:A:826:A2M:HM'3	2:A:929:A:C4	2.54	0.42
2:A:2424:U:H2'	2:A:2425:C:C6	2.54	0.42
15:Ja:171:GLU:HG3	15:Ja:235:TRP:CZ3	2.55	0.42
22:BS:225:LYS:NZ	86:BS:510:HOH:O	2.50	0.42
53:AA:76:ARG:NH2	78:AI:63:HIS:CE1	2.88	0.42
67:BB:69:ILE:HG22	67:BB:71:LEU:HG	2.01	0.42
68:AN:39:LEU:HD22	68:AN:69:ILE:HD12	2.01	0.42
10:Ma:65:PRO:HG3	65:Ua:128:ILE:O	2.20	0.42
25:BI:87:PRO:HA	25:BI:96:MET:O	2.20	0.42
26:AH:40:ALA:HB3	26:AH:43:MET:HG2	2.02	0.42
46:BJ:46:PHE:HB3	46:BJ:139:ARG:HG2	2.00	0.42
51:AB:126:HIS:O	51:AB:129:VAL:HG12	2.19	0.42
58:Wa:98:VAL:HG23	58:Wa:103:LEU:HD13	2.02	0.42
68:AN:27:LYS:N	68:AN:28:PRO:HD2	2.35	0.42
2:A:880:U:P	86:A:4110:HOH:O	2.77	0.42
2:A:989:A:N3	2:A:991:G:H1'	2.35	0.42
2:A:990:C:C3'	2:A:991:G:H5''	2.49	0.42
2:A:1026:A:N6	2:A:1029:G:OP2	2.53	0.42
31:BQ:82:MET:HA	31:BQ:86:GLN:OE1	2.20	0.42
46:BJ:53:VAL:HG22	46:BJ:164:LYS:O	2.20	0.42
75:h1:1545:A:C2	75:h1:1571:A:C8	3.07	0.42
77:Ba:78:ASN:ND2	86:Ba:202:HOH:O	2.52	0.42
2:A:1568:A:H5''	2:A:1568:A:N3	2.35	0.42
2:A:1682:U:H1'	2:A:1686:U:O4	2.20	0.42
21:BD:25:VAL:HG22	21:BD:72:LEU:HD22	2.02	0.42
45:BV:48:VAL:CG2	45:BV:61:LEU:HD21	2.49	0.42
59:Ta:32:LEU:HD11	59:Ta:54:GLY:HA2	2.02	0.42
66:Ya:129:LYS:HD3	75:h1:1183:U:H5''	2.01	0.42
75:h1:821:U:H2'	75:h1:822:U:C6	2.55	0.42
2:A:1223:G:H8	2:A:1223:G:H5''	1.85	0.41
11:Ia:12:ILE:HD11	11:Ia:58:LEU:HB2	2.01	0.41
44:Xa:68:ARG:CD	75:h1:114:U:H5'	2.50	0.41
50:Na:57:VAL:HG13	50:Na:62:GLN:O	2.20	0.41
51:AB:171:PRO:HB3	51:AB:175:LYS:HG2	2.02	0.41
60:AZ:24:LYS:HB3	60:AZ:69:LEU:CD2	2.50	0.41
65:Ua:137:ASP:OD1	75:h1:929:G:O3'	2.38	0.41
66:Ya:103:ASN:ND2	66:Ya:126:ILE:O	2.51	0.41
71:La:84:LEU:HB3	71:La:90:ILE:HG12	2.01	0.41
75:h1:1491:G:O2'	75:h1:1497:C:O2	2.30	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:h1:1676:U:H2'	75:h1:1677:G:C8	2.55	0.41
2:A:44:OMU:OP2	82:A:3401:TER:H102	2.20	0.41
2:A:673:G:N7	41:Ha:25:HIS:ND1	2.64	0.41
2:A:686:G:O6	30:AJ:56:LYS:NZ	2.52	0.41
2:A:843:U:C4	2:A:844:A:C6	3.08	0.41
2:A:3215:A:H2'	2:A:3216:A:O4'	2.19	0.41
6:BM:126:GLN:HB2	6:BM:142:SER:OG	2.20	0.41
19:Ka:21:ARG:HD3	19:Ka:76:LEU:HG	2.02	0.41
35:AT:27:THR:HG23	86:AT:201:HOH:O	2.20	0.41
53:AA:206:ASP:OD1	75:h1:1332:A:N3	2.53	0.41
62:Za:95:ALA:HB1	62:Za:100:ALA:O	2.20	0.41
62:Za:136:GLN:HB3	62:Za:137:PRO:HD3	2.02	0.41
75:h1:187:C:H2'	75:h1:188:U:O4'	2.20	0.41
75:h1:335:A:C6	75:h1:336:G:C6	3.08	0.41
43:BR:164:GLN:HG2	86:BR:464:HOH:O	2.19	0.41
45:BV:184:LEU:HG	45:BV:188:PHE:CZ	2.55	0.41
57:AF:57:LEU:HD13	57:AF:107:ILE:HD12	2.01	0.41
62:Za:84:ARG:NH2	62:Za:130:ASP:OD2	2.53	0.41
66:Ya:58:PRO:O	66:Ya:62:ILE:HG13	2.20	0.41
68:AN:23:ILE:HD11	68:AN:113:LEU:HG	2.02	0.41
73:AY:39:TYR:CD1	73:AY:40:PRO:HA	2.56	0.41
6:BM:37:ARG:O	6:BM:38:LYS:HB2	2.21	0.41
10:Ma:4:LYS:NZ	75:h1:1798:A:OP2	2.52	0.41
16:Ea:201:ARG:NH1	86:Ea:409:HOH:O	2.47	0.41
24:AC:53:MET:HE3	24:AC:158:LYS:HG2	2.01	0.41
42:BU:42:LEU:CD1	42:BU:127:MET:HE1	2.48	0.41
42:BU:164:TRP:CZ2	42:BU:168:LYS:HD3	2.55	0.41
59:Ta:133:ARG:NE	75:h1:164:C:OP1	2.53	0.41
64:Oa:28:VAL:HG11	64:Oa:51:LEU:HD12	2.01	0.41
75:h1:794:A2M:HM'3	75:h1:794:A2M:H1'	1.83	0.41
75:h1:1027:A:N7	75:h1:1776:C:O2'	2.51	0.41
75:h1:1316:U:H2'	75:h1:1317:C:O4'	2.20	0.41
2:A:2929:A:N7	86:A:3918:HOH:O	2.37	0.41
15:Ja:110:ARG:HH22	75:h1:790:G:P	2.44	0.41
15:Ja:181:VAL:HG12	15:Ja:227:THR:HA	2.01	0.41
29:AD:18:LEU:HD21	29:AD:69:VAL:HG11	2.02	0.41
30:AJ:41:ASN:C	86:AJ:351:HOH:O	2.62	0.41
31:BQ:108:PRO:HG3	61:BE:90:ILE:HD11	2.03	0.41
75:h1:502:C:O2'	75:h1:503:U:OP1	2.37	0.41
1:3:108:A:C8	1:3:109:A:C8	3.09	0.41
2:A:98:A:H5'	16:Ea:182:HIS:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:985:U:H2'	2:A:986:C:O4'	2.21	0.41
2:A:1155:C:H4'	2:A:1341:U:C4	2.56	0.41
2:A:1819:C:H2'	2:A:1820:C:O4'	2.21	0.41
2:A:2695:A:H2'	2:A:2696:A:C8	2.55	0.41
2:A:2711:U:H2'	2:A:2712:U:C6	2.56	0.41
51:AB:131:ILE:O	51:AB:144:ASN:HA	2.20	0.41
62:Za:168:ASN:O	62:Za:174:SER:OG	2.37	0.41
66:Ya:37:ASP:HA	66:Ya:40:LYS:HE3	2.02	0.41
2:A:7:C:H2'	2:A:8:C:O4'	2.20	0.41
2:A:1089:U:O2	34:BK:138:ARG:NH2	2.50	0.41
2:A:1119:C:H2'	2:A:1120:A:O4'	2.21	0.41
2:A:1200:C:H5''	32:BH:57:MET:HE1	2.02	0.41
26:AH:35:ARG:HD2	26:AH:47:GLN:OE1	2.20	0.41
53:AA:45:ARG:NH2	53:AA:87:TYR:OH	2.53	0.41
75:h1:969:U:H2'	75:h1:970:C:O4'	2.20	0.41
78:AI:71:GLU:OE2	78:AI:71:GLU:N	2.53	0.41
1:3:125:A:H2'	1:3:126:A:O4'	2.20	0.41
2:A:68:A:N1	2:A:310:G:O2'	2.48	0.41
2:A:1572:C:H42	2:A:1576:A:H61	1.69	0.41
2:A:1622:G:H2'	2:A:1623:U:C6	2.55	0.41
2:A:1658:G:H2'	2:A:1659:U:O4'	2.21	0.41
2:A:2189:PSU:H2'	2:A:2190:C:O4'	2.21	0.41
86:A:8516:HOH:O	61:BE:24:LYS:HG3	2.19	0.41
15:Ja:160:ILE:HG23	15:Ja:169:ILE:HG23	2.03	0.41
23:AM:105:PHE:CZ	23:AM:109:LYS:HE2	2.56	0.41
27:BT:54:ARG:NH2	86:BT:501:HOH:O	2.23	0.41
59:Ta:72:ARG:NH1	86:Ta:401:HOH:O	2.54	0.41
66:Ya:140:ALA:HB2	75:h1:1180:G:O2'	2.21	0.41
72:Aa:31:ARG:NH1	75:h1:334:U:OP1	2.41	0.41
75:h1:1567:C:H2'	75:h1:1568:U:O4'	2.20	0.41
2:A:462:G:H5'	63:AQ:74:LYS:HE3	2.02	0.41
2:A:774:U:N3	54:AG:182:LEU:HD21	2.36	0.41
2:A:1469:A:H5'	9:AU:55:VAL:O	2.20	0.41
2:A:1493:A:OP2	86:A:3825:HOH:O	2.22	0.41
2:A:1686:U:O2'	2:A:1688:U:H1'	2.21	0.41
2:A:1729:G:N3	2:A:1729:G:H5'	2.35	0.41
2:A:1917:A:H5'	49:AK:82:LYS:O	2.21	0.41
2:A:2503:U:H2'	2:A:2504:A:C8	2.56	0.41
2:A:2618:OMG:HM23	2:A:2618:OMG:H1'	1.81	0.41
2:A:2913:G:O2'	2:A:2933:A2M:N1	2.53	0.41
2:A:3114:G:N3	2:A:3114:G:H2'	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3317:A:H4'	22:BS:370:GLY:HA3	2.03	0.41
3:i:2:47:U:H3'	3:i:2:48:C:C5'	2.51	0.41
10:Ma:21:ILE:HD12	10:Ma:21:ILE:C	2.46	0.41
10:Ma:58:VAL:HG11	65:Ua:27:PHE:HZ	1.86	0.41
14:AP:24:VAL:C	14:AP:43:VAL:HG13	2.46	0.41
27:BT:365:LYS:HD3	27:BT:367:VAL:HB	2.03	0.41
42:BU:110:GLU:OE2	58:Wa:108:ARG:NH2	2.53	0.41
59:Ta:79:ARG:HG2	59:Ta:86:GLY:HA3	2.03	0.41
60:AZ:11:PHE:CZ	60:AZ:34:PHE:HB3	2.55	0.41
62:Za:95:ALA:HB2	62:Za:102:ALA:HB2	2.02	0.41
66:Ya:57:LYS:CB	66:Ya:58:PRO:HD3	2.51	0.41
67:BB:113:ASP:O	67:BB:114:THR:C	2.64	0.41
75:h1:1260:C:H2'	75:h1:1261:OMU:H6	2.03	0.41
2:A:1137:U:H2'	2:A:1138:A:O4'	2.21	0.41
2:A:2260:A:N1	75:h1:1762:U:O2'	2.47	0.41
2:A:2852:G:O2'	46:BJ:158:LYS:O	2.36	0.41
4:C3:28:C:OP1	42:BU:139:ARG:HD3	2.20	0.41
13:AX:44:ARG:HB2	86:AX:221:HOH:O	2.21	0.41
32:BH:130:LYS:HE3	32:BH:140:TYR:CZ	2.55	0.41
53:AA:76:ARG:HA	78:AI:22:PHE:CZ	2.56	0.41
53:AA:142:LEU:HD23	53:AA:182:LEU:HD11	2.02	0.41
59:Ta:12:CYS:HB3	59:Ta:126:LEU:HA	2.02	0.41
60:AZ:11:PHE:CE2	60:AZ:36:VAL:CG2	3.04	0.41
75:h1:627:C:O2	75:h1:975:A2M:N1	2.54	0.41
75:h1:1147:G:C6	75:h1:1148:A:C6	3.09	0.41
2:A:418:G:O6	2:A:2381:C:O2'	2.39	0.40
2:A:976:A:OP1	41:Ha:47:LYS:NZ	2.47	0.40
2:A:1356:G:H5''	27:BT:312:LYS:HD2	2.03	0.40
4:C3:111:U:H2'	4:C3:112:U:O4'	2.21	0.40
10:Ma:47:GLN:HA	10:Ma:50:ILE:HD12	2.03	0.40
59:Ta:7:ASN:HB3	59:Ta:12:CYS:SG	2.61	0.40
61:BE:30:GLU:O	61:BE:34:HIS:ND1	2.54	0.40
75:h1:1742:U:H2'	75:h1:1743:C:C6	2.57	0.40
75:h1:1766:A:O2'	75:h1:1787:C:H5'	2.21	0.40
2:A:1419:C:O2'	28:AV:96:GLU:OE1	2.33	0.40
2:A:1611:G:H2'	2:A:1612:G:O4'	2.20	0.40
2:A:3321:U:H4'	2:A:3322:A:H5'	2.03	0.40
15:Ja:66:MET:HG3	75:h1:456:A:O4'	2.22	0.40
24:AC:137:VAL:HG11	24:AC:182:PHE:HA	2.03	0.40
39:BG:127:LYS:NZ	86:BG:306:HOH:O	2.52	0.40
57:AF:42:GLN:HB3	57:AF:43:PRO:HD3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:AQ:94:PHE:N	63:AQ:95:PRO:CD	2.84	0.40
67:BB:5:ARG:O	67:BB:10:LYS:NZ	2.55	0.40
69:Ra:116:ASN:OD1	69:Ra:117:ARG:NH1	2.45	0.40
75:h1:1352:U:H2'	75:h1:1353:A:C8	2.56	0.40
2:A:693:A:N6	2:A:709:C:H2'	2.36	0.40
2:A:1421:G:H5''	28:AV:125:ALA:HB2	2.04	0.40
2:A:2860:U:H2'	2:A:2861:U:O4'	2.22	0.40
2:A:2881:U:H2'	2:A:2882:OMU:O4'	2.20	0.40
2:A:3191:C:H2'	2:A:3192:U:C6	2.57	0.40
15:Ja:104:ASP:OD1	15:Ja:110:ARG:HG3	2.21	0.40
16:Ea:68:ARG:HG2	16:Ea:126:THR:C	2.46	0.40
22:BS:56:ILE:HD12	22:BS:56:ILE:C	2.47	0.40
28:AV:65:ARG:O	28:AV:66:HIS:HB2	2.21	0.40
53:AA:27:ARG:NH2	75:h1:1439:A:OP1	2.54	0.40
57:AF:46:LEU:HB3	57:AF:80:VAL:HG21	2.03	0.40
67:BB:26:LEU:HD23	67:BB:58:MET:HB3	2.02	0.40
70:BL:15:PHE:CZ	70:BL:132:LEU:HD23	2.56	0.40
75:h1:1286:U:H4'	75:h1:1287:U:O4'	2.21	0.40
2:A:352:A:N1	27:BT:89:THR:CG2	2.85	0.40
2:A:1394:U:H4'	63:AQ:18:CYS:SG	2.62	0.40
2:A:2257:A:H2'	2:A:2258:PSU:O4'	2.22	0.40
2:A:2984:C:H2'	2:A:2985:U:O4'	2.22	0.40
23:AM:5:HIS:HD2	86:AM:374:HOH:O	2.04	0.40
28:AV:33:TRP:CZ2	28:AV:54:PRO:HD2	2.56	0.40
42:BU:55:THR:HG23	42:BU:62:ARG:HA	2.03	0.40
43:BR:136:GLU:HB3	43:BR:137:PRO:HD3	2.03	0.40
51:AB:136:ILE:O	51:AB:142:LEU:HD12	2.20	0.40
75:h1:522:A:H2'	75:h1:523:A:C8	2.56	0.40
2:A:1581:A:N3	2:A:1581:A:H2'	2.36	0.40
9:AU:33:ALA:HA	9:AU:71:PRO:HG3	2.04	0.40
9:AU:56:ASP:HB2	9:AU:98:THR:HG22	2.03	0.40
15:Ja:107:GLY:O	15:Ja:189:ARG:HD2	2.21	0.40
19:Ka:7:THR:HB	19:Ka:29:LEU:HB2	2.04	0.40
19:Ka:55:ASN:HB3	19:Ka:98:LEU:HD21	2.03	0.40
45:BV:179:CYS:SG	45:BV:187:LYS:HE3	2.61	0.40
46:BJ:139:ARG:HB2	46:BJ:173:PHE:CZ	2.56	0.40
58:Wa:11:HIS:O	58:Wa:22:GLY:N	2.47	0.40
58:Wa:88:LYS:HG2	66:Ya:23:ARG:HD2	2.03	0.40
67:BB:57:LEU:HD13	67:BB:69:ILE:HD11	2.03	0.40
75:h1:96:G:HO2'	75:h1:462:A:HO2'	1.56	0.40
75:h1:392:G:N7	75:h1:409:A:N1	2.70	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	
5	BC	23/25 (92%)	23 (100%)	0	0	100	100
6	BM	153/176 (87%)	149 (97%)	4 (3%)	0	100	100
7	BO	123/146 (84%)	122 (99%)	1 (1%)	0	100	100
8	AR	49/83 (59%)	45 (92%)	3 (6%)	1 (2%)	6	1
9	AU	107/119 (90%)	105 (98%)	2 (2%)	0	100	100
10	Ma	96/131 (73%)	93 (97%)	3 (3%)	0	100	100
11	Ia	188/194 (97%)	185 (98%)	3 (2%)	0	100	100
12	AE	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
13	AX	95/112 (85%)	94 (99%)	0	1 (1%)	11	4
14	AP	132/135 (98%)	127 (96%)	5 (4%)	0	100	100
15	Ja	256/262 (98%)	247 (96%)	6 (2%)	3 (1%)	10	3
16	Ea	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
17	AL	173/217 (80%)	170 (98%)	3 (2%)	0	100	100
18	Va	137/142 (96%)	133 (97%)	4 (3%)	0	100	100
19	Ka	118/133 (89%)	111 (94%)	7 (6%)	0	100	100
20	AW	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
21	BD	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
22	BS	383/389 (98%)	377 (98%)	6 (2%)	0	100	100
23	AM	161/164 (98%)	158 (98%)	3 (2%)	0	100	100
24	AC	213/284 (75%)	210 (99%)	3 (1%)	0	100	100
25	BI	129/140 (92%)	126 (98%)	3 (2%)	0	100	100
26	AH	126/134 (94%)	125 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	BT	389/406 (96%)	380 (98%)	9 (2%)	0	100	100
28	AV	124/133 (93%)	122 (98%)	2 (2%)	0	100	100
29	AD	180/207 (87%)	169 (94%)	10 (6%)	1 (1%)	21	11
30	AJ	184/187 (98%)	178 (97%)	6 (3%)	0	100	100
31	BQ	244/258 (95%)	235 (96%)	9 (4%)	0	100	100
32	BH	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
33	Da	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
34	BK	279/301 (93%)	273 (98%)	5 (2%)	1 (0%)	30	19
35	AT	92/112 (82%)	92 (100%)	0	0	100	100
36	Pa	45/62 (73%)	43 (96%)	2 (4%)	0	100	100
37	BP	118/123 (96%)	116 (98%)	2 (2%)	0	100	100
38	BN	115/154 (75%)	115 (100%)	0	0	100	100
39	BG	232/256 (91%)	224 (97%)	6 (3%)	2 (1%)	14	5
40	Fa	109/120 (91%)	108 (99%)	1 (1%)	0	100	100
41	Ha	143/146 (98%)	137 (96%)	5 (4%)	1 (1%)	18	8
42	BU	167/182 (92%)	165 (99%)	2 (1%)	0	100	100
43	BR	230/247 (93%)	226 (98%)	4 (2%)	0	100	100
44	Xa	144/160 (90%)	138 (96%)	5 (4%)	1 (1%)	18	8
45	BV	210/262 (80%)	204 (97%)	6 (3%)	0	100	100
46	BJ	203/221 (92%)	197 (97%)	6 (3%)	0	100	100
47	AO	60/164 (37%)	59 (98%)	1 (2%)	0	100	100
48	BW	71/82 (87%)	70 (99%)	0	1 (1%)	9	2
49	AK	176/214 (82%)	175 (99%)	1 (1%)	0	100	100
50	Na	81/86 (94%)	70 (86%)	11 (14%)	0	100	100
51	AB	178/197 (90%)	173 (97%)	5 (3%)	0	100	100
52	BF	184/233 (79%)	177 (96%)	7 (4%)	0	100	100
53	AA	206/250 (82%)	194 (94%)	10 (5%)	2 (1%)	12	4
54	AG	201/206 (98%)	196 (98%)	5 (2%)	0	100	100
55	Ga	49/128 (38%)	48 (98%)	1 (2%)	0	100	100
56	BA	48/51 (94%)	48 (100%)	0	0	100	100
57	AF	136/146 (93%)	127 (93%)	8 (6%)	1 (1%)	18	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	Wa	137/152 (90%)	133 (97%)	3 (2%)	1 (1%)	18	8
59	Ta	223/249 (90%)	203 (91%)	16 (7%)	4 (2%)	6	1
60	AZ	66/69 (96%)	61 (92%)	5 (8%)	0	100	100
61	BE	88/92 (96%)	83 (94%)	4 (4%)	1 (1%)	11	4
62	Za	196/298 (66%)	190 (97%)	6 (3%)	0	100	100
63	AQ	134/143 (94%)	123 (92%)	10 (8%)	1 (1%)	18	8
64	Oa	57/64 (89%)	57 (100%)	0	0	100	100
65	Ua	125/150 (83%)	120 (96%)	3 (2%)	2 (2%)	7	2
66	Ya	127/150 (85%)	118 (93%)	6 (5%)	3 (2%)	4	0
67	BB	117/141 (83%)	108 (92%)	7 (6%)	2 (2%)	7	1
68	AN	97/124 (78%)	90 (93%)	6 (6%)	1 (1%)	12	4
69	Ra	182/190 (96%)	163 (90%)	18 (10%)	1 (0%)	24	14
70	BL	134/143 (94%)	133 (99%)	1 (1%)	0	100	100
71	La	69/108 (64%)	67 (97%)	2 (3%)	0	100	100
72	Aa	181/222 (82%)	176 (97%)	5 (3%)	0	100	100
73	AY	85/95 (90%)	83 (98%)	1 (1%)	1 (1%)	10	3
74	Ca	53/56 (95%)	53 (100%)	0	0	100	100
77	Ba	99/122 (81%)	97 (98%)	2 (2%)	0	100	100
78	AI	90/177 (51%)	87 (97%)	3 (3%)	0	100	100
All	All	10403/11933 (87%)	10077 (97%)	294 (3%)	32 (0%)	37	26

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	Ja	151	ASP
34	BK	261	LYS
39	BG	218	ASP
59	Ta	14	LYS
59	Ta	139	ARG
67	BB	111	MET
8	AR	20	GLY
44	Xa	56	ASP
65	Ua	137	ASP
66	Ya	57	LYS
67	BB	94	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	Ja	3	ARG
59	Ta	151	LYS
13	AX	16	LYS
29	AD	79	HIS
48	BW	80	LYS
57	AF	68	ARG
61	BE	18	TYR
66	Ya	79	ALA
68	AN	76	GLN
69	Ra	48	GLN
73	AY	87	ARG
15	Ja	150	PRO
53	AA	5	ILE
58	Wa	11	HIS
63	AQ	21	VAL
65	Ua	149	ARG
39	BG	117	PRO
66	Ya	135	ARG
41	Ha	15	VAL
53	AA	43	PRO
59	Ta	42	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	BC	24/24 (100%)	24 (100%)	0	100	100
6	BM	131/148 (88%)	130 (99%)	1 (1%)	73	67
7	BO	116/133 (87%)	116 (100%)	0	100	100
8	AR	44/71 (62%)	44 (100%)	0	100	100
9	AU	96/105 (91%)	95 (99%)	1 (1%)	68	60
10	Ma	87/110 (79%)	87 (100%)	0	100	100
11	Ia	171/175 (98%)	171 (100%)	0	100	100
12	AE	111/112 (99%)	109 (98%)	2 (2%)	51	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	AX	84/94 (89%)	83 (99%)	1 (1%)	63	54
14	AP	116/117 (99%)	116 (100%)	0	100	100
15	Ja	225/227 (99%)	223 (99%)	2 (1%)	70	62
16	Ea	180/180 (100%)	179 (99%)	1 (1%)	78	74
17	AL	161/198 (81%)	159 (99%)	2 (1%)	63	54
18	Va	111/114 (97%)	110 (99%)	1 (1%)	70	62
19	Ka	104/114 (91%)	102 (98%)	2 (2%)	50	37
20	AW	97/98 (99%)	97 (100%)	0	100	100
21	BD	87/93 (94%)	87 (100%)	0	100	100
22	BS	326/329 (99%)	326 (100%)	0	100	100
23	AM	137/138 (99%)	137 (100%)	0	100	100
24	AC	183/225 (81%)	180 (98%)	3 (2%)	55	44
25	BI	104/110 (94%)	104 (100%)	0	100	100
26	AH	112/117 (96%)	112 (100%)	0	100	100
27	BT	323/331 (98%)	316 (98%)	7 (2%)	45	30
28	AV	114/121 (94%)	114 (100%)	0	100	100
29	AD	156/171 (91%)	152 (97%)	4 (3%)	40	23
30	AJ	157/158 (99%)	156 (99%)	1 (1%)	78	74
31	BQ	192/197 (98%)	191 (100%)	1 (0%)	81	77
32	BH	176/177 (99%)	176 (100%)	0	100	100
33	Da	132/133 (99%)	131 (99%)	1 (1%)	73	67
34	BK	238/254 (94%)	237 (100%)	1 (0%)	84	81
35	AT	81/97 (84%)	81 (100%)	0	100	100
36	Pa	40/49 (82%)	40 (100%)	0	100	100
37	BP	108/110 (98%)	108 (100%)	0	100	100
38	BN	108/136 (79%)	107 (99%)	1 (1%)	70	62
39	BG	200/219 (91%)	197 (98%)	3 (2%)	57	46
40	Fa	97/104 (93%)	97 (100%)	0	100	100
41	Ha	120/121 (99%)	119 (99%)	1 (1%)	73	67
42	BU	147/158 (93%)	145 (99%)	2 (1%)	59	49
43	BR	199/212 (94%)	198 (100%)	1 (0%)	81	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	Xa	124/135 (92%)	123 (99%)	1 (1%)	73	67
45	BV	187/226 (83%)	184 (98%)	3 (2%)	55	44
46	BJ	170/179 (95%)	168 (99%)	2 (1%)	63	54
47	AO	58/137 (42%)	58 (100%)	0	100	100
48	BW	60/68 (88%)	59 (98%)	1 (2%)	53	41
49	AK	158/181 (87%)	156 (99%)	2 (1%)	61	50
50	Na	76/78 (97%)	74 (97%)	2 (3%)	40	23
51	AB	161/172 (94%)	161 (100%)	0	100	100
52	BF	157/194 (81%)	157 (100%)	0	100	100
53	AA	174/207 (84%)	172 (99%)	2 (1%)	65	56
54	AG	174/177 (98%)	172 (99%)	2 (1%)	65	56
55	Ga	47/114 (41%)	47 (100%)	0	100	100
56	BA	47/48 (98%)	47 (100%)	0	100	100
57	AF	117/123 (95%)	116 (99%)	1 (1%)	70	62
58	Wa	121/132 (92%)	117 (97%)	4 (3%)	33	15
59	Ta	193/213 (91%)	189 (98%)	4 (2%)	47	32
60	AZ	64/65 (98%)	63 (98%)	1 (2%)	55	44
61	BE	72/73 (99%)	71 (99%)	1 (1%)	59	49
62	Za	166/228 (73%)	166 (100%)	0	100	100
63	AQ	116/122 (95%)	116 (100%)	0	100	100
64	Oa	52/57 (91%)	50 (96%)	2 (4%)	29	11
65	Ua	100/121 (83%)	100 (100%)	0	100	100
66	Ya	110/126 (87%)	109 (99%)	1 (1%)	70	62
67	BB	108/122 (88%)	108 (100%)	0	100	100
68	AN	88/104 (85%)	88 (100%)	0	100	100
69	Ra	165/169 (98%)	161 (98%)	4 (2%)	43	27
70	BL	110/113 (97%)	108 (98%)	2 (2%)	51	39
71	La	61/92 (66%)	61 (100%)	0	100	100
72	Aa	158/183 (86%)	155 (98%)	3 (2%)	50	37
73	AY	73/78 (94%)	73 (100%)	0	100	100
74	Ca	47/48 (98%)	47 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	Ba	93/110 (84%)	90 (97%)	3 (3%)	34	16
78	AI	87/139 (63%)	87 (100%)	0	100	100
All	All	9089/10114 (90%)	9009 (99%)	80 (1%)	68	62

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	BM	24	VAL
9	AU	90	LYS
12	AE	20	ARG
12	AE	74	VAL
13	AX	22	ARG
15	Ja	133	GLN
15	Ja	156	PRO
16	Ea	104	GLU
17	AL	26	ILE
17	AL	47	LEU
18	Va	28	LYS
19	Ka	60	PHE
19	Ka	76	LEU
24	AC	58	VAL
24	AC	130	VAL
24	AC	138	THR
27	BT	16	ASP
27	BT	222	LYS
27	BT	297	ARG
27	BT	332	LEU
27	BT	357	LYS
27	BT	380	LYS
27	BT	394	GLU
29	AD	23	THR
29	AD	122	ARG
29	AD	178	ILE
29	AD	197	GLU
30	AJ	75	ASP
31	BQ	208	GLU
33	Da	93	LYS
34	BK	282	GLU
38	BN	133	LYS
39	BG	116	LYS
39	BG	140	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	BG	217	ASN
41	Ha	60	TYR
42	BU	15	LYS
42	BU	46	THR
43	BR	100	ILE
44	Xa	119	LYS
45	BV	46	THR
45	BV	48	VAL
45	BV	143	THR
46	BJ	43	VAL
46	BJ	196	ASN
48	BW	61	GLN
49	AK	171	GLU
49	AK	174	HIS
50	Na	10	LEU
50	Na	48	VAL
53	AA	42	THR
53	AA	62	LYS
54	AG	68	VAL
54	AG	70	THR
57	AF	105	LYS
58	Wa	13	LEU
58	Wa	43	ILE
58	Wa	84	LEU
58	Wa	92	ASP
59	Ta	10	THR
59	Ta	31	ARG
59	Ta	81	THR
59	Ta	134	MET
60	AZ	36	VAL
61	BE	52	VAL
64	Oa	45	VAL
64	Oa	58	ARG
66	Ya	39	VAL
69	Ra	40	GLU
69	Ra	41	LEU
69	Ra	50	VAL
69	Ra	97	THR
70	BL	31	LEU
70	BL	123	LYS
72	Aa	45	ARG
72	Aa	138	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
72	Aa	150	GLN
77	Ba	35	LEU
77	Ba	52	ARG
77	Ba	100	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
6	BM	28	ASN
8	AR	6	ASN
8	AR	10	HIS
8	AR	19	ASN
8	AR	27	HIS
10	Ma	72	GLN
11	Ia	101	HIS
11	Ia	105	ASN
12	AE	98	GLN
15	Ja	67	GLN
15	Ja	96	ASN
15	Ja	133	GLN
15	Ja	157	ASN
15	Ja	201	HIS
16	Ea	15	GLN
17	AL	8	GLN
18	Va	72	GLN
18	Va	96	ASN
19	Ka	12	ASN
19	Ka	83	ASN
20	AW	36	GLN
20	AW	43	GLN
20	AW	47	ASN
27	BT	13	GLN
28	AV	78	HIS
31	BQ	21	HIS
32	BH	18	HIS
33	Da	105	ASN
34	BK	251	ASN
36	Pa	40	HIS
37	BP	7	HIS
37	BP	98	HIS
39	BG	143	GLN
39	BG	253	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	Fa	100	GLN
42	BU	22	ASN
42	BU	64	ASN
43	BR	118	ASN
43	BR	191	HIS
44	Xa	33	ASN
44	Xa	38	ASN
44	Xa	93	HIS
44	Xa	123	HIS
46	BJ	73	ASN
46	BJ	149	GLN
47	AO	60	GLN
49	AK	39	GLN
50	Na	40	GLN
51	AB	3	ASN
51	AB	83	ASN
51	AB	112	GLN
52	BF	41	ASN
53	AA	22	ASN
53	AA	162	GLN
54	AG	113	GLN
54	AG	147	GLN
55	Ga	104	HIS
55	Ga	117	HIS
59	Ta	7	ASN
59	Ta	65	GLN
59	Ta	78	HIS
59	Ta	148	ASN
62	Za	96	GLN
62	Za	101	ASN
64	Oa	25	GLN
66	Ya	109	GLN
66	Ya	119	HIS
68	AN	105	ASN
69	Ra	48	GLN
71	La	39	ASN
72	Aa	65	ASN
73	AY	83	GLN
74	Ca	46	ASN
78	AI	7	ASN
78	AI	28	ASN
78	AI	39	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	161/164 (98%)	20 (12%)	2 (1%)
2	A	3142/3385 (92%)	410 (13%)	51 (1%)
3	W2	75/76 (98%)	15 (20%)	1 (1%)
3	i2	75/76 (98%)	15 (20%)	0
4	C3	118/121 (97%)	6 (5%)	1 (0%)
75	h1	1604/1805 (88%)	238 (14%)	0
76	B1	11/12 (91%)	2 (18%)	0
All	All	5186/5639 (91%)	706 (13%)	55 (1%)

All (706) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	6	G
1	3	38	U
1	3	39	C
1	3	63	A
1	3	66	C
1	3	67	U
1	3	85	U
1	3	86	C
1	3	88	C
1	3	89	G
1	3	90	U
1	3	91	G
1	3	99	G
1	3	100	A
1	3	109	A
1	3	110	C
1	3	129	C
1	3	132	C
1	3	134	G
1	3	157	U
2	A	3	G
2	A	5	C
2	A	11	G
2	A	12	U
2	A	38	A
2	A	41	A
2	A	42	PSU
2	A	47	A
2	A	58	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	63	A
2	A	64	A
2	A	72	A
2	A	84	G
2	A	90	G
2	A	97	A
2	A	114	C
2	A	120	A
2	A	129	U
2	A	131	U
2	A	132	U
2	A	133	C
2	A	134	G
2	A	148	A
2	A	154	G
2	A	155	A
2	A	161	G
2	A	163	C
2	A	167	A
2	A	168	G
2	A	187	U
2	A	197	A
2	A	215	G
2	A	216	A
2	A	245	A
2	A	248	A
2	A	262	A
2	A	263	C
2	A	280	G
2	A	281	A
2	A	283	U
2	A	292	A
2	A	293	A
2	A	326	G
2	A	346	A
2	A	347	C
2	A	350	G
2	A	373	G
2	A	394	A
2	A	395	G
2	A	396	A
2	A	398	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	399	G
2	A	417	G
2	A	418	G
2	A	419	A
2	A	430	G
2	A	436	C
2	A	437	G
2	A	442	G
2	A	453	A
2	A	467	A
2	A	472	G
2	A	476	C
2	A	483	C
2	A	484	G
2	A	523	U
2	A	524	A
2	A	532	G
2	A	538	G
2	A	539	A
2	A	541	A
2	A	543	G
2	A	545	U
2	A	546	U
2	A	547	G
2	A	548	U
2	A	549	G
2	A	552	G
2	A	555	G
2	A	561	G
2	A	574	U
2	A	575	C
2	A	591	A
2	A	592	C
2	A	598	G
2	A	601	U
2	A	602	C
2	A	603	G
2	A	606	A
2	A	608	C
2	A	610	G
2	A	621	G
2	A	632	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	637	U
2	A	638	C
2	A	648	C
2	A	661	A2M
2	A	672	A
2	A	673	G
2	A	689	A
2	A	693	A
2	A	694	A
2	A	702	G
2	A	711	U
2	A	712	A
2	A	719	A
2	A	726	C
2	A	729	A
2	A	730	U
2	A	732	G
2	A	746	C
2	A	776	U
2	A	790	G
2	A	794	G
2	A	826	A2M
2	A	839	G
2	A	858	C
2	A	870	C
2	A	883	U
2	A	888	U
2	A	905	A
2	A	906	C
2	A	916	G
2	A	917	OMG
2	A	923	A
2	A	925	G
2	A	926	A
2	A	930	A
2	A	932	C
2	A	946	G
2	A	953	C
2	A	968	C
2	A	969	PSU
2	A	983	G
2	A	986	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	989	A
2	A	990	C
2	A	991	G
2	A	992	C
2	A	993	G
2	A	1004	G
2	A	1005	G
2	A	1012	C
2	A	1027	U
2	A	1035	G
2	A	1037	A
2	A	1039	C
2	A	1041	C
2	A	1042	C
2	A	1045	G
2	A	1046	A
2	A	1057	A
2	A	1074	A
2	A	1091	U
2	A	1092	U
2	A	1104	C
2	A	1105	G
2	A	1106	G
2	A	1107	A
2	A	1112	A
2	A	1126	G
2	A	1140	G
2	A	1162	A
2	A	1168	A
2	A	1183	G
2	A	1189	C
2	A	1190	U
2	A	1203	A
2	A	1211	C
2	A	1212	A
2	A	1219	G
2	A	1223	G
2	A	1293	C
2	A	1295	G
2	A	1297	A
2	A	1313	A
2	A	1314	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	1317	G
2	A	1319	U
2	A	1326	U
2	A	1327	A
2	A	1358	A
2	A	1359	A
2	A	1360	G
2	A	1361	A
2	A	1362	G
2	A	1363	C
2	A	1364	C
2	A	1408	A
2	A	1428	G
2	A	1443	G
2	A	1446	OMC
2	A	1455	A
2	A	1460	C
2	A	1461	A
2	A	1490	A
2	A	1492	G
2	A	1511	G
2	A	1545	G
2	A	1564	U
2	A	1568	A
2	A	1569	G
2	A	1575	A
2	A	1576	A
2	A	1581	A
2	A	1588	A
2	A	1590	A
2	A	1594	G
2	A	1621	C
2	A	1629	U
2	A	1645	G
2	A	1646	1MG
2	A	1657	C
2	A	1676	A
2	A	1692	G
2	A	1725	G
2	A	1744	G
2	A	1751	A
2	A	1752	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	1764	U
2	A	1766	G
2	A	1767	C
2	A	1768	G
2	A	1770	G
2	A	1799	A
2	A	1815	A
2	A	1816	G
2	A	1817	U
2	A	1818	G
2	A	1821	G
2	A	1823	U
2	A	1844	A
2	A	1845	OMC
2	A	1868	C
2	A	1880	G
2	A	1881	A
2	A	1882	U
2	A	1908	G
2	A	2091	A
2	A	2092	A
2	A	2095	G
2	A	2101	U
2	A	2110	G
2	A	2111	OMU
2	A	2121	G
2	A	2130	A
2	A	2139	U
2	A	2157	A
2	A	2208	G
2	A	2271	G
2	A	2277	A
2	A	2278	A
2	A	2305	G
2	A	2306	C
2	A	2308	U
2	A	2311	A
2	A	2313	G
2	A	2332	U
2	A	2333	G
2	A	2334	U
2	A	2370	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	2371	A
2	A	2372	C
2	A	2373	G
2	A	2391	G
2	A	2392	G
2	A	2395	A
2	A	2400	A
2	A	2401	G
2	A	2402	A
2	A	2409	U
2	A	2410	G
2	A	2437	A
2	A	2438	A
2	A	2441	A
2	A	2443	U
2	A	2446	A
2	A	2450	G
2	A	2451	U
2	A	2452	G
2	A	2453	U
2	A	2454	A
2	A	2455	G
2	A	2457	A
2	A	2458	U
2	A	2459	A
2	A	2460	A
2	A	2461	G
2	A	2495	U
2	A	2496	U
2	A	2497	U
2	A	2498	A
2	A	2499	A
2	A	2512	U
2	A	2513	A
2	A	2522	A
2	A	2550	U
2	A	2566	C
2	A	2573	G
2	A	2584	G
2	A	2590	G
2	A	2592	A
2	A	2605	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	2606	G
2	A	2613	G
2	A	2625	A
2	A	2635	A
2	A	2651	U
2	A	2655	A
2	A	2656	A
2	A	2673	A
2	A	2676	G
2	A	2680	U
2	A	2688	G
2	A	2689	G
2	A	2690	A
2	A	2693	A
2	A	2703	A
2	A	2713	G
2	A	2718	U
2	A	2728	U
2	A	2752	G
2	A	2761	A
2	A	2776	G
2	A	2777	G
2	A	2795	G
2	A	2798	A
2	A	2799	G
2	A	2800	A
2	A	2809	C
2	A	2816	A
2	A	2841	U
2	A	2844	A
2	A	2870	G
2	A	2886	A
2	A	2897	G
2	A	2898	C
2	A	2910	A2M
2	A	2922	PSU
2	A	2934	U
2	A	2935	A
2	A	2941	C
2	A	2946	G
2	A	2970	A
2	A	2971	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	2979	U
2	A	2989	G
2	A	2996	G
2	A	3010	A
2	A	3026	G
2	A	3028	G
2	A	3055	U
2	A	3056	C
2	A	3057	G
2	A	3076	G
2	A	3077	U
2	A	3090	C
2	A	3120	A
2	A	3128	A
2	A	3129	U
2	A	3140	A
2	A	3150	G
2	A	3152	G
2	A	3166	U
2	A	3167	G
2	A	3168	C
2	A	3172	C
2	A	3175	U
2	A	3181	G
2	A	3188	A
2	A	3189	G
2	A	3195	A
2	A	3202	C
2	A	3203	G
2	A	3205	G
2	A	3215	A
2	A	3218	U
2	A	3223	U
2	A	3224	U
2	A	3225	C
2	A	3226	G
2	A	3230	G
2	A	3231	A
2	A	3234	C
2	A	3242	G
2	A	3244	G
2	A	3248	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	3249	C
2	A	3251	U
2	A	3252	G
2	A	3263	A
2	A	3281	G
2	A	3291	C
2	A	3303	A
2	A	3304	U
2	A	3328	C
2	A	3332	G
2	A	3334	G
2	A	3338	U
2	A	3339	U
2	A	3341	C
2	A	3342	U
2	A	3343	G
2	A	3346	A
2	A	3356	G
2	A	3365	C
2	A	3369	U
2	A	3377	A
2	A	3379	G
2	A	3385	A
3	i2	2	C
3	i2	5	G
3	i2	6	G
3	i2	9	A
3	i2	17	U
3	i2	18	G
3	i2	20	G
3	i2	21	A
3	i2	22	G
3	i2	47	U
3	i2	48	C
3	i2	72	C
3	i2	73	A
3	i2	74	C
3	i2	76	A
4	C3	38	U
4	C3	42	A
4	C3	53	U
4	C3	54	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	C3	64	G
4	C3	110	G
75	h1	4	C
75	h1	17	C
75	h1	25	C
75	h1	26	A
75	h1	34	G
75	h1	42	G
75	h1	47	A
75	h1	56	U
75	h1	65	A
75	h1	68	A
75	h1	73	A
75	h1	75	U
75	h1	82	G
75	h1	83	U
75	h1	84	G
75	h1	101	A
75	h1	105	A
75	h1	115	A
75	h1	123	OMU
75	h1	127	G
75	h1	128	G
75	h1	129	U
75	h1	130	A
75	h1	132	C
75	h1	133	U
75	h1	135	C
75	h1	136	U
75	h1	139	U
75	h1	140	C
75	h1	151	A
75	h1	158	C
75	h1	174	C
75	h1	175	A
75	h1	176	A
75	h1	186	A
75	h1	189	U
75	h1	190	A
75	h1	191	U
75	h1	192	G
75	h1	193	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
75	h1	194	A
75	h1	214	A
75	h1	250	U
75	h1	251	C
75	h1	258	A
75	h1	263	A
75	h1	266	G
75	h1	272	A
75	h1	273	U
75	h1	276	C
75	h1	289	G
75	h1	316	C
75	h1	318	A
75	h1	322	U
75	h1	324	G
75	h1	335	A
75	h1	339	G
75	h1	340	C
75	h1	363	C
75	h1	372	A
75	h1	380	A
75	h1	382	U
75	h1	383	C
75	h1	402	A
75	h1	403	A
75	h1	404	C
75	h1	426	C
75	h1	427	A
75	h1	428	G
75	h1	436	G
75	h1	441	U
75	h1	446	C
75	h1	470	A
75	h1	479	A
75	h1	503	U
75	h1	509	U
75	h1	512	G
75	h1	517	A
75	h1	521	C
75	h1	536	A
75	h1	540	A
75	h1	544	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
75	h1	559	G
75	h1	561	C
75	h1	567	C
75	h1	580	OMU
75	h1	581	A
75	h1	583	PSU
75	h1	584	U
75	h1	585	C
75	h1	596	A
75	h1	597	OMG
75	h1	608	A
75	h1	621	A2M
75	h1	622	A
75	h1	624	A
75	h1	625	A
75	h1	626	G
75	h1	636	G
75	h1	641	U
75	h1	758	A
75	h1	759	A
75	h1	768	G
75	h1	769	C
75	h1	778	A2M
75	h1	781	C
75	h1	783	A
75	h1	784	C
75	h1	785	G
75	h1	789	U
75	h1	792	A
75	h1	815	A
75	h1	816	U
75	h1	817	A
75	h1	826	A
75	h1	830	U
75	h1	831	A
75	h1	833	U
75	h1	847	G
75	h1	857	A
75	h1	864	A
75	h1	865	C
75	h1	887	U
75	h1	934	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
75	h1	936	U
75	h1	945	A
75	h1	946	U
75	h1	952	A
75	h1	960	U
75	h1	961	U
75	h1	967	A
75	h1	1005	U
75	h1	1006	A
75	h1	1027	A
75	h1	1029	C
75	h1	1033	G
75	h1	1040	A
75	h1	1060	U
75	h1	1061	A
75	h1	1062	U
75	h1	1082	A
75	h1	1084	G
75	h1	1088	A
75	h1	1093	A
75	h1	1098	U
75	h1	1110	G
75	h1	1139	A
75	h1	1151	G
75	h1	1159	C
75	h1	1160	C
75	h1	1168	G
75	h1	1186	U
75	h1	1187	U
75	h1	1192	C4J
75	h1	1193	C
75	h1	1195	A
75	h1	1197	A
75	h1	1200	G
75	h1	1201	G
75	h1	1203	A
75	h1	1218	A
75	h1	1219	G
75	h1	1232	OMU
75	h1	1244	G
75	h1	1245	A
75	h1	1246	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
75	h1	1247	C
75	h1	1252	U
75	h1	1253	C
75	h1	1257	A
75	h1	1266	G
75	h1	1270	OMU
75	h1	1315	U
75	h1	1316	U
75	h1	1322	A
75	h1	1362	C
75	h1	1363	A
75	h1	1364	U
75	h1	1373	G
75	h1	1379	C
75	h1	1393	U
75	h1	1394	A
75	h1	1401	U
75	h1	1402	U
75	h1	1416	U
75	h1	1417	U
75	h1	1418	U
75	h1	1430	A
75	h1	1431	OMG
75	h1	1434	C
75	h1	1435	U
75	h1	1438	G
75	h1	1449	A
75	h1	1462	C
75	h1	1463	A
75	h1	1474	A
75	h1	1485	C
75	h1	1514	G
75	h1	1517	U
75	h1	1519	A
75	h1	1524	U
75	h1	1526	A
75	h1	1539	A
75	h1	1559	U
75	h1	1560	U
75	h1	1561	G
75	h1	1576	G
75	h1	1577	G7M

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
75	h1	1585	A
75	h1	1592	G
75	h1	1603	G
75	h1	1609	G
75	h1	1613	A
75	h1	1636	C
75	h1	1653	A
75	h1	1660	G
75	h1	1666	U
75	h1	1669	G
75	h1	1680	C
75	h1	1682	G
75	h1	1684	U
75	h1	1686	G
75	h1	1741	A
75	h1	1759	A
75	h1	1764	G
75	h1	1770	A
75	h1	1772	G
75	h1	1773	U
75	h1	1784	G
75	h1	1786	MA6
75	h1	1787	C
75	h1	1796	G
75	h1	1797	G
75	h1	1798	A
75	h1	1799	U
75	h1	1800	C
75	h1	1803	U
75	h1	1804	G
76	B1	19	U
76	B1	29	U
3	W2	3	G
3	W2	4	G
3	W2	5	G
3	W2	6	G
3	W2	8	U
3	W2	17	U
3	W2	18	G
3	W2	19	G
3	W2	20	G
3	W2	21	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	W2	22	G
3	W2	48	C
3	W2	70	C
3	W2	71	G
3	W2	76	A

All (55) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3	99	G
1	3	109	A
2	A	11	G
2	A	91	C
2	A	262	A
2	A	280	G
2	A	292	A
2	A	394	A
2	A	547	G
2	A	554	C
2	A	570	G
2	A	591	A
2	A	602	C
2	A	609	A
2	A	637	U
2	A	673	G
2	A	693	A
2	A	882	C
2	A	905	A
2	A	925	G
2	A	990	C
2	A	992	C
2	A	1004	G
2	A	1026	A
2	A	1313	A
2	A	1326	U
2	A	1460	C
2	A	1476	A
2	A	1606	A
2	A	1643	A
2	A	1645	G
2	A	1848	OMC
2	A	1881	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	2207	U
2	A	2304	C
2	A	2370	A
2	A	2372	C
2	A	2496	U
2	A	2592	A
2	A	2643	C
2	A	2655	A
2	A	2688	G
2	A	2713	G
2	A	2727	G
2	A	2897	G
2	A	3055	U
2	A	3119	U
2	A	3166	U
2	A	3179	U
2	A	3225	C
2	A	3230	G
2	A	3247	G
2	A	3303	A
4	C3	109	U
3	W2	70	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PSU	A	2134	2	18,21,22	0.88	1 (5%)	21,30,33	0.80	0
75	A2M	h1	1754	75	22,25,26	0.20	0	30,36,39	0.62	0
75	OMC	h1	416	75	19,22,23	0.28	0	25,31,34	0.55	0
2	PSU	A	1015	81,2	18,21,22	0.93	1 (5%)	21,30,33	0.70	0
2	OMU	A	2882	2	19,22,23	0.24	0	25,31,34	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	A	3290	2,80	23,26,27	0.35	0	32,38,41	0.74	2 (6%)
75	PSU	h1	761	75	18,21,22	0.94	1 (5%)	21,30,33	0.83	0
2	A2M	A	816	2	22,25,26	0.29	0	30,36,39	0.73	0
2	A2M	A	1458	2,80	22,25,26	0.29	0	30,36,39	0.61	0
75	OMG	h1	1272	81,75	23,26,27	0.31	0	32,38,41	0.46	0
2	UR3	A	2952	81,2	19,22,23	0.35	0	26,32,35	0.76	1 (3%)
2	OMC	A	2335	2	19,22,23	0.32	0	25,31,34	0.59	0
2	OMU	A	144	81,2	19,22,23	0.33	0	25,31,34	0.37	0
55	MLY	Ga	113	55	9,10,11	0.49	0	6,11,13	0.36	0
75	PSU	h1	1182	75	18,21,22	0.99	1 (5%)	21,30,33	0.85	0
75	A2M	h1	1327	75	22,25,26	0.20	0	30,36,39	0.40	0
2	PSU	A	2853	2	18,21,22	0.89	1 (5%)	21,30,33	0.77	0
2	OMC	A	2363	2	19,22,23	0.31	0	25,31,34	0.56	0
75	A2M	h1	621	75,80	22,25,26	0.29	0	30,36,39	0.73	0
75	PSU	h1	1783	75	18,21,22	1.08	1 (5%)	21,30,33	0.88	2 (9%)
2	PSU	A	2264	2	18,21,22	0.91	1 (5%)	21,30,33	0.72	0
2	OMG	A	1459	2,80	23,26,27	0.47	0	32,38,41	0.66	0
2	PSU	A	1133	2	18,21,22	0.87	1 (5%)	21,30,33	1.01	2 (9%)
1	A2M	3	47	1	22,25,26	0.24	0	30,36,39	0.72	1 (3%)
75	PSU	h1	948	75	18,21,22	0.98	1 (5%)	21,30,33	0.71	0
75	G7M	h1	1577	3,75	23,26,27	0.78	1 (4%)	34,39,42	0.57	1 (2%)
2	A2M	A	2212	2,80	22,25,26	0.22	0	30,36,39	0.69	1 (3%)
2	PSU	A	975	81,2	18,21,22	0.92	1 (5%)	21,30,33	0.87	0
2	PSU	A	150	81,2	18,21,22	0.97	1 (5%)	21,30,33	0.63	0
2	5MC	A	2869	81,2	19,22,23	0.85	1 (5%)	26,32,35	0.88	1 (3%)
75	4AC	h1	1281	75	21,24,25	0.37	0	28,34,37	0.63	0
1	PSU	3	78	1	18,21,22	1.03	1 (5%)	21,30,33	0.71	0
2	OMC	A	1848	2,80	19,22,23	0.29	0	25,31,34	0.50	0
75	A2M	h1	799	75	22,25,26	0.20	0	30,36,39	0.77	1 (3%)
2	PSU	A	2879	2	18,21,22	0.90	1 (5%)	21,30,33	0.79	0
2	PSU	A	2893	2	18,21,22	0.97	1 (5%)	21,30,33	0.84	0
75	PSU	h1	752	75	18,21,22	0.94	1 (5%)	21,30,33	0.72	0
75	PSU	h1	1104	75	18,21,22	0.88	1 (5%)	21,30,33	0.76	0
2	PSU	A	2256	2	18,21,22	0.94	1 (5%)	21,30,33	0.71	0
2	OMU	A	44	81,2	19,22,23	0.34	0	25,31,34	0.57	0
75	PSU	h1	121	75,80	18,21,22	0.85	1 (5%)	21,30,33	0.68	0
2	OMU	A	1066	2	19,22,23	0.30	0	25,31,34	0.74	0
2	1MG	A	1646	2	23,26,27	0.67	0	33,39,42	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	6MZ	h1	1767	81,75,80	22,25,26	0.35	0	29,36,39	0.72	0
2	PSU	A	969	2	18,21,22	0.88	1 (5%)	21,30,33	1.06	1 (4%)
2	OMC	A	2291	2	19,22,23	0.29	0	25,31,34	0.59	0
75	A2M	h1	778	75	22,25,26	0.19	0	30,36,39	0.42	0
2	PSU	A	2262	2	18,21,22	0.92	1 (5%)	21,30,33	0.80	0
75	PSU	h1	360	75	18,21,22	0.93	1 (5%)	21,30,33	0.79	0
2	OMC	A	2958	2,80	19,22,23	0.35	0	25,31,34	0.80	1 (4%)
2	PSU	A	277	2	18,21,22	1.03	1 (5%)	21,30,33	0.81	0
75	MA6	h1	1785	75	23,26,27	0.33	0	33,38,41	0.72	1 (3%)
75	PSU	h1	606	75	18,21,22	1.01	1 (5%)	21,30,33	0.74	0
2	A2M	A	1142	2	22,25,26	0.27	0	30,36,39	0.69	0
2	OMC	A	2947	2	19,22,23	0.32	0	25,31,34	0.51	0
2	PSU	A	3109	2	18,21,22	0.94	1 (5%)	21,30,33	0.97	0
2	A2M	A	945	2	22,25,26	0.32	0	30,36,39	0.88	1 (3%)
75	PSU	h1	1291	75	18,21,22	0.93	1 (5%)	21,30,33	0.69	0
2	OMU	A	2920	81,2	19,22,23	0.27	0	25,31,34	0.47	0
75	PSU	h1	1630	75	18,21,22	0.96	1 (5%)	21,30,33	0.75	0
2	A2M	A	2324	2	22,25,26	0.20	0	30,36,39	0.75	2 (6%)
2	OMC	A	1845	2	19,22,23	0.34	0	25,31,34	0.42	0
2	OMU	A	2345	2	19,22,23	0.32	0	25,31,34	0.51	0
75	A2M	h1	466	75	22,25,26	0.18	0	30,36,39	0.53	0
1	OMG	3	79	1	23,26,27	0.33	0	32,38,41	0.46	0
75	PSU	h1	415	75	18,21,22	0.93	1 (5%)	21,30,33	0.69	0
2	OMG	A	2650	2	23,26,27	0.35	0	32,38,41	0.52	0
2	OMU	A	2734	2,80	19,22,23	0.30	0	25,31,34	0.58	0
75	OMC	h1	38	75	19,22,23	0.29	0	25,31,34	0.62	0
2	PSU	A	228	2	18,21,22	0.96	1 (5%)	21,30,33	0.70	0
2	OMU	A	2408	81,2	19,22,23	0.30	0	25,31,34	0.35	0
75	PSU	h1	605	75	18,21,22	0.97	1 (5%)	21,30,33	0.79	0
2	OMG	A	2921	2	23,26,27	0.29	0	32,38,41	0.40	0
2	A2M	A	661	2	22,25,26	0.25	0	30,36,39	0.37	0
75	4AC	h1	1777	75	21,24,25	0.41	0	28,34,37	0.42	0
75	OMC	h1	471	75	19,22,23	0.29	0	25,31,34	0.55	0
2	OMG	A	2122	2	23,26,27	0.31	0	32,38,41	0.72	1 (3%)
2	PSU	A	2825	81,2	18,21,22	0.94	1 (5%)	21,30,33	0.71	0
1	OMG	3	155	2,1	23,26,27	0.34	0	32,38,41	0.36	0
75	PSU	h1	1188	75	18,21,22	0.89	1 (5%)	21,30,33	0.74	0
2	OMC	A	1478	2	19,22,23	0.32	0	25,31,34	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	A	2974	2	18,21,22	1.03	1 (5%)	21,30,33	1.00	2 (9%)
2	PSU	A	42	81,2	18,21,22	1.09	2 (11%)	21,30,33	1.06	3 (14%)
75	PSU	h1	337	81,75	18,21,22	0.93	1 (5%)	21,30,33	0.72	0
2	PSU	A	2430	2	18,21,22	0.84	1 (5%)	21,30,33	0.77	0
75	OMG	h1	390	81,75	23,26,27	0.33	0	32,38,41	0.54	0
75	A2M	h1	1575	75	22,25,26	0.24	0	30,36,39	0.64	1 (3%)
2	PSU	A	894	2	18,21,22	0.98	1 (5%)	21,30,33	0.94	0
75	PSU	h1	1000	75	18,21,22	0.94	1 (5%)	21,30,33	0.84	1 (4%)
2	OMU	A	2716	2	19,22,23	0.26	0	25,31,34	0.54	0
2	PSU	A	2258	2	18,21,22	0.92	1 (5%)	21,30,33	0.71	0
2	OMG	A	2286	2	23,26,27	0.33	0	32,38,41	0.32	0
2	OMC	A	2835	2	19,22,23	0.30	0	25,31,34	0.59	0
75	A2M	h1	543	75	22,25,26	0.23	0	30,36,39	0.62	0
2	PSU	A	2954	2	18,21,22	1.03	1 (5%)	21,30,33	0.81	1 (4%)
75	PSU	h1	468	75	18,21,22	1.00	1 (5%)	21,30,33	0.76	0
75	OMU	h1	1270	75,80	19,22,23	0.23	0	25,31,34	0.59	0
2	PSU	A	685	2	18,21,22	1.07	1 (5%)	21,30,33	0.91	1 (4%)
75	PSU	h1	1215	75	18,21,22	0.94	1 (5%)	21,30,33	0.64	0
75	PSU	h1	1302	75	18,21,22	0.92	1 (5%)	21,30,33	0.77	0
2	PSU	A	2922	2	18,21,22	0.92	1 (5%)	21,30,33	0.79	0
75	PSU	h1	1306	75	18,21,22	0.94	1 (5%)	21,30,33	0.62	0
75	UY1	h1	602	75	19,22,23	1.01	1 (5%)	21,31,34	0.82	0
75	PSU	h1	583	75	18,21,22	0.99	1 (5%)	21,30,33	0.72	0
2	PSU	A	2316	2,80	18,21,22	0.91	1 (5%)	21,30,33	0.70	0
2	OMG	A	2407	81,2	23,26,27	0.38	0	32,38,41	0.40	0
2	PSU	A	1132	2	18,21,22	0.94	1 (5%)	21,30,33	1.04	1 (4%)
75	OMU	h1	123	75	19,22,23	0.23	0	25,31,34	0.84	0
75	OMU	h1	1261	75	19,22,23	0.23	0	25,31,34	0.51	0
2	A2M	A	826	81,2,80	22,25,26	0.31	0	30,36,39	0.76	1 (3%)
75	PSU	h1	1025	75	18,21,22	0.99	1 (5%)	21,30,33	0.92	1 (4%)
2	OMC	A	675	2	19,22,23	0.35	0	25,31,34	0.68	0
75	PSU	h1	1531	75	18,21,22	0.98	1 (5%)	21,30,33	0.64	0
75	PSU	h1	1118	75	18,21,22	0.94	1 (5%)	21,30,33	0.85	0
75	PSU	h1	103	81,75	18,21,22	0.92	1 (5%)	21,30,33	0.80	0
2	A2M	A	2124	2	22,25,26	0.18	0	30,36,39	0.50	0
75	PSU	h1	1208	75	18,21,22	0.98	1 (5%)	21,30,33	0.71	0
75	A2M	h1	438	75	22,25,26	0.19	0	30,36,39	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	PSU	h1	449	81,75	18,21,22	0.98	1 (5%)	21,30,33	0.77	0
75	PSU	h1	1563	75	18,21,22	0.93	1 (5%)	21,30,33	0.71	0
2	PSU	A	2312	81,2	18,21,22	0.93	1 (5%)	21,30,33	0.83	0
75	OMU	h1	1445	75	19,22,23	0.23	0	25,31,34	0.50	0
22	HIC	BS	246	22	10,11,12	0.46	0	9,14,16	1.06	1 (11%)
2	OMU	A	3299	2	19,22,23	0.33	0	25,31,34	0.55	0
2	OMU	A	803	2	19,22,23	0.28	0	25,31,34	0.51	0
2	PSU	A	901	81,2	18,21,22	0.97	1 (5%)	21,30,33	0.85	0
75	OMC	h1	1216	75	19,22,23	0.29	0	25,31,34	0.38	0
2	PSU	A	1681	2	18,21,22	1.03	1 (5%)	21,30,33	0.79	0
75	A2M	h1	422	75	22,25,26	0.17	0	30,36,39	0.63	0
2	OMG	A	2234	2	23,26,27	0.34	0	32,38,41	0.49	0
75	PSU	h1	1611	75	18,21,22	0.99	1 (5%)	21,30,33	0.87	0
2	A2M	A	2933	2	22,25,26	0.22	0	30,36,39	0.50	0
2	OMG	A	2389	2	23,26,27	0.34	0	32,38,41	0.32	0
2	OMG	A	814	2	23,26,27	0.30	0	32,38,41	0.61	1 (3%)
75	OMC	h1	1641	75,80	19,22,23	0.33	0	25,31,34	0.55	0
75	OMU	h1	580	75	19,22,23	0.21	0	25,31,34	0.48	0
2	OMG	A	1853	2	23,26,27	0.38	0	32,38,41	0.65	1 (3%)
2	A2M	A	2279	2	22,25,26	0.37	0	30,36,39	0.78	1 (3%)
2	OMG	A	2814	2	23,26,27	0.31	0	32,38,41	0.27	0
2	OMC	A	2878	2	19,22,23	0.35	0	25,31,34	0.70	0
75	OMU	h1	1263	75	19,22,23	0.24	0	25,31,34	0.40	0
2	PSU	A	2943	81,2,80	18,21,22	0.93	1 (5%)	21,30,33	0.99	1 (4%)
75	OMU	h1	1381	75,80	19,22,23	0.23	0	25,31,34	0.54	0
2	OMG	A	2618	3,2	23,26,27	0.30	0	32,38,41	0.37	0
2	OMC	A	1858	2	19,22,23	0.39	0	25,31,34	0.60	0
2	PSU	A	1062	81,2	18,21,22	0.92	1 (5%)	21,30,33	0.82	0
2	OMU	A	1890	2	19,22,23	0.30	0	25,31,34	0.94	2 (8%)
2	A2M	A	2254	2	22,25,26	0.23	0	30,36,39	0.54	0
2	1MA	A	657	2,80	21,25,26	0.52	0	30,37,40	0.75	0
75	OMG	h1	597	75	23,26,27	0.31	0	32,38,41	0.55	0
75	OMG	h1	244	75	23,26,27	0.35	0	32,38,41	0.40	0
75	PSU	h1	604	75	18,21,22	0.93	1 (5%)	21,30,33	0.89	0
2	OMC	A	1517	2,80	19,22,23	0.33	0	25,31,34	0.68	0
75	OMG	h1	1431	75,80	23,26,27	0.37	0	32,38,41	0.42	0
2	PSU	A	509	2	18,21,22	1.02	1 (5%)	21,30,33	0.90	1 (4%)
2	PSU	A	2209	2	18,21,22	0.93	1 (5%)	21,30,33	0.72	0
2	OMU	A	2111	2	19,22,23	0.21	0	25,31,34	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMU	A	676	2	19,22,23	0.37	0	25,31,34	0.74	0
2	OMG	A	917	81,2	23,26,27	0.30	0	32,38,41	0.48	0
2	PSU	A	2252	2	18,21,22	0.91	1 (5%)	21,30,33	0.84	1 (4%)
2	PSU	A	1480	2	18,21,22	1.01	1 (5%)	21,30,33	0.76	0
2	PSU	A	2743	2	18,21,22	0.96	2 (11%)	21,30,33	0.74	0
2	PSU	A	2864	2	18,21,22	0.96	1 (5%)	21,30,33	0.81	0
2	PSU	A	785	2	18,21,22	0.91	1 (5%)	21,30,33	0.87	0
2	A2M	A	2639	2	22,25,26	0.18	0	30,36,39	0.36	0
2	PSU	A	828	2	18,21,22	0.93	1 (5%)	21,30,33	0.96	0
2	PSU	A	2189	81,2	18,21,22	0.97	1 (5%)	21,30,33	0.79	0
2	OMG	A	2393	2,80	23,26,27	0.36	0	32,38,41	0.68	1 (3%)
75	OMU	h1	1232	75	19,22,23	0.25	0	25,31,34	0.37	0
75	A2M	h1	162	75	22,25,26	0.21	0	30,36,39	0.63	0
2	OMU	A	2419	2	19,22,23	0.28	0	25,31,34	0.71	0
75	PSU	h1	808	75	18,21,22	0.96	1 (5%)	21,30,33	0.69	0
75	A2M	h1	28	75,80	22,25,26	0.20	0	30,36,39	0.59	0
2	PSU	A	34	2	18,21,22	1.04	1 (5%)	21,30,33	1.08	2 (9%)
2	PSU	A	1054	2	18,21,22	0.90	1 (5%)	21,30,33	0.83	0
75	PSU	h1	1483	75	18,21,22	0.91	1 (5%)	21,30,33	0.61	0
2	A2M	A	2319	2	22,25,26	0.27	0	30,36,39	0.67	1 (3%)
2	PSU	A	1001	2	18,21,22	1.01	1 (5%)	21,30,33	0.91	0
2	A2M	A	2945	2,80	22,25,26	0.24	0	30,36,39	0.66	1 (3%)
75	OMU	h1	613	75	19,22,23	0.28	0	25,31,34	0.45	0
75	PSU	h1	256	75	18,21,22	0.95	1 (5%)	21,30,33	0.72	0
75	C4J	h1	1192	75	25,29,30	1.05	2 (8%)	28,42,45	1.04	2 (7%)
2	A2M	A	2910	2	22,25,26	0.33	0	30,36,39	0.42	0
2	A2M	A	885	2	22,25,26	0.27	0	30,36,39	0.37	0
2	OMG	A	2790	2	23,26,27	0.31	0	32,38,41	0.37	0
75	PSU	h1	959	81,75	18,21,22	0.89	1 (5%)	21,30,33	0.75	0
75	PSU	h1	762	75	18,21,22	0.93	1 (5%)	21,30,33	0.67	0
2	PSU	A	2132	81,2	18,21,22	1.00	1 (5%)	21,30,33	0.92	0
2	A2M	A	1376	2,80	22,25,26	0.22	0	30,36,39	0.62	0
2	A2M	A	2359	2	22,25,26	0.25	0	30,36,39	0.44	0
75	PSU	h1	308	75	18,21,22	1.05	2 (11%)	21,30,33	0.96	1 (4%)
75	PSU	h1	1520	75	18,21,22	0.96	1 (5%)	21,30,33	0.63	0
2	PSU	A	2414	2,80	18,21,22	1.09	1 (5%)	21,30,33	0.89	1 (4%)
2	OMC	A	2681	2	19,22,23	0.27	0	25,31,34	0.59	0
2	OMG	A	2916	2	23,26,27	0.35	0	32,38,41	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	OMU	h1	1010	75	19,22,23	0.25	0	25,31,34	0.49	0
75	PSU	h1	95	75	18,21,22	1.04	1 (5%)	21,30,33	0.79	0
2	PSU	A	1131	2	18,21,22	0.97	1 (5%)	21,30,33	0.84	0
75	PSU	h1	634	75	18,21,22	1.02	1 (5%)	21,30,33	0.96	0
2	OMC	A	1446	2	19,22,23	0.36	0	25,31,34	0.68	1 (4%)
1	PSU	3	97	81,1	18,21,22	0.97	1 (5%)	21,30,33	0.77	0
2	PSU	A	311	81,2	18,21,22	1.18	2 (11%)	21,30,33	1.07	2 (9%)
2	PSU	A	1472	2	18,21,22	0.95	1 (5%)	21,30,33	0.73	0
2	OMC	A	2195	81,2	19,22,23	0.34	0	25,31,34	0.77	0
75	A2M	h1	975	75	22,25,26	0.19	0	30,36,39	0.47	0
2	PSU	A	965	2	18,21,22	1.12	2 (11%)	21,30,33	0.85	0
75	PSU	h1	304	75	18,21,22	0.93	1 (5%)	21,30,33	0.79	0
2	A2M	A	2218	2	22,25,26	0.18	0	30,36,39	0.62	1 (3%)
75	MA6	h1	1786	75	23,26,27	0.28	0	33,38,41	0.84	1 (3%)
2	OMG	A	2792	2	23,26,27	0.32	0	32,38,41	0.52	0
2	5MC	A	2276	2,80	19,22,23	0.68	1 (5%)	26,32,35	0.70	0
1	PSU	3	22	2,1	18,21,22	0.88	1 (5%)	21,30,33	0.72	0
2	OMU	A	48	2	19,22,23	0.37	0	25,31,34	0.60	0
2	UY1	A	2649	2	19,22,23	1.04	1 (5%)	21,31,34	1.01	2 (9%)
75	PSU	h1	1176	75	18,21,22	0.90	1 (5%)	21,30,33	0.90	0
75	A2M	h1	794	75	22,25,26	0.19	0	30,36,39	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	A	2134	2	-	0/7/25/26	0/2/2/2
75	A2M	h1	1754	75	-	0/9/27/28	0/3/3/3
75	OMC	h1	416	75	-	0/9/27/28	0/2/2/2
2	PSU	A	1015	81,2	-	0/7/25/26	0/2/2/2
2	OMU	A	2882	2	-	0/9/27/28	0/2/2/2
2	OMG	A	3290	2,80	-	0/9/27/28	0/3/3/3
75	PSU	h1	761	75	-	0/7/25/26	0/2/2/2
2	A2M	A	816	2	-	0/9/27/28	0/3/3/3
2	A2M	A	1458	2,80	-	0/9/27/28	0/3/3/3
75	OMG	h1	1272	81,75	-	0/9/27/28	0/3/3/3
2	UR3	A	2952	81,2	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	A	2335	2	-	0/9/27/28	0/2/2/2
2	OMU	A	144	81,2	-	0/9/27/28	0/2/2/2
55	MLY	Ga	113	55	-	0/8/9/11	-
75	PSU	h1	1182	75	-	0/7/25/26	0/2/2/2
75	A2M	h1	1327	75	-	0/9/27/28	0/3/3/3
2	PSU	A	2853	2	-	0/7/25/26	0/2/2/2
2	OMC	A	2363	2	-	1/9/27/28	0/2/2/2
75	A2M	h1	621	75,80	-	2/9/27/28	0/3/3/3
75	PSU	h1	1783	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2264	2	-	0/7/25/26	0/2/2/2
2	OMG	A	1459	2,80	-	0/9/27/28	0/3/3/3
2	PSU	A	1133	2	-	0/7/25/26	0/2/2/2
1	A2M	3	47	1	-	0/9/27/28	0/3/3/3
75	PSU	h1	948	75	-	0/7/25/26	0/2/2/2
75	G7M	h1	1577	3,75	-	0/7/25/26	0/3/3/3
2	A2M	A	2212	2,80	-	0/9/27/28	0/3/3/3
2	PSU	A	975	81,2	-	0/7/25/26	0/2/2/2
2	PSU	A	150	81,2	-	0/7/25/26	0/2/2/2
2	5MC	A	2869	81,2	-	4/7/25/26	0/2/2/2
75	4AC	h1	1281	75	-	0/11/29/30	0/2/2/2
1	PSU	3	78	1	-	0/7/25/26	0/2/2/2
2	OMC	A	1848	2,80	-	0/9/27/28	0/2/2/2
75	A2M	h1	799	75	-	0/9/27/28	0/3/3/3
2	PSU	A	2879	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2893	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	752	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1104	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2256	2	-	0/7/25/26	0/2/2/2
2	OMU	A	44	81,2	-	0/9/27/28	0/2/2/2
75	PSU	h1	121	75,80	-	0/7/25/26	0/2/2/2
2	OMU	A	1066	2	-	0/9/27/28	0/2/2/2
2	1MG	A	1646	2	-	0/7/25/26	0/3/3/3
75	6MZ	h1	1767	81,75,80	-	0/9/27/28	0/3/3/3
2	PSU	A	969	2	-	0/7/25/26	0/2/2/2
2	OMC	A	2291	2	-	0/9/27/28	0/2/2/2
75	A2M	h1	778	75	-	2/9/27/28	0/3/3/3
2	PSU	A	2262	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	360	75	-	0/7/25/26	0/2/2/2
2	OMC	A	2958	2,80	-	0/9/27/28	0/2/2/2
2	PSU	A	277	2	-	0/7/25/26	0/2/2/2
75	MA6	h1	1785	75	-	0/11/29/30	0/3/3/3
75	PSU	h1	606	75	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2M	A	1142	2	-	0/9/27/28	0/3/3/3
2	OMC	A	2947	2	-	0/9/27/28	0/2/2/2
2	PSU	A	3109	2	-	0/7/25/26	0/2/2/2
2	A2M	A	945	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	1291	75	-	0/7/25/26	0/2/2/2
2	OMU	A	2920	81,2	-	0/9/27/28	0/2/2/2
75	PSU	h1	1630	75	-	0/7/25/26	0/2/2/2
2	A2M	A	2324	2	-	0/9/27/28	0/3/3/3
2	OMC	A	1845	2	-	0/9/27/28	0/2/2/2
2	OMU	A	2345	2	-	0/9/27/28	0/2/2/2
75	A2M	h1	466	75	-	2/9/27/28	0/3/3/3
1	OMG	3	79	1	-	0/9/27/28	0/3/3/3
75	PSU	h1	415	75	-	0/7/25/26	0/2/2/2
2	OMG	A	2650	2	-	0/9/27/28	0/3/3/3
2	OMU	A	2734	2,80	-	0/9/27/28	0/2/2/2
75	OMC	h1	38	75	-	0/9/27/28	0/2/2/2
2	PSU	A	228	2	-	1/7/25/26	0/2/2/2
2	OMU	A	2408	81,2	-	0/9/27/28	0/2/2/2
75	PSU	h1	605	75	-	0/7/25/26	0/2/2/2
2	OMG	A	2921	2	-	0/9/27/28	0/3/3/3
2	A2M	A	661	2	-	1/9/27/28	0/3/3/3
75	4AC	h1	1777	75	-	0/11/29/30	0/2/2/2
75	OMC	h1	471	75	-	0/9/27/28	0/2/2/2
2	OMG	A	2122	2	-	0/9/27/28	0/3/3/3
2	PSU	A	2825	81,2	-	0/7/25/26	0/2/2/2
1	OMG	3	155	2,1	-	0/9/27/28	0/3/3/3
75	PSU	h1	1188	75	-	0/7/25/26	0/2/2/2
2	OMC	A	1478	2	-	0/9/27/28	0/2/2/2
2	PSU	A	2974	2	-	0/7/25/26	0/2/2/2
2	PSU	A	42	81,2	-	0/7/25/26	0/2/2/2
75	PSU	h1	337	81,75	-	0/7/25/26	0/2/2/2
2	PSU	A	2430	2	-	0/7/25/26	0/2/2/2
75	OMG	h1	390	81,75	-	0/9/27/28	0/3/3/3
75	A2M	h1	1575	75	-	0/9/27/28	0/3/3/3
2	PSU	A	894	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	1000	75	-	0/7/25/26	0/2/2/2
2	OMU	A	2716	2	-	0/9/27/28	0/2/2/2
2	PSU	A	2258	2	-	0/7/25/26	0/2/2/2
2	OMG	A	2286	2	-	0/9/27/28	0/3/3/3
2	OMC	A	2835	2	-	0/9/27/28	0/2/2/2
75	A2M	h1	543	75	-	1/9/27/28	0/3/3/3
2	PSU	A	2954	2	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
75	PSU	h1	468	75	-	0/7/25/26	0/2/2/2
75	OMU	h1	1270	75,80	-	2/9/27/28	0/2/2/2
2	PSU	A	685	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	1215	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1302	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2922	2	-	1/7/25/26	0/2/2/2
75	PSU	h1	1306	75	-	1/7/25/26	0/2/2/2
75	UY1	h1	602	75	-	0/9/27/28	0/2/2/2
75	PSU	h1	583	75	-	6/7/25/26	0/2/2/2
2	PSU	A	2316	2,80	-	0/7/25/26	0/2/2/2
2	OMG	A	2407	81,2	-	0/9/27/28	0/3/3/3
2	PSU	A	1132	2	-	0/7/25/26	0/2/2/2
75	OMU	h1	123	75	-	2/9/27/28	0/2/2/2
75	OMU	h1	1261	75	-	0/9/27/28	0/2/2/2
2	A2M	A	826	81,2,80	-	2/9/27/28	0/3/3/3
75	PSU	h1	1025	75	-	0/7/25/26	0/2/2/2
2	OMC	A	675	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	1531	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1118	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	103	81,75	-	0/7/25/26	0/2/2/2
2	A2M	A	2124	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	1208	75	-	1/7/25/26	0/2/2/2
75	A2M	h1	438	75	-	0/9/27/28	0/3/3/3
75	PSU	h1	449	81,75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1563	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2312	81,2	-	1/7/25/26	0/2/2/2
75	OMU	h1	1445	75	-	0/9/27/28	0/2/2/2
22	HIC	BS	246	22	-	0/5/6/8	0/1/1/1
2	OMU	A	3299	2	-	0/9/27/28	0/2/2/2
2	OMU	A	803	2	-	0/9/27/28	0/2/2/2
2	PSU	A	901	81,2	-	0/7/25/26	0/2/2/2
75	OMC	h1	1216	75	-	0/9/27/28	0/2/2/2
2	PSU	A	1681	2	-	0/7/25/26	0/2/2/2
75	A2M	h1	422	75	-	0/9/27/28	0/3/3/3
2	OMG	A	2234	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	1611	75	-	0/7/25/26	0/2/2/2
2	A2M	A	2933	2	-	0/9/27/28	0/3/3/3
2	OMG	A	2389	2	-	0/9/27/28	0/3/3/3
2	OMG	A	814	2	-	0/9/27/28	0/3/3/3
75	OMC	h1	1641	75,80	-	0/9/27/28	0/2/2/2
75	OMU	h1	580	75	-	2/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	A	1853	2	-	0/9/27/28	0/3/3/3
2	A2M	A	2279	2	-	3/9/27/28	0/3/3/3
2	OMG	A	2814	2	-	0/9/27/28	0/3/3/3
2	OMC	A	2878	2	-	0/9/27/28	0/2/2/2
75	OMU	h1	1263	75	-	1/9/27/28	0/2/2/2
2	PSU	A	2943	81,2,80	-	0/7/25/26	0/2/2/2
75	OMU	h1	1381	75,80	-	0/9/27/28	0/2/2/2
2	OMG	A	2618	3,2	-	1/9/27/28	0/3/3/3
2	OMC	A	1858	2	-	0/9/27/28	0/2/2/2
2	PSU	A	1062	81,2	-	0/7/25/26	0/2/2/2
2	OMU	A	1890	2	-	0/9/27/28	0/2/2/2
2	A2M	A	2254	2	-	0/9/27/28	0/3/3/3
2	1MA	A	657	2,80	-	0/7/25/26	0/3/3/3
75	OMG	h1	597	75	-	3/9/27/28	0/3/3/3
75	OMG	h1	244	75	-	0/9/27/28	0/3/3/3
75	PSU	h1	604	75	-	0/7/25/26	0/2/2/2
2	OMC	A	1517	2,80	-	2/9/27/28	0/2/2/2
75	OMG	h1	1431	75,80	-	1/9/27/28	0/3/3/3
2	PSU	A	509	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2209	2	-	0/7/25/26	0/2/2/2
2	OMU	A	2111	2	-	2/9/27/28	0/2/2/2
2	OMU	A	676	2	-	0/9/27/28	0/2/2/2
2	OMG	A	917	81,2	-	0/9/27/28	0/3/3/3
2	PSU	A	2252	2	-	0/7/25/26	0/2/2/2
2	PSU	A	1480	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2743	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2864	2	-	0/7/25/26	0/2/2/2
2	PSU	A	785	2	-	2/7/25/26	0/2/2/2
2	A2M	A	2639	2	-	0/9/27/28	0/3/3/3
2	PSU	A	828	2	-	0/7/25/26	0/2/2/2
2	PSU	A	2189	81,2	-	0/7/25/26	0/2/2/2
2	OMG	A	2393	2,80	-	0/9/27/28	0/3/3/3
75	OMU	h1	1232	75	-	2/9/27/28	0/2/2/2
75	A2M	h1	162	75	-	0/9/27/28	0/3/3/3
2	OMU	A	2419	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	808	75	-	0/7/25/26	0/2/2/2
75	A2M	h1	28	75,80	-	0/9/27/28	0/3/3/3
2	PSU	A	34	2	-	0/7/25/26	0/2/2/2
2	PSU	A	1054	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	1483	75	-	0/7/25/26	0/2/2/2
2	A2M	A	2319	2	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	A	1001	2	-	0/7/25/26	0/2/2/2
2	A2M	A	2945	2,80	-	0/9/27/28	0/3/3/3
75	OMU	h1	613	75	-	0/9/27/28	0/2/2/2
75	PSU	h1	256	75	-	0/7/25/26	0/2/2/2
75	C4J	h1	1192	75	-	5/16/34/35	0/2/2/2
2	A2M	A	2910	2	-	5/9/27/28	0/3/3/3
2	A2M	A	885	2	-	0/9/27/28	0/3/3/3
2	OMG	A	2790	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	959	81,75	-	0/7/25/26	0/2/2/2
75	PSU	h1	762	75	-	0/7/25/26	0/2/2/2
2	PSU	A	2132	81,2	-	0/7/25/26	0/2/2/2
2	A2M	A	1376	2,80	-	0/9/27/28	0/3/3/3
2	A2M	A	2359	2	-	0/9/27/28	0/3/3/3
75	PSU	h1	308	75	-	0/7/25/26	0/2/2/2
75	PSU	h1	1520	75	-	2/7/25/26	0/2/2/2
2	PSU	A	2414	2,80	-	0/7/25/26	0/2/2/2
2	OMC	A	2681	2	-	0/9/27/28	0/2/2/2
2	OMG	A	2916	2	-	0/9/27/28	0/3/3/3
75	OMU	h1	1010	75	-	0/9/27/28	0/2/2/2
75	PSU	h1	95	75	-	0/7/25/26	0/2/2/2
2	PSU	A	1131	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	634	75	-	0/7/25/26	0/2/2/2
2	OMC	A	1446	2	-	0/9/27/28	0/2/2/2
1	PSU	3	97	81,1	-	0/7/25/26	0/2/2/2
2	PSU	A	311	81,2	-	0/7/25/26	0/2/2/2
2	PSU	A	1472	2	-	0/7/25/26	0/2/2/2
2	OMC	A	2195	81,2	-	4/9/27/28	0/2/2/2
75	A2M	h1	975	75	-	0/9/27/28	0/3/3/3
2	PSU	A	965	2	-	0/7/25/26	0/2/2/2
75	PSU	h1	304	75	-	0/7/25/26	0/2/2/2
2	A2M	A	2218	2	-	0/9/27/28	0/3/3/3
75	MA6	h1	1786	75	-	1/11/29/30	0/3/3/3
2	OMG	A	2792	2	-	1/9/27/28	0/3/3/3
2	5MC	A	2276	2,80	-	0/7/25/26	0/2/2/2
1	PSU	3	22	2,1	-	0/7/25/26	0/2/2/2
2	OMU	A	48	2	-	0/9/27/28	0/2/2/2
2	UY1	A	2649	2	-	0/9/27/28	0/2/2/2
75	PSU	h1	1176	75	-	0/7/25/26	0/2/2/2
75	A2M	h1	794	75	-	1/9/27/28	0/3/3/3

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	311	PSU	C6-C5	4.14	1.39	1.35
2	A	2414	PSU	C6-C5	4.02	1.39	1.35
2	A	2954	PSU	C6-C5	4.01	1.39	1.35
75	h1	1783	PSU	C6-C5	3.96	1.39	1.35
1	3	78	PSU	C6-C5	3.93	1.39	1.35
2	A	2974	PSU	C6-C5	3.92	1.39	1.35
75	h1	583	PSU	C6-C5	3.91	1.39	1.35
75	h1	634	PSU	C6-C5	3.91	1.39	1.35
2	A	965	PSU	C6-C5	3.91	1.39	1.35
75	h1	1531	PSU	C6-C5	3.89	1.39	1.35
2	A	685	PSU	C6-C5	3.89	1.39	1.35
2	A	2649	UY1	C6-C5	3.88	1.39	1.35
2	A	1681	PSU	C6-C5	3.88	1.39	1.35
2	A	1480	PSU	C6-C5	3.87	1.39	1.35
75	h1	948	PSU	C6-C5	3.87	1.39	1.35
75	h1	1182	PSU	C6-C5	3.87	1.39	1.35
2	A	509	PSU	C6-C5	3.85	1.39	1.35
75	h1	602	UY1	C6-C5	3.83	1.39	1.35
75	h1	95	PSU	C6-C5	3.82	1.39	1.35
75	h1	468	PSU	C6-C5	3.82	1.39	1.35
2	A	1001	PSU	C6-C5	3.80	1.39	1.35
75	h1	449	PSU	C6-C5	3.78	1.39	1.35
2	A	1472	PSU	C6-C5	3.77	1.39	1.35
75	h1	808	PSU	C6-C5	3.77	1.39	1.35
2	A	2893	PSU	C6-C5	3.75	1.39	1.35
75	h1	1611	PSU	C6-C5	3.73	1.39	1.35
75	h1	1520	PSU	C6-C5	3.73	1.39	1.35
2	A	1131	PSU	C6-C5	3.73	1.39	1.35
75	h1	256	PSU	C6-C5	3.71	1.39	1.35
75	h1	606	PSU	C6-C5	3.70	1.39	1.35
75	h1	1025	PSU	C6-C5	3.69	1.39	1.35
75	h1	1215	PSU	C6-C5	3.69	1.39	1.35
75	h1	1563	PSU	C6-C5	3.68	1.39	1.35
2	A	2209	PSU	C6-C5	3.68	1.39	1.35
2	A	2316	PSU	C6-C5	3.66	1.39	1.35
2	A	42	PSU	C6-C5	3.66	1.39	1.35
2	A	2189	PSU	C6-C5	3.66	1.39	1.35
2	A	2825	PSU	C6-C5	3.65	1.39	1.35
75	h1	1630	PSU	C6-C5	3.65	1.39	1.35
2	A	2864	PSU	C6-C5	3.65	1.39	1.35
75	h1	761	PSU	C6-C5	3.65	1.39	1.35
2	A	228	PSU	C6-C5	3.64	1.39	1.35
2	A	1062	PSU	C6-C5	3.63	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	h1	1208	PSU	C6-C5	3.62	1.39	1.35
75	h1	360	PSU	C6-C5	3.62	1.39	1.35
2	A	785	PSU	C6-C5	3.61	1.39	1.35
2	A	2132	PSU	C6-C5	3.61	1.39	1.35
2	A	1015	PSU	C6-C5	3.60	1.39	1.35
75	h1	1483	PSU	C6-C5	3.60	1.39	1.35
75	h1	415	PSU	C6-C5	3.59	1.39	1.35
75	h1	1000	PSU	C6-C5	3.59	1.39	1.35
2	A	2256	PSU	C6-C5	3.59	1.39	1.35
75	h1	1118	PSU	C6-C5	3.59	1.39	1.35
2	A	901	PSU	C6-C5	3.58	1.39	1.35
75	h1	762	PSU	C6-C5	3.58	1.39	1.35
2	A	3109	PSU	C6-C5	3.58	1.39	1.35
2	A	277	PSU	C6-C5	3.57	1.39	1.35
2	A	1132	PSU	C6-C5	3.57	1.39	1.35
75	h1	337	PSU	C6-C5	3.57	1.39	1.35
75	h1	752	PSU	C6-C5	3.56	1.39	1.35
75	h1	103	PSU	C6-C5	3.54	1.39	1.35
75	h1	1176	PSU	C6-C5	3.54	1.39	1.35
2	A	2922	PSU	C6-C5	3.53	1.39	1.35
2	A	2262	PSU	C6-C5	3.53	1.39	1.35
2	A	2312	PSU	C6-C5	3.53	1.39	1.35
2	A	2258	PSU	C6-C5	3.52	1.39	1.35
75	h1	1291	PSU	C6-C5	3.51	1.39	1.35
2	A	34	PSU	C6-C5	3.50	1.39	1.35
75	h1	1306	PSU	C6-C5	3.50	1.39	1.35
2	A	2252	PSU	C6-C5	3.49	1.39	1.35
75	h1	959	PSU	C6-C5	3.47	1.39	1.35
75	h1	605	PSU	C6-C5	3.45	1.39	1.35
2	A	2264	PSU	C6-C5	3.45	1.39	1.35
75	h1	308	PSU	C6-C5	3.44	1.39	1.35
75	h1	304	PSU	C6-C5	3.44	1.39	1.35
2	A	1054	PSU	C6-C5	3.44	1.39	1.35
75	h1	1302	PSU	C6-C5	3.43	1.39	1.35
2	A	150	PSU	C6-C5	3.43	1.39	1.35
2	A	2879	PSU	C6-C5	3.42	1.39	1.35
1	3	97	PSU	C6-C5	3.41	1.39	1.35
75	h1	1188	PSU	C6-C5	3.40	1.39	1.35
75	h1	604	PSU	C6-C5	3.37	1.39	1.35
2	A	2869	5MC	C5-C4	-3.37	1.41	1.44
2	A	2134	PSU	C6-C5	3.34	1.39	1.35
75	h1	121	PSU	C6-C5	3.33	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	894	PSU	C6-C5	3.31	1.39	1.35
2	A	2853	PSU	C6-C5	3.28	1.38	1.35
2	A	1133	PSU	C6-C5	3.28	1.38	1.35
2	A	828	PSU	C6-C5	3.28	1.38	1.35
1	3	22	PSU	C6-C5	3.27	1.38	1.35
2	A	2943	PSU	C6-C5	3.26	1.38	1.35
2	A	975	PSU	C6-C5	3.21	1.38	1.35
75	h1	1104	PSU	C6-C5	3.21	1.38	1.35
2	A	2743	PSU	C6-C5	3.17	1.38	1.35
75	h1	1192	C4J	C4-C5	-3.17	1.40	1.47
75	h1	1192	C4J	C6-C5	3.10	1.39	1.35
2	A	969	PSU	C6-C5	3.02	1.38	1.35
2	A	2430	PSU	C6-C5	3.00	1.38	1.35
2	A	2276	5MC	C5-C4	-2.62	1.42	1.44
75	h1	1577	G7M	C8-N7	2.58	1.37	1.33
75	h1	308	PSU	C4-C5	-2.49	1.37	1.44
2	A	42	PSU	C4-C5	-2.26	1.38	1.44
2	A	311	PSU	C4-C5	-2.24	1.38	1.44
2	A	965	PSU	C4-C5	-2.19	1.38	1.44
2	A	2743	PSU	C4-C5	-2.14	1.38	1.44

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	945	A2M	O2'-C2'-C1'	-3.68	101.99	108.99
75	h1	1786	MA6	C2-N1-C6	3.10	119.40	111.83
75	h1	1785	MA6	C2-N1-C6	3.07	119.32	111.83
75	h1	799	A2M	O2'-C2'-C1'	2.74	114.19	108.99
2	A	2279	A2M	O4'-C1'-N9	2.68	113.24	108.09
2	A	814	OMG	C2'-C1'-N9	-2.63	109.25	114.24
2	A	1853	OMG	O2'-C2'-C1'	2.58	113.89	108.99
2	A	826	A2M	C3'-C2'-C1'	-2.58	97.87	102.81
2	A	311	PSU	C6-C5-C4	2.53	119.88	118.17
2	A	2252	PSU	C2'-C3'-C4'	-2.48	97.83	102.61
2	A	1890	OMU	O3'-C3'-C2'	2.47	118.10	111.19
2	A	2649	UY1	C6-C5-C4	2.45	119.83	118.17
2	A	2122	OMG	C2'-C1'-N9	-2.44	109.60	114.24
75	h1	1025	PSU	C3'-C2'-C1'	2.41	104.53	101.69
1	3	47	A2M	C2'-C1'-N9	-2.39	109.82	113.75
2	A	2324	A2M	O2'-C2'-C1'	2.37	113.50	108.99
2	A	42	PSU	C6-C5-C4	2.35	119.76	118.17
2	A	2393	OMG	C2'-C1'-N9	-2.34	109.79	114.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2218	A2M	O2'-C2'-C1'	2.34	113.43	108.99
2	A	34	PSU	C5-C6-N1	-2.34	118.90	122.14
2	A	2324	A2M	C2'-C1'-N9	-2.33	109.92	113.75
2	A	2954	PSU	C2'-C3'-C4'	-2.30	98.16	102.61
2	A	34	PSU	C6-C5-C4	2.28	119.71	118.17
2	A	2958	OMC	O2'-C2'-C1'	2.25	113.26	108.99
2	A	2649	UY1	C5-C6-N1	-2.23	119.04	122.14
2	A	2974	PSU	C2'-C3'-C4'	-2.22	98.31	102.61
2	A	1133	PSU	C2'-C3'-C4'	-2.21	98.33	102.61
2	A	685	PSU	C5-C6-N1	-2.19	119.09	122.14
75	h1	1192	C4J	C4-N3-C2	-2.17	122.94	125.62
2	A	42	PSU	C5-C6-N1	-2.16	119.14	122.14
75	h1	308	PSU	C2'-C3'-C4'	-2.16	98.44	102.61
2	A	1132	PSU	C5-C6-N1	-2.15	119.16	122.14
2	A	42	PSU	C2'-C3'-C4'	-2.13	98.49	102.61
75	h1	1577	G7M	N9-C8-N7	-2.12	107.32	112.48
2	A	2943	PSU	C5-C6-N1	-2.11	119.21	122.14
2	A	3290	OMG	O2'-C2'-C1'	2.10	112.98	108.99
2	A	311	PSU	C5-C6-N1	-2.10	119.22	122.14
2	A	2319	A2M	O2'-C2'-C1'	2.09	112.96	108.99
2	A	3290	OMG	C3'-C2'-C1'	-2.08	98.82	102.81
75	h1	1783	PSU	C6-C5-C4	2.07	119.57	118.17
2	A	2212	A2M	O2'-C2'-C1'	2.06	112.90	108.99
2	A	1133	PSU	C5-C6-N1	-2.06	119.28	122.14
2	A	2945	A2M	C2'-C1'-N9	-2.06	110.37	113.75
75	h1	1783	PSU	C5-C6-N1	-2.05	119.29	122.14
75	h1	1000	PSU	C5-C6-N1	-2.05	119.29	122.14
2	A	1446	OMC	C2'-C1'-N1	2.05	118.13	114.24
2	A	2869	5MC	C5-C6-N1	-2.05	121.09	123.31
2	A	2952	UR3	C4-N3-C2	-2.04	122.94	124.58
2	A	1890	OMU	O4'-C4'-C3'	-2.04	101.11	105.15
22	BS	246	HIC	NE2-CE1-ND1	-2.04	111.88	112.66
2	A	2414	PSU	C5-C6-N1	-2.02	119.33	122.14
75	h1	1575	A2M	C2'-C1'-N9	-2.02	110.42	113.75
2	A	509	PSU	C2'-C3'-C4'	-2.02	98.71	102.61
2	A	2974	PSU	C5-C6-N1	-2.01	119.35	122.14
75	h1	1192	C4J	O4'-C1'-C2'	-2.01	102.38	105.15
2	A	969	PSU	O2'-C2'-C1'	-2.00	106.46	111.21

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	785	PSU	C2'-C1'-C5-C4
2	A	2111	OMU	O4'-C4'-C5'-O5'
2	A	2195	OMC	C2'-C1'-N1-C6
2	A	2618	OMG	C1'-C2'-O2'-CM2
2	A	2910	A2M	O4'-C4'-C5'-O5'
75	h1	123	OMU	O4'-C4'-C5'-O5'
75	h1	583	PSU	C2'-C1'-C5-C4
75	h1	583	PSU	O4'-C1'-C5-C4
75	h1	583	PSU	O4'-C1'-C5-C6
75	h1	597	OMG	O4'-C4'-C5'-O5'
75	h1	778	A2M	O4'-C4'-C5'-O5'
75	h1	778	A2M	C3'-C4'-C5'-O5'
75	h1	794	A2M	C1'-C2'-O2'-CM'
75	h1	1232	OMU	C3'-C4'-C5'-O5'
75	h1	1232	OMU	O4'-C4'-C5'-O5'
2	A	2195	OMC	C2'-C1'-N1-C2
75	h1	123	OMU	C3'-C4'-C5'-O5'
75	h1	583	PSU	C3'-C4'-C5'-O5'
2	A	2910	A2M	C3'-C4'-C5'-O5'
75	h1	583	PSU	O4'-C4'-C5'-O5'
75	h1	1192	C4J	O4'-C4'-C5'-O5'
75	h1	1270	OMU	O4'-C4'-C5'-O5'
2	A	2111	OMU	C3'-C4'-C5'-O5'
75	h1	597	OMG	C3'-C4'-C5'-O5'
75	h1	1192	C4J	C3'-C4'-C5'-O5'
75	h1	466	A2M	O4'-C4'-C5'-O5'
75	h1	580	OMU	O4'-C4'-C5'-O5'
75	h1	621	A2M	C3'-C4'-C5'-O5'
2	A	2910	A2M	C2'-C1'-N9-C8
2	A	826	A2M	C3'-C2'-O2'-CM'
2	A	2279	A2M	O4'-C4'-C5'-O5'
75	h1	621	A2M	O4'-C4'-C5'-O5'
75	h1	1192	C4J	C4'-C5'-O5'-P
2	A	1517	OMC	O4'-C4'-C5'-O5'
2	A	2279	A2M	C3'-C4'-C5'-O5'
2	A	1517	OMC	C3'-C4'-C5'-O5'
75	h1	1270	OMU	C3'-C4'-C5'-O5'
2	A	2312	PSU	C4'-C5'-O5'-P
2	A	2869	5MC	O4'-C1'-N1-C6
2	A	2363	OMC	C3'-C2'-O2'-CM2
2	A	2922	PSU	C4'-C5'-O5'-P
2	A	2869	5MC	C2'-C1'-N1-C6
75	h1	1208	PSU	O4'-C1'-C5-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
75	h1	1306	PSU	O4'-C1'-C5-C4
2	A	2910	A2M	C2'-C1'-N9-C4
2	A	2195	OMC	O4'-C1'-N1-C6
2	A	2279	A2M	C2'-C1'-N9-C8
75	h1	1786	MA6	C4'-C5'-O5'-P
2	A	661	A2M	C4'-C5'-O5'-P
75	h1	466	A2M	C3'-C4'-C5'-O5'
75	h1	1263	OMU	C3'-C2'-O2'-CM2
2	A	826	A2M	C4'-C5'-O5'-P
75	h1	580	OMU	C3'-C4'-C5'-O5'
75	h1	597	OMG	C4'-C5'-O5'-P
2	A	2195	OMC	O4'-C1'-N1-C2
75	h1	1431	OMG	C4'-C5'-O5'-P
75	h1	1520	PSU	O4'-C1'-C5-C6
2	A	2792	OMG	C3'-C2'-O2'-CM2
2	A	2869	5MC	O4'-C1'-N1-C2
2	A	228	PSU	C3'-C4'-C5'-O5'
75	h1	583	PSU	C2'-C1'-C5-C6
75	h1	1520	PSU	C2'-C1'-C5-C6
2	A	2910	A2M	O4'-C1'-N9-C8
75	h1	543	A2M	O4'-C1'-N9-C8
75	h1	1192	C4J	C31-C32-C34-O35
2	A	785	PSU	O4'-C4'-C5'-O5'
75	h1	1192	C4J	C31-C32-C34-O36
2	A	2869	5MC	C2'-C1'-N1-C2

There are no ring outliers.

35 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2882	OMU	1	0
2	A	2879	PSU	1	0
2	A	44	OMU	1	0
75	h1	1767	6MZ	1	0
2	A	969	PSU	1	0
2	A	1142	A2M	1	0
2	A	2920	OMU	1	0
2	A	2324	A2M	1	0
2	A	2345	OMU	1	0
2	A	661	A2M	1	0
1	3	155	OMG	3	0
2	A	2258	PSU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2922	PSU	1	0
75	h1	1261	OMU	1	0
2	A	826	A2M	1	0
2	A	675	OMC	1	0
75	h1	1531	PSU	1	0
2	A	2312	PSU	1	0
2	A	2234	OMG	1	0
2	A	2933	A2M	2	0
2	A	2389	OMG	1	0
75	h1	1641	OMC	1	0
2	A	1853	OMG	1	0
2	A	2878	OMC	1	0
2	A	2618	OMG	1	0
2	A	2254	A2M	1	0
75	h1	244	OMG	1	0
2	A	2189	PSU	1	0
75	h1	1192	C4J	1	0
2	A	2790	OMG	1	0
2	A	1376	A2M	1	0
75	h1	95	PSU	1	0
2	A	1446	OMC	2	0
75	h1	975	A2M	1	0
75	h1	794	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 500 ligands modelled in this entry, 494 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	SPD	A	3403	-	9,9,9	0.29	0	8,8,8	0.55	0
84	EPE	A	3404	-	15,15,15	0.68	1 (6%)	19,20,20	0.63	0
83	SPD	A	3405	-	9,9,9	0.17	0	8,8,8	0.29	0
82	TER	A	3401	-	13,13,13	0.16	0	12,12,12	0.27	0
83	SPD	A	3402	-	9,9,9	0.18	0	8,8,8	0.15	0
83	SPD	A	3406	-	9,9,9	0.17	0	8,8,8	0.23	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	SPD	A	3403	-	-	5/7/7/7	-
84	EPE	A	3404	-	-	5/9/19/19	0/1/1/1
83	SPD	A	3405	-	-	1/7/7/7	-
82	TER	A	3401	-	-	1/11/11/11	-
83	SPD	A	3402	-	-	3/7/7/7	-
83	SPD	A	3406	-	-	2/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	A	3404	EPE	O3S-S	2.44	1.56	1.47

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	A	3406	SPD	C3-C4-C5-N6
83	A	3403	SPD	C3-C4-C5-N6
83	A	3405	SPD	C3-C4-C5-N6
83	A	3403	SPD	N6-C7-C8-C9
83	A	3402	SPD	C3-C4-C5-N6
83	A	3406	SPD	C8-C7-N6-C5
83	A	3403	SPD	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

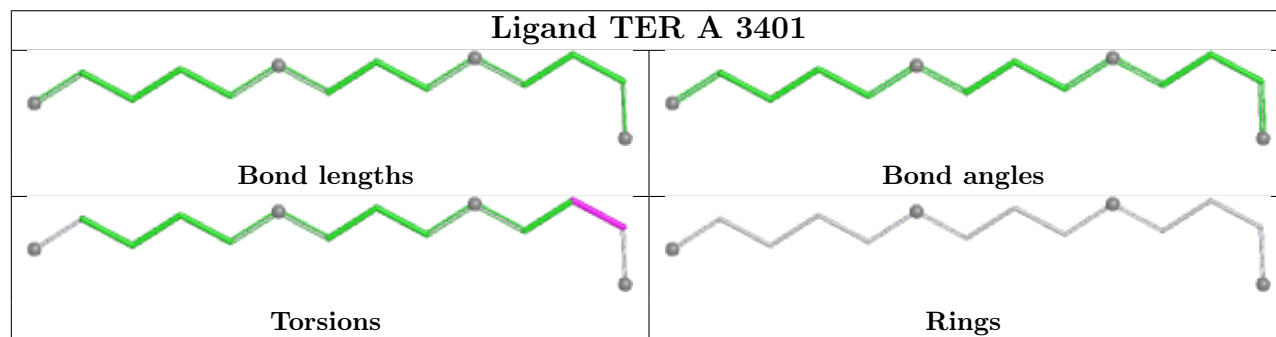
Mol	Chain	Res	Type	Atoms
83	A	3403	SPD	C8-C7-N6-C5
84	A	3404	EPE	C9-C10-S-O3S
84	A	3404	EPE	C8-C7-N4-C3
84	A	3404	EPE	C9-C10-S-O1S
84	A	3404	EPE	S-C10-C9-N1
84	A	3404	EPE	N4-C7-C8-O8
83	A	3403	SPD	C4-C5-N6-C7
82	A	3401	TER	N1-C2-C3-C4
83	A	3402	SPD	C7-C8-C9-N10
83	A	3402	SPD	N6-C7-C8-C9

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	A	3403	SPD	1	0
83	A	3405	SPD	1	0
82	A	3401	TER	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
74	Ca	1
73	AY	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ca	53:ILE	C	54:LYS	N	1.90
1	AY	76:THR	C	77:CYS	N	1.85

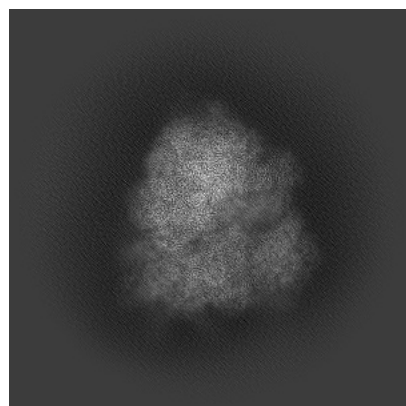
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51820. These allow visual inspection of the internal detail of the map and identification of artifacts.

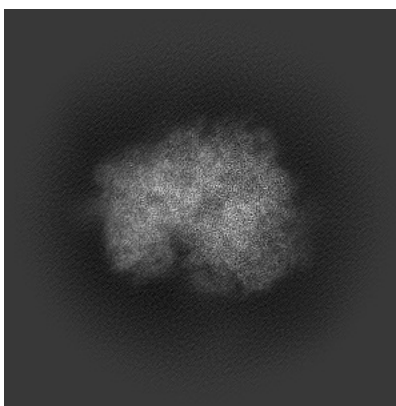
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

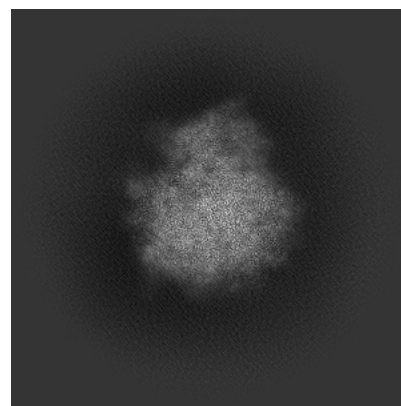
6.1.1 Primary map



X

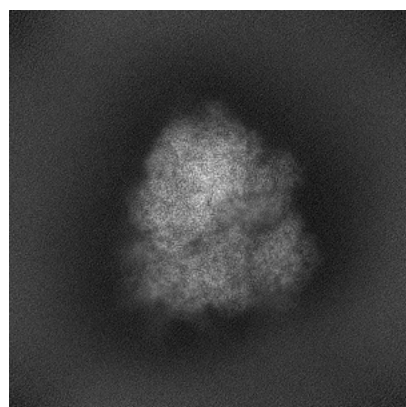


Y

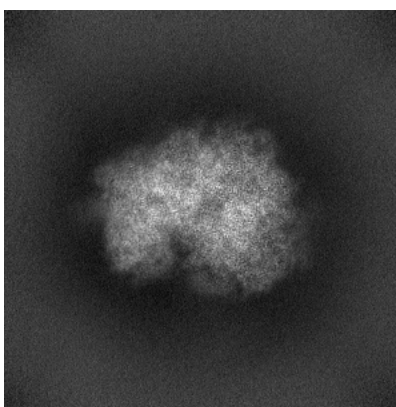


Z

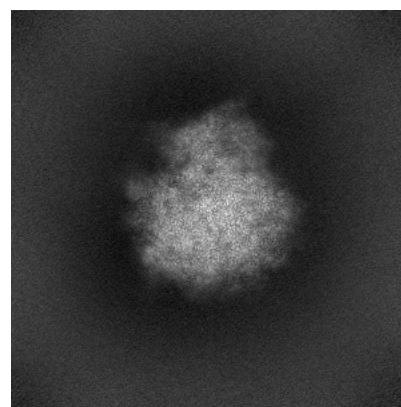
6.1.2 Raw map



X



Y

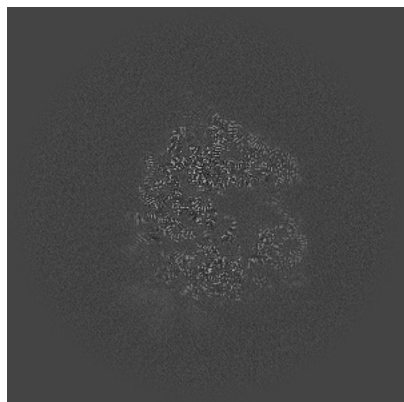


Z

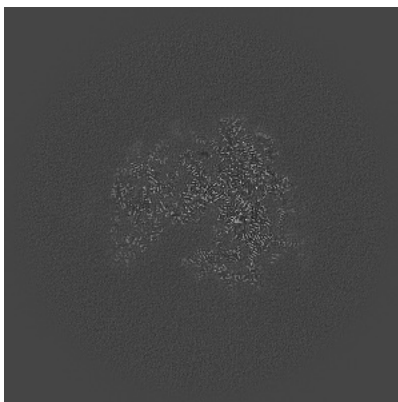
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

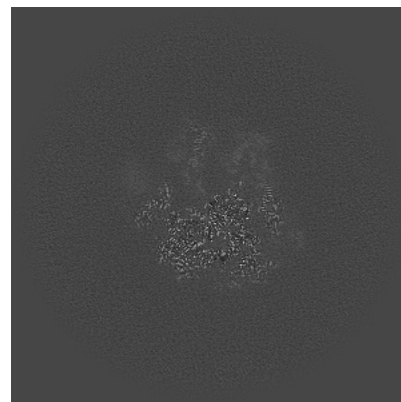
6.2.1 Primary map



X Index: 343

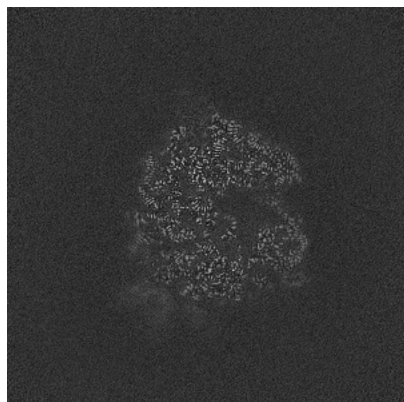


Y Index: 343

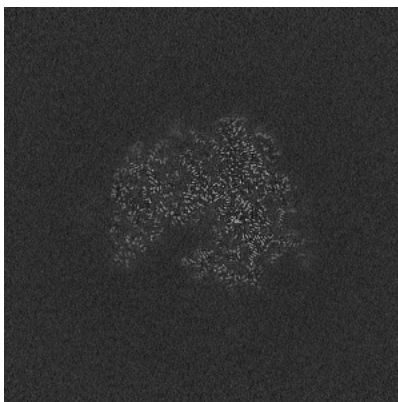


Z Index: 343

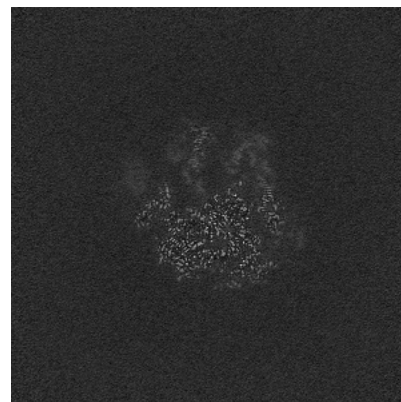
6.2.2 Raw map



X Index: 343



Y Index: 343

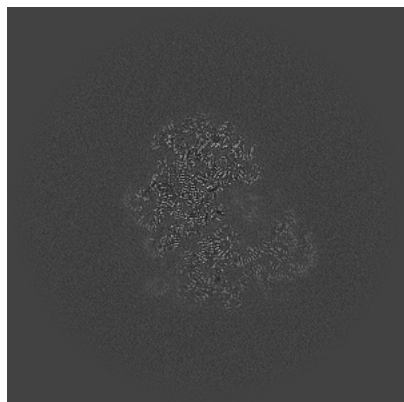


Z Index: 343

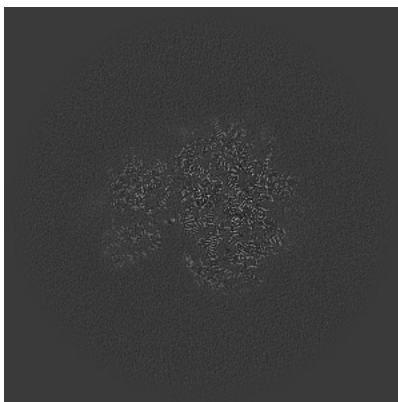
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

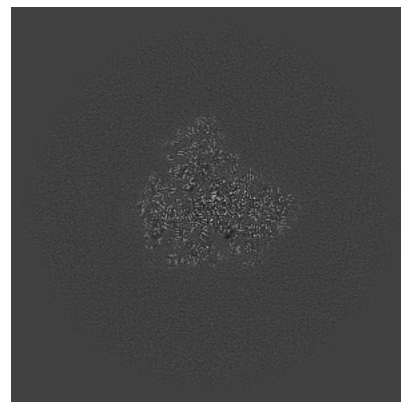
6.3.1 Primary map



X Index: 378

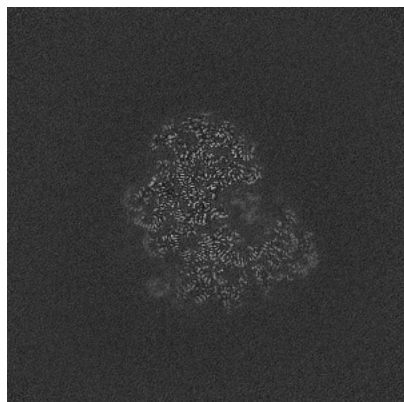


Y Index: 329

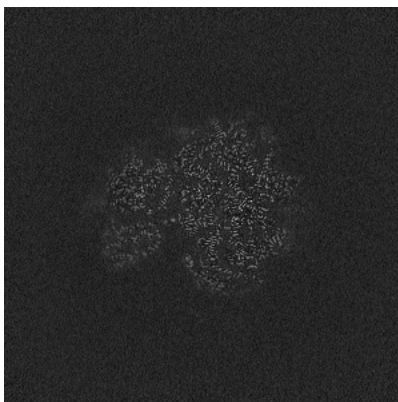


Z Index: 401

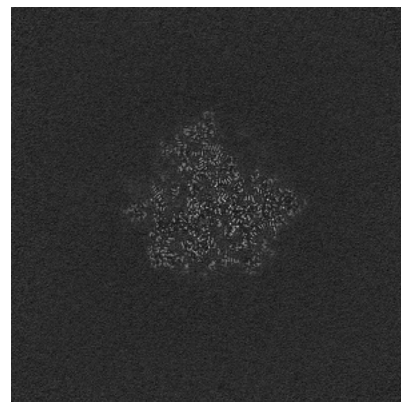
6.3.2 Raw map



X Index: 377



Y Index: 329

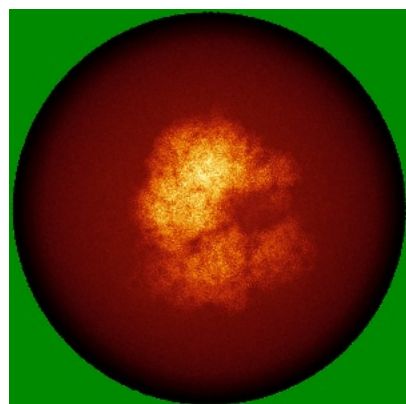


Z Index: 390

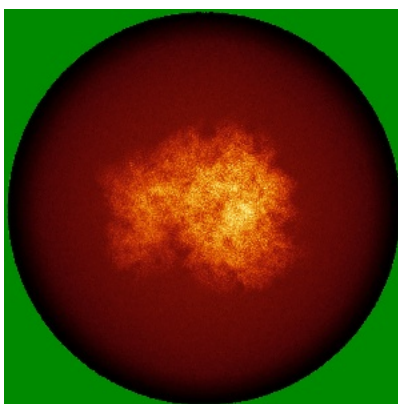
The images above show the largest variance slices of the map in three orthogonal directions.

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

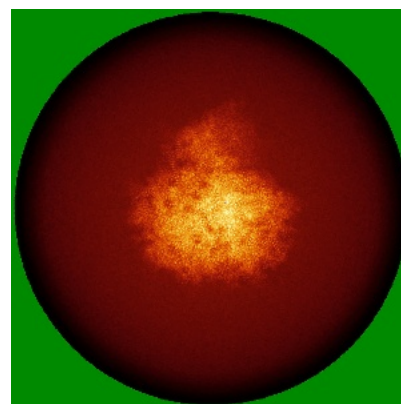
6.4.1 Primary map



X

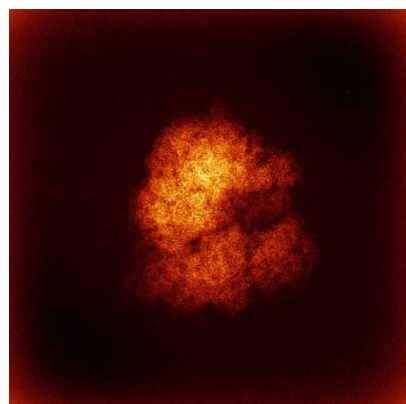


Y

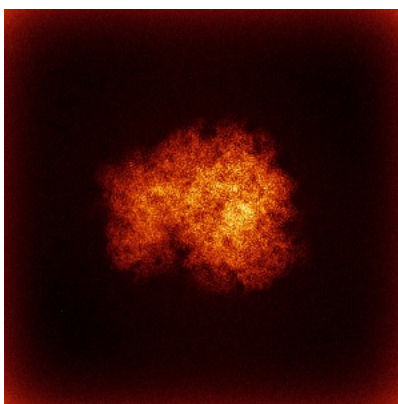


Z

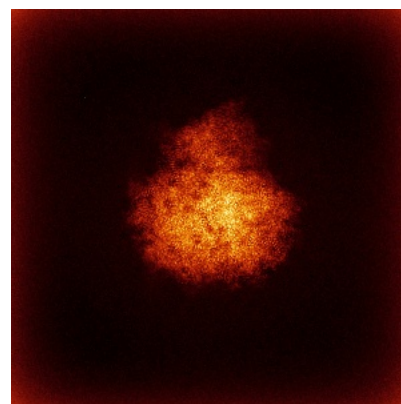
6.4.2 Raw map



X



Y

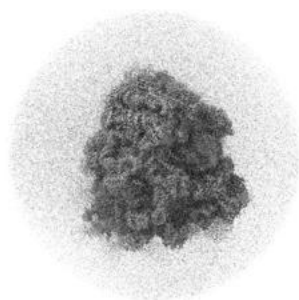


Z

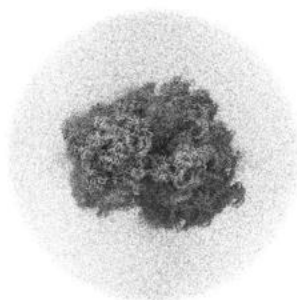
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

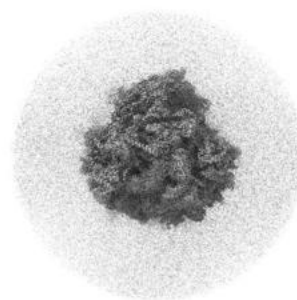
6.5.1 Primary map



X



Y



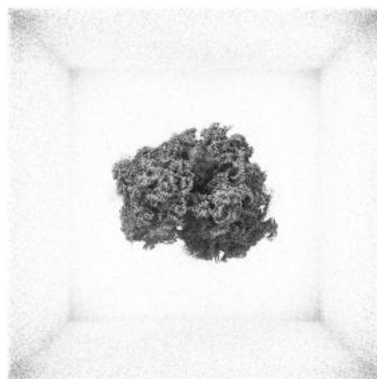
Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. 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



X



Y



Z

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

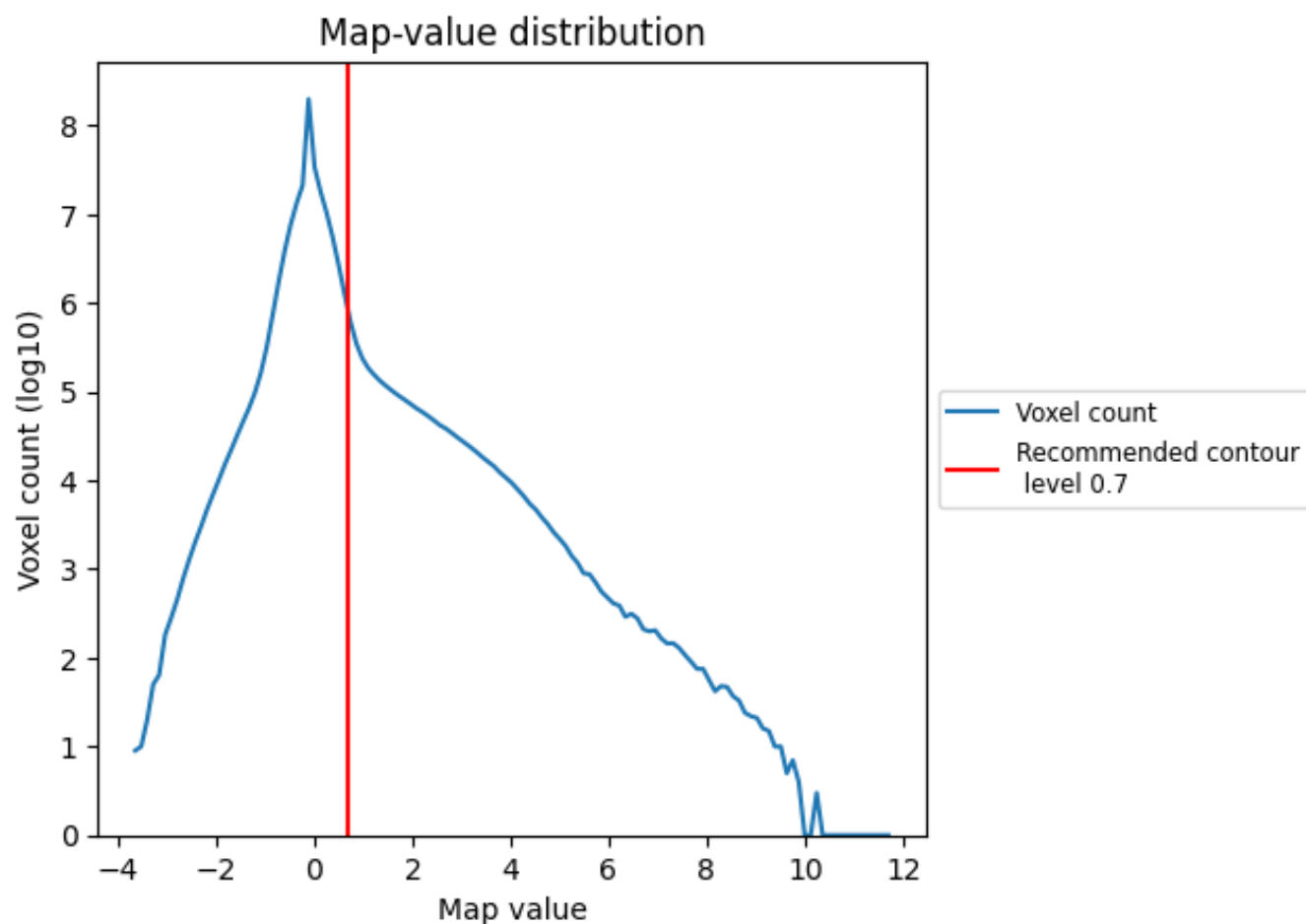
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

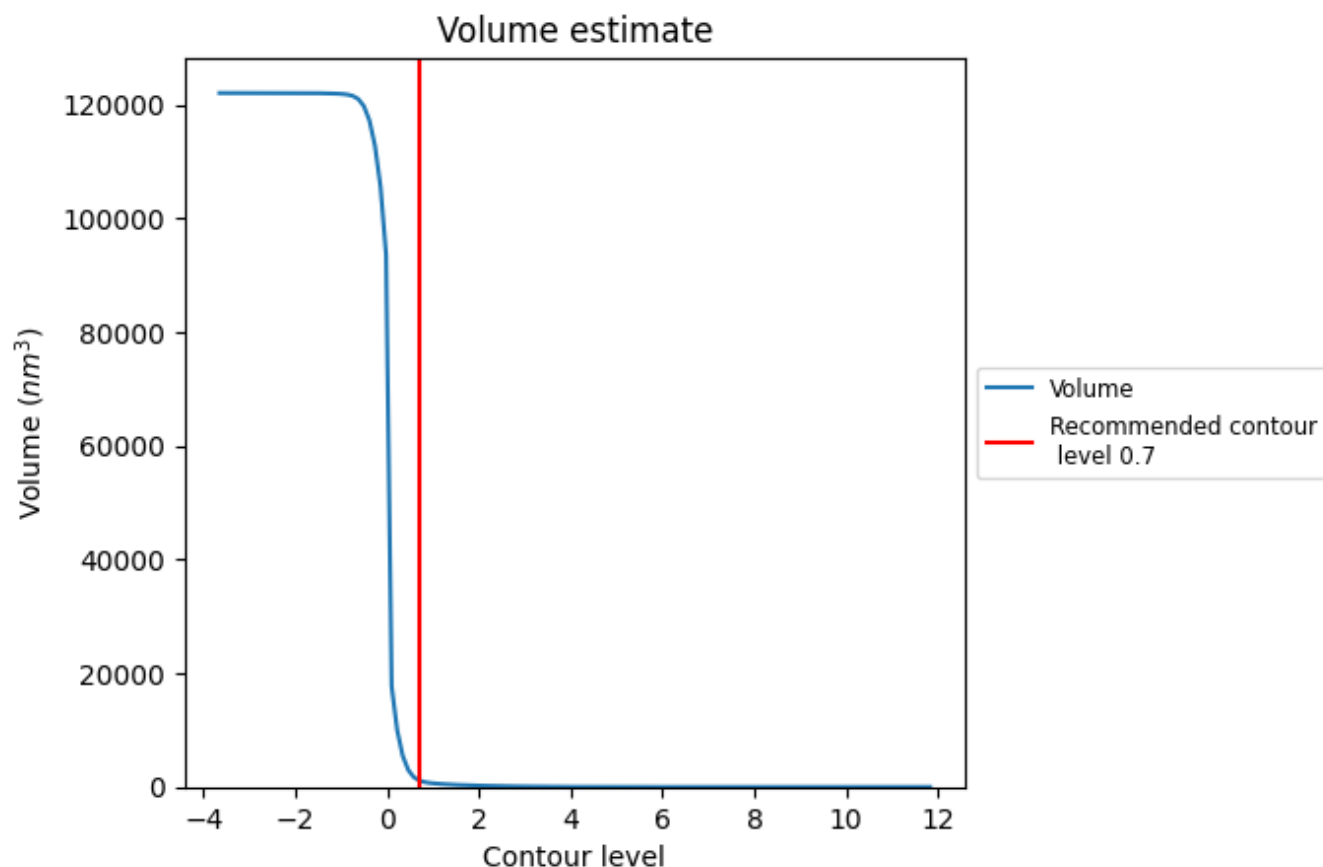
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

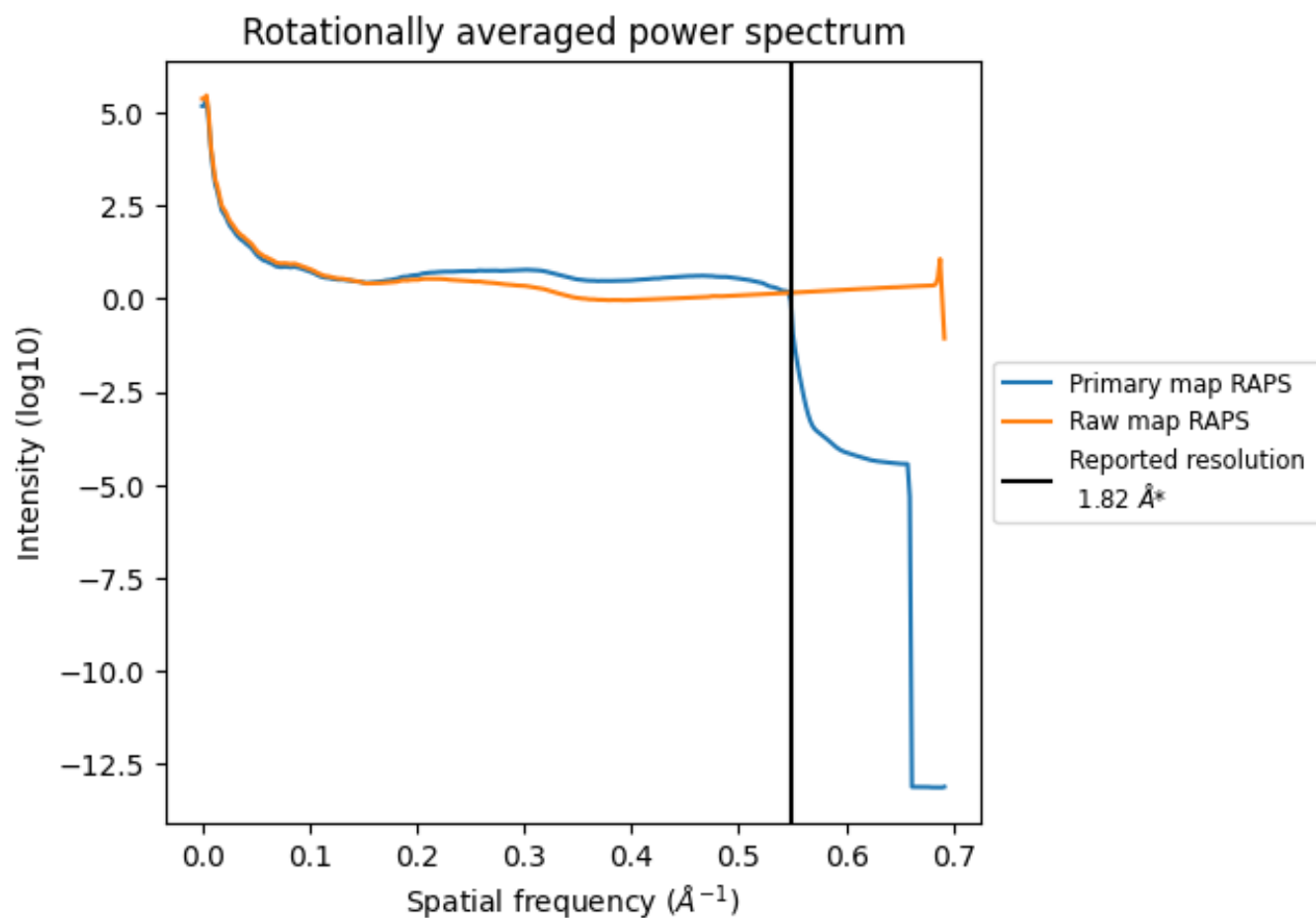
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1140 nm^3 ; this corresponds to an approximate mass of 1030 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 ⓘ

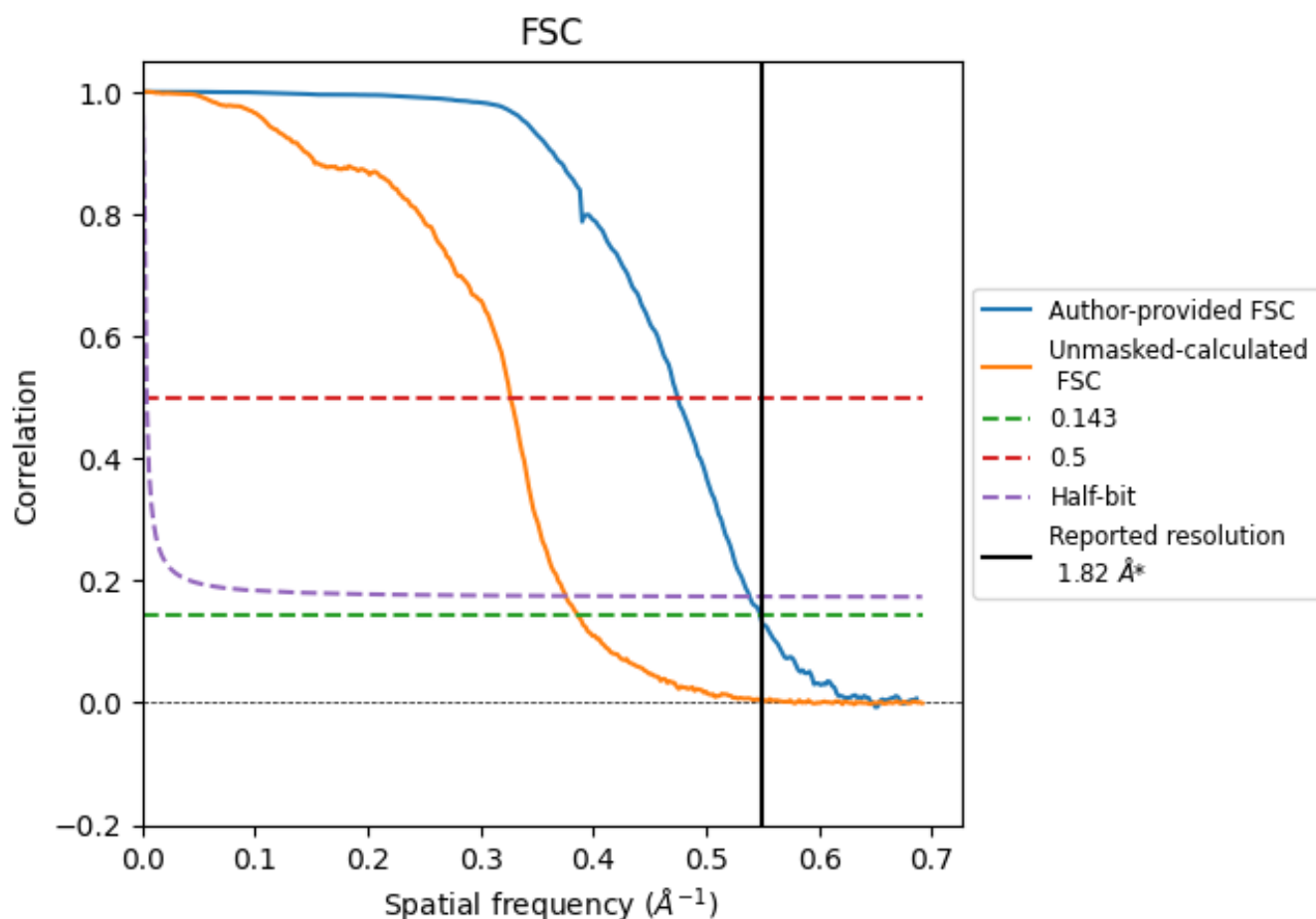


*Reported resolution corresponds to spatial frequency of 0.549 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.549 \AA^{-1}

8.2 Resolution estimates [i](#)

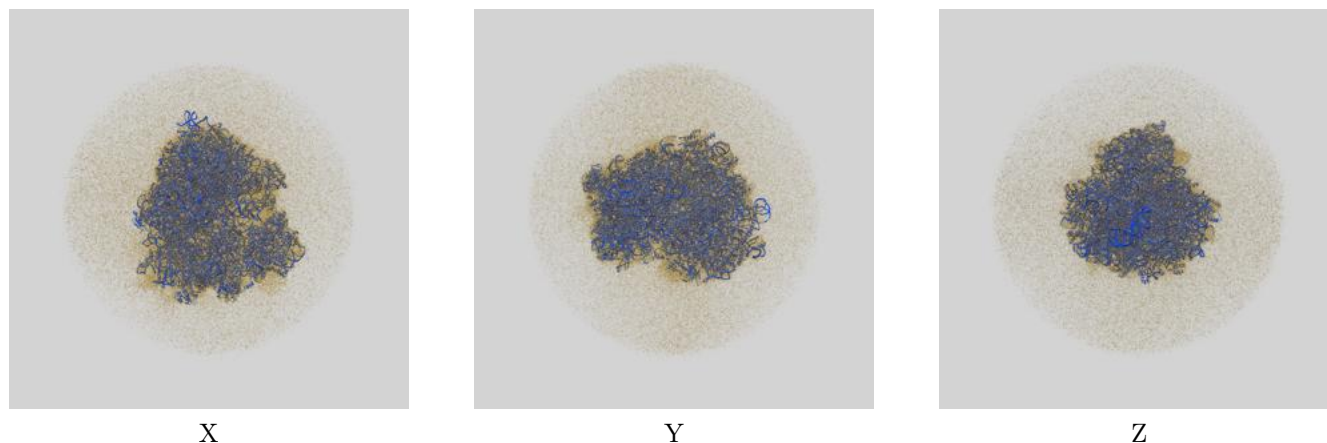
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.82	-	-
Author-provided FSC curve	1.82	2.11	1.86
Unmasked-calculated*	2.59	3.06	2.66

*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 2.59 differs from the reported value 1.82 by more than 10 %

9 Map-model fit [i](#)

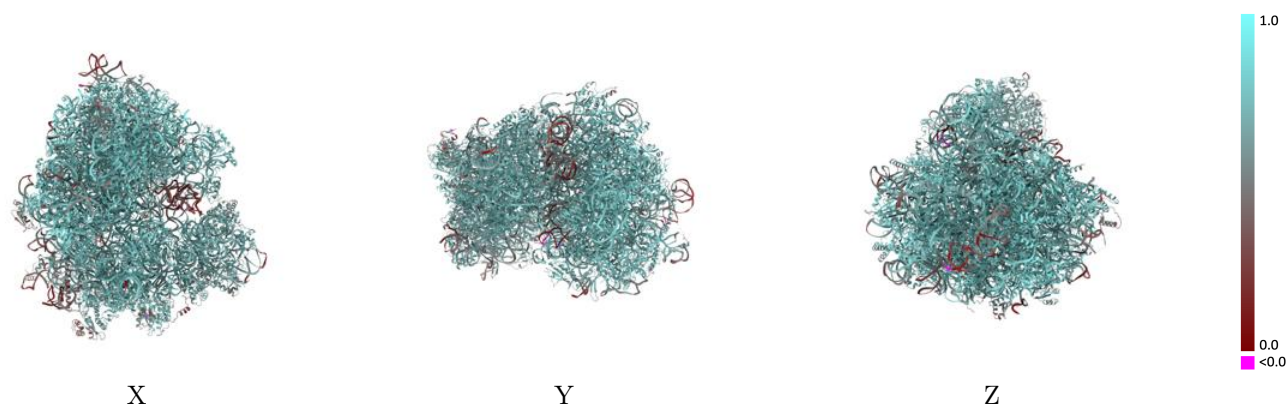
This section contains information regarding the fit between EMDB map EMD-51820 and PDB model 9H3G. Per-residue inclusion information can be found in section 3 on page 26.

9.1 Map-model overlay [i](#)



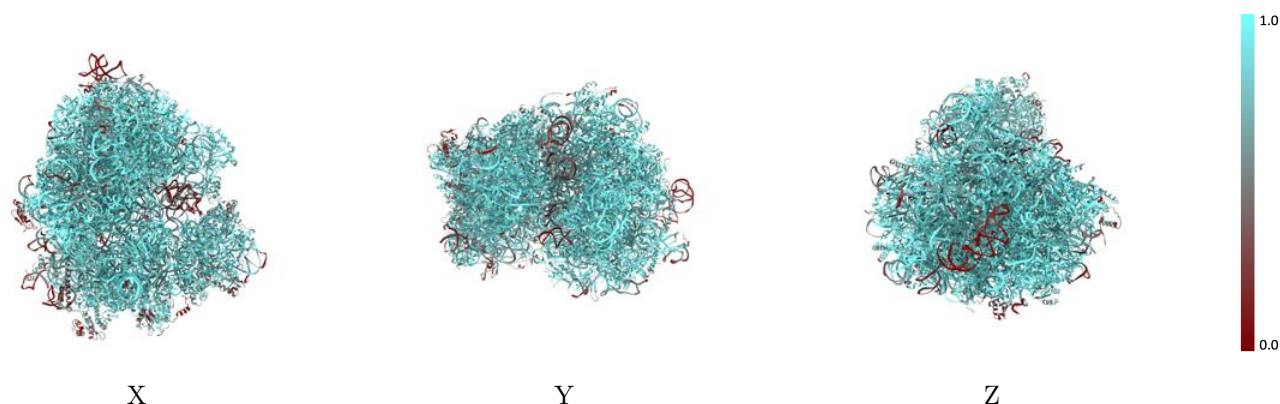
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



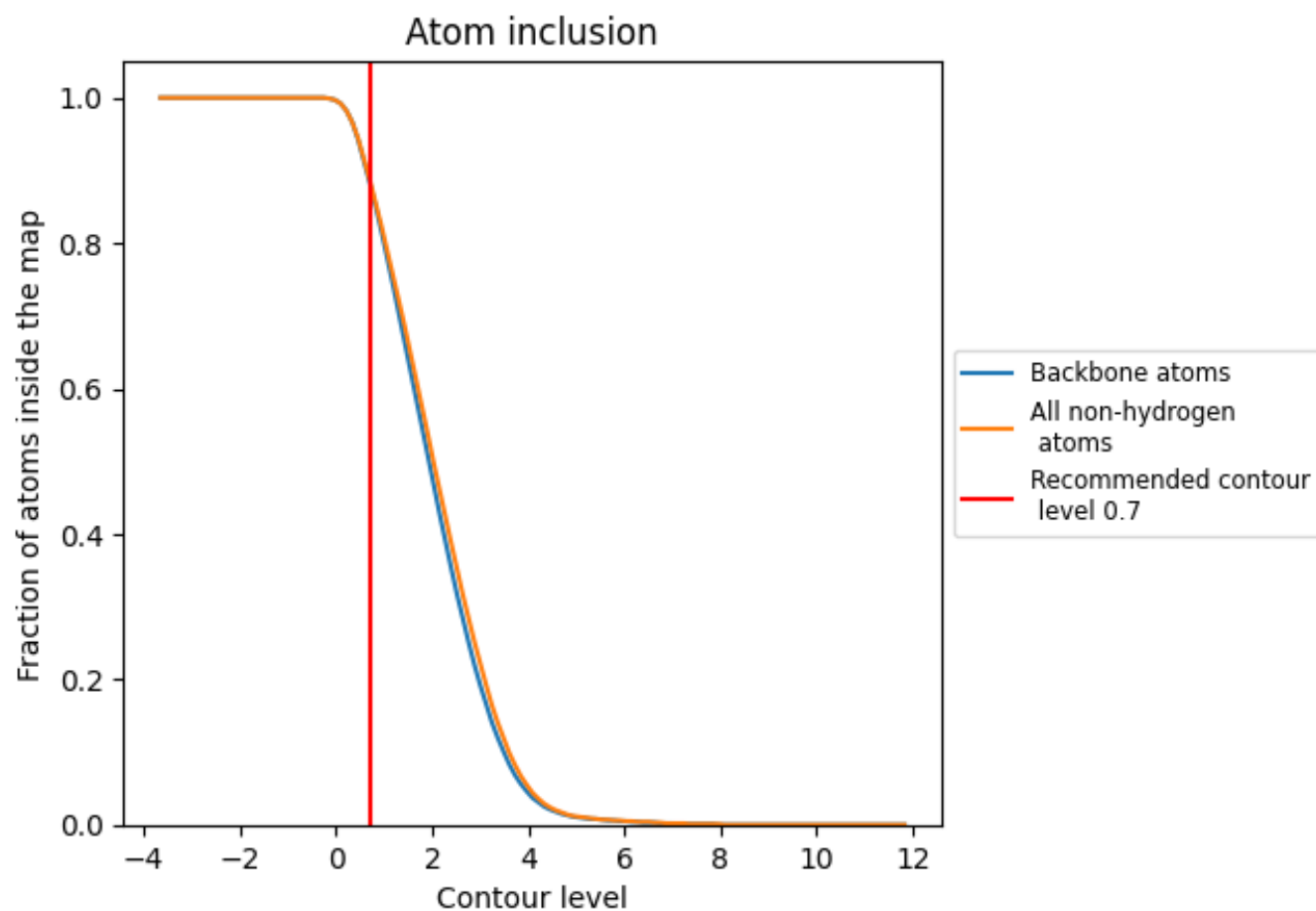
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.7).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 89% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8880	 0.7200
3	 0.9100	 0.7230
A	 0.9170	 0.7350
AA	 0.7410	 0.6400
AB	 0.8740	 0.7060
AC	 0.9420	 0.7610
AD	 0.8520	 0.6890
AE	 0.9760	 0.7920
AF	 0.8350	 0.6660
AG	 0.9130	 0.7590
AH	 0.9090	 0.7490
AI	 0.6240	 0.5820
AJ	 0.9850	 0.8130
AK	 0.8480	 0.7130
AL	 0.9620	 0.7880
AM	 0.9270	 0.7670
AN	 0.2300	 0.4770
AO	 0.9550	 0.7840
AP	 0.9330	 0.7550
AQ	 0.5680	 0.6590
AR	 0.9440	 0.7790
AT	 0.9290	 0.7560
AU	 0.8690	 0.7380
AV	 0.9790	 0.8020
AW	 0.9800	 0.8100
AX	 0.9090	 0.7420
AY	 0.9780	 0.8130
AZ	 0.8010	 0.6760
Aa	 0.8040	 0.6580
B1	 0.8630	 0.6720
BA	 0.9810	 0.8050
BB	 0.4740	 0.5180
BC	 0.9360	 0.7690
BD	 0.9680	 0.8040
BE	 0.9600	 0.7920







Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BF	 0.8500	 0.7060
BG	 0.8440	 0.7110
BH	 0.9540	 0.7920
BI	 0.9690	 0.8030
BJ	 0.9340	 0.7430
BK	 0.9050	 0.7470
BL	 0.8550	 0.6810
BM	 0.9560	 0.7990
BN	 0.9390	 0.7720
BO	 0.9640	 0.7860
BP	 0.9220	 0.7600
BQ	 0.9920	 0.8220
BR	 0.9330	 0.7830
BS	 0.9760	 0.8090
BT	 0.9220	 0.7750
BU	 0.8750	 0.7100
BV	 0.8960	 0.7220
BW	 0.8940	 0.7310
Ba	 0.6330	 0.6200
C3	 0.9930	 0.7660
Ca	 0.9080	 0.7380
Da	 0.8820	 0.7170
Ea	 0.9990	 0.8250
Fa	 0.9230	 0.7750
Ga	 0.9350	 0.7650
Ha	 0.9630	 0.8020
Ia	 0.9080	 0.7440
Ja	 0.8830	 0.7050
Ka	 0.7680	 0.6510
L3	 0.2430	 0.3620
La	 0.6740	 0.6000
Ma	 0.9180	 0.7510
Na	 0.7570	 0.6460
Oa	 0.8150	 0.6750
Pa	 0.7960	 0.6730
Ra	 0.5480	 0.5470
Ta	 0.6390	 0.5790
Ua	 0.9510	 0.7480
Va	 0.9600	 0.7790
W2	 0.5810	 0.4500
Wa	 0.8190	 0.6780
Xa	 0.8900	 0.7120

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Ya	 0.7050	 0.6230
Za	 0.8350	 0.6880
h1	 0.8930	 0.6910
i2	 0.6160	 0.4850