



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:24 PM UTC

PDB ID : 5GAN / pdb_00005gan
EMDB ID : EMD-8012
Title : The overall structure of the yeast spliceosomal U4/U6.U5 tri-snRNP at 3.7 Angstrom
Authors : Nguyen, T.H.D.; Galej, W.P.; Bai, X.C.; Oubridge, C.; Scheres, S.H.W.; Newman, A.J.; Nagai, K.
Deposited on : 2015-12-15
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

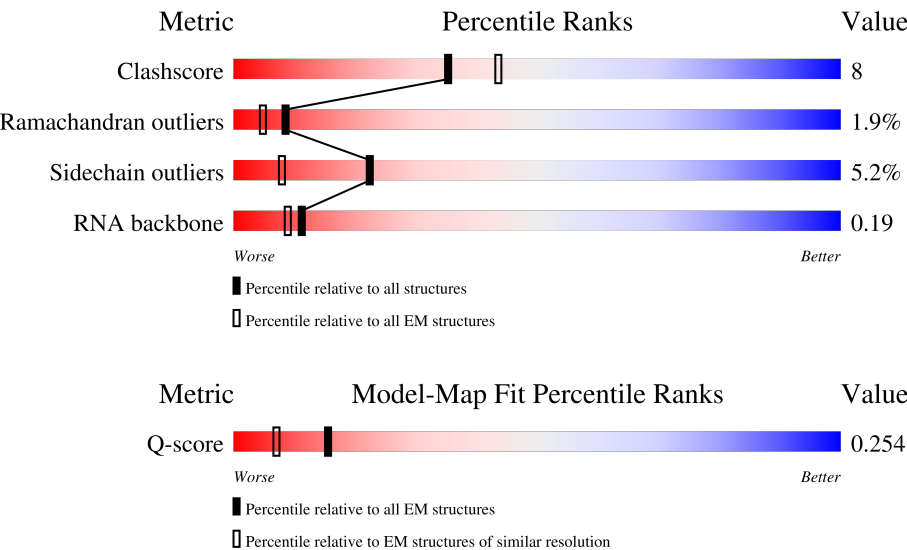
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.70 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.



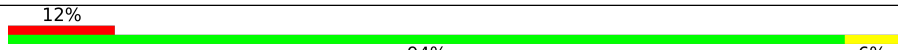
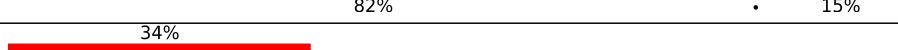
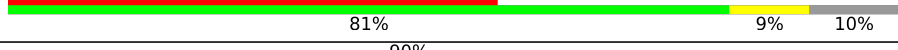
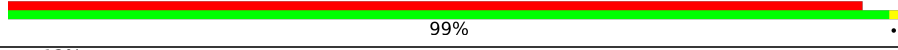
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11569 (3.20 - 4.20)

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 <=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	V	160	33% 26%37%12%•22%
2	W	112	13% 31%21%17%•29%
3	A	2413	15% 69%20%•9%

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Mol	Chain	Length	Quality of chain
4	H	465	
5	J	899	
6	D	143	
7	F	494	
8	G	469	
9	B	2163	
10	x	100	
11	b	196	
11	k	196	
12	h	146	
12	l	146	
13	j	110	
13	m	110	
14	d	101	
14	n	101	
15	e	94	
15	p	94	
16	f	86	
16	q	86	
17	g	77	
17	r	77	
18	E	328	
19	U	214	
20	K	126	
21	2	95	

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Mol	Chain	Length	Quality of chain
22	3	89	87%79%7%13%
23	4	187	40%37%60%
24	5	93	81%76%.19%
25	6	86	86%81%5%14%
26	7	115	57%55%.43%
27	8	109	59%58%.41%
28	C	1008	7%59%23%.15%

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 77370 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	V	124	Total	C	N	O	P	0	0
			2635	1179	459	873	124		

- Molecule 2 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	W	80	Total	C	N	O	P	0	0
			1697	759	293	565	80		

- Molecule 3 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	2196	Total	C	N	O	S	0	0
			17778	11444	3045	3226	63		

- Molecule 4 is a protein called U4/U6 small nuclear ribonucleoprotein PRP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	357	Total	C	N	O	S	0	0
			2789	1743	501	532	13		

- Molecule 5 is a protein called Pre-mRNA-splicing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	729	Total	C	N	O	S	0	0
			5822	3726	992	1079	25		

- Molecule 6 is a protein called Spliceosomal protein DIB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	140	Total	C	N	O	S	0	0
			1151	728	200	212	11		

- Molecule 7 is a protein called Pre-mRNA-processing factor 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	415	Total	C	N	O	S	0	0
			3218	2052	575	580	11		

- Molecule 8 is a protein called U4/U6 small nuclear ribonucleoprotein PRP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	318	Total	C	N	O	S	0	0
			2632	1659	469	488	16		

- Molecule 9 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	1781	Total	C	N	O	S	1	0
			14212	9098	2372	2685	57		

- Molecule 10 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	x	100	Total	C	N	O	0	0
			500	300	100	100		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
11	b	80	Total	C	N	O	S	0	0
			631	403	114	111	3		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	91	Total	C	N	O	S	0	0
			720	455	129	134	2		
12	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	94	Total	C	N	O	S	0	0
			737	474	140	119	4		
13	j	94	Total	C	N	O	S	0	0
			741	477	141	119	4		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
14	d	82	Total	C	N	O	S	0	0
			625	399	109	115	2		

- Molecule 15 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	p	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
15	e	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

- Molecule 16 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	q	72	Total	C	N	O	S	0	0
			573	368	101	103	1		
16	f	72	Total	C	N	O	S	0	0
			573	368	101	103	1		

- Molecule 17 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	r	69	Total	C	N	O	S	0	0
			526	336	93	95	2		
17	g	69	Total	C	N	O	S	0	0
			529	337	93	97	2		

- Molecule 18 is a protein called Snu66.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	328	Total	C	N	O		0	0
			1713	1033	342	338			

- Molecule 19 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	141	Total	C	N	O	P	0	0
			2999	1342	530	986	141		

- Molecule 20 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	K	124	Total	C	N	O	S	0	0
			936	597	161	174	4		

- Molecule 21 is a protein called U6 snRNA-associated Sm-like protein LSm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	2	90	Total	C	N	O	S	0	0
			735	469	124	139	3		

- Molecule 22 is a protein called U6 snRNA-associated Sm-like protein LSm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3	77	Total	C	N	O	S	0	0
			611	382	105	121	3		

- Molecule 23 is a protein called U6 snRNA-associated Sm-like protein LSm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	4	74	Total	C	N	O	S	0	0
			588	381	96	108	3		

- Molecule 24 is a protein called U6 snRNA-associated Sm-like protein LSm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	5	75	Total	C	N	O	S	0	0
			588	378	98	110	2		

- Molecule 25 is a protein called U6 snRNA-associated Sm-like protein LSm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	6	74	Total	C	N	O	S	0	0
			577	364	95	116	2		

- Molecule 26 is a protein called U6 snRNA-associated Sm-like protein LSm7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	7	66	Total	C	N	O	S	0	0
			504	325	85	91	3		

- Molecule 27 is a protein called U6 snRNA-associated Sm-like protein LSm8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	8	64	Total	C	N	O	S	0	0
			498	320	86	90	2		

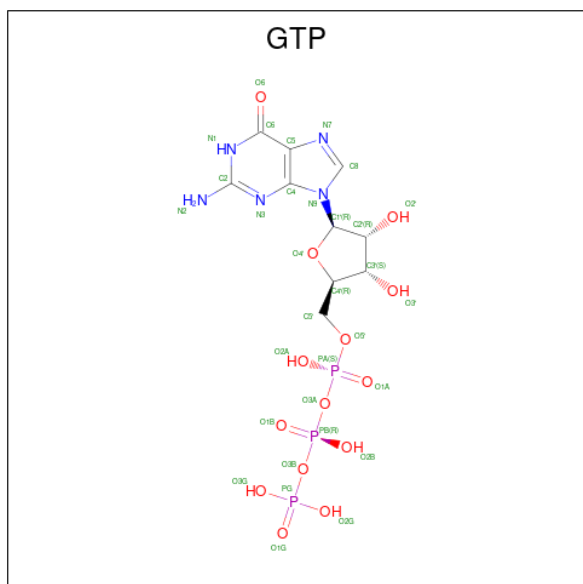
- Molecule 28 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C	855	Total	C	N	O	S	0	0
			6450	4195	1089	1143	23		

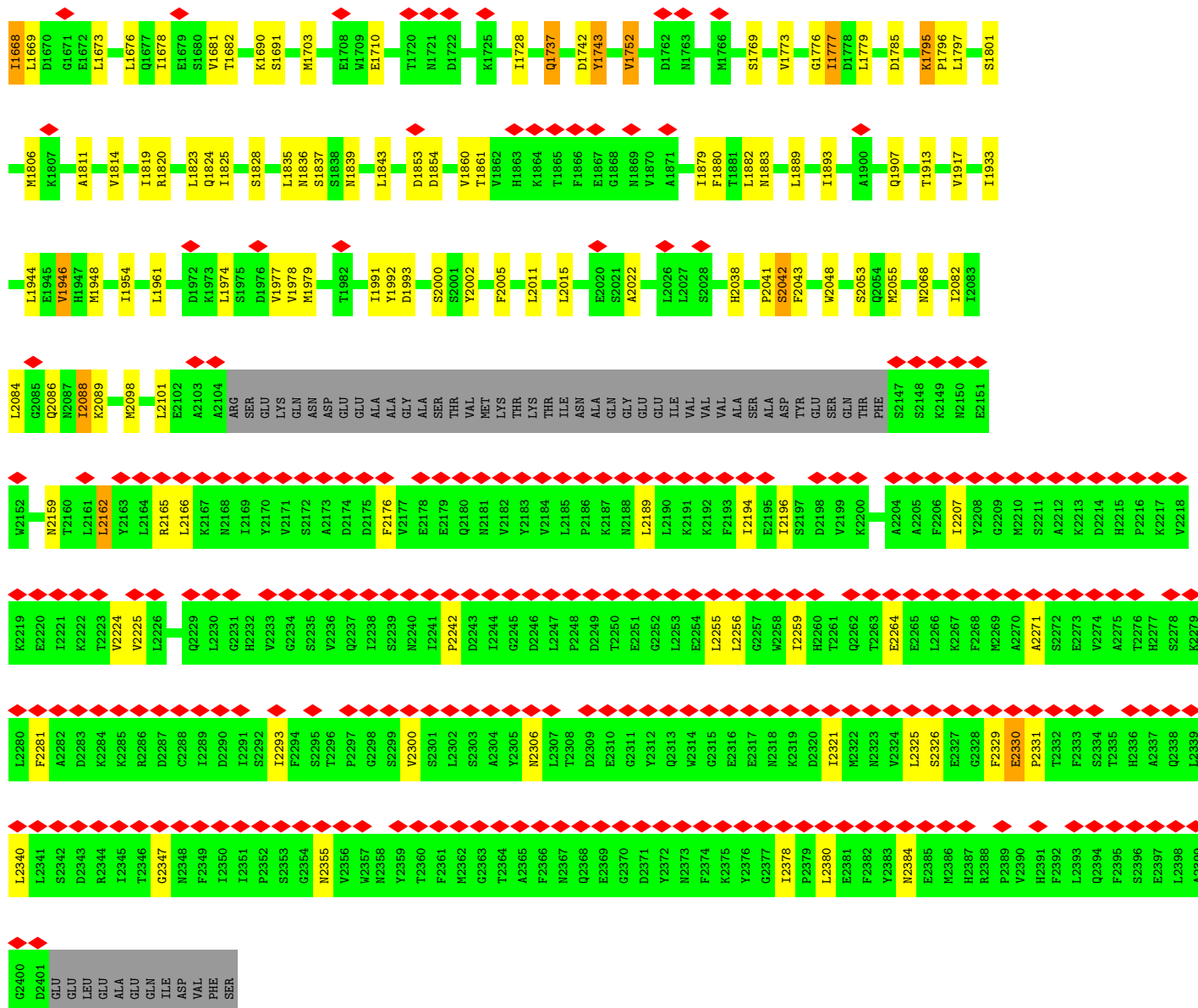
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	530	SER	GLU	conflict	UNP P36048
C	531	LYS	ASP	conflict	UNP P36048
C	532	THR	ASP	conflict	UNP P36048

- Molecule 29 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

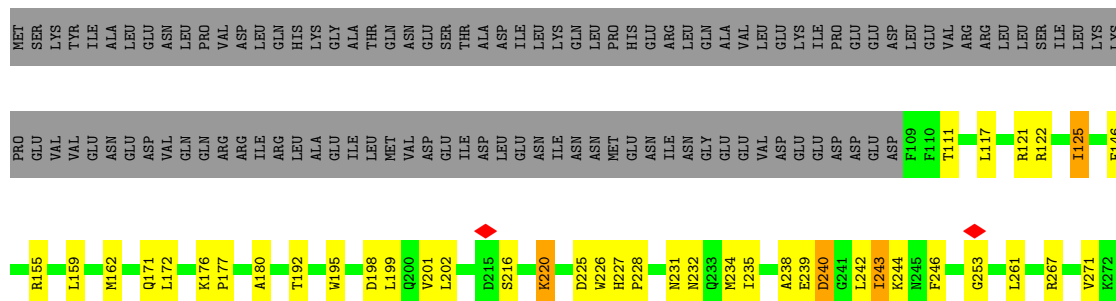


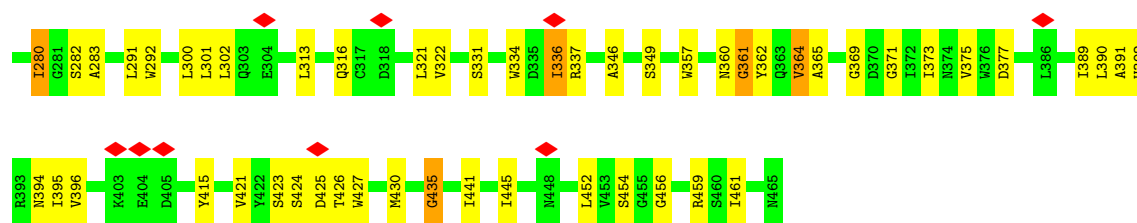




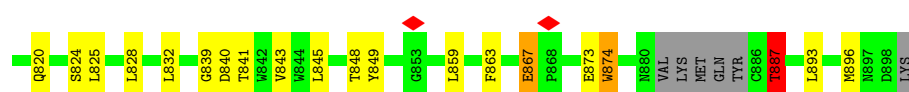
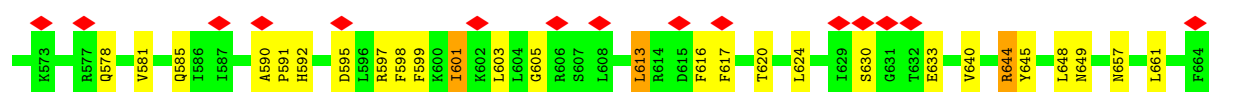
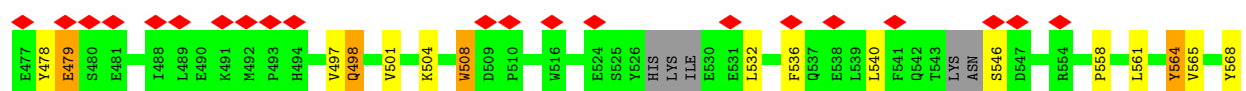
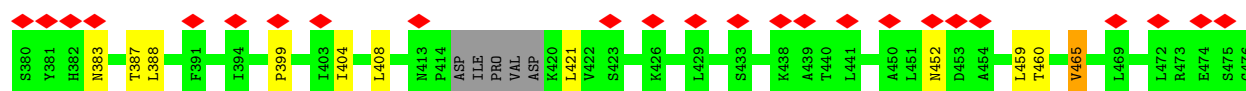
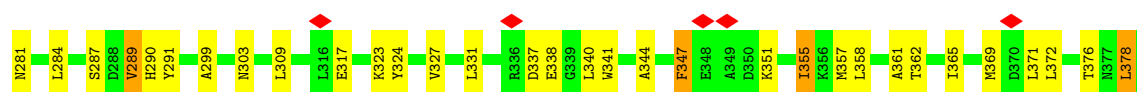
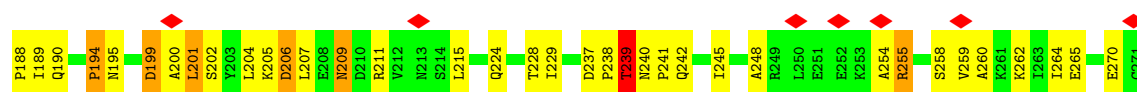
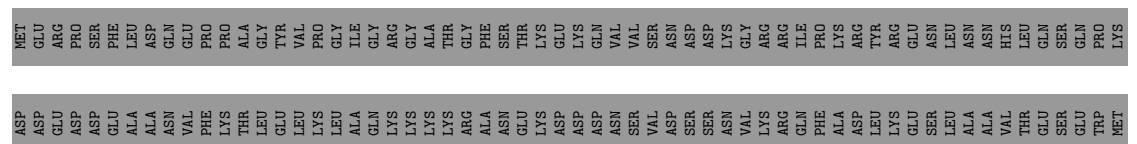
- Molecule 4: U4/U6 small nuclear ribonucleoprotein PRP4

Chain H: 57% 18% 23%



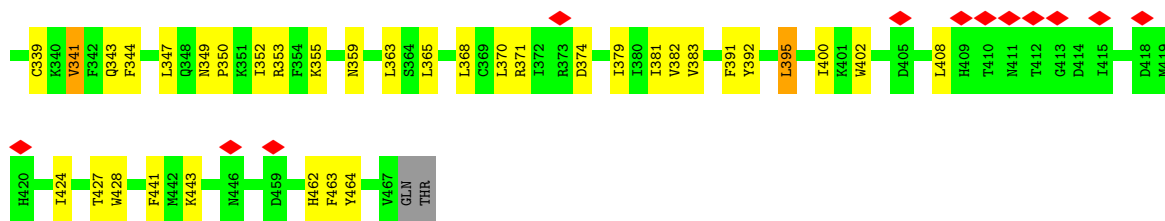


• Molecule 5: Pre-mRNA-splicing factor 6

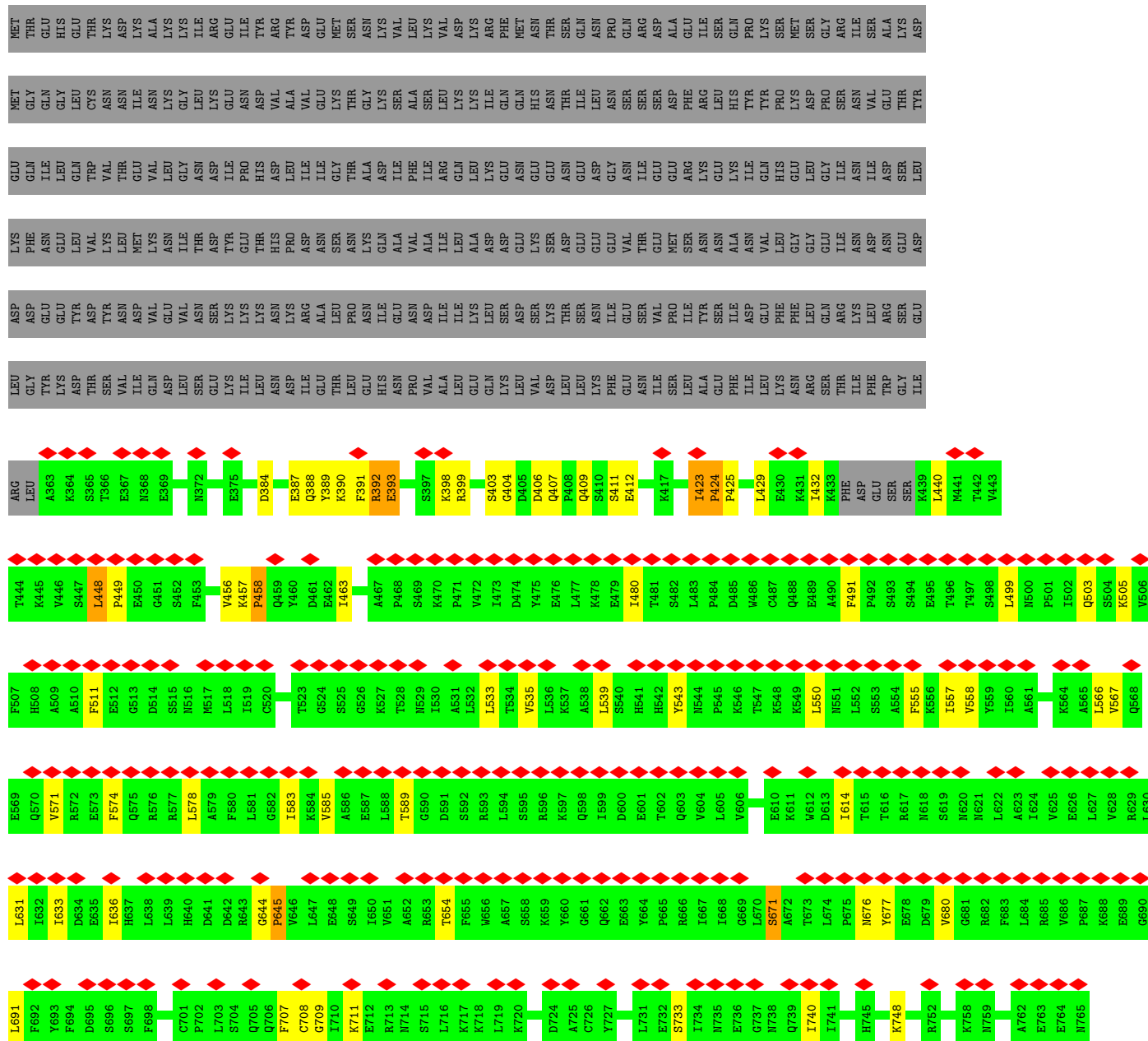


• Molecule 6: Spliceosomal protein DIB1

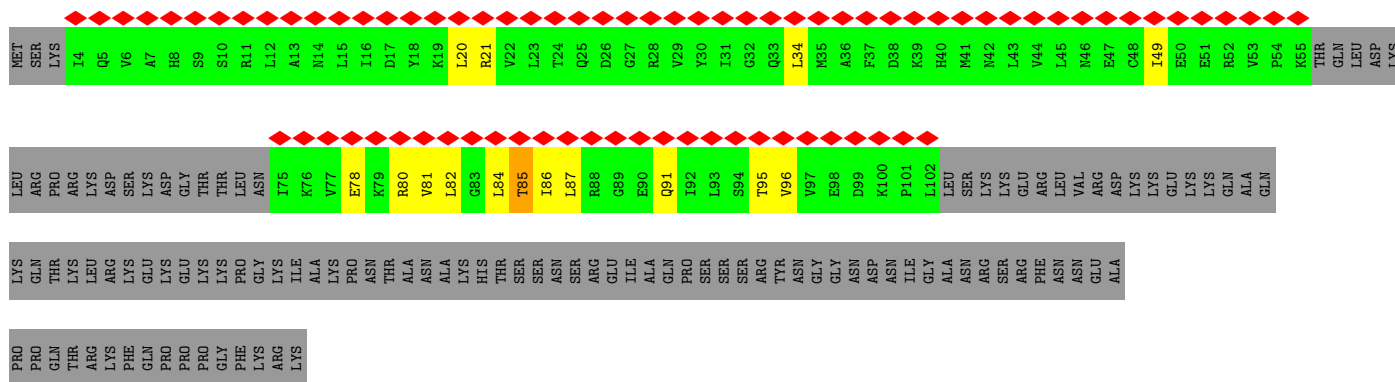




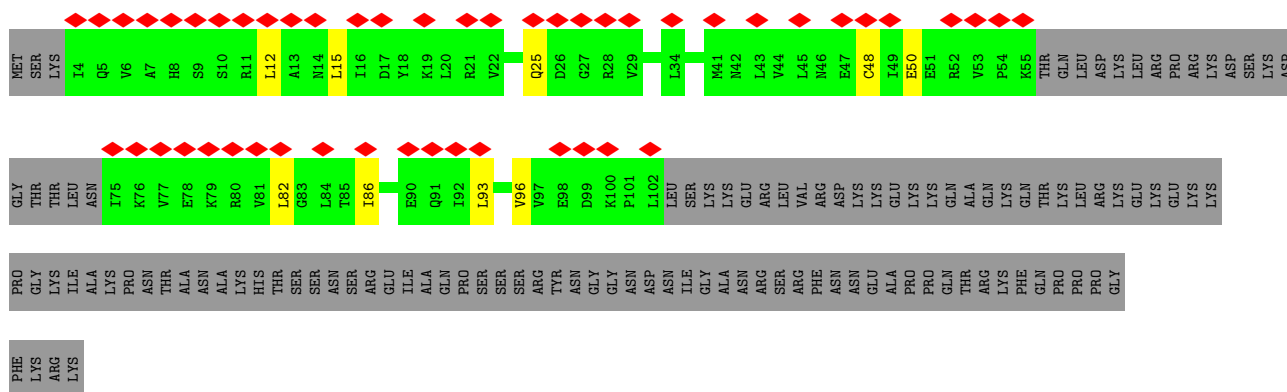
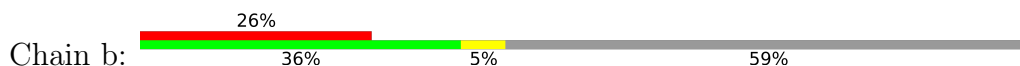
• Molecule 9: Pre-mRNA-splicing helicase BRR2



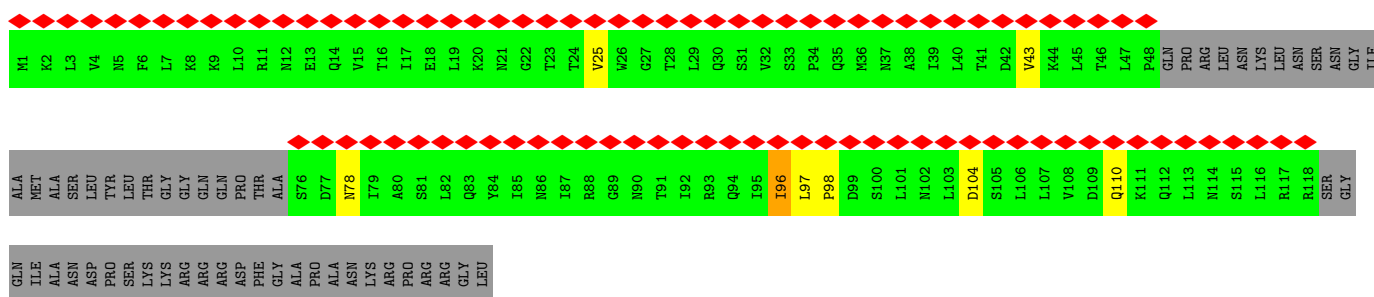
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V1483	Y1484	G1485	A1486	V1487	Y1488	E1489	T1490	L1491	S1492	R1493	R1494	M1495	I1496	F1497	I1498	A1499	T1500	Q1501	L1502	E1503	K1504	K1505	I1506	R1507	F1508	V1509	C1510	L1511	S1512	N1513	C1514	L1515	A1516	N1517	A1518	R1519	D1520	F1521	G1522	E1523	V1524	A1525	G1526	M1527	T1528	K1529	S1530	N1531	I1532	Y1533	N1534	F1535	S1536	P1537	S1538	R1539	K1600	F1601	E1542
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N1363	D1364	S1365	V1366	F1367	L1368	G1369	S1370	G1371	K1372	G1373	T1374	G1375	L1376	T1377	A1378	M1379	A1380	E1381	L1382	A1383	L1384	L1385	N1386	H1387	L1388	R1389	Q1390	N1391	L1392	G1393	R1394	A1395	V1396	Y1397	I1398	N1399	P1400	S1401	G1402	E1403	K1404	I1405	D1406	F1407	L1408	L1409	S1410	D1411	N1412	N1413	K1414	L1415	F1416	S1417	H1418	L1419	A1420	G1421	G1422
E1303	T1304	P1305	V1306	S1307	F1308	N1309	K1310	F1311	K1312	L1313	F1314	K1315	K1316	F1317	P1318	P1319	P1320	T1321	P1322	L1323	L1324	E1325	M1326	I1327	S1328	I1329	S1330	T1331	S1332	L1333	L1334	G1335	N1336	D1337	D1338	F1339	S1340	E1341	V1342	F1343	E1344	L1345	F1346	L1347	F1348	N1349	K1350	I1351	Q1352	S1353	Q1354	V1355	F1356	E1357	S1358	L1359	Y1360	N1361	S1362
L1243	E1244	D1245	T1246	D1247	G1248	D1249	S1250	L1251	L1252	Y1253	Y1254	L1255	V1256	L1257	F1258	I1259	T1260	K1261	D1262	L1263	V1264	G1265	H1266	E1267	F1268	T1269	L1270	S1271	F1272	T1273	Y1274	E1275	L1276	K1277	Q1278	N1280	Q1281	N1282	N1283	L1284	P1285	P1286	N1287	F1288	F1289	L1290	T1291	L1292	L1293	S1294	E1295	N1296	W1297	H1298	H1299	S1300	E1301	F1302	
E1303	T1304	P1305	V1306	S1307	F1308	N1309	K1310	F1311	K1312	L1313	F1314	K1315	K1316	F1317	P1318	P1319	P1320	T1321	P1322	L1323	L1324	E1325	M1326	I1327	S1328	I1329	S1330	T1331	S1332	L1333	L1334	G1335	N1336	D1337	D1338	F1339	S1340	E1341	V1342	F1343	E1344	L1345	F1346	L1347	F1348	N1349	K1350	I1351	Q1352	S1353	Q1354	V1355	F1356	E1357	S1358	L1359	Y1360	N1361	S1362
N1363	D1364	S1365	V1366	F1367	L1368	G1369	S1370	G1371	K1372	G1373	T1374	G1375	L1376	T1377	A1378	M1379	A1380	E1381	L1382	A1383	L1384	L1385	N1386	H1387	L1388	R1389	Q1390	N1391	L1392	G1393	R1394	A1395	V1396	Y1397	I1398	N1399	P1400	S1401	G1402	E1403	K1404	I1405	D1406	F1407	L1408	L1409	S1410	D1411	N1412	N1413	K1414	L1415	F1416	S1417	H1418	L1419	A1420	G1421	G1422
K1423	I1424	I1425	N1426	K1427	L1428	G1429	N1430	D1431	P1432	S1433	L1434	L1435	L1436	K1437	L1438	L1439	A1440	K1441	S1442	H1443	L1444	L1445	L1446	A1447	T1448	P1449	V1450	Q1451	F1452	E1453	L1454	L1455	S1456	R1457	R1458	W1459	R1460	Q1461	L1462	K1463	N1464	I1465	Q1466	S1467	L1468	E1469	L1470	M1471	L1472	Y1473	L1474	D1475	A1476	E1477	I1478	S1480	Q1481	G1482	



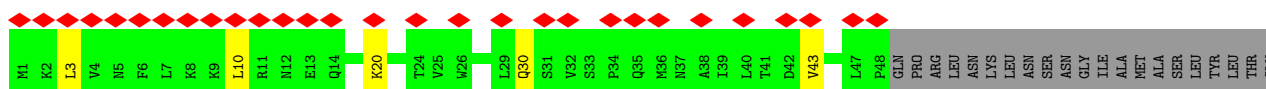
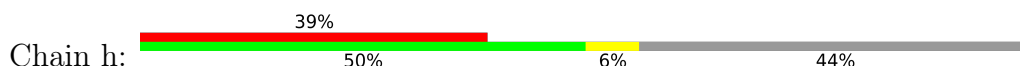
• Molecule 11: Small nuclear ribonucleoprotein-associated protein B

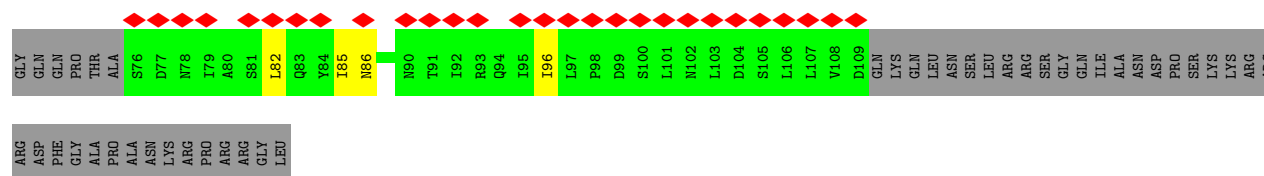


• Molecule 12: Small nuclear ribonucleoprotein Sm D1

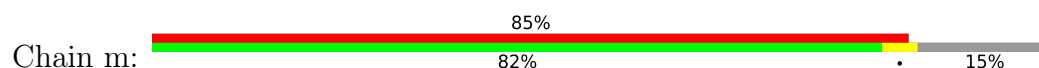


• Molecule 12: Small nuclear ribonucleoprotein Sm D1

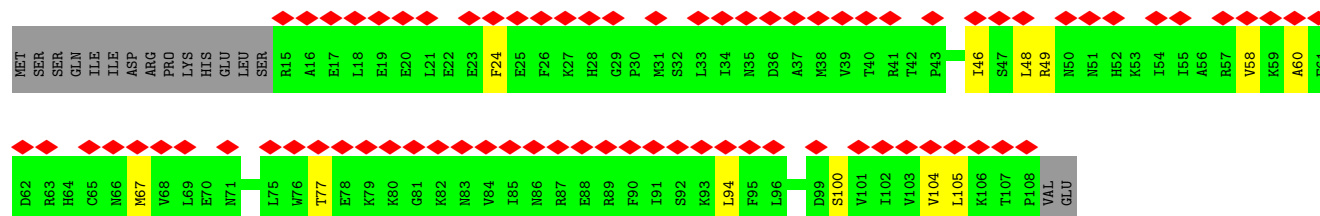
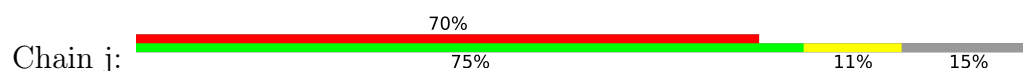




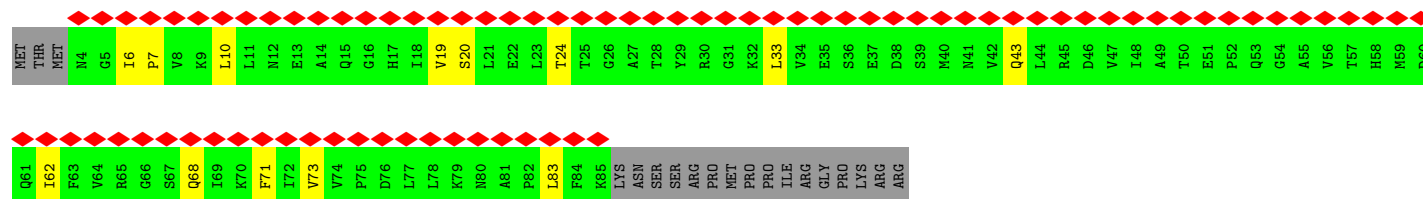
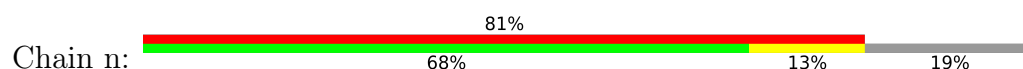
- Molecule 13: Small nuclear ribonucleoprotein Sm D2



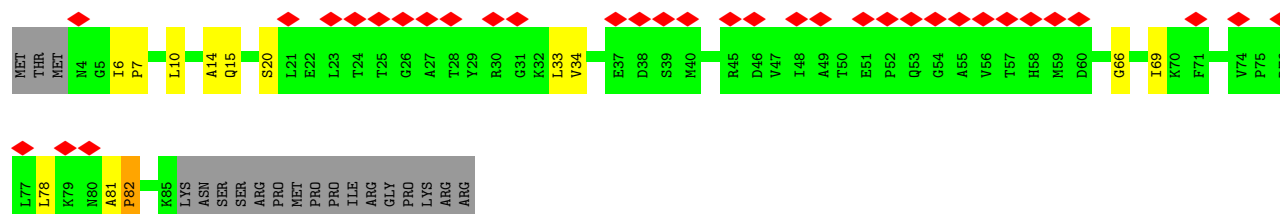
- Molecule 13: Small nuclear ribonucleoprotein Sm D2



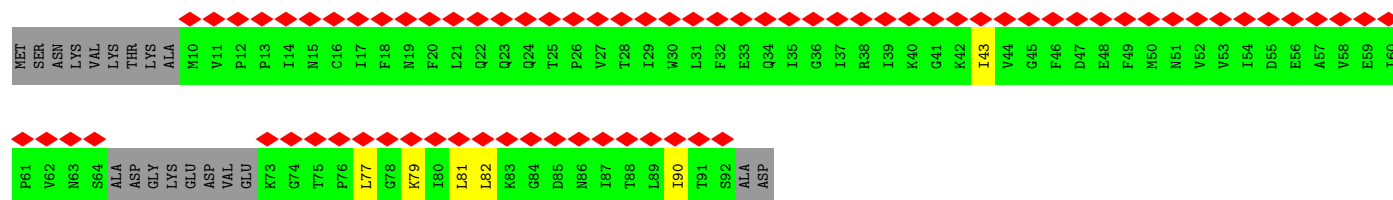
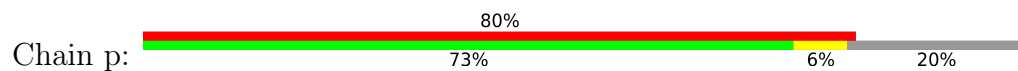
- Molecule 14: Small nuclear ribonucleoprotein Sm D3



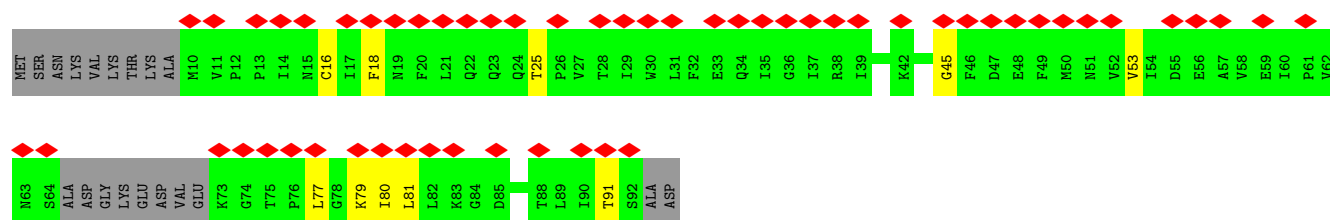
- Molecule 14: Small nuclear ribonucleoprotein Sm D3



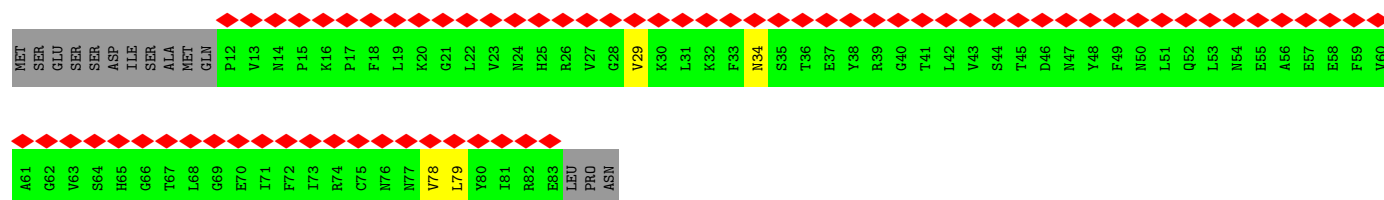
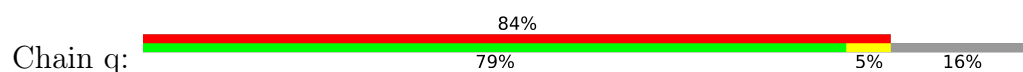
- Molecule 15: Small nuclear ribonucleoprotein E



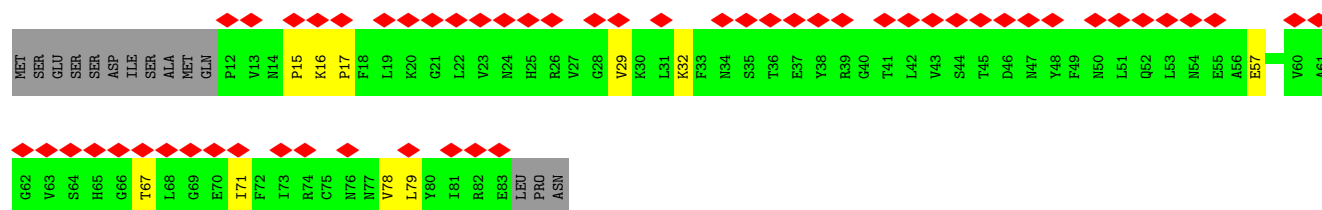
- Molecule 15: Small nuclear ribonucleoprotein E



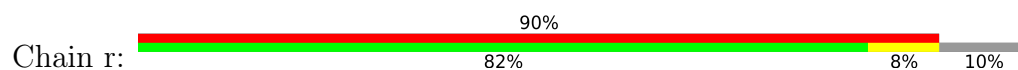
- Molecule 16: Small nuclear ribonucleoprotein F



- Molecule 16: Small nuclear ribonucleoprotein F



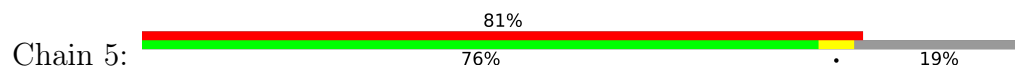
- Molecule 17: Small nuclear ribonucleoprotein G





SER
PRO
GLN
LYS
VAL
GLU
PHE

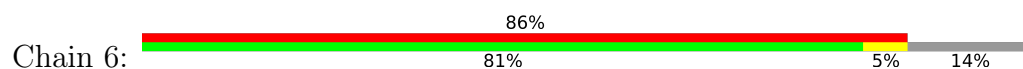
- Molecule 24: U6 snRNA-associated Sm-like protein LSm5



MET SER LEU P4 E5 T6 L7 P8 L9 E10 E11 V11 I12 D13 K14 T15 I16 I17 Q18 K19 V20 L21 L22 V23 L24 Q25 S26 S27 R28 E29 F30 E31 G32 T33 L34 V35 G36 F37 D38 D39 F40 V41 M42 V43 I44 L45 E46 D47 A48 V49 E50 W51 L52 I53 D54 PRO GLU ASP GLU SER ARG

N61 E62 K63 V64 M65 Q66 H67 H68 G69 M71 L72 L73 S74 G75 N76 M77 I78 A79 I80 V82 P83 G84 LYS LYS THR PRO THR ALA LEU

- Molecule 25: U6 snRNA-associated Sm-like protein LSm6



MET SER GLY LYS ALA SER THR GLY GLU SER V11 T12 T13 E14 F15 L16 S17 I18 I19 I20 Q21 K22 K23 V24 N25 V26 K27 L28 A29 G30 G31 L32 Y34 S35 G36 R37 L38 E39 S40 I41 D42 G43 F44 M45 M46 V47 A48 L49 S50 S51 A52 T53 E54 H55 Y56 E57 S58 N59 N60

N61 K62 L63 L64 M65 K66 F67 M68 S69 D70 V71 F72 L73 R74 G75 T76 Q77 V78 M79 I80 Y81 S82 S83 Q84 LYS ILE

- Molecule 26: U6 snRNA-associated Sm-like protein LSm7



MET HIS GLN GLN HIS SER LYS SER GLU ASN LYS PRO GLN GLN A26 I27 L28 D29 L30 A31 K32 Y33 K34 D35 S36 K37 I38 R39 V40 K41 L42 M43 G44 G45 K46 L47 V48 I49 G50 V51 VAL V52 L52 K53 G54 Y55 D56 Q57 L58 M59 N60

L61 V62 L63 D64 D65 T66 V67 E68 G69 M70 SER ASN PRO ASP ASP ASP ASP ASN ASN THR GLU LEU ILE SER N85 A86 R87 K88 L89 G90 L91 T92 V93 I94 R95 G96 T97 I98 L99 V100 S101 L102 S103 S104 A105 GLU GLY SER ASP VAL LEU TYR MET GLN LYS

- Molecule 27: U6 snRNA-associated Sm-like protein LSm8



MET SER ALA T4 L5 K6 D7 Y8 L9 M10 N11 K12 V13 V14 I15 I16 K17 V18 D19 G20 E21 C22 L23 L24 A25 S26 L27 N28 G29 F30 D31 K32 N33 T34 N35 L36 F37 T38 T39 N40 V41 F42 M43 N44 I45 S46 K47 E48 F49 I50 C51 K52 A53 Q54 L55 L56 H57 Q58 S59 E60

I61 A62 L63 V64 G65 L66 I67 ASP ASP ALA GLU ASN ASP ASP ASP LEU ALA PRO ILE ASP GLU LYS LYS VAL PRO MET LEU LYS ASP THR LYS ASN ILE GLU HIS VAL TRP LYS VAL TYR GLU SER LYS THR LYS

- Molecule 28: Pre-mRNA-splicing factor SNU114





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	140155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.243	Depositor
Minimum map value	-0.122	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.036	Depositor
Map size ($\text{\AA}$)	543.39996, 543.39996, 543.39996	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.43, 1.43, 1.43	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	V	0.44	0/2943	0.88	12/4577 (0.3%)
2	W	0.42	0/1891	0.94	11/2933 (0.4%)
3	A	0.61	2/18226 (0.0%)	1.09	36/24737 (0.1%)
4	H	0.58	0/2845	0.96	2/3843 (0.1%)
5	J	0.61	0/5934	1.24	10/8039 (0.1%)
6	D	0.61	0/1172	1.13	0/1578
7	F	0.65	1/3273 (0.0%)	1.24	7/4413 (0.2%)
8	G	0.60	0/2687	1.03	3/3611 (0.1%)
9	B	0.60	0/14518	0.96	8/19682 (0.0%)
11	b	0.58	0/636	0.72	0/856
11	k	0.64	0/636	0.75	1/856 (0.1%)
12	h	0.56	0/649	0.79	0/880
12	l	0.64	0/725	0.82	0/980
13	j	0.58	0/753	0.90	0/1013
13	m	0.64	0/749	0.84	0/1009
14	d	0.55	0/634	0.85	0/859
14	n	0.62	0/634	0.78	0/859
15	e	0.65	0/585	0.87	0/795
15	p	0.70	0/585	0.86	0/795
16	f	0.62	0/585	0.87	0/791
16	q	0.63	0/585	0.82	0/791
17	g	0.57	0/532	0.80	0/715
17	r	0.61	0/529	0.74	0/711
18	E	0.54	0/184	1.04	0/238
19	U	0.45	0/3350	0.89	7/5209 (0.1%)
20	K	0.69	0/949	1.20	3/1292 (0.2%)
21	2	0.68	0/745	0.91	0/1005
22	3	0.63	0/617	0.76	0/836
23	4	0.62	0/594	0.78	0/802
24	5	0.63	0/595	0.77	0/806
25	6	0.62	0/584	0.82	0/787
26	7	0.61	0/505	0.65	0/675

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	8	0.64	0/501	0.75	0/673
28	C	0.61	0/6590	1.10	11/8975 (0.1%)
All	All	0.59	3/77520 (0.0%)	1.02	111/106621 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	9
5	J	0	2
7	F	0	1
9	B	0	2
11	k	0	1
28	C	0	2
All	All	0	17

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	376	LYS	C-O	-6.12	1.16	1.24
3	A	1369	ASN	C-O	-5.35	1.17	1.24
3	A	719	ILE	CA-CB	5.35	1.56	1.54

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	719	ILE	O-C-N	8.92	126.13	120.42
1	V	17	A	C2'-C3'-O3'	8.89	127.03	113.70
5	J	199	ASP	N-CA-C	-8.69	97.16	110.10
1	V	19	U	C2'-C3'-O3'	8.39	122.09	109.50
3	A	404	ASN	N-CA-C	8.35	121.10	110.33
1	V	39	C	C2'-C3'-O3'	8.22	121.83	109.50
19	U	95	C	C4'-C3'-O3'	8.21	121.72	109.40
2	W	49	A	C2'-C3'-O3'	8.00	121.50	109.50
5	J	239	THR	N-CA-C	7.94	119.94	111.28
19	U	27	G	C4'-C3'-O3'	7.64	120.86	109.40
3	A	1285	VAL	N-CA-C	7.58	118.81	107.75
3	A	811	ILE	N-CA-CB	7.51	119.34	110.55
3	A	1361	VAL	N-CA-C	-7.34	102.59	110.23
19	U	129	G	C2'-C3'-O3'	7.34	120.51	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	379	ILE	O-C-N	7.20	125.03	120.42
2	W	45	A	C2'-C3'-O3'	7.10	124.35	113.70
3	A	1369	ASN	CA-C-O	-7.09	113.03	120.55
1	V	150	G	C4'-C3'-O3'	7.05	119.98	109.40
3	A	305	LEU	O-C-N	6.92	125.84	120.38
3	A	491	GLY	N-CA-C	6.85	119.80	110.69
28	C	360	ARG	CA-C-N	6.74	133.84	121.70
28	C	360	ARG	C-N-CA	6.74	133.84	121.70
3	A	719	ILE	N-CA-CB	6.61	114.95	110.52
2	W	62	A	C4'-C3'-O3'	-6.59	103.12	113.00
3	A	1752	VAL	N-CA-CB	6.54	119.43	110.54
9	B	1954	VAL	N-CA-C	6.46	119.13	111.05
2	W	83	A	C2'-C3'-O3'	6.40	119.10	109.50
5	J	564	TYR	CB-CA-C	-6.36	100.90	110.88
19	U	128	A	C2'-C3'-O3'	6.34	123.21	113.70
28	C	292	ILE	CB-CA-C	6.28	120.01	111.97
1	V	83	A	C2'-C3'-O3'	6.24	118.85	109.50
2	W	55	G	C2'-C3'-O3'	6.23	123.05	113.70
3	A	597	PHE	N-CA-C	6.19	123.99	110.80
3	A	558	GLN	N-CA-C	6.08	118.42	109.24
9	B	936	VAL	N-CA-CB	6.07	117.66	110.55
7	F	197	ILE	N-CA-CB	6.04	118.76	110.54
9	B	1807	VAL	N-CA-CB	6.04	117.62	110.55
19	U	31	G	C3'-C2'-O2'	5.96	119.63	110.70
1	V	75	U	N1-C1'-C2'	5.95	120.93	112.00
4	H	125	ILE	N-CA-CB	5.94	118.62	110.54
3	A	979	SER	C-N-CD	-5.93	107.55	120.60
3	A	1009	PHE	CA-C-N	5.90	125.91	119.89
3	A	1009	PHE	C-N-CA	5.90	125.91	119.89
2	W	84	C	C4'-C3'-O3'	5.90	118.25	109.40
9	B	1617	ILE	N-CA-C	5.88	116.61	110.62
2	W	48	C	C2'-C3'-O3'	5.85	122.47	113.70
3	A	1553	ILE	CB-CA-C	-5.83	104.41	111.88
3	A	1381	THR	N-CA-C	-5.82	104.84	111.07
19	U	78	A	C4'-C3'-O3'	5.79	121.68	113.00
8	G	247	ASN	CA-C-O	-5.78	114.37	120.55
5	J	887	THR	N-CA-C	5.77	122.57	109.81
3	A	816	ILE	N-CA-CB	5.77	118.39	110.54
5	J	624	LEU	N-CA-C	5.77	119.13	111.75
2	W	65	U	C3'-C2'-O2'	5.76	119.35	110.70
3	A	1522	ASN	N-CA-C	5.76	119.21	109.76
3	A	1795	LYS	O-C-N	5.75	125.60	120.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	174	VAL	N-CA-CB	5.73	118.33	110.54
7	F	117	ILE	N-CA-CB	5.73	118.33	110.54
9	B	733	SER	N-CA-C	5.71	117.19	110.97
28	C	370	TYR	CA-C-N	5.70	126.97	119.84
28	C	370	TYR	C-N-CA	5.70	126.97	119.84
3	A	1348	GLU	N-CA-C	-5.59	104.81	111.69
9	B	901	VAL	N-CA-CB	5.58	117.08	110.55
2	W	48	C	C3'-C2'-O2'	5.57	119.06	110.70
3	A	2002	TYR	CB-CA-C	-5.53	102.21	110.88
1	V	44	G	C2'-C3'-O3'	5.48	117.72	109.50
7	F	46	ILE	N-CA-C	5.46	117.88	111.05
3	A	287	GLU	N-CA-C	-5.43	103.92	111.52
1	V	73	A	C4'-C3'-O3'	5.40	121.11	113.00
5	J	355	ILE	CB-CA-C	-5.40	105.06	111.97
3	A	718	THR	N-CA-C	5.40	119.03	112.23
28	C	966	PHE	CB-CA-C	-5.37	102.45	110.88
3	A	1021	PRO	N-CA-C	5.36	117.24	110.70
3	A	1657	ILE	CB-CA-C	-5.35	105.13	111.97
4	H	364	VAL	CB-CA-C	-5.34	103.25	111.31
19	U	82	A	C3'-C2'-O2'	5.33	118.70	110.70
11	k	85	THR	N-CA-C	5.29	118.62	110.42
3	A	660	ILE	N-CA-C	-5.28	105.24	111.00
28	C	314	ALA	N-CA-C	5.28	116.31	108.60
3	A	1339	LEU	N-CA-C	-5.24	105.24	111.69
2	W	63	G	C3'-C2'-O2'	5.24	118.56	110.70
1	V	60	U	C4'-C3'-O3'	-5.20	105.20	113.00
3	A	1828	SER	N-CA-C	5.19	116.63	111.07
5	J	601	ILE	CB-CA-C	-5.18	105.34	111.97
7	F	109	ILE	N-CA-CB	5.18	116.61	110.55
5	J	289	VAL	N-CA-C	5.17	120.10	109.34
20	K	97	VAL	CA-C-N	-5.17	117.65	122.66
20	K	97	VAL	C-N-CA	-5.17	117.65	122.66
28	C	766	TRP	N-CA-C	5.15	117.36	110.35
28	C	259	ASN	N-CA-C	5.14	119.80	111.37
9	B	1157	ILE	N-CA-CB	5.13	117.52	110.54
3	A	1946	VAL	CB-CA-C	-5.13	105.40	111.97
3	A	2196	ILE	N-CA-CB	5.12	117.51	110.54
3	A	210	GLU	O-C-N	5.12	124.42	120.38
5	J	189	ILE	CB-CA-C	-5.12	105.42	111.97
3	A	927	VAL	CB-CA-C	-5.10	105.68	111.55
3	A	1029	THR	N-CA-CB	5.10	117.40	110.01
3	A	705	GLN	O-C-N	5.08	124.39	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	349	ASN	CA-C-N	5.07	124.38	118.85
8	G	349	ASN	C-N-CA	5.07	124.38	118.85
2	W	65	U	C4'-C3'-O3'	-5.07	105.40	113.00
3	A	205	THR	CB-CA-C	5.04	115.95	110.15
28	C	203	LEU	N-CA-C	-5.04	102.44	109.96
1	V	73	A	C2'-C3'-O3'	-5.04	106.14	113.70
1	V	39	C	O4'-C4'-C3'	-5.04	101.06	106.10
7	F	233	VAL	CB-CA-C	-5.03	107.43	111.71
1	V	17	A	C3'-C2'-O2'	5.03	118.24	110.70
20	K	125	LEU	N-CA-C	5.03	116.61	111.03
7	F	408	VAL	N-CA-C	5.03	115.47	108.84
9	B	671	SER	N-CA-C	5.02	116.15	108.42
5	J	595	ASP	N-CA-C	5.00	118.16	111.75

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	1096	SER	Peptide
3	A	1216	ILE	Peptide
3	A	1279	VAL	Peptide
3	A	1522	ASN	Peptide
3	A	286	LEU	Peptide
3	A	467	GLU	Peptide
3	A	557	PHE	Peptide
3	A	974	ASN	Peptide
3	A	979	SER	Peptide
9	B	423	ILE	Peptide
9	B	458	PRO	Peptide
28	C	607	LEU	Peptide
28	C	958	PRO	Peptide
7	F	154	SER	Peptide
5	J	201	LEU	Peptide
5	J	820	GLN	Peptide
11	k	84	LEU	Peptide

5.2 Too-close contacts [i](#)

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	V	2635	0	1328	40	0
2	W	1697	0	858	79	0
3	A	17778	0	17575	427	0
4	H	2789	0	2725	62	0
5	J	5822	0	5792	133	0
6	D	1151	0	1138	30	0
7	F	3218	0	3297	79	0
8	G	2632	0	2599	46	0
9	B	14212	0	14210	111	0
10	x	500	0	110	4	0
11	b	631	0	670	7	0
11	k	631	0	670	9	0
12	h	644	0	686	6	0
12	l	720	0	772	2	0
13	j	741	0	778	6	0
13	m	737	0	767	1	0
14	d	625	0	647	8	0
14	n	625	0	647	9	0
15	e	575	0	597	4	0
15	p	575	0	597	1	0
16	f	573	0	572	5	0
16	q	573	0	572	1	0
17	g	529	0	557	4	0
17	r	526	0	555	3	0
18	E	1713	0	567	1	0
19	U	2999	0	1516	56	0
20	K	936	0	987	44	0
21	2	735	0	744	11	0
22	3	611	0	620	4	0
23	4	588	0	602	2	0
24	5	588	0	594	3	0
25	6	577	0	572	2	0
26	7	504	0	557	1	0
27	8	498	0	533	1	0
28	C	6450	0	6419	174	0
29	C	32	0	12	0	0
All	All	77370	0	72442	1189	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1189) 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)
3:A:462:LEU:CD2	28:C:403:ASN:HD22	1.12	1.53
3:A:459:ALA:C	28:C:376:PHE:HE1	1.22	1.47
2:W:26:A:C5	3:A:671:TYR:CD1	2.10	1.39
3:A:462:LEU:CD2	28:C:403:ASN:ND2	1.77	1.38
3:A:459:ALA:C	28:C:376:PHE:CE1	2.03	1.35
3:A:462:LEU:HD21	28:C:403:ASN:ND2	1.35	1.32
2:W:26:A:C8	3:A:671:TYR:CE1	2.18	1.28
2:W:26:A:N3	3:A:667:TYR:O	1.66	1.27
3:A:459:ALA:O	28:C:376:PHE:HE1	1.13	1.26
2:W:26:A:C2	3:A:667:TYR:O	1.89	1.25
3:A:459:ALA:HB1	3:A:460:PRO:CD	1.67	1.22
3:A:459:ALA:O	28:C:376:PHE:CE1	1.94	1.20
3:A:459:ALA:CB	3:A:460:PRO:HD2	1.74	1.16
2:W:26:A:C4	3:A:671:TYR:CD1	2.34	1.14
3:A:462:LEU:HD22	28:C:403:ASN:ND2	1.63	1.11
2:W:26:A:C6	3:A:671:TYR:HB2	1.88	1.07
3:A:1578:ALA:HB1	3:A:1602:PRO:HB3	1.36	1.07
3:A:459:ALA:HB1	3:A:460:PRO:HD2	1.15	1.07
2:W:26:A:C6	3:A:671:TYR:CG	2.45	1.05
3:A:470:LEU:HB3	3:A:471:PRO:HD2	1.36	1.04
2:W:26:A:C8	3:A:671:TYR:CZ	2.45	1.03
3:A:461:LEU:HD21	28:C:380:PRO:HB3	1.40	1.03
2:W:26:A:C5	3:A:671:TYR:CE1	2.50	0.98
3:A:461:LEU:HD12	3:A:462:LEU:HG	1.47	0.97
2:W:26:A:N7	3:A:671:TYR:CE1	2.32	0.96
2:W:31:G:C5	3:A:1623:PHE:HD2	1.84	0.95
3:A:467:GLU:N	3:A:467:GLU:OE1	2.00	0.95
20:K:16:LEU:HD21	20:K:124:LEU:HD11	1.48	0.95
3:A:470:LEU:HB3	3:A:471:PRO:CD	1.96	0.95
3:A:1599:SER:O	3:A:1602:PRO:HD2	1.67	0.95
8:G:272:VAL:HG12	8:G:280:VAL:HG21	1.49	0.94
9:B:1700:ILE:HD11	9:B:1740:LEU:HD13	1.49	0.94
2:W:26:A:C4	3:A:671:TYR:CE1	2.55	0.94
2:W:26:A:C5	3:A:671:TYR:CG	2.56	0.94
3:A:461:LEU:CD1	3:A:462:LEU:HG	1.98	0.93
2:W:26:A:N9	3:A:671:TYR:CE1	2.36	0.92
2:W:26:A:C6	3:A:671:TYR:CB	2.53	0.92
2:W:26:A:C6	3:A:671:TYR:CD1	2.58	0.90
2:W:31:G:C6	3:A:1623:PHE:CD2	2.61	0.89
2:W:31:G:C6	3:A:1623:PHE:HD2	1.91	0.89
2:W:26:A:N7	3:A:671:TYR:CZ	2.42	0.88
3:A:461:LEU:HD12	3:A:462:LEU:N	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2259:ILE:HD11	3:A:2293:ILE:HD11	1.55	0.87
2:W:26:A:N6	3:A:671:TYR:HB2	1.90	0.86
3:A:468:LEU:HD11	28:C:382:TYR:HB3	1.58	0.85
7:F:112:MET:HE2	7:F:203:ILE:HD12	1.55	0.85
3:A:460:PRO:N	28:C:376:PHE:CE1	2.44	0.84
4:H:441:ILE:HG22	4:H:456:GLY:HA2	1.60	0.83
3:A:462:LEU:HD22	28:C:403:ASN:HD21	1.40	0.83
6:D:113:MET:HE3	6:D:117:LEU:HD21	1.61	0.83
2:W:26:A:N1	3:A:671:TYR:HB2	1.94	0.83
2:W:29:U:C2	19:U:98:U:C2	2.67	0.82
2:W:26:A:O2'	3:A:667:TYR:CE1	2.32	0.82
4:H:159:LEU:HD13	4:H:430:MET:HE2	1.62	0.81
2:W:31:G:C5	3:A:1623:PHE:CD2	2.67	0.81
3:A:1350:ILE:HG23	3:A:1356:LEU:HD23	1.63	0.80
3:A:164:ALA:HB1	3:A:199:ILE:HG21	1.62	0.80
3:A:673:VAL:HG22	3:A:714:PHE:CZ	2.18	0.79
3:A:468:LEU:O	3:A:468:LEU:HD23	1.82	0.79
28:C:323:THR:HG21	28:C:438:ALA:HB2	1.65	0.79
2:W:29:U:C4	19:U:98:U:C4	2.71	0.78
28:C:710:VAL:HG22	28:C:820:LEU:HD23	1.67	0.77
8:G:368:LEU:HD13	8:G:370:LEU:HD13	1.66	0.77
7:F:388:GLN:HG2	7:F:410:LEU:O	1.83	0.77
2:W:29:U:C4	19:U:98:U:N3	2.53	0.76
3:A:459:ALA:HB1	3:A:460:PRO:HD3	1.67	0.76
2:W:26:A:N6	3:A:671:TYR:CB	2.49	0.76
3:A:461:LEU:HD21	28:C:380:PRO:CB	2.15	0.75
9:B:1001:LEU:HD23	9:B:1015:MET:HE1	1.69	0.74
2:W:30:G:H5'	2:W:31:G:H5''	1.68	0.74
1:V:18:A:OP2	7:F:378:LYS:NZ	2.20	0.74
28:C:235:VAL:HG23	28:C:261:VAL:HG11	1.69	0.74
3:A:460:PRO:HA	28:C:376:PHE:CD1	2.22	0.73
3:A:460:PRO:CG	3:A:463:ALA:HB2	2.18	0.73
28:C:836:SER:O	28:C:840:PRO:HD2	1.87	0.73
2:W:88:U:H1'	21:2:80:ASN:HB3	1.71	0.72
5:J:199:ASP:O	5:J:201:LEU:N	2.22	0.72
15:e:77:LEU:HD21	15:e:80:ILE:HD12	1.71	0.72
3:A:715:LEU:O	3:A:719:ILE:HG23	1.89	0.72
3:A:461:LEU:HD12	3:A:461:LEU:C	2.14	0.72
3:A:1320:LEU:HD11	3:A:1366:ARG:HB3	1.70	0.72
3:A:470:LEU:CB	3:A:471:PRO:CD	2.68	0.72
5:J:299:ALA:HB1	5:J:309:LEU:HD13	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1206:CYS:SG	3:A:1207:TRP:N	2.63	0.71
28:C:345:THR:HA	28:C:348:LEU:HD12	1.71	0.71
5:J:361:ALA:HB1	5:J:371:LEU:HD13	1.73	0.71
6:D:46:LEU:HD21	6:D:113:MET:HE2	1.73	0.71
3:A:171:ALA:HB1	3:A:201:PHE:HB3	1.72	0.70
3:A:939:LEU:HD11	7:F:441:MET:HE2	1.73	0.70
2:W:26:A:O2'	3:A:667:TYR:HE1	1.71	0.70
3:A:1047:ALA:HB3	3:A:1251:TYR:HB3	1.72	0.70
3:A:1578:ALA:CB	3:A:1602:PRO:HB3	2.19	0.70
3:A:1335:TRP:CZ2	3:A:1339:LEU:HD13	2.26	0.70
2:W:31:G:N3	3:A:1636:GLY:HA2	1.83	0.69
12:h:3:LEU:HD11	13:j:60:ALA:HB1	1.74	0.69
7:F:233:VAL:HG11	7:F:237:ILE:HG21	1.73	0.69
1:V:50:G:H2'	1:V:51:U:O4'	1.93	0.69
2:W:27:U:C4'	3:A:668:ARG:HG2	2.23	0.68
3:A:330:LEU:HD21	3:A:386:ALA:HB2	1.74	0.68
7:F:347:ALA:HB1	7:F:348:PRO:CD	2.23	0.68
3:A:390:LEU:HD22	3:A:391:TYR:CE1	2.28	0.68
28:C:229:LEU:HD23	28:C:235:VAL:HG21	1.75	0.68
2:W:31:G:O6	3:A:1623:PHE:N	2.22	0.68
3:A:330:LEU:HD22	3:A:385:VAL:HG23	1.73	0.68
4:H:192:THR:HG21	4:H:461:ILE:CD1	2.24	0.68
5:J:597:ARG:HE	5:J:620:THR:HG22	1.59	0.67
28:C:866:ILE:HG22	28:C:868:VAL:HG13	1.76	0.67
19:U:41:A:H2'	19:U:42:A:C8	2.29	0.67
7:F:369:GLY:O	7:F:370:ARG:C	2.37	0.67
3:A:1603:ASN:C	3:A:1605:ARG:H	2.01	0.67
28:C:615:LEU:N	28:C:616:PRO:HD2	2.10	0.67
3:A:176:LEU:HD23	3:A:715:LEU:HD12	1.77	0.67
3:A:2330:GLU:CB	3:A:2331:PRO:CD	2.73	0.67
3:A:658:ASN:HD22	3:A:684:LYS:HB2	1.60	0.66
2:W:26:A:C4	3:A:671:TYR:HD1	2.09	0.66
3:A:1126:LEU:HD21	3:A:1161:TYR:CD2	2.30	0.66
6:D:86:TYR:CD2	6:D:124:ALA:HB1	2.30	0.66
3:A:1092:PHE:O	3:A:1093:LYS:C	2.38	0.66
5:J:264:ILE:HD13	5:J:284:LEU:HD11	1.76	0.66
5:J:327:VAL:HG11	5:J:344:ALA:HB2	1.77	0.66
7:F:253:ARG:HD2	20:K:70:LEU:HD13	1.76	0.66
5:J:598:PHE:HA	5:J:601:ILE:HD12	1.77	0.66
5:J:849:TYR:CD2	5:J:859:LEU:HD11	2.29	0.66
2:W:26:A:H1'	3:A:667:TYR:HD1	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:227:HIS:CD2	4:H:228:PRO:HD2	2.29	0.66
3:A:468:LEU:HD11	28:C:382:TYR:CB	2.25	0.65
20:K:98:ILE:HD12	20:K:99:ALA:N	2.11	0.65
3:A:1035:LEU:HD11	3:A:1160:LEU:HG	1.78	0.65
9:B:636:ILE:HG22	9:B:671:SER:HB2	1.78	0.65
3:A:960:THR:O	3:A:961:GLN:C	2.40	0.65
3:A:462:LEU:HD21	28:C:403:ASN:HD22	0.49	0.65
12:h:43:VAL:HG11	12:h:85:ILE:HD12	1.79	0.64
5:J:215:LEU:CD2	7:F:400:VAL:HG22	2.27	0.64
3:A:460:PRO:HG3	3:A:463:ALA:HB2	1.79	0.64
7:F:74:LEU:HB3	7:F:75:PRO:HD3	1.80	0.64
7:F:119:LEU:HD12	7:F:197:ILE:HG22	1.79	0.64
28:C:493:LEU:HB3	28:C:556:ALA:HB3	1.80	0.64
3:A:459:ALA:HB3	3:A:460:PRO:HD2	1.73	0.64
3:A:960:THR:HG21	7:F:455:PHE:CZ	2.33	0.64
3:A:1175:GLU:O	3:A:1177:ASP:N	2.31	0.63
19:U:129:G:H4'	19:U:130:A:H4'	1.80	0.63
2:W:26:A:N6	3:A:671:TYR:CG	2.66	0.63
3:A:461:LEU:HB3	28:C:332:TYR:OH	1.98	0.63
28:C:234:LEU:HD13	28:C:439:ILE:HG23	1.81	0.63
28:C:864:VAL:HG22	28:C:930:LEU:HD22	1.80	0.63
5:J:199:ASP:C	5:J:201:LEU:H	2.07	0.63
21:2:77:VAL:HG11	22:3:65:MET:HG2	1.79	0.63
3:A:1067:ASN:HB2	3:A:1083:THR:HG21	1.79	0.62
3:A:1387:VAL:HG12	3:A:1610:TRP:CD2	2.33	0.62
20:K:40:ALA:O	20:K:43:THR:OG1	2.16	0.62
3:A:876:PRO:HB2	7:F:157:LEU:HD13	1.80	0.62
8:G:368:LEU:HD11	8:G:381:ILE:HD12	1.81	0.62
28:C:251:GLN:HG2	28:C:933:TRP:CD2	2.35	0.62
4:H:425:ASP:HB2	8:G:174:LEU:HD23	1.82	0.62
14:n:68:GLN:HG3	17:r:69:ILE:HD12	1.82	0.62
8:G:276:ASN:O	8:G:278:MET:N	2.33	0.62
2:W:49:A:O2'	2:W:50:G:OP2	2.16	0.62
5:J:758:LEU:HD21	20:K:75:ASN:HB2	1.80	0.62
20:K:16:LEU:CD2	20:K:124:LEU:HD11	2.25	0.62
28:C:288:LEU:HD13	28:C:313:PHE:CE2	2.34	0.61
28:C:873:LEU:HD22	28:C:900:LEU:HD13	1.81	0.61
28:C:360:ARG:HA	28:C:361:THR:HG22	1.81	0.61
2:W:31:G:N7	3:A:1623:PHE:CE2	2.68	0.61
5:J:238:PRO:C	5:J:240:ASN:HA	2.26	0.61
5:J:465:VAL:HG11	5:J:501:VAL:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:737:VAL:HG22	5:J:767:PHE:CD2	2.35	0.61
9:B:1220:ILE:HD13	9:B:1241:LEU:HD11	1.82	0.61
3:A:813:GLU:O	3:A:816:ILE:HG13	1.99	0.61
5:J:351:LYS:O	5:J:355:ILE:HG13	2.01	0.61
3:A:175:LEU:HD13	3:A:571:LEU:HD12	1.82	0.61
3:A:939:LEU:HD21	7:F:445:ILE:HD11	1.82	0.61
7:F:347:ALA:HB1	7:F:348:PRO:HD2	1.81	0.61
2:W:26:A:O2'	3:A:667:TYR:CD1	2.50	0.61
2:W:26:A:N7	3:A:671:TYR:CD1	2.60	0.61
9:B:1022:LEU:HD23	9:B:1034:ILE:HD13	1.82	0.61
9:B:1544:LEU:HD21	9:B:1720:VAL:CG2	2.30	0.61
28:C:869:HIS:CD2	28:C:925:LEU:HD22	2.35	0.61
3:A:1835:LEU:HD21	3:A:1843:LEU:HD11	1.82	0.61
7:F:369:GLY:O	7:F:372:PHE:N	2.34	0.61
28:C:193:LEU:HD11	28:C:213:LEU:HB3	1.83	0.61
3:A:468:LEU:HD23	3:A:468:LEU:C	2.26	0.60
28:C:127:ALA:HB2	28:C:209:MET:HE3	1.83	0.60
28:C:659:LEU:CD2	28:C:668:ILE:HD13	2.31	0.60
14:d:81:ALA:HB1	14:d:82:PRO:HB3	1.82	0.60
20:K:23:VAL:HG21	20:K:117:VAL:HG21	1.83	0.60
2:W:27:U:H4'	3:A:668:ARG:HG2	1.83	0.60
3:A:714:PHE:CZ	3:A:718:THR:HG21	2.36	0.60
1:V:35:G:N2	1:V:43:C:C2	2.70	0.60
28:C:857:LEU:O	28:C:940:VAL:HG22	2.01	0.60
3:A:1603:ASN:O	3:A:1605:ARG:N	2.34	0.60
4:H:271:VAL:HG12	4:H:282:SER:HB3	1.84	0.60
5:J:341:TRP:CD1	5:J:365:ILE:HD11	2.37	0.60
5:J:613:LEU:O	5:J:617:PHE:CD2	2.55	0.60
9:B:391:PHE:O	9:B:392:ARG:C	2.45	0.60
3:A:963:VAL:C	3:A:964:PHE:CD1	2.80	0.60
3:A:1559:HIS:HB3	3:A:1613:THR:HG21	1.84	0.60
3:A:1603:ASN:C	3:A:1605:ARG:N	2.60	0.60
3:A:284:ARG:NH2	19:U:33:U:O4	2.35	0.59
3:A:1320:LEU:CD2	3:A:1367:ILE:HD13	2.32	0.59
9:B:1479:ILE:HG22	9:B:1488:TYR:HB3	1.84	0.59
3:A:330:LEU:HD12	28:C:920:LEU:HD21	1.84	0.59
20:K:37:ALA:HB2	20:K:98:ILE:HD11	1.83	0.59
9:B:1585:LEU:HD21	9:B:1683:LEU:HD23	1.84	0.59
3:A:1070:LEU:HD21	3:A:1113:ILE:CD1	2.31	0.59
3:A:1259:LEU:HD23	3:A:1268:ARG:HA	1.85	0.59
21:2:43:ILE:HD11	21:2:60:ILE:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:723:LEU:HB3	28:C:773:VAL:HG21	1.84	0.59
3:A:460:PRO:HG2	3:A:463:ALA:HB2	1.83	0.58
5:J:616:PHE:O	5:J:620:THR:HG23	2.02	0.58
28:C:615:LEU:H	28:C:616:PRO:HD2	1.68	0.58
28:C:712:ALA:HB1	28:C:816:VAL:CG1	2.33	0.58
28:C:868:VAL:HG11	28:C:876:VAL:HG21	1.85	0.58
5:J:190:GLN:O	5:J:194:PRO:HD2	2.03	0.58
9:B:1291:THR:HG23	9:B:1303:GLU:HB3	1.85	0.58
3:A:1668:ILE:HD13	3:A:1801:SER:HB3	1.83	0.58
4:H:121:ARG:O	4:H:125:ILE:HG23	2.03	0.58
5:J:204:LEU:HD23	7:F:433:ASN:HD22	1.68	0.58
28:C:712:ALA:HB2	28:C:818:TYR:CD1	2.38	0.58
1:V:58:G:H2'	1:V:59:C:O4'	2.04	0.58
8:G:274:LEU:HA	8:G:277:MET:HE3	1.84	0.58
11:b:12:LEU:HD12	11:b:15:LEU:HD11	1.85	0.58
2:W:27:U:H1'	3:A:668:ARG:O	2.03	0.58
3:A:1063:PHE:CZ	3:A:1086:ASN:HB3	2.38	0.58
9:B:948:MET:HB3	9:B:966:LEU:HD11	1.84	0.58
3:A:1598:LEU:HA	3:A:1601:ILE:HD12	1.86	0.58
15:p:43:ILE:HD11	15:p:90:ILE:HD12	1.86	0.58
3:A:1123:LEU:O	3:A:1127:GLY:N	2.37	0.58
5:J:843:VAL:HG21	5:J:896:MET:HE3	1.85	0.58
3:A:403:TYR:CD2	28:C:189:LEU:HD11	2.38	0.57
3:A:982:TYR:CD2	3:A:1104:ILE:HG23	2.38	0.57
3:A:1082:ILE:HD13	3:A:1113:ILE:HD11	1.86	0.57
8:G:365:LEU:HD22	8:G:382:VAL:HG12	1.85	0.57
4:H:392:HIS:HD2	4:H:396:VAL:HG22	1.68	0.57
22:3:26:LEU:HD13	22:3:68:ILE:HD11	1.85	0.57
3:A:470:LEU:CB	3:A:471:PRO:HD2	2.23	0.57
2:W:29:U:H2'	2:W:30:G:O4'	2.04	0.57
3:A:961:GLN:O	3:A:962:ARG:NH1	2.37	0.57
3:A:1207:TRP:O	3:A:1212:ARG:NH1	2.37	0.57
3:A:1405:ILE:HB	3:A:1437:ILE:HB	1.86	0.57
3:A:1614:ILE:HG22	3:A:1614:ILE:O	2.03	0.57
6:D:31:PHE:HB3	6:D:64:ILE:HD13	1.86	0.57
3:A:788:GLU:HB2	5:J:181:LEU:HD23	1.86	0.57
3:A:1063:PHE:CE1	3:A:1086:ASN:HB3	2.40	0.57
8:G:382:VAL:HG21	8:G:392:TYR:CD2	2.40	0.57
28:C:470:ALA:HB1	28:C:486:VAL:HG12	1.87	0.57
9:B:986:LEU:HD21	9:B:1015:MET:HE2	1.86	0.57
28:C:155:ILE:HA	28:C:161:ILE:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1023:LEU:HD13	3:A:1451:PHE:CD1	2.39	0.57
3:A:1033:ASN:HB2	3:A:1288:LEU:HD23	1.85	0.57
3:A:1447:TRP:HB3	3:A:1451:PHE:CE2	2.40	0.57
5:J:376:THR:HG22	5:J:388:LEU:HD13	1.86	0.57
7:F:106:LYS:O	7:F:109:ILE:HG22	2.05	0.57
2:W:26:A:N9	3:A:671:TYR:HE1	1.96	0.56
28:C:191:ILE:HG12	28:C:221:PHE:CZ	2.40	0.56
3:A:569:LEU:HD11	3:A:637:VAL:CG2	2.35	0.56
3:A:1560:THR:HG21	3:A:1609:TRP:NE1	2.20	0.56
5:J:702:PRO:O	5:J:706:VAL:HG23	2.05	0.56
28:C:602:VAL:HG11	28:C:908:VAL:HG21	1.86	0.56
28:C:862:TYR:CE2	28:C:908:VAL:HG13	2.40	0.56
3:A:670:LYS:O	3:A:673:VAL:HG23	2.06	0.56
5:J:323:LYS:O	5:J:327:VAL:HG23	2.06	0.56
5:J:590:ALA:HB3	5:J:591:PRO:HD3	1.87	0.56
7:F:298:VAL:HG12	7:F:302:MET:HB2	1.87	0.56
9:B:1804:SER:O	9:B:1807:VAL:HG22	2.06	0.56
28:C:200:CYS:HB3	28:C:436:VAL:HG21	1.87	0.56
2:W:84:C:H3'	8:G:350:PRO:HB3	1.88	0.56
3:A:467:GLU:CD	3:A:467:GLU:H	2.12	0.56
5:J:452:ASN:CB	5:J:497:VAL:HG21	2.36	0.56
5:J:824:SER:O	5:J:828:LEU:HG	2.05	0.56
2:W:31:G:O6	3:A:1623:PHE:CD2	2.58	0.56
3:A:811:ILE:HA	5:J:162:LEU:HD23	1.86	0.56
3:A:1335:TRP:CD1	3:A:1367:ILE:HG13	2.41	0.56
19:U:46:C:H4'	28:C:111:LYS:CG	2.36	0.56
3:A:874:ILE:HD13	3:A:1065:LEU:HD22	1.88	0.56
3:A:2082:ILE:HD12	8:G:288:THR:HA	1.87	0.56
5:J:778:ILE:HG23	5:J:794:PHE:CE1	2.41	0.56
1:V:55:U:OP2	5:J:201:LEU:HD11	2.06	0.56
3:A:2380:LEU:HB3	3:A:2384:ASN:HD22	1.70	0.56
4:H:261:LEU:HB3	4:H:292:TRP:CZ3	2.41	0.56
5:J:536:PHE:HB3	5:J:564:TYR:CZ	2.41	0.56
9:B:708:CYS:SG	9:B:709:GLY:N	2.78	0.56
28:C:680:SER:O	28:C:856:ILE:N	2.39	0.56
3:A:1210:ASP:CB	3:A:1278:VAL:HG11	2.37	0.55
28:C:472:VAL:HB	28:C:575:ALA:HB3	1.87	0.55
28:C:596:ASP:O	28:C:598:ILE:N	2.39	0.55
9:B:985:GLU:HG3	9:B:1001:LEU:HD22	1.87	0.55
20:K:64:LEU:O	20:K:66:HIS:N	2.39	0.55
24:5:15:THR:HG23	24:5:34:LEU:HD22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:26:LEU:HD21	6:D:120:ILE:HD11	1.88	0.55
3:A:459:ALA:O	28:C:376:PHE:CD1	2.54	0.55
3:A:460:PRO:CA	28:C:376:PHE:CE1	2.88	0.55
3:A:889:TRP:CH2	3:A:893:ARG:HD3	2.42	0.55
8:G:341:VAL:HG11	8:G:463:PHE:CD1	2.42	0.55
24:5:82:VAL:HG22	26:7:92:THR:HG22	1.89	0.55
3:A:1115:GLN:HA	3:A:1115:GLN:OE1	2.06	0.55
3:A:1946:VAL:HG21	5:J:229:ILE:HG21	1.88	0.55
9:B:1950:ILE:O	9:B:1954:VAL:HG13	2.07	0.55
20:K:108:SER:OG	20:K:110:ILE:N	2.39	0.55
28:C:235:VAL:CG2	28:C:261:VAL:HG11	2.37	0.55
3:A:639:PHE:HA	3:A:644:VAL:HG11	1.88	0.55
2:W:61:C:H2'	2:W:62:A:C8	2.42	0.55
3:A:673:VAL:HG22	3:A:714:PHE:CE1	2.42	0.55
9:B:1035:PHE:CD2	9:B:1080:LEU:HD22	2.42	0.55
3:A:1414:TRP:HA	3:A:1558:GLU:HG2	1.89	0.55
28:C:712:ALA:HB2	28:C:818:TYR:CE1	2.42	0.55
3:A:503:LYS:HA	3:A:506:PHE:CE2	2.42	0.54
3:A:1375:LEU:O	3:A:1638:ILE:HG23	2.07	0.54
5:J:617:PHE:CD2	5:J:644:ARG:CZ	2.90	0.54
28:C:659:LEU:HD21	28:C:668:ILE:HD13	1.89	0.54
3:A:390:LEU:HD22	3:A:391:TYR:CD1	2.41	0.54
3:A:819:LYS:O	3:A:823:TRP:HB2	2.06	0.54
3:A:1407:ILE:HG21	3:A:1412:LEU:HD21	1.90	0.54
28:C:223:ASP:OD2	28:C:631:GLY:N	2.40	0.54
3:A:1383:PHE:HE1	3:A:1614:ILE:HG23	1.72	0.54
3:A:1542:TYR:O	3:A:1546:VAL:HG23	2.07	0.54
5:J:248:ALA:HA	5:J:264:ILE:HD11	1.89	0.54
22:3:18:ILE:HD12	22:3:41:LEU:HD11	1.89	0.54
24:5:42:ASN:HB2	25:6:12:THR:HG21	1.90	0.54
28:C:656:LEU:HD22	28:C:670:ILE:HD11	1.90	0.54
3:A:883:PHE:O	3:A:887:VAL:HG23	2.08	0.54
3:A:1578:ALA:HB1	3:A:1602:PRO:CB	2.25	0.54
7:F:98:PHE:HA	7:F:101:ILE:HG22	1.89	0.54
20:K:54:MET:HG2	20:K:64:LEU:HD12	1.89	0.54
4:H:291:LEU:HD22	4:H:336:ILE:HG21	1.89	0.54
5:J:183:LYS:CG	7:F:350:ILE:HG22	2.38	0.54
6:D:80:MET:SD	6:D:80:MET:N	2.81	0.54
6:D:94:ASP:HB2	6:D:130:LEU:HD11	1.90	0.54
19:U:98:U:H2'	19:U:99:U:O4'	2.07	0.54
28:C:856:ILE:HG21	28:C:939:LYS:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1853:ASP:HB3	3:A:1880:PHE:HB3	1.90	0.54
5:J:159:LEU:O	5:J:163:THR:HG23	2.08	0.54
20:K:24:VAL:HG13	20:K:33:LEU:CD1	2.38	0.54
3:A:656:ILE:O	3:A:660:ILE:HD12	2.08	0.53
3:A:1854:ASP:HB3	3:A:1913:THR:HG21	1.90	0.53
19:U:40:C:N3	19:U:115:G:C6	2.77	0.53
28:C:108:GLN:O	28:C:111:LYS:HD3	2.08	0.53
9:B:1139:MET:HE2	9:B:1139:MET:N	2.22	0.53
11:b:50:GLU:HB2	11:b:82:LEU:HD11	1.90	0.53
28:C:385:PHE:CE1	28:C:425:LEU:HD11	2.44	0.53
1:V:33:A:C8	1:V:45:A:C6	2.96	0.53
3:A:1222:LEU:O	3:A:1226:VAL:HG23	2.09	0.53
3:A:1286:TRP:CE2	3:A:1302:LEU:HD11	2.43	0.53
3:A:1342:LEU:CD2	3:A:1360:LEU:HD21	2.38	0.53
5:J:239:THR:N	5:J:240:ASN:HA	2.23	0.53
28:C:318:LEU:HB3	28:C:425:LEU:HD12	1.90	0.53
28:C:685:SER:CB	28:C:711:ALA:HB1	2.38	0.53
3:A:1014:LYS:HB3	3:A:1015:PRO:HA	1.90	0.53
5:J:207:LEU:HD12	7:F:382:SER:HB2	1.90	0.53
7:F:218:ILE:O	7:F:222:ILE:HG23	2.08	0.53
9:B:981:LEU:HD23	9:B:986:LEU:HD12	1.91	0.53
9:B:1782:ILE:HD11	9:B:1791:VAL:HG21	1.90	0.53
3:A:1340:ILE:HD11	3:A:1400:ILE:CD1	2.39	0.53
4:H:226:TRP:CE3	4:H:234:MET:HB3	2.43	0.53
4:H:235:ILE:HD11	4:H:243:ILE:HG13	1.91	0.53
5:J:337:ASP:HB3	5:J:340:LEU:HD12	1.89	0.53
9:B:1101:ILE:O	9:B:1105:ALA:N	2.41	0.53
9:B:1402:GLY:HA2	9:B:1405:ILE:HD12	1.89	0.53
19:U:99:U:C5	19:U:100:A:C4	2.97	0.53
28:C:856:ILE:HD13	28:C:939:LYS:HG3	1.90	0.53
3:A:305:LEU:HD21	3:A:476:ALA:HB2	1.91	0.53
3:A:901:PRO:HD3	3:A:1078:ILE:HD11	1.91	0.53
3:A:1394:LEU:HD11	3:A:1553:ILE:CD1	2.39	0.53
3:A:1669:LEU:HB3	3:A:1681:VAL:HG21	1.91	0.53
3:A:1580:GLY:HA3	7:F:389:ASN:CG	2.33	0.53
5:J:260:ALA:HB1	5:J:264:ILE:HD12	1.90	0.53
9:B:933:ASN:O	9:B:936:VAL:HG22	2.08	0.53
9:B:1456:SER:HA	9:B:1465:ILE:HD13	1.90	0.53
9:B:1930:LEU:HD22	9:B:1983:LEU:HD21	1.89	0.53
20:K:36:GLY:N	20:K:99:ALA:O	2.38	0.53
28:C:774:LEU:HD22	28:C:803:VAL:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1354:GLU:N	3:A:1355:PRO:CD	2.72	0.53
3:A:1820:ARG:O	3:A:1824:GLN:N	2.40	0.53
9:B:1398:ILE:HD13	9:B:1491:LEU:HD21	1.91	0.53
28:C:761:ALA:O	28:C:765:VAL:HG13	2.09	0.53
3:A:1879:ILE:HG12	3:A:1913:THR:HG23	1.91	0.53
5:J:204:LEU:CD1	7:F:381:LEU:HD23	2.39	0.53
5:J:687:SER:O	5:J:690:THR:OG1	2.23	0.52
3:A:461:LEU:HB3	28:C:332:TYR:CZ	2.44	0.52
3:A:461:LEU:O	3:A:462:LEU:HD23	2.09	0.52
3:A:1125:LEU:HD13	3:A:1168:ILE:HD12	1.91	0.52
4:H:125:ILE:HG22	4:H:337:ARG:HB3	1.91	0.52
14:d:66:GLY:HA2	14:d:69:ILE:HD12	1.91	0.52
2:W:29:U:N3	19:U:98:U:C2	2.78	0.52
3:A:284:ARG:N	3:A:285:PRO:HA	2.25	0.52
3:A:1913:THR:O	3:A:1917:VAL:HG23	2.09	0.52
5:J:498:GLN:HE21	5:J:498:GLN:N	2.07	0.52
9:B:1399:ASN:O	9:B:1405:ILE:HD11	2.09	0.52
19:U:15:A:H4'	19:U:15:A:OP1	2.08	0.52
3:A:405:ASN:C	3:A:405:ASN:HD22	2.16	0.52
3:A:459:ALA:CB	3:A:460:PRO:CD	2.37	0.52
28:C:219:VAL:HG11	28:C:931:TYR:HB3	1.91	0.52
1:V:74:U:OP2	10:x:45:UNK:HA	2.10	0.52
12:l:96:ILE:HG23	13:m:94:LEU:HA	1.92	0.52
1:V:99:G:H5''	9:B:1177:ALA:HB2	1.92	0.52
2:W:30:G:H5'	2:W:31:G:C5'	2.38	0.52
4:H:459:ARG:NH2	20:K:72:GLU:O	2.43	0.52
6:D:86:TYR:CG	6:D:124:ALA:HB1	2.43	0.52
7:F:57:LEU:HD21	7:F:108:ASN:HA	1.91	0.52
17:r:63:ILE:HB	17:r:68:ILE:HD11	1.90	0.52
21:2:6:PHE:CZ	21:2:10:LEU:HD11	2.45	0.52
1:V:20:A:H2'	1:V:21:C:O4'	2.09	0.52
7:F:123:ARG:NH1	7:F:145:GLU:OE2	2.42	0.52
9:B:1095:ASN:O	9:B:1098:ILE:HG22	2.10	0.52
3:A:2189:LEU:HD13	3:A:2224:VAL:HG23	1.91	0.52
7:F:102:ILE:N	7:F:103:PRO:CD	2.73	0.52
9:B:574:PHE:CB	9:B:585:VAL:HG11	2.40	0.52
21:2:25:ILE:HD12	27:8:63:LEU:HD11	1.91	0.52
3:A:790:TRP:CZ3	3:A:793:TRP:CE3	2.98	0.52
6:D:121:PHE:CE2	6:D:125:ARG:HD2	2.45	0.52
9:B:404:GLY:O	9:B:407:GLN:HB2	2.10	0.52
15:e:77:LEU:HD21	15:e:80:ILE:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:31:G:N7	3:A:1623:PHE:CD2	2.78	0.51
3:A:1893:ILE:HD12	3:A:1978:VAL:HG22	1.91	0.51
5:J:849:TYR:CE2	5:J:859:LEU:HD11	2.45	0.51
2:W:30:G:C2	19:U:97:U:C2	2.99	0.51
3:A:379:ILE:HG23	3:A:379:ILE:O	2.11	0.51
3:A:562:ILE:HG22	3:A:563:ASP:O	2.10	0.51
3:A:1026:TYR:HA	3:A:1286:TRP:CZ3	2.45	0.51
3:A:2330:GLU:CB	3:A:2331:PRO:HD3	2.40	0.51
5:J:209:ASN:CG	5:J:209:ASN:O	2.54	0.51
19:U:40:C:C2	19:U:115:G:N1	2.78	0.51
20:K:39:GLU:O	20:K:43:THR:HG23	2.10	0.51
28:C:723:LEU:HD12	28:C:773:VAL:HG11	1.92	0.51
2:W:31:G:N7	3:A:1623:PHE:HE2	2.09	0.51
3:A:460:PRO:HA	28:C:376:PHE:CE1	2.46	0.51
3:A:1318:GLY:O	3:A:1321:MET:O	2.27	0.51
3:A:1992:TYR:OH	3:A:2005:PHE:HA	2.10	0.51
8:G:392:TYR:HA	8:G:395:LEU:HD23	1.93	0.51
2:W:29:U:O4	19:U:98:U:C4	2.63	0.51
3:A:1678:ILE:HG12	3:A:1703:MET:HE2	1.92	0.51
3:A:2041:PRO:O	3:A:2042:SER:C	2.54	0.51
4:H:371:GLY:HA2	4:H:396:VAL:HG23	1.92	0.51
9:B:1032:PHE:CD2	9:B:1080:LEU:HD23	2.45	0.51
3:A:1183:THR:HG23	3:A:1221:ASN:HB3	1.92	0.51
3:A:1654:TRP:HA	3:A:1657:ILE:HD12	1.92	0.51
3:A:1657:ILE:HA	3:A:1811:ALA:CB	2.40	0.51
4:H:192:THR:HG21	4:H:461:ILE:HD13	1.92	0.51
7:F:373:ARG:O	7:F:374:LYS:C	2.53	0.51
9:B:423:ILE:HG23	9:B:424:PRO:HD3	1.93	0.51
3:A:1676:LEU:HD12	3:A:1678:ILE:HD11	1.92	0.51
3:A:2084:LEU:HB3	3:A:2086:GLN:HB3	1.92	0.51
7:F:381:LEU:HD22	7:F:385:ARG:HB3	1.92	0.51
28:C:470:ALA:HB3	28:C:577:LEU:CD1	2.40	0.51
2:W:26:A:H1'	3:A:667:TYR:CD1	2.43	0.51
3:A:632:ILE:HG23	3:A:656:ILE:HG21	1.92	0.51
3:A:919:LEU:CD1	3:A:990:ILE:HD13	2.41	0.51
4:H:243:ILE:HG13	4:H:261:LEU:HD13	1.92	0.51
5:J:372:LEU:O	5:J:376:THR:HG23	2.11	0.51
5:J:601:ILE:HG12	5:J:617:PHE:CE1	2.46	0.51
6:D:120:ILE:HG22	6:D:131:VAL:HG11	1.93	0.51
19:U:12:C:H2'	19:U:13:A:C8	2.45	0.51
3:A:1387:VAL:HG12	3:A:1610:TRP:CE3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1562:PHE:O	3:A:1565:THR:OG1	2.25	0.51
5:J:873:GLU:HB3	5:J:896:MET:HE1	1.92	0.51
28:C:864:VAL:HG22	28:C:930:LEU:CD2	2.41	0.51
3:A:461:LEU:HD12	3:A:462:LEU:CG	2.29	0.50
8:G:379:ILE:HD12	8:G:464:TYR:HA	1.93	0.50
28:C:879:LEU:HD11	28:C:921:SER:OG	2.11	0.50
3:A:919:LEU:HD13	3:A:990:ILE:HD13	1.92	0.50
5:J:863:PHE:CE1	5:J:893:LEU:HD11	2.47	0.50
9:B:535:VAL:HG13	9:B:557:ILE:HD13	1.93	0.50
4:H:171:GLN:NE2	4:H:172:LEU:O	2.44	0.50
4:H:201:VAL:C	4:H:202:LEU:HD12	2.36	0.50
5:J:465:VAL:CG1	5:J:501:VAL:HG22	2.42	0.50
8:G:195:LYS:HB2	8:G:196:LEU:HD12	1.92	0.50
28:C:360:ARG:HA	28:C:361:THR:CB	2.41	0.50
3:A:971:MET:SD	3:A:979:SER:OG	2.58	0.50
3:A:1454:SER:HA	3:A:1487:GLY:HA2	1.92	0.50
5:J:540:LEU:O	5:J:546:SER:N	2.45	0.50
3:A:1933:ILE:HD12	3:A:1948:MET:HE2	1.94	0.50
7:F:135:LEU:HD22	7:F:208:TRP:CD1	2.46	0.50
10:x:30:UNK:O	10:x:34:UNK:N	2.44	0.50
19:U:23:C:H2'	19:U:24:G:O4'	2.11	0.50
28:C:360:ARG:HA	28:C:361:THR:CG2	2.41	0.50
28:C:911:SER:OG	28:C:912:ALA:N	2.39	0.50
1:V:22:G:C2	1:V:23:C:C2	2.99	0.50
2:W:26:A:N7	3:A:671:TYR:CE2	2.79	0.50
1:V:7:A:H2'	1:V:8:U:O4'	2.10	0.50
3:A:390:LEU:HD21	28:C:605:ILE:HD11	1.94	0.50
3:A:756:LEU:HD13	6:D:44:GLU:HG3	1.92	0.50
3:A:770:MET:HE1	3:A:782:ILE:CD1	2.42	0.50
3:A:1413:SER:N	3:A:1743:TYR:OH	2.44	0.50
4:H:243:ILE:HG12	4:H:261:LEU:HB2	1.92	0.50
19:U:98:U:C4	19:U:99:U:C5	3.00	0.50
8:G:352:ILE:HD12	8:G:400:ILE:HG23	1.94	0.50
9:B:1982:MET:O	9:B:1986:GLY:N	2.45	0.50
11:b:86:ILE:HG23	14:d:7:PRO:HB3	1.93	0.50
19:U:38:A:H2'	19:U:39:U:C6	2.47	0.50
1:V:19:U:O2	1:V:19:U:O5'	2.30	0.50
20:K:35:LYS:HG2	20:K:91:CYS:HB3	1.94	0.50
1:V:30:G:C8	20:K:35:LYS:HD2	2.47	0.49
2:W:86:G:C6	2:W:87:U:C5	3.00	0.49
3:A:630:LYS:O	3:A:634:ASP:N	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:708:TRP:CZ2	3:A:712:LEU:HD11	2.47	0.49
6:D:81:THR:HG21	6:D:102:LYS:HD2	1.94	0.49
28:C:872:LEU:HD13	28:C:922:THR:HG22	1.93	0.49
2:W:34:A:C6	2:W:50:G:C6	3.01	0.49
3:A:403:TYR:CE2	28:C:650:LEU:HD13	2.47	0.49
4:H:390:LEU:HB3	8:G:428:TRP:CE3	2.47	0.49
7:F:112:MET:HE2	7:F:203:ILE:CD1	2.35	0.49
28:C:966:PHE:O	28:C:970:THR:HG23	2.11	0.49
1:V:58:G:C6	1:V:59:C:C4	3.01	0.49
3:A:786:LEU:HG	3:A:815:TYR:CE2	2.47	0.49
3:A:1811:ALA:HA	3:A:2101:LEU:HD13	1.95	0.49
6:D:5:LEU:HD13	6:D:47:SER:HB2	1.93	0.49
8:G:250:LYS:HG2	8:G:251:MET:HE2	1.94	0.49
15:e:91:THR:HB	17:g:61:THR:HG22	1.94	0.49
19:U:74:U:H2'	19:U:75:A:H4'	1.95	0.49
3:A:1098:VAL:HG21	7:F:276:GLU:N	2.27	0.49
7:F:194:ARG:O	7:F:197:ILE:HG13	2.12	0.49
28:C:193:LEU:HD21	28:C:213:LEU:HD13	1.95	0.49
3:A:857:ILE:CG2	3:A:1095:MET:HE2	2.42	0.49
3:A:857:ILE:HG21	3:A:1095:MET:HE2	1.95	0.49
5:J:686:MET:O	5:J:690:THR:HG23	2.13	0.49
28:C:621:ALA:CB	28:C:664:ALA:HB2	2.43	0.49
3:A:1394:LEU:HD11	3:A:1553:ILE:HD13	1.95	0.49
7:F:298:VAL:HG13	7:F:344:LEU:HD13	1.93	0.49
8:G:293:TRP:O	8:G:297:VAL:HG13	2.13	0.49
9:B:574:PHE:HB3	9:B:585:VAL:HG11	1.94	0.49
9:B:1544:LEU:HD21	9:B:1720:VAL:HG23	1.94	0.49
19:U:46:C:H4'	28:C:111:LYS:HG3	1.95	0.49
2:W:30:G:C2	19:U:97:U:O2	2.66	0.49
3:A:468:LEU:C	3:A:468:LEU:CD2	2.86	0.49
3:A:963:VAL:C	3:A:964:PHE:CG	2.90	0.49
3:A:1836:ASN:N	3:A:1839:ASN:OD1	2.46	0.49
3:A:2207:ILE:HD12	3:A:2256:LEU:HB2	1.95	0.49
4:H:180:ALA:O	4:H:192:THR:HA	2.13	0.49
5:J:781:PHE:CE2	5:J:793:ILE:HG13	2.48	0.49
20:K:21:LEU:HD13	20:K:90:ALA:HB2	1.95	0.49
28:C:154:VAL:HG11	28:C:177:TYR:CD2	2.47	0.49
28:C:236:LEU:HD23	28:C:264:CYS:HB3	1.95	0.49
1:V:58:G:N1	1:V:59:C:C2	2.81	0.49
3:A:209:ILE:HB	3:A:212:VAL:HB	1.93	0.49
3:A:308:MET:HE3	3:A:489:THR:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:170:LEU:HD13	5:J:175:ASP:OD2	2.13	0.49
5:J:183:LYS:HG2	7:F:350:ILE:HG22	1.95	0.49
28:C:320:PHE:CE1	28:C:425:LEU:HD13	2.48	0.49
3:A:405:ASN:C	3:A:405:ASN:ND2	2.71	0.49
5:J:378:LEU:C	5:J:378:LEU:HD13	2.38	0.49
6:D:9:LEU:HD13	6:D:15:VAL:HA	1.95	0.49
20:K:67:LEU:N	20:K:68:PRO:CD	2.75	0.49
28:C:471:HIS:HB2	28:C:592:PHE:CZ	2.48	0.49
1:V:35:G:C2	1:V:43:C:C2	3.01	0.48
3:A:172:ILE:HA	3:A:571:LEU:HD11	1.95	0.48
3:A:1372:LYS:HG2	3:A:1383:PHE:CE2	2.48	0.48
5:J:763:ALA:HB1	5:J:773:LEU:CD1	2.42	0.48
9:B:1273:THR:HG21	9:B:1731:TYR:CD1	2.48	0.48
3:A:331:PHE:CD2	3:A:336:PHE:HZ	2.31	0.48
3:A:816:ILE:HD12	3:A:817:LYS:N	2.28	0.48
4:H:125:ILE:HG22	4:H:337:ARG:CB	2.43	0.48
5:J:260:ALA:HB1	5:J:264:ILE:CD1	2.43	0.48
5:J:331:LEU:HD13	5:J:341:TRP:CH2	2.47	0.48
7:F:105:ILE:HD13	7:F:210:LEU:HD21	1.95	0.48
9:B:499:LEU:HD23	9:B:503:GLN:HB3	1.95	0.48
28:C:621:ALA:HB2	28:C:664:ALA:HB2	1.95	0.48
3:A:831:ARG:HD2	3:A:831:ARG:HA	1.70	0.48
3:A:1073:ILE:HD13	3:A:1116:TYR:CE1	2.48	0.48
28:C:270:LEU:HD11	28:C:313:PHE:HB3	1.95	0.48
4:H:195:TRP:CG	4:H:220:LYS:HG3	2.49	0.48
4:H:390:LEU:HD13	8:G:428:TRP:HB2	1.95	0.48
6:D:112:GLU:CD	6:D:137:TYR:OH	2.57	0.48
9:B:567:VAL:O	9:B:571:VAL:HG23	2.12	0.48
9:B:1367:PHE:HB3	9:B:1532:ILE:HA	1.95	0.48
9:B:1707:VAL:N	9:B:1708:GLY:HA3	2.28	0.48
3:A:2189:LEU:HD11	3:A:2347:GLY:HA3	1.95	0.48
16:f:57:GLU:HG2	16:f:67:THR:HG22	1.94	0.48
19:U:125:C:H2'	19:U:126:A:O4'	2.14	0.48
2:W:61:C:H2'	2:W:62:A:O4'	2.14	0.48
3:A:1312:PHE:CE2	3:A:1360:LEU:HD23	2.49	0.48
28:C:227:VAL:HG11	28:C:474:LYS:HD3	1.95	0.48
3:A:172:ILE:HD11	3:A:626:LEU:CD2	2.43	0.48
3:A:1088:VAL:HG22	3:A:1104:ILE:HD11	1.95	0.48
7:F:277:SER:HB2	7:F:279:VAL:HG12	1.94	0.48
9:B:1291:THR:HG22	9:B:1293:ILE:HD11	1.96	0.48
9:B:2113:ALA:HB2	9:B:2130:PHE:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:234:LEU:HD21	28:C:264:CYS:HB2	1.96	0.48
28:C:567:ILE:HG22	28:C:571:TYR:CE1	2.49	0.48
3:A:789:ALA:HB2	3:A:799:TRP:CE2	2.49	0.48
3:A:972:MET:HE2	3:A:1522:ASN:HB2	1.96	0.48
21:2:8:LYS:O	21:2:11:VAL:HG23	2.13	0.48
3:A:268:LEU:HD13	3:A:277:LYS:HB3	1.96	0.48
3:A:920:LYS:O	3:A:921:ASP:C	2.57	0.48
3:A:1598:LEU:O	3:A:1602:PRO:HD3	2.12	0.48
5:J:561:LEU:O	5:J:565:VAL:HG23	2.14	0.48
3:A:239:PHE:HA	3:A:240:PRO:C	2.38	0.48
4:H:369:GLY:O	4:H:395:ILE:HG22	2.13	0.48
7:F:374:LYS:O	7:F:375:TYR:C	2.57	0.48
9:B:836:TRP:HA	9:B:836:TRP:CE3	2.49	0.48
19:U:87:G:H2'	19:U:88:U:C6	2.49	0.48
19:U:93:G:C6	19:U:94:C:N4	2.82	0.48
23:4:17:ILE:HD13	23:4:79:ILE:HG23	1.96	0.48
2:W:29:U:C5	19:U:98:U:N3	2.82	0.47
8:G:276:ASN:O	8:G:277:MET:C	2.57	0.47
9:B:631:LEU:HD22	9:B:654:THR:HG21	1.96	0.47
20:K:121:ILE:HA	20:K:124:LEU:HD12	1.96	0.47
28:C:869:HIS:HB2	28:C:872:LEU:HD12	1.96	0.47
1:V:50:G:OP1	5:J:188:PRO:HG2	2.14	0.47
3:A:173:LEU:HD13	3:A:715:LEU:HB3	1.95	0.47
3:A:383:TYR:O	3:A:386:ALA:N	2.47	0.47
3:A:925:SER:HA	7:F:408:VAL:HG21	1.97	0.47
3:A:1795:LYS:N	3:A:1796:PRO:CD	2.77	0.47
4:H:176:LYS:HB3	4:H:177:PRO:HD2	1.96	0.47
5:J:674:LEU:CD2	5:J:690:THR:HG21	2.44	0.47
20:K:64:LEU:HD21	20:K:98:ILE:HB	1.96	0.47
3:A:569:LEU:HD11	3:A:637:VAL:HG22	1.96	0.47
3:A:1230:ILE:HD13	3:A:1230:ILE:HA	1.80	0.47
3:A:1946:VAL:HG21	5:J:229:ILE:CG2	2.44	0.47
6:D:79:PRO:O	6:D:81:THR:HG23	2.15	0.47
28:C:219:VAL:HG13	28:C:933:TRP:CH2	2.49	0.47
28:C:864:VAL:HG21	28:C:906:VAL:CG2	2.44	0.47
9:B:1977:MET:HE1	9:B:2102:VAL:HG22	1.95	0.47
15:e:45:GLY:HA3	15:e:53:VAL:HG12	1.96	0.47
2:W:65:U:H2'	2:W:66:C:C6	2.49	0.47
3:A:1383:PHE:CE1	3:A:1614:ILE:HG23	2.48	0.47
4:H:271:VAL:HG12	4:H:282:SER:CB	2.43	0.47
5:J:691:TYR:CE2	5:J:711:ILE:HD11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:543:TYR:HB2	9:B:550:LEU:HD12	1.96	0.47
9:B:558:VAL:HB	9:B:631:LEU:HD12	1.96	0.47
1:V:18:A:C5'	1:V:19:U:OP1	2.63	0.47
3:A:466:GLU:HG2	3:A:467:GLU:N	2.28	0.47
3:A:657:LEU:HD13	3:A:708:TRP:HA	1.97	0.47
3:A:1654:TRP:CZ3	3:A:1779:LEU:HD12	2.49	0.47
3:A:1961:LEU:HG	3:A:2084:LEU:HG	1.95	0.47
7:F:57:LEU:O	7:F:59:LEU:HD23	2.15	0.47
14:n:62:ILE:HD11	17:r:70:SER:OG	2.14	0.47
23:4:29:LEU:HD21	23:4:32:VAL:CG2	2.45	0.47
1:V:5:U:H2'	1:V:6:U:C6	2.50	0.47
3:A:792:CYS:SG	5:J:184:ASN:HB2	2.55	0.47
3:A:1795:LYS:HB3	3:A:1796:PRO:HD3	1.97	0.47
4:H:155:ARG:HD3	8:G:174:LEU:HD22	1.97	0.47
6:D:39:CYS:SG	6:D:40:MET:N	2.87	0.47
7:F:244:HIS:CD2	7:F:262:ILE:HG23	2.50	0.47
3:A:943:ALA:O	3:A:947:PRO:HA	2.15	0.47
6:D:97:THR:O	6:D:141:ARG:NH2	2.46	0.47
7:F:102:ILE:HG22	7:F:103:PRO:HD3	1.96	0.47
7:F:283:GLY:O	7:F:284:TYR:C	2.58	0.47
9:B:384:ASP:O	9:B:387:GLU:HB3	2.14	0.47
3:A:161:PHE:CE2	3:A:198:ALA:HB2	2.50	0.47
3:A:966:PRO:HB3	3:A:1089:VAL:HB	1.95	0.47
3:A:1605:ARG:HG2	3:A:1823:LEU:HA	1.97	0.47
3:A:2084:LEU:HD22	3:A:2086:GLN:CD	2.40	0.47
5:J:617:PHE:CE2	5:J:644:ARG:NH1	2.83	0.47
5:J:645:TYR:O	5:J:649:ASN:N	2.47	0.47
5:J:843:VAL:HG21	5:J:896:MET:CE	2.45	0.47
6:D:6:LEU:HD22	6:D:59:ILE:CG2	2.44	0.47
9:B:1482:GLY:O	9:B:1483:VAL:HG13	2.15	0.47
19:U:79:C:C2	19:U:114:G:N2	2.82	0.47
28:C:274:ILE:HG21	28:C:385:PHE:CD2	2.50	0.47
1:V:8:U:H2'	1:V:9:G:C8	2.50	0.47
4:H:234:MET:HE2	4:H:246:PHE:CD2	2.50	0.47
5:J:229:ILE:HD12	7:F:417:LEU:HD21	1.97	0.47
11:k:49:ILE:HG23	11:k:80:ARG:O	2.15	0.47
19:U:132:A:O2'	19:U:133:C:OP1	2.28	0.47
25:6:52:ALA:HB3	25:6:71:VAL:HG21	1.97	0.47
28:C:133:ILE:HG23	28:C:209:MET:SD	2.55	0.47
28:C:320:PHE:CD1	28:C:425:LEU:HD13	2.50	0.47
28:C:539:VAL:HG13	28:C:564:ILE:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:823:TRP:NE1	3:A:851:ARG:HD3	2.30	0.46
3:A:882:ILE:CD1	3:A:1238:LEU:HD21	2.46	0.46
3:A:1974:LEU:O	3:A:1977:VAL:HG22	2.15	0.46
4:H:424:SER:HA	4:H:427:TRP:CZ3	2.51	0.46
14:n:6:ILE:N	14:n:7:PRO:CD	2.78	0.46
28:C:374:VAL:HG12	28:C:379:ILE:HG12	1.97	0.46
1:V:58:G:C2	1:V:59:C:C2	3.04	0.46
2:W:26:A:H2	3:A:667:TYR:O	1.78	0.46
3:A:1353:THR:HG23	3:A:1356:LEU:HB3	1.97	0.46
9:B:820:PHE:CD1	9:B:840:LEU:HD21	2.50	0.46
11:b:96:VAL:HG11	12:h:82:LEU:HD13	1.98	0.46
28:C:628:TYR:O	28:C:630:PRO:HD3	2.16	0.46
1:V:77:U:H3'	9:B:833:THR:HG22	1.96	0.46
2:W:31:G:OP1	3:A:1377:SER:OG	2.24	0.46
3:A:176:LEU:HD13	3:A:632:ILE:CD1	2.46	0.46
5:J:195:ASN:O	5:J:199:ASP:N	2.48	0.46
6:D:121:PHE:CZ	6:D:125:ARG:HD2	2.50	0.46
11:k:91:GLN:NE2	14:n:24:THR:HG22	2.29	0.46
28:C:473:LEU:HB2	28:C:485:LEU:HD23	1.98	0.46
28:C:873:LEU:N	28:C:874:PRO:CD	2.79	0.46
3:A:140:ARG:NE	3:A:255:ILE:HD11	2.31	0.46
3:A:1607:THR:O	3:A:1611:SER:N	2.48	0.46
3:A:2015:LEU:HD23	3:A:2022:ALA:HB3	1.96	0.46
4:H:239:GLU:HA	4:H:267:ARG:CB	2.45	0.46
9:B:1409:LEU:HD22	9:B:1427:LYS:HB2	1.97	0.46
19:U:40:C:O2	19:U:115:G:C2	2.69	0.46
2:W:88:U:C1'	21:2:80:ASN:HB3	2.44	0.46
9:B:1226:TRP:CH2	9:B:1259:ILE:HG21	2.51	0.46
11:k:85:THR:HG21	14:n:71:PHE:CD1	2.50	0.46
12:h:82:LEU:HD12	12:h:85:ILE:HD11	1.98	0.46
28:C:231:ALA:O	28:C:487:ARG:NH1	2.49	0.46
3:A:208:VAL:CG1	3:A:496:ALA:HB2	2.46	0.46
4:H:395:ILE:HD11	4:H:415:TYR:CD1	2.51	0.46
5:J:358:LEU:O	5:J:362:THR:HG23	2.15	0.46
9:B:936:VAL:HG11	9:B:971:GLU:CD	2.40	0.46
1:V:35:G:C2	1:V:36:A:C8	3.04	0.46
3:A:193:TYR:CE1	3:A:560:THR:HG23	2.51	0.46
3:A:459:ALA:C	28:C:376:PHE:CZ	2.83	0.46
3:A:819:LYS:O	3:A:823:TRP:N	2.47	0.46
3:A:1676:LEU:HD11	3:A:1797:LEU:HD22	1.97	0.46
4:H:357:TRP:CZ3	4:H:364:VAL:HG22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:601:ILE:HD13	5:J:640:VAL:HG11	1.96	0.46
8:G:193:GLU:O	8:G:196:LEU:N	2.49	0.46
3:A:138:HIS:NE2	3:A:142:ILE:HD11	2.30	0.46
3:A:550:SER:OG	3:A:558:GLN:NE2	2.49	0.46
3:A:672:LYS:N	19:U:101:C:OP1	2.43	0.46
3:A:1214:ARG:N	3:A:1255:ASN:OD1	2.47	0.46
19:U:129:G:H4'	19:U:130:A:C4'	2.46	0.46
2:W:27:U:H2'	2:W:28:U:C6	2.51	0.46
3:A:168:LEU:HD23	3:A:622:MET:HE3	1.98	0.46
3:A:329:TYR:CD1	3:A:330:LEU:HG	2.51	0.46
3:A:404:ASN:CG	3:A:405:ASN:N	2.73	0.46
3:A:1070:LEU:HD11	3:A:1113:ILE:HD12	1.97	0.46
5:J:792:THR:OG1	20:K:46:ARG:NE	2.49	0.46
8:G:264:LEU:HD12	9:B:458:PRO:HA	1.97	0.46
9:B:845:VAL:HG21	9:B:874:ARG:O	2.16	0.46
9:B:1656:TYR:CZ	9:B:1677:THR:HG22	2.50	0.46
28:C:615:LEU:N	28:C:616:PRO:CD	2.77	0.46
28:C:762:SER:O	28:C:765:VAL:HG22	2.15	0.46
1:V:57:U:O2'	1:V:58:G:H5'	2.16	0.45
3:A:355:LEU:HD13	3:A:355:LEU:O	2.16	0.45
3:A:1933:ILE:CD1	3:A:1948:MET:HE2	2.46	0.45
9:B:480:ILE:HD12	9:B:491:PHE:CD1	2.52	0.45
28:C:862:TYR:N	28:C:906:VAL:O	2.46	0.45
28:C:866:ILE:HB	28:C:902:VAL:HG13	1.98	0.45
3:A:268:LEU:HD13	3:A:277:LYS:CB	2.46	0.45
5:J:254:ALA:N	5:J:255:ARG:HA	2.31	0.45
9:B:932:ARG:O	9:B:936:VAL:HG13	2.17	0.45
28:C:222:MET:HE3	28:C:225:THR:HB	1.97	0.45
28:C:389:LEU:HD21	28:C:421:LEU:HD12	1.99	0.45
3:A:666:ILE:CG2	3:A:673:VAL:HG21	2.46	0.45
3:A:788:GLU:CB	5:J:181:LEU:HD23	2.46	0.45
3:A:819:LYS:O	3:A:823:TRP:CB	2.64	0.45
5:J:404:ILE:O	5:J:408:LEU:HG	2.16	0.45
5:J:561:LEU:HD23	5:J:585:GLN:HE21	1.82	0.45
5:J:601:ILE:HG12	5:J:617:PHE:HE1	1.81	0.45
8:G:402:TRP:CD1	8:G:424:ILE:HG21	2.51	0.45
9:B:793:LEU:HD12	9:B:803:THR:HG23	1.98	0.45
11:k:20:LEU:HD23	11:k:95:THR:HB	1.96	0.45
20:K:64:LEU:HD21	20:K:98:ILE:HD13	1.98	0.45
2:W:26:A:HO2'	3:A:667:TYR:HD1	1.50	0.45
3:A:1032:ILE:HG21	3:A:1258:LEU:CD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1066:LEU:HD11	3:A:1113:ILE:HG23	1.99	0.45
3:A:1933:ILE:HG21	3:A:1944:LEU:HD21	1.98	0.45
3:A:2271:ALA:HB2	3:A:2326:SER:OG	2.16	0.45
4:H:283:ALA:HB2	4:H:313:LEU:HG	1.97	0.45
5:J:187:ASN:N	5:J:188:PRO:CD	2.79	0.45
9:B:539:LEU:HD11	9:B:555:PHE:CE1	2.51	0.45
9:B:633:ILE:HG21	9:B:636:ILE:HD13	1.99	0.45
3:A:305:LEU:HD22	28:C:390:SER:HA	1.99	0.45
3:A:1122:ASP:CG	3:A:1163:ARG:HE	2.23	0.45
5:J:211:ARG:CB	7:F:400:VAL:HG21	2.47	0.45
5:J:242:GLN:HA	5:J:245:ILE:HD12	1.99	0.45
5:J:536:PHE:HB3	5:J:564:TYR:CE2	2.51	0.45
6:D:82:VAL:CG2	6:D:103:LEU:HG	2.46	0.45
7:F:309:LYS:HG3	7:F:337:LEU:HD21	1.97	0.45
28:C:360:ARG:HA	28:C:361:THR:HB	1.99	0.45
28:C:685:SER:HB2	28:C:711:ALA:HB1	1.98	0.45
3:A:208:VAL:HG13	3:A:496:ALA:HB2	1.98	0.45
3:A:1385:PRO:O	3:A:1386:ALA:C	2.58	0.45
4:H:243:ILE:HD11	4:H:261:LEU:HD22	1.99	0.45
7:F:400:VAL:HG23	7:F:410:LEU:HG	1.99	0.45
19:U:115:G:H2'	19:U:116:U:C6	2.52	0.45
21:2:83:GLN:HG2	22:3:12:LEU:HD22	1.98	0.45
28:C:844:LYS:O	28:C:848:VAL:HG23	2.17	0.45
2:W:5:G:C6	2:W:6:C:N4	2.85	0.45
3:A:484:PHE:CD1	3:A:484:PHE:C	2.94	0.45
3:A:656:ILE:HA	3:A:663:LEU:HD12	1.98	0.45
3:A:1208:PRO:O	3:A:1209:LYS:C	2.58	0.45
3:A:1320:LEU:HD21	3:A:1367:ILE:HD13	1.99	0.45
3:A:1752:VAL:HG11	3:A:1785:ASP:O	2.17	0.45
5:J:224:GLN:O	5:J:228:THR:HG23	2.17	0.45
5:J:605:GLY:HA3	5:J:887:THR:HG21	1.99	0.45
8:G:355:LYS:O	8:G:359:ASN:ND2	2.50	0.45
28:C:241:VAL:HG11	28:C:273:LEU:HD23	1.99	0.45
3:A:212:VAL:HA	3:A:311:LEU:HD22	1.99	0.45
3:A:526:LEU:HD23	3:A:526:LEU:HA	1.90	0.45
3:A:885:VAL:HG21	3:A:1124:LEU:CD2	2.47	0.45
5:J:204:LEU:HD11	7:F:381:LEU:HD23	1.98	0.45
20:K:64:LEU:CD2	20:K:98:ILE:HD13	2.46	0.45
3:A:1599:SER:O	3:A:1602:PRO:CD	2.53	0.45
4:H:198:ASP:OD1	4:H:198:ASP:N	2.50	0.45
7:F:253:ARG:CD	20:K:70:LEU:HD13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:391:MET:C	7:F:392:GLU:O	2.59	0.45
28:C:161:ILE:HD12	28:C:164:MET:SD	2.57	0.45
28:C:861:ILE:HD12	28:C:936:ILE:CG2	2.47	0.45
1:V:10:C:H2'	1:V:11:A:O4'	2.16	0.45
3:A:805:PRO:HD3	5:J:178:LEU:CD2	2.47	0.45
3:A:1461:TYR:CE1	3:A:1475:LEU:HD23	2.52	0.45
11:k:20:LEU:HD22	11:k:34:LEU:HD12	1.99	0.45
28:C:210:ILE:HD11	28:C:436:VAL:HG13	1.98	0.45
28:C:634:ILE:HG13	28:C:644:ILE:HG23	1.99	0.45
4:H:159:LEU:CD1	4:H:430:MET:HE2	2.40	0.44
5:J:259:VAL:HA	5:J:262:LYS:HD2	1.99	0.44
5:J:674:LEU:HD22	5:J:690:THR:HG21	1.99	0.44
8:G:264:LEU:HD13	9:B:711:LYS:HD3	1.98	0.44
9:B:1084:PHE:CE2	9:B:1131:LEU:HD13	2.52	0.44
11:k:21:ARG:N	11:k:96:VAL:O	2.50	0.44
4:H:316:GLN:HE21	4:H:361:GLY:HA3	1.82	0.44
6:D:49:ILE:HG23	6:D:114:ILE:HG12	1.99	0.44
7:F:154:SER:HB2	7:F:155:ASP:C	2.42	0.44
8:G:347:LEU:HD11	8:G:371:ARG:CD	2.47	0.44
3:A:173:LEU:HA	3:A:715:LEU:HD13	1.98	0.44
3:A:461:LEU:CD1	3:A:461:LEU:C	2.85	0.44
3:A:1063:PHE:HD2	7:F:272:LEU:HD11	1.82	0.44
3:A:1536:LEU:HD23	3:A:1536:LEU:HA	1.84	0.44
7:F:434:GLN:O	7:F:435:ALA:C	2.61	0.44
8:G:363:LEU:HD11	8:G:391:PHE:CD2	2.52	0.44
19:U:73:U:H2'	19:U:74:U:N1	2.32	0.44
20:K:53:ILE:HD11	20:K:102:ILE:HG12	1.99	0.44
28:C:655:LEU:C	28:C:655:LEU:HD23	2.42	0.44
2:W:77:G:H2'	2:W:78:G:O4'	2.17	0.44
3:A:628:MET:HE1	3:A:664:THR:HB	2.00	0.44
5:J:199:ASP:C	5:J:201:LEU:N	2.70	0.44
5:J:215:LEU:HD22	7:F:400:VAL:HG22	1.99	0.44
8:G:347:LEU:HD11	8:G:371:ARG:HD3	2.00	0.44
14:d:82:PRO:HD3	28:C:122:TYR:CE2	2.52	0.44
19:U:6:G:C6	19:U:7:C:N4	2.86	0.44
28:C:774:LEU:HD13	28:C:803:VAL:HG23	2.00	0.44
2:W:85:C:OP2	8:G:353:ARG:CZ	2.65	0.44
3:A:1557:LEU:O	3:A:1560:THR:N	2.49	0.44
5:J:201:LEU:HD23	7:F:379:PHE:CZ	2.52	0.44
7:F:305:MET:HE3	7:F:340:LYS:HB3	1.99	0.44
16:f:16:LYS:N	16:f:17:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:75:U:O2	1:V:75:U:C2'	2.65	0.44
2:W:84:C:C2	2:W:85:C:C5	3.05	0.44
3:A:674:MET:HA	3:A:677:ILE:HD12	2.00	0.44
3:A:1350:ILE:HG23	3:A:1356:LEU:CD2	2.38	0.44
5:J:568:TYR:CZ	5:J:581:VAL:HG21	2.53	0.44
7:F:84:LEU:C	7:F:84:LEU:HD12	2.42	0.44
9:B:708:CYS:SG	9:B:889:ILE:HA	2.58	0.44
9:B:1703:LEU:O	9:B:1707:VAL:HG22	2.18	0.44
14:d:33:LEU:HD23	14:d:34:VAL:N	2.33	0.44
19:U:32:G:O6	19:U:120:G:O6	2.35	0.44
28:C:341:ILE:O	28:C:345:THR:HG23	2.17	0.44
1:V:59:C:H5''	1:V:59:C:H6	1.83	0.44
3:A:326:ASN:ND2	3:A:404:ASN:OD1	2.49	0.44
3:A:591:LEU:HD22	3:A:599:LEU:HD21	1.99	0.44
3:A:1335:TRP:CH2	3:A:1339:LEU:HD13	2.52	0.44
5:J:160:ASN:O	5:J:163:THR:OG1	2.30	0.44
5:J:204:LEU:HD22	7:F:380:ARG:O	2.18	0.44
12:l:25:VAL:HG13	12:l:43:VAL:HG13	2.00	0.44
28:C:322:PHE:CE2	28:C:381:LEU:HD11	2.52	0.44
28:C:656:LEU:HD13	28:C:670:ILE:HD13	2.00	0.44
3:A:703:PHE:CE2	3:A:706:PRO:HD3	2.53	0.44
3:A:1320:LEU:HD23	3:A:1367:ILE:HD13	1.98	0.44
3:A:1603:ASN:OD1	3:A:1603:ASN:N	2.51	0.44
5:J:698:VAL:HG23	5:J:698:VAL:O	2.18	0.44
7:F:77:ILE:HG22	7:F:78:VAL:HG23	2.00	0.44
9:B:740:ILE:HD11	9:B:846:ILE:HD12	1.99	0.44
20:K:98:ILE:HD12	20:K:99:ALA:CB	2.48	0.44
3:A:459:ALA:CA	28:C:376:PHE:CE1	2.97	0.44
5:J:780:LEU:O	5:J:783:HIS:HB2	2.18	0.44
6:D:93:CYS:SG	6:D:120:ILE:HG21	2.58	0.44
6:D:109:ASP:HB2	6:D:112:GLU:CB	2.48	0.44
7:F:47:LEU:HD13	7:F:97:PHE:HB3	1.99	0.44
28:C:872:LEU:HB3	28:C:922:THR:HG23	2.00	0.44
3:A:308:MET:CG	3:A:479:LEU:HD21	2.48	0.43
3:A:534:LEU:HD23	3:A:535:HIS:CE1	2.53	0.43
9:B:1001:LEU:HD23	9:B:1015:MET:CE	2.43	0.43
19:U:74:U:C2	19:U:75:A:H4'	2.53	0.43
20:K:117:VAL:O	20:K:121:ILE:HG13	2.18	0.43
1:V:75:U:O2	1:V:75:U:H2'	2.17	0.43
3:A:1860:VAL:HA	3:A:1861:THR:HA	2.00	0.43
4:H:357:TRP:CH2	4:H:364:VAL:HG22	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:339:CYS:HB2	8:G:383:VAL:HG22	2.00	0.43
9:B:1183:ILE:HD11	9:B:1192:VAL:HG11	1.98	0.43
14:d:14:ALA:HA	14:d:78:LEU:HD21	1.99	0.43
19:U:132:A:C2'	19:U:133:C:OP1	2.66	0.43
28:C:227:VAL:HG22	28:C:595:LEU:HD12	2.00	0.43
28:C:492:LEU:HD12	28:C:492:LEU:O	2.18	0.43
28:C:774:LEU:HD21	28:C:813:ILE:HG21	2.01	0.43
2:W:50:G:N3	2:W:50:G:C2'	2.81	0.43
4:H:162:MET:HB3	4:H:421:VAL:HG21	2.00	0.43
5:J:289:VAL:HG23	5:J:290:HIS:N	2.33	0.43
5:J:324:TYR:CD1	5:J:347:PHE:CE2	3.07	0.43
9:B:589:THR:HG23	9:B:589:THR:O	2.18	0.43
19:U:22:G:N1	19:U:131:A:C2	2.86	0.43
21:2:25:ILE:HD11	21:2:52:PRO:HG3	1.99	0.43
3:A:808:ILE:HA	3:A:811:ILE:HG22	2.00	0.43
3:A:1737:GLN:HE21	3:A:1737:GLN:HA	1.83	0.43
8:G:289:ASP:O	8:G:290:PRO:C	2.61	0.43
28:C:314:ALA:CB	28:C:321:THR:HG22	2.48	0.43
2:W:5:G:C2	2:W:6:C:C2	3.05	0.43
3:A:338:ASN:OD1	3:A:399:ARG:N	2.51	0.43
4:H:172:LEU:HD22	5:J:755:GLN:HG3	2.01	0.43
4:H:243:ILE:CG1	4:H:261:LEU:HD13	2.49	0.43
4:H:445:ILE:HA	4:H:452:LEU:HD23	2.00	0.43
5:J:764:LEU:HD13	5:J:774:TRP:CZ2	2.53	0.43
8:G:287:ILE:HD12	8:G:287:ILE:N	2.32	0.43
19:U:41:A:C2	19:U:42:A:N1	2.86	0.43
1:V:30:G:O2'	20:K:97:VAL:HG22	2.18	0.43
3:A:200:THR:N	3:A:574:GLN:OE1	2.46	0.43
3:A:883:PHE:CZ	3:A:1072:LEU:HD11	2.54	0.43
3:A:1054:LEU:HD13	3:A:1121:ILE:HG21	2.00	0.43
3:A:1204:ARG:O	3:A:1206:CYS:N	2.51	0.43
3:A:2000:SER:HB3	8:G:277:MET:HE1	2.01	0.43
5:J:205:LYS:O	5:J:206:ASP:C	2.61	0.43
7:F:52:GLU:O	7:F:56:THR:HG23	2.19	0.43
9:B:1109:LEU:HD22	9:B:1131:LEU:HD12	2.00	0.43
20:K:71:CYS:O	20:K:75:ASN:N	2.52	0.43
28:C:197:THR:O	28:C:198:LEU:HD23	2.19	0.43
1:V:31:U:O4'	20:K:63:ILE:HD12	2.19	0.43
2:W:29:U:N3	19:U:98:U:N3	2.67	0.43
3:A:141:LYS:O	3:A:145:THR:HG23	2.19	0.43
3:A:172:ILE:HD11	3:A:626:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:614:ARG:C	3:A:615:LEU:HD13	2.43	0.43
3:A:708:TRP:CE2	3:A:712:LEU:HD11	2.54	0.43
3:A:1203:ASN:ND2	3:A:1213:MET:O	2.50	0.43
3:A:1598:LEU:O	3:A:1601:ILE:HB	2.18	0.43
3:A:1676:LEU:HD11	3:A:1797:LEU:CD2	2.49	0.43
14:n:19:VAL:HG11	14:n:33:LEU:HD12	2.01	0.43
17:g:64:ARG:NH2	19:U:169:U:O4'	2.52	0.43
19:U:43:G:C2'	19:U:44:A:H5'	2.49	0.43
1:V:74:U:O2	1:V:74:U:C2'	2.66	0.43
3:A:831:ARG:HH11	3:A:848:ASN:HD21	1.66	0.43
3:A:889:TRP:CZ2	3:A:893:ARG:HD3	2.54	0.43
7:F:120:TYR:CE1	7:F:141:ILE:HG23	2.53	0.43
19:U:20:U:H2'	19:U:21:G:C1'	2.48	0.43
20:K:20:ILE:HD13	20:K:79:VAL:HG21	2.01	0.43
28:C:234:LEU:HD23	28:C:235:VAL:N	2.34	0.43
3:A:1158:ILE:HG22	3:A:1158:ILE:O	2.19	0.43
3:A:1561:LEU:O	3:A:1564:GLY:N	2.47	0.43
5:J:504:LYS:HG3	5:J:508:TRP:CZ3	2.54	0.43
7:F:229:VAL:HG23	7:F:317:ASP:OD2	2.18	0.43
9:B:644:GLY:N	9:B:645:PRO:HD2	2.33	0.43
9:B:707:PHE:CZ	9:B:902:LEU:HD12	2.54	0.43
17:g:28:ILE:HG22	17:g:41:ASP:HB3	2.00	0.43
19:U:133:C:H2'	19:U:133:C:O2	2.19	0.43
20:K:54:MET:CG	20:K:64:LEU:HD12	2.48	0.43
28:C:472:VAL:HA	28:C:486:VAL:HG22	2.01	0.43
3:A:172:ILE:HG23	3:A:629:MET:HG3	2.00	0.43
3:A:461:LEU:N	28:C:332:TYR:OH	2.52	0.43
3:A:905:TYR:HB3	3:A:908:ASP:HB2	2.01	0.43
3:A:1354:GLU:N	3:A:1355:PRO:HD2	2.34	0.43
5:J:702:PRO:HA	5:J:739:PHE:CZ	2.54	0.43
5:J:839:GLY:O	5:J:841:THR:N	2.52	0.43
5:J:845:LEU:O	5:J:848:THR:OG1	2.30	0.43
9:B:677:TYR:HB2	9:B:691:LEU:HD11	2.01	0.43
9:B:1774:THR:HG21	18:E:412:UNK:HA	2.01	0.43
9:B:1803:LEU:O	9:B:1807:VAL:HG13	2.19	0.43
16:f:29:VAL:HG13	16:f:78:VAL:HG13	2.01	0.43
14:d:14:ALA:O	14:d:15:GLN:C	2.61	0.43
3:A:365:ASN:OD1	3:A:365:ASN:N	2.52	0.42
4:H:390:LEU:HD13	8:G:428:TRP:CG	2.54	0.42
4:H:435:GLY:N	5:J:731:LEU:HD13	2.34	0.42
5:J:341:TRP:CE3	5:J:361:ALA:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:737:VAL:HG13	5:J:773:LEU:HD11	1.99	0.42
7:F:233:VAL:CG1	7:F:237:ILE:HG21	2.46	0.42
9:B:1157:ILE:HD12	9:B:1158:LYS:N	2.34	0.42
9:B:1273:THR:HG21	9:B:1731:TYR:CE1	2.54	0.42
19:U:20:U:H2'	19:U:21:G:O4'	2.19	0.42
19:U:46:C:C5'	28:C:111:LYS:HG2	2.50	0.42
3:A:857:ILE:CD1	3:A:969:ILE:HD11	2.49	0.42
3:A:2165:ARG:HB3	3:A:2300:VAL:HG13	2.00	0.42
5:J:327:VAL:O	5:J:331:LEU:HG	2.19	0.42
5:J:344:ALA:HB3	5:J:357:MET:HE2	2.01	0.42
5:J:369:MET:HG3	5:J:404:ILE:HD11	2.00	0.42
8:G:200:ILE:HG23	8:G:200:ILE:O	2.19	0.42
9:B:448:LEU:N	9:B:449:PRO:HA	2.34	0.42
28:C:577:LEU:C	28:C:577:LEU:HD12	2.44	0.42
3:A:913:VAL:HG21	10:x:105:UNK:HA	2.01	0.42
3:A:1063:PHE:CD2	7:F:272:LEU:HD11	2.54	0.42
3:A:1120:VAL:O	3:A:1124:LEU:HG	2.20	0.42
3:A:1168:ILE:C	3:A:1169:TYR:CD1	2.97	0.42
4:H:365:ALA:HB2	4:H:375:VAL:HG13	2.01	0.42
4:H:445:ILE:HG23	4:H:452:LEU:CD2	2.50	0.42
5:J:737:VAL:HG22	5:J:767:PHE:CG	2.54	0.42
7:F:233:VAL:HG11	7:F:237:ILE:CG2	2.44	0.42
28:C:483:TRP:CH2	28:C:550:VAL:HG11	2.54	0.42
4:H:235:ILE:HD12	4:H:244:LYS:C	2.45	0.42
4:H:426:THR:OG1	4:H:427:TRP:N	2.52	0.42
6:D:112:GLU:HG2	6:D:135:TYR:CE1	2.54	0.42
9:B:578:LEU:HB3	9:B:583:ILE:HD12	2.01	0.42
1:V:33:A:H1'	1:V:45:A:C2	2.55	0.42
3:A:930:ASN:OD1	3:A:930:ASN:C	2.62	0.42
3:A:1651:ALA:O	3:A:1652:HIS:C	2.62	0.42
3:A:1946:VAL:CG2	5:J:229:ILE:HG21	2.48	0.42
4:H:117:LEU:HD13	4:H:301:LEU:HD12	2.01	0.42
5:J:561:LEU:O	5:J:564:TYR:HB2	2.19	0.42
7:F:311:SER:O	7:F:315:ARG:HG2	2.19	0.42
7:F:347:ALA:CB	7:F:348:PRO:CD	2.96	0.42
8:G:286:ASN:OD1	8:G:293:TRP:NE1	2.52	0.42
9:B:429:LEU:HA	9:B:432:ILE:HD12	2.02	0.42
9:B:1224:ALA:HB1	9:B:1226:TRP:CZ3	2.53	0.42
11:k:87:LEU:HD12	14:n:71:PHE:HB3	2.00	0.42
3:A:1032:ILE:HG21	3:A:1258:LEU:HD23	2.01	0.42
3:A:1752:VAL:CG1	3:A:1776:GLY:HA3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1835:LEU:CD2	3:A:1843:LEU:HD11	2.49	0.42
9:B:1978:ASP:O	9:B:1982:MET:HG3	2.20	0.42
20:K:23:VAL:HG21	20:K:117:VAL:CG2	2.48	0.42
20:K:33:LEU:C	20:K:33:LEU:HD23	2.45	0.42
28:C:271:ASP:CB	28:C:318:LEU:HD12	2.50	0.42
28:C:288:LEU:HD13	28:C:313:PHE:HE2	1.83	0.42
28:C:774:LEU:HD21	28:C:813:ILE:CG2	2.50	0.42
2:W:87:U:C5	8:G:441:PHE:CD1	3.08	0.42
3:A:198:ALA:HA	3:A:574:GLN:HG2	2.02	0.42
3:A:330:LEU:HD21	3:A:386:ALA:CB	2.47	0.42
3:A:885:VAL:HG21	3:A:1124:LEU:HD23	2.02	0.42
3:A:1170:MET:HE1	3:A:1230:ILE:HG21	2.02	0.42
3:A:1993:ASP:HB2	3:A:2038:HIS:CG	2.54	0.42
4:H:373:ILE:HG13	4:H:391:ALA:HB2	2.00	0.42
9:B:391:PHE:O	9:B:393:GLU:N	2.53	0.42
9:B:836:TRP:HA	9:B:836:TRP:HE3	1.83	0.42
9:B:1139:MET:HE3	9:B:1298:TRP:NE1	2.35	0.42
19:U:70:A:H3'	19:U:71:A:H5''	2.02	0.42
20:K:24:VAL:HG22	20:K:53:ILE:HD13	2.02	0.42
28:C:241:VAL:CG1	28:C:273:LEU:HD23	2.49	0.42
1:V:31:U:OP1	20:K:98:ILE:HG13	2.20	0.42
3:A:591:LEU:HA	3:A:601:PRO:HA	2.01	0.42
3:A:1028:TRP:NE1	3:A:1032:ILE:HD11	2.34	0.42
3:A:1186:TYR:CE2	3:A:1224:ARG:HB3	2.55	0.42
4:H:195:TRP:O	4:H:220:LYS:HA	2.20	0.42
4:H:238:ALA:HB3	4:H:240:ASP:HB3	2.01	0.42
5:J:873:GLU:CB	5:J:896:MET:HE1	2.49	0.42
6:D:29:ILE:HG21	6:D:31:PHE:CE1	2.55	0.42
7:F:70:THR:HA	7:F:73:ILE:HD12	2.01	0.42
7:F:171:GLN:O	7:F:174:VAL:HG22	2.19	0.42
28:C:634:ILE:O	28:C:634:ILE:HG22	2.19	0.42
3:A:2041:PRO:O	3:A:2043:PHE:N	2.53	0.42
5:J:265:GLU:HG2	5:J:281:ASN:HD21	1.84	0.42
9:B:398:LYS:O	9:B:399:ARG:CB	2.68	0.42
19:U:93:G:C2	19:U:94:C:N3	2.87	0.42
28:C:127:ALA:O	28:C:133:ILE:HD11	2.20	0.42
28:C:468:LEU:C	28:C:468:LEU:HD12	2.45	0.42
3:A:171:ALA:CB	3:A:201:PHE:HB3	2.44	0.42
3:A:1092:PHE:O	3:A:1095:MET:N	2.52	0.42
3:A:1126:LEU:O	3:A:1130:ARG:HB3	2.19	0.42
3:A:2225:VAL:HG11	3:A:2242:PRO:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:122:ARG:O	4:H:125:ILE:HG12	2.20	0.42
9:B:978:LEU:HD23	9:B:981:LEU:HD12	2.02	0.42
9:B:1812:ASN:HA	9:B:1815:VAL:HG22	2.02	0.42
11:b:25:GLN:HG2	11:b:93:LEU:HD21	2.01	0.42
16:f:71:ILE:HG22	13:j:105:LEU:CB	2.50	0.42
20:K:87:LEU:HD13	20:K:87:LEU:C	2.45	0.42
3:A:377:VAL:HG21	28:C:912:ALA:HB3	2.01	0.41
3:A:999:LEU:HD13	3:A:1112:PHE:CE1	2.55	0.41
3:A:1948:MET:HE1	3:A:1954:ILE:HD12	2.02	0.41
5:J:578:GLN:HE21	5:J:603:LEU:CD2	2.33	0.41
9:B:633:ILE:HD12	9:B:633:ILE:N	2.35	0.41
11:b:48:CYS:SG	11:b:82:LEU:HD12	2.60	0.41
17:g:56:GLN:C	17:g:57:LEU:HD22	2.45	0.41
28:C:617:LYS:CB	28:C:666:ILE:HD11	2.49	0.41
28:C:768:PHE:HB3	28:C:775:ILE:HA	2.02	0.41
2:W:29:U:C2	19:U:98:U:O2	2.70	0.41
3:A:596:ASN:O	3:A:598:ASN:N	2.46	0.41
3:A:785:HIS:CD2	5:J:181:LEU:HD22	2.55	0.41
3:A:852:LEU:HD23	3:A:852:LEU:C	2.45	0.41
3:A:2255:LEU:HD21	3:A:2281:PHE:CE1	2.54	0.41
5:J:383:ASN:O	5:J:387:THR:HG23	2.20	0.41
6:D:137:TYR:O	6:D:138:ASN:CB	2.68	0.41
8:G:344:PHE:HB3	8:G:424:ILE:HD13	2.03	0.41
9:B:406:ASP:O	9:B:409:GLN:N	2.53	0.41
9:B:491:PHE:HZ	9:B:533:LEU:HD21	1.86	0.41
9:B:1728:MET:HA	9:B:1728:MET:HE2	2.01	0.41
14:d:6:ILE:N	14:d:7:PRO:CD	2.83	0.41
20:K:79:VAL:HG13	20:K:121:ILE:HG23	2.01	0.41
28:C:108:GLN:O	28:C:111:LYS:CD	2.68	0.41
28:C:255:GLN:HG3	28:C:598:ILE:HD13	2.02	0.41
3:A:644:VAL:HG22	3:A:645:ASP:H	1.85	0.41
3:A:895:PHE:CZ	3:A:1008:LEU:HB2	2.55	0.41
3:A:1206:CYS:SG	3:A:1207:TRP:CD1	3.13	0.41
3:A:1814:VAL:HG23	3:A:2098:MET:HG2	2.01	0.41
5:J:185:ALA:O	5:J:187:ASN:N	2.53	0.41
5:J:733:ASN:OD1	5:J:739:PHE:CE1	2.74	0.41
6:D:84:PHE:HB3	6:D:120:ILE:HD12	2.03	0.41
7:F:320:GLN:HE22	7:F:326:ASN:HB3	1.86	0.41
8:G:214:ILE:O	8:G:214:ILE:HG22	2.19	0.41
9:B:676:ASN:O	9:B:680:VAL:HG23	2.20	0.41
9:B:809:THR:HA	9:B:1092:PHE:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:85:THR:HG22	14:n:73:VAL:HG22	2.01	0.41
13:j:58:VAL:HG13	13:j:67:MET:HE2	2.02	0.41
19:U:41:A:C2	19:U:42:A:C6	3.08	0.41
28:C:418:GLN:HB3	28:C:419:PRO:HD3	2.01	0.41
28:C:470:ALA:HB3	28:C:577:LEU:HD11	2.02	0.41
1:V:36:A:C2	1:V:37:U:C6	3.08	0.41
2:W:62:A:C4	2:W:63:G:C8	3.09	0.41
3:A:1673:LEU:HA	3:A:1678:ILE:HD12	2.01	0.41
5:J:867:GLU:HB2	5:J:874:TRP:CZ3	2.55	0.41
9:B:1095:ASN:O	9:B:1099:VAL:HG23	2.19	0.41
12:h:96:ILE:HG12	13:j:94:LEU:HD12	2.02	0.41
28:C:342:ASP:O	28:C:345:THR:OG1	2.30	0.41
3:A:279:TRP:HB2	3:A:286:LEU:HB3	2.02	0.41
3:A:875:THR:HB	3:A:876:PRO:HD2	2.01	0.41
3:A:2159:ASN:HA	3:A:2162:LEU:HD13	2.03	0.41
3:A:2378:ILE:N	3:A:2378:ILE:HD12	2.35	0.41
4:H:321:LEU:HD12	4:H:334:TRP:C	2.45	0.41
5:J:341:TRP:CE3	5:J:357:MET:HE1	2.56	0.41
5:J:781:PHE:CZ	5:J:793:ILE:HG13	2.56	0.41
7:F:45:GLU:O	7:F:48:PRO:HD2	2.21	0.41
8:G:260:ILE:HD12	8:G:266:PRO:HG2	2.02	0.41
9:B:779:GLN:O	9:B:783:THR:HG23	2.21	0.41
10:x:46:UNK:O	10:x:48:UNK:N	2.54	0.41
1:V:22:G:N2	1:V:23:C:C2	2.89	0.41
3:A:914:LEU:HD22	3:A:1505:ASP:HB2	2.03	0.41
3:A:1000:TRP:NE1	3:A:1112:PHE:HB2	2.36	0.41
4:H:227:HIS:HA	4:H:273:TYR:CD2	2.55	0.41
5:J:190:GLN:O	5:J:194:PRO:CD	2.66	0.41
7:F:315:ARG:HD2	20:K:66:HIS:CE1	2.56	0.41
9:B:491:PHE:CZ	9:B:533:LEU:HD21	2.56	0.41
28:C:120:ARG:HD3	28:C:551:TYR:CE1	2.55	0.41
28:C:251:GLN:HG2	28:C:933:TRP:CG	2.55	0.41
28:C:324:ILE:HG23	28:C:377:ILE:HD11	2.01	0.41
28:C:328:VAL:HG21	28:C:345:THR:HG22	2.03	0.41
1:V:57:U:C4	2:W:63:G:C2	3.09	0.41
3:A:1405:ILE:HG21	3:A:1437:ILE:HG13	2.02	0.41
5:J:565:VAL:HG11	5:J:599:PHE:CB	2.50	0.41
5:J:845:LEU:O	5:J:849:TYR:HD2	2.04	0.41
6:D:91:MET:HE1	6:D:128:LYS:O	2.20	0.41
7:F:291:ILE:CD1	7:F:306:LEU:HD22	2.51	0.41
8:G:263:GLY:N	9:B:458:PRO:HG2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:1770:VAL:O	9:B:1774:THR:HG23	2.21	0.41
19:U:128:A:N3	19:U:128:A:H2'	2.35	0.41
28:C:469:TRP:CZ3	28:C:590:LYS:HG2	2.56	0.41
28:C:599:THR:HA	28:C:933:TRP:HA	2.02	0.41
1:V:6:U:H2'	1:V:7:A:C8	2.55	0.41
1:V:37:U:H2'	1:V:39:C:C5	2.56	0.41
3:A:1375:LEU:CD2	3:A:1607:THR:HG23	2.51	0.41
3:A:1882:LEU:HD12	3:A:1883:ASN:N	2.35	0.41
9:B:809:THR:HA	9:B:1092:PHE:CD1	2.56	0.41
9:B:1873:THR:HG22	9:B:2109:LYS:HD2	2.03	0.41
21:2:19:LEU:HD12	21:2:23:ILE:CG2	2.50	0.41
28:C:242:VAL:HG22	28:C:277:LEU:HD11	2.02	0.41
1:V:17:A:C2	1:V:18:A:C4	3.09	0.41
2:W:60:G:H2'	2:W:61:C:O4'	2.21	0.41
3:A:963:VAL:HG21	7:F:280:ARG:NH2	2.35	0.41
3:A:1609:TRP:CZ3	3:A:1823:LEU:HD13	2.56	0.41
3:A:1777:ILE:HG12	3:A:1806:MET:HE1	2.01	0.41
5:J:682:GLY:O	5:J:683:ASN:C	2.63	0.41
5:J:763:ALA:HB1	5:J:773:LEU:HD13	2.02	0.41
6:D:79:PRO:HA	6:D:80:MET:CE	2.51	0.41
7:F:285:LEU:HD13	7:F:306:LEU:HD23	2.02	0.41
19:U:45:A:H2'	19:U:45:A:N3	2.35	0.41
20:K:81:VAL:HB	20:K:82:PRO:HD2	2.03	0.41
28:C:139:ILE:O	28:C:237:ILE:HA	2.21	0.41
28:C:227:VAL:HG22	28:C:595:LEU:CD1	2.51	0.41
28:C:856:ILE:HG22	28:C:857:LEU:O	2.20	0.41
3:A:1021:PRO:N	3:A:1022:PRO:CD	2.84	0.41
3:A:2011:LEU:HD22	3:A:2055:MET:HE3	2.02	0.41
4:H:172:LEU:HD13	5:J:755:GLN:HG3	2.03	0.41
4:H:395:ILE:CD1	20:K:126:ILE:CD1	2.99	0.41
7:F:135:LEU:HD22	7:F:208:TRP:NE1	2.35	0.41
7:F:369:GLY:O	7:F:371:LYS:N	2.54	0.41
9:B:412:GLU:N	9:B:412:GLU:OE1	2.54	0.41
9:B:924:VAL:HG12	9:B:998:ALA:HB2	2.02	0.41
9:B:1746:LEU:O	9:B:1750:ILE:HG23	2.20	0.41
9:B:2113:ALA:HB2	9:B:2130:PHE:CB	2.51	0.41
16:q:29:VAL:HG13	16:q:78:VAL:HG13	2.03	0.41
11:b:12:LEU:HD13	12:h:86:ASN:HD22	1.86	0.41
16:f:71:ILE:HG22	13:j:105:LEU:HB3	2.03	0.41
19:U:24:G:H2'	19:U:25:G:O5'	2.21	0.41
28:C:142:LEU:HD22	28:C:143:HIS:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:394:ARG:HD3	28:C:610:LEU:HD13	2.04	0.40
3:A:466:GLU:HG2	3:A:467:GLU:C	2.46	0.40
3:A:576:HIS:CD2	3:A:580:ASN:HD21	2.40	0.40
3:A:1710:GLU:HG2	3:A:1728:ILE:HD12	2.03	0.40
4:H:155:ARG:NE	8:G:174:LEU:HD22	2.35	0.40
5:J:299:ALA:O	5:J:303:ASN:N	2.46	0.40
5:J:478:TYR:O	5:J:479:GLU:CB	2.69	0.40
9:B:940:ALA:HB2	9:B:970:ARG:NH1	2.36	0.40
19:U:17:C:H2'	19:U:18:A:C8	2.56	0.40
21:2:10:LEU:HD22	21:2:13:GLN:HE21	1.85	0.40
28:C:220:ASN:HB3	28:C:651:TYR:HB2	2.03	0.40
28:C:446:PHE:HA	28:C:449:PHE:HB3	2.03	0.40
1:V:81:C:C4	1:V:82:C:C4	3.09	0.40
3:A:330:LEU:CD2	3:A:385:VAL:HG23	2.48	0.40
3:A:461:LEU:HD11	3:A:462:LEU:HG	1.94	0.40
4:H:321:LEU:HD22	8:G:195:LYS:CD	2.51	0.40
11:k:86:ILE:HD11	14:n:10:LEU:HD22	2.03	0.40
19:U:96:U:C4	19:U:97:U:C5	3.09	0.40
28:C:219:VAL:O	28:C:221:PHE:N	2.54	0.40
2:W:27:U:H1'	3:A:668:ARG:HA	2.02	0.40
3:A:1889:LEU:HD22	3:A:1991:ILE:HD12	2.04	0.40
3:A:2166:LEU:HD11	3:A:2194:ILE:HG21	2.03	0.40
8:G:365:LEU:HD22	8:G:382:VAL:CG1	2.51	0.40
8:G:428:TRP:CE3	8:G:428:TRP:HA	2.57	0.40
9:B:1428:LEU:HB2	9:B:1447:ALA:HB2	2.02	0.40
20:K:20:ILE:O	20:K:24:VAL:HG23	2.21	0.40
20:K:95:ARG:HG3	20:K:96:PRO:HD2	2.03	0.40
3:A:881:THR:O	3:A:885:VAL:HG23	2.21	0.40
3:A:1837:SER:N	3:A:2084:LEU:HD21	2.37	0.40
4:H:273:TYR:CD1	4:H:280:ILE:HG23	2.56	0.40
9:B:1773:PHE:CD2	9:B:1803:LEU:HD21	2.56	0.40
19:U:93:G:N2	19:U:94:C:C2	2.90	0.40
28:C:941:PRO:O	28:C:963:SER:HB3	2.22	0.40
3:A:324:ASP:HB3	3:A:407:VAL:HG21	2.04	0.40
3:A:632:ILE:CG2	3:A:656:ILE:HG21	2.51	0.40
3:A:852:LEU:O	3:A:855:LEU:HG	2.21	0.40
3:A:1048:VAL:HG11	3:A:1226:VAL:HG11	2.03	0.40
3:A:1624:LEU:HD23	3:A:1633:PHE:CG	2.57	0.40
13:j:46:ILE:HG12	13:j:104:VAL:HG13	2.04	0.40
28:C:962:LEU:O	28:C:963:SER:C	2.64	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	
3	A	2182/2413 (90%)	1924 (88%)	217 (10%)	41 (2%)	6	33
4	H	355/465 (76%)	301 (85%)	43 (12%)	11 (3%)	3	26
5	J	719/899 (80%)	643 (89%)	59 (8%)	17 (2%)	4	29
6	D	138/143 (96%)	124 (90%)	9 (6%)	5 (4%)	2	23
7	F	413/494 (84%)	361 (87%)	35 (8%)	17 (4%)	2	20
8	G	316/469 (67%)	274 (87%)	34 (11%)	8 (2%)	4	29
9	B	1776/2163 (82%)	1623 (91%)	132 (7%)	21 (1%)	10	40
11	b	76/196 (39%)	67 (88%)	9 (12%)	0	100	100
11	k	76/196 (39%)	70 (92%)	5 (7%)	1 (1%)	9	38
12	h	78/146 (53%)	73 (94%)	4 (5%)	1 (1%)	9	38
12	l	87/146 (60%)	76 (87%)	9 (10%)	2 (2%)	5	30
13	j	92/110 (84%)	87 (95%)	5 (5%)	0	100	100
13	m	92/110 (84%)	87 (95%)	5 (5%)	0	100	100
14	d	80/101 (79%)	72 (90%)	7 (9%)	1 (1%)	9	38
14	n	80/101 (79%)	73 (91%)	7 (9%)	0	100	100
15	e	71/94 (76%)	65 (92%)	6 (8%)	0	100	100
15	p	71/94 (76%)	64 (90%)	7 (10%)	0	100	100
16	f	70/86 (81%)	64 (91%)	4 (6%)	2 (3%)	3	26
16	q	70/86 (81%)	63 (90%)	7 (10%)	0	100	100
17	g	65/77 (84%)	63 (97%)	2 (3%)	0	100	100
17	r	65/77 (84%)	58 (89%)	7 (11%)	0	100	100
18	E	21/328 (6%)	20 (95%)	1 (5%)	0	100	100
20	K	122/126 (97%)	113 (93%)	7 (6%)	2 (2%)	7	35
21	2	88/95 (93%)	76 (86%)	11 (12%)	1 (1%)	11	42
22	3	75/89 (84%)	71 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	4	70/187 (37%)	65 (93%)	5 (7%)	0	100	100
24	5	71/93 (76%)	66 (93%)	5 (7%)	0	100	100
25	6	72/86 (84%)	67 (93%)	4 (6%)	1 (1%)	9	37
26	7	62/115 (54%)	57 (92%)	5 (8%)	0	100	100
27	8	62/109 (57%)	59 (95%)	3 (5%)	0	100	100
28	C	847/1008 (84%)	734 (87%)	82 (10%)	31 (4%)	2	22
All	All	8462/10902 (78%)	7560 (89%)	740 (9%)	162 (2%)	8	33

All (162) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	247	PRO
3	A	470	LEU
3	A	471	PRO
3	A	597	PHE
3	A	796	ASN
3	A	980	PRO
3	A	1093	LYS
3	A	1176	GLU
3	A	1209	LYS
3	A	1562	PHE
3	A	2042	SER
3	A	2088	ILE
3	A	2330	GLU
4	H	360	ASN
4	H	361	GLY
4	H	362	TYR
5	J	186	SER
5	J	592	HIS
6	D	54	ARG
7	F	59	LEU
7	F	148	ASN
7	F	407	GLU
8	G	194	GLU
8	G	277	MET
9	B	388	GLN
9	B	392	ARG
9	B	393	GLU
9	B	424	PRO
9	B	448	LEU

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Mol	Chain	Res	Type
9	B	843	HIS
9	B	1264	VAL
9	B	1483	VAL
20	K	65	LEU
28	C	164	MET
28	C	367	VAL
28	C	598	ILE
3	A	495	ARG
3	A	921	ASP
3	A	961	GLN
3	A	1102	GLY
3	A	1159	ARG
3	A	1604	ARG
3	A	2068	ASN
4	H	216	SER
4	H	240	ASP
5	J	200	ALA
5	J	479	GLU
5	J	683	ASN
6	D	127	ASN
7	F	58	ALA
7	F	79	ASP
7	F	146	ASN
7	F	353	THR
7	F	363	PRO
7	F	370	ARG
7	F	435	ALA
8	G	462	HIS
11	k	81	VAL
12	l	78	ASN
16	f	32	LYS
21	2	55	GLY
28	C	175	LEU
28	C	269	LYS
28	C	361	THR
28	C	568	SER
28	C	830	ASN
28	C	963	SER
3	A	360	GLU
3	A	598	ASN
3	A	802	PRO
3	A	839	HIS

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Mol	Chain	Res	Type
3	A	1386	ALA
3	A	1530	SER
3	A	1743	TYR
3	A	2321	ILE
5	J	237	ASP
5	J	633	GLU
5	J	867	GLU
7	F	365	LYS
9	B	875	ALA
9	B	1301	GLU
28	C	220	ASN
28	C	432	GLN
28	C	446	PHE
28	C	535	PRO
28	C	600	GLU
28	C	884	ARG
3	A	262	ASP
3	A	539	PRO
3	A	615	LEU
3	A	703	PHE
3	A	1205	LYS
4	H	346	ALA
4	H	377	ASP
4	H	394	ASN
5	J	206	ASP
5	J	287	SER
5	J	840	ASP
6	D	97	THR
6	D	101	ASN
7	F	74	LEU
7	F	165	ALA
8	G	266	PRO
8	G	288	THR
9	B	411	SER
9	B	1422	GLY
9	B	1586	PRO
9	B	1637	VAL
12	h	10	LEU
25	6	57	GLU
28	C	162	PRO
28	C	180	ASN
28	C	371	PRO

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Mol	Chain	Res	Type
28	C	464	PRO
28	C	573	LYS
28	C	597	TYR
28	C	923	ASN
3	A	199	ILE
3	A	260	PRO
3	A	644	VAL
3	A	1165	LEU
3	A	1347	ARG
3	A	2089	LYS
4	H	231	ASN
5	J	202	SER
5	J	241	PRO
5	J	258	SER
6	D	78	ASP
9	B	389	TYR
9	B	791	PRO
9	B	958	PRO
20	K	82	PRO
28	C	369	LYS
28	C	428	ILE
28	C	770	ASN
28	C	886	SER
28	C	949	ALA
5	J	887	THR
7	F	392	GLU
8	G	374	ASP
9	B	1482	GLY
28	C	807	PRO
28	C	951	ILE
3	A	979	SER
4	H	435	GLY
8	G	263	GLY
8	G	268	PRO
9	B	1327	ILE
5	J	558	PRO
7	F	132	PRO
7	F	347	ALA
14	d	82	PRO
5	J	399	PRO
16	f	15	PRO
28	C	547	GLY

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Mol	Chain	Res	Type
28	C	829	VAL
4	H	253	GLY
7	F	89	ILE
9	B	425	PRO
9	B	1062	PRO
3	A	509	HIS
12	l	98	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	1918/2182 (88%)	1827 (95%)	91 (5%)	23	48
4	H	305/410 (74%)	287 (94%)	18 (6%)	18	44
5	J	627/813 (77%)	594 (95%)	33 (5%)	20	46
6	D	129/132 (98%)	118 (92%)	11 (8%)	10	35
7	F	346/445 (78%)	303 (88%)	43 (12%)	4	22
8	G	289/436 (66%)	277 (96%)	12 (4%)	26	51
9	B	1592/1955 (81%)	1531 (96%)	61 (4%)	29	53
11	b	70/176 (40%)	70 (100%)	0	100	100
11	k	70/176 (40%)	68 (97%)	2 (3%)	37	57
12	h	77/129 (60%)	75 (97%)	2 (3%)	40	60
12	l	85/129 (66%)	81 (95%)	4 (5%)	23	48
13	j	79/103 (77%)	74 (94%)	5 (6%)	16	43
13	m	78/103 (76%)	75 (96%)	3 (4%)	29	53
14	d	69/89 (78%)	67 (97%)	2 (3%)	37	57
14	n	69/89 (78%)	66 (96%)	3 (4%)	26	50
15	e	65/83 (78%)	60 (92%)	5 (8%)	12	38
15	p	65/83 (78%)	61 (94%)	4 (6%)	16	44
16	f	63/77 (82%)	62 (98%)	1 (2%)	55	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	q	63/77 (82%)	61 (97%)	2 (3%)	34	56
17	g	58/66 (88%)	57 (98%)	1 (2%)	53	67
17	r	57/66 (86%)	55 (96%)	2 (4%)	32	54
18	E	20/20 (100%)	19 (95%)	1 (5%)	22	48
20	K	102/104 (98%)	91 (89%)	11 (11%)	6	27
21	2	85/91 (93%)	76 (89%)	9 (11%)	6	27
22	3	71/81 (88%)	69 (97%)	2 (3%)	38	58
23	4	64/172 (37%)	64 (100%)	0	100	100
24	5	66/84 (79%)	66 (100%)	0	100	100
25	6	66/75 (88%)	66 (100%)	0	100	100
26	7	56/103 (54%)	54 (96%)	2 (4%)	31	54
27	8	56/99 (57%)	55 (98%)	1 (2%)	51	67
28	C	673/910 (74%)	617 (92%)	56 (8%)	10	35
All	All	7433/9558 (78%)	7046 (95%)	387 (5%)	22	47

All (387) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	124	ARG
3	A	129	THR
3	A	175	LEU
3	A	205	THR
3	A	210	GLU
3	A	228	LYS
3	A	229	ARG
3	A	249	LEU
3	A	254	HIS
3	A	276	VAL
3	A	282	ASP
3	A	284	ARG
3	A	287	GLU
3	A	288	GLU
3	A	331	PHE
3	A	340	LYS
3	A	351	LYS
3	A	355	LEU
3	A	365	ASN

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Mol	Chain	Res	Type
3	A	402	TRP
3	A	405	ASN
3	A	493	MET
3	A	523	GLN
3	A	526	LEU
3	A	571	LEU
3	A	615	LEU
3	A	622	MET
3	A	631	LEU
3	A	660	ILE
3	A	666	ILE
3	A	690	LYS
3	A	701	CYS
3	A	721	LEU
3	A	753	TYR
3	A	760	ASN
3	A	812	ILE
3	A	848	ASN
3	A	855	LEU
3	A	909	THR
3	A	913	VAL
3	A	937	LEU
3	A	950	THR
3	A	965	LYS
3	A	971	MET
3	A	972	MET
3	A	979	SER
3	A	1004	ASP
3	A	1024	LEU
3	A	1049	LEU
3	A	1099	ASN
3	A	1121	ILE
3	A	1210	ASP
3	A	1222	LEU
3	A	1230	ILE
3	A	1239	THR
3	A	1267	VAL
3	A	1276	GLU
3	A	1277	GLU
3	A	1331	VAL
3	A	1337	THR
3	A	1339	LEU

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Mol	Chain	Res	Type
3	A	1358	ASP
3	A	1373	LEU
3	A	1510	ILE
3	A	1512	ARG
3	A	1603	ASN
3	A	1624	LEU
3	A	1668	ILE
3	A	1682	THR
3	A	1690	LYS
3	A	1691	SER
3	A	1737	GLN
3	A	1742	ASP
3	A	1769	SER
3	A	1773	VAL
3	A	1777	ILE
3	A	1819	ILE
3	A	1825	ILE
3	A	1907	GLN
3	A	1979	MET
3	A	2048	TRP
3	A	2053	SER
3	A	2088	ILE
3	A	2162	LEU
3	A	2176	PHE
3	A	2264	GLU
3	A	2306	ASN
3	A	2325	LEU
3	A	2329	PHE
3	A	2340	LEU
3	A	2355	ASN
4	H	111	THR
4	H	146	PHE
4	H	199	LEU
4	H	220	LYS
4	H	225	ASP
4	H	232	ASN
4	H	242	LEU
4	H	243	ILE
4	H	280	ILE
4	H	300	LEU
4	H	302	LEU
4	H	322	VAL

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Mol	Chain	Res	Type
4	H	331	SER
4	H	336	ILE
4	H	349	SER
4	H	389	ILE
4	H	423	SER
4	H	454	SER
5	J	159	LEU
5	J	194	PRO
5	J	209	ASN
5	J	239	THR
5	J	255	ARG
5	J	270	GLU
5	J	291	TYR
5	J	317	GLU
5	J	338	GLU
5	J	347	PHE
5	J	378	LEU
5	J	421	LEU
5	J	459	LEU
5	J	460	THR
5	J	465	VAL
5	J	498	GLN
5	J	508	TRP
5	J	532	LEU
5	J	613	LEU
5	J	630	SER
5	J	644	ARG
5	J	648	LEU
5	J	657	ASN
5	J	661	LEU
5	J	708	LEU
5	J	733	ASN
5	J	743	LYS
5	J	767	PHE
5	J	788	SER
5	J	809	LEU
5	J	825	LEU
5	J	832	LEU
5	J	874	TRP
6	D	14	HIS
6	D	38	GLN
6	D	39	CYS

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Mol	Chain	Res	Type
6	D	41	ILE
6	D	43	ASP
6	D	49	ILE
6	D	76	LEU
6	D	80	MET
6	D	107	VAL
6	D	119	THR
6	D	139	HIS
7	F	57	LEU
7	F	59	LEU
7	F	63	ASP
7	F	67	LEU
7	F	74	LEU
7	F	77	ILE
7	F	81	LYS
7	F	82	ARG
7	F	84	LEU
7	F	85	GLN
7	F	111	LEU
7	F	116	LEU
7	F	117	ILE
7	F	119	LEU
7	F	120	TYR
7	F	130	LEU
7	F	142	SER
7	F	144	LEU
7	F	153	GLU
7	F	156	GLU
7	F	210	LEU
7	F	232	LEU
7	F	254	ILE
7	F	276	GLU
7	F	280	ARG
7	F	288	SER
7	F	304	ARG
7	F	305	MET
7	F	307	CYS
7	F	332	LYS
7	F	337	LEU
7	F	364	LYS
7	F	371	LYS
7	F	376	LYS

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Mol	Chain	Res	Type
7	F	384	VAL
7	F	388	GLN
7	F	392	GLU
7	F	397	GLU
7	F	401	LEU
7	F	404	TYR
7	F	407	GLU
7	F	412	MET
7	F	454	GLU
8	G	189	THR
8	G	244	LEU
8	G	278	MET
8	G	285	GLN
8	G	329	MET
8	G	332	GLU
8	G	341	VAL
8	G	343	GLN
8	G	395	LEU
8	G	408	LEU
8	G	427	THR
8	G	443	LYS
9	B	390	LYS
9	B	403	SER
9	B	440	LEU
9	B	456	VAL
9	B	457	LYS
9	B	463	ILE
9	B	505	LYS
9	B	511	PHE
9	B	566	LEU
9	B	614	ILE
9	B	645	PRO
9	B	748	LYS
9	B	778	LYS
9	B	782	LYS
9	B	793	LEU
9	B	836	TRP
9	B	870	GLN
9	B	872	LEU
9	B	901	VAL
9	B	902	LEU
9	B	928	ASN

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Mol	Chain	Res	Type
9	B	942	THR
9	B	944	LEU
9	B	956	LYS
9	B	1015	MET
9	B	1016	ASP
9	B	1039	GLU
9	B	1049	GLU
9	B	1054	LEU
9	B	1065	ILE
9	B	1077	ASN
9	B	1086	GLN
9	B	1088	LYS
9	B	1131	LEU
9	B	1137	THR
9	B	1139	MET
9	B	1160	LEU
9	B	1198	ARG
9	B	1220	ILE
9	B	1240	LEU
9	B	1280	ASN
9	B	1284	LEU
9	B	1408	LEU
9	B	1453	GLU
9	B	1483	VAL
9	B	1491	LEU
9	B	1515	LEU
9	B	1519	ARG
9	B	1578	ARG
9	B	1610	LEU
9	B	1651	ILE
9	B	1687	LEU
9	B	1689	ASP
9	B	1696	MET
9	B	1724	THR
9	B	1743	GLU
9	B	1849	ASN
9	B	1917	THR
9	B	1928	LEU
9	B	1975	THR
9	B	2011	ILE
11	k	78	GLU
11	k	82	LEU

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Mol	Chain	Res	Type
12	l	96	ILE
12	l	97	LEU
12	l	104	ASP
12	l	110	GLN
13	m	41	ARG
13	m	48	LEU
13	m	52	HIS
14	n	20	SER
14	n	43	GLN
14	n	83	LEU
15	p	77	LEU
15	p	79	LYS
15	p	81	LEU
15	p	82	LEU
16	q	34	ASN
16	q	79	LEU
17	r	40	LEU
17	r	71	LEU
18	E	550	GLN
15	e	16	CYS
15	e	18	PHE
15	e	25	THR
15	e	79	LYS
15	e	81	LEU
16	f	79	LEU
17	g	71	LEU
14	d	10	LEU
14	d	20	SER
12	h	20	LYS
12	h	30	GLN
13	j	24	PHE
13	j	48	LEU
13	j	49	ARG
13	j	77	THR
13	j	100	SER
20	K	11	LEU
20	K	21	LEU
20	K	22	ASP
20	K	30	LEU
20	K	33	LEU
20	K	35	LYS
20	K	46	ARG

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Mol	Chain	Res	Type
20	K	73	ASP
20	K	93	VAL
20	K	120	LYS
20	K	125	LEU
21	2	12	ASP
21	2	13	GLN
21	2	32	VAL
21	2	45	CYS
21	2	63	ARG
21	2	66	THR
21	2	68	ARG
21	2	72	LEU
21	2	90	VAL
22	3	26	LEU
22	3	55	GLU
26	7	67	VAL
26	7	85	ASN
27	8	63	LEU
28	C	111	LYS
28	C	113	ILE
28	C	142	LEU
28	C	160	ARG
28	C	170	LEU
28	C	176	ARG
28	C	179	ASP
28	C	183	GLN
28	C	255	GLN
28	C	260	ASN
28	C	264	CYS
28	C	272	ARG
28	C	315	SER
28	C	361	THR
28	C	367	VAL
28	C	400	LEU
28	C	406	VAL
28	C	407	ASN
28	C	418	GLN
28	C	421	LEU
28	C	431	GLN
28	C	458	ILE
28	C	474	LYS
28	C	475	THR

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Mol	Chain	Res	Type
28	C	478	TYR
28	C	534	THR
28	C	537	CYS
28	C	576	THR
28	C	577	LEU
28	C	590	LYS
28	C	605	ILE
28	C	615	LEU
28	C	619	LEU
28	C	625	ILE
28	C	634	ILE
28	C	643	VAL
28	C	655	LEU
28	C	674	LEU
28	C	681	CYS
28	C	707	SER
28	C	723	LEU
28	C	767	SER
28	C	770	ASN
28	C	772	ASN
28	C	784	SER
28	C	791	TYR
28	C	808	LEU
28	C	851	LEU
28	C	883	ARG
28	C	909	ILE
28	C	916	THR
28	C	928	CYS
28	C	933	TRP
28	C	936	ILE
28	C	971	ARG
28	C	988	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	155	ASN
3	A	170	HIS
3	A	216	GLN
3	A	310	ASN
3	A	326	ASN
3	A	344	ASN

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Mol	Chain	Res	Type
3	A	404	ASN
3	A	405	ASN
3	A	472	ASN
3	A	481	HIS
3	A	543	ASN
3	A	558	GLN
3	A	580	ASN
3	A	596	ASN
3	A	620	HIS
3	A	638	GLN
3	A	654	HIS
3	A	692	ASN
3	A	705	GLN
3	A	828	HIS
3	A	848	ASN
3	A	1005	GLN
3	A	1218	GLN
3	A	1254	ASN
3	A	1368	GLN
3	A	1369	ASN
3	A	1531	HIS
3	A	1540	ASN
3	A	1559	HIS
3	A	1677	GLN
3	A	1695	ASN
3	A	1737	GLN
3	A	1831	GLN
3	A	1869	ASN
3	A	1985	GLN
3	A	2018	ASN
3	A	2068	ASN
3	A	2159	ASN
3	A	2168	ASN
3	A	2373	ASN
3	A	2391	HIS
4	H	203	ASN
4	H	306	HIS
4	H	316	GLN
4	H	374	ASN
4	H	385	GLN
4	H	392	HIS
4	H	450	HIS

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Mol	Chain	Res	Type
4	H	465	ASN
5	J	190	GLN
5	J	240	ASN
5	J	281	ASN
5	J	397	GLN
5	J	498	GLN
5	J	537	GLN
5	J	578	GLN
5	J	585	GLN
5	J	673	GLN
5	J	733	ASN
5	J	752	ASN
7	F	136	GLN
7	F	148	ASN
7	F	244	HIS
7	F	270	HIS
7	F	292	GLN
7	F	299	HIS
7	F	320	GLN
7	F	331	HIS
7	F	398	GLN
7	F	414	ASN
7	F	433	ASN
8	G	276	ASN
8	G	308	HIS
8	G	316	HIS
8	G	394	ASN
9	B	570	GLN
9	B	621	ASN
9	B	804	HIS
9	B	903	ASN
9	B	921	ASN
9	B	928	ASN
9	B	1003	ASN
9	B	1019	ASN
9	B	1025	HIS
9	B	1056	GLN
9	B	1086	GLN
9	B	1191	GLN
9	B	1281	GLN
9	B	1349	ASN
9	B	1451	GLN

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Mol	Chain	Res	Type
9	B	1517	ASN
9	B	1534	ASN
9	B	1579	ASN
9	B	1686	ASN
9	B	1693	HIS
9	B	1726	HIS
9	B	1727	ASN
9	B	1747	GLN
9	B	1767	GLN
9	B	1959	ASN
9	B	1968	ASN
9	B	1992	ASN
9	B	1996	GLN
9	B	2037	GLN
9	B	2040	GLN
9	B	2058	ASN
9	B	2069	GLN
9	B	2161	ASN
12	l	110	GLN
12	l	112	GLN
15	p	23	GLN
15	p	86	ASN
16	q	14	ASN
16	q	25	HIS
16	q	34	ASN
15	e	15	ASN
15	e	34	GLN
15	e	86	ASN
16	f	25	HIS
16	f	77	ASN
17	g	18	ASN
17	g	20	ASN
17	g	66	ASN
12	h	86	ASN
13	j	28	HIS
13	j	64	HIS
20	K	45	ASN
20	K	105	ASN
20	K	113	GLN
21	2	13	GLN
22	3	53	ASN
23	4	9	ASN

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Mol	Chain	Res	Type
23	4	82	GLN
24	5	25	GLN
24	5	61	ASN
24	5	77	ASN
28	C	112	ASN
28	C	143	HIS
28	C	180	ASN
28	C	183	GLN
28	C	194	ASN
28	C	218	HIS
28	C	259	ASN
28	C	290	HIS
28	C	403	ASN
28	C	432	GLN
28	C	514	GLN
28	C	623	ASN
28	C	776	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	V	122/160 (76%)	63 (51%)	13 (10%)
19	U	138/214 (64%)	77 (55%)	21 (15%)
2	W	77/112 (68%)	35 (45%)	12 (15%)
All	All	337/486 (69%)	175 (51%)	46 (13%)

All (175) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	V	2	U
1	V	11	A
1	V	15	G
1	V	17	A
1	V	18	A
1	V	19	U
1	V	20	A
1	V	22	G
1	V	25	U
1	V	26	A
1	V	31	U
1	V	32	G

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Mol	Chain	Res	Type
1	V	33	A
1	V	36	A
1	V	37	U
1	V	39	C
1	V	40	G
1	V	41	U
1	V	44	G
1	V	45	A
1	V	46	G
1	V	53	U
1	V	55	U
1	V	56	U
1	V	57	U
1	V	59	C
1	V	64	U
1	V	65	G
1	V	66	A
1	V	67	A
1	V	74	U
1	V	75	U
1	V	78	A
1	V	81	C
1	V	82	C
1	V	83	A
1	V	84	G
1	V	85	A
1	V	86	C
1	V	87	C
1	V	88	G
1	V	89	U
1	V	90	C
1	V	91	U
1	V	94	U
1	V	98	G
1	V	101	C
1	V	102	A
1	V	103	A
1	V	104	U
1	V	129	A
1	V	130	A
1	V	131	G
1	V	132	A

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Mol	Chain	Res	Type
1	V	137	G
1	V	143	A
1	V	144	A
1	V	145	U
1	V	146	U
1	V	147	U
1	V	149	U
1	V	151	G
1	V	152	A
2	W	2	U
2	W	7	G
2	W	8	A
2	W	17	U
2	W	25	C
2	W	26	A
2	W	27	U
2	W	28	U
2	W	29	U
2	W	30	G
2	W	31	G
2	W	32	U
2	W	33	C
2	W	34	A
2	W	38	U
2	W	45	A
2	W	46	U
2	W	47	A
2	W	48	C
2	W	49	A
2	W	50	G
2	W	56	A
2	W	61	C
2	W	63	G
2	W	75	A
2	W	76	A
2	W	83	A
2	W	84	C
2	W	85	C
2	W	86	G
2	W	87	U
2	W	88	U
2	W	109	U

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Mol	Chain	Res	Type
2	W	110	U
2	W	111	U
19	U	12	C
19	U	13	A
19	U	14	G
19	U	15	A
19	U	16	U
19	U	17	C
19	U	18	A
19	U	21	G
19	U	22	G
19	U	23	C
19	U	25	G
19	U	26	A
19	U	27	G
19	U	28	G
19	U	30	A
19	U	32	G
19	U	33	U
19	U	34	C
19	U	35	A
19	U	38	A
19	U	39	U
19	U	40	C
19	U	41	A
19	U	43	G
19	U	44	A
19	U	45	A
19	U	53	C
19	U	65	U
19	U	67	U
19	U	68	A
19	U	69	G
19	U	70	A
19	U	71	A
19	U	72	C
19	U	73	U
19	U	74	U
19	U	75	A
19	U	76	U
19	U	77	A
19	U	78	A

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Mol	Chain	Res	Type
19	U	79	C
19	U	80	G
19	U	81	A
19	U	82	A
19	U	83	C
19	U	84	A
19	U	87	G
19	U	94	C
19	U	95	C
19	U	96	U
19	U	97	U
19	U	101	C
19	U	103	A
19	U	104	G
19	U	108	C
19	U	112	C
19	U	115	G
19	U	119	U
19	U	120	G
19	U	121	U
19	U	122	C
19	U	123	U
19	U	125	C
19	U	126	A
19	U	128	A
19	U	129	G
19	U	130	A
19	U	133	C
19	U	134	A
19	U	135	G
19	U	142	C
19	U	143	U
19	U	167	A
19	U	170	U
19	U	171	U
19	U	172	U
19	U	173	U

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	V	17	A

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Mol	Chain	Res	Type
1	V	19	U
1	V	31	U
1	V	39	C
1	V	44	G
1	V	73	A
1	V	74	U
1	V	83	A
1	V	88	G
1	V	129	A
1	V	143	A
1	V	145	U
1	V	150	G
2	W	16	C
2	W	25	C
2	W	26	A
2	W	27	U
2	W	31	G
2	W	32	U
2	W	45	A
2	W	48	C
2	W	49	A
2	W	55	G
2	W	83	A
2	W	84	C
19	U	25	G
19	U	26	A
19	U	27	G
19	U	32	G
19	U	40	C
19	U	44	A
19	U	68	A
19	U	75	A
19	U	78	A
19	U	80	G
19	U	82	A
19	U	83	C
19	U	95	C
19	U	103	A
19	U	114	G
19	U	124	C
19	U	128	A
19	U	129	G

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Mol	Chain	Res	Type
19	U	132	A
19	U	133	C
19	U	172	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
29	GTP	C	1101	-	33,34,34	1.12	4 (12%)	50,54,54	1.69	7 (14%)

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
29	GTP	C	1101	-	-	4/22/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	1101	GTP	C5-C4	3.00	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	1101	GTP	C5-N7	-2.49	1.34	1.39
29	C	1101	GTP	C6-N1	-2.21	1.34	1.38
29	C	1101	GTP	C4-N9	-2.09	1.32	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	1101	GTP	C5-C4-N3	-5.64	119.41	128.39
29	C	1101	GTP	C2-N3-C4	4.75	120.48	112.30
29	C	1101	GTP	N9-C4-N3	4.40	134.74	125.95
29	C	1101	GTP	C6-C5-N7	3.20	136.11	130.29
29	C	1101	GTP	O6-C6-C5	-2.64	119.57	126.53
29	C	1101	GTP	C4-C5-N7	-2.21	107.17	110.67
29	C	1101	GTP	C5-C6-N1	2.08	118.55	113.25

There are no chirality outliers.

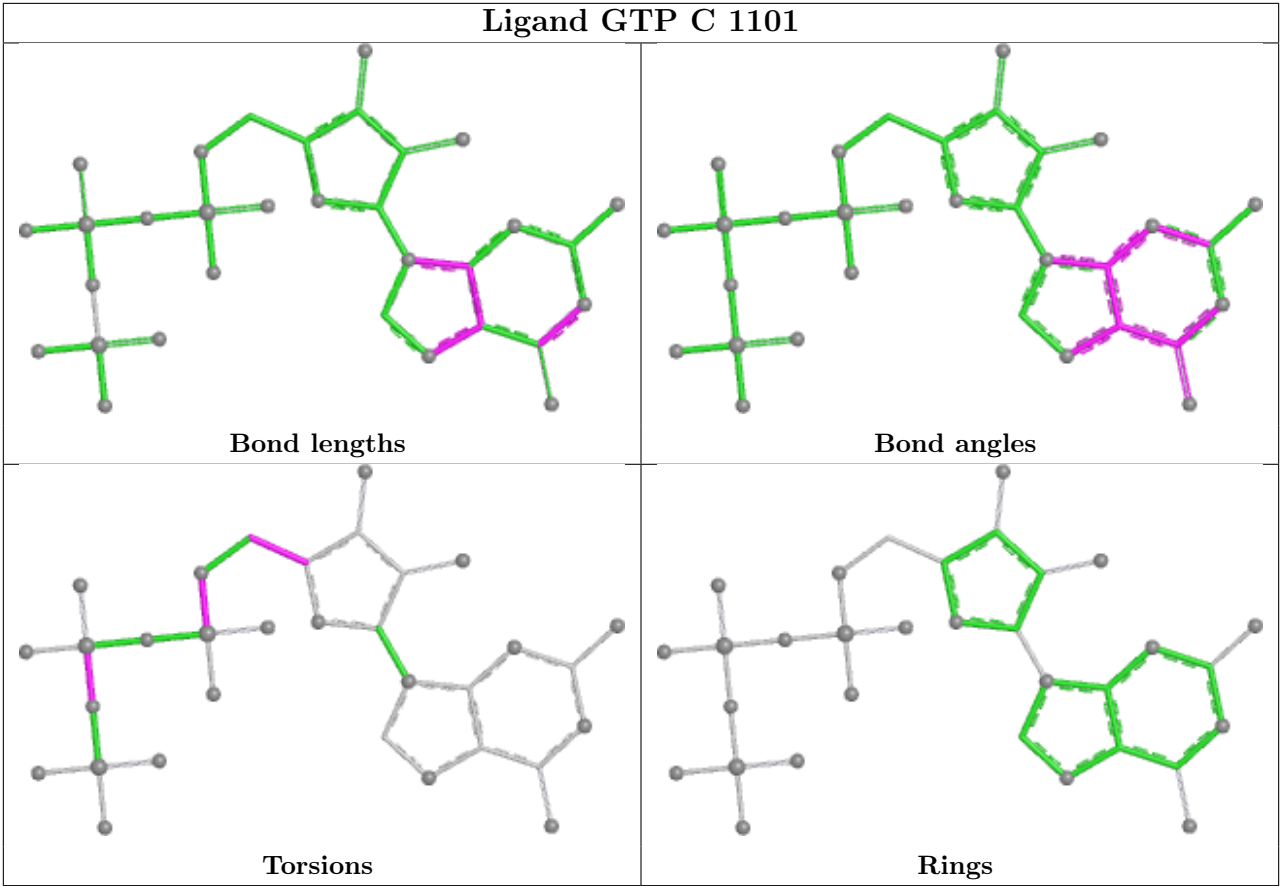
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	C	1101	GTP	C5'-O5'-PA-O1A
29	C	1101	GTP	O4'-C4'-C5'-O5'
29	C	1101	GTP	C3'-C4'-C5'-O5'
29	C	1101	GTP	PG-O3B-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	E	13
10	x	2
3	A	1
19	U	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	120:UNK	C	201:UNK	N	117.38
1	x	62:UNK	C	101:UNK	N	54.41
1	E	132:UNK	C	150:UNK	N	36.51

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	170:UNK	C	180:UNK	N	34.13
1	E	102:UNK	C	120:UNK	N	31.43
1	E	226:UNK	C	240:UNK	N	25.24
1	E	250:UNK	C	270:UNK	N	25.14
1	E	420:UNK	C	487:UNK	N	24.41
1	E	280:UNK	C	310:UNK	N	16.17
1	E	194:UNK	C	210:UNK	N	13.89
1	E	318:UNK	C	330:UNK	N	13.76
1	E	57:UNK	C	70:UNK	N	11.67
1	E	25:UNK	C	40:UNK	N	8.61
1	E	91:UNK	C	96:UNK	N	7.62
1	E	79:UNK	C	82:UNK	N	5.98
1	A	1860:VAL	C	1861:THR	N	4.45
1	U	166:U	O3'	167:A	P	3.43

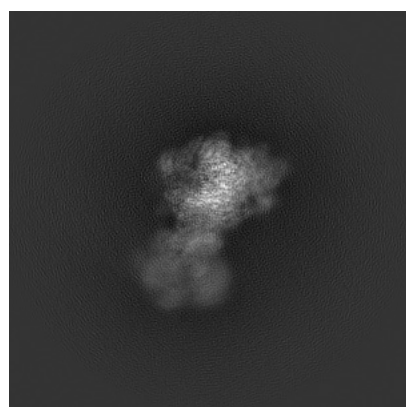
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8012. These allow visual inspection of the internal detail of the map and identification of artifacts.

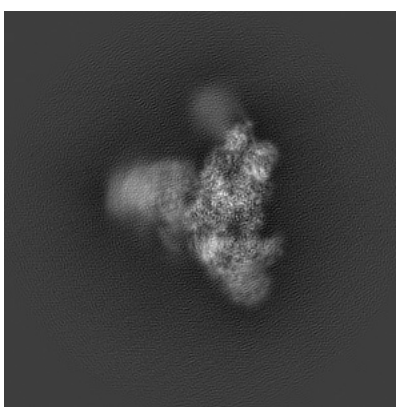
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

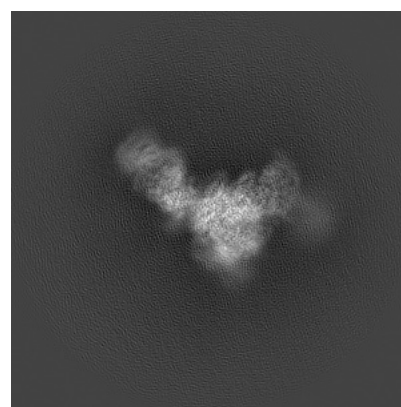
6.1.1 Primary map



X



Y

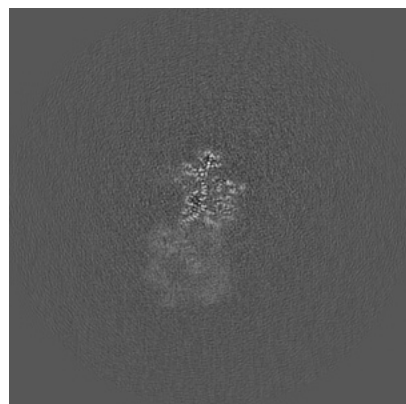


Z

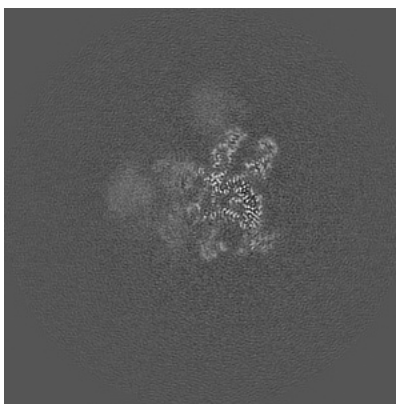
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

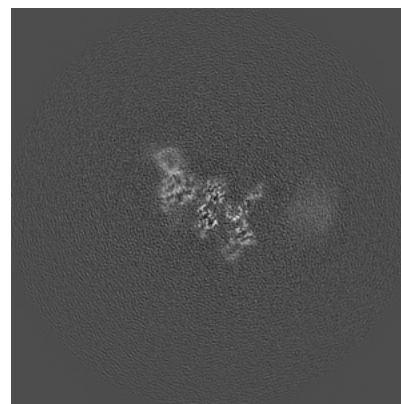
6.2.1 Primary map



X Index: 190



Y Index: 190

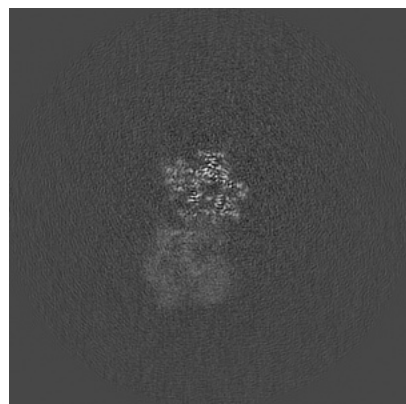


Z Index: 190

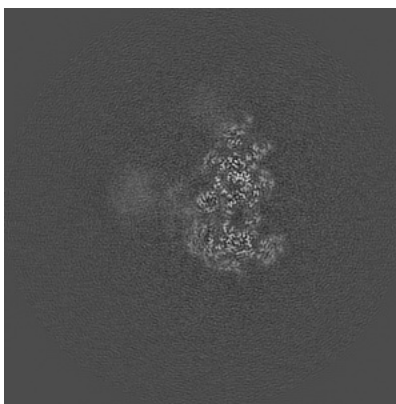
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

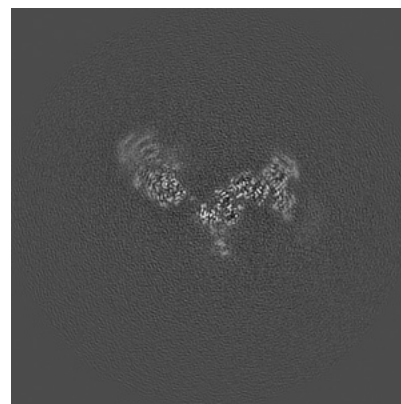
6.3.1 Primary map



X Index: 196



Y Index: 202

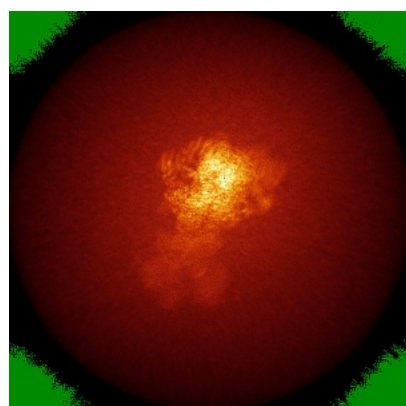


Z Index: 221

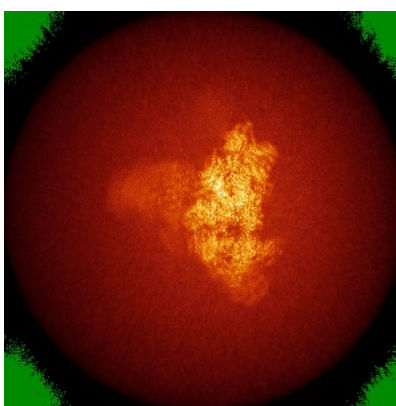
The images above show the largest variance slices of the map in three orthogonal directions.

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

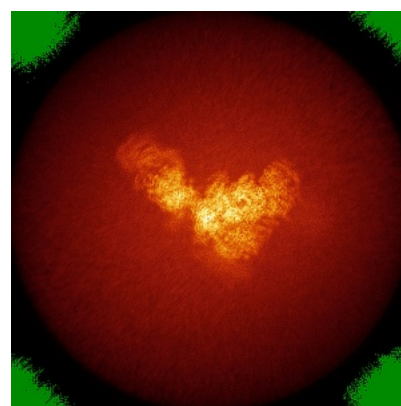
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

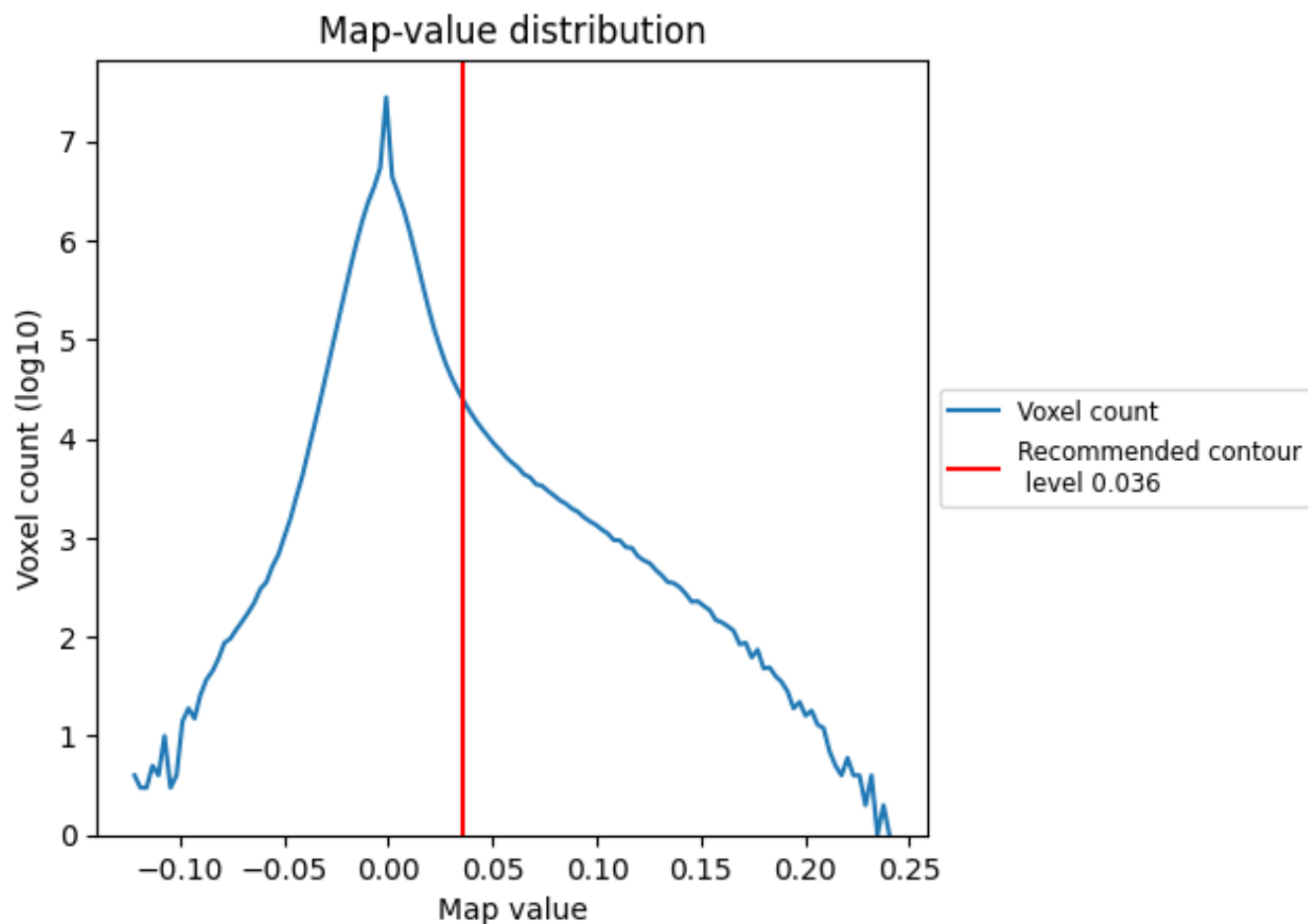
6.6 Mask visualisation

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

7 Map analysis [i](#)

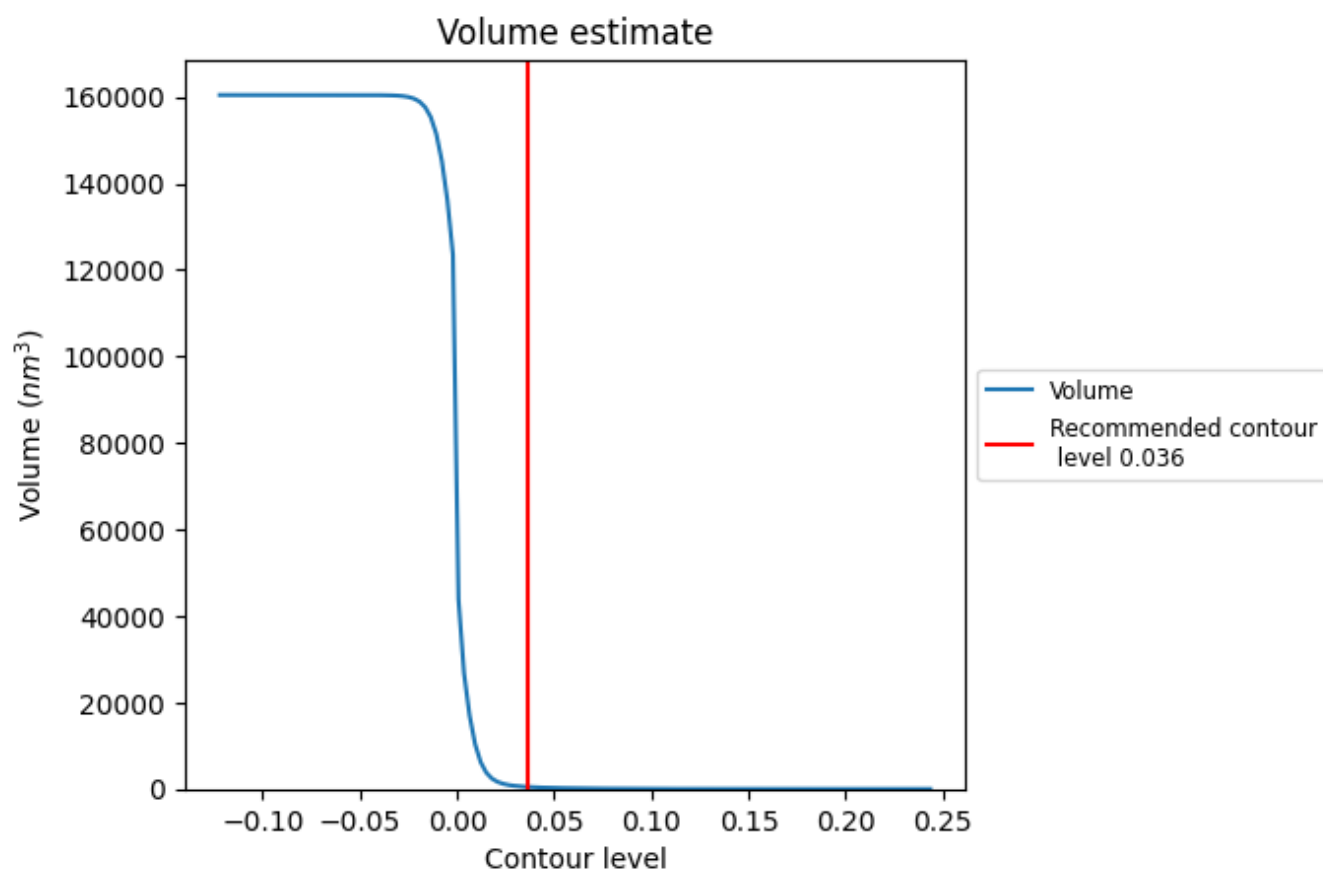
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

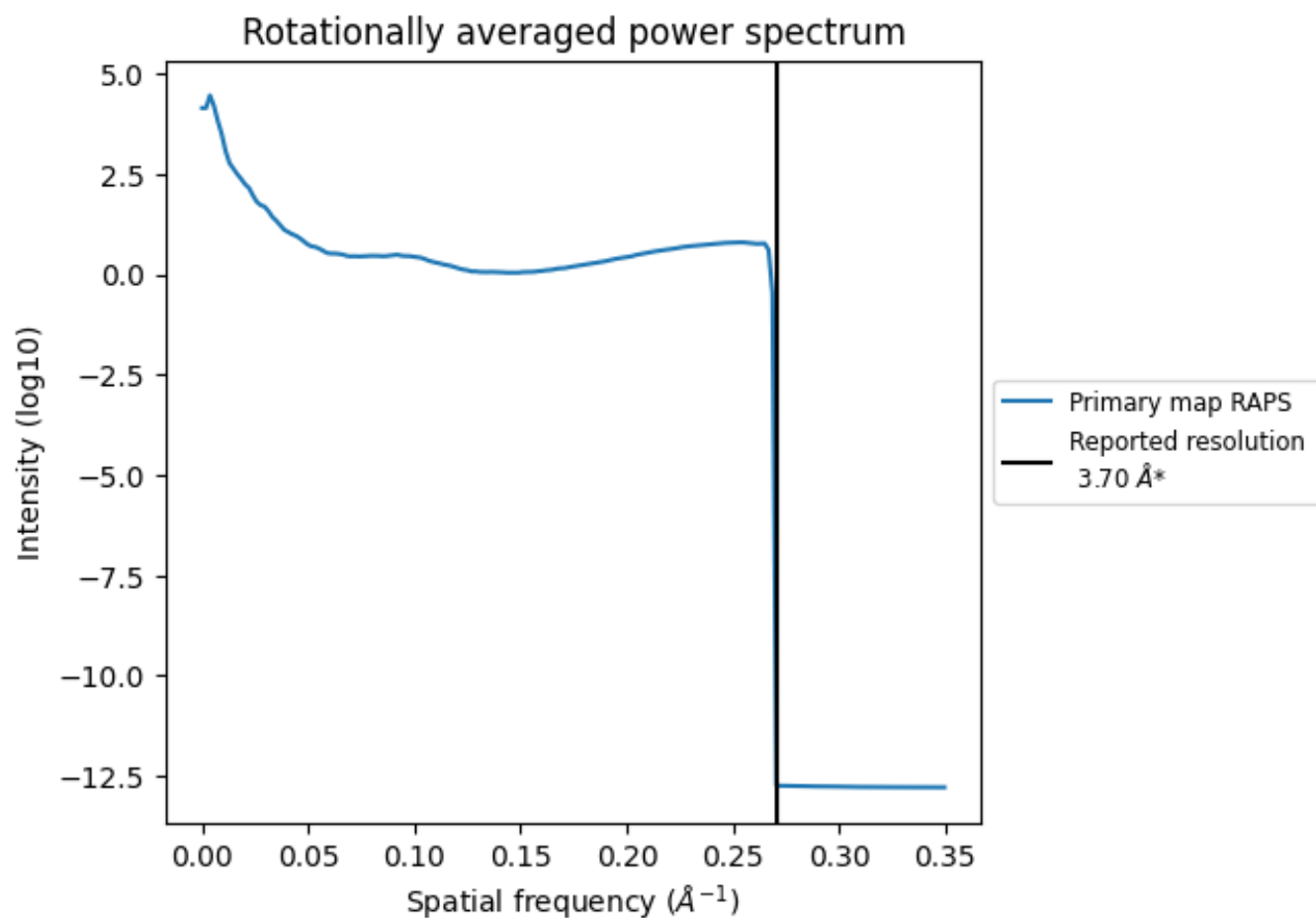
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 478 nm³; this corresponds to an approximate mass of 432 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 ⓘ

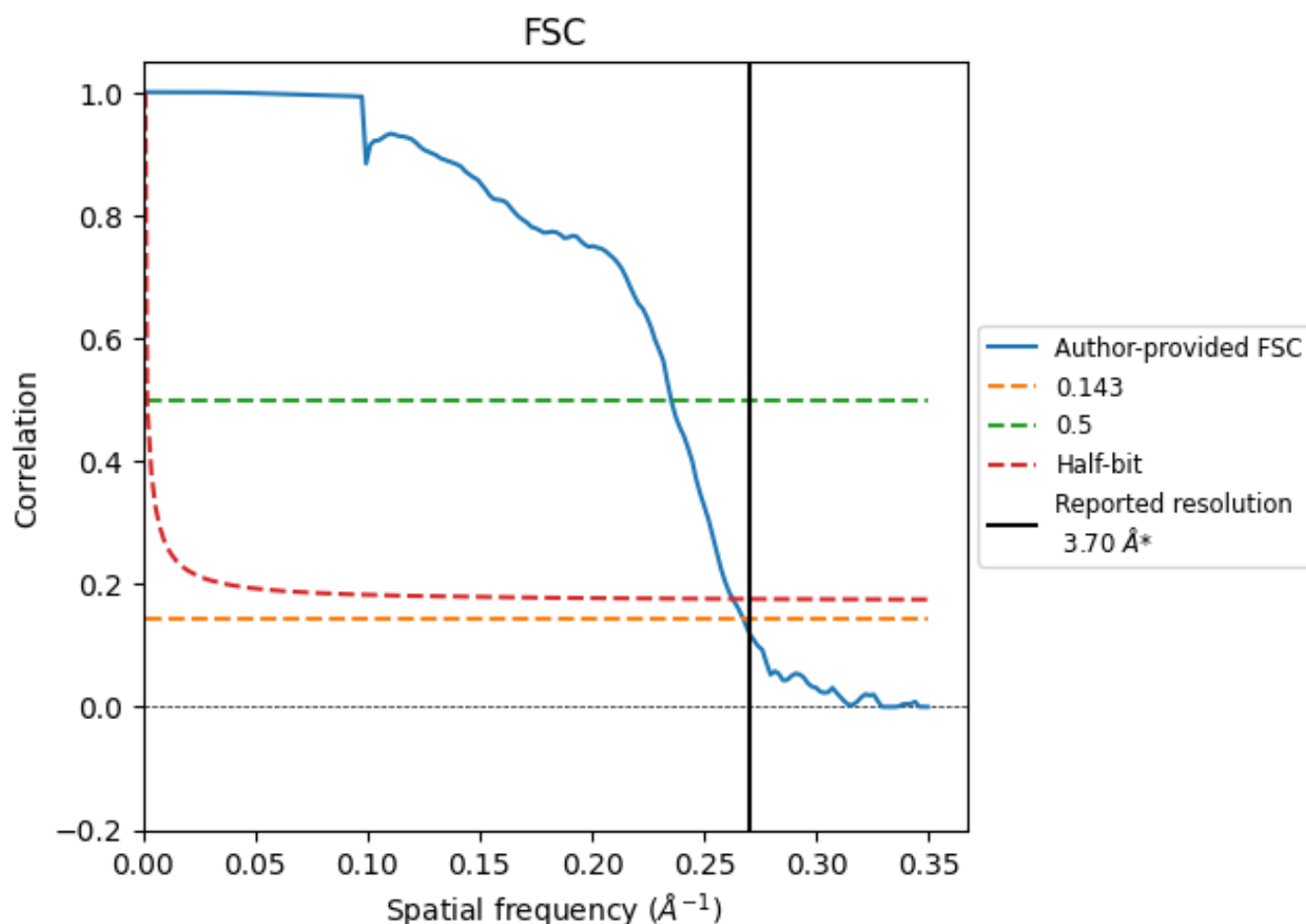


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

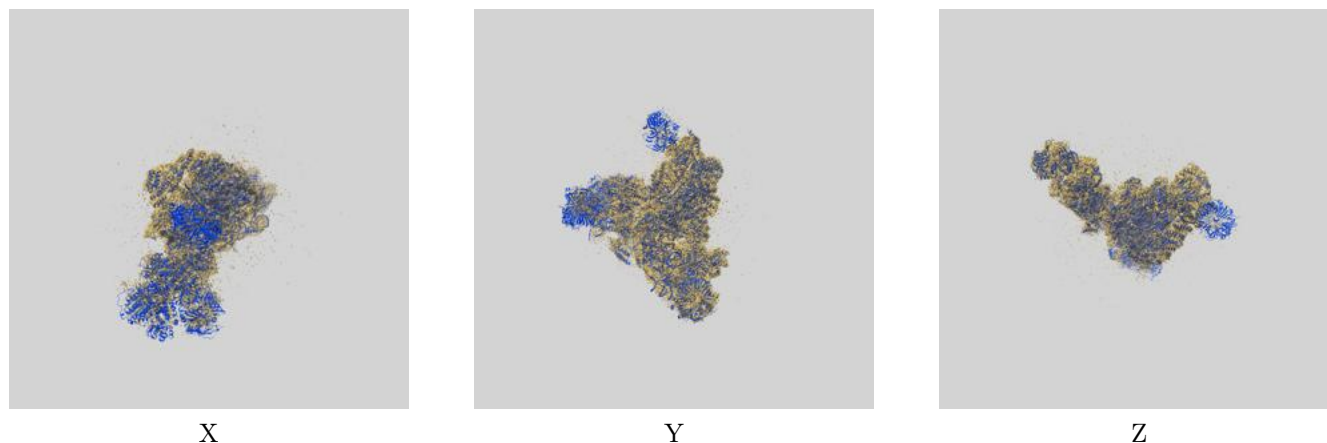
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.74	4.25	3.81
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

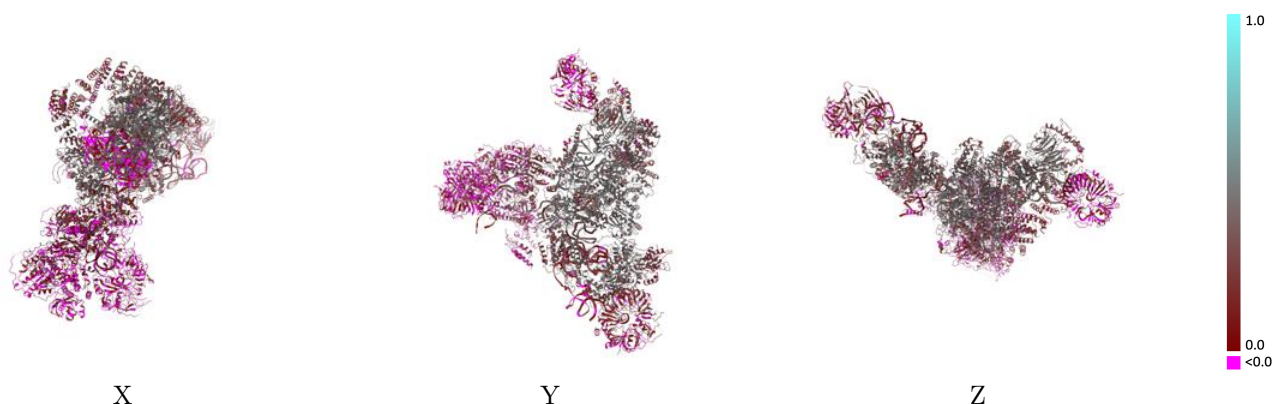
This section contains information regarding the fit between EMDB map EMD-8012 and PDB model 5GAN. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



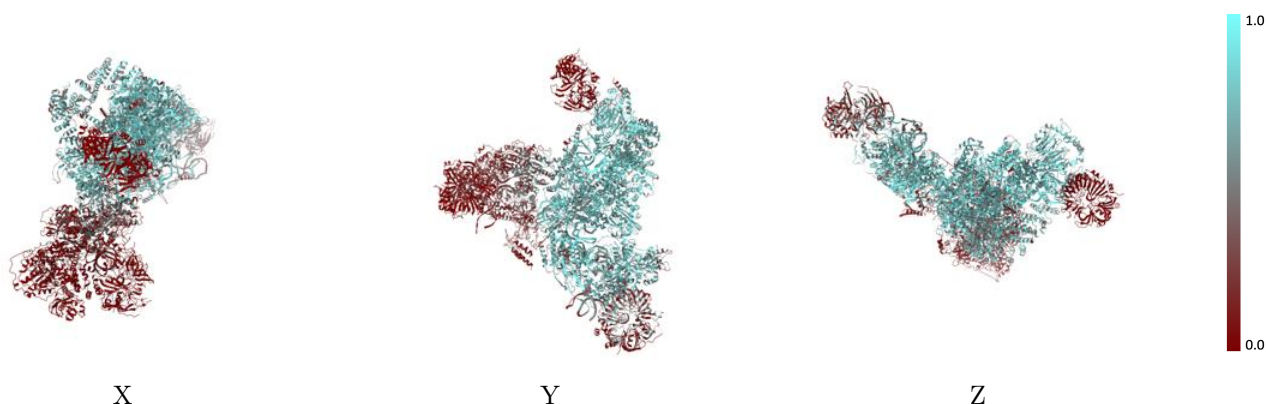
The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



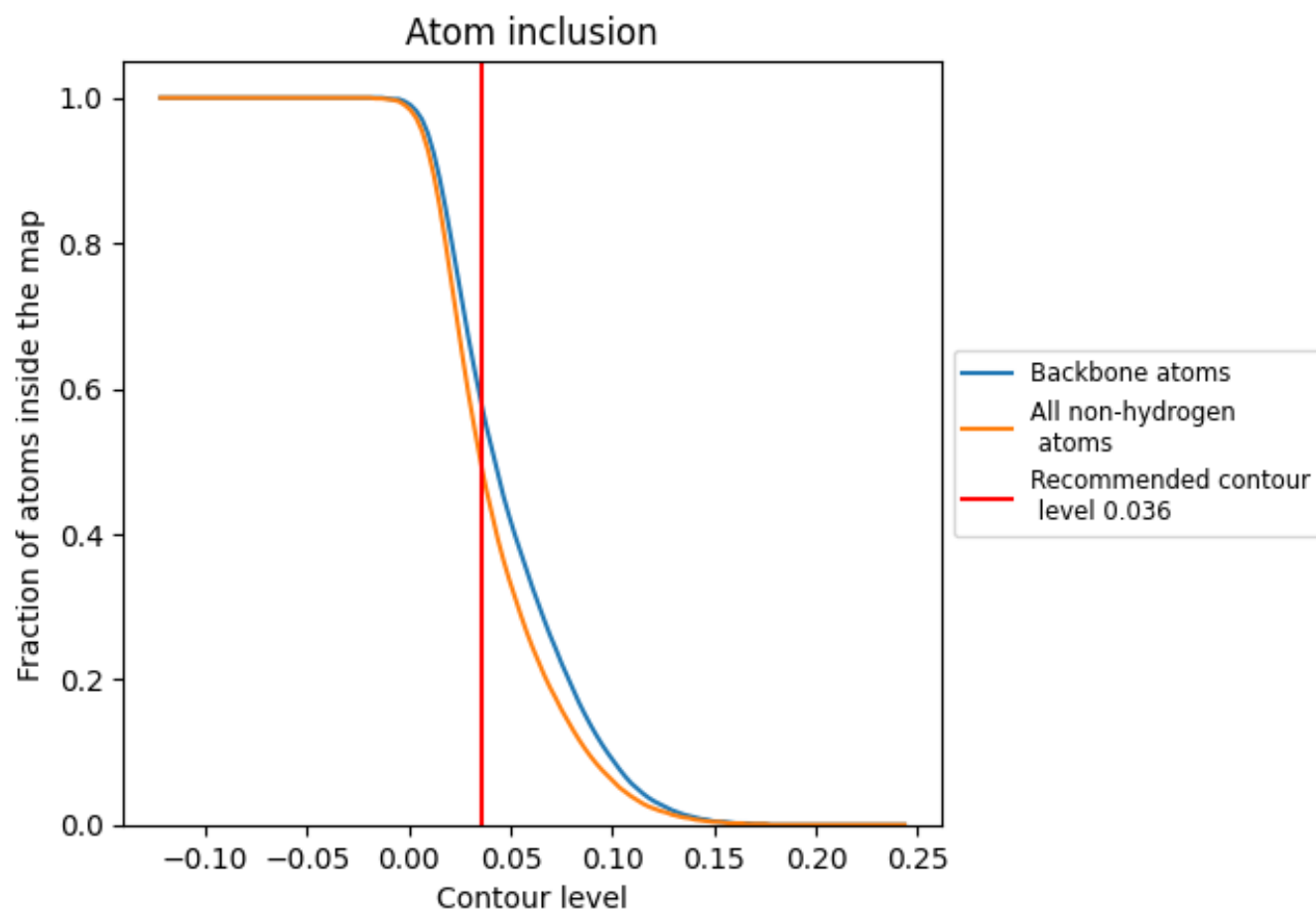
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.036).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4890	 0.2540
2	 0.0220	 0.0760
3	 0.0080	 0.0640
4	 0.0190	 0.0770
5	 0.0000	 0.0550
6	 0.0040	 0.0430
7	 0.0100	 0.0630
8	 0.0100	 0.0410
A	 0.6810	 0.3630
B	 0.1810	 0.1170
C	 0.7240	 0.3730
D	 0.7460	 0.4020
E	 0.0850	 0.0850
F	 0.7670	 0.4080
G	 0.6910	 0.3490
H	 0.7420	 0.3860
J	 0.6790	 0.3010
K	 0.8000	 0.4520
U	 0.6440	 0.2000
V	 0.5710	 0.2740
W	 0.7070	 0.2760
b	 0.3310	 0.1900
d	 0.4320	 0.2390
e	 0.2380	 0.1230
f	 0.2310	 0.0880
g	 0.3300	 0.1810
h	 0.2890	 0.1520
j	 0.2060	 0.1110
k	 0.0310	 0.0540
l	 0.0340	 0.0340
m	 0.0370	 0.0270
n	 0.0100	 0.0140
p	 0.0070	 0.0770
q	 0.0180	 0.0120
r	 0.0080	 0.0270
x	 0.7280	 0.3730

