



Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 03:20 pm BST

PDB ID : 8PJ5 / pdb_00008pj5
EMDB ID : EMD-17700
Title : Structure of human 48S translation initiation complex after eIF2 release prior
60S subunit joining (48S-5)
Authors : Petrychenko, V.; Yi, S.-H.; Liedtke, D.; Peng, B.Z.; Rodnina, M.V.; Fischer,
N.
Deposited on : 2023-06-22
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

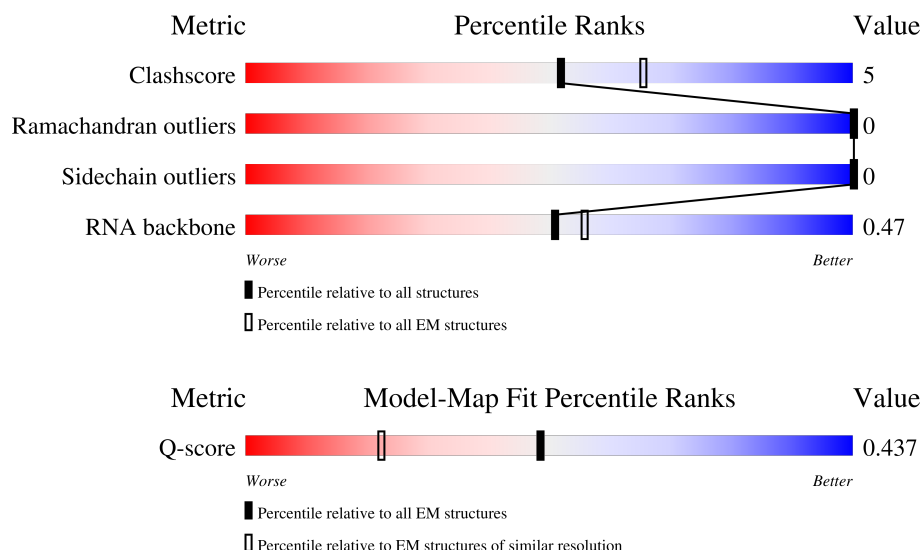
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



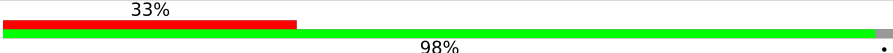
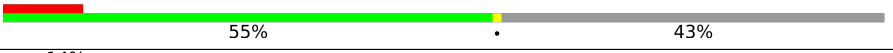
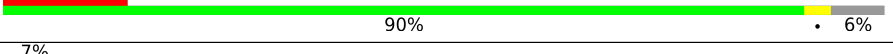
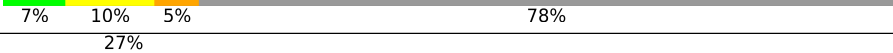
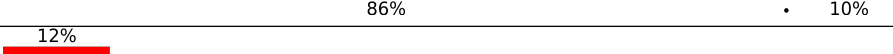
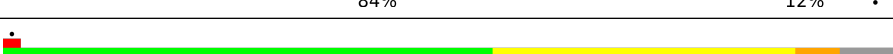
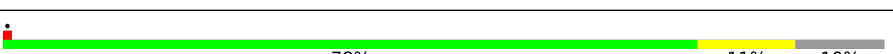
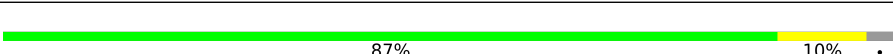
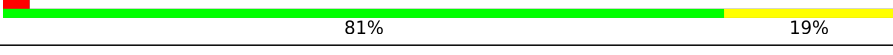
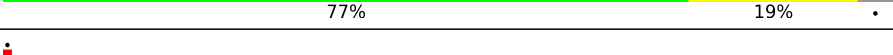
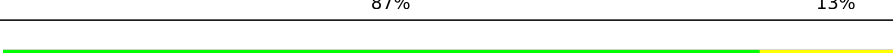
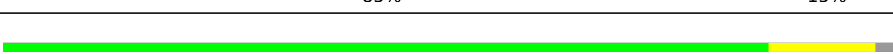
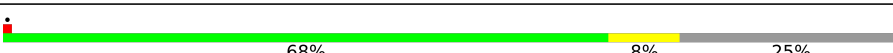
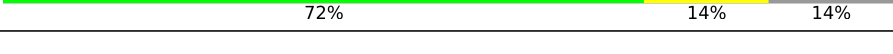
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	0	1220	
2	1	814	
3	2	325	

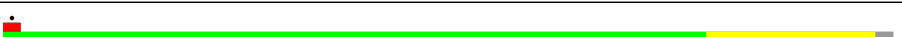
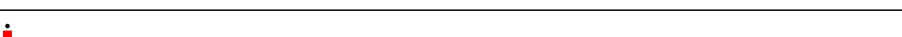
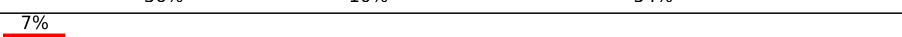
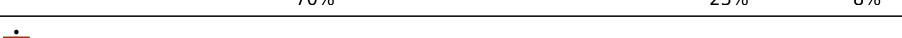
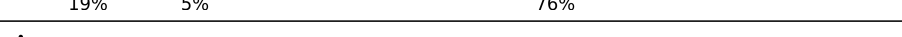
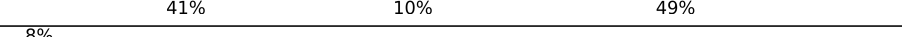
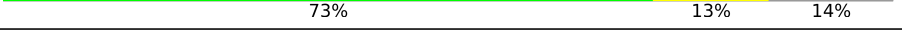
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Mol	Chain	Length	Quality of chain
4	3	218	
5	4	357	
6	5	564	
7	6	374	
8	7	255	
9	8	352	
10	9	25	
11	A	1869	
12	B	158	
13	C	263	
14	D	194	
15	E	143	
16	F	59	
17	G	194	
18	H	84	
19	I	151	
20	J	130	
21	K	83	
22	L	293	
23	M	135	
24	N	295	
25	O	264	
26	P	151	
27	Q	115	
28	R	208	

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Mol	Chain	Length	Quality of chain
29	S	249	
30	T	133	
31	V	204	
32	Y	146	
33	Z	243	
34	a	165	
35	b	145	
36	c	317	
37	d	145	
38	e	125	
39	f	152	
40	h	119	
41	i	56	
42	k	156	
43	m	132	
44	n	69	
45	o	320	
46	q	144	
47	u	1382	
48	v	445	
49	w	75	
50	x	548	
51	y	913	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 113033 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Eukaryotic translation initiation factor 5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	622	Total	C	N	O	S	0	0
			4928	3141	851	914	22		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	588	Total	C	N	O	S	0	0
			3258	1986	633	634	5		

- Molecule 3 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	2	304	Total	C	N	O	0	0
			1493	885	304	304		

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	3	213	Total	C	N	O	0	0
			1057	631	213	213		

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	4	257	Total	C	N	O	0	0
			1272	757	257	258		

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5	319	Total	C	N	O	0	0
			1581	943	319	319		

- Molecule 7 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	350	Total	C	N	O	S	0	0
			1917	1159	376	380	2		

- Molecule 8 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	56	Total	C	N	O	P	5	0
			1300	584	245	410	61		

- Molecule 9 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	8	317	Total	C	N	O	0	0
			1571	936	317	318		

- Molecule 10 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 11 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1754	Total	C	N	O	P	0	0
			37429	16718	6714	12244	1753		

- Molecule 12 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	142	Total	C	N	O	S	0	0
			1166	743	218	199	6		

- Molecule 13 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	256	Total	C	N	O	S	0	0
			2035	1302	378	347	8		

- Molecule 14 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	177	Total	C	N	O	S	0	0
			1477	941	295	239	2		

- Molecule 15 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	140	Total	C	N	O	S	0	0
			1087	687	215	182	3		

- Molecule 16 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	59	Total	C	N	O	S	0	0
			461	285	100	75	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	125	PRO	LYS	conflict	UNP P62861
F	126	GLY	LYS	conflict	UNP P62861

- Molecule 17 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	177	Total	C	N	O	S	0	0
			1430	917	260	252	1		

- Molecule 18 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	H	81	Total	C	N	O	S	0	0
			631	397	116	111	7		

- Molecule 19 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 20 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 21 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 22 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	220	Total	C	N	O	S	0	0
			1707	1104	292	301	10		

- Molecule 23 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 24 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	207	Total	C	N	O	S	0	0
			1633	1040	288	297	8		

- Molecule 25 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

- Molecule 26 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	P	133	Total	C	N	O	S	0	0
			997	610	196	185	6		

- Molecule 27 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 28 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	R	198	Total	C	N	O	S	0	0
			1627	1021	322	279	5		

- Molecule 29 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	S	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 30 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	T	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 31 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 32 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 33 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 34 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	99	Total	C	N	O	S	0	0
			834	544	149	135	6		

- Molecule 35 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	131	Total	C	N	O	S	0	0
			1072	682	201	182	7		

- Molecule 36 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 37 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	142	Total	C	N	O	S	0	0
			1105	692	213	197	3		

- Molecule 38 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	82	Total	C	N	O	S	0	0
			658	426	121	110	1		

- Molecule 39 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	149	Total	C	N	O	S	0	0
			1227	770	249	207	1		

- Molecule 40 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 41 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	50	Total	C	N	O	S	0	0
			419	262	85	67	5		

- Molecule 42 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	71	Total	C	N	O	S	0	0
			581	367	109	98	7		

- Molecule 43 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 44 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	o	77	Total	C	N	O	0	0
			616	389	111	116		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	117	Total	C	N	O	S	1	0
			951	590	183	174	4		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	u	706	Total	C	N	O	S	1	0
			5383	3379	982	999	23		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	384	Total	C	N	O	S	0	0
			2635	1657	477	489	12		

- Molecule 49 is a RNA chain called Initiator Met-tRNA-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	w	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	x	421	Total	C	N	O	S	0	0
			2831	1746	521	555	9		

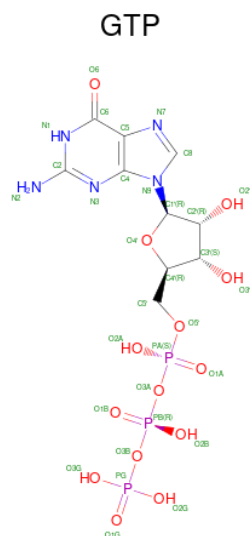
- Molecule 51 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	y	531	Total	C	N	O	S	0	0
			4305	2711	764	797	33		

- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
52	0	1	Total	Mg	0
			1	1	
52	A	87	Total	Mg	0
			87	87	
52	P	1	Total	Mg	0
			1	1	
52	S	1	Total	Mg	0
			1	1	
52	f	1	Total	Mg	0
			1	1	

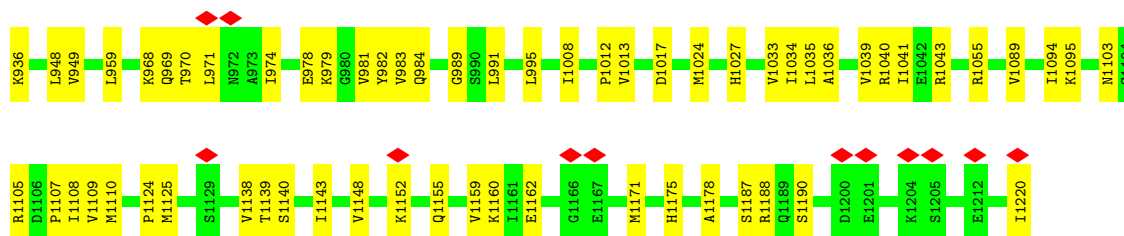
- Molecule 53 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



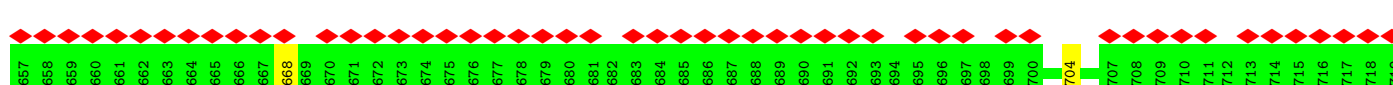
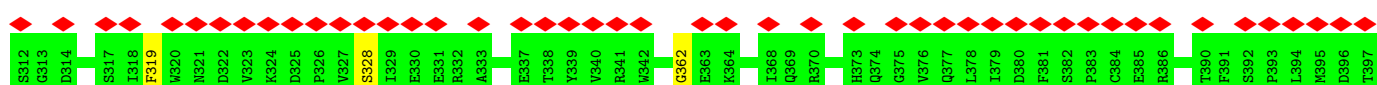
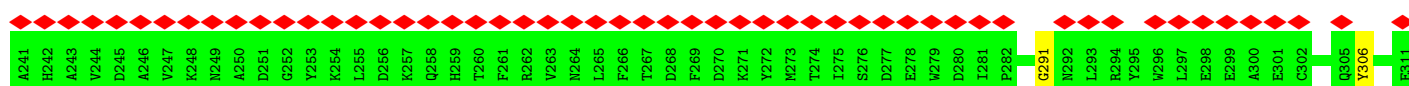
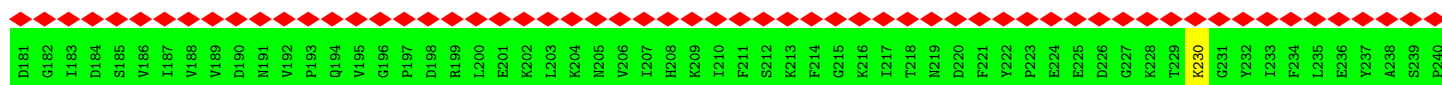
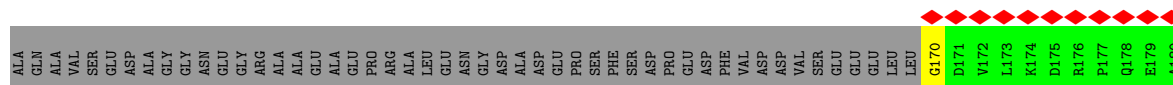
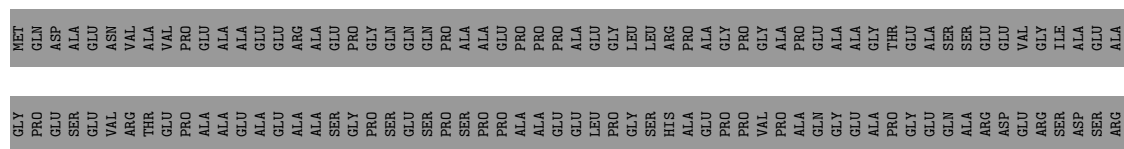
Mol	Chain	Residues	Atoms					AltConf
53	0	1	Total	C	N	O	P	0
			32	10	5	14	3	

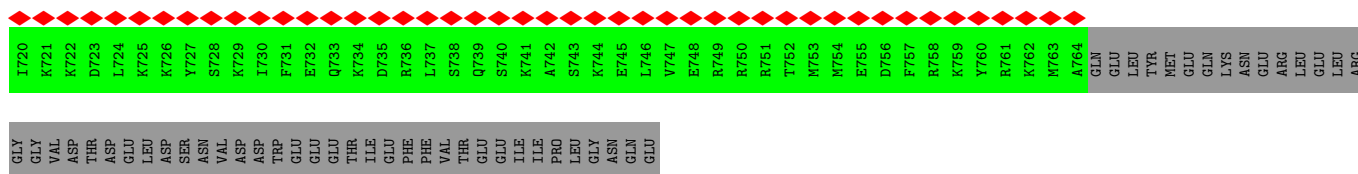
- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
54	Q	1	Total Zn 1 1	0
54	k	1	Total Zn 1 1	0

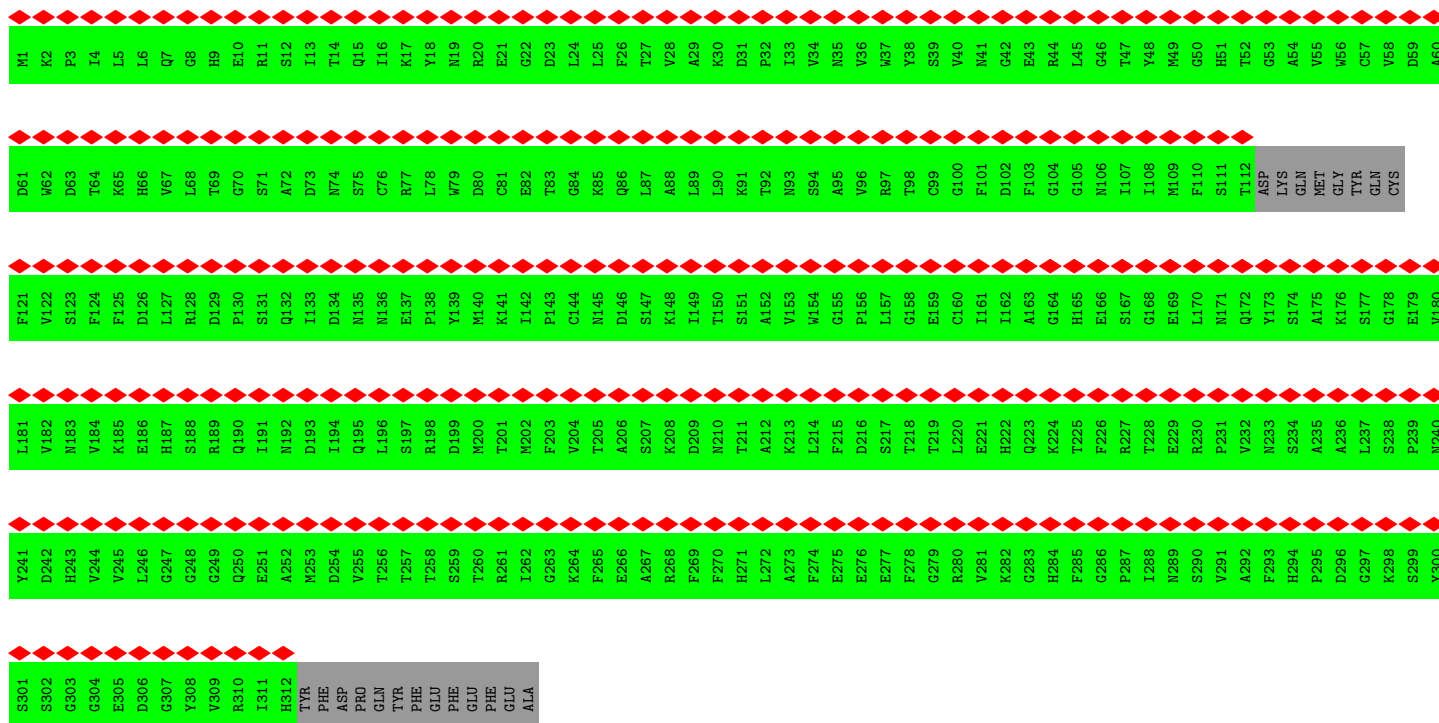


• Molecule 2: Eukaryotic translation initiation factor 3 subunit B

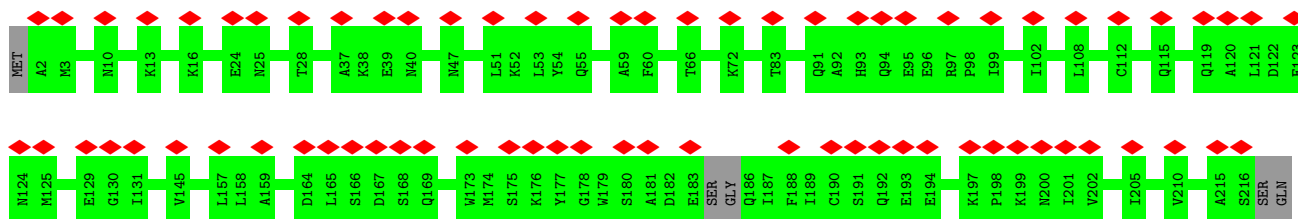




- Molecule 3: Eukaryotic translation initiation factor 3 subunit I

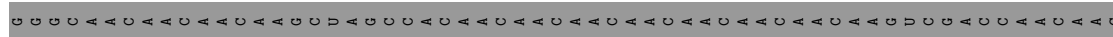


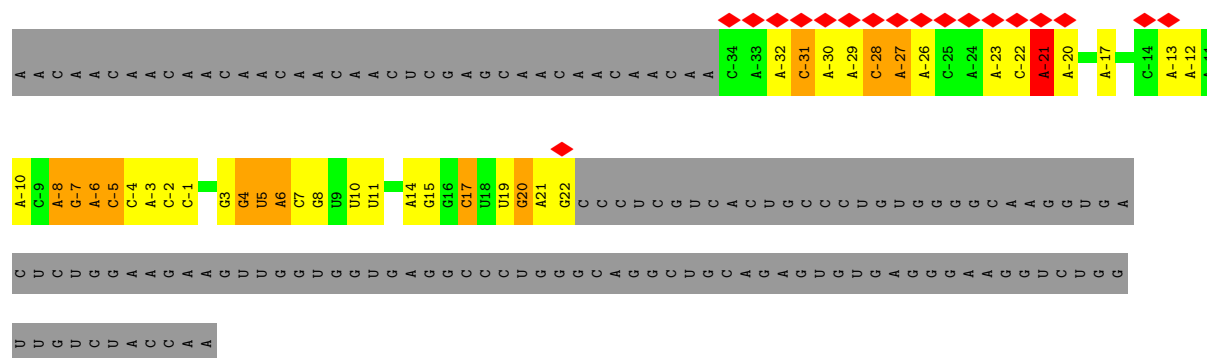
- Molecule 4: Eukaryotic translation initiation factor 3 subunit K



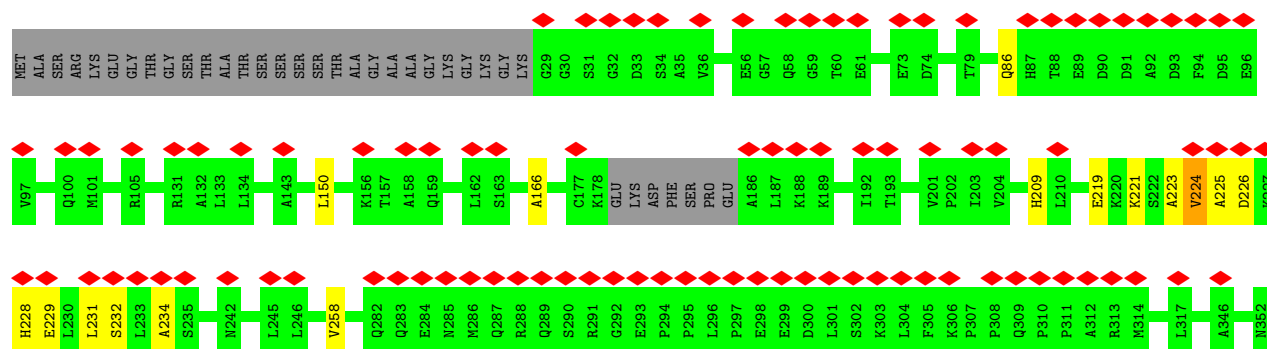
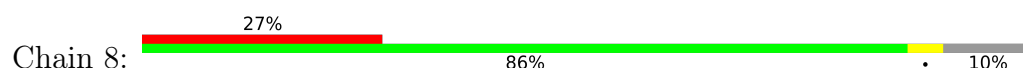
- Molecule 5: Eukaryotic translation initiation factor 3 subunit F



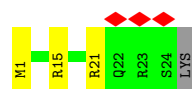
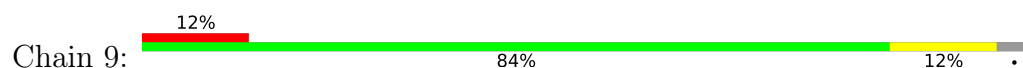




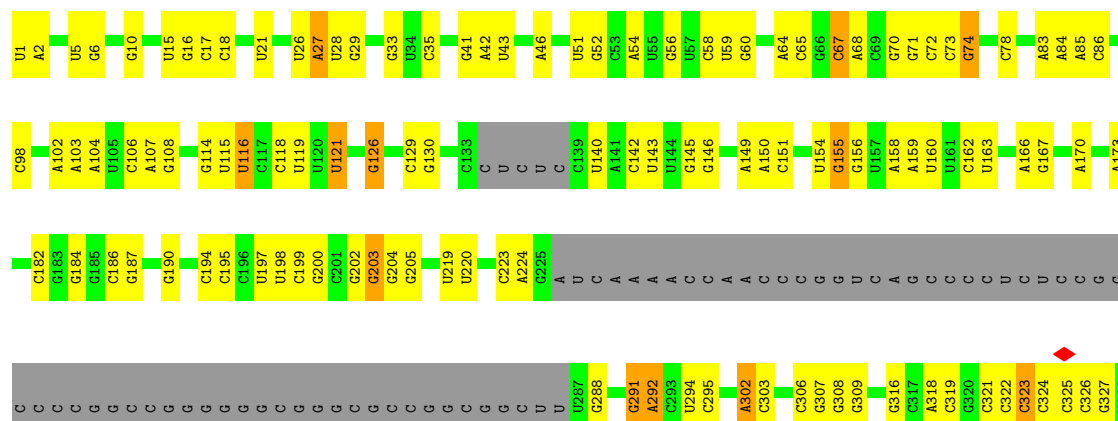
• Molecule 9: Eukaryotic translation initiation factor 3 subunit H



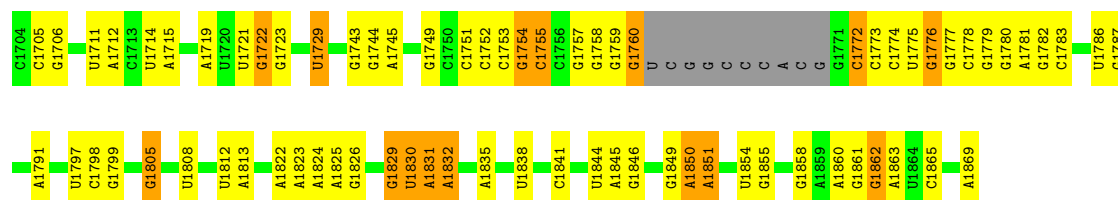
• Molecule 10: 60S ribosomal protein L41



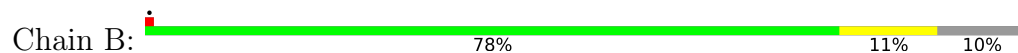
• Molecule 11: 18S rRNA



U1621	U1622	A1623	U1624	C1629	A1634	G1635	G1636	G1639	U1643	C1644	C1645	C1646	A1647	U1648	U1649	A1650	A1651	U1652	U1653	G1654	G1655	G1656	G1659	U1660	A1661	U1662	A1664	C1665	C1666	G1669	C1670	U1671	U1672	U1673	A1674	A1675	U1676	U1677	A1678	G1686	C1687	C1688	U1692	G1693	A1699	C1700	C1701	G1702	C1703				
G1520	C1521	A1522	G1526	C1527	G1528	A1533	U1535	U1536	A1537	U1543	C1544	U1545	U1550	U1551	G1552	C1553	A1556	C1557	C1558	C1559	U1560	A1561	C1562	C1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1578	A1579	A1580	U1585	U1586	G1587	U1588	A1589	C1593	A1594	C1597	U1598	U1599	G1600	A1601	U1602	G1605	G1606	C1700	G1612	U1615	
A1386	G1387	A1388	A1396	U1397	G1398	A1401	A1402	G1413	G1414	C1415	C1416	C1417	C1418	C1419	G1420	A1421	C1422	C1423	G1424	G1425	C1433	C1434	C1435	C1436	C1437	A1438	A1439	U1442	A1454	U1463	C1468	A1469	A1487	C1488	A1489	G1490	G1491	C1493	U1494	G1495	U1496	G1497	A1498	A1507	A1508	C1513	G1514						
A1195	G1274	G1275	A1276	C1277	A1278	G1279	G1280	G1281	C1282	C1283	A1284	G1285	U1288	U1289	C1290	A1291	C1292	A1293	G1294	A1295	A1301	G1302	C1303	U1308	C1309	U1310	C1322	U1326	U1327	A1332	U1333	C1341	U1342	G1345	G1348	G1354	C1355	G1356	U1360	U1371	U1372	A1378	A1379	A1382	G1289	G1270							
G1092	A1093	C1094	C1098	G991	A992	G999	U1002	U1003	U1004	G1005	C1007	A1008	A1009	A1010	A1011	U1012	U1013	U1016	U1017	U1018	G1130	A1133	C1138	A1143	A1144	A1145	C1146	C1153	U1154	U1155	U1156	U1160	G1166	A1170	U1171	U1172	A1173	U1174	A1183	G1187	A1190	U1193	A1194										
A983	C989	A990	G991	A992	G999	U1002	U1003	U1004	G1005	C1006	C1007	A1008	A1009	A1010	A1011	U1012	U1013	U1016	U1017	U1018	A1023	A1030	A1031	C1032	G1033	A1143	A1144	A1145	C1146	C1153	U1154	U1155	U1156	U1160	G1166	A1170	U1171	U1172	A1173	U1174	A1183	G1187	A1190	U1193	A1194								
A886	U887	U888	U889	U890	G891	G895	U896	U897	U898	U899	C900	G901	G902	A903	A904	A908	A913	A919	A920	G921	A922	G923	G924	G925	G928	G929	C930	G931	G932	G933	G934	U940	C941	G942	U943	C948	G949	G952	C953	G961	A962	A963	A972	C973	G976	G982							
C729	C730	G731	U732	C733	C734	C735	C736	G737	C738	C739	C740	C	U	U	U	C	C746	U747	C748	U749	C750	C751	G752	C753	G	C	C	C	C	C	U	U	U	U	A	C	C	U	G	A	U	U	U	U	U	C	C	C	G788				
A655	C860	G861	C862	C863	A664	A668	U669	A670	A671	A672	G673	U681	U688	U689	G690	G691	G692	A693	G694	C695	C696	C697	G698	G699	G700	G701	G702	C703	G704	G705	U706	C707	C708	C709	C710	C711	C712	C713	G714	A715	G716	G717	C718	G719	A720	G721	C722	C723	A724	C725	C726	G727	C728
G474	C475	A476	G477	G482	C483	A484	A485	A486	U487	U488	C492	A493	U495	A500	G507	A508	G509	C517	A520	A521	A522	A525	A526	C527	A528	A531	G534	G535	A536	C537	U538	C539	U540	U541	C542	C543	A544	A545	G546	G547	C550	U551	G552	U553	A554	A555	U556	U557					
G329	G332	G347	C350	C362	A363	A364	U367	U368	C369	G370	A371	G377	U378	C379	G380	C381	C382	C383	U384	C385	C386	C409	A418	C426	G431	C441	C442	A445	G446	A447	A448	A449	C450	G451	G452	C453	U454	A455	C459	A460	A465	G471	C472	A473									



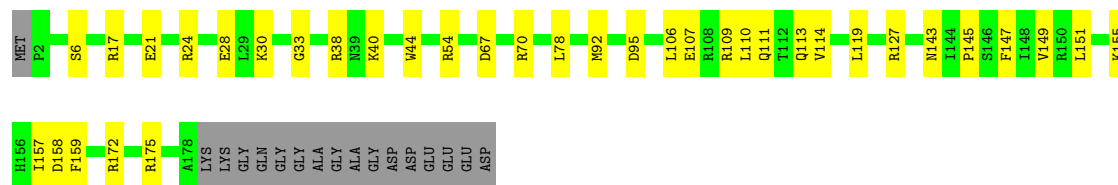
- Molecule 12: 40S ribosomal protein S11



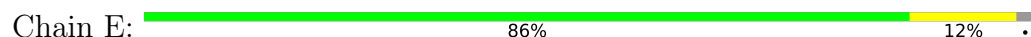
- Molecule 13: 40S ribosomal protein S4, X isoform



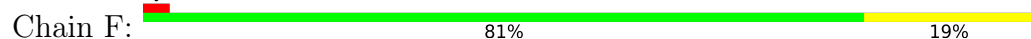
- Molecule 14: 40S ribosomal protein S9



- Molecule 15: 40S ribosomal protein S23



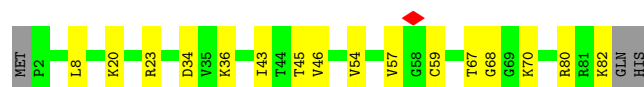
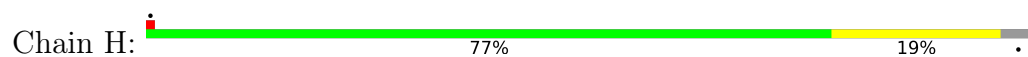
- Molecule 16: 40S ribosomal protein S30



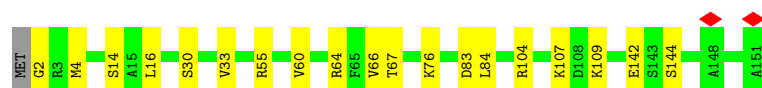
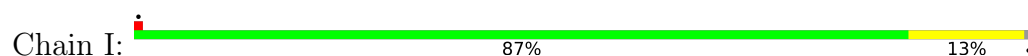
- Molecule 17: 40S ribosomal protein S7



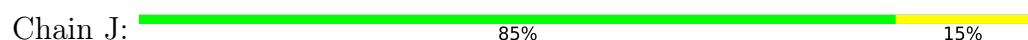
- Molecule 18: 40S ribosomal protein S27



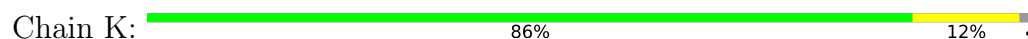
- Molecule 19: 40S ribosomal protein S13



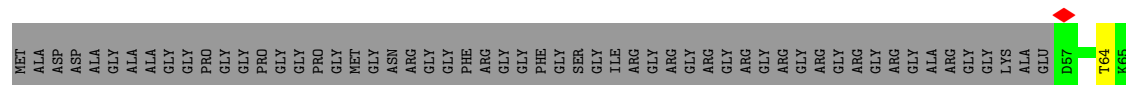
- Molecule 20: 40S ribosomal protein S15a



- Molecule 21: 40S ribosomal protein S21

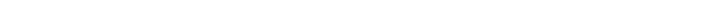


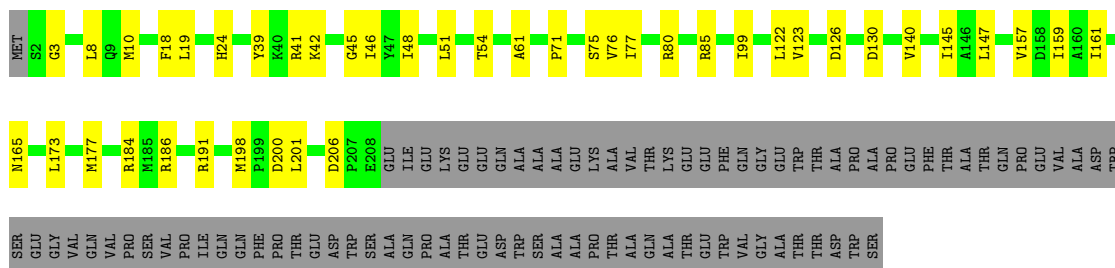
- Molecule 22: 40S ribosomal protein S2



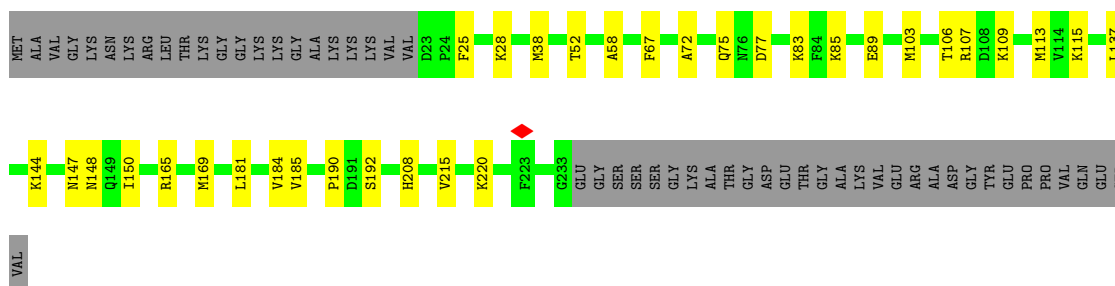
- Molecule 23: 40S ribosomal protein S17

MET	G2	I17	E36	I41	R47	V54	M58	Q62	R81	T102	L106	K107	L108	L109	R132	GLY	PRO	VAL
-----	----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	-----	-----	-----

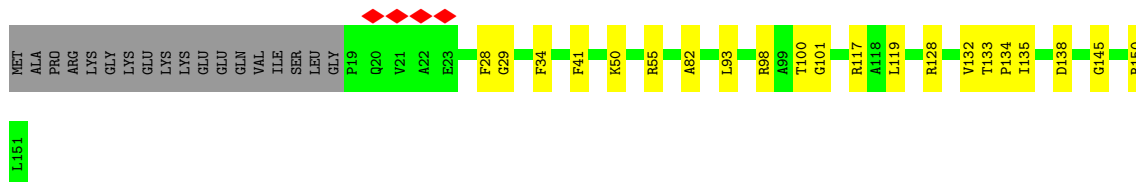
- Chain N:  56% 14% 30%



- Chain 0:  67% 12% 20%



- Chain P: 74% 14% 12%

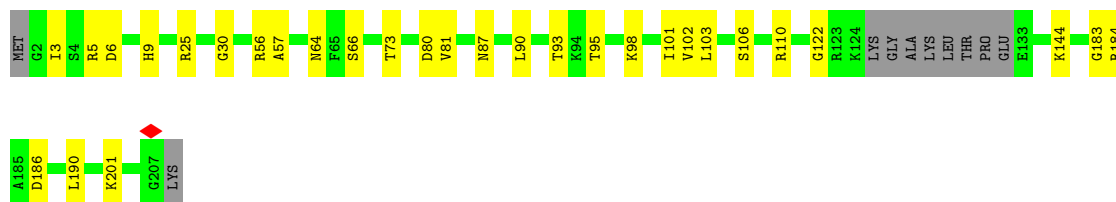


- Chain Q:  72% 14% 14%



- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

Chain R:  81% 14% 5%



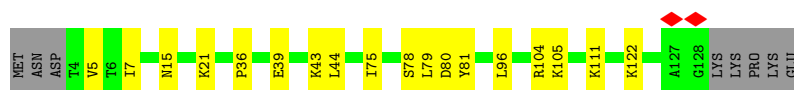
- Molecule 29: 40S ribosomal protein S6

Chain S:  82% 11% 8%



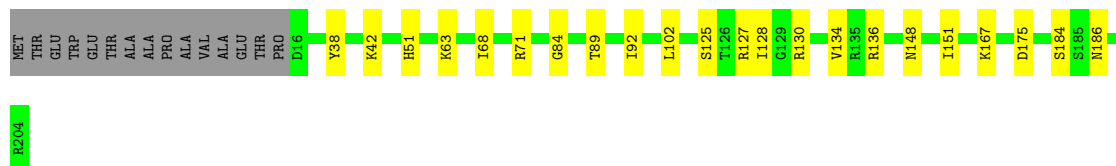
- Molecule 30: 40S ribosomal protein S24

Chain T:  80% 14% 6%



- Molecule 31: 40S ribosomal protein S5

Chain V:  82% 11% 7%



- Molecule 32: 40S ribosomal protein S16

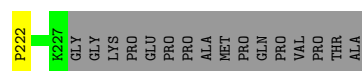
Chain Y:  86% 11% 3%



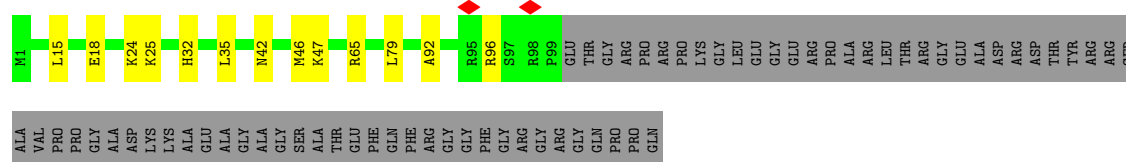
- Molecule 33: 40S ribosomal protein S3

Chain Z:  81% 12% 7%

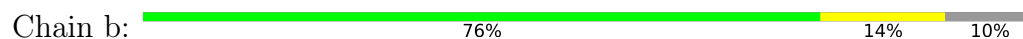




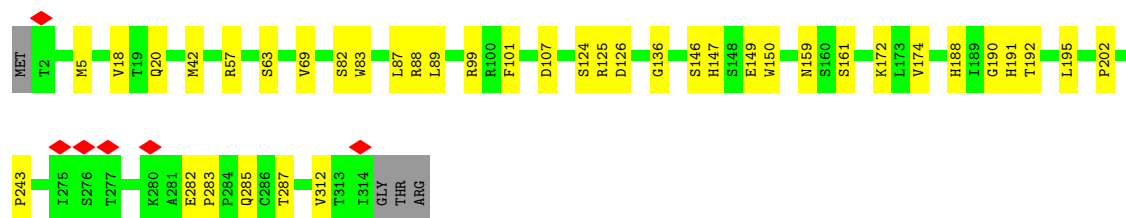
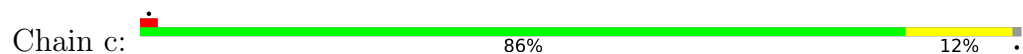
- Molecule 34: 40S ribosomal protein S10



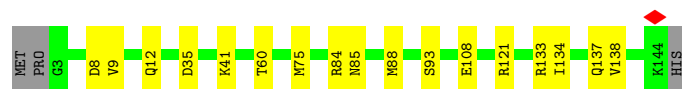
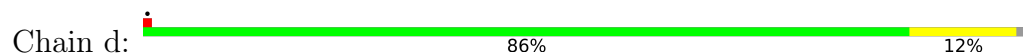
- Molecule 35: 40S ribosomal protein S15



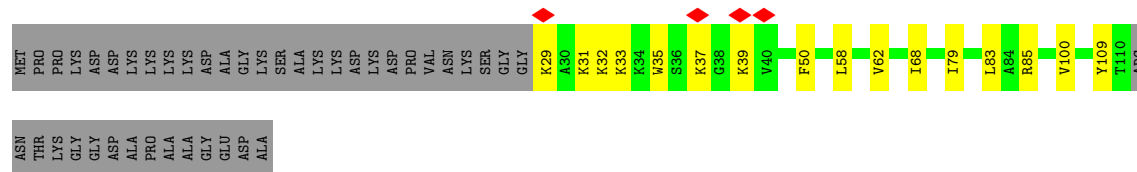
- Molecule 36: Receptor of activated protein C kinase 1



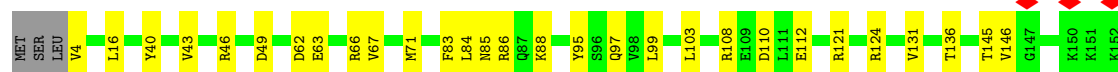
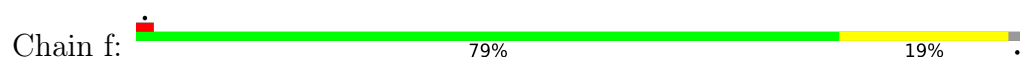
- Molecule 37: 40S ribosomal protein S19



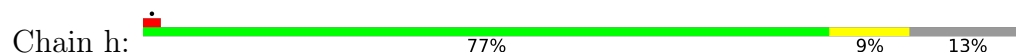
- Molecule 38: 40S ribosomal protein S25



- Molecule 39: 40S ribosomal protein S18



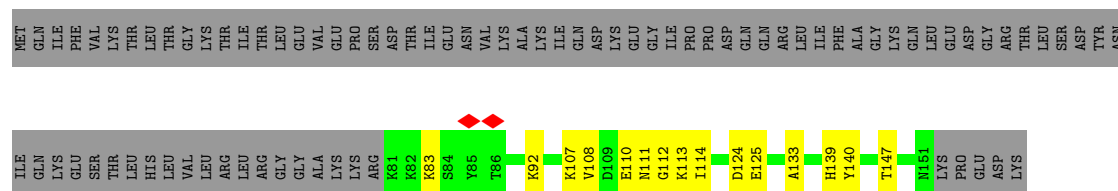
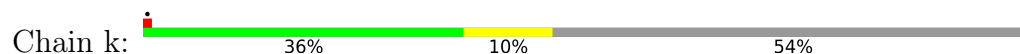
- Molecule 40: 40S ribosomal protein S20



- Molecule 41: 40S ribosomal protein S29



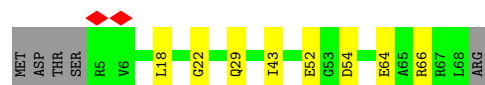
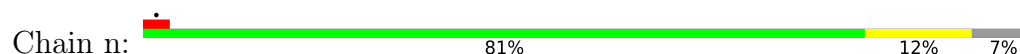
- Molecule 42: Ubiquitin



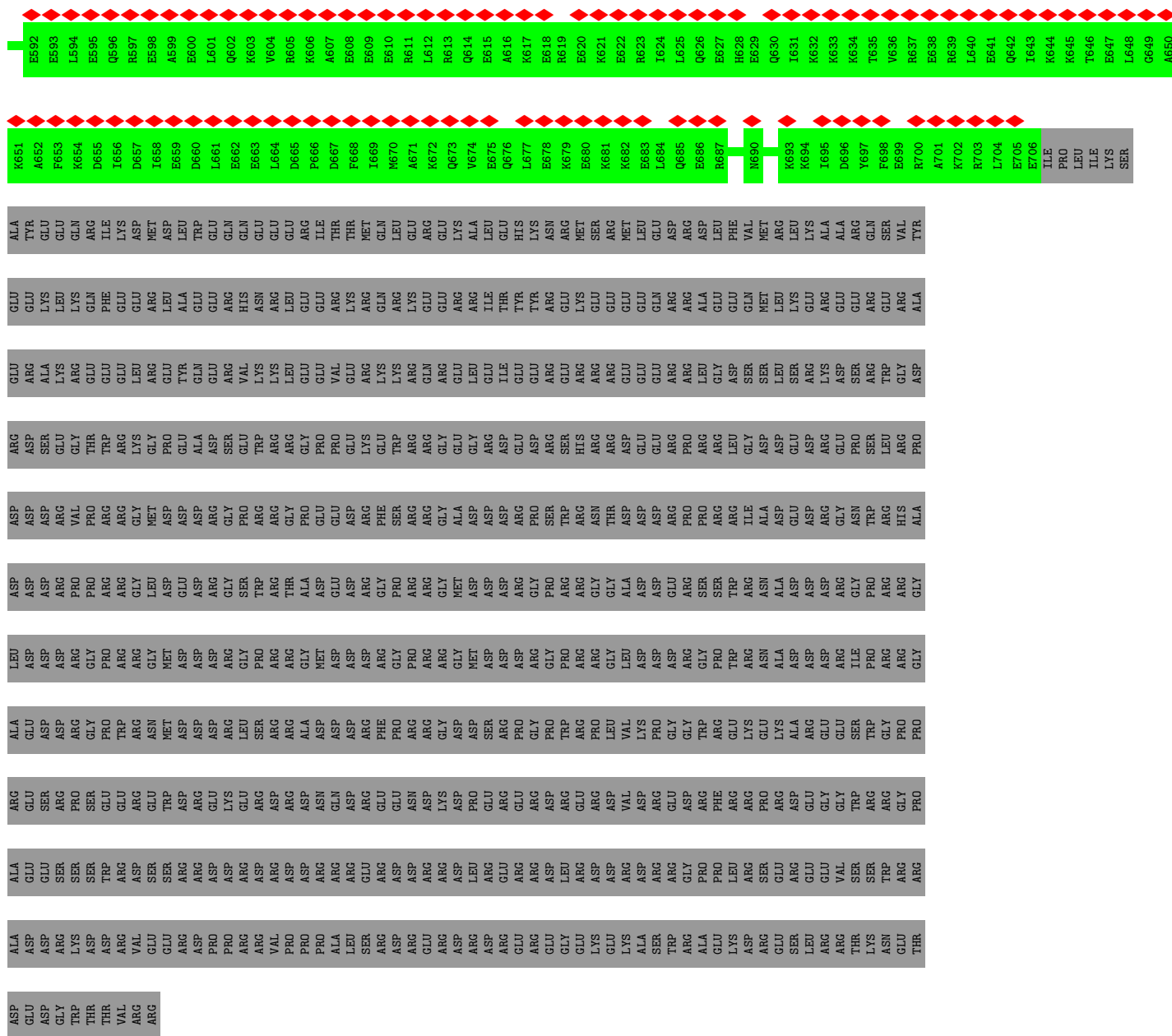
- Molecule 43: 40S ribosomal protein S12



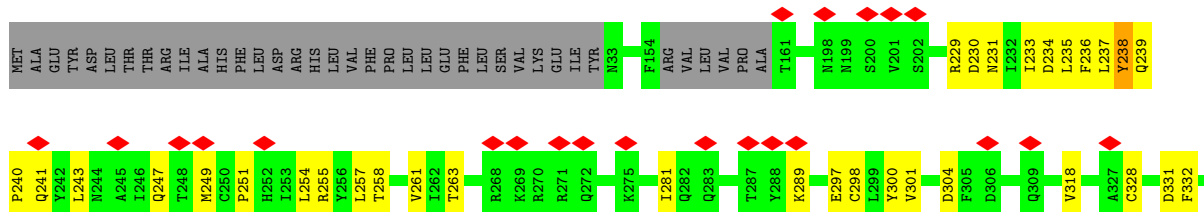
- Molecule 44: 40S ribosomal protein S28

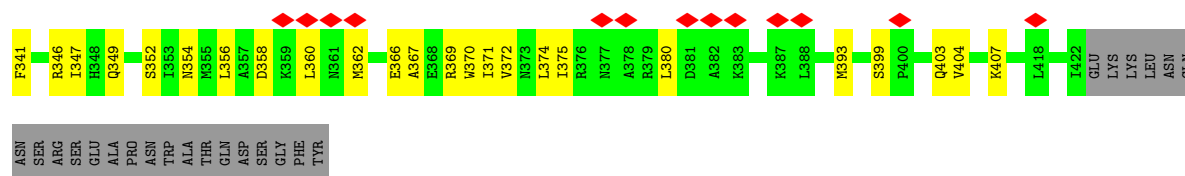


- Molecule 45: Eukaryotic translation initiation factor 3 subunit G



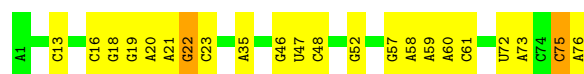
- Molecule 48: Eukaryotic translation initiation factor 3 subunit E





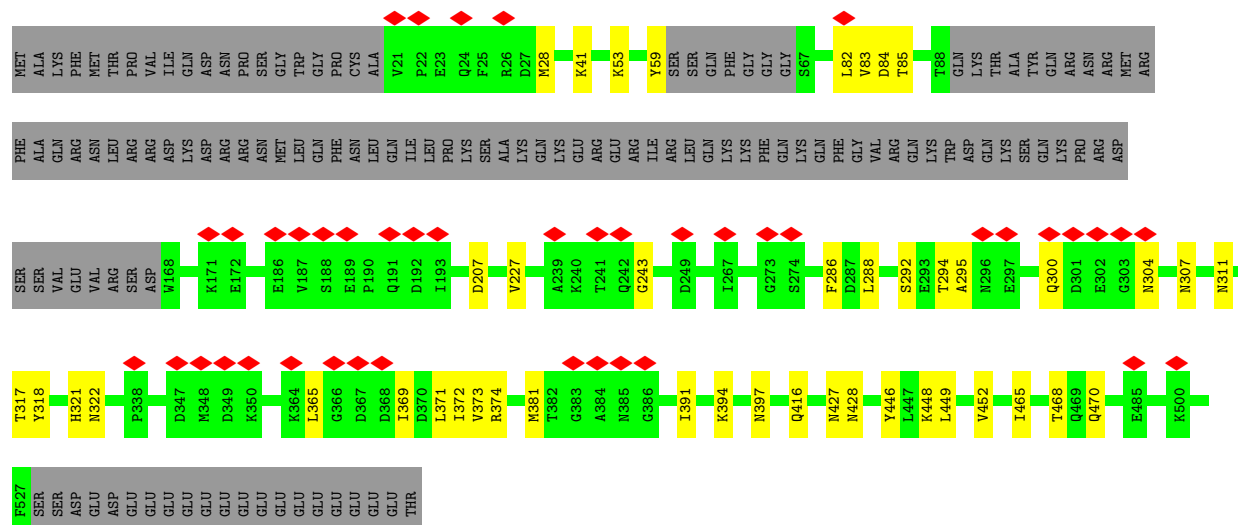
• Molecule 49: Initiator Met-tRNA-i

Chain w: 71% 27%



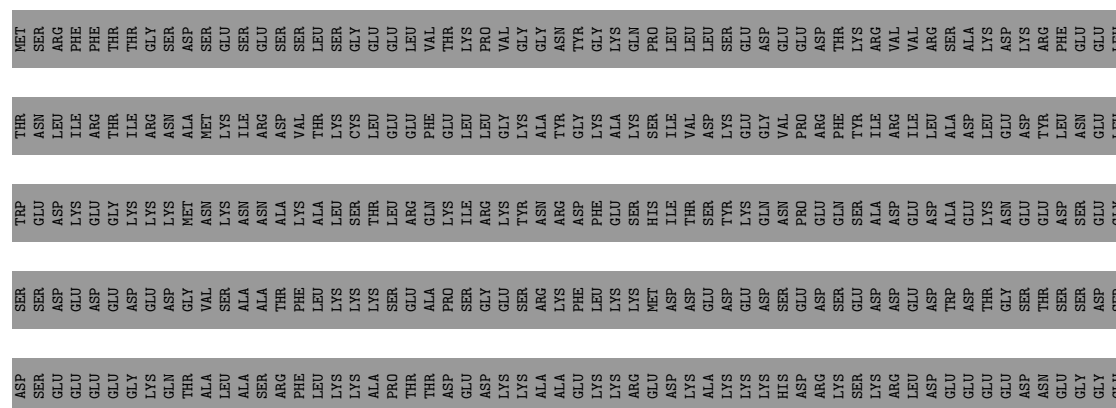
• Molecule 50: Eukaryotic translation initiation factor 3 subunit D

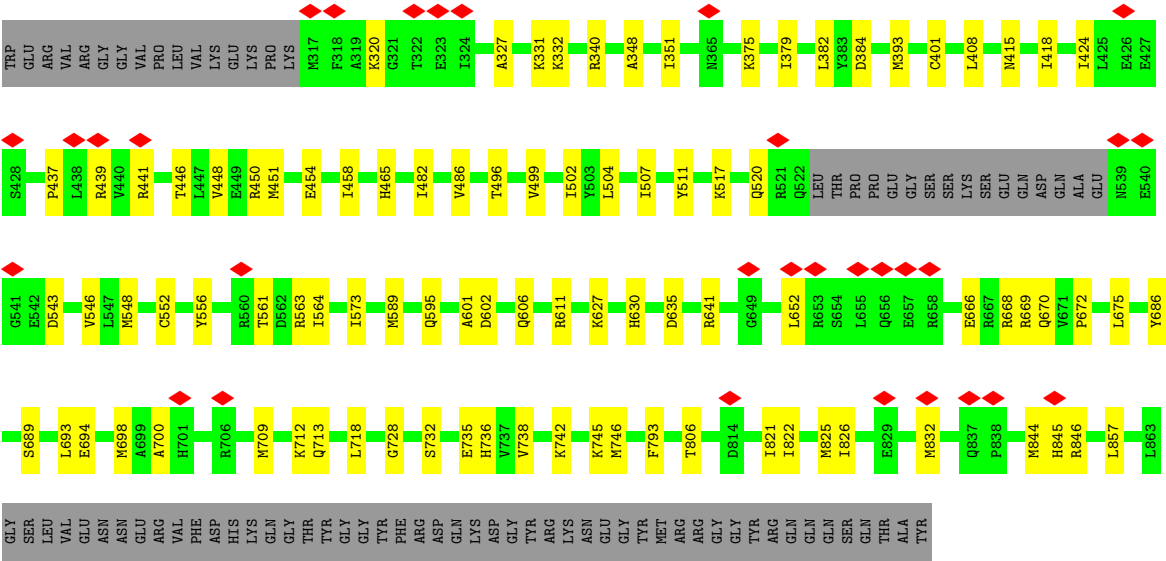
Chain x: 8% 69% 8% 23%



• Molecule 51: Eukaryotic translation initiation factor 3 subunit C

Chain y: 48% 10% 42%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	238019	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	26.872	Depositor
Minimum map value	-7.142	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3	Depositor
Map size (Å)	417.74402, 417.74402, 417.74402	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96700007, 0.96700007, 0.96700007	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, OMG, B8N, UR3, OMC, A2M, OMU, MG, 5MC, JMH, 6MZ, MA6, 5MU, ZN, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.21	0/5010	0.47	0/6754
2	1	0.17	0/3279	0.46	0/4534
3	2	0.15	0/1491	0.37	0/2068
4	3	0.11	0/1055	0.33	0/1469
5	4	0.13	0/1269	0.34	0/1762
6	5	0.13	0/1575	0.32	0/2187
7	6	0.14	0/1926	0.42	0/2669
8	7	0.17	0/1456	0.37	1/2265 (0.0%)
9	8	0.18	0/1569	0.47	1/2183 (0.0%)
10	9	0.18	0/231	0.45	0/294
11	A	0.17	1/41130 (0.0%)	0.31	0/64100
12	B	0.14	0/1186	0.32	0/1585
13	C	0.15	0/2077	0.43	2/2796 (0.1%)
14	D	0.17	0/1502	0.43	0/2008
15	E	0.16	0/1105	0.42	0/1476
16	F	0.16	0/468	0.47	0/618
17	G	0.19	0/1451	0.47	0/1942
18	H	0.16	0/644	0.41	0/864
19	I	0.18	0/1232	0.41	0/1656
20	J	0.18	0/1051	0.41	0/1406
21	K	0.18	0/623	0.42	0/833
22	L	0.19	0/1743	0.45	0/2354
23	M	0.20	0/1078	0.52	0/1447
24	N	0.18	0/1670	0.40	0/2271
25	O	0.18	0/1742	0.45	0/2330
26	P	0.20	0/1010	0.48	0/1353
27	Q	0.19	0/805	0.41	0/1079
28	R	0.15	0/1654	0.38	0/2203
29	S	0.16	0/1885	0.42	0/2510
30	T	0.17	0/1032	0.41	0/1371
31	V	0.19	0/1516	0.54	2/2037 (0.1%)
32	Y	0.21	0/1142	0.51	1/1528 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Z	0.18	0/1793	0.42	0/2414
34	a	0.18	0/859	0.46	0/1159
35	b	0.18	0/1094	0.42	0/1464
36	c	0.18	0/2493	0.48	0/3394
37	d	0.19	0/1123	0.43	0/1504
38	e	0.27	0/666	0.46	0/889
39	f	0.17	0/1245	0.46	2/1665 (0.1%)
40	h	0.21	0/827	0.55	0/1110
41	i	0.17	0/429	0.37	0/568
42	k	0.19	0/593	0.60	0/786
43	m	0.21	0/960	0.59	0/1286
44	n	0.37	1/508 (0.2%)	0.54	0/680
45	o	0.18	0/628	0.48	0/846
46	q	0.23	0/965	0.55	0/1282
47	u	0.21	0/5475	0.56	1/7432 (0.0%)
48	v	0.21	0/2672	0.53	1/3647 (0.0%)
49	w	0.15	0/1795	0.34	1/2798 (0.0%)
50	x	0.18	0/2874	0.46	0/3925
51	y	0.18	0/4380	0.48	0/5911
All	All	0.18	2/117986 (0.0%)	0.41	12/168712 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	n	29	GLN	C-N	-5.52	1.26	1.33
11	A	1830	UR3	O3'-P	5.03	1.61	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	v	238	TYR	N-CA-C	-9.06	100.15	111.75
31	V	42	LYS	CA-C-N	6.24	133.45	121.54
31	V	42	LYS	C-N-CA	6.24	133.45	121.54
47	u	353	ARG	CA-CB-CG	5.43	124.96	114.10
13	C	114	ILE	CA-C-N	5.40	136.61	120.69
13	C	114	ILE	C-N-CA	5.40	136.61	120.69
9	8	224	VAL	N-CA-C	-5.26	107.26	113.42
49	w	22	G	P-O3'-C3'	5.13	127.89	120.20
32	Y	107	GLU	N-CA-CB	5.11	118.20	110.28
39	f	145	THR	CA-C-N	5.07	127.48	120.49
39	f	145	THR	C-N-CA	5.07	127.48	120.49
8	7	-21	A	P-O3'-C3'	5.01	127.71	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4928	0	5112	84	0
2	1	3258	0	1917	24	0
3	2	1493	0	677	0	0
4	3	1057	0	475	0	0
5	4	1272	0	564	5	0
6	5	1581	0	689	3	0
7	6	1917	0	1096	10	0
8	7	1300	0	664	30	0
9	8	1571	0	683	18	0
10	9	230	0	276	3	0
11	A	37429	0	18911	325	0
12	B	1166	0	1233	10	0
13	C	2035	0	2138	16	0
14	D	1477	0	1589	28	0
15	E	1087	0	1154	12	0
16	F	461	0	500	10	0
17	G	1430	0	1520	18	0
18	H	631	0	657	11	0
19	I	1208	0	1294	15	0
20	J	1034	0	1080	15	0
21	K	617	0	622	7	0
22	L	1707	0	1794	15	0
23	M	1064	0	1118	9	0
24	N	1633	0	1640	28	0
25	O	1715	0	1785	21	0
26	P	997	0	1021	16	0
27	Q	792	0	843	16	0
28	R	1627	0	1706	21	0
29	S	1862	0	2017	21	0
30	T	1015	0	1086	13	0
31	V	1495	0	1549	14	0
32	Y	1124	0	1193	9	0
33	Z	1765	0	1865	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	a	834	0	861	9	0
35	b	1072	0	1121	17	0
36	c	2436	0	2393	23	0
37	d	1105	0	1138	12	0
38	e	658	0	737	14	0
39	f	1227	0	1298	21	0
40	h	817	0	882	8	0
41	i	419	0	415	8	0
42	k	581	0	595	10	0
43	m	950	0	987	17	0
44	n	506	0	536	6	0
45	o	616	0	600	9	0
46	q	951	0	981	17	0
47	u	5383	0	5085	90	0
48	v	2635	0	2207	75	0
49	w	1604	0	816	2	0
50	x	2831	0	2199	30	0
51	y	4305	0	4321	60	0
52	0	1	0	0	0	0
52	A	87	0	0	0	0
52	P	1	0	0	0	0
52	S	1	0	0	0	0
52	f	1	0	0	0	0
53	0	32	0	12	1	0
54	Q	1	0	0	0	0
54	k	1	0	0	0	0
All	All	113033	0	87652	1051	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 5.

All (1051) 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)
48:v:231:ASN:CB	48:v:235:LEU:HD22	1.82	1.08
9:8:225:ALA:HA	9:8:229:GLU:CB	1.84	1.06
48:v:230:ASP:C	48:v:235:LEU:HD13	1.81	1.05
48:v:231:ASN:HA	48:v:235:LEU:HD13	1.38	1.04
9:8:225:ALA:CA	9:8:229:GLU:CB	2.36	1.03
48:v:231:ASN:CA	48:v:235:LEU:HD13	1.89	1.02
8:7:-5:C:O2'	8:7:-4[B]:C:OP2	1.78	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:v:235:LEU:HD23	48:v:238:TYR:OH	1.60	1.00
48:v:231:ASN:CA	48:v:235:LEU:HD22	1.93	0.99
48:v:231:ASN:HA	48:v:235:LEU:CD1	1.93	0.98
48:v:231:ASN:HA	48:v:235:LEU:CG	1.96	0.95
48:v:231:ASN:N	48:v:235:LEU:HD13	1.81	0.94
48:v:231:ASN:HA	48:v:235:LEU:HD22	1.47	0.93
48:v:231:ASN:HA	48:v:235:LEU:CD2	1.99	0.92
11:A:925:G:H1	11:A:1017:U:H3	1.19	0.90
48:v:236:PHE:O	48:v:240:PRO:HD2	1.71	0.90
48:v:235:LEU:CD2	48:v:238:TYR:OH	2.19	0.89
8:7:-5:C:O2'	8:7:-4[B]:C:P	2.30	0.89
9:8:225:ALA:HB1	9:8:229:GLU:CB	2.06	0.85
9:8:225:ALA:CB	9:8:229:GLU:CB	2.55	0.85
48:v:231:ASN:HB3	48:v:235:LEU:HD22	1.57	0.85
11:A:878:G:H1	11:A:908:A:H61	1.25	0.84
47:u:100:LYS:O	47:u:104:ALA:HB3	1.81	0.80
48:v:230:ASP:O	48:v:235:LEU:HD13	1.86	0.76
35:b:141:PHE:CE2	35:b:143:PRO:HB3	2.22	0.73
48:v:236:PHE:CE2	48:v:238:TYR:HB3	2.23	0.73
8:7:4:G:H5''	35:b:145:LYS:HB2	1.72	0.72
48:v:231:ASN:O	48:v:235:LEU:HB2	1.90	0.71
48:v:235:LEU:HB3	48:v:238:TYR:HE1	1.55	0.71
11:A:1652:G:H1	11:A:1672:U:H3	1.37	0.70
48:v:230:ASP:C	48:v:235:LEU:CD1	2.64	0.69
7:6:308:VAL:HA	7:6:311:PHE:HB3	1.74	0.69
2:1:469:ASP:HB3	2:1:482:TRP:HB3	1.73	0.69
11:A:1033:G:H1	11:A:1080:A:HO2'	1.39	0.69
48:v:233:ILE:HB	48:v:257:LEU:HD21	1.73	0.69
11:A:851:C:H5''	11:A:852:G:H5'	1.75	0.69
48:v:237:LEU:HD23	48:v:240:PRO:HB2	1.75	0.69
11:A:1228:A:C5'	38:e:31:LYS:HZ3	2.06	0.69
14:D:127:ARG:HD3	16:F:105:ARG:HD3	1.75	0.68
17:G:154:ILE:HB	17:G:185:VAL:HG12	1.75	0.68
24:N:173:LEU:HG	24:N:177:MET:HE2	1.77	0.67
11:A:1533:A:H62	11:A:1602:U:H3	1.43	0.67
22:L:64:THR:HG23	22:L:67:GLY:H	1.60	0.67
48:v:233:ILE:HG23	48:v:234:ASP:H	1.60	0.67
9:8:225:ALA:O	9:8:229:GLU:CB	2.43	0.67
11:A:878:G:H1	11:A:908:A:N6	1.92	0.67
11:A:919:A:H5''	19:I:16:LEU:HD12	1.76	0.66
11:A:1743:G:H21	11:A:1791:A:H62	1.41	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:f:85:ASN:ND2	39:f:97:GLN:OE1	2.29	0.66
24:N:77:ILE:HG12	24:N:99:ILE:HB	1.78	0.65
11:A:888:U:O4	11:A:900:C:N3	2.30	0.65
8:7:-5:C:HO2'	8:7:-4[B]:C:P	2.07	0.65
47:u:100:LYS:O	47:u:104:ALA:CB	2.44	0.65
51:y:439:ARG:HH12	51:y:441:ARG:HE	1.46	0.64
1:0:719:LEU:HD23	1:0:876:ILE:HD12	1.79	0.64
48:v:263:THR:HG21	48:v:328:CYS:HB2	1.79	0.64
1:0:1103:ASN:HB2	1:0:1109:VAL:HG22	1.77	0.64
11:A:940:U:H3	11:A:1002:U:H3	1.45	0.64
48:v:231:ASN:HA	48:v:235:LEU:CB	2.28	0.64
11:A:563:G:N7	14:D:172:ARG:NH1	2.43	0.63
23:M:109:LEU:HD21	24:N:10:MET:HE1	1.80	0.63
25:O:107:ARG:NH1	26:P:133:THR:O	2.31	0.63
47:u:301:HIS:HB3	47:u:376:ARG:HH21	1.63	0.63
51:y:694:GLU:HG2	51:y:698:MET:HE2	1.79	0.63
8:7:-21:A:H62	47:u:192:ALA:HB1	1.64	0.63
23:M:58:MET:O	23:M:62:GLN:NE2	2.32	0.63
28:R:110:ARG:HH21	28:R:122:GLY:HA3	1.64	0.63
2:1:548:ARG:HB3	2:1:555:PRO:HD2	1.79	0.63
47:u:185:CYS:O	47:u:188:TYR:O	2.17	0.63
51:y:821:ILE:HG22	51:y:825:MET:HE1	1.80	0.63
34:a:92:ALA:HA	34:a:96:ARG:HD3	1.80	0.63
50:x:82:LEU:HG	50:x:84:ASP:HB3	1.81	0.63
47:u:289:ALA:HB3	47:u:330:PRO:HD3	1.79	0.63
25:O:72:ALA:HB3	26:P:128:ARG:HH12	1.63	0.62
47:u:234:LEU:HD11	47:u:275:TYR:HA	1.81	0.62
47:u:267:PRO:HB2	47:u:272:MET:HE3	1.82	0.62
18:H:59:CYS:HB3	51:y:446:THR:HG21	1.80	0.62
11:A:801:U:O4	17:G:106:ARG:NH1	2.32	0.62
51:y:709:MET:HE2	51:y:712:LYS:HD3	1.81	0.62
1:0:984:GLN:HG3	1:0:1013:VAL:HG22	1.81	0.62
11:A:614:C:OP1	46:q:62:ARG:NH2	2.32	0.62
1:0:968:LYS:HA	1:0:971:LEU:HG	1.81	0.61
1:0:978:GLU:O	15:E:97:ASN:ND2	2.32	0.61
1:0:1095:LYS:NZ	1:0:1178:ALA:O	2.33	0.61
13:C:11:ARG:HA	13:C:28:ALA:HB2	1.82	0.61
30:T:5:VAL:O	30:T:43:LYS:NZ	2.34	0.61
43:m:52:LEU:HD13	43:m:65:VAL:HG11	1.82	0.61
31:V:71:ARG:NH2	31:V:148:ASN:OD1	2.32	0.61
11:A:1086:G:OP2	27:Q:12:LYS:NZ	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:M:36:GLU:OE1	23:M:47:ARG:NH1	2.34	0.61
1:0:1094:ILE:HD12	1:0:1125:MET:HE2	1.81	0.61
13:C:176:ASP:OD1	13:C:179:ASN:ND2	2.34	0.61
33:Z:16:ILE:HD11	41:i:36:LEU:HD23	1.83	0.61
34:a:32:HIS:HB3	34:a:35:LEU:HB2	1.83	0.61
1:0:712:LEU:HD21	1:0:989:GLY:HA3	1.83	0.61
27:Q:64:LEU:HD12	27:Q:65:PRO:HD2	1.82	0.61
14:D:54:ARG:NH2	22:L:200:ARG:O	2.32	0.61
9:8:225:ALA:C	9:8:229:GLU:CB	2.73	0.60
51:y:507:ILE:O	51:y:511:TYR:HB3	2.00	0.60
11:A:874:G:H2'	11:A:875:A:H8	1.67	0.60
9:8:219:GLU:O	9:8:223:ALA:N	2.34	0.60
1:0:982:TYR:O	1:0:1034:ILE:HA	2.01	0.59
11:A:1016:U:OP2	18:H:20:LYS:NZ	2.34	0.59
37:d:85:ASN:HB2	37:d:88:MET:HB2	1.83	0.59
45:o:302:GLY:HA2	45:o:309:ILE:HG23	1.83	0.59
24:N:42:LYS:HD3	24:N:46:ILE:HB	1.84	0.59
48:v:231:ASN:HA	48:v:235:LEU:HB2	1.84	0.59
15:E:98:ASP:OD2	15:E:140:ARG:NH2	2.34	0.59
47:u:405:GLU:HA	47:u:408:THR:HG22	1.85	0.59
25:O:77:ASP:OD2	47:u:14[B]:ARG:NH1	2.35	0.59
8:7:-5:C:H1'	8:7:-4[A]:C:C6	2.38	0.59
11:A:507:G:OP2	30:T:104:ARG:NH2	2.36	0.59
50:x:452:VAL:HG22	50:x:465:ILE:HG22	1.84	0.59
51:y:735:GLU:HA	51:y:738:VAL:HG12	1.83	0.59
33:Z:62:LYS:O	33:Z:67:ARG:NH2	2.36	0.59
18:H:57:VAL:HG23	18:H:59:CYS:H	1.66	0.58
26:P:117:ARG:NH2	44:n:64:GLU:OE2	2.35	0.58
2:1:565:ILE:HD11	2:1:579:VAL:HB	1.84	0.58
12:B:104:LYS:O	15:E:11:ARG:NH2	2.36	0.58
22:L:191:VAL:HG11	22:L:236:PHE:HA	1.85	0.58
48:v:231:ASN:CG	48:v:235:LEU:HD22	2.28	0.58
14:D:28:GLU:OE2	14:D:44:TRP:NE1	2.36	0.58
11:A:1563:G:OP1	37:d:121:ARG:NH1	2.37	0.58
1:0:888:ILE:HG22	1:0:949:VAL:HG22	1.84	0.58
1:0:725:LEU:HD21	1:0:737:THR:HG23	1.84	0.58
48:v:375:ILE:HG12	48:v:380:LEU:HD22	1.84	0.58
51:y:627:LYS:HA	51:y:693:LEU:HD11	1.84	0.58
11:A:43:U:OP2	11:A:485:A:N6	2.36	0.58
11:A:303:C:O2	28:R:184:ARG:NH1	2.36	0.58
16:F:110:MET:HE3	16:F:114:ARG:HH21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:660:GLU:OE2	1:0:914:ARG:NH1	2.36	0.58
11:A:1677:U:H2'	11:A:1678:A2M:H8	1.86	0.58
47:u:329:ILE:O	47:u:367:ARG:NH1	2.37	0.58
51:y:382:LEU:HD13	51:y:401:CYS:HA	1.85	0.58
11:A:1204:A:O2'	11:A:1700:C:OP2	2.22	0.58
13:C:54:TYR:O	30:T:15:ASN:ND2	2.36	0.58
38:e:50:PHE:HB2	39:f:4:VAL:HG12	1.85	0.58
11:A:1396:A:O2'	11:A:1398:G:N7	2.35	0.58
48:v:235:LEU:HD22	48:v:238:TYR:OH	2.02	0.58
50:x:381:MET:HE3	50:x:391:ILE:HG21	1.86	0.58
1:0:983:VAL:HG12	1:0:1035:LEU:HB2	1.86	0.57
11:A:377:G:H5'	28:R:98:LYS:HB3	1.86	0.57
11:A:546:G:N2	11:A:547:G:O6	2.36	0.57
11:A:28:U:H2'	11:A:29:G:H8	1.69	0.57
11:A:1605:G:OP1	37:d:84:ARG:NH2	2.37	0.57
29:S:159:ARG:NH2	29:S:171:THR:O	2.36	0.57
44:n:18:LEU:HD11	44:n:43:ILE:HD12	1.86	0.57
11:A:922:A:OP2	20:J:28:ARG:NH1	2.38	0.57
11:A:1593:C:O2	37:d:12:GLN:NE2	2.33	0.57
35:b:81:ARG:NH2	35:b:120:SER:O	2.37	0.57
31:V:127:ARG:HA	31:V:136:ARG:HG2	1.87	0.57
39:f:67:VAL:HG12	39:f:71:MET:HE2	1.87	0.57
13:C:100:ARG:HB2	13:C:114:ILE:HD13	1.86	0.57
48:v:240:PRO:HA	48:v:243:LEU:HB2	1.87	0.57
1:0:657:GLN:NE2	1:0:658:ASP:OD1	2.38	0.57
43:m:47:ALA:HA	43:m:112:LYS:HA	1.87	0.57
48:v:230:ASP:O	48:v:235:LEU:CD1	2.52	0.57
11:A:871:U:OP2	19:I:76:LYS:NZ	2.37	0.57
50:x:448:LYS:HD2	50:x:470:GLN:HG2	1.86	0.57
51:y:450:ARG:NH2	51:y:454:GLU:OE2	2.38	0.57
31:V:167:LYS:NZ	31:V:175:ASP:OD2	2.38	0.57
1:0:707:GLU:HA	1:0:713:ARG:HH22	1.68	0.57
11:A:1550:G:H3'	11:A:1579:A:H61	1.70	0.57
27:Q:45:VAL:HG11	27:Q:53:ILE:HG13	1.86	0.57
31:V:130:ARG:HH12	31:V:134:VAL:HG12	1.69	0.56
8:7:4:G:O2'	8:7:6:A:OP1	2.22	0.56
11:A:507:G:O6	30:T:105:LYS:NZ	2.38	0.56
25:O:67:PHE:O	25:O:85:LYS:HA	2.05	0.56
1:0:902:ARG:HE	1:0:936:LYS:HD2	1.71	0.56
8:7:17:C:O2	33:Z:54:ARG:NH2	2.38	0.56
11:A:606:G:N3	16:F:132:ASN:ND2	2.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1199:A:H5''	27:Q:2:THR:HB	1.88	0.56
11:A:1658:G:OP2	11:A:1660:C:N4	2.38	0.56
11:A:322:C:N4	11:A:323:C:O2	2.38	0.56
11:A:1854:U:OP1	26:P:150:ARG:NH1	2.38	0.56
15:E:60:LYS:H	15:E:114:ASP:HB2	1.70	0.56
1:O:1033:VAL:HG12	1:O:1055:ARG:HB2	1.86	0.56
11:A:67:C:N4	29:S:168:LYS:O	2.39	0.56
11:A:379:C:O2	28:R:5:ARG:NE	2.38	0.56
36:c:42:MET:HE2	36:c:57:ARG:HB3	1.88	0.56
48:v:297:GLU:HA	48:v:300:TYR:HD2	1.70	0.56
51:y:561:THR:HG22	51:y:563:ARG:H	1.70	0.56
11:A:72:C:O2'	11:A:74:G:N2	2.39	0.56
11:A:976:G:H21	26:P:50:LYS:HE2	1.71	0.56
11:A:1032:C:H5''	19:I:109:LYS:HD2	1.87	0.56
48:v:249:MET:HB3	48:v:254:LEU:HD11	1.87	0.56
51:y:448:VAL:HG11	51:y:486:VAL:HG21	1.87	0.56
47:u:52:LEU:HD22	47:u:89:VAL:HG23	1.88	0.55
47:u:185:CYS:O	47:u:188:TYR:C	2.49	0.55
47:u:540:ALA:HA	47:u:543:LEU:HB2	1.88	0.55
48:v:371:ILE:HD13	48:v:374:LEU:HD21	1.88	0.55
28:R:101:ILE:HD12	28:R:190:LEU:HD11	1.89	0.55
48:v:237:LEU:O	48:v:238:TYR:C	2.44	0.55
8:7:-3[A]:A:H2	11:A:1056:U:HO2'	1.53	0.55
47:u:340:ARG:HH22	51:y:742:LYS:HA	1.71	0.55
11:A:551:U:H5'	16:F:117:VAL:HG11	1.89	0.55
11:A:1291:A:N3	42:k:140:TYR:OH	2.39	0.55
27:Q:12:LYS:HG2	27:Q:15:ARG:HB2	1.88	0.55
36:c:87:LEU:HB2	36:c:101:PHE:HB2	1.88	0.55
43:m:33:ARG:HD2	43:m:91:LEU:HD23	1.87	0.55
47:u:296:LEU:HB3	47:u:322:VAL:HG22	1.87	0.55
8:7:5:U:H5'	46:q:11:ASN:HB3	1.88	0.55
11:A:1497:G:N7	34:a:25:LYS:NZ	2.43	0.55
1:O:991:LEU:HD21	1:O:1008:ILE:HB	1.88	0.55
8:7:-29:A:H5''	51:y:712:LYS:HE3	1.89	0.55
11:A:913:A:N6	17:G:119:SER:O	2.40	0.55
43:m:49:LEU:HD12	43:m:75:ASN:HB3	1.87	0.55
8:7:-7:G:N2	44:n:66:ARG:O	2.40	0.55
11:A:60:G:H22	11:A:316:G:H21	1.54	0.55
11:A:1124:C:H5''	25:O:150:ILE:HG12	1.88	0.55
34:a:65:ARG:NH1	41:i:20:SER:OG	2.40	0.55
11:A:1129:G:H3'	11:A:1130:G:H21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:E:39:ASN:ND2	15:E:42:GLY:O	2.37	0.54
35:b:145:LYS:HA	46:q:70:TRP:CH2	2.41	0.54
47:u:324:LEU:HD12	47:u:424:LEU:HD22	1.89	0.54
12:B:135:SER:O	12:B:139:ARG:NH1	2.40	0.54
21:K:38:GLU:OE1	21:K:51:LYS:NZ	2.33	0.54
5:4:163:VAL:HA	9:8:86:GLN:HA	1.89	0.54
11:A:1650:A:H5''	32:Y:139:ALA:HB2	1.90	0.54
17:G:144:ILE:HB	20:J:52:ILE:HB	1.89	0.54
28:R:93:THR:HG23	28:R:95:THR:HG23	1.88	0.54
47:u:95:LYS:NZ	47:u:99:GLU:OE1	2.40	0.54
1:0:902:ARG:NH1	11:A:477:G:O2'	2.41	0.54
11:A:528:A:N1	11:A:557:U:O2'	2.40	0.54
25:O:89:GLU:OE1	25:O:220:LYS:NZ	2.40	0.54
50:x:243:GLY:HA3	50:x:372:ILE:HD11	1.88	0.54
1:0:673:VAL:HB	1:0:698:MET:HB2	1.89	0.54
11:A:1228:A:H2'	11:A:1229:G:C8	2.42	0.54
24:N:41:ARG:HE	24:N:45:GLY:HA2	1.73	0.54
26:P:145:GLY:O	27:Q:22:ARG:NH2	2.37	0.54
11:A:948:C:H2'	11:A:949:G:H8	1.72	0.54
11:A:1398:G:H1'	36:c:63:SER:HB3	1.89	0.54
25:O:75:GLN:NE2	47:u:17:GLU:OE2	2.41	0.54
8:7:-5:C:C2'	8:7:-4[B]:C:OP2	2.43	0.54
11:A:973:C:N3	26:P:55:ARG:NH2	2.55	0.54
36:c:124:SER:OG	36:c:126:ASP:OD1	2.24	0.54
1:0:630:ARG:NH1	1:0:721:ASP:OD2	2.37	0.54
1:0:647:ILE:O	1:0:651:LEU:HG	2.08	0.54
11:A:1597:C:OP2	38:e:85:ARG:NH2	2.41	0.54
47:u:330:PRO:HB2	47:u:333:PRO:HG3	1.89	0.54
11:A:643:A:OP1	14:D:38:ARG:NH1	2.41	0.53
11:A:860:G:N2	20:J:107:SER:OG	2.41	0.53
28:R:87:ASN:HB3	28:R:90:LEU:HG	1.90	0.53
50:x:28:MET:HE1	51:y:556:TYR:HD2	1.73	0.53
11:A:624:C:N4	15:E:63:ASN:OD1	2.34	0.53
11:A:1160:U:O4	15:E:2:GLY:N	2.41	0.53
43:m:82:ASN:ND2	43:m:107:SER:OG	2.39	0.53
1:0:1013:VAL:HB	1:0:1041:ILE:HG23	1.90	0.53
11:A:1242:U:OP1	46:q:23:LYS:NZ	2.41	0.53
26:P:29:GLY:O	26:P:93:LEU:HA	2.09	0.53
26:P:98:ARG:HB3	26:P:132:VAL:HG23	1.90	0.53
47:u:135:GLU:OE2	51:y:465:HIS:ND1	2.36	0.53
11:A:649:U:H2'	11:A:650:A:H8	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:u:43:TRP:HZ3	47:u:46:ILE:HG22	1.73	0.53
11:A:664:A:O2'	11:A:670:A:N1	2.41	0.53
11:A:1013:U:OP1	11:A:1129:G:O2'	2.26	0.53
31:V:89:THR:HA	31:V:92:ILE:HG12	1.90	0.53
47:u:571:ARG:HB3	47:u:577:GLU:HA	1.89	0.53
11:A:84:A:H5''	30:T:122:LYS:HD3	1.91	0.53
11:A:1228:A:H2'	11:A:1229:G:H8	1.73	0.53
35:b:141:PHE:CZ	35:b:143:PRO:HB3	2.43	0.53
48:v:352:SER:O	48:v:356:LEU:HB2	2.08	0.53
47:u:499:TYR:O	47:u:518:GLN:NE2	2.42	0.53
26:P:101:GLY:HA3	26:P:134:PRO:HG2	1.91	0.53
47:u:18:PHE:HA	47:u:21:VAL:HG12	1.91	0.53
47:u:109:GLN:HA	47:u:112:VAL:HG12	1.91	0.53
7:6:313:ILE:HD11	47:u:401:LEU:HD13	1.91	0.52
8:7:-31:C:N4	51:y:635:ASP:OD1	2.42	0.52
15:E:105:PHE:HD1	15:E:121:LYS:HB3	1.74	0.52
47:u:84:LYS:NZ	47:u:88:ASP:OD1	2.42	0.52
50:x:317:THR:O	50:x:321:HIS:ND1	2.42	0.52
11:A:612:PSU:O2'	16:F:85:LYS:NZ	2.42	0.52
29:S:43:GLU:OE1	29:S:119:LYS:NZ	2.42	0.52
32:Y:85:ARG:NH2	32:Y:118:THR:OG1	2.42	0.52
47:u:380:LEU:O	47:u:388:LYS:HG2	2.09	0.52
48:v:366:GLU:OE2	48:v:369:ARG:NH1	2.42	0.52
11:A:1589:A:N3	11:A:1653:U:O2'	2.42	0.52
14:D:21:GLU:OE1	14:D:24:ARG:NH1	2.41	0.52
20:J:39:THR:HG22	20:J:43:LYS:HE2	1.91	0.52
51:y:666:GLU:OE1	51:y:669:ARG:NH2	2.43	0.52
40:h:28:ASN:OD1	40:h:31:SER:OG	2.24	0.52
47:u:93:TYR:HA	47:u:96:MET:HE2	1.91	0.52
44:n:52:GLU:O	50:x:416:GLN:NE2	2.42	0.52
47:u:105:LYS:HA	47:u:108:SER:HB3	1.90	0.52
50:x:391:ILE:HG22	50:x:446:TYR:HB2	1.92	0.52
1:0:893:VAL:HG22	1:0:974:ILE:HG21	1.92	0.52
11:A:752:G:N2	11:A:793:G:O2'	2.41	0.52
25:O:52:THR:HG22	25:O:58:ALA:H	1.75	0.52
6:5:387:HIS:O	6:5:391:ARG:N	2.42	0.52
14:D:158:ASP:OD1	14:D:159:PHE:N	2.42	0.52
48:v:235:LEU:HB3	48:v:238:TYR:CE1	2.42	0.52
51:y:340:ARG:NH1	51:y:384:ASP:OD2	2.40	0.52
9:8:223:ALA:O	47:u:551:GLN:NE2	2.42	0.52
11:A:106:C:H2'	11:A:107:A:H8	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:D:30:LYS:HD2	16:F:112:TYR:HE1	1.74	0.52
24:N:126:ASP:O	24:N:130:ASP:HB2	2.09	0.52
42:k:111:ASN:OD1	42:k:112:GLY:N	2.43	0.52
47:u:403:LEU:HA	47:u:406:ARG:HB2	1.90	0.52
10:9:15:ARG:NH1	11:A:1183:A:OP1	2.39	0.52
11:A:1190:A:N3	11:A:1714:U:O2'	2.43	0.52
12:B:121:GLN:OE1	12:B:147:LYS:NZ	2.43	0.52
42:k:133:ALA:N	42:k:140:TYR:O	2.41	0.52
43:m:12:MET:HE2	43:m:119:GLN:HG3	1.92	0.52
1:0:707:GLU:OE1	1:0:736:GLN:NE2	2.43	0.52
2:1:543:ASN:ND2	2:1:545:GLU:OE2	2.42	0.52
11:A:1092:G:OP1	19:I:2:GLY:N	2.43	0.52
11:A:1310:U:OP1	43:m:36:ARG:NH2	2.43	0.52
43:m:42:LEU:HD23	43:m:68:LEU:HB3	1.92	0.52
1:0:706:HIS:O	1:0:713:ARG:NH1	2.33	0.51
1:0:863:VAL:HG12	1:0:873:ILE:HG22	1.92	0.51
8:7:-3[A]:A:H2'	8:7:-2[A]:C:O4'	2.10	0.51
11:A:1228:A:H5'	38:e:31:LYS:HZ3	1.74	0.51
39:f:49:ASP:OD1	39:f:66:ARG:NH1	2.43	0.51
39:f:86:ARG:NH1	39:f:110:ASP:OD2	2.43	0.51
45:o:259:PHE:HB2	45:o:265:ILE:HD11	1.93	0.51
1:0:948:LEU:HB3	1:0:959:LEU:HD13	1.92	0.51
1:0:1089:VAL:HG11	1:0:1124:PRO:HD2	1.91	0.51
11:A:1669:G:OP1	40:h:79:ARG:NH1	2.42	0.51
11:A:1285:G:H5'	43:m:61:TYR:HE2	1.74	0.51
11:A:1345:G:OP1	11:A:1688:C:O2'	2.28	0.51
24:N:76:VAL:HG12	24:N:123:VAL:HB	1.92	0.51
29:S:192:ILE:HG22	29:S:196:LYS:HE3	1.92	0.51
46:q:70:TRP:CD1	46:q:70:TRP:N	2.79	0.51
48:v:237:LEU:C	48:v:239:GLN:N	2.60	0.51
9:8:221:LYS:O	9:8:225:ALA:HA	2.09	0.51
11:A:219:U:H1'	28:R:184:ARG:HD2	1.92	0.51
13:C:21:ASP:OD2	13:C:24:THR:OG1	2.28	0.51
28:R:6:ASP:OD1	28:R:9:HIS:ND1	2.44	0.51
1:0:1040:ARG:NH1	11:A:460:A:OP1	2.44	0.51
11:A:1831:A:H2'	11:A:1832:6MZ:H8	1.92	0.51
36:c:282:GLU:OE2	36:c:285:GLN:NE2	2.43	0.51
11:A:1829:G:H1'	11:A:1850:MA6:H2	1.93	0.51
29:S:1:MET:HE1	29:S:106:LEU:HB2	1.92	0.51
48:v:362:MET:HE1	48:v:367:ALA:HA	1.93	0.51
1:0:1187:SER:N	1:0:1190:SER:OG	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:9:1:MET:HB2	11:A:1706:G:H5'	1.93	0.51
11:A:70:G:OP2	29:S:167:LYS:NZ	2.39	0.51
11:A:1217:A:H2'	11:A:1218:C:H6	1.75	0.51
24:N:80:ARG:NH2	24:N:165:ASN:O	2.43	0.51
11:A:941:C:H2'	11:A:942:G:H8	1.76	0.51
11:A:1332:A:O2'	33:Z:145:GLN:O	2.27	0.51
17:G:20:GLU:OE2	17:G:24:SER:OG	2.29	0.51
21:K:39:VAL:HG11	24:N:8:LEU:HD11	1.92	0.51
47:u:384:VAL:HB	47:u:387:VAL:HG22	1.92	0.51
47:u:449:SER:HA	47:u:492:SER:HA	1.93	0.51
5:4:122:GLY:HA3	5:4:131:VAL:HA	1.93	0.51
24:N:85:ARG:NH2	24:N:201:LEU:O	2.44	0.51
47:u:19:LEU:HD21	47:u:57:LEU:HD21	1.91	0.51
51:y:672:PRO:HD2	51:y:675:LEU:HD12	1.93	0.51
11:A:64:A:N6	11:A:83:A:OP2	2.44	0.51
11:A:84:A:N3	11:A:150:A:O2'	2.43	0.51
11:A:1156:U:OP1	20:J:71:LYS:NZ	2.42	0.51
11:A:943:U:H3	26:P:138:ASP:HB2	1.74	0.50
12:B:66:VAL:HG11	12:B:141:ASN:HD22	1.76	0.50
14:D:67:ASP:HB3	14:D:70:ARG:HB3	1.93	0.50
2:1:490:PRO:HG3	14:D:159:PHE:HE2	1.77	0.50
11:A:1705:C:H2'	11:A:1706:G:C8	2.46	0.50
11:A:1825:A:N6	46:q:65:LEU:O	2.44	0.50
1:0:1103:ASN:ND2	49:w:75:C:O4'	2.38	0.50
2:1:493:VAL:HG22	2:1:507:ARG:HB3	1.93	0.50
11:A:17:C:O2'	11:A:1194:A:N1	2.40	0.50
31:V:102:LEU:HD11	38:e:100:VAL:HG21	1.93	0.50
50:x:41:LYS:HG3	51:y:595:GLN:HB3	1.93	0.50
1:0:842:THR:HA	1:0:846:LEU:HB2	1.93	0.50
11:A:350:C:O2'	11:A:383:G:N1	2.45	0.50
11:A:924:G:H1	11:A:1018:U:H3	1.59	0.50
11:A:1264:C:OP1	41:i:28:HIS:NE2	2.34	0.50
11:A:1760:G:H21	11:A:1772:C:H5''	1.76	0.50
11:A:5:U:H2'	11:A:6:G:H8	1.76	0.50
11:A:520:A:O2'	11:A:825:A:N3	2.38	0.50
20:J:87:GLU:OE2	20:J:117:ARG:NH1	2.44	0.50
47:u:286:SER:HA	51:y:728:GLY:HA2	1.93	0.50
50:x:300:GLN:HG2	50:x:307:ASN:HD21	1.76	0.50
1:0:1143:ILE:HG13	1:0:1148:VAL:HG11	1.94	0.50
11:A:1147:C:OP1	27:Q:6:ARG:NH1	2.42	0.50
11:A:205:G:N7	28:R:144:LYS:NZ	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1016:U:H5''	19:I:14:SER:HB2	1.93	0.50
28:R:81:VAL:HG22	28:R:102:VAL:HG12	1.94	0.50
33:Z:167:TYR:OH	33:Z:202:LYS:O	2.27	0.50
43:m:81:ASP:HB3	43:m:84:LYS:HB2	1.93	0.50
47:u:303:SER:OG	47:u:307:ARG:NH2	2.44	0.50
11:A:1248:B8N:O2	11:A:1701:C:N4	2.45	0.50
23:M:41:ILE:HD12	23:M:47:ARG:HG2	1.93	0.50
35:b:17:TYR:HB3	35:b:25:LEU:HD11	1.94	0.50
47:u:526:MET:HA	47:u:529:VAL:HG22	1.94	0.50
11:A:531:A:N1	11:A:552:G:C6	2.80	0.50
11:A:1612:G:OP1	35:b:18:ARG:NH2	2.45	0.50
48:v:298:CYS:HA	48:v:301:VAL:HG12	1.93	0.50
11:A:693:A:H2'	11:A:694:G:C8	2.47	0.49
11:A:1360:U:O2'	11:A:1379:A:OP2	2.29	0.49
37:d:134:ILE:HA	37:d:137:GLN:HG2	1.94	0.49
42:k:107:LYS:NZ	42:k:108:VAL:O	2.43	0.49
8:7:20:G:N2	45:o:269:TYR:OH	2.46	0.49
11:A:1674:G:OP1	31:V:51:HIS:NE2	2.40	0.49
17:G:46:THR:HG23	17:G:65:PRO:HD3	1.94	0.49
2:1:319:PHE:HA	2:1:328:SER:HA	1.95	0.49
11:A:562:U:H2'	11:A:563:G:C8	2.47	0.49
11:A:1513:C:H2'	11:A:1514:G:H8	1.78	0.49
1:0:1188:ARG:NH1	1:0:1220:ILE:O	2.45	0.49
11:A:1560:U:H2'	11:A:1561:A:H8	1.77	0.49
11:A:1636:G:H8	38:e:39:LYS:HD2	1.76	0.49
36:c:82:SER:OG	36:c:83:TRP:N	2.44	0.49
38:e:79:ILE:HB	38:e:83:LEU:HD23	1.94	0.49
11:A:126:G:OP2	29:S:195:LYS:NZ	2.36	0.49
11:A:1550:G:O2'	11:A:1558:C:O2	2.27	0.49
14:D:114:VAL:HG13	14:D:119:LEU:HB2	1.93	0.49
18:H:67:THR:OG1	18:H:70:LYS:O	2.30	0.49
35:b:123:TYR:OH	39:f:124:ARG:NH1	2.43	0.49
45:o:243:VAL:HB	45:o:283:ALA:HB3	1.94	0.49
6:5:224:VAL:O	6:5:228:LEU:N	2.43	0.49
8:7:-3[A]:A:H2	11:A:1056:U:O2'	1.95	0.49
11:A:726:C:N4	11:A:727:G:O6	2.46	0.49
11:A:1101:U:H2'	11:A:1102:G:H8	1.78	0.49
11:A:1629:C:O2'	39:f:83:PHE:O	2.25	0.49
22:L:210:PRO:HD3	22:L:236:PHE:CE2	2.47	0.49
38:e:32:LYS:O	38:e:33:LYS:C	2.53	0.49
47:u:483:ARG:HH22	51:y:845:HIS:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:948:LEU:HD13	1:0:959:LEU:HD22	1.94	0.49
8:7:-8:A:OP1	27:Q:100:ARG:NH2	2.46	0.49
9:8:150:LEU:HA	9:8:166:ALA:HA	1.94	0.49
11:A:1729:U:H3	11:A:1805:G:H1	1.61	0.49
12:B:42:LEU:HD13	12:B:72:ILE:HD11	1.93	0.49
14:D:24:ARG:NE	14:D:28:GLU:OE1	2.44	0.49
36:c:18:VAL:O	36:c:287:THR:OG1	2.29	0.49
47:u:253:VAL:HG12	47:u:358:LEU:HD23	1.94	0.49
11:A:71:G:O6	29:S:170:ARG:NH1	2.46	0.49
11:A:1536:G:H2'	11:A:1537:A:C8	2.47	0.49
23:M:17:ILE:HD11	23:M:54:VAL:HA	1.94	0.49
35:b:62:LYS:HA	35:b:65:LYS:HG2	1.95	0.49
37:d:108:GLU:OE1	37:d:121:ARG:NE	2.35	0.49
43:m:19:GLN:HE22	43:m:88:TRP:CG	2.31	0.49
51:y:499:VAL:HA	51:y:502:ILE:HG22	1.95	0.49
2:1:549:MET:HA	2:1:554:VAL:HG12	1.93	0.49
11:A:1206:G:O2'	11:A:1208:A:OP1	2.30	0.49
18:H:45:THR:OG1	18:H:82:LYS:NZ	2.40	0.49
47:u:55:LEU:HD11	47:u:71:LEU:HD21	1.95	0.49
6:5:241:ASN:O	6:5:436:HIS:N	2.46	0.49
11:A:928:G:N2	18:H:68:GLY:O	2.40	0.49
11:A:1171:G:O2'	11:A:1187:G:O6	2.28	0.49
22:L:87:PRO:HG3	24:N:140:VAL:HA	1.95	0.49
22:L:180:VAL:HG22	22:L:219:ILE:HD13	1.95	0.49
24:N:147:LEU:O	24:N:165:ASN:ND2	2.46	0.49
33:Z:138:VAL:HG22	33:Z:184:ILE:HG12	1.95	0.49
48:v:231:ASN:CG	48:v:235:LEU:CD2	2.85	0.49
11:A:1745:A:O3'	29:S:31:ARG:NH1	2.42	0.48
51:y:504:LEU:HD22	51:y:564:ILE:HG23	1.95	0.48
11:A:1424:G:H2'	11:A:1425:G:H8	1.78	0.48
14:D:149:VAL:HG11	14:D:157:ILE:HD11	1.95	0.48
18:H:23:ARG:O	20:J:60:LYS:NZ	2.46	0.48
1:0:670:ALA:HB3	1:0:913:LEU:HD13	1.95	0.48
1:0:1140:SER:HB3	1:0:1160:LYS:HB3	1.95	0.48
11:A:696:G:H4'	11:A:697:G:H5'	1.94	0.48
11:A:1528:G:O2'	11:A:1666:C:OP1	2.28	0.48
17:G:84:GLU:O	17:G:88:SER:HA	2.14	0.48
26:P:34:PHE:HB3	26:P:41:PHE:HB2	1.96	0.48
46:q:20:GLU:O	46:q:24[B]:ARG:NH2	2.42	0.48
11:A:544:G:H2'	11:A:545:A:C8	2.48	0.48
11:A:931:C:H2'	11:A:932:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1092:G:H2'	11:A:1093:A:H8	1.78	0.48
11:A:1094:C:O2	20:J:16:ASN:ND2	2.46	0.48
11:A:1416:C:OP1	37:d:133:ARG:NH2	2.46	0.48
25:O:192:SER:HB2	47:u:23:LYS:HG3	1.96	0.48
32:Y:42:ILE:HG22	32:Y:44:PRO:HD2	1.95	0.48
46:q:71:ILE:HG23	46:q:77:ILE:HG21	1.94	0.48
11:A:1084:A:OP1	11:A:1858:G:O2'	2.29	0.48
11:A:1825:A:N6	46:q:69:VAL:O	2.45	0.48
17:G:36:LEU:HB3	17:G:40:LEU:HD22	1.95	0.48
23:M:106:LEU:HD11	24:N:19:LEU:HD11	1.96	0.48
41:i:46:TYR:O	41:i:50:ILE:HD12	2.14	0.48
47:u:372:ASN:HA	47:u:375:VAL:HG12	1.95	0.48
51:y:641:ARG:HA	51:y:652:LEU:HD21	1.94	0.48
1:0:670:ALA:HB2	1:0:861:MET:HE1	1.96	0.48
8:7:-2[B]:C:H2'	8:7:-1[B]:C:H6	1.79	0.48
11:A:35:C:H5''	11:A:579:C:H5''	1.96	0.48
11:A:1231:C:O2'	11:A:1253:A:N6	2.46	0.48
11:A:1521:C:OP2	39:f:136:THR:OG1	2.25	0.48
21:K:16:LYS:NZ	22:L:257:LYS:O	2.42	0.48
26:P:34:PHE:HE1	26:P:100:THR:HA	1.78	0.48
32:Y:19:ALA:HB2	32:Y:75:GLY:HA3	1.96	0.48
47:u:19:LEU:HD11	47:u:53:LYS:HD2	1.95	0.48
47:u:405:GLU:OE2	47:u:406:ARG:NH1	2.46	0.48
1:0:652:ARG:NH1	1:0:671:THR:OG1	2.47	0.48
2:1:569:ALA:HB3	2:1:578:ALA:HB3	1.96	0.48
5:4:314:GLN:HA	7:6:334:VAL:HG13	1.96	0.48
11:A:1398:G:O2'	36:c:88:ARG:NH2	2.44	0.48
1:0:722:ILE:HD11	1:0:841:LEU:HD23	1.96	0.48
8:7:-3[A]:A:H1'	11:A:961:G:C5	2.49	0.48
8:7:5:U:H4'	8:7:6:A:H5'	1.95	0.48
11:A:620:G:N2	11:A:647:U:OP1	2.47	0.48
15:E:134:TYR:O	16:F:87:ARG:NH2	2.45	0.48
25:O:144:LYS:HA	25:O:208:HIS:HD2	1.79	0.48
38:e:58:LEU:HD12	38:e:62:VAL:HG21	1.96	0.48
47:u:24:LYS:NZ	47:u:60:ASP:OD2	2.47	0.48
51:y:601:ALA:O	51:y:606:GLN:NE2	2.47	0.48
11:A:613:G:N2	11:A:626:G:OP1	2.43	0.48
11:A:1199:A:OP1	27:Q:2:THR:N	2.47	0.48
33:Z:124:ARG:NH1	33:Z:128:GLU:OE1	2.47	0.48
47:u:96:MET:HA	47:u:99:GLU:HG2	1.95	0.48
51:y:573:ILE:HD13	51:y:589:MET:SD	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:y:641:ARG:HG2	51:y:652:LEU:HD11	1.95	0.48
1:0:1036:ALA:HB1	1:0:1039:VAL:HB	1.96	0.47
9:8:258:VAL:HA	51:y:857:LEU:HD13	1.96	0.47
11:A:5:U:H2'	11:A:6:G:C8	2.49	0.47
29:S:57:ASP:OD1	29:S:58:LYS:N	2.43	0.47
36:c:107:ASP:HB2	36:c:125:ARG:HG3	1.96	0.47
40:h:78:ASP:OD1	41:i:54:LYS:NZ	2.31	0.47
48:v:240:PRO:O	48:v:243:LEU:N	2.47	0.47
1:0:665:THR:HG23	1:0:704:PRO:HA	1.96	0.47
1:0:678:ILE:HD11	1:0:698:MET:HG3	1.95	0.47
11:A:941:C:H2'	11:A:942:G:C8	2.49	0.47
11:A:1755:C:O2'	11:A:1778:C:O2	2.28	0.47
36:c:5:MET:HG2	36:c:312:VAL:HA	1.95	0.47
11:A:640:A:H2'	11:A:641:A:C8	2.48	0.47
11:A:1284:A:HO2'	43:m:106:CYS:HG	1.61	0.47
17:G:146:VAL:HG12	20:J:42:MET:HE1	1.96	0.47
32:Y:97:GLN:HB2	32:Y:105:LYS:HG3	1.96	0.47
33:Z:193:ASP:OD1	33:Z:193:ASP:N	2.47	0.47
40:h:80:PHE:HB3	41:i:52:PHE:HB3	1.95	0.47
47:u:340:ARG:HH21	51:y:745:LYS:HB2	1.78	0.47
50:x:295:ALA:HB2	50:x:427:ASN:HA	1.97	0.47
2:1:306:TYR:HA	2:1:704:TRP:HA	1.95	0.47
11:A:1235:G:H4'	46:q:3:LYS:HD2	1.96	0.47
11:A:1743:G:N2	11:A:1791:A:H62	2.09	0.47
5:4:289:TYR:HA	7:6:348:GLN:HB3	1.95	0.47
11:A:928:G:H2'	11:A:929:G:C8	2.49	0.47
11:A:992:A:N7	27:Q:15:ARG:NH2	2.62	0.47
11:A:1588:A:H2'	11:A:1589:A:C8	2.49	0.47
11:A:1757:G:O2'	11:A:1776:G:N1	2.47	0.47
13:C:192:ILE:HD13	13:C:238:LEU:HD22	1.97	0.47
17:G:37:LYS:O	17:G:41:ARG:NH1	2.47	0.47
1:0:1108:ILE:HG22	1:0:1110:MET:HE1	1.96	0.47
11:A:145:G:H2'	11:A:146:G:C8	2.49	0.47
47:u:404:CYS:SG	47:u:405:GLU:N	2.88	0.47
11:A:1017:U:H5'	19:I:55:ARG:HD3	1.97	0.47
11:A:1244:U:H2'	11:A:1245:G:H8	1.80	0.47
17:G:51:ILE:HD11	17:G:176:VAL:HG22	1.95	0.47
24:N:18:PHE:CE1	24:N:177:MET:HE1	2.49	0.47
25:O:190:PRO:HA	47:u:14[B]:ARG:HH21	1.80	0.47
29:S:181:THR:HG23	29:S:184:VAL:H	1.80	0.47
47:u:321:ARG:HD2	47:u:423:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:v:237:LEU:HA	48:v:240:PRO:HB2	1.96	0.47
48:v:399:SER:HA	48:v:403:GLN:HB2	1.97	0.47
51:y:424:ILE:HD11	51:y:437:PRO:HB2	1.96	0.47
51:y:602:ASP:OD1	51:y:602:ASP:N	2.48	0.47
1:0:724:ILE:HD11	1:0:838:LEU:HD21	1.96	0.47
2:1:527:CYS:SG	2:1:570:TRP:NE1	2.88	0.47
11:A:1678:A2M:OP2	31:V:63:LYS:NZ	2.44	0.47
34:a:42:ASN:O	34:a:46:MET:HG3	2.14	0.47
11:A:1010:G:H2'	11:A:1011:A:C8	2.49	0.47
1:0:753:VAL:O	1:0:820:LEU:HA	2.14	0.47
5:4:229:GLY:HA2	7:6:9:ILE:H	1.80	0.47
7:6:316:VAL:HG23	7:6:321:VAL:HG12	1.96	0.47
11:A:380:G:OP1	28:R:56:ARG:NH2	2.45	0.47
11:A:704:G:H2'	11:A:705:G:C8	2.50	0.47
17:G:145:ARG:NH1	20:J:51:GLU:OE2	2.48	0.47
40:h:81:GLN:HE21	41:i:55:LEU:HD12	1.78	0.47
43:m:89:VAL:HG11	43:m:109:VAL:HG11	1.97	0.47
47:u:451:GLU:HG2	47:u:454:ARG:H	1.80	0.47
51:y:826:ILE:HG12	51:y:832:MET:HB2	1.97	0.47
1:0:969:GLN:OE1	1:0:970:THR:OG1	2.34	0.46
11:A:1388:A:H61	33:Z:161:GLY:HA3	1.80	0.46
47:u:146:LEU:HD21	47:u:188:TYR:HE1	1.79	0.46
1:0:1027:HIS:NE2	15:E:52:LEU:O	2.48	0.46
2:1:570:TRP:CD2	2:1:577:PHE:HB3	2.51	0.46
11:A:98:C:H2'	11:A:426:A:H4'	1.97	0.46
11:A:555:A:N6	11:A:557:U:O2	2.49	0.46
20:J:37:PHE:O	20:J:41:MET:HG3	2.15	0.46
8:7:-28:C:O2'	8:7:-27:A:O4'	2.30	0.46
12:B:38:LYS:NZ	12:B:64:GLY:O	2.49	0.46
23:M:81:ARG:NH2	24:N:206:ASP:O	2.48	0.46
24:N:42:LYS:HD2	24:N:48:ILE:HD11	1.96	0.46
30:T:78:SER:OG	30:T:80:ASP:OD1	2.31	0.46
48:v:231:ASN:HB3	48:v:238:TYR:OH	2.16	0.46
48:v:237:LEU:HD13	50:x:59:TYR:CZ	2.51	0.46
11:A:1221:G:H2'	11:A:1222:G:C8	2.50	0.46
37:d:9:VAL:HG21	37:d:138:VAL:HG13	1.96	0.46
47:u:564:GLU:HA	47:u:572:ARG:HH21	1.80	0.46
50:x:394:LYS:HG3	50:x:449:LEU:HD23	1.97	0.46
51:y:517:LYS:HA	51:y:520:GLN:HG3	1.98	0.46
11:A:1355:C:O2	22:L:235:ASN:ND2	2.42	0.46
32:Y:33:LYS:NZ	37:d:8:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:v:255:ARG:NH2	48:v:318:VAL:O	2.48	0.46
11:A:197:U:H2'	11:A:203:G:H21	1.80	0.46
11:A:1722:G:H1	11:A:1812:U:H3	1.64	0.46
14:D:110:LEU:HB2	14:D:147:PHE:HB3	1.96	0.46
30:T:80:ASP:OD1	30:T:81:TYR:N	2.48	0.46
39:f:108:ARG:O	39:f:112:GLU:HG2	2.15	0.46
8:7:-8:A:H2	27:Q:43:ASN:H	1.62	0.46
11:A:1236:G:O2'	35:b:131:PRO:O	2.28	0.46
25:O:103:MET:HG3	25:O:215:VAL:HB	1.97	0.46
51:y:844:MET:HB3	51:y:846:ARG:HD3	1.98	0.46
1:0:842:THR:HG22	1:0:846:LEU:HD12	1.98	0.46
11:A:1098:C:H2'	11:A:1099:G:C8	2.51	0.46
11:A:1277:C:H2'	11:A:1278:A:C8	2.51	0.46
45:o:266:SER:HB3	45:o:288:HIS:HB2	1.98	0.46
11:A:383:G:H21	12:B:133:PRO:HG2	1.80	0.46
11:A:639:C:H2'	11:A:640:A:C8	2.51	0.46
11:A:919:A:OP2	19:I:64:ARG:NH2	2.40	0.46
11:A:1520:G:OP1	39:f:136:THR:N	2.49	0.46
14:D:107:GLU:O	14:D:113:GLN:NE2	2.43	0.46
16:F:79:SER:HB3	16:F:82:ARG:HD3	1.98	0.46
17:G:35:ASP:O	17:G:39:GLN:NE2	2.41	0.46
42:k:124:ASP:OD1	42:k:125:GLU:N	2.49	0.46
50:x:83:VAL:HG22	50:x:85:THR:HG23	1.97	0.46
13:C:44:LEU:HD13	13:C:72:ILE:HD11	1.98	0.46
18:H:34:ASP:OD2	18:H:80:ARG:NH2	2.49	0.46
45:o:247:SER:OG	45:o:249:ASP:OD1	2.32	0.46
1:0:905:LEU:HB3	1:0:919:TYR:HB3	1.99	0.45
11:A:476:A:N3	11:A:488:U:O2'	2.36	0.45
11:A:649:U:H2'	11:A:650:A:C8	2.51	0.45
17:G:25:GLN:HA	17:G:28:LEU:HB2	1.98	0.45
28:R:66:SER:HA	28:R:73:THR:HA	1.98	0.45
40:h:97:ILE:O	40:h:101:ILE:HG12	2.15	0.45
48:v:237:LEU:O	48:v:241:GLN:HB3	2.16	0.45
50:x:292:SER:N	50:x:428:ASN:OD1	2.49	0.45
50:x:304:ASN:OD1	50:x:311:ASN:ND2	2.49	0.45
11:A:106:C:H2'	11:A:107:A:C8	2.51	0.45
11:A:447:A:H4'	13:C:3:ARG:HB2	1.97	0.45
11:A:1228:A:O2'	11:A:1634:A:N3	2.41	0.45
12:B:75:GLY:HA3	12:B:88:ILE:HD12	1.98	0.45
17:G:69:LEU:HD22	17:G:96:ALA:HB2	1.99	0.45
24:N:145:ILE:HG12	24:N:159:ILE:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:v:258:THR:HA	48:v:261:VAL:HG22	1.98	0.45
1:0:995:LEU:HD11	1:0:1008:ILE:HG21	1.97	0.45
9:8:231:LEU:O	9:8:232:SER:C	2.59	0.45
11:A:1075:C:OP1	19:I:107:LYS:NZ	2.41	0.45
11:A:1101:U:H2'	11:A:1102:G:C8	2.52	0.45
11:A:1277:C:H2'	11:A:1278:A:H8	1.79	0.45
11:A:1845:A:H2'	11:A:1846:G:C8	2.51	0.45
21:K:3:ASN:ND2	21:K:7:GLU:OE2	2.43	0.45
22:L:66:LEU:HD11	22:L:81:ILE:HG12	1.97	0.45
22:L:212:LYS:HA	22:L:215:MET:HE2	1.97	0.45
47:u:518:GLN:HA	47:u:521:ASN:HB2	1.97	0.45
48:v:347:ILE:HA	51:y:826:ILE:HG21	1.97	0.45
2:1:656:ASP:O	2:1:668:THR:HA	2.16	0.45
11:A:367:U:H4'	11:A:371:A:C8	2.52	0.45
11:A:553:U:O4	11:A:555:A:N6	2.50	0.45
11:A:703:C:H2'	11:A:704:G:H8	1.80	0.45
11:A:1245:G:O2'	11:A:1492:U:OP1	2.32	0.45
11:A:1253:A:OP2	11:A:1526:G:N2	2.40	0.45
11:A:1265:A:O2'	11:A:1327:G:OP2	2.28	0.45
13:C:247:THR:N	13:C:250:GLU:OE2	2.48	0.45
24:N:75:SER:HB3	24:N:122:LEU:HD12	1.99	0.45
33:Z:192:TRP:NE1	33:Z:201:LYS:O	2.42	0.45
7:6:344:LYS:HG3	7:6:351:TYR:HE2	1.82	0.45
11:A:708:C:H2'	11:A:709:G:H8	1.81	0.45
11:A:1221:G:O2'	11:A:1676:U:O2	2.30	0.45
11:A:1263:U:H4'	41:i:27:ARG:HD2	1.98	0.45
18:H:46:VAL:HG12	18:H:54:VAL:HG11	1.97	0.45
26:P:82:ALA:HB2	26:P:119:LEU:HD23	1.96	0.45
28:R:80:ASP:HB3	28:R:103:LEU:HD12	1.99	0.45
35:b:21:ASP:OD1	35:b:22:LEU:N	2.44	0.45
47:u:51:MET:HB3	47:u:89:VAL:HG21	1.98	0.45
47:u:297:HIS:HE1	47:u:326:THR:HB	1.82	0.45
47:u:316:GLN:O	47:u:320:THR:HG23	2.16	0.45
47:u:335:ARG:HH12	47:u:350:GLU:HA	1.81	0.45
47:u:440:LEU:HA	47:u:443:VAL:HG12	1.99	0.45
48:v:346:ARG:HH21	48:v:393:MET:HG3	1.82	0.45
1:0:982:TYR:HE2	1:0:1017:ASP:HB3	1.82	0.45
11:A:928:G:H1	11:A:1013:U:H3	1.64	0.45
1:0:642:THR:N	53:0:1302:GTP:O1B	2.50	0.45
10:9:21:ARG:NH1	11:A:1174:U:OP1	2.49	0.45
11:A:704:G:H2'	11:A:705:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:823:PSU:N3	14:D:143:ASN:OD1	2.48	0.45
11:A:1413:G:H2'	11:A:1414:A:H8	1.81	0.45
43:m:18:LEU:HA	43:m:21:VAL:HG12	1.98	0.45
47:u:1:MET:HE1	47:u:39:LYS:HZ1	1.81	0.45
48:v:233:ILE:HG23	48:v:234:ASP:N	2.31	0.45
11:A:495:U:O2'	13:C:27:PHE:O	2.34	0.45
11:A:1221:G:H2'	11:A:1222:G:H8	1.82	0.45
11:A:1860:A:N7	27:Q:34:LYS:NZ	2.65	0.45
18:H:8:LEU:HD23	18:H:8:LEU:HA	1.78	0.45
1:0:755:LEU:HD22	1:0:794:ILE:HD13	1.98	0.45
1:0:1105:ARG:HH11	49:w:72:U:H5	1.64	0.45
13:C:124:CYS:HB3	13:C:141:THR:HB	1.98	0.45
48:v:231:ASN:CA	48:v:235:LEU:CD1	2.68	0.45
48:v:304:ASP:N	48:v:304:ASP:OD1	2.48	0.45
51:y:320:LYS:HA	51:y:332:LYS:HE2	1.99	0.45
51:y:451:MET:HE1	51:y:482:ILE:HG21	1.99	0.45
14:D:95:ASP:OD2	22:L:172:ASN:ND2	2.41	0.45
35:b:22:LEU:HA	35:b:25:LEU:HD12	1.99	0.45
51:y:327:ALA:O	51:y:331:LYS:NZ	2.47	0.45
51:y:511:TYR:OH	51:y:611:ARG:NH1	2.49	0.45
1:0:745:LYS:NZ	1:0:801:GLN:O	2.46	0.44
11:A:1722:G:H2'	11:A:1723:G:C8	2.52	0.44
39:f:40:TYR:CZ	39:f:97:GLN:HG2	2.52	0.44
47:u:186:LEU:HD12	47:u:239:SER:HA	1.97	0.44
47:u:268:LYS:HD3	47:u:269:PRO:HD2	1.99	0.44
47:u:380:LEU:HA	47:u:383:VAL:HG22	1.99	0.44
8:7:-31:C:H5'	50:x:53:LYS:HD3	1.99	0.44
11:A:882:U:O4	11:A:904:A:N6	2.51	0.44
13:C:45:ILE:HA	13:C:61:VAL:HG11	2.00	0.44
13:C:148:ARG:NH2	29:S:202:ASN:OD1	2.50	0.44
23:M:102:THR:HG21	24:N:24:HIS:CD2	2.51	0.44
31:V:125:SER:OG	31:V:136:ARG:NH2	2.50	0.44
43:m:54:SER:HB2	43:m:80:ASP:HA	2.00	0.44
47:u:384:VAL:O	47:u:388:LYS:N	2.46	0.44
48:v:341:PHE:HD2	48:v:370:TRP:HE1	1.64	0.44
51:y:496:THR:HA	51:y:499:VAL:HG12	1.98	0.44
11:A:102:A:H4'	11:A:104:A:C8	2.52	0.44
11:A:116:OMU:HM23	11:A:116:OMU:H1'	1.67	0.44
11:A:151:C:O2'	29:S:132:ARG:NH1	2.50	0.44
11:A:641:A:OP1	14:D:40:LYS:NZ	2.35	0.44
11:A:1166:G:H1	11:A:1193:U:H3	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1232:U:H2'	11:A:1233:G:C8	2.52	0.44
11:A:1798:C:H2'	11:A:1799:G:O4'	2.17	0.44
24:N:198:MET:HG2	24:N:200:ASP:H	1.83	0.44
33:Z:222:PRO:HA	36:c:190:GLY:HA2	1.99	0.44
36:c:146:SER:OG	36:c:147:HIS:N	2.50	0.44
1:0:981:VAL:HG13	1:0:1033:VAL:HG23	1.98	0.44
2:1:291:GLY:HA3	2:1:362:GLY:HA2	2.00	0.44
11:A:106:C:OP1	11:A:431:G:O2'	2.30	0.44
12:B:128:VAL:HG12	12:B:142:VAL:HA	1.98	0.44
24:N:51:LEU:HA	24:N:54:THR:HG22	1.99	0.44
37:d:60:THR:OG1	37:d:75:MET:SD	2.71	0.44
39:f:43:VAL:HG21	39:f:83:PHE:HE2	1.81	0.44
45:o:244:THR:HG23	45:o:282:PHE:HE1	1.83	0.44
11:A:453:C:O2'	29:S:92:ARG:O	2.29	0.44
11:A:639:C:H2'	11:A:640:A:H8	1.82	0.44
11:A:1536:G:H2'	11:A:1537:A:H8	1.82	0.44
33:Z:28:GLU:HG2	33:Z:69:LEU:HD21	1.99	0.44
33:Z:216:GLU:OE1	36:c:172:LYS:NZ	2.50	0.44
36:c:202:PRO:HG2	36:c:243:PRO:HA	2.00	0.44
39:f:84:LEU:HD12	39:f:95:TYR:HB3	2.00	0.44
47:u:309:ASN:HB2	47:u:311:THR:HG22	1.99	0.44
48:v:231:ASN:C	48:v:235:LEU:HB2	2.42	0.44
51:y:822:ILE:O	51:y:826:ILE:HG13	2.18	0.44
1:0:1012:PRO:HA	1:0:1039:VAL:HG13	1.99	0.44
2:1:485:GLU:OE1	2:1:491:ALA:N	2.49	0.44
11:A:1010:G:H2'	11:A:1011:A:H8	1.83	0.44
23:M:108:LEU:HD13	24:N:39:TYR:HE1	1.82	0.44
26:P:28:PHE:HZ	27:Q:58:VAL:HG21	1.83	0.44
47:u:230:LEU:HB3	47:u:271:LEU:HD21	2.00	0.44
1:0:646:LYS:HB3	1:0:825:ALA:HB1	1.99	0.44
1:0:1103:ASN:O	1:0:1107:PRO:HD2	2.18	0.44
9:8:224:VAL:O	9:8:225:ALA:HB3	2.17	0.44
13:C:175:PHE:HE2	13:C:198:ARG:HD2	1.82	0.44
20:J:86:LEU:O	20:J:90:GLN:HG3	2.18	0.44
46:q:38:VAL:HG21	46:q:71:ILE:HG22	2.00	0.44
1:0:639:HIS:CG	1:0:640:VAL:H	2.35	0.44
36:c:149:GLU:HG3	36:c:150:TRP:H	1.83	0.44
37:d:41:LYS:HE3	37:d:93:SER:HB2	2.00	0.44
48:v:249:MET:HB2	48:v:281:ILE:HG12	2.00	0.44
11:A:609:U:H2'	11:A:610:G:H8	1.83	0.44
11:A:1030:A:H2'	11:A:1031:A2M:H8	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:E:54:LYS:HB2	46:q:84:TYR:HB2	1.99	0.44
18:H:36:LYS:HG3	18:H:43:ILE:HG22	2.00	0.44
48:v:237:LEU:HD13	50:x:59:TYR:OH	2.18	0.44
2:1:520:GLN:HG2	2:1:525:TYR:HB2	2.00	0.43
2:1:555:PRO:HB3	14:D:155:LYS:HB3	2.00	0.43
11:A:107:A:H2'	11:A:108:G:C8	2.52	0.43
11:A:636:C:H5''	16:F:96:GLN:HE21	1.83	0.43
11:A:1543:U:OP1	32:Y:37:ARG:NH2	2.51	0.43
14:D:111:GLN:NE2	14:D:127:ARG:HB2	2.33	0.43
15:E:71:ARG:HH22	15:E:80:LYS:HD3	1.82	0.43
25:O:165:ARG:HG2	25:O:169:MET:HE3	1.98	0.43
28:R:3:ILE:O	28:R:30:GLY:N	2.51	0.43
30:T:21:LYS:HB2	30:T:75:ILE:HB	2.00	0.43
50:x:227:VAL:O	50:x:374:ARG:NH2	2.51	0.43
1:0:979:LYS:HA	1:0:1024:MET:HE1	2.00	0.43
1:0:1171:MET:H	1:0:1175:HIS:HB2	1.83	0.43
11:A:160:U:O2'	11:A:162:C:OP2	2.28	0.43
11:A:703:C:H2'	11:A:704:G:C8	2.53	0.43
11:A:888:U:C4	11:A:900:C:N3	2.86	0.43
11:A:943:U:O2'	26:P:135:ILE:O	2.36	0.43
17:G:63:PHE:HA	17:G:95:ILE:O	2.18	0.43
36:c:159:ASN:OD1	36:c:161:SER:OG	2.31	0.43
42:k:113:LYS:HG3	42:k:114:ILE:H	1.83	0.43
46:q:116:ASN:HB3	46:q:118:THR:HG23	2.00	0.43
51:y:393:MET:HB3	51:y:458:ILE:HD11	2.00	0.43
8:7:17:C:H2'	33:Z:94:ARG:HH22	1.83	0.43
11:A:877:C:H2'	11:A:878:G:C8	2.53	0.43
11:A:897:U:N3	11:A:899:U:O4	2.51	0.43
11:A:1144:A:H2'	11:A:1145:A:C8	2.53	0.43
25:O:83:LYS:HD3	25:O:106:THR:HG22	1.99	0.43
31:V:184:SER:OG	31:V:186:ASN:OD1	2.36	0.43
35:b:85:ILE:HG22	35:b:112:ILE:HD13	2.00	0.43
39:f:63:GLU:HG2	39:f:66:ARG:HH21	1.84	0.43
48:v:352:SER:OG	48:v:354:ASN:OD1	2.29	0.43
11:A:952:G:H2'	11:A:953:C:C6	2.53	0.43
24:N:71:PRO:HB3	24:N:186:ARG:HH22	1.83	0.43
47:u:204:HIS:O	47:u:208:ILE:HG13	2.19	0.43
47:u:469:ARG:NH1	51:y:746:MET:O	2.51	0.43
47:u:544:GLN:O	47:u:548:GLU:HB2	2.18	0.43
1:0:646:LYS:HB3	1:0:646:LYS:HE3	1.61	0.43
1:0:711:ASN:OD1	1:0:711:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:855:GLU:O	1:0:857:ARG:NH1	2.52	0.43
1:0:886:ASP:HB2	1:0:901:ILE:HD12	2.00	0.43
11:A:121:OMU:H1'	11:A:121:OMU:HM23	1.73	0.43
11:A:962:A:N1	11:A:1055:A:O2'	2.51	0.43
11:A:1004:U:H2'	11:A:1005:G:H8	1.84	0.43
11:A:1280:G:H2'	11:A:1281:G:H8	1.82	0.43
19:I:142:GLU:OE1	19:I:144:SER:OG	2.37	0.43
25:O:147:ASN:OD1	25:O:148:ASN:N	2.52	0.43
33:Z:51:LEU:HD13	33:Z:89:GLU:HB3	2.01	0.43
34:a:24:LYS:O	34:a:42:ASN:ND2	2.47	0.43
48:v:251:PRO:HG2	48:v:289:LYS:HD2	2.01	0.43
51:y:375:LYS:HB3	51:y:408:LEU:HD13	1.99	0.43
11:A:155:G:H4'	29:S:15:LEU:HD13	2.00	0.43
11:A:441:C:H2'	11:A:442:C:C6	2.53	0.43
11:A:1007:C:O2'	19:I:104:ARG:NH2	2.51	0.43
20:J:112:ASP:OD1	20:J:112:ASP:N	2.47	0.43
1:0:764:TRP:HD1	1:0:766:LYS:HD3	1.83	0.43
1:0:1043:ARG:HH22	11:A:459:C:H5'	1.84	0.43
30:T:79:LEU:HD11	30:T:96:LEU:HD21	2.01	0.43
32:Y:49:TYR:O	32:Y:53:GLU:HG3	2.18	0.43
48:v:237:LEU:HD22	50:x:59:TYR:OH	2.18	0.43
2:1:467:ILE:HA	2:1:483:VAL:HG22	2.01	0.43
8:7:-6:A:H2'	8:7:-5:C:C5	2.53	0.43
11:A:492:C:H5	30:T:104:ARG:HH21	1.67	0.43
11:A:539:C:N4	11:A:542:U:OP1	2.51	0.43
11:A:692:G:H2'	11:A:693:A:C8	2.54	0.43
11:A:1037:G:H4'	11:A:1845:A:H4'	2.00	0.43
11:A:1754:G:H8	11:A:1755:C:H4'	1.83	0.43
13:C:151:ASP:OD2	29:S:216:ARG:NH2	2.52	0.43
17:G:128:ALA:HA	17:G:131:GLU:HG2	1.99	0.43
21:K:65:SER:OG	24:N:157:VAL:O	2.36	0.43
29:S:56:ASN:HB2	29:S:108:VAL:HG12	2.01	0.43
31:V:128:ILE:HD12	44:n:22:GLY:HA2	2.00	0.43
33:Z:123:LEU:HD22	33:Z:152:PHE:HB3	2.00	0.43
48:v:369:ARG:HA	48:v:372:VAL:HG12	2.01	0.43
2:1:548:ARG:NH2	2:1:596:ASN:O	2.52	0.43
11:A:551:U:O2'	11:A:552:G:O4'	2.34	0.43
11:A:1128:C:H2'	11:A:1129:G:H8	1.83	0.43
33:Z:142:LEU:HD12	33:Z:148:LYS:HG3	2.00	0.43
34:a:47:LYS:HA	34:a:47:LYS:HD3	1.88	0.43
1:0:647:ILE:HD12	1:0:726:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:525:A:H2'	11:A:526:A:C8	2.53	0.43
11:A:750:C:H2'	11:A:752:G:H5'	2.01	0.43
42:k:83:LYS:NZ	46:q:23:LYS:O	2.47	0.43
48:v:358:ASP:HB3	48:v:360:LEU:HD13	2.00	0.43
48:v:404:VAL:HA	48:v:407:LYS:HE3	2.01	0.43
1:0:718:SER:HB2	1:0:747:LYS:HZ3	1.84	0.42
11:A:10:G:O2'	22:L:113:GLN:OE1	2.36	0.42
11:A:167:G:H4'	29:S:131:ARG:HH21	1.84	0.42
11:A:1303:C:O2	42:k:92:LYS:NZ	2.46	0.42
11:A:1386:A:OP2	33:Z:160:SER:OG	2.32	0.42
11:A:1830:UR3:H6	11:A:1831:A:H62	1.84	0.42
30:T:36:PRO:HD2	30:T:39:GLU:OE2	2.18	0.42
48:v:231:ASN:CB	48:v:235:LEU:CD2	2.74	0.42
50:x:207:ASP:O	50:x:468:THR:OG1	2.37	0.42
1:0:1220:ILE:HD13	46:q:52:PHE:HD1	1.85	0.42
7:6:204:ALA:HB2	7:6:233:GLU:H	1.84	0.42
7:6:316:VAL:HG13	47:u:398:PHE:HE2	1.83	0.42
8:7:-1[A]:C:H2'	8:7:-1[A]:C:O2	2.18	0.42
11:A:1711:U:H2'	11:A:1712:A:C8	2.54	0.42
31:V:68:ILE:HD11	31:V:151:ILE:HD11	2.01	0.42
35:b:60:LEU:HD22	35:b:92:SER:HB3	2.00	0.42
36:c:174:VAL:HB	36:c:188:HIS:HB2	2.01	0.42
40:h:26:SER:HB3	40:h:32:LEU:HD22	2.00	0.42
47:u:175:HIS:ND1	47:u:228:MET:HE3	2.33	0.42
47:u:489:ARG:HH22	51:y:806:THR:HG21	1.83	0.42
48:v:237:LEU:HA	48:v:240:PRO:CB	2.48	0.42
51:y:686:TYR:HE2	51:y:713:GLN:HB2	1.84	0.42
9:8:231:LEU:O	9:8:234:ALA:N	2.52	0.42
11:A:26:U:H2'	11:A:27:A2M:H8	2.01	0.42
11:A:472:C:O2	11:A:475:C:N4	2.52	0.42
11:A:834:C:HO2'	11:A:836:G:H1	1.67	0.42
11:A:1673:U:O2'	31:V:84:GLY:O	2.33	0.42
32:Y:96:TYR:HA	32:Y:100:VAL:HG22	2.01	0.42
33:Z:218:LEU:HD22	36:c:192:THR:HB	2.01	0.42
45:o:272:LYS:HA	45:o:279:SER:HA	2.01	0.42
48:v:231:ASN:CA	48:v:235:LEU:CD2	2.71	0.42
1:0:1013:VAL:HG23	1:0:1039:VAL:HG11	2.01	0.42
11:A:1438:A:H2'	11:A:1439:A:C8	2.54	0.42
11:A:1615:U:O4	35:b:40:ARG:NH2	2.52	0.42
19:I:83:ASP:OD1	19:I:84:LEU:N	2.52	0.42
27:Q:44:ILE:HD12	27:Q:65:PRO:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:V:38:TYR:OH	44:n:54:ASP:OD1	2.24	0.42
36:c:20:GLN:HG2	36:c:69:VAL:H	1.84	0.42
42:k:108:VAL:HG22	42:k:110:GLU:H	1.85	0.42
47:u:91:ARG:HH21	47:u:173:LEU:HD13	1.85	0.42
51:y:718:LEU:HD13	51:y:738:VAL:HG23	2.00	0.42
51:y:732:SER:O	51:y:736:HIS:ND1	2.37	0.42
11:A:484:A2M:O5'	11:A:484:A2M:H8	2.19	0.42
14:D:78:LEU:HD22	14:D:92:MET:HA	2.01	0.42
43:m:18:LEU:HD21	43:m:51:VAL:HG21	2.00	0.42
2:1:524:ASP:OD2	2:1:550:ARG:NH2	2.51	0.42
37:d:35:ASP:HB2	39:f:46:ARG:HG2	2.01	0.42
47:u:94:LEU:O	47:u:98:GLU:HG2	2.20	0.42
48:v:229:ARG:O	48:v:230:ASP:C	2.63	0.42
2:1:471:SER:HB3	2:1:519:TRP:HE1	1.85	0.42
51:y:415:ASN:HD22	51:y:418:ILE:HD11	1.85	0.42
11:A:155:G:H2'	11:A:156:G:H8	1.85	0.42
11:A:525:A:H2'	11:A:526:A:H8	1.84	0.42
11:A:674:C:H2'	11:A:675:U:C6	2.55	0.42
11:A:1172:U:H2'	11:A:1173:A:H8	1.84	0.42
19:I:60:VAL:HG13	19:I:66:VAL:HG21	2.01	0.42
24:N:61:ALA:HB2	24:N:161:ILE:HD11	2.02	0.42
24:N:147:LEU:HD13	24:N:161:ILE:HB	2.02	0.42
36:c:101:PHE:CE1	36:c:136:GLY:HA2	2.55	0.42
48:v:231:ASN:CA	48:v:235:LEU:HB2	2.49	0.42
51:y:543:ASP:HB2	51:y:546:VAL:HG22	2.02	0.42
11:A:186:C:H2'	11:A:187:G:H8	1.85	0.42
11:A:920:A:O2'	11:A:922:A:OP1	2.28	0.42
11:A:1083:A:N7	11:A:1841:C:O2'	2.38	0.42
28:R:64:ASN:O	28:R:186:ASP:HA	2.20	0.42
11:A:913:A:OP2	17:G:99:ARG:NH2	2.50	0.42
11:A:1036:A:N3	11:A:1844:U:O2'	2.53	0.42
11:A:1513:C:H2'	11:A:1514:G:C8	2.55	0.42
11:A:1562:C:H2'	11:A:1563:G:H8	1.83	0.42
25:O:38:MET:SD	25:O:185:VAL:HG11	2.60	0.42
38:e:29:LYS:HD3	39:f:146:VAL:HA	2.02	0.42
48:v:238:TYR:CZ	48:v:239:GLN:HG2	2.54	0.42
50:x:28:MET:HE1	51:y:556:TYR:CD2	2.55	0.42
1:0:1109:VAL:HG12	1:0:1160:LYS:HA	2.01	0.41
11:A:15:U:H2'	11:A:16:G:O4'	2.20	0.41
11:A:448:A:H5''	28:R:25:ARG:HA	2.02	0.41
19:I:30:SER:HB2	19:I:67:THR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:33:VAL:HG21	19:I:66:VAL:HG11	2.02	0.41
22:L:69:LEU:HD11	22:L:273:LEU:HD11	2.01	0.41
29:S:58:LYS:HA	29:S:107:SER:HB2	2.01	0.41
34:a:15:LEU:HD23	34:a:79:LEU:HD11	2.01	0.41
39:f:16:LEU:HD13	39:f:99:LEU:HD13	2.01	0.41
42:k:139:HIS:O	42:k:147:THR:HA	2.19	0.41
47:u:30:VAL:O	47:u:34:VAL:HG23	2.20	0.41
1:0:1139:THR:HG21	1:0:1162:GLU:HB3	2.02	0.41
2:1:575:SER:O	2:1:575:SER:OG	2.38	0.41
8:7:4:G:O6	46:q:6:GLY:HA3	2.20	0.41
11:A:28:U:H2'	11:A:29:G:C8	2.52	0.41
11:A:1213:C:H2'	11:A:1214:A:H8	1.86	0.41
21:K:79:VAL:HA	24:N:3:GLY:H	1.85	0.41
47:u:86:LEU:HA	47:u:89:VAL:HG12	2.02	0.41
47:u:278:LYS:HA	47:u:281:THR:HG22	2.03	0.41
11:A:16:G:H2'	11:A:17:C:C6	2.55	0.41
11:A:194:C:H2'	11:A:195:C:C6	2.55	0.41
13:C:23:LEU:HD11	14:D:6:SER:HB2	2.02	0.41
35:b:83:MET:HB3	35:b:116:LEU:HD12	2.01	0.41
38:e:37:LYS:HD3	38:e:37:LYS:HA	1.88	0.41
43:m:66:GLU:HA	43:m:69:CYS:SG	2.60	0.41
47:u:55:LEU:HD13	47:u:93:TYR:HB2	2.03	0.41
47:u:392:ASN:HA	47:u:396:VAL:HB	2.02	0.41
47:u:398:PHE:HD1	47:u:511:LEU:HB3	1.85	0.41
47:u:499:TYR:H	47:u:518:GLN:HG3	1.85	0.41
51:y:668:ARG:NH2	51:y:670:GLN:OE1	2.53	0.41
9:8:228:HIS:O	9:8:232:SER:N	2.45	0.41
11:A:60:G:N2	11:A:316:G:H21	2.19	0.41
11:A:600:G:H2'	11:A:601:G:C8	2.55	0.41
11:A:681:U:O2'	11:A:1160:U:OP1	2.38	0.41
11:A:1144:A:H5'	11:A:1355:C:H41	1.85	0.41
50:x:318:TYR:O	50:x:322:ASN:ND2	2.53	0.41
50:x:397:ASN:OD1	50:x:397:ASN:N	2.54	0.41
1:0:673:VAL:HG22	1:0:910:MET:HE1	2.03	0.41
11:A:223:C:H2'	11:A:224:A:C8	2.55	0.41
11:A:746:C:N4	11:A:797:C:O2	2.54	0.41
11:A:924:G:H5'	19:I:4:MET:HE3	2.03	0.41
12:B:111:VAL:HG12	12:B:140:PHE:HB2	2.02	0.41
25:O:137:LEU:HG	25:O:215:VAL:HG22	2.02	0.41
28:R:201:LYS:HD2	28:R:201:LYS:HA	1.88	0.41
46:q:77:ILE:HG22	46:q:94:LYS:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6:316:VAL:HG11	47:u:446:ILE:HD13	2.03	0.41
8:7:-4[A]:C:OP1	11:A:961:G:H5'	2.20	0.41
11:A:156:G:OP1	29:S:2:LYS:NZ	2.43	0.41
11:A:522:A:H5''	14:D:145:PRO:HD2	2.01	0.41
11:A:527:C:H2'	11:A:528:A:C8	2.55	0.41
20:J:42:MET:HE2	20:J:42:MET:HB3	1.78	0.41
39:f:121:ARG:HG3	39:f:131:VAL:HB	2.01	0.41
48:v:239:GLN:CB	48:v:240:PRO:CD	2.98	0.41
48:v:243:LEU:HA	48:v:247:GLN:HB3	2.01	0.41
51:y:700:ALA:HB2	51:y:793:PHE:CG	2.55	0.41
9:8:224:VAL:C	9:8:226:ASP:H	2.27	0.41
11:A:1722:G:H2'	11:A:1723:G:H8	1.85	0.41
36:c:89:LEU:HB3	36:c:99:ARG:HB2	2.02	0.41
47:u:44:GLN:HG3	47:u:82:ASN:HD21	1.86	0.41
47:u:521:ASN:HA	47:u:524:THR:HG23	2.03	0.41
11:A:85:A:H2'	11:A:86:C:H6	1.86	0.41
11:A:934:G:H22	11:A:1008:A:H2	1.68	0.41
11:A:1215:C:O2'	11:A:1645:C:OP2	2.38	0.41
11:A:1797:U:H2'	11:A:1798:C:C6	2.55	0.41
14:D:33:GLY:HA3	16:F:112:TYR:CG	2.56	0.41
20:J:80:ASP:OD1	20:J:124:LYS:NZ	2.53	0.41
2:1:170:GLY:N	2:1:230:LYS:O	2.54	0.41
8:7:-4[A]:C:O3'	8:7:-3[A]:A:H4'	2.21	0.41
11:A:17:C:H2'	11:A:18:C:H6	1.86	0.41
11:A:51:U:H2'	11:A:52:G:C8	2.55	0.41
11:A:982:G:H2'	11:A:983:A:C8	2.56	0.41
11:A:1004:U:H2'	11:A:1005:G:C8	2.56	0.41
11:A:1113:A:O2'	11:A:1114:U:O4'	2.26	0.41
11:A:1643:U:H2'	11:A:1644:C:C6	2.56	0.41
11:A:1692:U:H2'	11:A:1693:G:C8	2.56	0.41
22:L:102:LEU:HD23	22:L:102:LEU:HA	1.94	0.41
25:O:109:LYS:O	25:O:113:MET:HG3	2.20	0.41
25:O:181:LEU:HA	25:O:184:VAL:HG12	2.03	0.41
28:R:57:ALA:HB2	28:R:183:GLY:HA2	2.03	0.41
33:Z:75:LYS:HD2	34:a:18:GLU:HG2	2.03	0.41
35:b:18:ARG:NH1	39:f:88:LYS:HE3	2.36	0.41
39:f:99:LEU:O	39:f:103:LEU:N	2.49	0.41
45:o:279:SER:OG	45:o:280:LYS:N	2.53	0.41
47:u:266:PRO:HA	47:u:267:PRO:HD3	1.80	0.41
48:v:349:GLN:OE1	48:v:393:MET:N	2.45	0.41
50:x:294:THR:O	50:x:294:THR:OG1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:x:371:LEU:HB3	50:x:373:VAL:HG23	2.03	0.41
1:0:646:LYS:HG2	1:0:657:GLN:HG2	2.03	0.41
1:0:1138:VAL:HG23	1:0:1159:VAL:HB	2.03	0.41
11:A:868:G:OP2	11:A:868:G:N2	2.35	0.41
11:A:1844:U:H3	11:A:1855:G:H1	1.69	0.41
25:O:25:PHE:HA	25:O:28:LYS:HD2	2.03	0.41
51:y:630:HIS:HB2	51:y:689:SER:HB3	2.02	0.41
21:K:66:ASP:OD1	21:K:67:ASP:N	2.54	0.40
29:S:2:LYS:HB3	29:S:15:LEU:HD21	2.02	0.40
48:v:347:ILE:HG23	51:y:826:ILE:HD12	2.02	0.40
51:y:375:LYS:O	51:y:379:ILE:HG12	2.22	0.40
11:A:21:U:O2'	14:D:17:ARG:O	2.37	0.40
11:A:291:G:H2'	11:A:292:A:C8	2.56	0.40
11:A:1227:G:H4'	38:e:35:TRP:HE1	1.86	0.40
11:A:1786:U:H2'	11:A:1787:G:H8	1.85	0.40
14:D:106:LEU:HD23	14:D:109:ARG:HD2	2.02	0.40
14:D:151:LEU:HD23	14:D:151:LEU:HA	1.96	0.40
38:e:31:LYS:HD3	38:e:32:LYS:N	2.37	0.40
39:f:62:ASP:OD1	39:f:63:GLU:N	2.54	0.40
40:h:26:SER:HB2	40:h:110:VAL:HG22	2.03	0.40
47:u:452:PHE:HA	47:u:455:LEU:HB2	2.03	0.40
48:v:331:ASP:OD1	48:v:332:PHE:N	2.55	0.40
50:x:286:PHE:HB3	50:x:288:LEU:HD22	2.02	0.40
50:x:448:LYS:HE3	50:x:448:LYS:HB3	1.89	0.40
51:y:348:ALA:HA	51:y:351:ILE:HG12	2.03	0.40
1:0:645:THR:O	1:0:648:LEU:N	2.54	0.40
1:0:679:ASN:HB3	1:0:690:ARG:HH21	1.86	0.40
1:0:877:LEU:HD11	1:0:882:LEU:HD12	2.03	0.40
11:A:17:C:H2'	11:A:18:C:C6	2.56	0.40
11:A:54:A:OP1	30:T:111:LYS:NZ	2.40	0.40
11:A:710:C:H2'	11:A:711:C:C6	2.56	0.40
11:A:1129:G:H3'	11:A:1130:G:N2	2.34	0.40
14:D:172:ARG:HA	14:D:175:ARG:HG2	2.04	0.40
22:L:165:VAL:HG13	22:L:244:ILE:HG23	2.03	0.40
27:Q:33:ASP:OD1	27:Q:33:ASP:N	2.54	0.40
28:R:106:SER:O	28:R:110:ARG:HB3	2.22	0.40
30:T:7:ILE:HD12	30:T:44:LEU:HD23	2.04	0.40
36:c:191:HIS:CD2	36:c:195:LEU:HD21	2.56	0.40
36:c:282:GLU:HA	36:c:283:PRO:HD3	1.94	0.40
51:y:548:MET:HE3	51:y:552:CYS:SG	2.62	0.40
1:0:723:ALA:O	1:0:751:PHE:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1152:LYS:HB2	1:0:1155:GLN:HB2	2.04	0.40
2:1:481:PHE:HB2	2:1:494:THR:HB	2.02	0.40
11:A:116:OMU:H6	11:A:116:OMU:O5'	2.22	0.40
11:A:118:C:H1'	11:A:445:A:C5	2.57	0.40
11:A:302:A:N3	28:R:64:ASN:ND2	2.70	0.40
11:A:1217:A:H2'	11:A:1218:C:C6	2.55	0.40
11:A:1235:G:H5'	11:A:1247:C:H42	1.86	0.40
11:A:1468:C:H2'	11:A:1469:A:C8	2.57	0.40
11:A:1862:G:H22	27:Q:76:SER:HB3	1.87	0.40
11:A:1869:A:C5	25:O:115:LYS:HG2	2.56	0.40
47:u:559:LYS:HA	47:u:559:LYS:HD3	1.95	0.40
9:8:209:HIS:O	47:u:572:ARG:NH1	2.54	0.40
11:A:600:G:H2'	11:A:601:G:H8	1.87	0.40
11:A:1269:G:H2'	11:A:1270:G:C8	2.56	0.40
11:A:1413:G:H2'	11:A:1414:A:C8	2.55	0.40
11:A:1593:C:H2'	11:A:1594:A:C8	2.57	0.40
24:N:184:ARG:NH1	24:N:191:ARG:O	2.54	0.40
38:e:68:ILE:HB	38:e:109:TYR:HB2	2.04	0.40
50:x:365:LEU:HD22	50:x:369:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	620/1220 (51%)	593 (96%)	27 (4%)	0	100	100
2	1	584/814 (72%)	551 (94%)	33 (6%)	0	100	100
3	2	300/325 (92%)	296 (99%)	4 (1%)	0	100	100
4	3	209/218 (96%)	204 (98%)	5 (2%)	0	100	100
5	4	251/357 (70%)	235 (94%)	16 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	5	307/564 (54%)	293 (95%)	14 (5%)	0	100	100
7	6	348/374 (93%)	322 (92%)	26 (8%)	0	100	100
9	8	313/352 (89%)	286 (91%)	27 (9%)	0	100	100
10	9	22/25 (88%)	22 (100%)	0	0	100	100
12	B	138/158 (87%)	137 (99%)	1 (1%)	0	100	100
13	C	254/263 (97%)	249 (98%)	5 (2%)	0	100	100
14	D	175/194 (90%)	173 (99%)	2 (1%)	0	100	100
15	E	138/143 (96%)	132 (96%)	6 (4%)	0	100	100
16	F	57/59 (97%)	52 (91%)	5 (9%)	0	100	100
17	G	171/194 (88%)	166 (97%)	5 (3%)	0	100	100
18	H	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
19	I	148/151 (98%)	147 (99%)	1 (1%)	0	100	100
20	J	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
21	K	79/83 (95%)	73 (92%)	6 (8%)	0	100	100
22	L	218/293 (74%)	215 (99%)	3 (1%)	0	100	100
23	M	129/135 (96%)	123 (95%)	6 (5%)	0	100	100
24	N	205/295 (70%)	199 (97%)	6 (3%)	0	100	100
25	O	209/264 (79%)	205 (98%)	4 (2%)	0	100	100
26	P	131/151 (87%)	124 (95%)	7 (5%)	0	100	100
27	Q	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
28	R	194/208 (93%)	190 (98%)	4 (2%)	0	100	100
29	S	228/249 (92%)	223 (98%)	5 (2%)	0	100	100
30	T	123/133 (92%)	122 (99%)	1 (1%)	0	100	100
31	V	187/204 (92%)	178 (95%)	9 (5%)	0	100	100
32	Y	139/146 (95%)	134 (96%)	5 (4%)	0	100	100
33	Z	225/243 (93%)	221 (98%)	4 (2%)	0	100	100
34	a	97/165 (59%)	93 (96%)	4 (4%)	0	100	100
35	b	129/145 (89%)	126 (98%)	3 (2%)	0	100	100
36	c	311/317 (98%)	291 (94%)	20 (6%)	0	100	100
37	d	140/145 (97%)	135 (96%)	5 (4%)	0	100	100
38	e	80/125 (64%)	76 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	f	147/152 (97%)	136 (92%)	11 (8%)	0	100	100
40	h	101/119 (85%)	95 (94%)	6 (6%)	0	100	100
41	i	48/56 (86%)	48 (100%)	0	0	100	100
42	k	69/156 (44%)	60 (87%)	9 (13%)	0	100	100
43	m	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
44	n	62/69 (90%)	56 (90%)	6 (10%)	0	100	100
45	o	75/320 (23%)	71 (95%)	4 (5%)	0	100	100
46	q	116/144 (81%)	110 (95%)	6 (5%)	0	100	100
47	u	705/1382 (51%)	666 (94%)	39 (6%)	0	100	100
48	v	380/445 (85%)	363 (96%)	17 (4%)	0	100	100
50	x	415/548 (76%)	391 (94%)	24 (6%)	0	100	100
51	y	527/913 (58%)	506 (96%)	21 (4%)	0	100	100
All	All	9927/13477 (74%)	9494 (96%)	433 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	547/1081 (51%)	547 (100%)	0	100	100
2	1	97/702 (14%)	97 (100%)	0	100	100
7	6	49/335 (15%)	49 (100%)	0	100	100
10	9	23/24 (96%)	23 (100%)	0	100	100
12	B	129/142 (91%)	129 (100%)	0	100	100
13	C	220/225 (98%)	220 (100%)	0	100	100
14	D	158/168 (94%)	158 (100%)	0	100	100
15	E	112/115 (97%)	112 (100%)	0	100	100
16	F	47/47 (100%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	G	159/174 (91%)	159 (100%)	0	100	100
18	H	73/76 (96%)	73 (100%)	0	100	100
19	I	130/131 (99%)	130 (100%)	0	100	100
20	J	112/113 (99%)	112 (100%)	0	100	100
21	K	65/67 (97%)	65 (100%)	0	100	100
22	L	186/225 (83%)	186 (100%)	0	100	100
23	M	119/122 (98%)	119 (100%)	0	100	100
24	N	173/243 (71%)	173 (100%)	0	100	100
25	O	192/231 (83%)	192 (100%)	0	100	100
26	P	104/119 (87%)	104 (100%)	0	100	100
27	Q	86/98 (88%)	86 (100%)	0	100	100
28	R	172/180 (96%)	172 (100%)	0	100	100
29	S	200/218 (92%)	200 (100%)	0	100	100
30	T	107/115 (93%)	107 (100%)	0	100	100
31	V	159/170 (94%)	159 (100%)	0	100	100
32	Y	117/121 (97%)	117 (100%)	0	100	100
33	Z	190/202 (94%)	190 (100%)	0	100	100
34	a	90/136 (66%)	90 (100%)	0	100	100
35	b	117/130 (90%)	117 (100%)	0	100	100
36	c	272/275 (99%)	272 (100%)	0	100	100
37	d	112/115 (97%)	112 (100%)	0	100	100
38	e	72/103 (70%)	72 (100%)	0	100	100
39	f	129/132 (98%)	129 (100%)	0	100	100
40	h	94/107 (88%)	94 (100%)	0	100	100
41	i	44/49 (90%)	44 (100%)	0	100	100
42	k	64/140 (46%)	64 (100%)	0	100	100
43	m	104/108 (96%)	104 (100%)	0	100	100
44	n	57/62 (92%)	57 (100%)	0	100	100
45	o	64/277 (23%)	64 (100%)	0	100	100
46	q	100/123 (81%)	100 (100%)	0	100	100
47	u	528/1259 (42%)	528 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	v	206/406 (51%)	206 (100%)	0	100	100
50	x	206/494 (42%)	206 (100%)	0	100	100
51	y	473/811 (58%)	473 (100%)	0	100	100
All	All	6458/10171 (64%)	6458 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	655	HIS
1	0	1118	GLN
12	B	19	ASN
12	B	141	ASN
13	C	50	ASN
13	C	142	HIS
16	F	111	GLN
17	G	33	ASN
19	I	36	GLN
19	I	58	HIS
19	I	105	ASN
23	M	83	ASN
24	N	164	ASN
25	O	43	ASN
25	O	95	ASN
25	O	158	HIS
25	O	202	GLN
26	P	79	GLN
28	R	168	GLN
28	R	181	GLN
32	Y	11	GLN
32	Y	24	HIS
34	a	73	ASN
35	b	46	ASN
35	b	137	HIS
36	c	285	GLN
38	e	45	ASN
39	f	85	ASN
39	f	97	GLN
40	h	18	HIS
43	m	28	HIS

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Mol	Chain	Res	Type
43	m	46	GLN
46	q	11	ASN
46	q	60	HIS
47	u	207	GLN
47	u	236	GLN
47	u	498	ASN
48	v	395	ASN
48	v	416	GLN
50	x	392	ASN
51	y	334	ASN
51	y	436	GLN
51	y	600	HIS
51	y	753	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1746/1869 (93%)	379 (21%)	8 (0%)
49	w	74/75 (98%)	21 (28%)	0
8	7	50/255 (19%)	33 (66%)	2 (4%)
All	All	1870/2199 (85%)	433 (23%)	10 (0%)

All (433) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	-32	A
8	7	-31	C
8	7	-30	A
8	7	-28	C
8	7	-27	A
8	7	-26	A
8	7	-23	A
8	7	-22	C
8	7	-21	A
8	7	-20	A
8	7	-17	A
8	7	-13	A
8	7	-12	A
8	7	-10	A
8	7	-8	A
8	7	-7	G

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Mol	Chain	Res	Type
8	7	-6	A
8	7	-5	C
8	7	3	G
8	7	4	G
8	7	5	U
8	7	6	A
8	7	7	C
8	7	8	G
8	7	10	U
8	7	11	U
8	7	14	A
8	7	15	G
8	7	17	C
8	7	19	U
8	7	20	G
8	7	21	A
8	7	22	G
11	A	2	A
11	A	33	G
11	A	41	G
11	A	42	A
11	A	46	A
11	A	56	G
11	A	58	C
11	A	59	U
11	A	65	C
11	A	67	C
11	A	68	A
11	A	73	C
11	A	74	G
11	A	78	C
11	A	103	A
11	A	114	G
11	A	115	U
11	A	126	G
11	A	129	C
11	A	130	G
11	A	140	U
11	A	142	C
11	A	143	U
11	A	149	A
11	A	154	U

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Mol	Chain	Res	Type
11	A	155	G
11	A	158	A
11	A	163	U
11	A	170	A
11	A	173	A
11	A	182	C
11	A	184	G
11	A	190	G
11	A	198	U
11	A	199	C
11	A	200	G
11	A	202	G
11	A	203	G
11	A	204	G
11	A	220	U
11	A	288	G
11	A	291	G
11	A	292	A
11	A	294	U
11	A	295	C
11	A	302	A
11	A	306	C
11	A	307	G
11	A	308	G
11	A	309	G
11	A	318	A
11	A	319	C
11	A	321	C
11	A	323	C
11	A	324	C
11	A	325	C
11	A	326	C
11	A	327	G
11	A	329	G
11	A	332	G
11	A	347	G
11	A	362	C
11	A	364	A
11	A	368	U
11	A	369	C
11	A	370	G
11	A	381	C

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Mol	Chain	Res	Type
11	A	384	U
11	A	385	G
11	A	386	C
11	A	409	C
11	A	418	A
11	A	448	A
11	A	450	C
11	A	452	G
11	A	455	A
11	A	465	A
11	A	471	G
11	A	472	C
11	A	473	A
11	A	474	G
11	A	476	A
11	A	482	G
11	A	487	U
11	A	492	C
11	A	493	A
11	A	500	A
11	A	508	A
11	A	509	OMG
11	A	534	G
11	A	536	A
11	A	537	C
11	A	538	U
11	A	539	C
11	A	540	U
11	A	541	U
11	A	542	U
11	A	543	C
11	A	544	G
11	A	545	A
11	A	546	G
11	A	550	C
11	A	553	U
11	A	554	A
11	A	556	U
11	A	557	U
11	A	558	G
11	A	563	G
11	A	564	A

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Mol	Chain	Res	Type
11	A	566	U
11	A	568	C
11	A	576	A
11	A	589	G
11	A	590	A
11	A	591	U
11	A	594	A
11	A	604	A
11	A	606	G
11	A	607	U
11	A	614	C
11	A	617	G
11	A	628	A
11	A	631	U
11	A	643	A
11	A	655	A
11	A	660	C
11	A	662	G
11	A	668	A2M
11	A	669	A
11	A	671	A
11	A	672	A
11	A	673	G
11	A	688	U
11	A	689	U
11	A	691	G
11	A	692	G
11	A	695	C
11	A	696	G
11	A	697	G
11	A	698	G
11	A	699	C
11	A	700	G
11	A	707	C
11	A	710	C
11	A	713	C
11	A	715	A
11	A	717	G
11	A	720	A
11	A	721	G
11	A	722	C
11	A	729	C

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Mol	Chain	Res	Type
11	A	731	G
11	A	732	U
11	A	734	C
11	A	735	C
11	A	737	G
11	A	738	C
11	A	739	C
11	A	748	C
11	A	749	U
11	A	751	G
11	A	752	G
11	A	753	C
11	A	791	C
11	A	795	A
11	A	798	G
11	A	799	U
11	A	810	A
11	A	821	G
11	A	822	PSU
11	A	827	A
11	A	830	A
11	A	835	C
11	A	836	G
11	A	837	A
11	A	838	G
11	A	839	C
11	A	840	C
11	A	841	G
11	A	845	G
11	A	847	A
11	A	870	A
11	A	872	A
11	A	873	G
11	A	880	G
11	A	886	A
11	A	887	U
11	A	888	U
11	A	890	U
11	A	891	G
11	A	895	G
11	A	896	U
11	A	897	U

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Mol	Chain	Res	Type
11	A	898	U
11	A	899	U
11	A	900	C
11	A	901	G
11	A	903	A
11	A	908	A
11	A	913	A
11	A	920	A
11	A	922	A
11	A	933	G
11	A	963	A
11	A	972	A
11	A	989	C
11	A	990	A
11	A	992	A
11	A	999	G
11	A	1002	U
11	A	1017	U
11	A	1023	A
11	A	1045	U
11	A	1047	C
11	A	1061	U
11	A	1062	A
11	A	1078	C
11	A	1083	A
11	A	1085	C
11	A	1089	G
11	A	1109	C
11	A	1113	A
11	A	1115	U
11	A	1117	C
11	A	1120	U
11	A	1123	C
11	A	1133	A
11	A	1138	C
11	A	1143	A
11	A	1153	C
11	A	1154	U
11	A	1155	U
11	A	1170	A
11	A	1195	A
11	A	1207	G

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Mol	Chain	Res	Type
11	A	1208	A
11	A	1211	G
11	A	1215	C
11	A	1216	C
11	A	1217	A
11	A	1220	A
11	A	1224	G
11	A	1242	U
11	A	1248	B8N
11	A	1249	C
11	A	1251	A
11	A	1253	A
11	A	1256	G
11	A	1257	G
11	A	1259	A
11	A	1264	C
11	A	1274	G
11	A	1275	G
11	A	1283	C
11	A	1288	U
11	A	1290	G
11	A	1292	C
11	A	1294	G
11	A	1295	A
11	A	1301	A
11	A	1302	G
11	A	1303	C
11	A	1308	U
11	A	1322	G
11	A	1326	U
11	A	1333	U
11	A	1341	C
11	A	1342	U
11	A	1348	G
11	A	1354	G
11	A	1356	G
11	A	1371	U
11	A	1372	U
11	A	1378	A
11	A	1382	A
11	A	1397	U
11	A	1398	G

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Mol	Chain	Res	Type
11	A	1401	A
11	A	1402	A
11	A	1417	C
11	A	1418	C
11	A	1419	C
11	A	1420	G
11	A	1421	A
11	A	1422	G
11	A	1423	C
11	A	1424	G
11	A	1433	C
11	A	1435	C
11	A	1436	C
11	A	1437	C
11	A	1438	A
11	A	1442	U
11	A	1454	A
11	A	1463	U
11	A	1487	A
11	A	1489	A
11	A	1490	G
11	A	1494	U
11	A	1495	G
11	A	1497	G
11	A	1498	A
11	A	1507	G
11	A	1508	A
11	A	1521	C
11	A	1522	A
11	A	1533	A
11	A	1534	C
11	A	1544	C
11	A	1552	G
11	A	1553	C
11	A	1556	A
11	A	1560	U
11	A	1570	G
11	A	1578	U
11	A	1580	A
11	A	1585	U
11	A	1587	G
11	A	1588	A

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Mol	Chain	Res	Type
11	A	1598	G
11	A	1600	G
11	A	1601	A
11	A	1606	G
11	A	1621	U
11	A	1623	A
11	A	1624	U
11	A	1639	G
11	A	1646	C
11	A	1648	G
11	A	1654	G
11	A	1661	A
11	A	1663	A
11	A	1665	G
11	A	1671	G
11	A	1686	G
11	A	1699	A
11	A	1715	A
11	A	1719	A
11	A	1721	U
11	A	1722	G
11	A	1729	U
11	A	1744	G
11	A	1749	G
11	A	1751	C
11	A	1752	C
11	A	1753	C
11	A	1754	G
11	A	1755	C
11	A	1758	G
11	A	1759	G
11	A	1760	G
11	A	1772	C
11	A	1773	C
11	A	1774	C
11	A	1775	U
11	A	1776	G
11	A	1777	G
11	A	1779	G
11	A	1780	G
11	A	1781	A
11	A	1782	G

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Mol	Chain	Res	Type
11	A	1783	C
11	A	1805	G
11	A	1808	U
11	A	1813	A
11	A	1822	A
11	A	1823	A
11	A	1824	A
11	A	1826	G
11	A	1829	G
11	A	1831	A
11	A	1835	A
11	A	1838	U
11	A	1849	G
11	A	1851	MA6
11	A	1861	G
11	A	1862	G
11	A	1863	A
11	A	1865	C
49	w	13	C
49	w	16	C
49	w	18	G
49	w	19	G
49	w	20	A
49	w	21	A
49	w	22	G
49	w	23	C
49	w	35	A
49	w	46	G
49	w	47	U
49	w	48	C
49	w	52	G
49	w	57	G
49	w	58	A
49	w	59	A
49	w	60	A
49	w	61	C
49	w	73	A
49	w	75	C
49	w	76	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	7	-21	A
8	7	4	G
11	A	1	U
11	A	291	G
11	A	368	U
11	A	688	U
11	A	694	G
11	A	731	G
11	A	797	C
11	A	1600	G

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

29 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
11	A2M	A	166	11	22,25,26	3.95	10 (45%)	31,36,39	3.40	14 (45%)
11	OMG	A	509	52,11	23,26,27	0.52	0	33,38,41	0.46	0
11	A2M	A	668	52,11	22,25,26	3.91	11 (50%)	31,36,39	3.30	14 (45%)
11	PSU	A	822	11	18,21,22	1.05	1 (5%)	22,30,33	1.76	5 (22%)
11	OMC	A	1703	52,11	19,22,23	0.54	0	26,31,34	0.72	1 (3%)
11	A2M	A	1678	11	22,25,26	3.96	11 (50%)	31,36,39	3.46	14 (45%)
11	JMH	A	1219	52,11	18,22,23	2.92	5 (27%)	21,32,35	1.71	4 (19%)
11	PSU	A	1081	11	18,21,22	1.06	1 (5%)	22,30,33	1.75	4 (18%)
11	B8N	A	1248	11	24,29,30	3.04	7 (29%)	29,42,45	1.79	5 (17%)
11	OMG	A	644	11	23,26,27	0.50	0	33,38,41	0.46	0
11	PSU	A	119	11	18,21,22	1.02	1 (5%)	22,30,33	1.56	4 (18%)
11	MA6	A	1851	11	23,26,27	1.56	3 (13%)	34,38,41	3.18	12 (35%)
11	A2M	A	159	11	22,25,26	3.90	10 (45%)	31,36,39	3.39	13 (41%)
11	MA6	A	1850	11	23,26,27	1.57	3 (13%)	34,38,41	3.12	12 (35%)
11	OMC	A	517	11	19,22,23	0.55	0	26,31,34	0.77	1 (3%)
11	PSU	A	823	11	18,21,22	1.10	1 (5%)	22,30,33	1.69	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	PSU	A	1243	11	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
11	5MU	A	814	11	19,22,23	0.42	0	28,32,35	0.82	1 (3%)
11	UR3	A	1830	11	19,22,23	2.83	8 (42%)	26,32,35	1.57	4 (15%)
11	A2M	A	27	52,11	22,25,26	3.91	11 (50%)	31,36,39	3.33	12 (38%)
11	5MC	A	1374	11	18,22,23	0.56	0	26,32,35	0.68	0
11	OMU	A	116	11	19,22,23	3.02	6 (31%)	26,31,34	1.58	4 (15%)
11	PSU	A	612	11	18,21,22	1.02	1 (5%)	22,30,33	1.71	5 (22%)
11	A2M	A	1031	11	22,25,26	3.94	11 (50%)	31,36,39	3.40	13 (41%)
11	A2M	A	484	11	22,25,26	3.86	11 (50%)	31,36,39	3.30	12 (38%)
11	OMC	A	174	52,11	19,22,23	0.53	0	26,31,34	0.66	0
11	6MZ	A	1832	52,11	22,25,26	2.39	5 (22%)	30,36,39	2.31	10 (33%)
11	OMG	A	683	11	23,26,27	0.51	0	33,38,41	0.53	0
11	OMU	A	121	11	19,22,23	3.01	6 (31%)	26,31,34	1.60	5 (19%)

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
11	A2M	A	166	11	-	0/9/27/28	0/3/3/3
11	OMG	A	509	52,11	-	2/9/27/28	0/3/3/3
11	A2M	A	668	52,11	-	3/9/27/28	0/3/3/3
11	PSU	A	822	11	-	2/7/25/26	0/2/2/2
11	OMC	A	1703	52,11	-	0/9/27/28	0/2/2/2
11	A2M	A	1678	11	-	1/9/27/28	0/3/3/3
11	JMH	A	1219	52,11	-	1/7/25/26	0/2/2/2
11	PSU	A	1081	11	-	1/7/25/26	0/2/2/2
11	B8N	A	1248	11	-	6/16/34/35	0/2/2/2
11	OMG	A	644	11	-	1/9/27/28	0/3/3/3
11	PSU	A	119	11	-	0/7/25/26	0/2/2/2
11	MA6	A	1851	11	-	3/11/29/30	0/3/3/3
11	A2M	A	159	11	-	3/9/27/28	0/3/3/3
11	MA6	A	1850	11	-	0/11/29/30	0/3/3/3
11	OMC	A	517	11	-	0/9/27/28	0/2/2/2
11	PSU	A	823	11	-	0/7/25/26	0/2/2/2
11	PSU	A	1243	11	-	2/7/25/26	0/2/2/2
11	5MU	A	814	11	-	0/7/25/26	0/2/2/2
11	UR3	A	1830	11	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	A2M	A	27	52,11	-	2/9/27/28	0/3/3/3
11	5MC	A	1374	11	-	0/7/25/26	0/2/2/2
11	OMU	A	116	11	-	1/9/27/28	0/2/2/2
11	PSU	A	612	11	-	0/7/25/26	0/2/2/2
11	A2M	A	1031	11	-	1/9/27/28	0/3/3/3
11	A2M	A	484	11	-	1/9/27/28	0/3/3/3
11	OMC	A	174	52,11	-	0/9/27/28	0/2/2/2
11	6MZ	A	1832	52,11	-	2/9/27/28	0/3/3/3
11	OMG	A	683	11	-	2/9/27/28	0/3/3/3
11	OMU	A	121	11	-	1/9/27/28	0/2/2/2

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	166	A2M	C3'-C2'	-12.81	1.24	1.52
11	A	1031	A2M	C3'-C2'	-12.80	1.24	1.52
11	A	1678	A2M	C3'-C2'	-12.74	1.24	1.52
11	A	27	A2M	C3'-C2'	-12.66	1.24	1.52
11	A	159	A2M	C3'-C2'	-12.49	1.25	1.52
11	A	484	A2M	C3'-C2'	-12.35	1.25	1.52
11	A	668	A2M	C3'-C2'	-12.33	1.25	1.52
11	A	1832	6MZ	C6-N6	9.50	1.44	1.34
11	A	1219	JMH	C2-N1	8.26	1.50	1.38
11	A	1248	B8N	C4-N3	-8.11	1.25	1.40
11	A	1830	UR3	C2-N1	7.63	1.49	1.38
11	A	1248	B8N	C6-N1	7.50	1.55	1.36
11	A	116	OMU	C2-N3	7.14	1.50	1.38
11	A	116	OMU	C2-N1	7.13	1.49	1.38
11	A	121	OMU	C2-N3	7.03	1.50	1.38
11	A	121	OMU	C2-N1	7.01	1.49	1.38
11	A	668	A2M	O4'-C4'	-6.93	1.29	1.45
11	A	159	A2M	O4'-C4'	-6.76	1.29	1.45
11	A	1678	A2M	O4'-C4'	-6.74	1.29	1.45
11	A	484	A2M	O4'-C4'	-6.56	1.30	1.45
11	A	27	A2M	O4'-C4'	-6.54	1.30	1.45
11	A	166	A2M	O4'-C4'	-6.51	1.30	1.45
11	A	1031	A2M	O4'-C4'	-6.49	1.30	1.45
11	A	121	OMU	C6-C5	6.20	1.49	1.35
11	A	116	OMU	C6-C5	6.14	1.49	1.35
11	A	1830	UR3	C6-C5	6.10	1.49	1.35
11	A	1219	JMH	C6-C5	5.94	1.48	1.35
11	A	1248	B8N	C6-C5	5.43	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1219	JMH	C2-N3	5.37	1.49	1.39
11	A	484	A2M	C3'-C4'	5.28	1.66	1.53
11	A	1678	A2M	C3'-C4'	5.23	1.66	1.53
11	A	668	A2M	C3'-C4'	5.22	1.66	1.53
11	A	27	A2M	C3'-C4'	5.19	1.66	1.53
11	A	159	A2M	C3'-C4'	5.16	1.66	1.53
11	A	1248	B8N	C2-N1	5.13	1.54	1.39
11	A	1850	MA6	C6-N6	5.10	1.51	1.36
11	A	1830	UR3	C2-N3	5.10	1.48	1.39
11	A	1851	MA6	C6-N6	5.06	1.51	1.36
11	A	1031	A2M	C3'-C4'	5.03	1.65	1.53
11	A	166	A2M	C3'-C4'	4.90	1.65	1.53
11	A	1678	A2M	C6-N6	4.56	1.45	1.34
11	A	159	A2M	C6-N6	4.55	1.45	1.34
11	A	166	A2M	C6-N6	4.54	1.45	1.34
11	A	27	A2M	C6-N6	4.53	1.45	1.34
11	A	484	A2M	C6-N6	4.53	1.45	1.34
11	A	668	A2M	C6-N6	4.53	1.45	1.34
11	A	1031	A2M	C6-N6	4.50	1.45	1.34
11	A	166	A2M	O4'-C1'	4.45	1.52	1.42
11	A	1031	A2M	O4'-C1'	4.41	1.52	1.42
11	A	166	A2M	C1'-N9	-4.39	1.33	1.46
11	A	1678	A2M	C1'-N9	-4.38	1.33	1.46
11	A	1031	A2M	C1'-N9	-4.33	1.34	1.46
11	A	1678	A2M	O4'-C1'	4.28	1.52	1.42
11	A	27	A2M	C1'-N9	-4.28	1.34	1.46
11	A	159	A2M	C1'-N9	-4.27	1.34	1.46
11	A	668	A2M	C1'-N9	-4.22	1.34	1.46
11	A	116	OMU	C4-N3	4.15	1.46	1.38
11	A	27	A2M	O4'-C1'	4.12	1.51	1.42
11	A	121	OMU	C4-N3	4.09	1.45	1.38
11	A	159	A2M	O4'-C1'	4.07	1.51	1.42
11	A	484	A2M	O4'-C1'	4.04	1.51	1.42
11	A	484	A2M	C1'-N9	-4.00	1.35	1.46
11	A	668	A2M	O4'-C1'	3.72	1.50	1.42
11	A	1248	B8N	C1'-C5	3.63	1.58	1.50
11	A	1243	PSU	C6-C5	3.55	1.39	1.35
11	A	823	PSU	C6-C5	3.53	1.39	1.35
11	A	159	A2M	O2'-C2'	3.49	1.51	1.42
11	A	119	PSU	C6-C5	3.48	1.39	1.35
11	A	1031	A2M	O2'-C2'	3.46	1.51	1.42
11	A	27	A2M	O2'-C2'	3.44	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	484	A2M	O2'-C2'	3.44	1.51	1.42
11	A	1678	A2M	O2'-C2'	3.42	1.51	1.42
11	A	668	A2M	O2'-C2'	3.41	1.51	1.42
11	A	822	PSU	C6-C5	3.39	1.39	1.35
11	A	166	A2M	O2'-C2'	3.39	1.51	1.42
11	A	1081	PSU	C6-C5	3.39	1.39	1.35
11	A	1248	B8N	O2-C2	-3.37	1.16	1.22
11	A	668	A2M	C2'-C1'	3.35	1.61	1.53
11	A	612	PSU	C6-C5	3.20	1.39	1.35
11	A	1830	UR3	C6-N1	3.11	1.45	1.38
11	A	166	A2M	C2'-C1'	3.07	1.61	1.53
11	A	484	A2M	C2'-C1'	3.04	1.60	1.53
11	A	1832	6MZ	C5-N7	-3.00	1.33	1.39
11	A	159	A2M	C2'-C1'	2.98	1.60	1.53
11	A	1851	MA6	C5-C4	-2.96	1.33	1.39
11	A	1031	A2M	C2'-C1'	2.96	1.60	1.53
11	A	1219	JMH	C6-N1	2.94	1.45	1.38
11	A	1850	MA6	C5-C4	-2.91	1.33	1.39
11	A	166	A2M	C5-C4	-2.89	1.33	1.39
11	A	668	A2M	C5-C4	-2.86	1.33	1.39
11	A	1678	A2M	C5-C4	-2.86	1.33	1.39
11	A	1031	A2M	C5-C4	-2.85	1.33	1.39
11	A	27	A2M	C5-C4	-2.84	1.33	1.39
11	A	27	A2M	C2'-C1'	2.78	1.60	1.53
11	A	159	A2M	C5-C4	-2.75	1.33	1.39
11	A	484	A2M	C5-C4	-2.72	1.33	1.39
11	A	121	OMU	C6-N1	2.65	1.44	1.38
11	A	1678	A2M	C2'-C1'	2.61	1.59	1.53
11	A	116	OMU	C6-N1	2.61	1.44	1.38
11	A	668	A2M	C5-N7	-2.53	1.34	1.39
11	A	1219	JMH	C5-C4	2.53	1.48	1.42
11	A	484	A2M	C5-N7	-2.52	1.34	1.39
11	A	1678	A2M	C5-N7	-2.47	1.34	1.39
11	A	27	A2M	C5-N7	-2.46	1.34	1.39
11	A	1031	A2M	C5-N7	-2.45	1.34	1.39
11	A	159	A2M	C5-N7	-2.45	1.34	1.39
11	A	166	A2M	C5-N7	-2.44	1.34	1.39
11	A	1830	UR3	O4-C4	-2.25	1.18	1.23
11	A	484	A2M	O3'-C3'	2.25	1.48	1.43
11	A	668	A2M	O3'-C3'	2.23	1.48	1.43
11	A	1830	UR3	O2-C2	-2.21	1.18	1.22
11	A	1248	B8N	C2-N3	2.21	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1678	A2M	C8-N9	-2.20	1.33	1.37
11	A	1830	UR3	C4-N3	2.20	1.45	1.40
11	A	1832	6MZ	C5-C4	-2.19	1.34	1.39
11	A	1830	UR3	C5-C4	2.18	1.49	1.43
11	A	121	OMU	C5-C4	2.13	1.48	1.43
11	A	1832	6MZ	C6-N1	-2.12	1.31	1.35
11	A	116	OMU	C5-C4	2.11	1.48	1.43
11	A	1851	MA6	C4-N3	2.08	1.38	1.34
11	A	1031	A2M	O3'-C3'	2.06	1.47	1.43
11	A	1850	MA6	C4-N3	2.06	1.38	1.34
11	A	27	A2M	O3'-C3'	2.04	1.47	1.43
11	A	1832	6MZ	C8-N9	-2.01	1.33	1.37

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1851	MA6	N1-C6-N6	-12.13	103.83	117.08
11	A	1850	MA6	N1-C6-N6	-11.89	104.08	117.08
11	A	1678	A2M	C1'-N9-C8	-9.56	105.55	127.14
11	A	159	A2M	C1'-N9-C8	-9.37	105.99	127.14
11	A	1031	A2M	C1'-N9-C8	-9.07	106.65	127.14
11	A	27	A2M	C1'-N9-C8	-8.91	107.02	127.14
11	A	166	A2M	C1'-N9-C8	-8.88	107.07	127.14
11	A	484	A2M	C1'-N9-C8	-8.85	107.15	127.14
11	A	668	A2M	C1'-N9-C8	-8.67	107.55	127.14
11	A	159	A2M	C4-N9-C1'	8.02	145.69	126.59
11	A	1678	A2M	C4-N9-C1'	7.93	145.48	126.59
11	A	484	A2M	C4-N9-C1'	7.75	145.06	126.59
11	A	1031	A2M	C4-N9-C1'	7.66	144.86	126.59
11	A	27	A2M	C4-N9-C1'	7.56	144.61	126.59
11	A	166	A2M	C4-N9-C1'	7.48	144.42	126.59
11	A	668	A2M	C4-N9-C1'	7.39	144.19	126.59
11	A	1850	MA6	C5-C6-N6	6.52	136.66	125.30
11	A	1851	MA6	C5-C6-N6	6.46	136.56	125.30
11	A	166	A2M	N3-C2-N1	-5.75	119.61	128.60
11	A	27	A2M	N3-C2-N1	-5.74	119.62	128.60
11	A	1832	6MZ	N1-C2-N3	-5.74	119.62	128.60
11	A	1678	A2M	N3-C2-N1	-5.66	119.75	128.60
11	A	668	A2M	N6-C6-N1	-5.65	105.97	118.35
11	A	1031	A2M	N3-C2-N1	-5.61	119.83	128.60
11	A	1851	MA6	N1-C2-N3	-5.59	119.86	128.60
11	A	1031	A2M	N6-C6-N1	-5.59	106.11	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	166	A2M	N6-C6-N1	-5.58	106.12	118.35
11	A	484	A2M	N6-C6-N1	-5.56	106.18	118.35
11	A	159	A2M	N6-C6-N1	-5.52	106.26	118.35
11	A	27	A2M	N6-C6-N1	-5.51	106.28	118.35
11	A	1678	A2M	N6-C6-N1	-5.51	106.29	118.35
11	A	484	A2M	N3-C2-N1	-5.47	120.04	128.60
11	A	1850	MA6	N1-C2-N3	-5.44	120.09	128.60
11	A	159	A2M	N3-C2-N1	-5.43	120.11	128.60
11	A	668	A2M	N3-C2-N1	-5.39	120.17	128.60
11	A	1248	B8N	C5-C4-N3	5.34	126.06	116.17
11	A	1832	6MZ	C5-C4-N3	-5.28	119.87	126.75
11	A	484	A2M	C5-C4-N3	-5.20	119.96	126.75
11	A	159	A2M	C5-C4-N3	-5.11	120.08	126.75
11	A	1031	A2M	C5-C4-N3	-5.06	120.16	126.75
11	A	668	A2M	C5-C4-N3	-5.03	120.18	126.75
11	A	1219	JMH	C1'-N1-C2	5.00	125.42	116.99
11	A	27	A2M	C5-C4-N3	-4.98	120.26	126.75
11	A	1851	MA6	C5-C4-N3	-4.97	120.26	126.75
11	A	1678	A2M	C5-C4-N3	-4.97	120.27	126.75
11	A	166	A2M	C5-C4-N3	-4.88	120.38	126.75
11	A	668	A2M	C5-C6-N6	4.88	134.04	123.43
11	A	1248	B8N	C4-N3-C2	-4.83	119.35	125.46
11	A	121	OMU	C4-N3-C2	-4.81	120.24	126.58
11	A	1678	A2M	N9-C8-N7	-4.80	107.35	113.91
11	A	166	A2M	C5-C6-N6	4.79	133.86	123.43
11	A	159	A2M	C5-C6-N6	4.77	133.82	123.43
11	A	484	A2M	C5-C6-N6	4.77	133.80	123.43
11	A	27	A2M	C5-C6-N6	4.76	133.80	123.43
11	A	1031	A2M	C5-C6-N6	4.76	133.78	123.43
11	A	1678	A2M	C5-C6-N6	4.76	133.78	123.43
11	A	1850	MA6	C5-C4-N3	-4.74	120.57	126.75
11	A	166	A2M	N9-C8-N7	-4.67	107.53	113.91
11	A	1243	PSU	N1-C2-N3	4.65	120.40	115.13
11	A	1851	MA6	N9-C8-N7	-4.63	107.58	113.91
11	A	1031	A2M	N9-C8-N7	-4.61	107.61	113.91
11	A	1081	PSU	C4-N3-C2	-4.59	119.72	126.34
11	A	116	OMU	C4-N3-C2	-4.59	120.53	126.58
11	A	1850	MA6	N9-C8-N7	-4.56	107.68	113.91
11	A	822	PSU	N1-C2-N3	4.50	120.23	115.13
11	A	27	A2M	N9-C8-N7	-4.46	107.82	113.91
11	A	823	PSU	C4-N3-C2	-4.43	119.96	126.34
11	A	1243	PSU	C4-N3-C2	-4.42	119.97	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1081	PSU	N1-C2-N3	4.42	120.14	115.13
11	A	159	A2M	N9-C8-N7	-4.42	107.87	113.91
11	A	668	A2M	N9-C8-N7	-4.41	107.88	113.91
11	A	1830	UR3	C4-N3-C2	-4.38	120.44	124.56
11	A	822	PSU	C4-N3-C2	-4.38	120.03	126.34
11	A	612	PSU	N1-C2-N3	4.36	120.07	115.13
11	A	1832	6MZ	N9-C8-N7	-4.34	107.98	113.91
11	A	612	PSU	C4-N3-C2	-4.33	120.10	126.34
11	A	823	PSU	N1-C2-N3	4.29	119.99	115.13
11	A	484	A2M	N9-C8-N7	-4.10	108.31	113.91
11	A	1830	UR3	C1'-N1-C2	4.01	123.76	116.99
11	A	119	PSU	N1-C2-N3	4.01	119.67	115.13
11	A	119	PSU	C4-N3-C2	-3.99	120.59	126.34
11	A	27	A2M	O4'-C1'-N9	3.87	115.69	108.06
11	A	166	A2M	O4'-C1'-N9	3.84	115.63	108.06
11	A	1031	A2M	O4'-C1'-N9	3.82	115.59	108.06
11	A	1219	JMH	C6-N1-C2	-3.78	118.40	121.79
11	A	1850	MA6	C2-N1-C6	3.74	120.60	111.75
11	A	1678	A2M	O4'-C1'-N9	3.69	115.34	108.06
11	A	1851	MA6	C2-N1-C6	3.66	120.41	111.75
11	A	121	OMU	N3-C2-N1	3.66	119.74	114.89
11	A	1832	6MZ	C2-N3-C4	3.65	120.38	111.75
11	A	1832	6MZ	C5-N7-C8	3.63	108.67	103.51
11	A	1851	MA6	C2-N3-C4	3.55	120.14	111.75
11	A	1031	A2M	C2-N3-C4	3.53	120.10	111.75
11	A	27	A2M	C2-N3-C4	3.53	120.09	111.75
11	A	1850	MA6	C4-C5-C6	3.53	119.83	115.88
11	A	1832	6MZ	C4-C5-C6	3.52	119.53	116.81
11	A	166	A2M	C2-N3-C4	3.52	120.06	111.75
11	A	484	A2M	C2-N3-C4	3.51	120.05	111.75
11	A	116	OMU	N3-C2-N1	3.51	119.55	114.89
11	A	1678	A2M	C2-N3-C4	3.51	120.03	111.75
11	A	159	A2M	C2-N3-C4	3.46	119.92	111.75
11	A	1851	MA6	C4-C5-C6	3.43	119.72	115.88
11	A	668	A2M	C2-N3-C4	3.42	119.83	111.75
11	A	1850	MA6	C2-N3-C4	3.35	119.67	111.75
11	A	484	A2M	O4'-C1'-N9	3.34	114.63	108.06
11	A	1678	A2M	C5-N7-C8	3.32	108.23	103.51
11	A	1851	MA6	C5-N7-C8	3.24	108.12	103.51
11	A	166	A2M	C5-N7-C8	3.23	108.09	103.51
11	A	1031	A2M	C5-N7-C8	3.23	108.09	103.51
11	A	1678	A2M	N3-C4-N9	3.20	132.36	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	159	A2M	N3-C4-N9	3.16	132.28	127.08
11	A	1850	MA6	C5-N7-C8	3.14	107.97	103.51
11	A	1031	A2M	N3-C4-N9	3.13	132.25	127.08
11	A	159	A2M	C5-N7-C8	3.13	107.96	103.51
11	A	121	OMU	C5-C4-N3	3.10	119.48	114.84
11	A	668	A2M	C5-N7-C8	3.10	107.91	103.51
11	A	27	A2M	C5-N7-C8	3.09	107.89	103.51
11	A	484	A2M	N3-C4-N9	3.08	132.16	127.08
11	A	116	OMU	C5-C4-N3	3.06	119.42	114.84
11	A	27	A2M	N3-C4-N9	3.06	132.12	127.08
11	A	668	A2M	C2'-C1'-N9	3.05	118.67	113.53
11	A	1832	6MZ	N3-C4-N9	3.03	132.08	127.08
11	A	484	A2M	C5-N7-C8	3.02	107.79	103.51
11	A	668	A2M	N3-C4-N9	3.01	132.04	127.08
11	A	1830	UR3	C6-N1-C2	-3.00	119.10	121.79
11	A	159	A2M	O4'-C1'-N9	2.99	113.96	108.06
11	A	1248	B8N	N3-C2-N1	2.99	120.98	116.76
11	A	1678	A2M	C4'-O4'-C1'	-2.98	102.89	109.47
11	A	166	A2M	N3-C4-N9	2.98	131.99	127.08
11	A	1219	JMH	O2-C2-N3	-2.96	117.17	121.34
11	A	1678	A2M	C4-N9-C8	2.93	108.90	105.73
11	A	1851	MA6	N3-C4-N9	2.89	131.85	127.08
11	A	668	A2M	C4'-O4'-C1'	-2.83	103.22	109.47
11	A	116	OMU	O4-C4-C5	-2.78	120.27	125.16
11	A	1243	PSU	O2-C2-N1	-2.77	119.74	122.79
11	A	166	A2M	C4'-O4'-C1'	-2.76	103.37	109.47
11	A	822	PSU	O2-C2-N1	-2.75	119.76	122.79
11	A	1850	MA6	N3-C4-N9	2.75	131.61	127.08
11	A	612	PSU	O2-C2-N1	-2.74	119.78	122.79
11	A	166	A2M	C2'-C1'-N9	-2.74	108.92	113.53
11	A	1031	A2M	C4'-O4'-C1'	-2.73	103.46	109.47
11	A	121	OMU	O4-C4-C5	-2.67	120.47	125.16
11	A	1850	MA6	C4-N9-C8	2.61	108.55	105.73
11	A	1851	MA6	C4-N9-C8	2.58	108.52	105.73
11	A	166	A2M	C4-N9-C8	2.56	108.50	105.73
11	A	1031	A2M	C4-N9-C8	2.55	108.49	105.73
11	A	1243	PSU	C6-N1-C2	-2.55	120.08	122.68
11	A	1248	B8N	O4-C4-N3	-2.54	115.66	119.98
11	A	1832	6MZ	C4-C5-N7	-2.54	107.52	110.62
11	A	823	PSU	O2-C2-N1	-2.53	120.00	122.79
11	A	27	A2M	C4-N9-C8	2.44	108.37	105.73
11	A	822	PSU	C6-N1-C2	-2.39	120.24	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	159	A2M	C4-N9-C8	2.39	108.32	105.73
11	A	1830	UR3	O2-C2-N3	-2.36	118.02	121.34
11	A	159	A2M	C4'-O4'-C1'	-2.34	104.31	109.47
11	A	612	PSU	C6-N1-C2	-2.32	120.32	122.68
11	A	1081	PSU	O2-C2-N1	-2.31	120.25	122.79
11	A	119	PSU	O2-C2-N1	-2.29	120.27	122.79
11	A	668	A2M	C4-N9-C8	2.28	108.20	105.73
11	A	119	PSU	C6-N1-C2	-2.25	120.39	122.68
11	A	1851	MA6	C4-C5-N7	-2.24	107.90	110.62
11	A	823	PSU	C6-N1-C2	-2.23	120.40	122.68
11	A	822	PSU	O4'-C1'-C2'	2.21	108.26	105.14
11	A	1850	MA6	C4-C5-N7	-2.16	107.98	110.62
11	A	668	A2M	C3'-C2'-C1'	2.15	106.93	102.89
11	A	1219	JMH	C1'-N1-C6	-2.14	116.17	120.84
11	A	1832	6MZ	C4-N9-C1'	-2.14	121.49	126.59
11	A	1248	B8N	C31-N3-C2	2.10	120.82	117.67
11	A	1832	6MZ	C9-N6-C6	2.10	124.68	122.87
11	A	612	PSU	O4'-C1'-C2'	2.09	108.09	105.14
11	A	1081	PSU	O4'-C1'-C2'	2.08	108.07	105.14
11	A	814	5MU	C1'-N1-C2	2.08	121.33	117.57
11	A	121	OMU	O2-C2-N1	-2.06	120.05	122.79
11	A	1678	A2M	C4-C5-N7	-2.03	108.14	110.62
11	A	1703	OMC	C1'-N1-C2	2.02	122.94	118.42
11	A	484	A2M	C2'-C3'-C4'	2.02	106.37	101.99
11	A	517	OMC	C1'-N1-C2	2.00	122.89	118.42

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	27	A2M	C1'-C2'-O2'-CM'
11	A	116	OMU	C1'-C2'-O2'-CM2
11	A	121	OMU	C1'-C2'-O2'-CM2
11	A	159	A2M	C1'-C2'-O2'-CM'
11	A	484	A2M	C1'-C2'-O2'-CM'
11	A	668	A2M	O4'-C4'-C5'-O5'
11	A	668	A2M	C3'-C4'-C5'-O5'
11	A	1031	A2M	C1'-C2'-O2'-CM'
11	A	1830	UR3	O4'-C1'-N1-C6
11	A	1830	UR3	O4'-C1'-N1-C2
11	A	1832	6MZ	C5-C6-N6-C9
11	A	1832	6MZ	N1-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
11	A	1851	MA6	O4'-C4'-C5'-O5'
11	A	1248	B8N	O4'-C1'-C5-C6
11	A	1248	B8N	C2'-C1'-C5-C6
11	A	1248	B8N	C2'-C1'-C5-C4
11	A	1851	MA6	C3'-C4'-C5'-O5'
11	A	683	OMG	O4'-C4'-C5'-O5'
11	A	1248	B8N	O4'-C4'-C5'-O5'
11	A	1248	B8N	C3'-C4'-C5'-O5'
11	A	822	PSU	C3'-C4'-C5'-O5'
11	A	1243	PSU	O4'-C4'-C5'-O5'
11	A	683	OMG	C3'-C4'-C5'-O5'
11	A	822	PSU	O4'-C4'-C5'-O5'
11	A	1243	PSU	C3'-C4'-C5'-O5'
11	A	668	A2M	C1'-C2'-O2'-CM'
11	A	159	A2M	C4'-C5'-O5'-P
11	A	509	OMG	O4'-C4'-C5'-O5'
11	A	644	OMG	C4'-C5'-O5'-P
11	A	1851	MA6	C4'-C5'-O5'-P
11	A	1248	B8N	O4'-C1'-C5-C4
11	A	27	A2M	O4'-C4'-C5'-O5'
11	A	1678	A2M	C1'-C2'-O2'-CM'
11	A	1081	PSU	C4'-C5'-O5'-P
11	A	1219	JMH	C2'-C1'-N1-C2
11	A	159	A2M	C3'-C4'-C5'-O5'
11	A	509	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1678	A2M	2	0
11	A	1248	B8N	1	0
11	A	1850	MA6	1	0
11	A	823	PSU	1	0
11	A	1830	UR3	1	0
11	A	27	A2M	1	0
11	A	116	OMU	2	0
11	A	612	PSU	1	0
11	A	1031	A2M	1	0
11	A	484	A2M	1	0
11	A	1832	6MZ	1	0
11	A	121	OMU	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 94 ligands modelled in this entry, 93 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	GTP	0	1302	52	30,34,34	0.83	1 (3%)	46,54,54	1.71	10 (21%)

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
53	GTP	0	1302	52	-	5/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	0	1302	GTP	C2-N3	2.19	1.38	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	0	1302	GTP	C5-C4-N3	-4.98	120.38	128.46
53	0	1302	GTP	C2-N3-C4	4.42	120.17	112.30
53	0	1302	GTP	PB-O3B-PG	-3.75	119.97	132.83
53	0	1302	GTP	N9-C4-N3	3.26	132.48	125.94
53	0	1302	GTP	C2-N1-C6	-2.84	119.92	125.10
53	0	1302	GTP	N9-C8-N7	-2.55	108.58	113.39
53	0	1302	GTP	C5-C6-N1	2.47	119.47	113.19
53	0	1302	GTP	C8-N7-C5	2.44	108.66	104.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	0	1302	GTP	O6-C6-C5	-2.36	120.33	126.60
53	0	1302	GTP	C3'-C2'-C1'	2.12	105.46	101.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

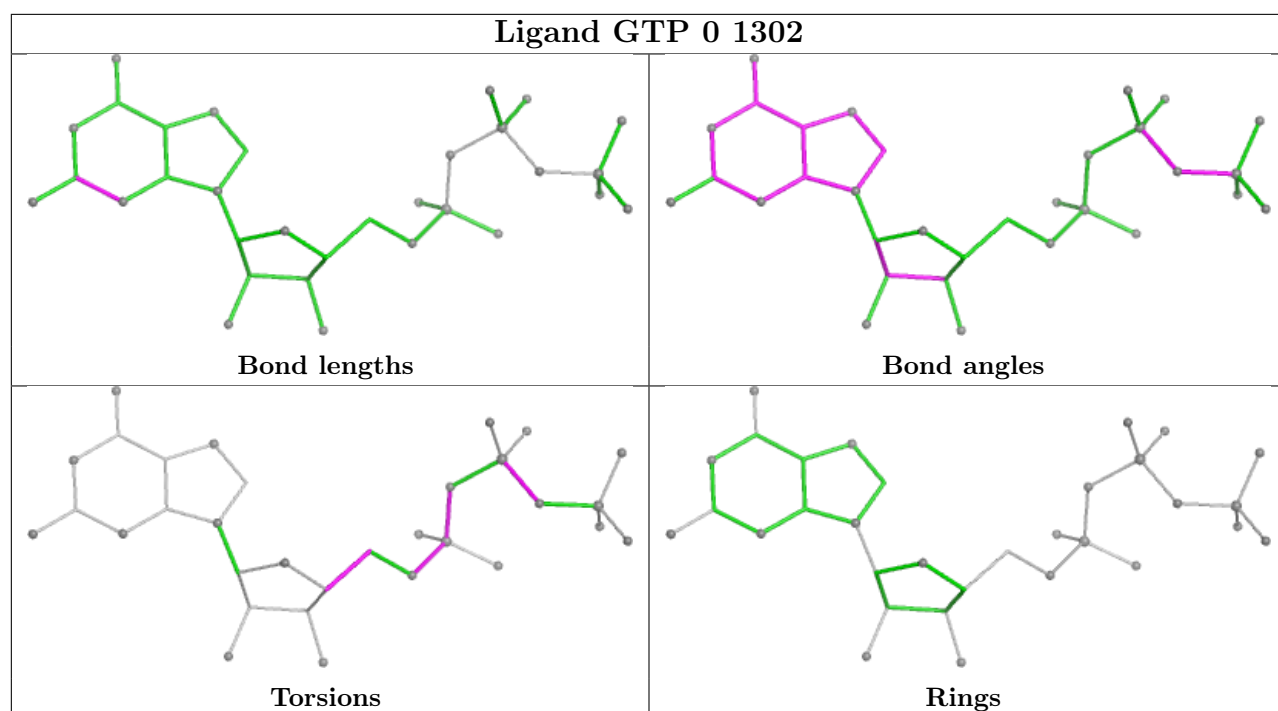
Mol	Chain	Res	Type	Atoms
53	0	1302	GTP	PB-O3A-PA-O1A
53	0	1302	GTP	PG-O3B-PB-O2B
53	0	1302	GTP	O4'-C4'-C5'-O5'
53	0	1302	GTP	C5'-O5'-PA-O3A
53	0	1302	GTP	PG-O3B-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	0	1302	GTP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

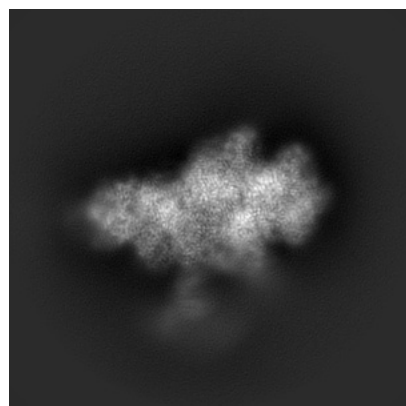
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17700. These allow visual inspection of the internal detail of the map and identification of artifacts.

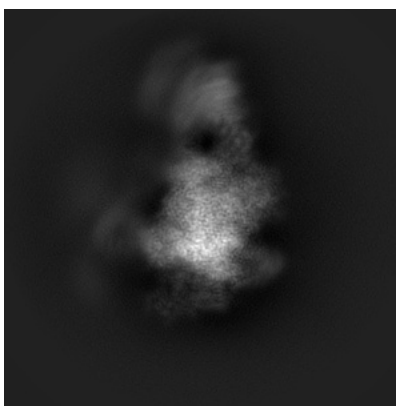
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

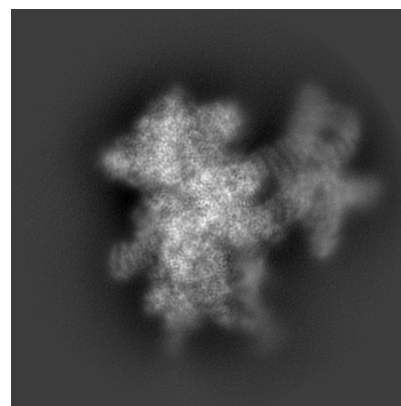
6.1.1 Primary map



X

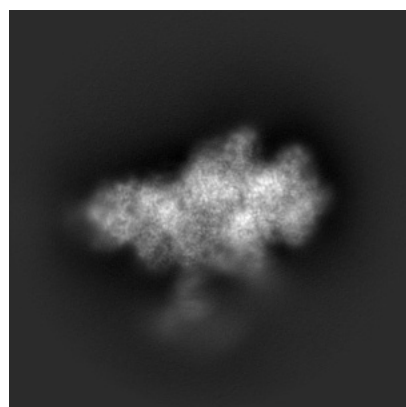


Y

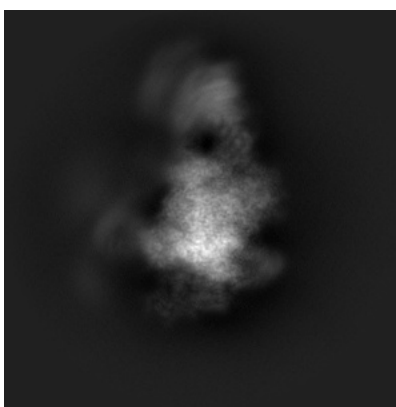


Z

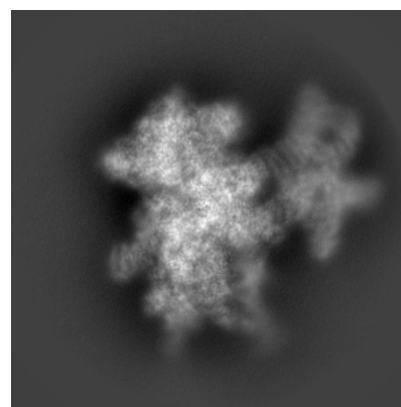
6.1.2 Raw map



X



Y

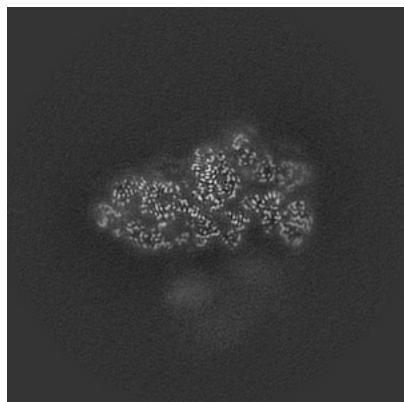


Z

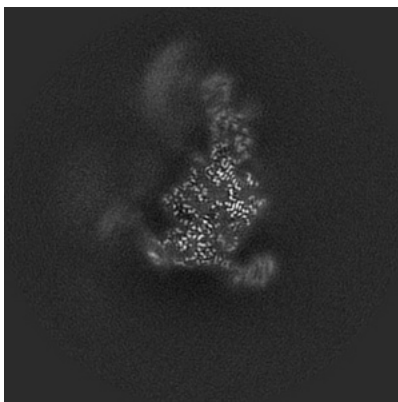
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

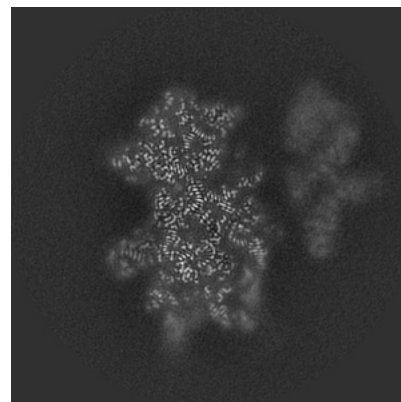
6.2.1 Primary map



X Index: 216

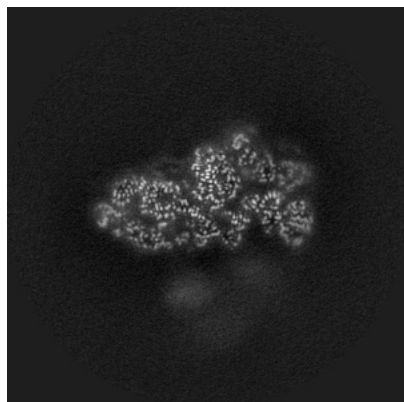


Y Index: 216

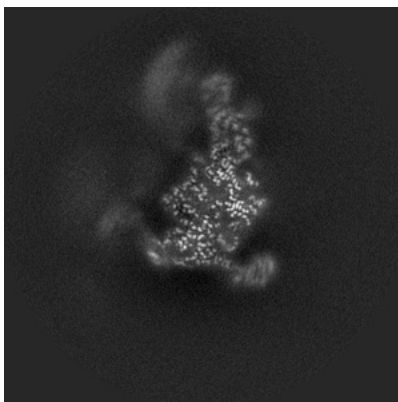


Z Index: 216

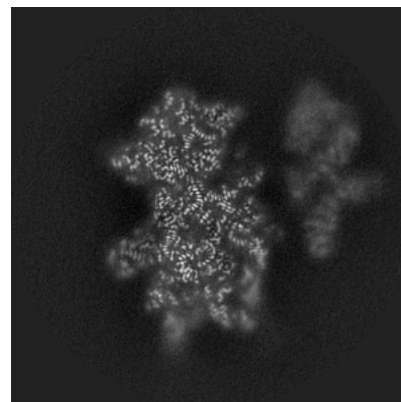
6.2.2 Raw map



X Index: 180



Y Index: 180

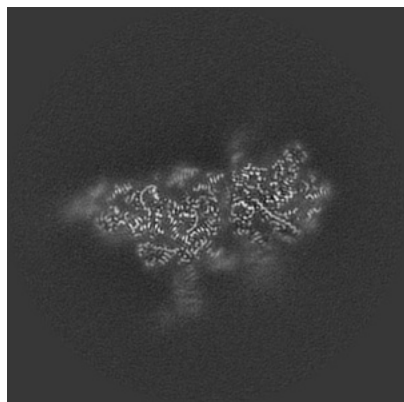


Z Index: 180

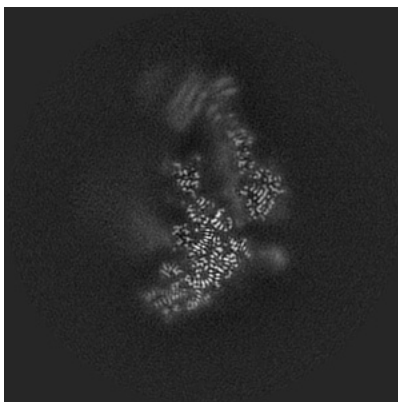
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

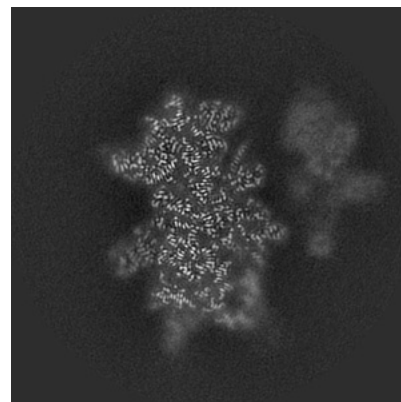
6.3.1 Primary map



X Index: 176

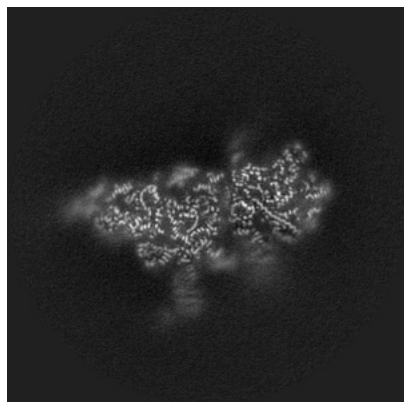


Y Index: 259

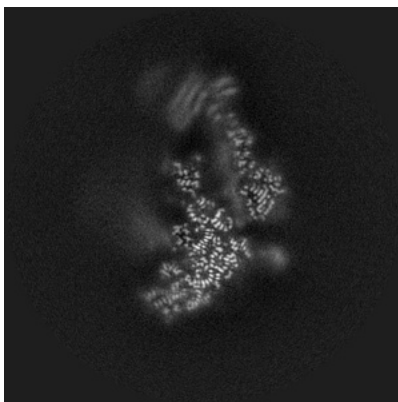


Z Index: 210

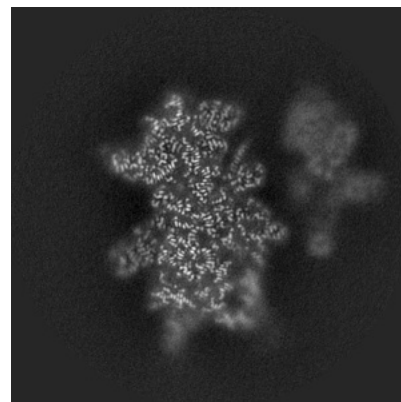
6.3.2 Raw map



X Index: 147



Y Index: 216

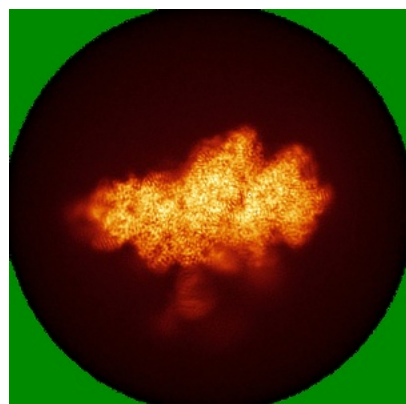


Z Index: 175

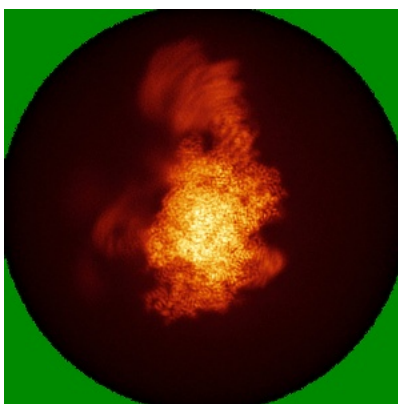
The images above show the largest variance slices of the map in three orthogonal directions.

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

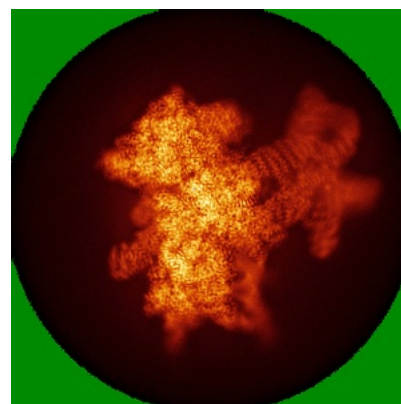
6.4.1 Primary map



X

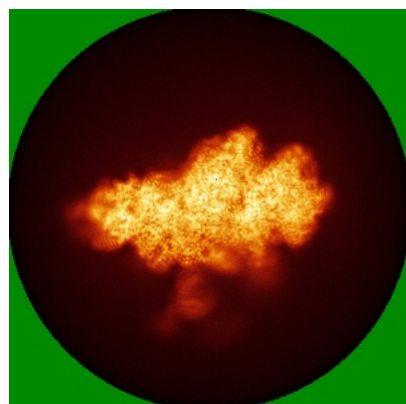


Y

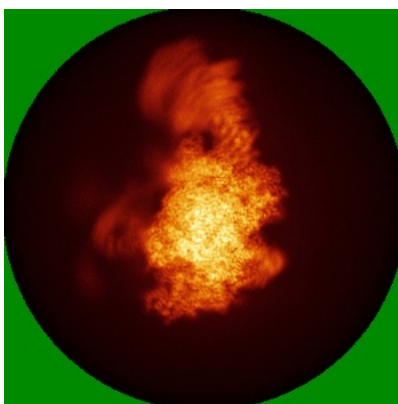


Z

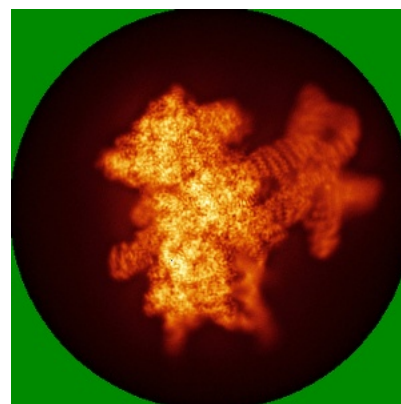
6.4.2 Raw map



X



Y

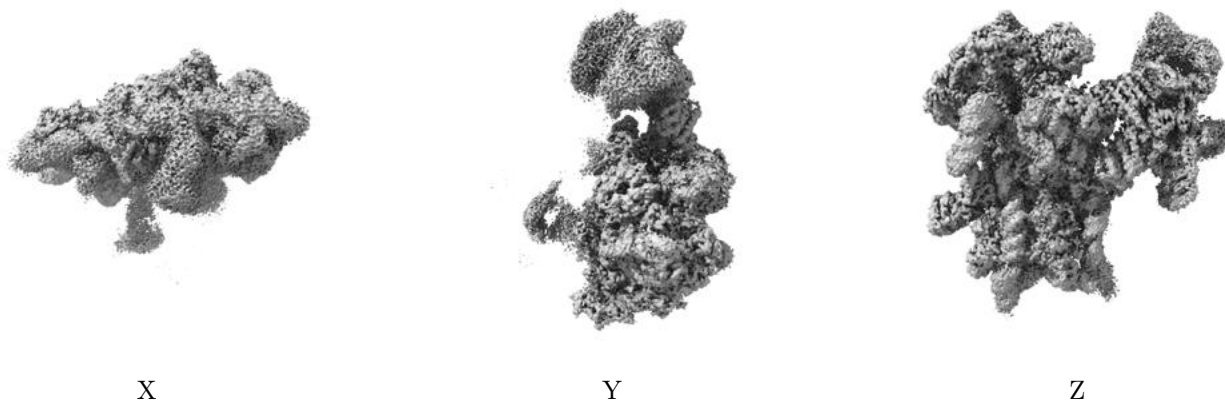


Z

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

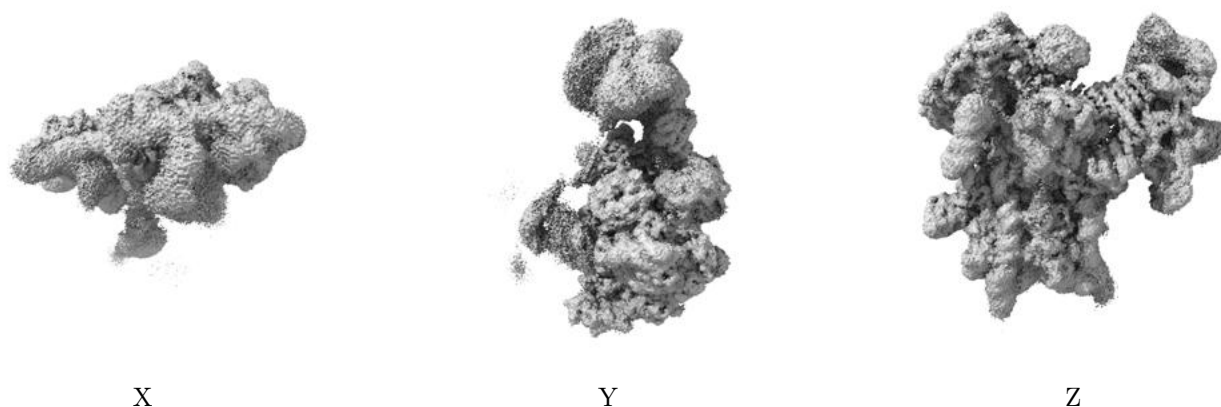
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

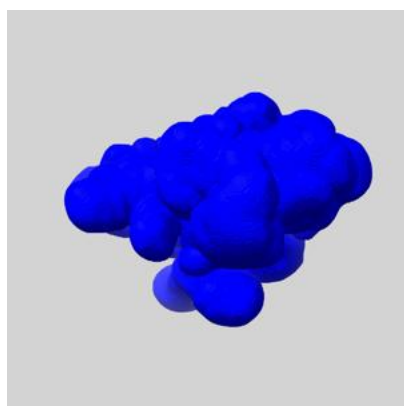
6.6 Mask visualisation [i](#)

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

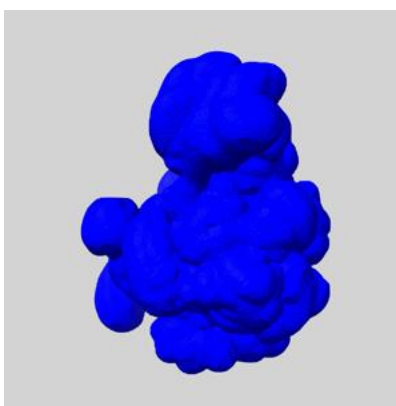
A mask typically either:

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

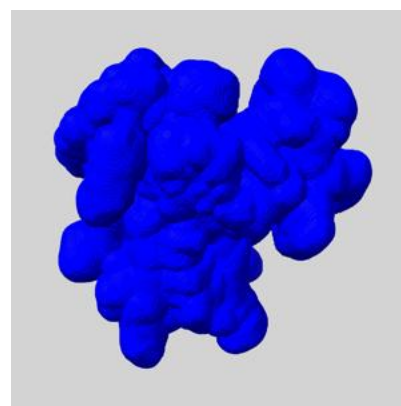
6.6.1 emd_17700_msk_1.map [i](#)



X



Y

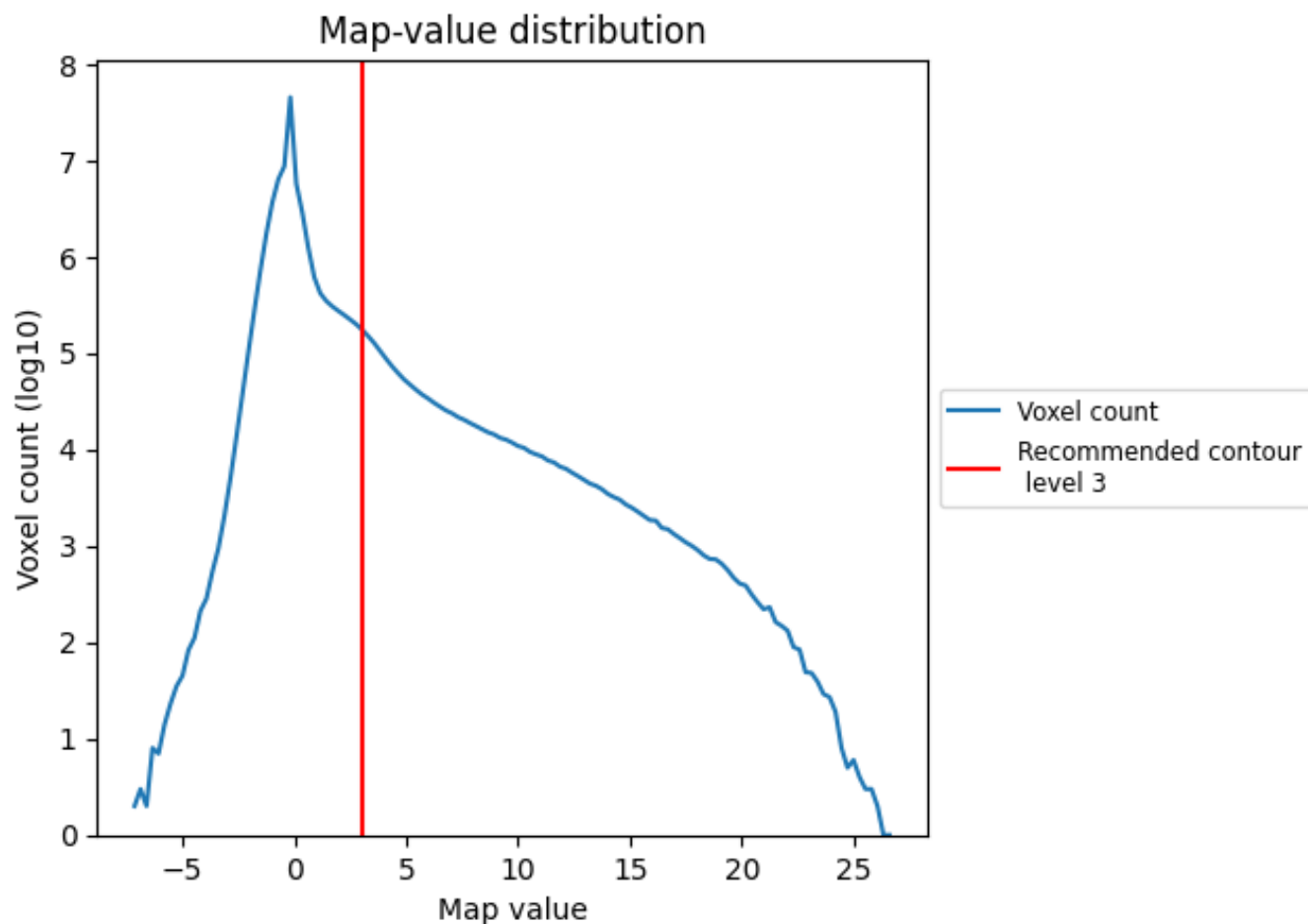


Z

7 Map analysis [i](#)

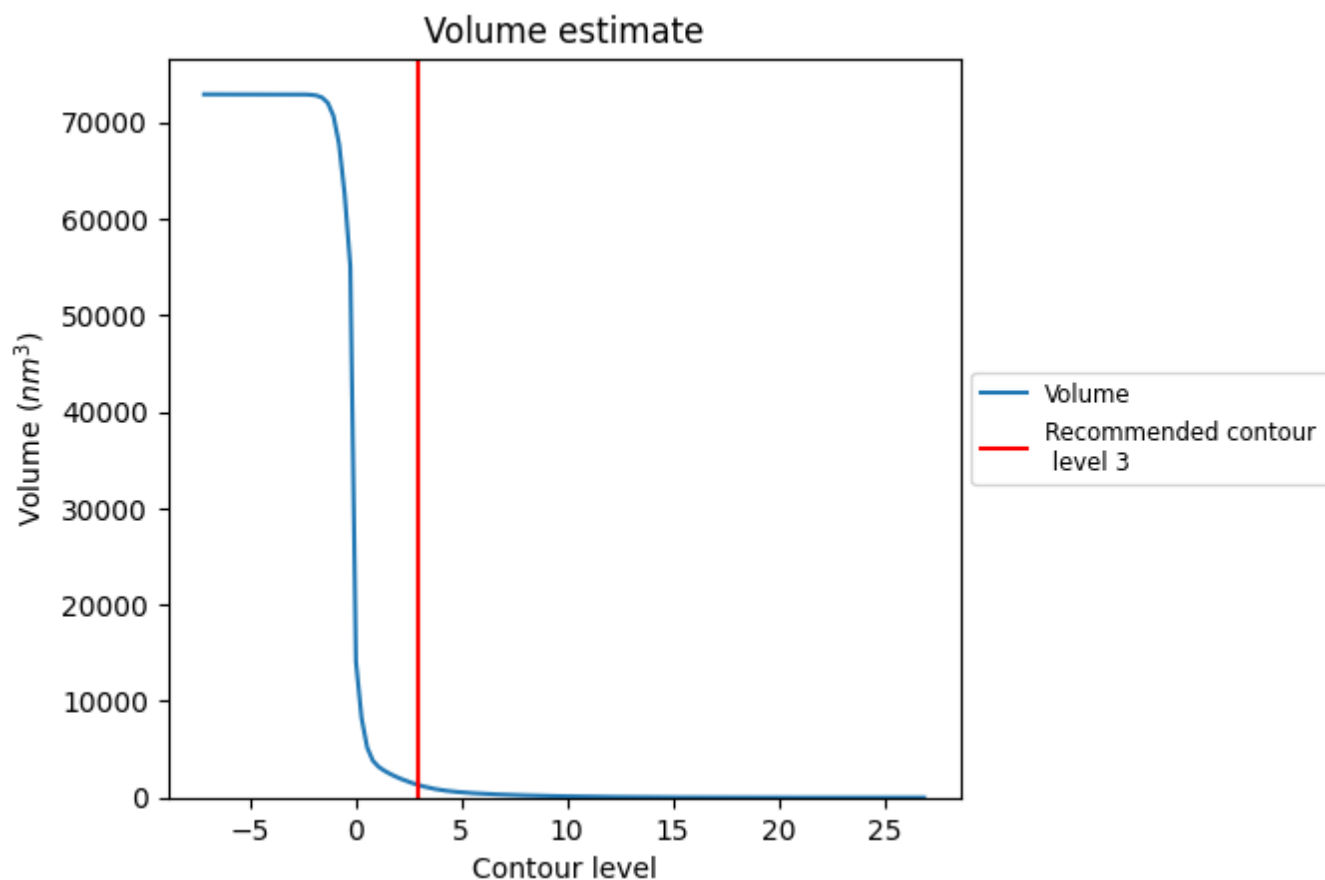
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

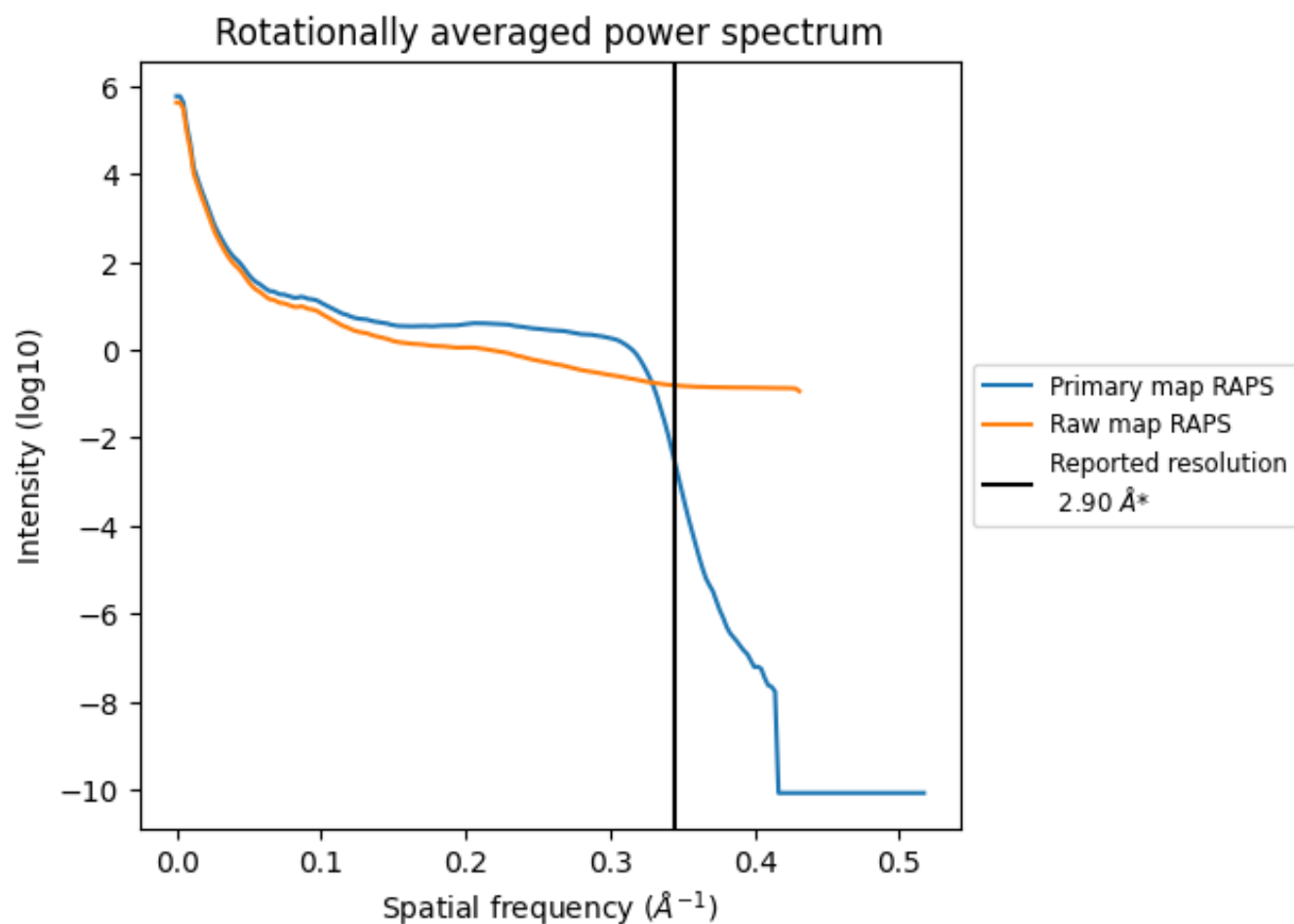
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1292 nm³; this corresponds to an approximate mass of 1167 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 ⓘ

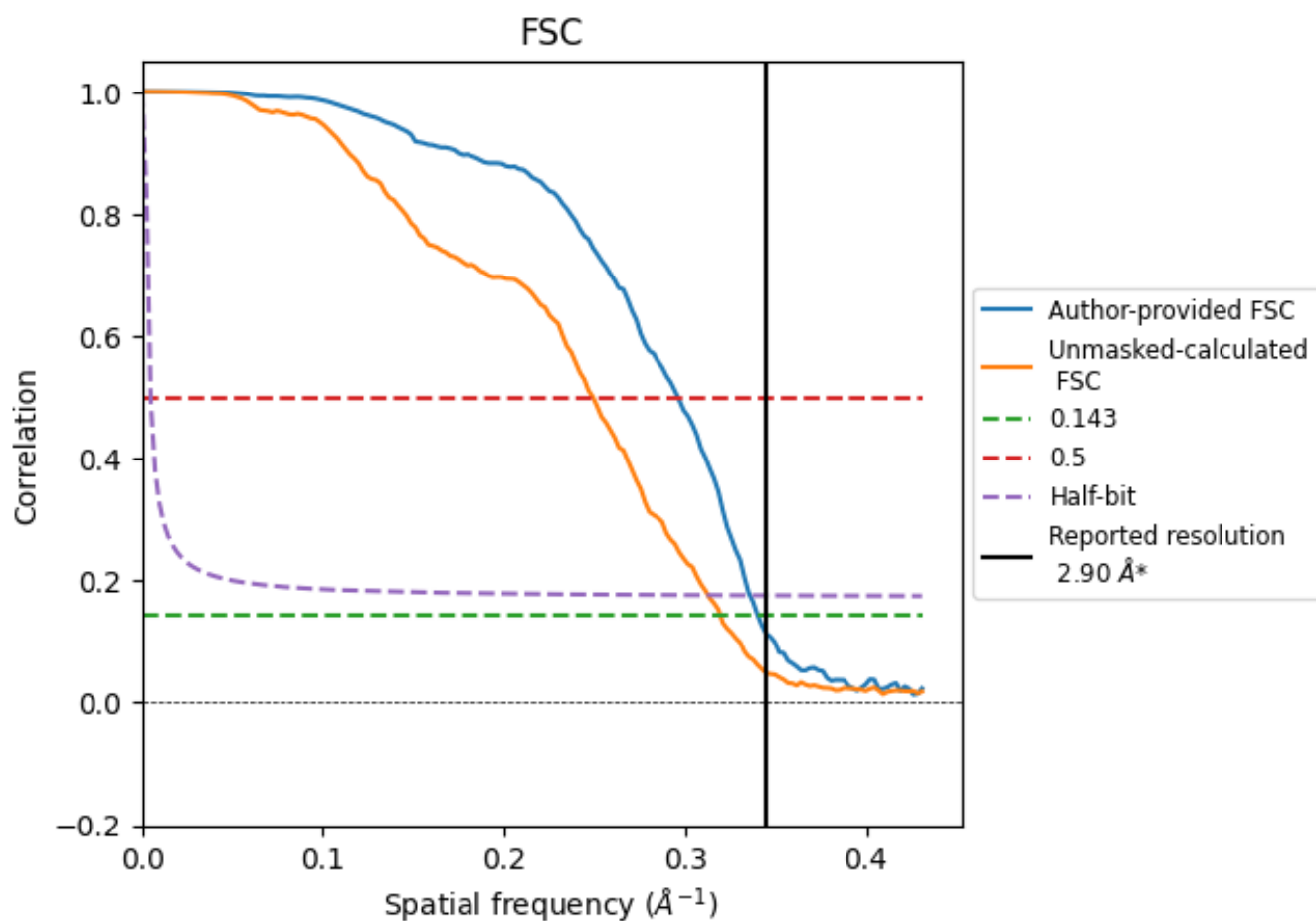


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

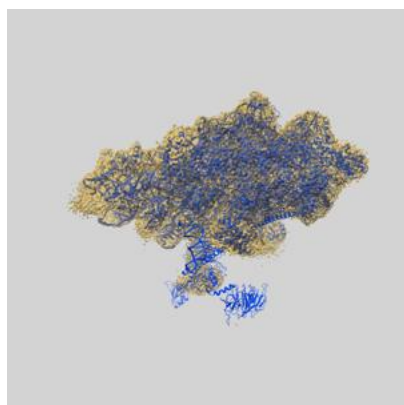
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.94	3.38	2.98
Unmasked-calculated*	3.13	4.01	3.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

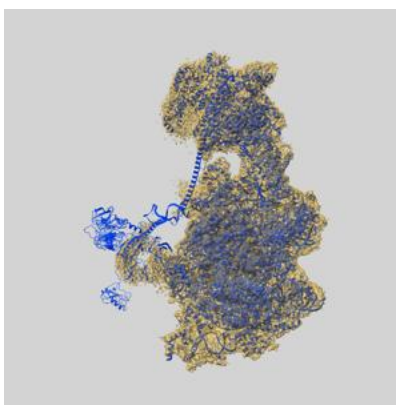
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17700 and PDB model 8PJ5. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

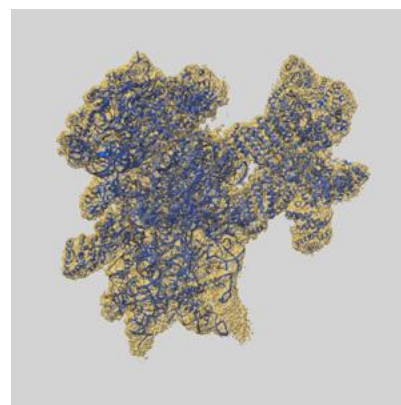
9.1 Map-model overlay [i](#)



X



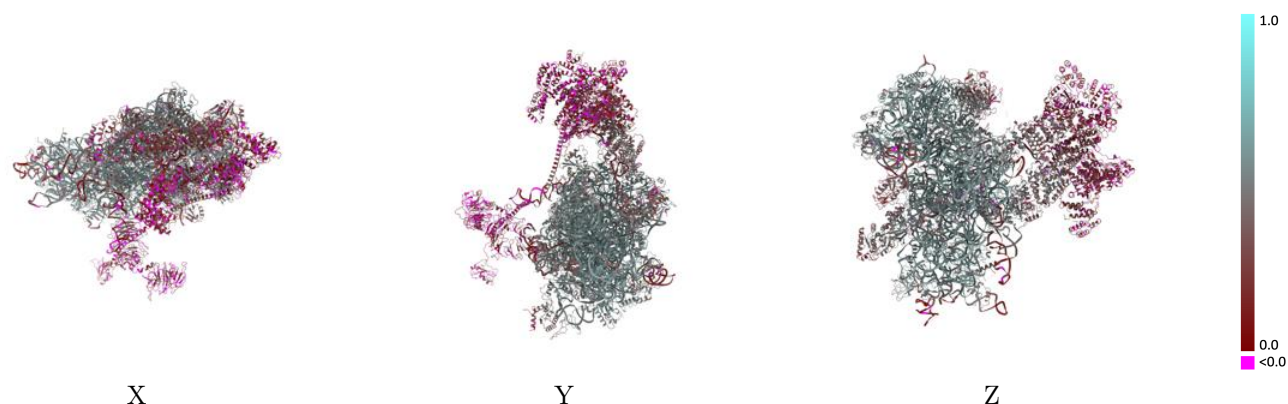
Y



Z

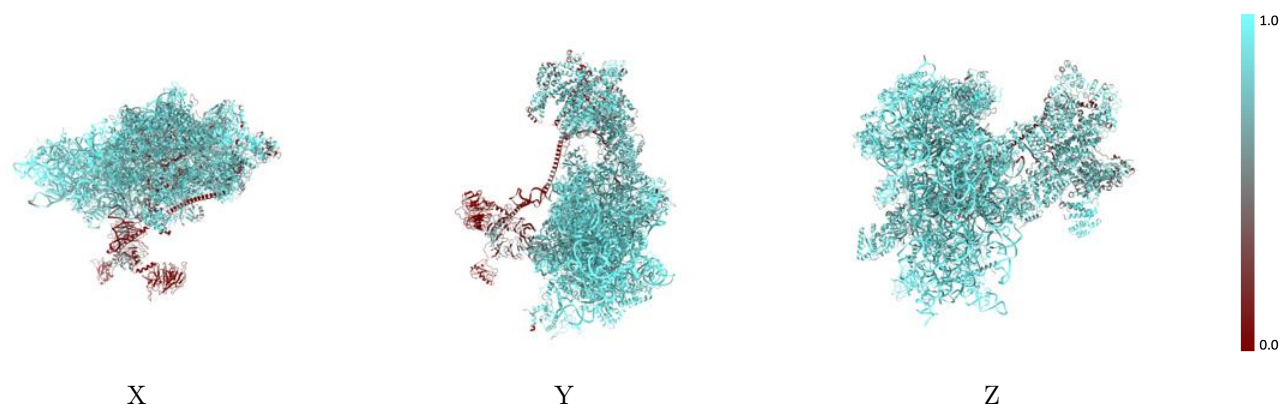
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



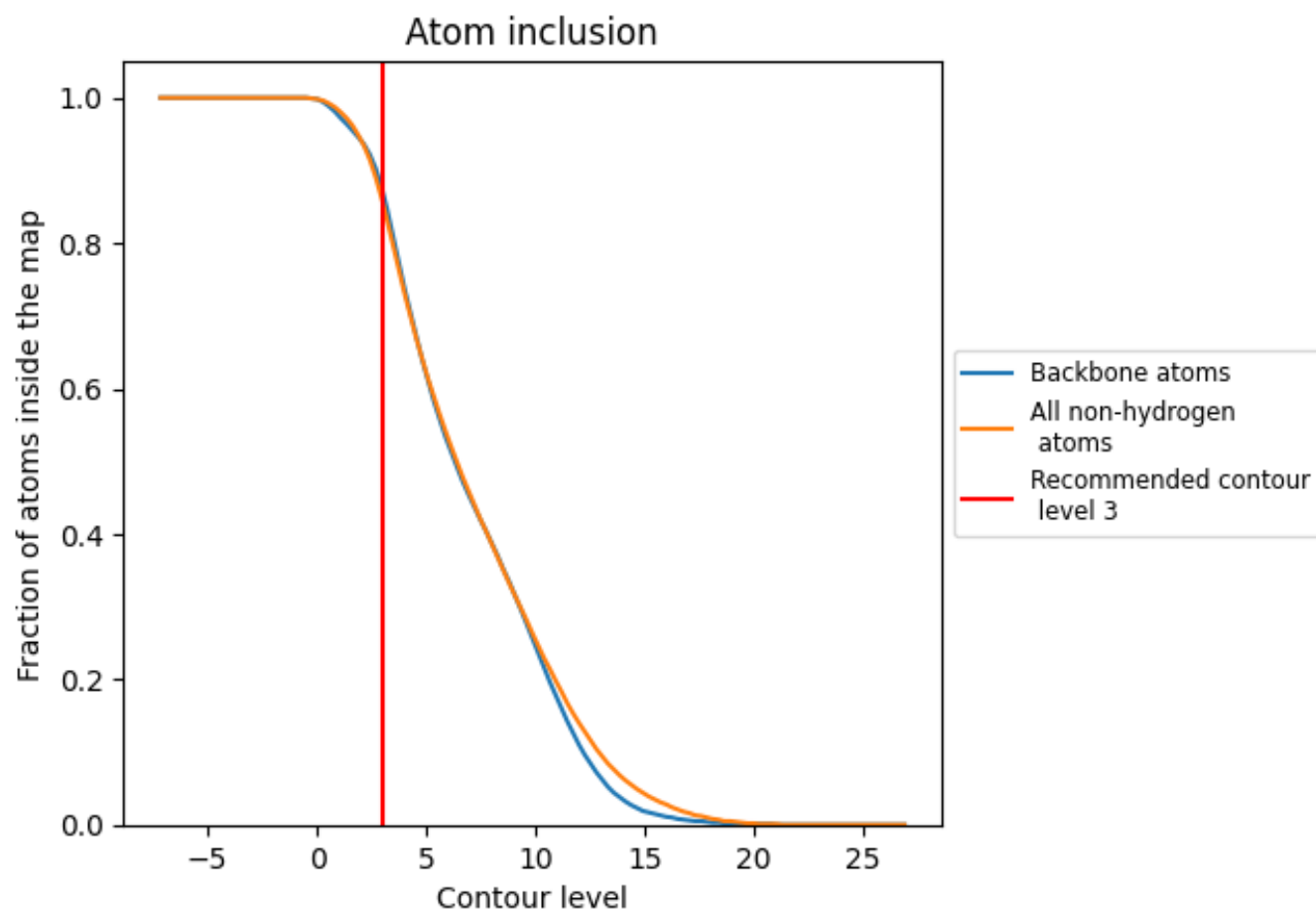
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8580	 0.4370
0	 0.8160	 0.3900
1	 0.2300	 0.1250
2	 0.0000	 0.0810
3	 0.6210	 0.1340
4	 0.7700	 0.1600
5	 0.7550	 0.1450
6	 0.7550	 0.1630
7	 0.6480	 0.2570
8	 0.6660	 0.1550
9	 0.8660	 0.5070
A	 0.9680	 0.5180
B	 0.9480	 0.5560
C	 0.9540	 0.5540
D	 0.9310	 0.5420
E	 0.9480	 0.5580
F	 0.8610	 0.5050
G	 0.8570	 0.4660
H	 0.9110	 0.5190
I	 0.9260	 0.5370
J	 0.9510	 0.5600
K	 0.9190	 0.5250
L	 0.9100	 0.5470
M	 0.8670	 0.5120
N	 0.9380	 0.5440
O	 0.9280	 0.5270
P	 0.9150	 0.5250
Q	 0.9300	 0.5430
R	 0.9570	 0.5250
S	 0.9460	 0.4950
T	 0.9430	 0.5270
V	 0.9240	 0.5360
Y	 0.9670	 0.5570
Z	 0.8790	 0.5170
a	 0.9360	 0.5160



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Chain	Atom inclusion	Q-score
b	 0.9380	 0.5370
c	 0.9230	 0.4990
d	 0.9560	 0.5470
e	 0.8760	 0.5080
f	 0.9140	 0.5130
h	 0.9110	 0.4910
i	 0.9580	 0.5670
k	 0.8590	 0.3870
m	 0.8110	 0.3500
n	 0.8540	 0.4940
o	 0.6480	 0.3030
q	 0.8250	 0.5010
u	 0.6850	 0.2860
v	 0.7430	 0.1900
w	 0.9360	 0.3200
x	 0.7740	 0.3550
y	 0.7960	 0.3640