



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 04:38 PM UTC

PDB ID : 8QPA / pdb_00008qpa
EMDB ID : EMD-18546
Title : Cryo-EM Structure of Pre-B+5'ssLNG Complex (core part)
Authors : Zhang, Z.; Kumar, V.; Dybkov, O.; Will, C.L.; Zhong, J.; Ludwig, S.; Urlaub, H.; Kastner, B.; Stark, H.; Luehrmann, R.
Deposited on : 2023-10-01
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:

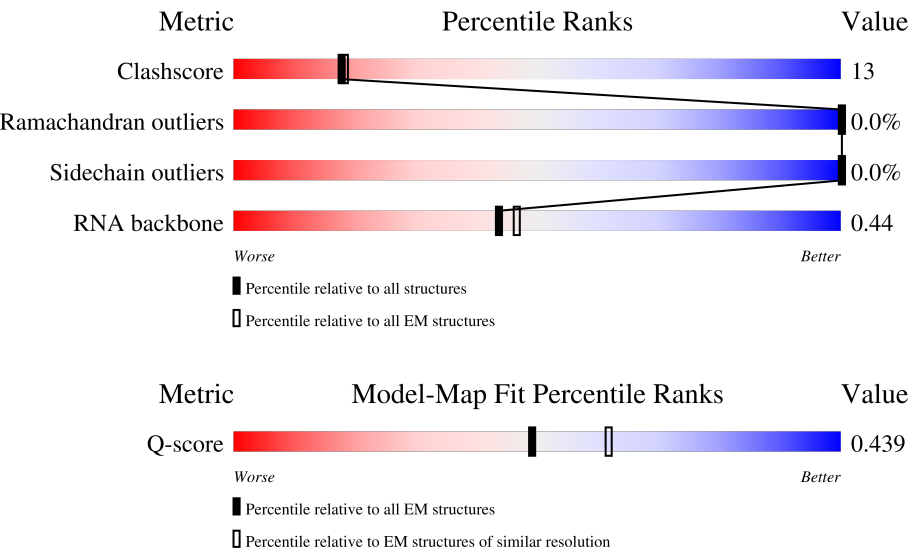
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	2136	99%
2	G	820	85%
3	J	683	88%

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Mol	Chain	Length	Quality of chain
4	L	499	
5	F	522	
6	N	941	
7	A	2335	
8	U	565	
9	S	800	
10	C	972	
11	M	128	
12	D	142	
13	5	117	
14	z	18	
15	7	793	
16	4	144	
17	6	106	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 43455 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	22	Total	C	N	O	S	0	0
			158	97	28	32	1		

- Molecule 2 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	122	Total	C	N	O	S	0	0
			1077	673	205	197	2		

- Molecule 3 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	85	Total	C	N	O	S	0	0
			678	416	139	120	3		

- Molecule 4 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	376	Total	C	N	O	S	0	0
			2874	1788	524	550	12		

- Molecule 5 is a protein called U4/U6 small nuclear ribonucleoprotein Prp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	61	Total	C	N	O	S	0	0
			488	297	97	93	1		

- Molecule 6 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	457	Total	C	N	O	S	0	0
			3095	1902	591	595	7		

- Molecule 7 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1971	Total	C	N	O	S	0	0
			16383	10554	2858	2901	70		

- Molecule 8 is a protein called Ubiquitin carboxyl-terminal hydrolase 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	456	Total	C	N	O	S	0	0
			3749	2427	635	673	14		

- Molecule 9 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	148	Total	C	N	O	S	0	0
			1167	727	216	222	2		

- Molecule 10 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	836	Total	C	N	O	S	0	0
			6592	4211	1110	1238	33		

- Molecule 11 is a protein called NHP2-like protein 1, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	124	Total	C	N	O	S	0	0
			962	608	171	178	5		

- Molecule 12 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	141	Total	C	N	O	S	0	0
			1170	751	194	215	10		

- Molecule 13 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	5	79	Total	C	N	O	P	0	0
			1660	744	275	562	79		

- Molecule 14 is a RNA chain called 5'ss oligo.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	z	18	Total	C	N	O	P	0	0
			384	172	69	125	18		

- Molecule 15 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	7	81	Total	C	N	O	S	0	0
			650	405	115	128	2		

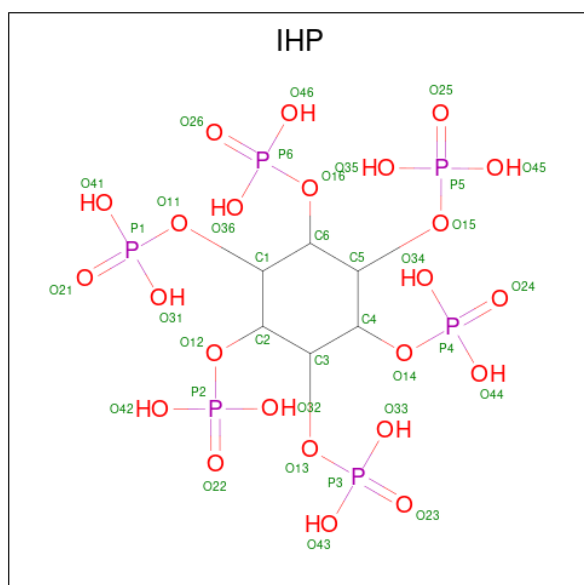
- Molecule 16 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	62	Total	C	N	O	P	0	0
			1322	590	233	437	62		

- Molecule 17 is a RNA chain called U6 snRNA.

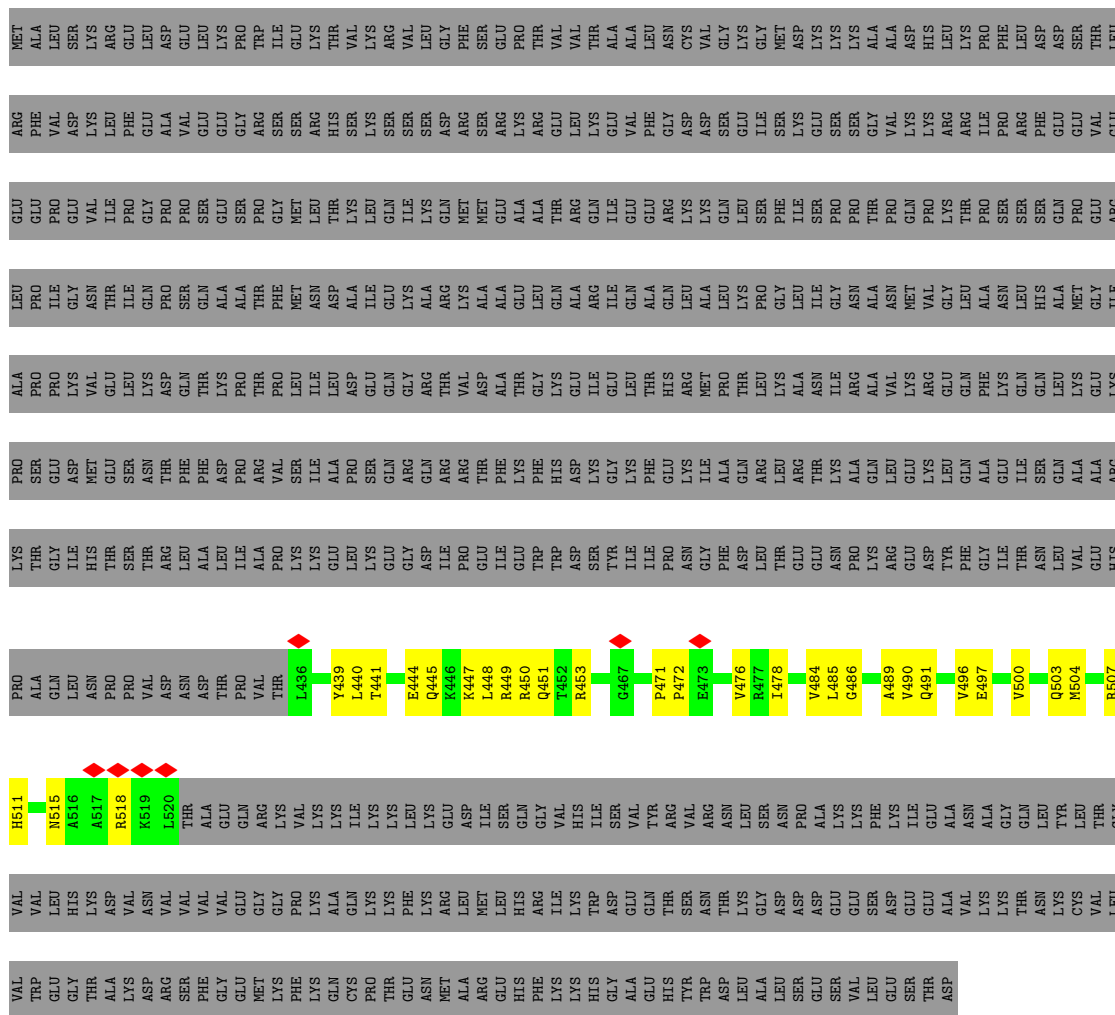
Mol	Chain	Residues	Atoms					AltConf	Trace
17	6	47	Total	C	N	O	P	0	0
			1010	453	194	317	46		

- Molecule 18 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).

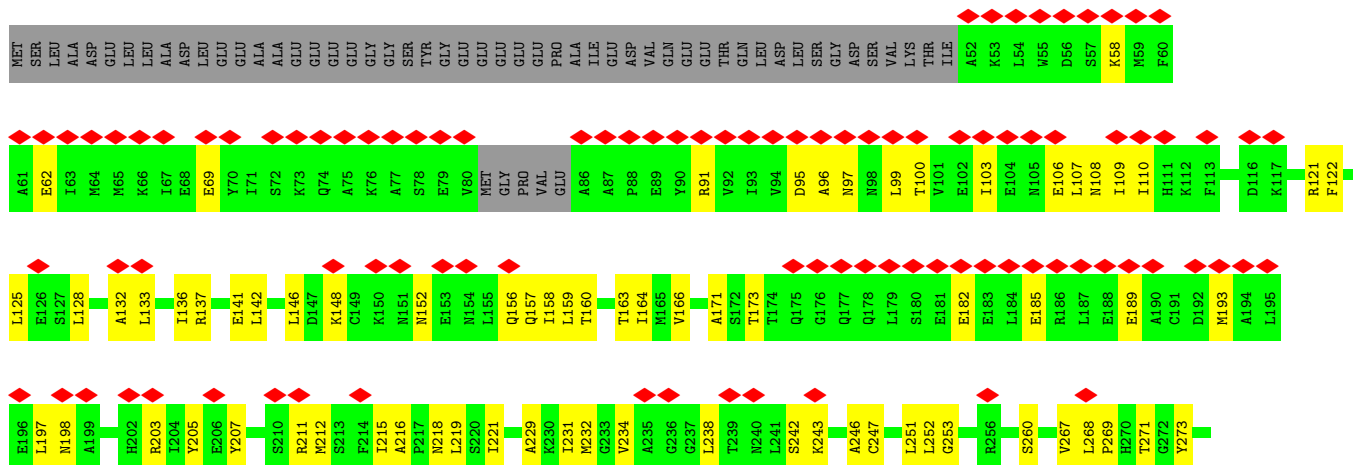


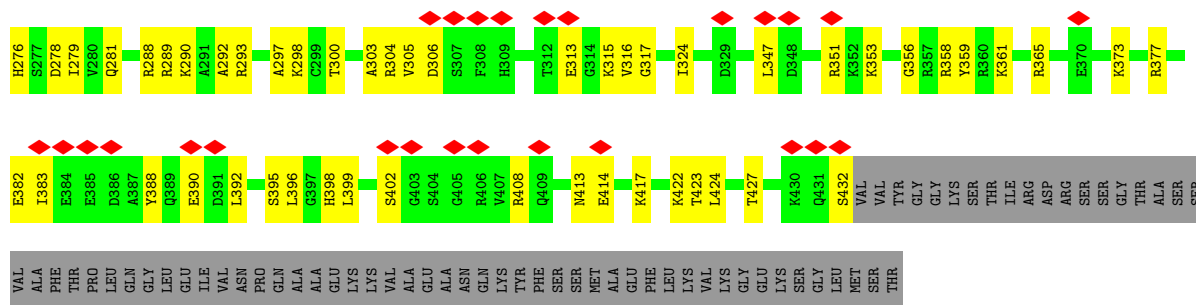
Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			36	6	24	6	



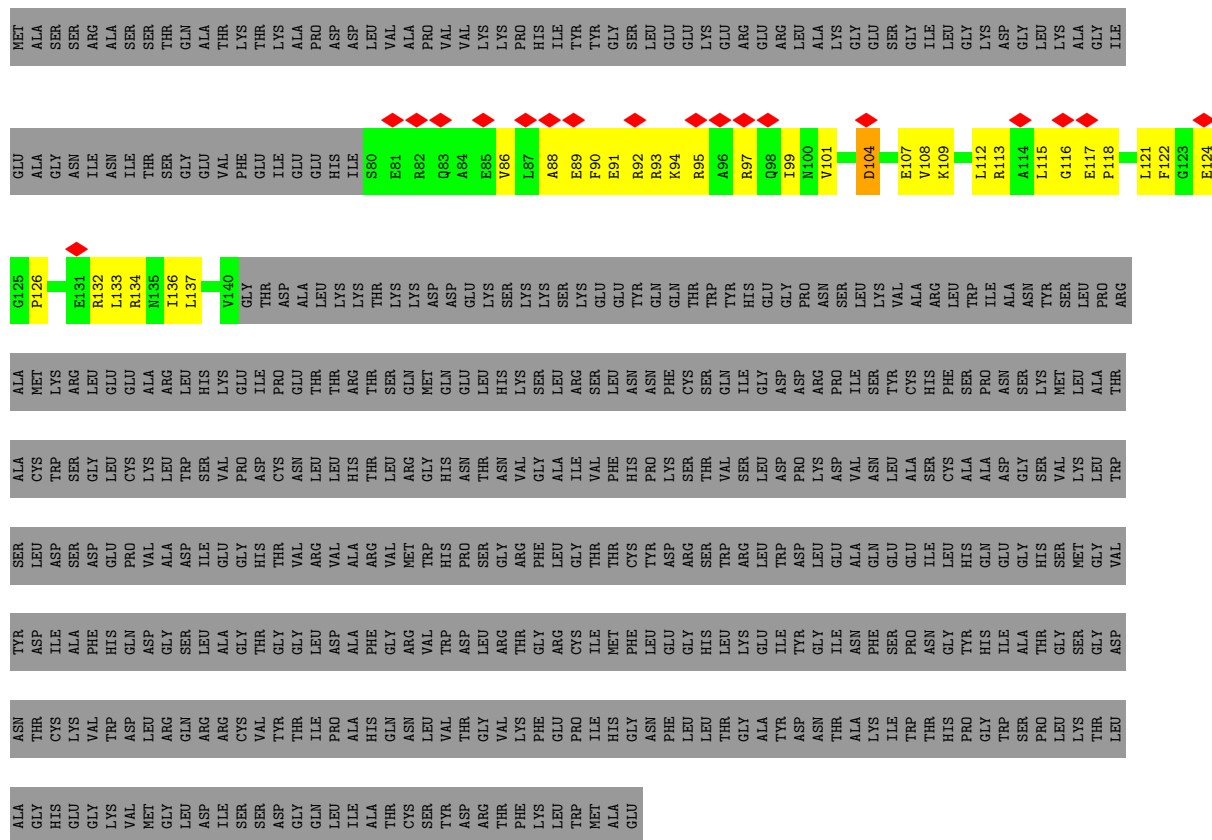


Chain L:

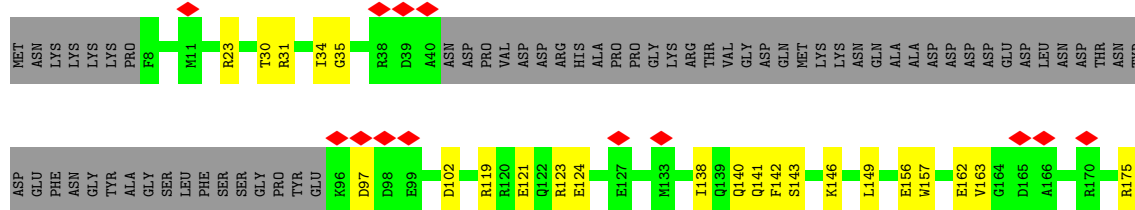
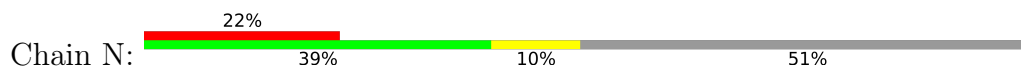




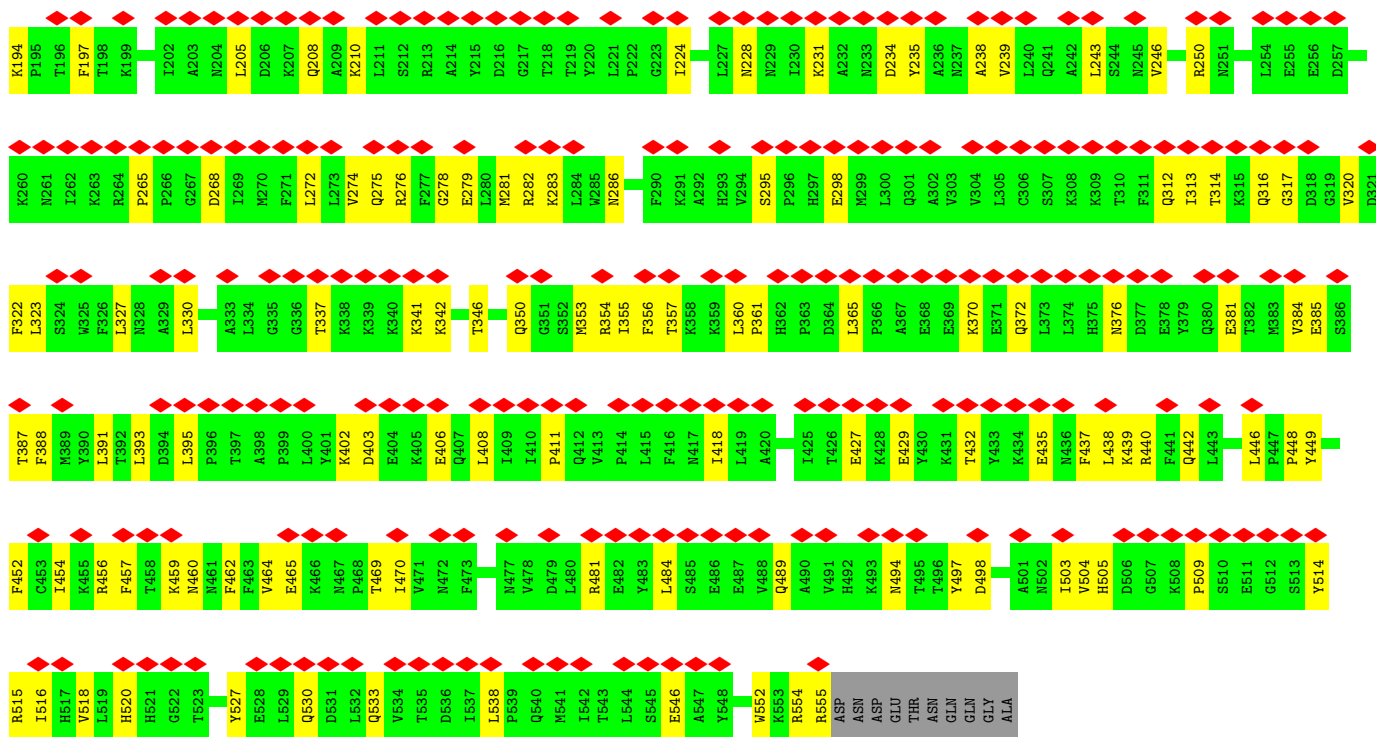
• Molecule 5: U4/U6 small nuclear ribonucleoprotein Prp4



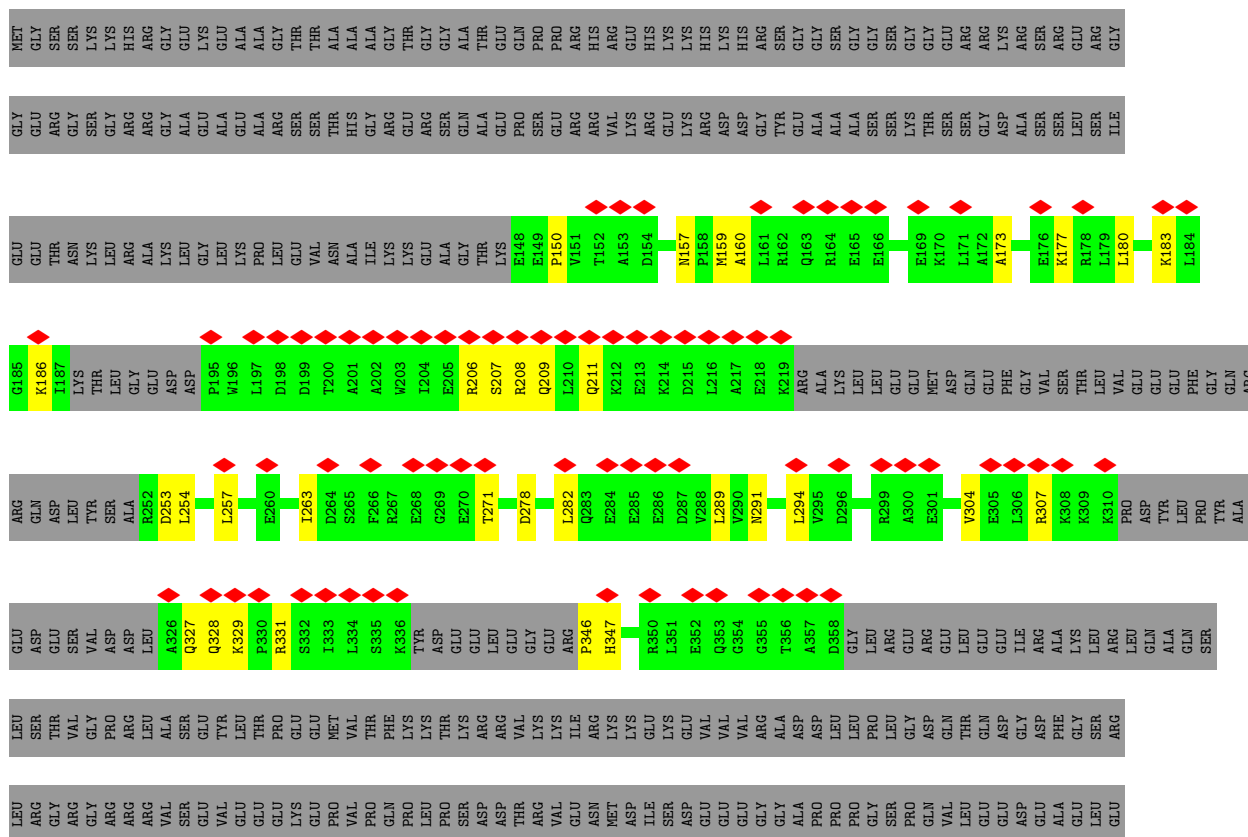
• Molecule 6: Pre-mRNA-processing factor 6



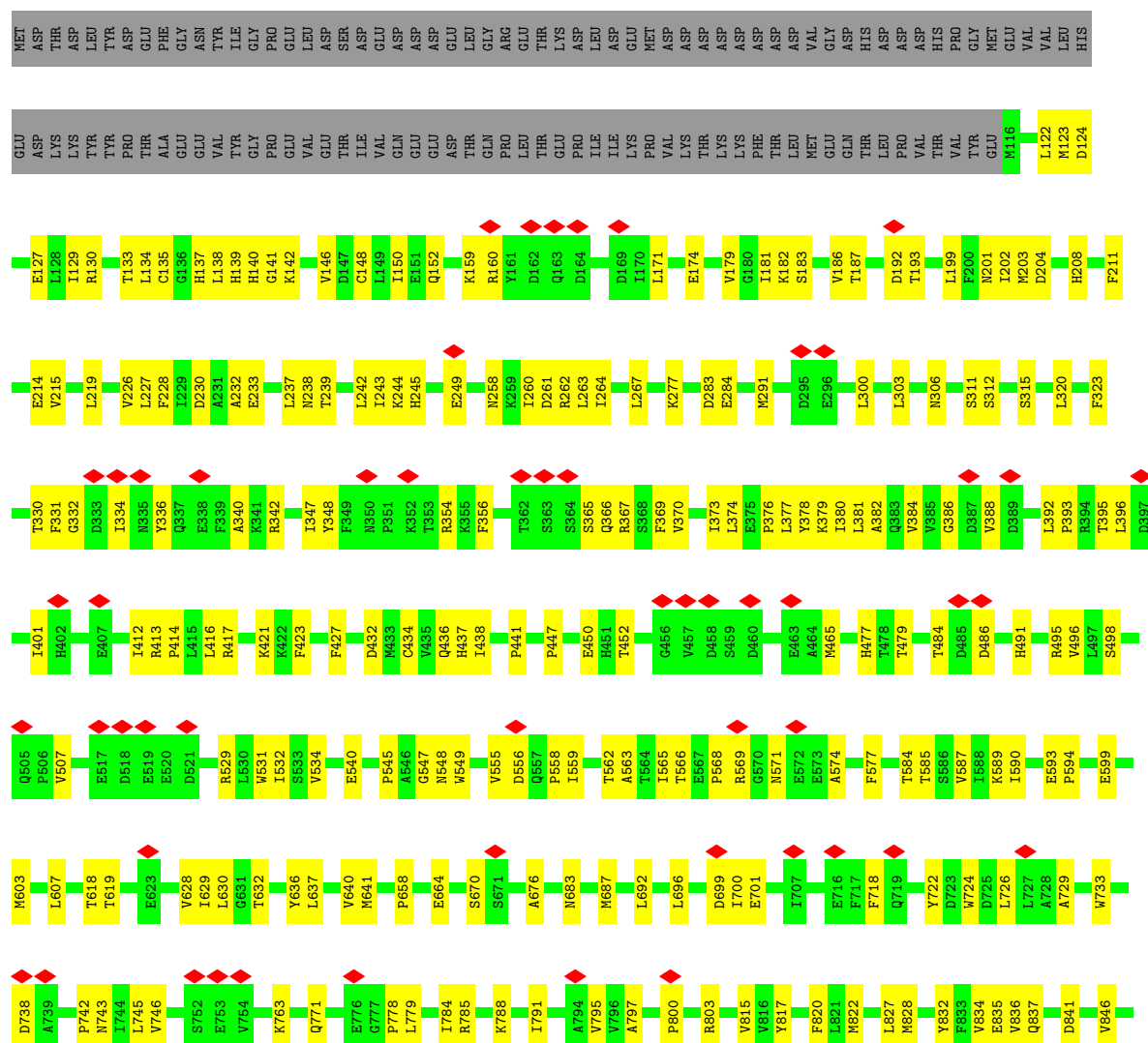
P1417	R1418	Q1424	D1426	R1427	H1428	T1429	R1437	V1438	R1439	F1442	N1451	P1452	W1455	T1456	Q1457	Q1458	R1459	W1465	N1466	N1468	N1469	D1473	V1481	L1485	E1486	H1487	F1490	T1493	Y1494	F1495	W1503	E1504	G1508	F1509	E1510	S1512	M1513	K1514	W1515	K1516	T1519	R153	E154	R155	D157	R158	F161	M164	R165	F166	P167	P168	F169	D170	D171	E172	E173	D180	M181	L182	L183	D184	P187	L193	E194	L195	E198	E199	V203	V206	F207	Q211	R214	N221	G222	S223	Q226	R227	M234	M235	A242	L245	L246	T247	D248																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
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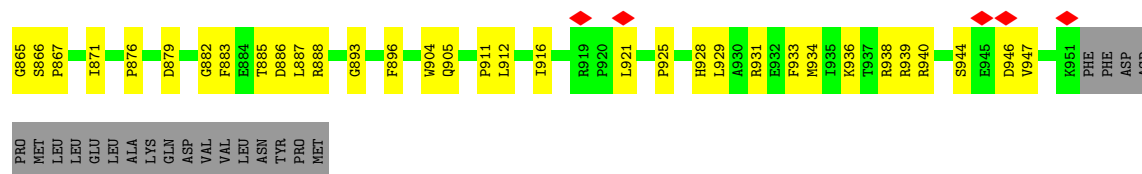


- Molecule 9: U4/U6.U5 tri-snRNP-associated protein 1

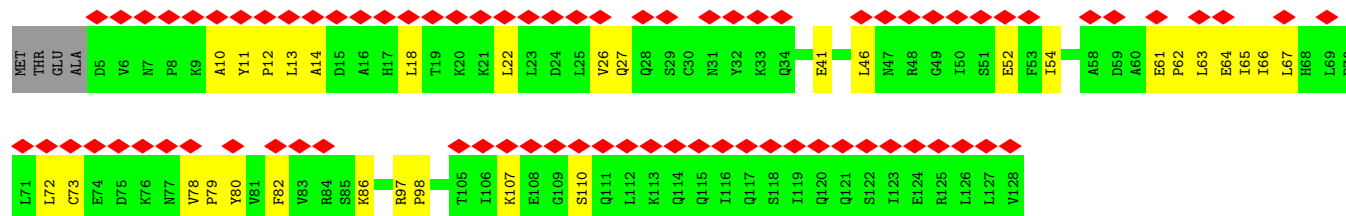


- Molecule 10: 116 kDa U5 small nuclear ribonucleoprotein component

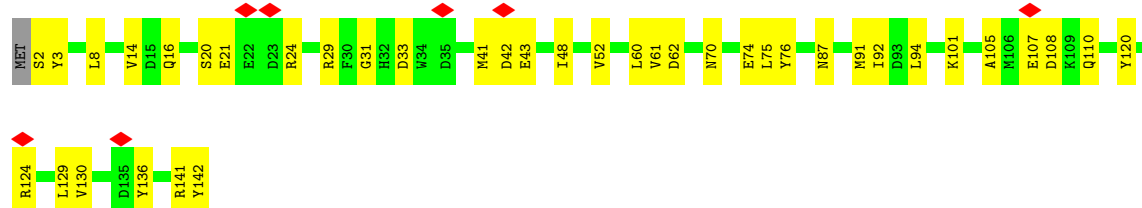




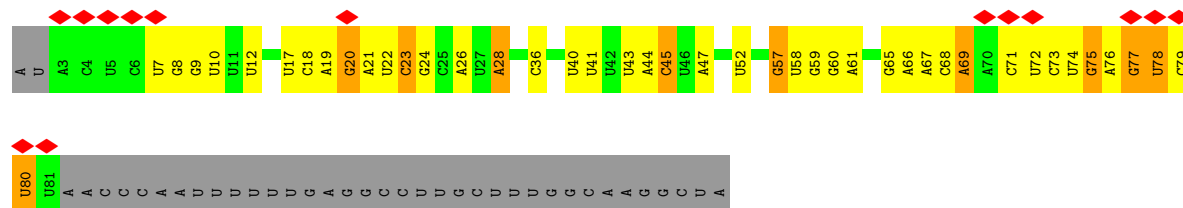
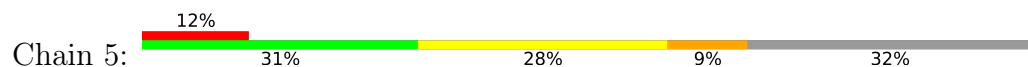
- Molecule 11: NHP2-like protein 1, N-terminally processed



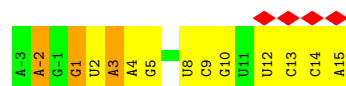
- Molecule 12: Thioredoxin-like protein 4A



- Molecule 13: U5 snRNA

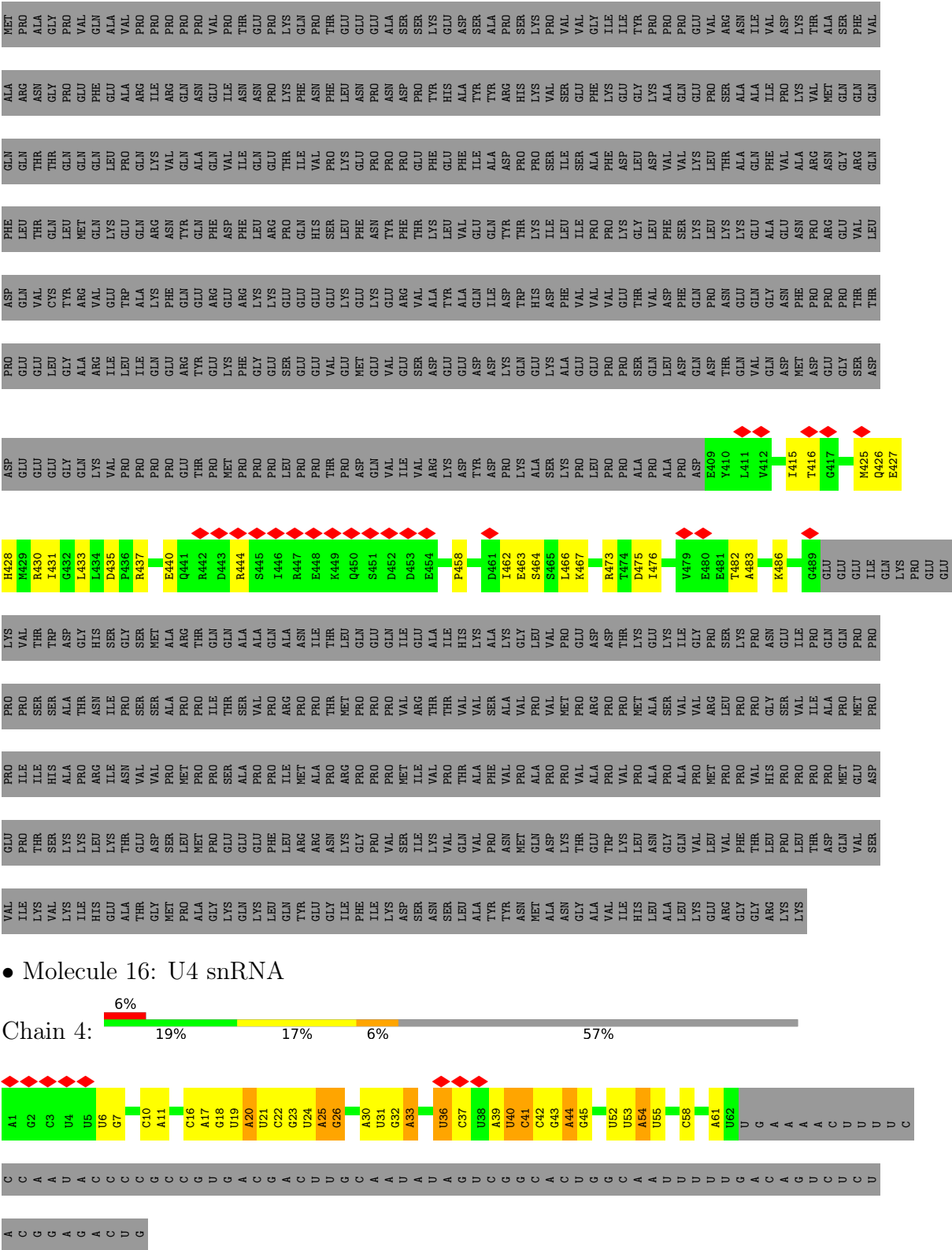


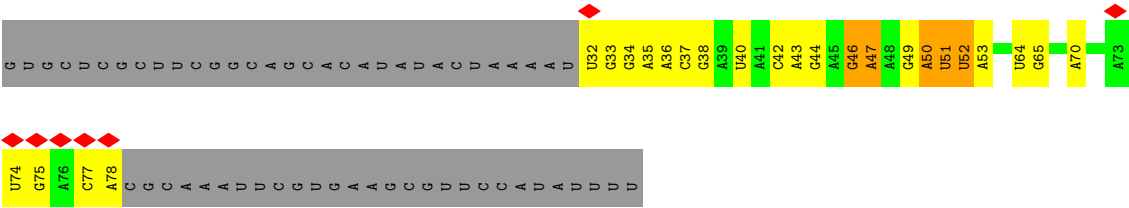
- Molecule 14: 5'ss oligo



- Molecule 15: Splicing factor 3A subunit 1







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136333	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.144	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.031	Depositor
Map size (Å)	556.8, 556.8, 556.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IHP

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	B	0.11	0/158	0.42	0/209
2	G	0.12	0/1096	0.34	0/1455
3	J	0.14	0/685	0.34	0/911
4	L	0.17	0/2912	0.34	0/3924
5	F	0.21	0/491	0.47	0/657
6	N	0.12	0/3136	0.33	0/4273
7	A	0.15	0/16830	0.35	1/22831 (0.0%)
8	U	0.12	0/3845	0.34	0/5208
9	S	0.11	0/1175	0.30	0/1571
10	C	0.14	0/6739	0.33	0/9151
11	M	0.13	0/974	0.33	0/1316
12	D	0.13	0/1199	0.32	0/1620
13	5	0.11	0/1850	0.23	0/2875
14	z	0.09	0/429	0.18	0/666
15	7	0.14	0/659	0.40	0/884
16	4	0.09	0/1477	0.17	0/2300
17	6	0.16	0/1133	0.30	0/1766
All	All	0.14	0/44788	0.33	1/61617 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1756	SER	CB-CA-C	-5.23	110.52	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	158	0	166	9	0
2	G	1077	0	1066	30	0
3	J	678	0	711	24	0
4	L	2874	0	2856	98	0
5	F	488	0	499	30	0
6	N	3095	0	2612	82	0
7	A	16383	0	16318	517	0
8	U	3749	0	3769	111	0
9	S	1167	0	1182	25	0
10	C	6592	0	6615	192	0
11	M	962	0	1012	31	0
12	D	1170	0	1141	30	0
13	5	1660	0	842	25	0
14	z	384	0	194	11	0
15	7	650	0	655	18	0
16	4	1322	0	666	28	0
17	6	1010	0	512	19	0
18	A	36	0	6	0	0
All	All	43455	0	40822	1117	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 13.

All (1117) 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)
6:N:378:ARG:O	6:N:382:LEU:HB2	1.72	0.89
7:A:752:ASN:HD22	8:U:462:PHE:HB3	1.39	0.88
7:A:942:PRO:HG2	7:A:1042:GLN:HE22	1.40	0.87
8:U:460:ASN:HD21	8:U:465:GLU:HG2	1.45	0.81
17:6:42:C:H2'	17:6:43:A:C8	2.16	0.80
7:A:941:LYS:HB2	7:A:944:ASP:HB2	1.61	0.80
3:J:478:ILE:HG12	3:J:504:MET:HE1	1.64	0.79
7:A:1212:GLY:HA2	7:A:1276:GLU:HB3	1.64	0.79
7:A:1889:LEU:HD23	7:A:2014:MET:HE3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:SER:HA	7:A:1289:VAL:HG21	1.64	0.78
7:A:690:MET:HE2	7:A:710:LEU:HD12	1.66	0.77
7:A:300:ASN:HB3	10:C:939:ARG:HE	1.50	0.75
7:A:583:ALA:HB1	7:A:609:LYS:CD	2.18	0.74
5:F:117:GLU:HG3	5:F:136:ILE:HD13	1.69	0.73
7:A:947:PRO:HD2	7:A:950:LEU:HD23	1.70	0.73
4:L:141:GLU:OE2	4:L:152:ASN:ND2	2.22	0.72
4:L:247:CYS:HB2	16:4:41:C:H41	1.53	0.72
8:U:174:CYS:O	8:U:178:ASN:N	2.22	0.72
17:6:42:C:H2'	17:6:43:A:H8	1.53	0.72
7:A:465:LYS:O	13:5:23:C:N4	2.22	0.72
7:A:1781:ASP:HB3	7:A:1808:PHE:HB2	1.71	0.72
3:J:489:ALA:HA	3:J:496:VAL:HG21	1.72	0.72
7:A:145:GLY:HA2	7:A:245:LEU:HD23	1.70	0.72
7:A:281:PRO:HG2	7:A:284:ARG:HE	1.52	0.72
8:U:231:LYS:HE2	8:U:313:ILE:HG13	1.72	0.72
7:A:92:LEU:HD13	7:A:503:MET:HG3	1.71	0.71
8:U:250:ARG:HA	8:U:281:MET:HE1	1.71	0.71
10:C:300:LEU:HA	10:C:306:ASN:HD22	1.54	0.71
13:5:7:U:O2	13:5:74:U:N3	2.24	0.71
15:7:482:THR:HG22	15:7:483:ALA:H	1.55	0.71
7:A:1700:GLY:H	7:A:1717:ASN:HB2	1.53	0.71
7:A:1345:GLN:NE2	7:A:1712:HIS:O	2.23	0.70
7:A:425:PRO:HB2	7:A:428:LYS:HB2	1.73	0.70
7:A:387:PHE:HE1	10:C:330:THR:HG21	1.56	0.70
4:L:396:LEU:HD12	4:L:399:LEU:HD23	1.72	0.70
7:A:1641:ARG:HH22	7:A:1651:VAL:H	1.40	0.70
4:L:163:THR:HA	4:L:166:VAL:HG12	1.73	0.70
10:C:683:ASN:HA	10:C:795:VAL:O	1.91	0.70
4:L:373:LYS:HD2	7:A:1759:THR:HG21	1.74	0.70
7:A:291:GLU:O	7:A:1136:ARG:NH1	2.25	0.70
10:C:187:THR:HG21	10:C:532:ILE:HG13	1.72	0.70
7:A:1863:VAL:HG11	7:A:1868:MET:HB3	1.74	0.69
10:C:237:LEU:HB2	10:C:835:GLU:HG2	1.73	0.69
10:C:127:GLU:O	10:C:130:ARG:NH2	2.26	0.69
7:A:683:LEU:HD21	12:D:43:GLU:HG2	1.75	0.69
6:N:369:LEU:HB3	6:N:373:VAL:HG11	1.74	0.69
4:L:148:LYS:O	4:L:152:ASN:ND2	2.26	0.69
7:A:1737:ASN:HD22	7:A:1740:LEU:HD13	1.57	0.68
10:C:779:LEU:O	10:C:938:ARG:NH1	2.25	0.68
6:N:201:ASP:H	7:A:1427:ARG:HH22	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:107:PRO:HD3	7:A:489:TRP:CD2	2.28	0.68
8:U:353:MET:HE3	8:U:355:ILE:HD11	1.75	0.68
7:A:1839:TRP:CD1	7:A:1871:PRO:HB3	2.28	0.68
10:C:381:LEU:HA	10:C:384:VAL:HG22	1.75	0.68
5:F:121:LEU:HD12	5:F:122:PHE:H	1.59	0.68
7:A:1183:PRO:HB3	7:A:1201:ARG:NH1	2.09	0.68
10:C:529:ARG:HB2	10:C:531:TRP:HZ3	1.59	0.68
3:J:476:VAL:HG23	3:J:500:VAL:HG23	1.76	0.67
7:A:832:TYR:HB3	7:A:835:ASP:HB2	1.76	0.67
5:F:94:LYS:HG3	5:F:95:ARG:HE	1.60	0.67
7:A:1340:LEU:HD23	7:A:1355:SER:HB3	1.75	0.67
7:A:357:ASN:ND2	10:C:866:SER:O	2.28	0.67
7:A:683:LEU:HD11	12:D:43:GLU:HB3	1.77	0.67
7:A:1608:THR:HG22	7:A:1632:PHE:HB2	1.76	0.67
2:G:271:LYS:HG3	2:G:273:VAL:HG13	1.77	0.67
7:A:1995:ASN:O	9:S:307:ARG:NH2	2.28	0.67
4:L:305:VAL:HG11	4:L:316:VAL:HG11	1.78	0.66
7:A:1865:ARG:HD2	9:S:278:ASP:HB3	1.76	0.66
12:D:70:ASN:HA	12:D:75:LEU:HB2	1.77	0.66
2:G:332:GLU:HB2	2:G:335:GLN:HE22	1.60	0.66
7:A:1271:MET:SD	7:A:1330:MET:HE1	2.36	0.66
8:U:350:GLN:HA	8:U:388:PHE:O	1.95	0.66
10:C:718:PHE:HB3	10:C:724:TRP:HB2	1.77	0.66
7:A:1641:ARG:HH22	7:A:1651:VAL:HG12	1.60	0.66
8:U:126:ILE:HD12	8:U:151:HIS:HB3	1.77	0.66
7:A:1260:VAL:O	7:A:1264:ASN:ND2	2.29	0.66
10:C:742:PRO:HG2	10:C:785:ARG:HG3	1.78	0.66
8:U:224:ILE:HD11	8:U:520:HIS:HB2	1.78	0.66
4:L:122:PHE:HD2	4:L:125:LEU:HB2	1.61	0.66
7:A:523:ASN:OD1	7:A:552:ARG:NH1	2.29	0.66
7:A:1582:TRP:O	7:A:1585:ILE:HG22	1.96	0.66
7:A:301:LYS:NZ	10:C:939:ARG:O	2.28	0.65
7:A:1849:ILE:HD11	7:A:1861:ILE:HD11	1.79	0.65
4:L:212:MET:HA	4:L:215:ILE:HG12	1.79	0.65
7:A:470:ARG:NH2	13:5:17:U:OP2	2.30	0.65
7:A:1183:PRO:HB3	7:A:1201:ARG:HD3	1.79	0.65
6:N:200:VAL:HA	7:A:1427:ARG:HH12	1.62	0.65
7:A:758:ARG:O	7:A:762:ARG:HG2	1.97	0.65
10:C:938:ARG:NH2	10:C:944:SER:OG	2.29	0.65
7:A:635:ARG:HA	7:A:638:LEU:HD12	1.78	0.64
7:A:1821:ILE:HG22	7:A:1906:ILE:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:122:PHE:CD2	4:L:125:LEU:HB2	2.32	0.64
7:A:583:ALA:HB1	7:A:609:LYS:HD3	1.79	0.64
8:U:360:LEU:HG	8:U:435:GLU:HG2	1.79	0.64
3:J:497:GLU:HB3	7:A:1931:THR:HG21	1.80	0.64
6:N:908:HIS:O	6:N:912:TRP:N	2.30	0.64
10:C:491:HIS:CD2	10:C:531:TRP:HZ2	2.16	0.64
11:M:86:LYS:NZ	16:4:31:U:O4	2.30	0.64
7:A:1555:LEU:HD23	7:A:1560:ILE:HG23	1.79	0.64
10:C:137:HIS:HA	10:C:238:ASN:HD22	1.61	0.64
6:N:293:LYS:NZ	7:A:1870:ASP:OD1	2.31	0.64
7:A:843:LEU:HD22	7:A:867:ILE:HG23	1.80	0.63
10:C:479:THR:HG23	10:C:562:THR:HG22	1.80	0.63
6:N:141:GLN:O	7:A:741:ARG:NH2	2.31	0.63
7:A:66:VAL:HG11	7:A:487:LEU:HD11	1.79	0.63
4:L:377:ARG:HB3	4:L:398:HIS:HD2	1.61	0.63
7:A:113:ILE:HD11	7:A:187:PRO:HG3	1.81	0.63
7:A:457:ASN:ND2	13:5:28:A:OP2	2.30	0.63
15:7:431:ILE:HD11	16:4:25:A:C5	2.33	0.63
6:N:326:GLN:NE2	6:N:330:ASN:OD1	2.32	0.63
3:J:447:LYS:O	3:J:451:GLN:HG2	1.98	0.62
7:A:943:ALA:HB1	7:A:1437:ARG:HB3	1.81	0.62
7:A:1052:VAL:O	7:A:1160:ARG:NH1	2.32	0.62
6:N:119:ARG:NH2	13:5:19:A:OP2	2.33	0.62
7:A:776:LEU:HD13	7:A:900:ASP:HB3	1.80	0.62
7:A:1298:ARG:NH1	12:D:142:TYR:OH	2.33	0.62
10:C:133:THR:HG22	10:C:203:MET:HB3	1.80	0.62
5:F:94:LYS:HA	5:F:97:ARG:HE	1.64	0.62
7:A:1544:ARG:HB3	7:A:1547:VAL:HG22	1.82	0.62
10:C:637:LEU:HA	10:C:640:VAL:HG12	1.80	0.62
7:A:391:THR:O	10:C:379:LYS:NZ	2.32	0.62
7:A:468:LYS:NZ	13:5:18:C:OP2	2.32	0.62
8:U:243:LEU:HD11	8:U:327:LEU:HD21	1.82	0.62
10:C:836:VAL:HG21	10:C:846:VAL:HG11	1.81	0.61
7:A:1146:ASP:OD2	7:A:1182:ASN:ND2	2.33	0.61
6:N:359:LYS:HA	6:N:362:VAL:HG12	1.82	0.61
7:A:1872:LEU:O	7:A:1876:LEU:N	2.32	0.61
8:U:172:PHE:HE2	8:U:186:LEU:HB3	1.64	0.61
8:U:246:VAL:O	8:U:250:ARG:N	2.32	0.61
3:J:511:HIS:O	3:J:515:ASN:ND2	2.32	0.61
7:A:1792:LYS:NZ	7:A:1793:THR:O	2.31	0.61
7:A:723:ASN:ND2	7:A:788:GLN:OE1	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1050:LEU:O	7:A:1054:GLY:N	2.22	0.61
5:F:113:ARG:NH1	5:F:117:GLU:O	2.34	0.61
7:A:1193:GLU:HG3	7:A:1233:ASP:HB3	1.82	0.61
7:A:1690:ASP:OD1	7:A:1691:ASN:N	2.33	0.61
7:A:168:PRO:HB2	7:A:563:GLN:HG3	1.83	0.61
6:N:811:GLY:HA3	6:N:841:PRO:HG2	1.83	0.61
7:A:1519:THR:OG1	7:A:1522:GLN:NE2	2.34	0.61
10:C:827:LEU:HD11	10:C:934:MET:HB3	1.81	0.61
7:A:1169:GLN:NE2	7:A:1171:GLU:OE2	2.33	0.60
10:C:192:ASP:OD1	10:C:193:THR:N	2.31	0.60
7:A:106:MET:HG3	7:A:107:PRO:HD2	1.83	0.60
7:A:715:GLU:OE2	7:A:718:ARG:NH2	2.34	0.60
7:A:1890:GLN:O	7:A:1941:ARG:NH2	2.33	0.60
10:C:529:ARG:HB2	10:C:531:TRP:CZ3	2.36	0.60
4:L:395:SER:OG	7:A:1320:LYS:NZ	2.30	0.60
6:N:157:TRP:CE3	7:A:697:MET:HG3	2.36	0.60
7:A:300:ASN:HB3	10:C:939:ARG:NE	2.16	0.60
10:C:201:ASN:HB3	10:C:549:TRP:CE3	2.37	0.60
7:A:942:PRO:HG2	7:A:1042:GLN:NE2	2.15	0.60
7:A:1640:SER:O	7:A:1717:ASN:ND2	2.34	0.60
7:A:1730:MET:HA	7:A:1733:ILE:HG22	1.84	0.60
10:C:778:PRO:HD3	10:C:784:ILE:HD11	1.82	0.60
6:N:178:LYS:O	7:A:861:ARG:NH1	2.35	0.59
7:A:1738:PRO:HD3	9:S:331:ARG:HH12	1.67	0.59
10:C:836:VAL:HG22	10:C:871:ILE:HB	1.84	0.59
4:L:121:ARG:O	4:L:121:ARG:NH1	2.35	0.59
4:L:108:ASN:OD1	4:L:109:ILE:N	2.35	0.59
4:L:424:LEU:HD21	7:A:866:LEU:HD11	1.85	0.59
7:A:1386:TRP:HE1	7:A:1417:PRO:HD2	1.68	0.59
7:A:1130:ASN:HA	7:A:1174:PHE:HE1	1.67	0.59
6:N:163:VAL:HG21	7:A:715:GLU:HG2	1.84	0.59
7:A:606:LYS:HA	7:A:609:LYS:HE2	1.84	0.59
7:A:1763:LEU:HD22	7:A:1862:ILE:HG21	1.84	0.59
9:S:157:ASN:HB3	9:S:160:ALA:HB3	1.83	0.59
10:C:687:MET:HG2	10:C:791:ILE:HG12	1.83	0.59
7:A:1676:ILE:HD13	7:A:1706:ASP:HB2	1.85	0.59
10:C:743:ASN:ND2	10:C:784:ILE:O	2.36	0.59
15:7:415:ILE:HG13	15:7:416:THR:HG23	1.84	0.59
5:F:118:PRO:O	5:F:132:ARG:NH2	2.35	0.59
7:A:211:GLN:OE1	7:A:214:ARG:NH1	2.35	0.59
7:A:605:CYS:O	7:A:609:LYS:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:766:THR:HG22	12:D:141:ARG:HB3	1.83	0.59
10:C:746:VAL:HG21	10:C:788:LYS:HE3	1.85	0.59
7:A:823:SER:OG	7:A:933:ARG:NH1	2.36	0.58
7:A:787:GLU:OE2	7:A:790:ARG:NH2	2.36	0.58
8:U:454:ILE:HG22	8:U:456:ARG:HG2	1.85	0.58
4:L:422:LYS:HE2	16:4:20:A:H5'	1.84	0.58
7:A:816:TRP:HD1	7:A:817:LEU:HD22	1.67	0.58
7:A:1044:TYR:O	7:A:1047:VAL:HB	2.02	0.58
6:N:354:PRO:O	6:N:357:THR:OG1	2.21	0.58
10:C:377:LEU:HD23	10:C:380:ILE:HD11	1.85	0.58
7:A:1134:TRP:O	7:A:1139:ARG:NH1	2.37	0.58
7:A:2009:ASP:HB3	7:A:2014:MET:HB2	1.85	0.58
7:A:811:THR:HA	7:A:814:VAL:HG22	1.86	0.58
10:C:632:THR:H	10:C:636:TYR:HD2	1.52	0.58
16:4:33:A:N6	16:4:43:G:O2'	2.37	0.58
4:L:156:GLN:HA	4:L:164:ILE:HD11	1.84	0.58
7:A:1128:TYR:HE2	7:A:1140:MET:HE1	1.68	0.58
7:A:1146:ASP:HB3	7:A:1177:VAL:HG11	1.85	0.58
8:U:316:GLN:NE2	8:U:317:GLY:O	2.37	0.58
2:G:245:LYS:HB3	2:G:286:TYR:HB2	1.85	0.57
7:A:1344:LYS:HG2	7:A:1353:PHE:HE1	1.69	0.57
8:U:497:TYR:HB3	8:U:552:TRP:HB3	1.85	0.57
10:C:441:PRO:HB3	10:C:495:ARG:HH21	1.69	0.57
8:U:484:LEU:O	8:U:489:GLN:NE2	2.34	0.57
3:J:491:GLN:HB3	7:A:1984:LYS:HD3	1.86	0.57
2:G:327:ARG:NH2	7:A:357:ASN:OD1	2.37	0.57
3:J:518:ARG:NH2	16:4:10:C:O2	2.37	0.57
10:C:260:ILE:HG22	10:C:311:SER:HB2	1.86	0.57
10:C:227:LEU:HD11	10:C:243:ILE:HG22	1.87	0.57
10:C:828:MET:HE2	10:C:904:TRP:HB2	1.87	0.57
10:C:916:ILE:HD12	10:C:928:HIS:CD2	2.39	0.57
6:N:156:GLU:HG2	7:A:732:PRO:HG3	1.86	0.57
7:A:104:GLU:HG3	7:A:422:LEU:HD21	1.87	0.57
13:5:12:U:H3	13:5:65:G:H1	1.53	0.57
7:A:515:TYR:HA	7:A:527:VAL:HG22	1.87	0.57
7:A:1265:THR:HG22	7:A:1452:PRO:HG3	1.86	0.57
8:U:187:GLU:O	8:U:190:THR:OG1	2.22	0.57
3:J:440:LEU:HB2	3:J:444:GLU:HG3	1.86	0.57
10:C:159:LYS:NZ	10:C:160:ARG:O	2.33	0.56
11:M:64:GLU:HA	11:M:67:LEU:HB2	1.87	0.56
7:A:1557:LEU:HD21	7:A:1580:HIS:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:291:ILE:HD12	6:N:322:THR:HG21	1.86	0.56
6:N:304:THR:OG1	7:A:1832:ARG:NH2	2.38	0.56
7:A:142:SER:HA	7:A:242:ALA:HB2	1.86	0.56
7:A:539:ARG:NH1	14:z:-2:A:O2'	2.38	0.56
7:A:1645:LEU:HD13	7:A:1714:ALA:HB3	1.88	0.56
7:A:235:MET:HE1	7:A:411:PHE:HA	1.88	0.56
7:A:422:LEU:HD22	7:A:638:LEU:HD13	1.87	0.56
7:A:939:TRP:NE1	7:A:1049:ASP:OD2	2.36	0.56
8:U:170:LEU:HD22	8:U:190:THR:HG22	1.86	0.56
8:U:504:VAL:HG23	8:U:515:ARG:HB2	1.86	0.56
4:L:212:MET:HE1	4:L:229:ALA:HA	1.87	0.56
7:A:1667:ARG:NH2	7:A:1706:ASP:OD2	2.36	0.56
7:A:1740:LEU:HB3	7:A:1744:ARG:HH21	1.71	0.56
7:A:1537:TRP:HE3	7:A:1751:LEU:HD13	1.70	0.56
7:A:1809:ILE:HB	7:A:1818:PHE:HB2	1.88	0.56
8:U:316:GLN:HE21	8:U:514:TYR:HE1	1.53	0.56
12:D:8:LEU:HD13	12:D:14:VAL:HA	1.88	0.56
2:G:343:LEU:HA	2:G:346:LYS:HG2	1.87	0.56
7:A:1504:GLU:HB2	7:A:1752:GLN:HB3	1.86	0.56
7:A:1945:VAL:HG12	7:A:1946:ASN:HD22	1.70	0.56
7:A:198:GLU:HG2	7:A:199:GLU:HG3	1.87	0.56
7:A:430:TRP:HB3	7:A:611:LEU:HD11	1.86	0.56
7:A:1495:PHE:HE2	7:A:1755:SER:HB3	1.71	0.56
8:U:279:GLU:O	8:U:283:LYS:HG3	2.06	0.56
12:D:21:GLU:OE2	12:D:24:ARG:N	2.25	0.56
6:N:146:LYS:HE2	7:A:692:ASP:HA	1.87	0.56
15:7:483:ALA:HB3	15:7:486:LYS:HB2	1.88	0.56
7:A:1761:PRO:HB2	7:A:1885:LYS:HG2	1.88	0.56
7:A:1786:TYR:HE1	9:S:289:LEU:HD21	1.71	0.56
10:C:484:THR:OG1	10:C:486:ASP:OD1	2.23	0.56
2:G:248:HIS:NE2	2:G:252:GLU:OE2	2.40	0.55
3:J:439:TYR:HD2	11:M:27:GLN:HG3	1.72	0.55
4:L:361:LYS:HD3	16:4:18:G:H22	1.71	0.55
7:A:309:ARG:NE	7:A:311:GLU:OE2	2.35	0.55
7:A:962:LEU:HD13	7:A:1086:ARG:HD3	1.88	0.55
7:A:1224:ARG:NH1	7:A:1226:ALA:O	2.40	0.55
14:z:13:C:H42	17:6:34:G:H1	1.54	0.55
6:N:35:GLY:HA2	12:D:76:TYR:CE2	2.41	0.55
7:A:1270:LEU:O	7:A:1274:PHE:N	2.35	0.55
7:A:1354:ARG:HG3	9:S:150:PRO:HG2	1.87	0.55
10:C:186:VAL:HB	10:C:202:ILE:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:497:GLU:HA	3:J:500:VAL:HG12	1.88	0.55
7:A:95:MET:HE1	7:A:496:VAL:HG22	1.89	0.55
7:A:1171:GLU:OE1	7:A:1171:GLU:N	2.28	0.55
8:U:265:PRO:HD2	8:U:268:ASP:HB2	1.87	0.55
7:A:546:LEU:HD22	7:A:648:LEU:HD11	1.88	0.55
4:L:353:LYS:O	17:6:53:A:N6	2.37	0.55
11:M:65:ILE:HG13	11:M:66:ILE:HG23	1.87	0.55
8:U:460:ASN:ND2	8:U:465:GLU:HG2	2.17	0.55
7:A:1495:PHE:CE2	7:A:1755:SER:HB3	2.41	0.55
7:A:1622:MET:O	7:A:1687:TYR:OH	2.25	0.55
10:C:701:GLU:OE2	10:C:785:ARG:NH1	2.40	0.55
3:J:450:ARG:NH1	16:4:23:G:OP1	2.40	0.55
4:L:298:LYS:NZ	16:4:32:G:OP1	2.39	0.55
7:A:863:GLU:O	7:A:867:ILE:HD12	2.07	0.55
7:A:1667:ARG:NH1	7:A:1673:SER:O	2.39	0.55
7:A:1869:LEU:HD11	7:A:1886:GLY:HA3	1.89	0.55
7:A:1919:LEU:HD13	7:A:1936:LEU:HD11	1.87	0.55
10:C:123:MET:HE3	10:C:548:ASN:HD22	1.71	0.55
10:C:589:LYS:HG3	10:C:628:VAL:HG13	1.89	0.55
11:M:46:LEU:HD11	11:M:54:ILE:HD13	1.88	0.55
16:4:6:U:H2'	16:4:7:G:C8	2.42	0.55
2:G:277:ASP:OD1	2:G:278:ALA:N	2.40	0.55
7:A:108:MET:HE3	7:A:109:PRO:HD2	1.88	0.55
7:A:1354:ARG:NH1	7:A:1356:GLY:O	2.39	0.55
10:C:593:GLU:HG3	10:C:594:PRO:HD2	1.87	0.55
4:L:305:VAL:HA	11:M:64:GLU:HG3	1.89	0.54
7:A:845:ARG:NH1	7:A:1439:ARG:HD3	2.22	0.54
7:A:1791:HIS:HB3	9:S:271:THR:HA	1.89	0.54
10:C:171:LEU:HB2	10:C:174:GLU:OE1	2.08	0.54
10:C:263:LEU:HD23	10:C:267:LEU:HD12	1.88	0.54
6:N:142:PHE:HE1	7:A:741:ARG:HB3	1.72	0.54
7:A:102:LEU:CD2	7:A:496:VAL:HG11	2.38	0.54
7:A:1705:ILE:HD11	7:A:1730:MET:HE1	1.88	0.54
8:U:174:CYS:O	8:U:178:ASN:CA	2.56	0.54
7:A:939:TRP:CD1	7:A:940:ILE:HG13	2.43	0.54
9:S:180:LEU:HA	9:S:183:LYS:HB2	1.90	0.54
10:C:384:VAL:HG21	10:C:416:LEU:HD13	1.90	0.54
10:C:916:ILE:HB	10:C:931:ARG:HG2	1.89	0.54
5:F:104:ASP:N	5:F:104:ASP:OD1	2.41	0.54
7:A:1738:PRO:HB3	7:A:2023:ARG:HG3	1.90	0.54
8:U:124:CYS:HB3	8:U:129:SER:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:316:ALA:HB2	6:N:332:ILE:HD11	1.90	0.54
7:A:107:PRO:HG2	7:A:561:HIS:CE1	2.43	0.54
10:C:124:ASP:HA	10:C:545:PRO:HG3	1.90	0.54
10:C:347:ILE:HD12	10:C:356:PHE:HB3	1.89	0.54
4:L:166:VAL:HG23	7:A:995:ARG:HD2	1.89	0.54
4:L:432:SER:HA	7:A:883:ARG:HH12	1.72	0.54
7:A:542:ASN:OD1	13:5:43:U:O2'	2.25	0.54
7:A:1892:PRO:HD2	7:A:1937:ILE:HD11	1.90	0.54
17:6:34:G:H2'	17:6:35:A:C8	2.43	0.54
7:A:150:MET:HE1	7:A:193:LEU:HB2	1.90	0.54
10:C:632:THR:O	10:C:832:TYR:OH	2.21	0.54
10:C:846:VAL:HG22	10:C:887:LEU:HD11	1.88	0.54
4:L:218:ASN:ND2	4:L:306:ASP:OD1	2.37	0.54
5:F:133:LEU:HD12	5:F:137:LEU:HD23	1.89	0.54
1:B:44:VAL:HG13	7:A:1282:GLN:HG2	1.90	0.53
10:C:370:VAL:HA	10:C:374:LEU:HB2	1.89	0.53
13:5:78:U:O2'	13:5:80:U:OP1	2.20	0.53
7:A:1671:TYR:O	7:A:1674:HIS:ND1	2.40	0.53
15:7:425:MET:HA	15:7:428:HIS:HB3	1.89	0.53
7:A:147:MET:O	7:A:151:MET:HG3	2.08	0.53
14:z:13:C:H2'	14:z:14:C:O4'	2.09	0.53
6:N:202:PRO:O	7:A:1393:ARG:NH1	2.34	0.53
7:A:955:TRP:HE1	7:A:976:MET:HE1	1.72	0.53
7:A:1317:TYR:CE1	7:A:1329:SER:HB3	2.43	0.53
8:U:372:GLN:NE2	8:U:376:ASN:OD1	2.42	0.53
4:L:402:SER:HA	6:N:290:ASP:HA	1.90	0.53
6:N:102:ASP:OD2	7:A:658:ARG:NH2	2.42	0.53
6:N:253:MET:HB3	6:N:274:LEU:HB2	1.90	0.53
7:A:109:PRO:HD3	7:A:630:TRP:HZ2	1.73	0.53
10:C:876:PRO:HB2	10:C:879:ASP:HB2	1.91	0.53
6:N:200:VAL:HA	7:A:1427:ARG:NH1	2.24	0.53
6:N:252:ASP:OD1	6:N:253:MET:N	2.42	0.53
7:A:150:MET:CE	7:A:193:LEU:HB2	2.39	0.53
7:A:972:GLU:HG3	7:A:1100:ARG:HH21	1.73	0.53
7:A:1560:ILE:HG12	7:A:1573:LEU:HD13	1.89	0.53
8:U:365:LEU:HD22	8:U:370:LYS:HZ3	1.72	0.53
7:A:121:HIS:HB2	7:A:126:ILE:HG22	1.91	0.53
7:A:1821:ILE:HG12	7:A:1913:GLN:H	1.74	0.53
4:L:276:HIS:HA	4:L:281:GLN:HE21	1.74	0.53
7:A:256:TYR:HE2	10:C:885:THR:HG23	1.74	0.53
7:A:678:GLU:HA	7:A:749:TRP:HZ2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:74:GLU:O	12:D:101:LYS:NZ	2.42	0.53
2:G:367:ASP:OD1	2:G:368:ARG:N	2.41	0.52
10:C:186:VAL:HG13	10:C:534:VAL:HG23	1.90	0.52
10:C:559:ILE:HG23	10:C:563:ALA:HB2	1.90	0.52
15:7:463:GLU:HG2	15:7:467:LYS:HE3	1.89	0.52
1:B:43:LEU:HD13	1:B:47:LEU:HD21	1.92	0.52
3:J:503:GLN:OE1	3:J:507:ARG:NH1	2.43	0.52
4:L:408:ARG:HG3	7:A:1873:GLU:HB3	1.90	0.52
7:A:169:PHE:HE1	7:A:563:GLN:HG2	1.75	0.52
7:A:293:TRP:NE1	7:A:298:ASP:OD1	2.40	0.52
7:A:1565:LYS:HD3	14:z:1:G:H4'	1.91	0.52
8:U:272:LEU:HA	8:U:275:GLN:HG2	1.92	0.52
7:A:598:LEU:HD11	7:A:640:PHE:CE1	2.44	0.52
7:A:720:TRP:O	7:A:785:LYS:NZ	2.43	0.52
7:A:1988:LEU:HD21	7:A:2007:ILE:HD13	1.92	0.52
17:6:51:U:O2'	17:6:52:U:OP1	2.26	0.52
7:A:257:LEU:HD13	7:A:311:GLU:HB2	1.92	0.52
8:U:188:ASP:OD1	8:U:189:ILE:N	2.42	0.52
8:U:239:VAL:HG21	8:U:322:PHE:CD2	2.45	0.52
10:C:607:LEU:HD22	10:C:629:ILE:HD11	1.89	0.52
10:C:618:THR:HB	10:C:630:LEU:HB2	1.90	0.52
4:L:347:LEU:HD23	17:6:50:A:C4	2.43	0.52
6:N:34:ILE:HD11	12:D:76:TYR:HB2	1.92	0.52
7:A:72:ASP:O	7:A:78:ASN:ND2	2.41	0.52
2:G:243:LYS:O	2:G:247:LEU:HD13	2.09	0.52
5:F:115:LEU:HD22	5:F:117:GLU:HG2	1.92	0.52
6:N:146:LYS:NZ	7:A:695:ASP:OD2	2.41	0.52
7:A:299:ILE:HD12	10:C:921:LEU:HD21	1.92	0.52
7:A:1923:TRP:O	7:A:1927:ILE:HG22	2.09	0.52
3:J:511:HIS:CD2	3:J:515:ASN:HD21	2.27	0.52
7:A:387:PHE:CE1	10:C:330:THR:HG21	2.42	0.52
7:A:1839:TRP:NE1	7:A:1871:PRO:HB3	2.23	0.52
8:U:457:PHE:HD1	8:U:509:PRO:HG3	1.75	0.52
8:U:459:LYS:HA	8:U:464:VAL:HA	1.92	0.52
7:A:443:VAL:HG12	7:A:610:HIS:HB3	1.92	0.52
7:A:1384:ARG:O	7:A:1388:GLU:HG3	2.10	0.52
10:C:888:ARG:O	10:C:893:GLY:N	2.38	0.52
13:5:58:U:H2'	13:5:59:G:H8	1.75	0.52
7:A:155:LYS:NZ	7:A:622:GLY:O	2.43	0.52
7:A:909:TYR:HB2	7:A:1033:GLY:HA3	1.93	0.52
7:A:919:ASP:HB3	7:A:1035:GLN:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1188:ASN:HB3	7:A:1193:GLU:HG2	1.91	0.52
7:A:1734:MET:HA	7:A:1734:MET:HE3	1.90	0.52
8:U:353:MET:HB2	8:U:388:PHE:CD2	2.45	0.52
9:S:253:ASP:OD1	9:S:254:LEU:N	2.43	0.52
7:A:441:VAL:HB	7:A:444:ARG:HH21	1.75	0.51
7:A:1323:GLY:HA3	7:A:1537:TRP:NE1	2.26	0.51
7:A:1570:LYS:NZ	17:6:46:G:N7	2.58	0.51
7:A:1645:LEU:O	7:A:1727:GLN:NE2	2.43	0.51
10:C:232:ALA:HB3	10:C:262:ARG:HE	1.75	0.51
11:M:41:GLU:HG3	16:4:32:G:H1	1.74	0.51
11:M:107:LYS:HB3	11:M:110:SER:HB2	1.92	0.51
2:G:318:ARG:HH11	2:G:322:ASP:HB3	1.75	0.51
4:L:132:ALA:O	4:L:136:ILE:HD12	2.10	0.51
6:N:301:VAL:HA	6:N:304:THR:HB	1.91	0.51
7:A:1611:LYS:NZ	7:A:2065:GLN:O	2.39	0.51
7:A:1776:ILE:HG22	7:A:1813:ARG:HG3	1.92	0.51
7:A:1951:LYS:O	7:A:1955:LYS:HG2	2.11	0.51
4:L:383:ILE:HD13	7:A:1321:GLU:OE2	2.10	0.51
7:A:878:LEU:O	7:A:882:LYS:HG2	2.10	0.51
8:U:172:PHE:HD2	8:U:186:LEU:HD23	1.75	0.51
10:C:778:PRO:HG2	10:C:820:PHE:HD2	1.76	0.51
12:D:29:ARG:HH21	12:D:60:LEU:HD13	1.76	0.51
6:N:348:GLU:HA	6:N:351:ARG:HG2	1.92	0.51
8:U:456:ARG:NH1	8:U:469:THR:O	2.36	0.51
12:D:120:TYR:CZ	12:D:124:ARG:HD3	2.45	0.51
4:L:383:ILE:HB	9:S:159:MET:HE3	1.92	0.51
7:A:120:TYR:CZ	7:A:483:GLN:HB2	2.46	0.51
7:A:980:ARG:HH11	7:A:1093:ASP:HB2	1.75	0.51
7:A:994:ASN:HB2	7:A:1010:THR:HG21	1.92	0.51
7:A:1052:VAL:HG23	7:A:1161:LEU:HD21	1.93	0.51
7:A:1513:MET:HA	7:A:1516:LYS:HD3	1.92	0.51
8:U:432:THR:HB	8:U:437:PHE:HE2	1.75	0.51
4:L:269:PRO:HD2	4:L:289:ARG:HH22	1.76	0.51
10:C:778:PRO:HG3	10:C:817:TYR:CD1	2.45	0.51
15:7:430:ARG:HH12	16:4:25:A:H5'	1.76	0.51
5:F:113:ARG:NH1	5:F:113:ARG:HA	2.25	0.51
8:U:172:PHE:CE2	8:U:186:LEU:HB3	2.46	0.51
13:5:74:U:H2'	13:5:75:G:C8	2.45	0.51
4:L:137:ARG:HB3	4:L:158:ILE:HD13	1.92	0.51
7:A:1220:VAL:HG23	7:A:1221:THR:HG23	1.93	0.51
4:L:106:GLU:O	4:L:110:ILE:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:142:LEU:HD23	4:L:146:LEU:HD22	1.91	0.51
4:L:159:LEU:HB3	4:L:163:THR:HG23	1.93	0.51
7:A:285:ASP:HB3	7:A:288:LEU:HB2	1.93	0.51
8:U:137:LEU:HD21	8:U:165:LEU:HB2	1.93	0.51
8:U:391:LEU:HD12	8:U:452:PHE:HE1	1.76	0.51
7:A:89:LEU:HA	7:A:92:LEU:HG	1.93	0.51
7:A:686:ARG:NE	12:D:3:TYR:OH	2.41	0.51
7:A:1823:HIS:HB2	7:A:1912:PRO:HG3	1.93	0.51
8:U:238:ALA:HB1	8:U:503:ILE:HD12	1.93	0.50
2:G:368:ARG:HH21	7:A:154:GLU:HG3	1.76	0.50
8:U:112:ASN:ND2	8:U:138:VAL:O	2.44	0.50
3:J:439:TYR:CD2	11:M:27:GLN:HG3	2.46	0.50
6:N:288:ILE:HG13	7:A:1877:LEU:HD11	1.91	0.50
7:A:942:PRO:HA	7:A:1091:TYR:HA	1.92	0.50
8:U:127:SER:OG	8:U:151:HIS:NE2	2.36	0.50
8:U:429:GLU:HG3	8:U:438:LEU:HD13	1.92	0.50
7:A:169:PHE:HZ	7:A:562:VAL:CG1	2.24	0.50
1:B:43:LEU:HD21	7:A:1330:MET:HG2	1.93	0.50
7:A:384:VAL:HA	10:C:331:PHE:CE1	2.47	0.50
7:A:441:VAL:HA	7:A:444:ARG:HE	1.76	0.50
7:A:1889:LEU:HD13	7:A:2012:LEU:HD12	1.92	0.50
7:A:1889:LEU:HD22	7:A:2012:LEU:HB3	1.94	0.50
8:U:395:LEU:HD23	8:U:469:THR:HB	1.93	0.50
10:C:388:VAL:HG13	10:C:392:LEU:HD22	1.93	0.50
1:B:50:THR:O	1:B:51:ARG:NE	2.44	0.50
7:A:372:PRO:HG3	10:C:342:ARG:HG2	1.94	0.50
7:A:548:ARG:NH1	7:A:549:GLU:OE2	2.45	0.50
8:U:105:CYS:HB3	8:U:181:ILE:HD12	1.93	0.50
14:z:9:C:H2'	14:z:10:G:H8	1.77	0.50
2:G:294:HIS:CD2	2:G:297:GLN:HE22	2.30	0.50
7:A:1468:ASN:OD1	7:A:1469:ASN:N	2.44	0.50
10:C:134:LEU:HD23	10:C:226:VAL:HB	1.93	0.50
6:N:201:ASP:N	7:A:1427:ARG:HH22	2.09	0.50
7:A:443:VAL:HG11	7:A:614:TYR:CE1	2.46	0.50
7:A:1321:GLU:O	7:A:1503:TRP:NE1	2.44	0.50
7:A:1494:TYR:HB2	7:A:1710:ASN:ND2	2.27	0.50
7:A:1853:PRO:HB2	7:A:1855:GLU:OE2	2.12	0.50
10:C:946:ASP:OD1	10:C:947:VAL:N	2.36	0.50
11:M:12:PRO:HG3	11:M:80:TYR:CE2	2.46	0.50
7:A:1609:VAL:HG22	7:A:1631:LEU:HD22	1.93	0.50
10:C:135:CYS:HB2	10:C:242:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:33:ASP:N	12:D:33:ASP:OD1	2.45	0.50
7:A:468:LYS:O	7:A:470:ARG:NH1	2.45	0.49
7:A:639:PHE:O	13:5:28:A:O2'	2.29	0.49
7:A:1426:ASP:HB2	7:A:1429:THR:HG22	1.94	0.49
16:4:20:A:H2'	16:4:21:U:C6	2.47	0.49
7:A:640:PHE:CZ	7:A:644:ILE:HD13	2.47	0.49
7:A:1641:ARG:NH2	7:A:1651:VAL:H	2.10	0.49
8:U:274:VAL:HG22	8:U:330:LEU:HD13	1.94	0.49
10:C:204:ASP:OD1	10:C:204:ASP:N	2.45	0.49
10:C:925:PRO:HD2	10:C:928:HIS:ND1	2.28	0.49
6:N:343:GLU:HG3	6:N:375:ILE:HD11	1.94	0.49
14:z:12:U:H2'	14:z:13:C:C6	2.48	0.49
15:7:464:SER:HA	15:7:467:LYS:HD2	1.93	0.49
7:A:1183:PRO:HB3	7:A:1201:ARG:HH11	1.76	0.49
10:C:837:GLN:HE21	10:C:896:PHE:HB3	1.78	0.49
3:J:486:GLY:O	3:J:490:VAL:HG23	2.13	0.49
6:N:97:ASP:OD1	6:N:97:ASP:N	2.44	0.49
7:A:380:LEU:HD12	7:A:384:VAL:HG21	1.95	0.49
7:A:697:MET:HE2	7:A:702:LYS:HG3	1.93	0.49
7:A:1174:PHE:CE2	7:A:1176:SER:HB2	2.48	0.49
7:A:1304:ASN:OD1	7:A:1305:SER:N	2.45	0.49
4:L:351:ARG:HB2	17:6:50:A:C8	2.47	0.49
6:N:200:VAL:HG22	7:A:1403:LEU:HB2	1.94	0.49
7:A:962:LEU:HB2	7:A:965:VAL:HB	1.95	0.49
7:A:975:VAL:HG12	7:A:1099:PHE:HB2	1.94	0.49
7:A:1189:MET:HE2	7:A:1189:MET:HA	1.95	0.49
7:A:1790:ILE:HG13	7:A:1800:THR:HG22	1.94	0.49
7:A:1962:THR:HA	7:A:1966:HIS:HE1	1.76	0.49
9:S:206:ARG:O	9:S:209:GLN:HG3	2.13	0.49
17:6:64:U:H2'	17:6:65:G:C8	2.48	0.49
4:L:396:LEU:HB3	4:L:399:LEU:HB3	1.94	0.49
7:A:1840:LYS:O	7:A:1844:GLU:HG2	2.13	0.49
8:U:276:ARG:NH1	8:U:298:GLU:O	2.45	0.49
6:N:157:TRP:CZ3	7:A:735:ILE:HD11	2.48	0.49
6:N:313:ILE:HG13	6:N:344:ASP:OD2	2.13	0.49
7:A:158:ARG:NH2	7:A:570:ASP:OD2	2.46	0.49
7:A:1763:LEU:HD22	7:A:1862:ILE:HD13	1.95	0.49
2:G:299:LEU:HA	2:G:320:TYR:CE2	2.48	0.49
7:A:384:VAL:HG12	10:C:331:PHE:CB	2.43	0.49
11:M:14:ALA:HB1	11:M:18:LEU:HD21	1.95	0.49
7:A:533:LYS:NZ	14:z:2:U:O2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:111:ILE:HG23	8:U:137:LEU:HB3	1.95	0.48
8:U:183:ASP:HB2	8:U:186:LEU:HD22	1.95	0.48
10:C:182:LYS:HA	10:C:214:GLU:HG2	1.94	0.48
6:N:327:VAL:HG22	9:S:173:ALA:HB2	1.95	0.48
7:A:1087:LEU:HB2	7:A:1098:PHE:HB3	1.95	0.48
4:L:128:LEU:HD23	4:L:166:VAL:HG13	1.94	0.48
6:N:911:LEU:O	6:N:915:VAL:N	2.40	0.48
7:A:926:LEU:HD11	7:A:1009:MET:HE2	1.95	0.48
7:A:1098:PHE:HE1	7:A:1185:LEU:HD21	1.77	0.48
7:A:1771:LEU:HD11	7:A:1779:PHE:HZ	1.78	0.48
8:U:346:THR:O	8:U:350:GLN:HB3	2.13	0.48
8:U:353:MET:HB2	8:U:388:PHE:HD2	1.77	0.48
10:C:934:MET:O	10:C:938:ARG:N	2.35	0.48
4:L:358:ARG:HH22	16:4:54:A:H3'	1.78	0.48
6:N:23:ARG:HB2	12:D:87:ASN:HD21	1.79	0.48
6:N:140:GLN:HA	6:N:143:SER:HB3	1.95	0.48
6:N:252:ASP:OD2	6:N:254:ARG:NH2	2.46	0.48
10:C:676:ALA:HB3	10:C:815:VAL:HB	1.96	0.48
7:A:1614:ILE:HD12	7:A:1618:LYS:HD2	1.96	0.48
7:A:1792:LYS:HA	7:A:1798:LEU:HA	1.95	0.48
8:U:174:CYS:O	8:U:178:ASN:HA	2.13	0.48
7:A:258:PHE:HZ	7:A:275:GLY:HA3	1.78	0.48
7:A:1081:ALA:HA	7:A:1086:ARG:NH2	2.28	0.48
7:A:1641:ARG:NH2	7:A:1651:VAL:HG12	2.29	0.48
8:U:149:LYS:NZ	10:C:738:ASP:OD1	2.37	0.48
11:M:62:PRO:HG2	11:M:65:ILE:HD13	1.94	0.48
10:C:258:ASN:ND2	10:C:312:SER:OG	2.45	0.48
10:C:585:THR:O	10:C:587:VAL:HG23	2.13	0.48
13:5:23:C:O2	13:5:57:G:N1	2.47	0.48
3:J:476:VAL:HG12	3:J:484:VAL:HG21	1.95	0.48
4:L:304:ARG:HB3	11:M:65:ILE:HA	1.95	0.48
7:A:881:ILE:HG23	7:A:918:THR:HG23	1.96	0.48
7:A:978:GLU:HG3	7:A:1174:PHE:HB3	1.96	0.48
8:U:205:LEU:HB3	8:U:250:ARG:HH22	1.77	0.48
10:C:332:GLY:O	10:C:334:ILE:HG13	2.14	0.48
2:G:248:HIS:O	2:G:252:GLU:HG3	2.14	0.48
5:F:126:PRO:HB2	16:4:25:A:C5	2.49	0.48
7:A:92:LEU:HB3	7:A:503:MET:SD	2.54	0.48
5:F:89:GLU:O	5:F:92:ARG:HG3	2.13	0.48
7:A:171:ASP:C	7:A:173:GLU:H	2.22	0.48
7:A:246:LEU:HD22	7:A:408:PRO:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1668:TRP:CD1	7:A:1708:ALA:HB2	2.49	0.48
8:U:156:SER:HB2	8:U:176:PRO:HG3	1.94	0.48
10:C:140:HIS:NE2	10:C:233:GLU:OE1	2.44	0.48
4:L:260:SER:O	7:A:991:THR:HG22	2.14	0.47
4:L:382:GLU:H	7:A:1321:GLU:HG3	1.79	0.47
6:N:313:ILE:HD11	6:N:345:VAL:HA	1.96	0.47
7:A:1369:TYR:CD2	7:A:1370:ARG:HG3	2.48	0.47
7:A:102:LEU:HD21	7:A:496:VAL:HG11	1.96	0.47
7:A:153:ARG:O	7:A:157:ASP:N	2.46	0.47
7:A:335:PRO:HG3	10:C:139:HIS:HB3	1.95	0.47
7:A:1808:PHE:HD1	7:A:1817:LEU:HD11	1.79	0.47
7:A:2003:THR:O	7:A:2007:ILE:HG13	2.14	0.47
7:A:2022:GLN:H	7:A:2022:GLN:CD	2.22	0.47
8:U:149:LYS:HD2	10:C:771:GLN:HB3	1.94	0.47
12:D:108:ASP:OD1	12:D:110:GLN:N	2.40	0.47
15:7:435:ASP:OD2	15:7:437:ARG:HG2	2.13	0.47
4:L:182:GLU:O	4:L:185:GLU:HG3	2.15	0.47
4:L:388:TYR:HE2	7:A:852:VAL:HB	1.79	0.47
7:A:639:PHE:HA	7:A:642:ARG:HG2	1.96	0.47
7:A:1963:GLU:HG2	7:A:1966:HIS:NE2	2.29	0.47
8:U:341:LYS:HG3	8:U:342:LYS:HG2	1.97	0.47
2:G:318:ARG:HD2	2:G:318:ARG:O	2.14	0.47
4:L:290:LYS:HG3	4:L:293:ARG:HH21	1.79	0.47
4:L:298:LYS:HB2	4:L:324:ILE:HD11	1.96	0.47
7:A:206:TRP:HZ2	7:A:234:MET:HE3	1.78	0.47
7:A:941:LYS:NZ	7:A:1071:PHE:HB2	2.28	0.47
7:A:952:VAL:HG22	7:A:1189:MET:HB3	1.95	0.47
7:A:1976:TRP:HA	7:A:1979:VAL:HG12	1.96	0.47
10:C:122:LEU:HG	10:C:199:LEU:HB2	1.96	0.47
4:L:246:ALA:HB2	4:L:300:THR:HG21	1.96	0.47
4:L:267:VAL:O	4:L:268:LEU:C	2.57	0.47
4:L:288:ARG:O	4:L:292:ALA:N	2.41	0.47
10:C:315:SER:OG	10:C:421:LYS:HG3	2.15	0.47
10:C:413:ARG:HB2	10:C:414:PRO:HD3	1.95	0.47
17:6:43:A:H2'	17:6:44:G:C8	2.48	0.47
4:L:103:ILE:HB	4:L:197:LEU:HD22	1.97	0.47
8:U:481:ARG:O	8:U:489:GLN:NE2	2.46	0.47
9:S:291:ASN:HD22	9:S:294:LEU:HD13	1.79	0.47
12:D:107:GLU:N	12:D:107:GLU:OE1	2.48	0.47
6:N:269:ASP:HB2	7:A:1916:LEU:HB3	1.97	0.47
7:A:494:LEU:HD21	7:A:562:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:634:TRP:NE1	7:A:638:LEU:HD11	2.30	0.47
7:A:691:HIS:HA	15:7:466:LEU:HD13	1.96	0.47
8:U:276:ARG:HA	8:U:279:GLU:HG2	1.95	0.47
8:U:515:ARG:HG2	8:U:530:GLN:HB2	1.97	0.47
10:C:135:CYS:SG	10:C:242:LEU:HD23	2.55	0.47
10:C:392:LEU:HB3	10:C:393:PRO:HD3	1.95	0.47
10:C:507:VAL:HG11	10:C:565:ILE:HD11	1.97	0.47
4:L:189:GLU:O	4:L:193:MET:HG2	2.15	0.47
4:L:243:LYS:HD2	11:M:72:LEU:HD13	1.97	0.47
5:F:121:LEU:N	5:F:124:GLU:OE1	2.48	0.47
6:N:914:ALA:O	6:N:918:ASP:N	2.48	0.47
7:A:384:VAL:HG12	10:C:331:PHE:CG	2.50	0.47
7:A:1314:VAL:HG21	7:A:1487:HIS:CG	2.50	0.47
7:A:1821:ILE:HG12	7:A:1913:GLN:O	2.15	0.47
10:C:215:VAL:O	10:C:219:LEU:HB2	2.15	0.47
10:C:566:THR:OG1	10:C:571:ASN:ND2	2.46	0.47
12:D:16:GLN:O	12:D:20:SER:N	2.46	0.47
4:L:242:SER:O	4:L:304:ARG:NE	2.33	0.47
5:F:88:ALA:HA	5:F:91:GLU:HG3	1.97	0.47
7:A:246:LEU:HD11	7:A:411:PHE:CE2	2.50	0.47
7:A:1090:ARG:HD3	7:A:1091:TYR:O	2.15	0.47
8:U:395:LEU:HD11	8:U:454:ILE:HG23	1.96	0.47
9:S:304:VAL:HG22	9:S:307:ARG:HH21	1.80	0.47
13:5:73:C:H2'	13:5:74:U:C6	2.49	0.47
6:N:265:GLN:HA	7:A:1965:HIS:HD2	1.80	0.47
7:A:1308:PRO:HG3	7:A:1548:TYR:CZ	2.50	0.47
10:C:828:MET:HA	10:C:905:GLN:O	2.15	0.47
4:L:99:LEU:O	4:L:103:ILE:HG23	2.15	0.46
7:A:166:PHE:HA	7:A:167:PRO:C	2.41	0.46
11:M:10:ALA:HB1	11:M:13:LEU:HB2	1.96	0.46
11:M:98:PRO:HD3	15:7:426:GLN:NE2	2.30	0.46
3:J:441:THR:O	3:J:445:GLN:HG2	2.16	0.46
5:F:109:LYS:O	5:F:113:ARG:HG2	2.15	0.46
7:A:331:TRP:O	7:A:333:HIS:N	2.44	0.46
7:A:988:ILE:HG12	7:A:1044:TYR:CE2	2.50	0.46
7:A:1190:CYS:O	7:A:1273:TYR:OH	2.28	0.46
4:L:215:ILE:HG13	4:L:216:ALA:N	2.31	0.46
6:N:30:THR:OG1	12:D:74:GLU:OE1	2.33	0.46
7:A:1275:ARG:NH1	7:A:1378:GLU:OE2	2.48	0.46
7:A:1629:ILE:HG23	7:A:1662:ILE:HB	1.97	0.46
7:A:1809:ILE:HG21	7:A:1848:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:470:ILE:HD13	8:U:546:GLU:HB3	1.97	0.46
10:C:369:PHE:CE2	10:C:374:LEU:HG	2.51	0.46
10:C:401:ILE:HD11	10:C:423:PHE:HB2	1.98	0.46
3:J:485:LEU:O	3:J:489:ALA:N	2.48	0.46
4:L:95:ASP:OD1	4:L:96:ALA:N	2.48	0.46
7:A:352:PHE:HZ	7:A:358:PRO:HA	1.81	0.46
7:A:1269:GLY:HA3	7:A:1452:PRO:HB2	1.97	0.46
8:U:448:PRO:C	8:U:449:TYR:HD1	2.24	0.46
1:B:47:LEU:HD13	7:A:1279:VAL:HG13	1.96	0.46
4:L:58:LYS:O	4:L:62:GLU:N	2.43	0.46
5:F:95:ARG:O	5:F:99:ILE:HG12	2.14	0.46
5:F:104:ASP:O	5:F:108:VAL:HG23	2.16	0.46
7:A:384:VAL:HG11	10:C:334:ILE:HD11	1.98	0.46
7:A:955:TRP:HE1	7:A:976:MET:CE	2.28	0.46
7:A:1586:HIS:NE2	7:A:1664:ILE:HG23	2.30	0.46
8:U:402:LYS:HE3	8:U:408:LEU:HG	1.98	0.46
10:C:181:ILE:HG13	10:C:182:LYS:N	2.29	0.46
10:C:534:VAL:O	10:C:534:VAL:HG13	2.15	0.46
17:6:47:A:OP2	17:6:47:A:H8	1.98	0.46
6:N:293:LYS:O	6:N:297:LEU:HG	2.15	0.46
7:A:318:TYR:HE2	7:A:329:LEU:HD21	1.81	0.46
7:A:1086:ARG:HD2	7:A:1100:ARG:HB3	1.96	0.46
7:A:1199:LYS:HE3	7:A:1199:LYS:HB3	1.83	0.46
7:A:1667:ARG:HD3	7:A:1679:TYR:CD2	2.50	0.46
10:C:142:LYS:O	10:C:146:VAL:HG23	2.16	0.46
10:C:245:HIS:O	10:C:249:GLU:HG2	2.16	0.46
10:C:664:GLU:HB3	10:C:820:PHE:CZ	2.51	0.46
12:D:8:LEU:HB2	12:D:61:VAL:HG22	1.97	0.46
1:B:41:LEU:O	7:A:1332:HIS:N	2.44	0.46
6:N:162:GLU:N	6:N:162:GLU:OE2	2.47	0.46
6:N:301:VAL:HG11	7:A:1839:TRP:CE3	2.51	0.46
7:A:1183:PRO:CB	7:A:1201:ARG:HD3	2.45	0.46
7:A:1625:SER:OG	7:A:1663:ASP:OD2	2.31	0.46
11:M:12:PRO:HG3	11:M:80:TYR:CD2	2.51	0.46
5:F:113:ARG:HA	5:F:113:ARG:CZ	2.45	0.46
6:N:138:ILE:HD12	15:7:476:ILE:HD12	1.98	0.46
6:N:247:ARG:HG2	6:N:282:PRO:HG2	1.96	0.46
6:N:374:ARG:O	6:N:377:ILE:HG22	2.16	0.46
7:A:169:PHE:CD1	7:A:559:ASP:HB3	2.51	0.46
7:A:331:TRP:HZ3	10:C:179:VAL:HB	1.81	0.46
7:A:750:TRP:HH2	7:A:781:ARG:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:170:LEU:HD21	8:U:193:LEU:HD11	1.98	0.46
10:C:396:LEU:HB3	10:C:401:ILE:O	2.15	0.46
12:D:94:LEU:HD12	12:D:136:TYR:CD1	2.51	0.46
17:6:32:U:H2'	17:6:33:G:H8	1.81	0.46
2:G:290:TYR:O	2:G:293:ARG:NH1	2.49	0.46
7:A:318:TYR:CE2	7:A:329:LEU:HD21	2.51	0.46
7:A:1317:TYR:HE1	7:A:1329:SER:HB3	1.80	0.46
8:U:538:LEU:HD23	8:U:538:LEU:H	1.80	0.46
10:C:129:ILE:HD11	10:C:201:ASN:HD21	1.81	0.46
10:C:148:CYS:SG	10:C:417:ARG:NH2	2.82	0.46
7:A:146:SER:O	7:A:149:ILE:HG22	2.16	0.46
7:A:1345:GLN:HB2	7:A:1711:LEU:HD22	1.98	0.46
7:A:1493:THR:HG22	7:A:1747:ILE:HG22	1.98	0.46
10:C:447:PRO:HA	10:C:450:GLU:HG2	1.98	0.46
16:4:6:U:H2'	16:4:7:G:H8	1.81	0.46
16:4:24:U:H1'	16:4:26:G:N7	2.31	0.46
4:L:160:THR:O	4:L:164:ILE:HG13	2.16	0.45
4:L:232:MET:HE2	4:L:238:LEU:HD13	1.98	0.45
4:L:269:PRO:HD2	4:L:289:ARG:NH2	2.31	0.45
6:N:181:PRO:HB3	7:A:1515:TRP:CZ2	2.51	0.45
7:A:516:LEU:HD22	7:A:524:LEU:HG	1.98	0.45
8:U:193:LEU:HD12	8:U:194:LYS:HB2	1.97	0.45
10:C:146:VAL:HG11	10:C:186:VAL:HG21	1.97	0.45
10:C:374:LEU:HD23	10:C:374:LEU:HA	1.82	0.45
10:C:584:THR:OG1	10:C:585:THR:N	2.49	0.45
7:A:89:LEU:HD13	7:A:656:LEU:HG	1.98	0.45
7:A:762:ARG:NH2	7:A:903:SER:O	2.50	0.45
7:A:1779:PHE:HE1	7:A:1812:PRO:HG3	1.81	0.45
10:C:726:LEU:HA	10:C:729:ALA:HB3	1.98	0.45
17:6:37:C:H2'	17:6:38:G:C8	2.51	0.45
4:L:141:GLU:OE1	4:L:142:LEU:HD12	2.16	0.45
6:N:278:ASN:HB2	6:N:344:ASP:OD1	2.17	0.45
6:N:309:PRO:N	6:N:310:PRO:HD2	2.31	0.45
7:A:380:LEU:HB2	10:C:354:ARG:HB3	1.99	0.45
7:A:598:LEU:HD11	7:A:640:PHE:HE1	1.81	0.45
7:A:974:ASN:OD1	7:A:1100:ARG:HD3	2.17	0.45
7:A:1644:LEU:HD23	7:A:1715:TYR:HB2	1.98	0.45
8:U:504:VAL:HG12	8:U:546:GLU:O	2.17	0.45
4:L:107:LEU:HA	4:L:110:ILE:HG12	1.99	0.45
4:L:361:LYS:HD3	16:4:18:G:N2	2.30	0.45
4:L:402:SER:HB2	6:N:292:LYS:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:91:GLU:HA	5:F:94:LYS:HG2	1.97	0.45
10:C:183:SER:OG	10:C:214:GLU:HB3	2.15	0.45
12:D:2:SER:HA	12:D:42:ASP:HB3	1.99	0.45
13:5:58:U:H2'	13:5:59:G:C8	2.52	0.45
5:F:101:VAL:HG21	5:F:134:ARG:HB2	1.98	0.45
6:N:123:ARG:NH2	13:5:52:U:OP1	2.49	0.45
7:A:844:GLU:O	7:A:848:GLU:HG2	2.16	0.45
7:A:1892:PRO:HD3	7:A:1941:ARG:NH2	2.31	0.45
8:U:265:PRO:HG3	8:U:337:THR:HG23	1.98	0.45
8:U:354:ARG:HB3	8:U:442:GLN:HB3	1.98	0.45
8:U:356:PHE:HD2	8:U:381:GLU:HB3	1.81	0.45
6:N:306:PRO:HB3	6:N:338:MET:HE3	1.98	0.45
7:A:109:PRO:HD3	7:A:630:TRP:CZ2	2.50	0.45
7:A:899:MET:HG3	7:A:906:VAL:HB	1.98	0.45
7:A:1790:ILE:HD11	7:A:1798:LEU:HD12	1.98	0.45
6:N:149:LEU:HD23	7:A:734:PRO:HB2	1.98	0.45
7:A:929:GLU:O	7:A:933:ARG:HG2	2.17	0.45
7:A:1077:ILE:HA	7:A:1080:GLU:OE1	2.16	0.45
7:A:1598:ASP:HA	7:A:1601:LEU:HD23	1.99	0.45
10:C:778:PRO:HG3	10:C:817:TYR:CG	2.51	0.45
17:6:51:U:HO2'	17:6:52:U:P	2.37	0.45
2:G:307:ILE:HB	2:G:312:GLN:NE2	2.32	0.45
7:A:86:ARG:NH1	7:A:89:LEU:HD11	2.32	0.45
7:A:353:ASP:OD1	7:A:353:ASP:N	2.49	0.45
10:C:384:VAL:HG12	10:C:392:LEU:HD11	1.98	0.45
14:z:14:C:H2'	14:z:15:A:H8	1.82	0.45
4:L:247:CYS:HB2	16:4:41:C:N4	2.29	0.45
5:F:104:ASP:HB2	5:F:107:GLU:HG2	1.99	0.45
6:N:324:LYS:HA	6:N:324:LYS:HD3	1.70	0.45
7:A:927:TRP:CD1	7:A:1439:ARG:HH21	2.35	0.45
7:A:1354:ARG:O	7:A:1357:MET:HE3	2.17	0.45
7:A:1863:VAL:CG1	7:A:1868:MET:HB3	2.44	0.45
7:A:1969:PRO:HB2	7:A:1971:LEU:HD11	1.99	0.45
10:C:129:ILE:HD11	10:C:201:ASN:ND2	2.31	0.45
1:B:51:ARG:NH1	7:A:1209:HIS:O	2.50	0.45
4:L:173:THR:HG23	4:L:173:THR:O	2.17	0.45
4:L:205:TYR:HE1	4:L:229:ALA:HB3	1.82	0.45
7:A:161:PHE:HZ	7:A:573:GLN:HA	1.82	0.45
7:A:164:MET:HE2	7:A:168:PRO:HB3	1.98	0.45
7:A:1592:ASP:O	9:S:328:GLN:NE2	2.50	0.45
7:A:1661:TRP:CE2	7:A:1700:GLY:HA3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1889:LEU:HA	7:A:2014:MET:HE3	1.98	0.45
8:U:457:PHE:CD1	8:U:509:PRO:HG3	2.52	0.45
10:C:797:ALA:HB3	10:C:803:ARG:HB3	1.99	0.45
10:C:834:VAL:HG11	10:C:883:PHE:HE2	1.82	0.45
2:G:303:PHE:HB3	2:G:312:GLN:OE1	2.17	0.44
7:A:684:GLU:OE2	15:7:473:ARG:NH2	2.38	0.44
7:A:1645:LEU:HG	7:A:1727:GLN:NE2	2.32	0.44
7:A:1701:VAL:HA	7:A:1716:GLY:HA3	1.98	0.44
8:U:122:LYS:NZ	8:U:298:GLU:OE2	2.49	0.44
8:U:459:LYS:HG3	8:U:464:VAL:HG22	1.99	0.44
10:C:152:GLN:OE1	10:C:427:PHE:HB2	2.17	0.44
10:C:243:ILE:HG13	10:C:244:LYS:N	2.32	0.44
10:C:936:LYS:O	10:C:940:ARG:N	2.44	0.44
5:F:113:ARG:HH12	5:F:116:GLY:C	2.25	0.44
7:A:1661:TRP:NE1	7:A:1699:THR:O	2.50	0.44
10:C:465:MET:HE1	10:C:498:SER:HB3	1.99	0.44
12:D:29:ARG:HB3	12:D:60:LEU:HD22	1.99	0.44
4:L:359:TYR:OH	17:6:53:A:OP2	2.31	0.44
6:N:178:LYS:N	16:4:19:U:O4	2.51	0.44
7:A:784:LEU:HB2	7:A:1022:MET:HE3	1.98	0.44
7:A:839:LEU:HD22	7:A:878:LEU:HG	1.98	0.44
7:A:1308:PRO:HB2	7:A:1310:ARG:O	2.18	0.44
7:A:2020:SER:HA	7:A:2022:GLN:HE22	1.81	0.44
8:U:246:VAL:HG13	8:U:449:TYR:CD2	2.52	0.44
8:U:278:GLY:O	8:U:282:ARG:HG3	2.18	0.44
8:U:516:ILE:HG22	8:U:518:VAL:HG13	1.99	0.44
9:S:186:LYS:HD2	9:S:186:LYS:HA	1.81	0.44
10:C:365:SER:OG	10:C:366:GLN:N	2.50	0.44
10:C:477:HIS:HB2	10:C:577:PHE:CE2	2.52	0.44
10:C:571:ASN:HB3	10:C:574:ALA:HB2	2.00	0.44
10:C:683:ASN:OD1	10:C:797:ALA:N	2.50	0.44
4:L:91:ARG:NE	4:L:91:ARG:HA	2.31	0.44
4:L:413:ASN:OD1	4:L:414:GLU:N	2.50	0.44
6:N:121:GLU:O	6:N:124:GLU:HG2	2.18	0.44
7:A:419:ARG:NH2	7:A:423:ASP:O	2.49	0.44
7:A:1455:TRP:H	7:A:1455:TRP:CD1	2.34	0.44
8:U:208:GLN:NE2	8:U:210:LYS:O	2.34	0.44
8:U:403:ASP:HB3	8:U:406:GLU:O	2.18	0.44
10:C:261:ASP:OD1	10:C:262:ARG:N	2.49	0.44
11:M:10:ALA:HA	11:M:82:PHE:HE2	1.83	0.44
11:M:52:GLU:O	11:M:79:PRO:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:61:GLU:HG2	11:M:62:PRO:HD3	2.00	0.44
7:A:1636:LYS:HB3	7:A:1656:THR:OG1	2.18	0.44
8:U:128:LEU:HD22	10:C:619:THR:HG21	1.98	0.44
6:N:250:LEU:HD21	7:A:1847:ALA:HB2	1.99	0.44
6:N:375:ILE:H	6:N:375:ILE:HD12	1.82	0.44
7:A:119:LEU:HD21	7:A:476:PHE:HB3	2.00	0.44
8:U:239:VAL:HG21	8:U:322:PHE:CE2	2.53	0.44
10:C:556:ASP:OD1	10:C:556:ASP:N	2.51	0.44
8:U:144:GLN:NE2	8:U:150:SER:HB3	2.33	0.44
8:U:356:PHE:HB3	8:U:381:GLU:HB3	1.98	0.44
4:L:417:LYS:HG3	7:A:868:GLU:OE2	2.18	0.44
7:A:73:HIS:HA	7:A:81:PHE:CZ	2.52	0.44
10:C:174:GLU:HB2	10:C:179:VAL:O	2.18	0.44
10:C:670:SER:HB2	10:C:822:MET:HB3	2.00	0.44
6:N:302:ARG:HD3	6:N:312:TRP:CZ3	2.52	0.44
7:A:943:ALA:HB3	7:A:1438:VAL:HG22	2.00	0.44
7:A:975:VAL:HG11	7:A:1153:VAL:HG21	2.00	0.44
7:A:1180:LYS:O	7:A:1201:ARG:NH2	2.51	0.44
16:4:16:C:H2'	16:4:17:A:C8	2.52	0.44
2:G:250:ILE:HG12	7:A:307:PRO:HB3	2.00	0.43
2:G:347:GLU:O	2:G:351:ARG:HG3	2.18	0.43
4:L:423:THR:O	4:L:427:THR:HG23	2.18	0.43
8:U:355:ILE:HB	8:U:384:VAL:HB	2.00	0.43
4:L:267:VAL:O	4:L:267:VAL:HG13	2.18	0.43
6:N:319:GLU:HB3	6:N:328:ALA:HB2	2.00	0.43
7:A:103:LEU:HB3	7:A:638:LEU:HD21	1.99	0.43
7:A:927:TRP:CH2	7:A:1042:GLN:HG3	2.53	0.43
8:U:228:ASN:HB2	8:U:295:SER:HA	1.99	0.43
9:S:257:LEU:HD13	9:S:289:LEU:HD13	1.99	0.43
10:C:140:HIS:CE1	10:C:230:ASP:H	2.36	0.43
11:M:11:TYR:HB3	11:M:12:PRO:HD3	2.01	0.43
13:5:77:G:H4'	13:5:78:U:OP1	2.18	0.43
4:L:133:LEU:HG	4:L:198:ASN:HD22	1.83	0.43
6:N:313:ILE:O	6:N:317:ARG:HG2	2.18	0.43
7:A:226:GLN:NE2	13:5:59:G:OP1	2.49	0.43
7:A:251:ASP:HB3	7:A:337:VAL:HG22	2.00	0.43
8:U:498:ASP:OD2	8:U:555:ARG:NH1	2.52	0.43
9:S:207:SER:OG	9:S:211:GLN:NE2	2.51	0.43
10:C:733:TRP:HB2	10:C:745:LEU:HD22	2.00	0.43
10:C:800:PRO:HA	10:C:803:ARG:HE	1.83	0.43
17:6:36:A:H2'	17:6:37:C:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:221:ILE:HD11	4:L:317:GLY:HA3	2.00	0.43
7:A:902:TYR:HB2	7:A:1242:ASN:ND2	2.34	0.43
8:U:393:LEU:HB3	8:U:418:ILE:HG21	1.99	0.43
10:C:183:SER:HB3	10:C:203:MET:SD	2.58	0.43
10:C:208:HIS:HB3	10:C:211:PHE:HD1	1.82	0.43
10:C:348:TYR:HE1	10:C:367:ARG:HD2	1.83	0.43
10:C:434:CYS:O	10:C:438:ILE:HG12	2.18	0.43
6:N:31:ARG:HG2	6:N:34:ILE:HG22	2.01	0.43
7:A:443:VAL:HG11	7:A:614:TYR:CZ	2.54	0.43
7:A:1808:PHE:HZ	7:A:1897:LEU:HB2	1.82	0.43
8:U:146:ARG:HG2	8:U:175:LEU:HD11	2.00	0.43
8:U:224:ILE:HD13	8:U:527:TYR:CD2	2.53	0.43
8:U:530:GLN:HB3	8:U:533:GLN:HG2	2.01	0.43
10:C:369:PHE:CD1	10:C:373:ILE:HD12	2.53	0.43
10:C:692:LEU:HD22	10:C:696:LEU:HD23	2.00	0.43
10:C:779:LEU:HD22	10:C:912:LEU:HD21	2.00	0.43
4:L:219:LEU:HD21	4:L:231:ILE:HD11	2.01	0.43
7:A:902:TYR:CE2	7:A:1246:GLN:HB3	2.54	0.43
7:A:955:TRP:NE1	7:A:959:ILE:HD11	2.34	0.43
7:A:1757:GLU:N	7:A:1758:PRO:HD3	2.34	0.43
8:U:205:LEU:HB3	8:U:250:ARG:NH2	2.33	0.43
10:C:192:ASP:OD1	10:C:432:ASP:HB3	2.18	0.43
11:M:22:LEU:O	11:M:26:VAL:HG23	2.19	0.43
15:7:458:PRO:O	15:7:462:ILE:HD12	2.19	0.43
7:A:161:PHE:CZ	7:A:573:GLN:HA	2.54	0.43
7:A:479:THR:HG22	7:A:481:PHE:H	1.82	0.43
8:U:234:ASP:N	8:U:234:ASP:OD1	2.52	0.43
8:U:411:PRO:HG2	8:U:469:THR:HA	2.01	0.43
8:U:494:ASN:O	8:U:554:ARG:NH2	2.51	0.43
10:C:834:VAL:HG11	10:C:883:PHE:CE2	2.54	0.43
2:G:308:ASP:HB2	7:A:152:ARG:NH2	2.33	0.43
7:A:1371:TYR:OH	7:A:1473:ASP:OD2	2.30	0.43
7:A:1424:GLN:OE1	7:A:1459:ARG:NE	2.45	0.43
7:A:1456:THR:OG1	7:A:1457:HIS:N	2.52	0.43
7:A:1945:VAL:HG12	7:A:1946:ASN:ND2	2.33	0.43
8:U:129:SER:OG	8:U:131:ILE:HG12	2.19	0.43
8:U:197:PHE:HZ	8:U:286:ASN:HA	1.83	0.43
11:M:61:GLU:CD	11:M:62:PRO:HD3	2.43	0.43
7:A:76:MET:HE1	7:A:85:LYS:HD2	2.00	0.43
7:A:442:LYS:HE3	7:A:614:TYR:OH	2.19	0.43
7:A:1125:ILE:HG13	7:A:1147:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:696:LEU:O	10:C:700:ILE:HG12	2.19	0.43
11:M:13:LEU:HA	11:M:82:PHE:HB2	2.00	0.43
12:D:31:GLY:O	12:D:62:ASP:HA	2.18	0.43
2:G:306:GLY:HA3	7:A:615:ARG:HD2	2.00	0.43
4:L:100:THR:HA	4:L:103:ILE:HG12	2.00	0.43
6:N:308:HIS:CD2	6:N:310:PRO:HG2	2.54	0.43
7:A:960:ASN:ND2	7:A:1216:LEU:HB3	2.34	0.43
7:A:1017:ILE:HD11	7:A:1031:ILE:HD11	1.99	0.43
7:A:1670:ASP:O	7:A:1674:HIS:HB3	2.18	0.43
7:A:1806:ALA:HB1	7:A:1819:LEU:HG	2.00	0.43
7:A:1846:ALA:HB2	7:A:1875:HIS:HB3	2.00	0.43
10:C:336:TYR:O	10:C:340:ALA:HB2	2.19	0.43
10:C:568:PRO:O	10:C:569:ARG:HG2	2.19	0.43
11:M:18:LEU:HD23	11:M:18:LEU:H	1.84	0.43
2:G:324:MET:HE1	7:A:355:LEU:HA	2.01	0.42
4:L:97:ASN:O	4:L:100:THR:HG22	2.19	0.42
6:N:364:GLN:HG2	6:N:367:ARG:HD2	2.00	0.42
7:A:943:ALA:HB1	7:A:1437:ARG:CB	2.49	0.42
7:A:1481:VAL:HG12	7:A:1485:LEU:HD22	2.01	0.42
7:A:1667:ARG:N	7:A:1705:ILE:O	2.52	0.42
8:U:101:ARG:O	8:U:101:ARG:HG3	2.19	0.42
10:C:277:LYS:HD3	10:C:865:GLY:HA3	2.00	0.42
10:C:452:THR:HG22	10:C:577:PHE:HD1	1.84	0.42
10:C:743:ASN:HD21	10:C:784:ILE:C	2.27	0.42
4:L:219:LEU:HD12	4:L:303:ALA:HB2	2.00	0.42
6:N:297:LEU:HD23	9:S:282:LEU:HD21	2.01	0.42
7:A:221:ASN:OD1	7:A:222:GLY:N	2.52	0.42
7:A:384:VAL:HA	10:C:331:PHE:CD1	2.54	0.42
7:A:533:LYS:NZ	14:z:4:A:OP1	2.51	0.42
7:A:1961:ILE:HD12	7:A:1961:ILE:H	1.84	0.42
8:U:353:MET:O	8:U:385:GLU:HA	2.18	0.42
10:C:323:PHE:CD2	10:C:373:ILE:HG12	2.54	0.42
13:5:60:G:H2'	13:5:61:A:C8	2.54	0.42
15:7:440:GLU:O	15:7:444:ARG:N	2.52	0.42
4:L:251:LEU:HD12	16:4:40:U:H5'	2.00	0.42
4:L:356:GLY:H	4:L:359:TYR:HB3	1.84	0.42
5:F:91:GLU:O	5:F:95:ARG:HG2	2.19	0.42
5:F:112:LEU:HD22	5:F:117:GLU:HB2	2.01	0.42
7:A:1137:ASP:OD1	7:A:1138:ALA:N	2.52	0.42
7:A:1415:GLY:O	7:A:1418:ARG:HD3	2.20	0.42
7:A:1842:ALA:HA	7:A:1845:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:356:PHE:HB2	8:U:440:ARG:CG	2.49	0.42
10:C:159:LYS:HG2	10:C:160:ARG:O	2.19	0.42
10:C:227:LEU:HD22	10:C:239:THR:HG23	2.00	0.42
2:G:348:ALA:HB2	2:G:351:ARG:HH21	1.83	0.42
7:A:235:MET:HE3	7:A:235:MET:HB3	1.79	0.42
7:A:515:TYR:CZ	7:A:534:GLU:HB3	2.55	0.42
10:C:925:PRO:HD2	10:C:928:HIS:HD1	1.83	0.42
11:M:97:ARG:HD2	11:M:97:ARG:HA	1.83	0.42
16:4:22:C:H2'	16:4:23:G:C8	2.54	0.42
4:L:157:GLN:HG2	4:L:158:ILE:HG13	2.00	0.42
7:A:136:ILE:HB	7:A:139:VAL:HB	2.00	0.42
7:A:510:ARG:HG3	7:A:511:LYS:HG2	2.01	0.42
7:A:1140:MET:HB2	7:A:1186:LEU:HD13	2.02	0.42
7:A:1692:MET:SD	7:A:1692:MET:N	2.92	0.42
7:A:1903:GLY:O	7:A:1907:LEU:HG	2.19	0.42
8:U:320:VAL:HA	8:U:323:LEU:CD2	2.50	0.42
10:C:641:MET:HE3	10:C:641:MET:HB3	1.73	0.42
7:A:171:ASP:C	7:A:173:GLU:N	2.77	0.42
7:A:1667:ARG:HD3	7:A:1679:TYR:CE2	2.54	0.42
7:A:1771:LEU:HD11	7:A:1779:PHE:CZ	2.54	0.42
9:S:263:ILE:HD12	9:S:263:ILE:H	1.84	0.42
12:D:92:ILE:HG13	12:D:130:VAL:HG23	2.00	0.42
4:L:193:MET:HE3	4:L:193:MET:HB2	1.89	0.42
7:A:223:SER:OG	13:5:12:U:H5''	2.20	0.42
7:A:549:GLU:OE1	7:A:552:ARG:NH2	2.47	0.42
7:A:750:TRP:CZ2	7:A:778:ARG:HG2	2.54	0.42
7:A:817:LEU:HD12	7:A:822:PHE:CD2	2.55	0.42
7:A:1019:TYR:CG	7:A:1020:LYS:N	2.87	0.42
7:A:1650:ASP:N	7:A:1650:ASP:OD1	2.53	0.42
7:A:1957:ASP:O	7:A:1960:THR:OG1	2.29	0.42
8:U:350:GLN:HE21	8:U:387:THR:HB	1.85	0.42
10:C:590:ILE:HG22	10:C:658:PRO:HA	2.02	0.42
11:M:63:LEU:HD12	11:M:63:LEU:H	1.84	0.42
13:5:19:A:H4'	13:5:20:G:C8	2.55	0.42
7:A:137:GLU:N	7:A:138:PRO:HD2	2.35	0.42
7:A:180:ASP:OD1	7:A:181:ASN:N	2.52	0.42
7:A:881:ILE:HG21	7:A:921:TYR:CD2	2.55	0.42
7:A:901:LEU:O	7:A:1242:ASN:ND2	2.50	0.42
7:A:1594:CYS:SG	7:A:1629:ILE:HD12	2.59	0.42
7:A:1830:GLN:HG3	7:A:1836:LEU:HD13	2.02	0.42
10:C:134:LEU:HD22	10:C:228:PHE:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:61:GLU:CD	11:M:61:GLU:H	2.28	0.42
11:M:73:CYS:HB3	11:M:78:VAL:O	2.20	0.42
12:D:29:ARG:HE	12:D:42:ASP:CG	2.28	0.42
12:D:48:ILE:O	12:D:52:VAL:HG22	2.20	0.42
3:J:489:ALA:HB2	3:J:496:VAL:HG11	2.02	0.42
6:N:309:PRO:O	6:N:313:ILE:HG12	2.20	0.42
7:A:439:GLN:OE1	7:A:614:TYR:HD2	2.03	0.42
7:A:583:ALA:HB1	7:A:609:LYS:HD2	2.01	0.42
7:A:1486:GLU:O	7:A:1709:TYR:OH	2.23	0.42
7:A:1773:SER:OG	7:A:1774:ASN:N	2.53	0.42
10:C:283:ASP:OD1	10:C:284:GLU:N	2.53	0.42
10:C:291:MET:N	10:C:291:MET:HE2	2.34	0.42
10:C:496:VAL:O	10:C:547:GLY:N	2.40	0.42
16:4:30:A:N6	16:4:44:A:H2'	2.35	0.42
4:L:234:VAL:HG13	4:L:252:LEU:HD22	2.02	0.42
4:L:390:GLU:OE1	7:A:1451:ASN:ND2	2.46	0.42
6:N:146:LYS:O	7:A:696:MET:HE3	2.20	0.42
7:A:816:TRP:CD1	7:A:817:LEU:HD22	2.49	0.42
7:A:1699:THR:HA	7:A:1717:ASN:OD1	2.20	0.42
7:A:1788:VAL:HG12	7:A:1802:PRO:HA	2.02	0.42
10:C:593:GLU:HG3	10:C:594:PRO:CD	2.50	0.42
14:z:3:A:H2'	14:z:4:A:C8	2.55	0.42
15:7:475:ASP:N	15:7:475:ASP:OD1	2.52	0.42
3:J:448:LEU:HD12	15:7:433:LEU:HD21	2.01	0.41
4:L:69:GLU:HA	4:L:203:ARG:HH12	1.85	0.41
4:L:122:PHE:CE1	4:L:171:ALA:HA	2.55	0.41
6:N:206:GLN:HB3	7:A:1386:TRP:CZ3	2.55	0.41
7:A:246:LEU:HD11	7:A:411:PHE:CD2	2.55	0.41
7:A:331:TRP:HH2	10:C:138:LEU:HD21	1.85	0.41
7:A:942:PRO:HB3	7:A:1092:ILE:N	2.34	0.41
7:A:1038:SER:HA	7:A:1442:PHE:CE2	2.55	0.41
7:A:1051:LEU:HB2	7:A:1161:LEU:HD23	2.02	0.41
7:A:1564:GLY:H	14:z:1:G:N2	2.18	0.41
7:A:1637:TRP:O	7:A:1656:THR:HA	2.19	0.41
7:A:1973:ASP:O	7:A:1977:ILE:HG12	2.20	0.41
10:C:342:ARG:O	10:C:347:ILE:HD11	2.20	0.41
10:C:531:TRP:HB3	10:C:540:GLU:HA	2.02	0.41
3:J:471:PRO:HA	3:J:472:PRO:HD3	1.94	0.41
4:L:278:ASP:OD1	4:L:279:ILE:N	2.54	0.41
5:F:112:LEU:O	5:F:116:GLY:N	2.41	0.41
7:A:287:ASN:OD1	7:A:287:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1940:LEU:HD13	7:A:1940:LEU:HA	1.95	0.41
8:U:457:PHE:HZ	8:U:505:HIS:CD2	2.38	0.41
9:S:329:LYS:HA	9:S:329:LYS:HD3	1.88	0.41
10:C:699:ASP:OD2	10:C:722:TYR:OH	2.34	0.41
1:B:40:VAL:HG12	7:A:1289:VAL:HG13	2.02	0.41
2:G:338:ALA:O	2:G:341:ARG:HG2	2.20	0.41
4:L:100:THR:O	4:L:103:ILE:HG12	2.20	0.41
5:F:88:ALA:O	5:F:91:GLU:HG3	2.21	0.41
6:N:358:ALA:HB1	6:N:382:LEU:HD21	2.02	0.41
7:A:136:ILE:HG22	7:A:138:PRO:HD2	2.03	0.41
7:A:355:LEU:O	10:C:867:PRO:HB3	2.20	0.41
7:A:993:LEU:HD11	7:A:1040:ILE:HG23	2.02	0.41
7:A:1508:GLY:HA2	7:A:1511:GLU:HG2	2.02	0.41
7:A:1788:VAL:HA	7:A:1802:PRO:HA	2.01	0.41
9:S:346:PRO:HB2	9:S:347:HIS:H	1.72	0.41
10:C:137:HIS:HB3	10:C:140:HIS:CE1	2.55	0.41
10:C:203:MET:HB2	10:C:549:TRP:CH2	2.55	0.41
12:D:41:MET:HE2	12:D:41:MET:HB3	1.86	0.41
12:D:41:MET:HB2	12:D:105:ALA:HB1	2.02	0.41
16:4:19:U:H5'	16:4:54:A:O2'	2.21	0.41
2:G:253:ARG:HD2	7:A:313:LYS:HZ3	1.85	0.41
3:J:497:GLU:HG2	7:A:1927:ILE:HD11	2.01	0.41
7:A:203:VAL:O	7:A:207:PHE:HB2	2.20	0.41
7:A:720:TRP:CZ2	7:A:747:ALA:HB1	2.56	0.41
7:A:1537:TRP:CE3	7:A:1751:LEU:HD13	2.53	0.41
13:5:67:A:H3'	13:5:69:A:OP1	2.21	0.41
4:L:313:GLU:HG2	4:L:315:LYS:HG2	2.03	0.41
7:A:428:LYS:HD2	7:A:431:TYR:OH	2.21	0.41
7:A:724:ILE:HD13	7:A:724:ILE:HA	1.91	0.41
7:A:964:ASP:C	7:A:1100:ARG:HH12	2.28	0.41
10:C:733:TRP:CD1	10:C:763:LYS:HE2	2.54	0.41
13:5:75:G:H2'	13:5:76:A:C8	2.55	0.41
6:N:142:PHE:HB3	7:A:738:MET:HE3	2.01	0.41
7:A:118:VAL:HG21	7:A:487:LEU:HB2	2.03	0.41
7:A:169:PHE:HZ	7:A:562:VAL:HG11	1.84	0.41
7:A:331:TRP:CZ3	10:C:179:VAL:HB	2.56	0.41
7:A:370:PRO:HD2	10:C:303:LEU:HD11	2.02	0.41
7:A:1807:ILE:HD13	7:A:1841:THR:HA	2.02	0.41
8:U:312:GLN:NE2	10:C:599:GLU:OE2	2.53	0.41
8:U:427:GLU:HB3	8:U:440:ARG:HB3	2.03	0.41
10:C:354:ARG:HA	10:C:354:ARG:HD3	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:594:PRO:HD3	10:C:603:MET:SD	2.61	0.41
4:L:253:GLY:HA3	4:L:273:TYR:CE2	2.55	0.41
4:L:365:ARG:HH22	16:4:18:G:P	2.44	0.41
7:A:816:TRP:O	7:A:820:ARG:HG2	2.21	0.41
8:U:360:LEU:N	8:U:361:PRO:HD3	2.36	0.41
10:C:264:ILE:HG12	10:C:378:TYR:CE1	2.55	0.41
2:G:298:LEU:HD21	7:A:248:ASP:O	2.20	0.41
3:J:449:ARG:NH1	3:J:453:ARG:HG3	2.36	0.41
4:L:207:TYR:CE1	4:L:211:ARG:HG3	2.55	0.41
7:A:366:LYS:HG3	7:A:368:GLN:HG2	2.03	0.41
7:A:384:VAL:HG12	10:C:331:PHE:HB3	2.03	0.41
7:A:388:LEU:HD21	10:C:395:THR:OG1	2.21	0.41
7:A:1044:TYR:CD2	7:A:1048:MET:HE1	2.56	0.41
7:A:1732:LYS:NZ	9:S:327:GLN:O	2.47	0.41
10:C:841:ASP:N	10:C:841:ASP:OD1	2.53	0.41
15:7:427:GLU:O	15:7:431:ILE:HG22	2.21	0.41
17:6:74:U:H2'	17:6:75:G:C8	2.55	0.41
2:G:368:ARG:HA	2:G:371:ARG:HE	1.86	0.41
4:L:159:LEU:HB2	4:L:164:ILE:HG12	2.02	0.41
5:F:94:LYS:O	5:F:97:ARG:HG2	2.21	0.41
7:A:86:ARG:HH12	7:A:89:LEU:HD11	1.86	0.41
7:A:89:LEU:HB2	7:A:656:LEU:HD21	2.02	0.41
7:A:95:MET:CE	7:A:551:LEU:HD11	2.50	0.41
7:A:106:MET:HE1	7:A:582:PHE:HE2	1.86	0.41
7:A:164:MET:HE1	7:A:560:SER:HA	2.03	0.41
7:A:488:ASP:OD1	7:A:489:TRP:N	2.53	0.41
7:A:596:TYR:HB3	13:5:45:C:H4'	2.01	0.41
7:A:888:GLN:O	7:A:889:ARG:NH1	2.47	0.41
7:A:928:TYR:CZ	7:A:932:LYS:HD2	2.55	0.41
7:A:985:TYR:CG	7:A:1032:ARG:HD3	2.56	0.41
7:A:1128:TYR:CD1	7:A:1147:VAL:HG13	2.56	0.41
7:A:1299:ILE:HG21	7:A:1316:PHE:HE1	1.86	0.41
7:A:1490:PHE:O	7:A:1493:THR:OG1	2.32	0.41
7:A:1642:PRO:HA	7:A:1716:GLY:C	2.46	0.41
7:A:1672:ASP:OD1	7:A:1672:ASP:N	2.53	0.41
8:U:231:LYS:HE3	8:U:314:THR:HA	2.03	0.41
8:U:235:TYR:O	8:U:239:VAL:HG22	2.21	0.41
8:U:446:LEU:HD23	8:U:446:LEU:HA	1.95	0.41
9:S:208:ARG:HD3	9:S:208:ARG:HA	1.82	0.41
10:C:303:LEU:HA	10:C:320:LEU:HD12	2.03	0.41
11:M:10:ALA:HA	11:M:82:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:392:LEU:HD11	7:A:1264:ASN:HB2	2.02	0.41
6:N:175:ARG:HD3	16:4:52:U:C4	2.56	0.41
7:A:171:ASP:O	7:A:173:GLU:N	2.54	0.41
7:A:537:LYS:HE3	7:A:537:LYS:HB2	1.79	0.41
7:A:1663:ASP:OD2	7:A:1695:TYR:OH	2.36	0.41
8:U:170:LEU:HD23	8:U:170:LEU:HA	1.93	0.41
10:C:141:GLY:HA3	10:C:258:ASN:ND2	2.36	0.41
10:C:882:GLY:O	10:C:886:ASP:N	2.43	0.41
12:D:91:MET:O	12:D:129:LEU:HA	2.21	0.41
5:F:89:GLU:O	5:F:93:ARG:HG3	2.21	0.40
5:F:108:VAL:O	5:F:112:LEU:HG	2.21	0.40
6:N:250:LEU:HD21	6:N:252:ASP:HB3	2.03	0.40
7:A:100:LEU:HD13	7:A:641:MET:HB3	2.03	0.40
7:A:405:LEU:HD21	10:C:412:ILE:HG21	2.02	0.40
7:A:835:ASP:OD1	7:A:878:LEU:HD22	2.21	0.40
10:C:146:VAL:O	10:C:150:ILE:HG12	2.21	0.40
10:C:382:ALA:O	10:C:386:GLY:N	2.53	0.40
10:C:929:LEU:HD22	10:C:933:PHE:CZ	2.55	0.40
2:G:276:TRP:CE2	7:A:449:LYS:HG3	2.56	0.40
5:F:86:VAL:HG22	5:F:90:PHE:CE1	2.57	0.40
7:A:67:ARG:HH12	7:A:183:LEU:HD22	1.86	0.40
7:A:270:ASN:ND2	7:A:281:PRO:HB3	2.36	0.40
7:A:927:TRP:HH2	7:A:1042:GLN:HG3	1.86	0.40
7:A:1311:PHE:HA	7:A:1312:PRO:HD3	1.92	0.40
7:A:1465:TRP:CE3	7:A:1467:LEU:HD13	2.56	0.40
2:G:363:ASP:OD1	2:G:363:ASP:N	2.52	0.40
7:A:422:LEU:CD2	7:A:638:LEU:HD13	2.51	0.40
7:A:1260:VAL:HG12	7:A:1264:ASN:HD21	1.86	0.40
8:U:357:THR:HG23	8:U:439:LYS:HG2	2.03	0.40
10:C:555:VAL:O	10:C:558:PRO:HD2	2.21	0.40
13:5:66:A:H2'	13:5:67:A:H8	1.86	0.40
16:4:36:U:H2'	16:4:37:C:C6	2.56	0.40
7:A:270:ASN:HD22	7:A:281:PRO:HB3	1.86	0.40
7:A:1922:ASP:O	7:A:1925:LYS:HB2	2.22	0.40
4:L:297:ALA:O	4:L:300:THR:HG22	2.20	0.40
6:N:326:GLN:NE2	9:S:177:LYS:HB2	2.37	0.40
7:A:850:TYR:CE1	7:A:860:GLN:HG2	2.57	0.40
10:C:373:ILE:C	10:C:376:PRO:HD2	2.46	0.40
10:C:436:GLN:HG3	10:C:437:HIS:ND1	2.36	0.40
10:C:911:PRO:HB2	10:C:934:MET:SD	2.62	0.40
11:M:62:PRO:O	11:M:65:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:6:43:A:H2'	17:6:44:G:O4'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	20/2136 (1%)	20 (100%)	0	0	100	100
2	G	118/820 (14%)	117 (99%)	1 (1%)	0	100	100
3	J	83/683 (12%)	83 (100%)	0	0	100	100
4	L	372/499 (74%)	364 (98%)	8 (2%)	0	100	100
5	F	59/522 (11%)	56 (95%)	3 (5%)	0	100	100
6	N	447/941 (48%)	433 (97%)	14 (3%)	0	100	100
7	A	1965/2335 (84%)	1899 (97%)	65 (3%)	1 (0%)	48	78
8	U	454/565 (80%)	435 (96%)	19 (4%)	0	100	100
9	S	138/800 (17%)	138 (100%)	0	0	100	100
10	C	834/972 (86%)	803 (96%)	31 (4%)	0	100	100
11	M	122/128 (95%)	118 (97%)	4 (3%)	0	100	100
12	D	139/142 (98%)	131 (94%)	8 (6%)	0	100	100
15	7	79/793 (10%)	78 (99%)	1 (1%)	0	100	100
All	All	4830/11336 (43%)	4675 (97%)	154 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	172	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	17/1908 (1%)	17 (100%)	0	100	100
2	G	113/721 (16%)	113 (100%)	0	100	100
3	J	70/599 (12%)	70 (100%)	0	100	100
4	L	299/424 (70%)	298 (100%)	1 (0%)	86	83
5	F	52/442 (12%)	51 (98%)	1 (2%)	50	65
6	N	233/792 (29%)	233 (100%)	0	100	100
7	A	1786/2108 (85%)	1786 (100%)	0	100	100
8	U	418/511 (82%)	418 (100%)	0	100	100
9	S	121/681 (18%)	121 (100%)	0	100	100
10	C	738/866 (85%)	738 (100%)	0	100	100
11	M	108/111 (97%)	108 (100%)	0	100	100
12	D	129/130 (99%)	129 (100%)	0	100	100
15	7	71/709 (10%)	71 (100%)	0	100	100
All	All	4155/10002 (42%)	4153 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	271	THR
5	F	104	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	350	GLN
3	J	511	HIS
3	J	515	ASN
4	L	97	ASN
4	L	398	HIS

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Mol	Chain	Res	Type
6	N	278	ASN
6	N	307	HIS
6	N	326	GLN
7	A	521	ASN
7	A	573	GLN
7	A	723	ASN
7	A	752	ASN
7	A	873	ASN
7	A	963	GLN
7	A	1522	GLN
7	A	1580	HIS
7	A	1583	GLN
7	A	1599	GLN
7	A	1737	ASN
7	A	1830	GLN
7	A	1965	HIS
7	A	1966	HIS
7	A	2004	GLN
7	A	2022	GLN
8	U	112	ASN
8	U	144	GLN
8	U	251	ASN
8	U	275	GLN
8	U	316	GLN
8	U	372	GLN
8	U	380	GLN
8	U	460	ASN
9	S	211	GLN
9	S	291	ASN
10	C	210	ASN
10	C	238	ASN
10	C	248	GLN
10	C	702	ASN
10	C	719	GLN
10	C	890	HIS
10	C	924	GLN
12	D	7	HIS

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	5	78/117 (66%)	25 (32%)	2 (2%)
14	z	17/18 (94%)	5 (29%)	0
16	4	61/144 (42%)	17 (27%)	0
17	6	46/106 (43%)	10 (21%)	3 (6%)
All	All	202/385 (52%)	57 (28%)	5 (2%)

All (57) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	5	8	G
13	5	9	G
13	5	10	U
13	5	20	G
13	5	21	A
13	5	22	U
13	5	23	C
13	5	24	G
13	5	26	A
13	5	28	A
13	5	36	C
13	5	40	U
13	5	41	U
13	5	44	A
13	5	45	C
13	5	47	A
13	5	57	G
13	5	68	C
13	5	69	A
13	5	71	C
13	5	72	U
13	5	75	G
13	5	78	U
13	5	79	C
13	5	80	U
14	z	-2	A
14	z	1	G
14	z	3	A
14	z	5	G
14	z	8	U
16	4	11	A
16	4	20	A

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Mol	Chain	Res	Type
16	4	25	A
16	4	26	G
16	4	33	A
16	4	36	U
16	4	39	A
16	4	40	U
16	4	41	C
16	4	42	C
16	4	44	A
16	4	45	G
16	4	53	U
16	4	54	A
16	4	55	U
16	4	58	C
16	4	61	A
17	6	40	U
17	6	46	G
17	6	47	A
17	6	49	G
17	6	50	A
17	6	51	U
17	6	52	U
17	6	70	A
17	6	77	C
17	6	78	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
13	5	77	G
13	5	78	U
17	6	46	G
17	6	51	U
17	6	77	C

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

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	$\# Z > 2$
18	IHP	A	2401	-	36,36,36	0.74	0	60,60,60	1.11	2 (3%)

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
18	IHP	A	2401	-	-	2/30/54/54	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	2401	IHP	O14-C4-C5	2.41	113.88	108.76
18	A	2401	IHP	C3-C2-C1	2.02	114.86	110.43

There are no chirality outliers.

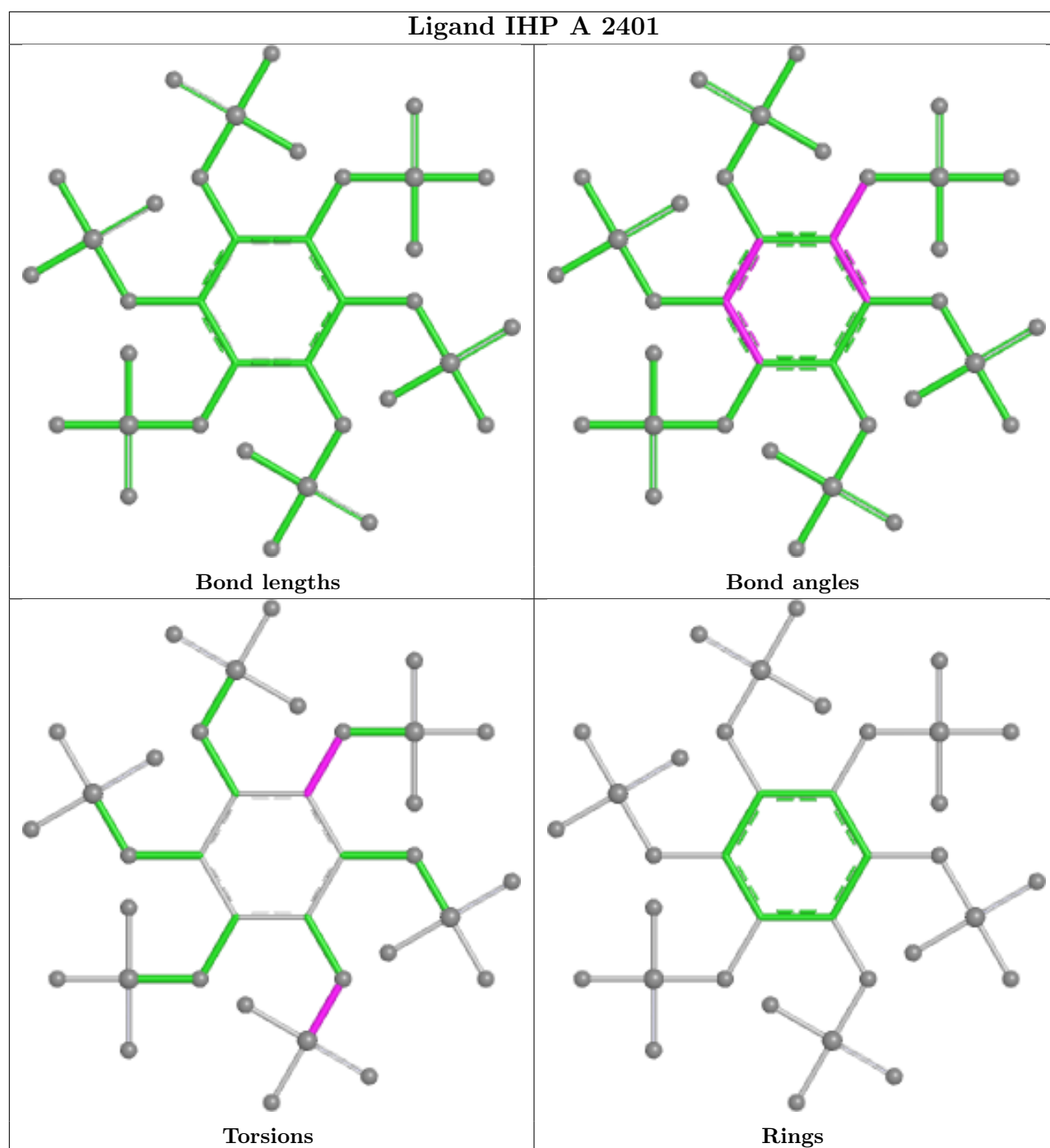
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	2401	IHP	C5-C4-O14-P4
18	A	2401	IHP	C6-O16-P6-O36

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

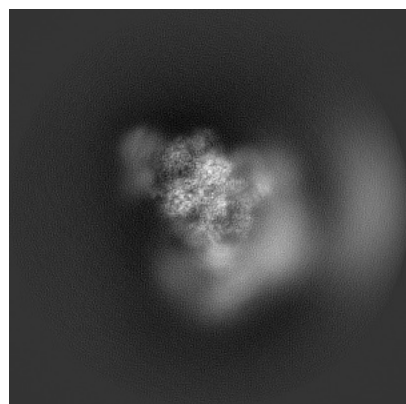
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18546. These allow visual inspection of the internal detail of the map and identification of artifacts.

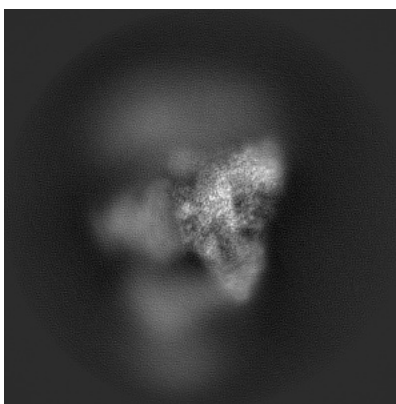
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

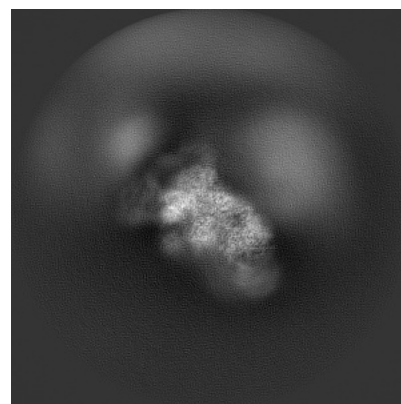
6.1.1 Primary map



X

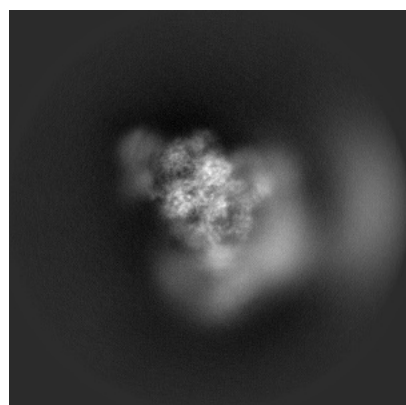


Y

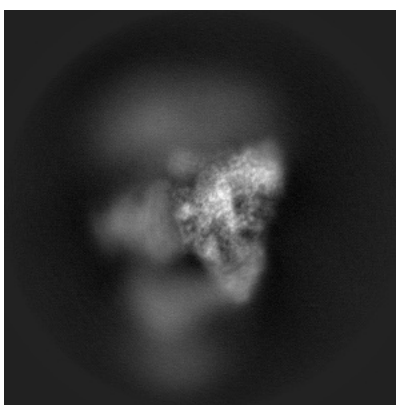


Z

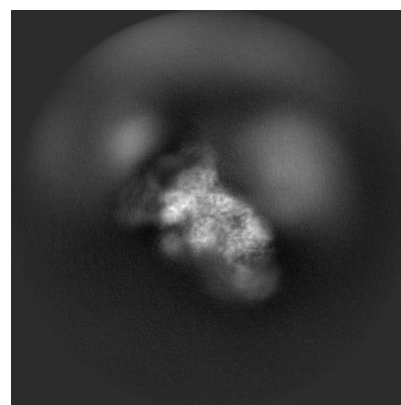
6.1.2 Raw map



X



Y

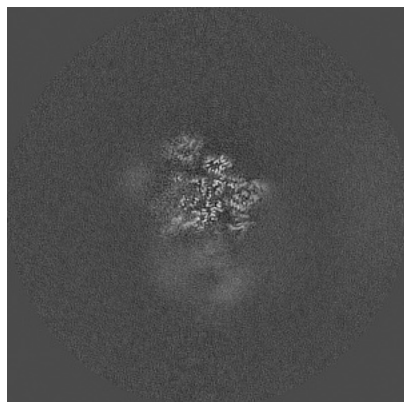


Z

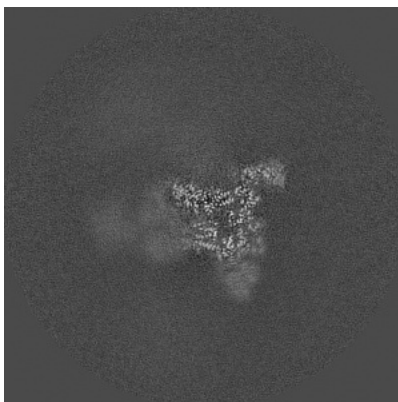
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

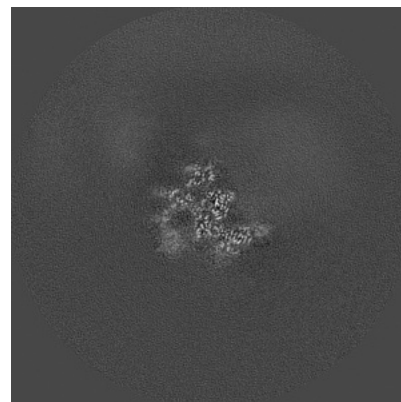
6.2.1 Primary map



X Index: 240

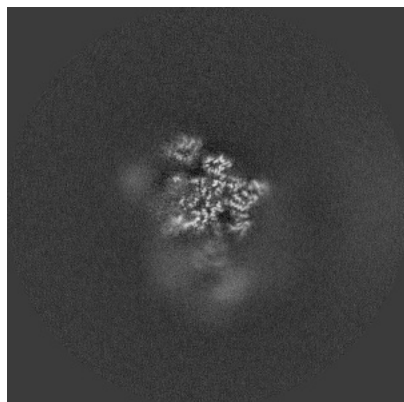


Y Index: 240

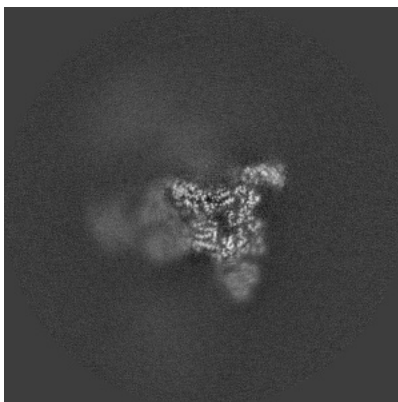


Z Index: 240

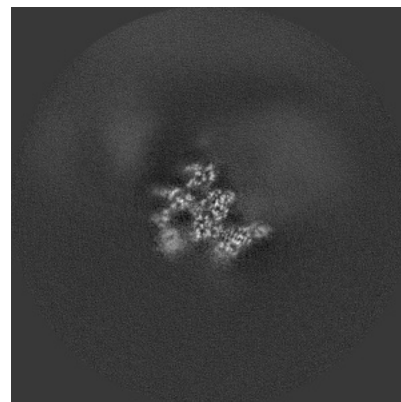
6.2.2 Raw map



X Index: 240



Y Index: 240

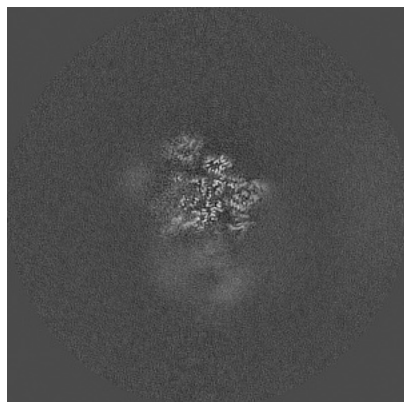


Z Index: 240

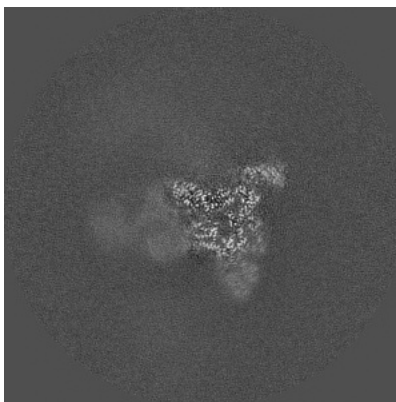
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

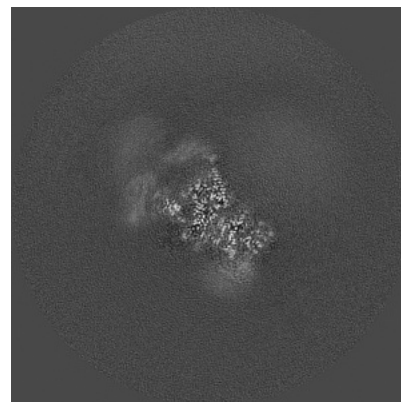
6.3.1 Primary map



X Index: 240

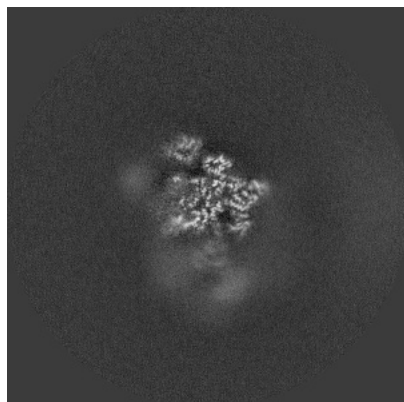


Y Index: 241

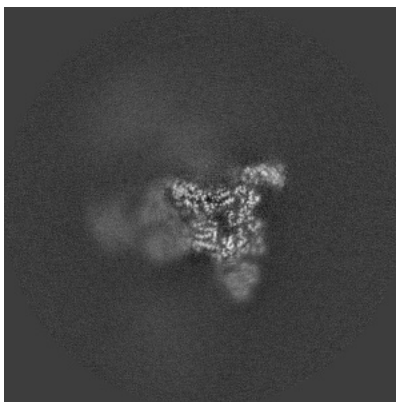


Z Index: 270

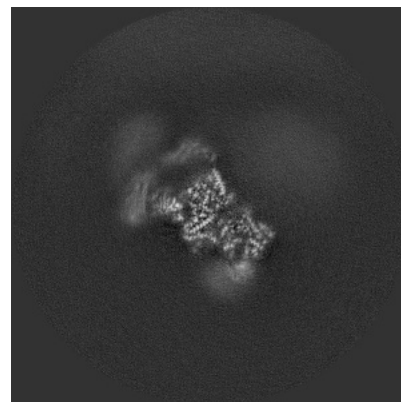
6.3.2 Raw map



X Index: 240



Y Index: 240

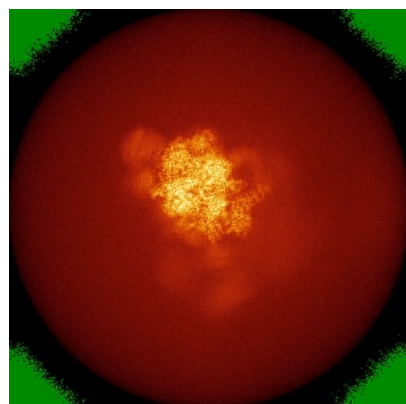


Z Index: 272

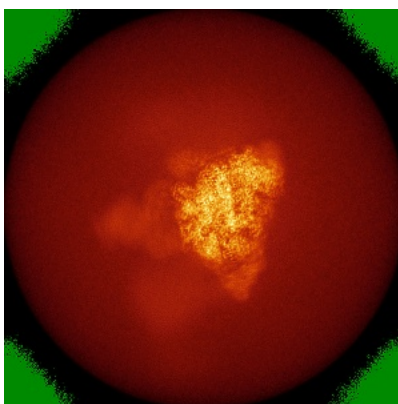
The images above show the largest variance slices of the map in three orthogonal directions.

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

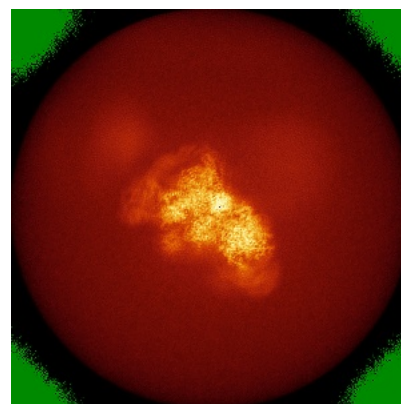
6.4.1 Primary map



X

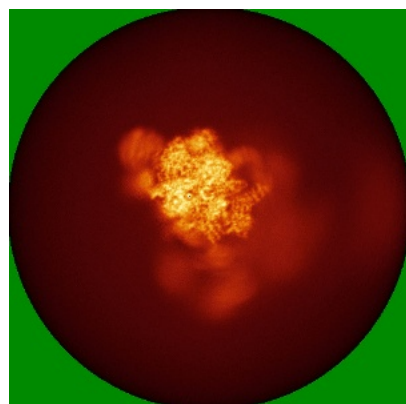


Y

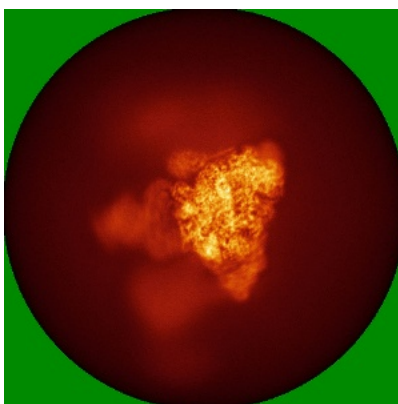


Z

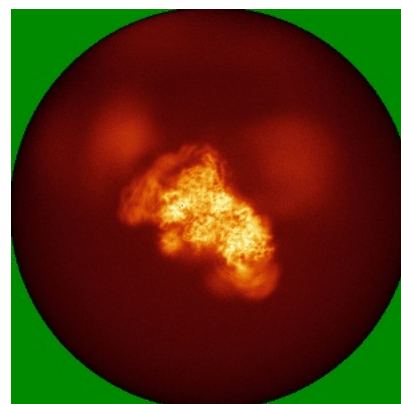
6.4.2 Raw map



X



Y



Z

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

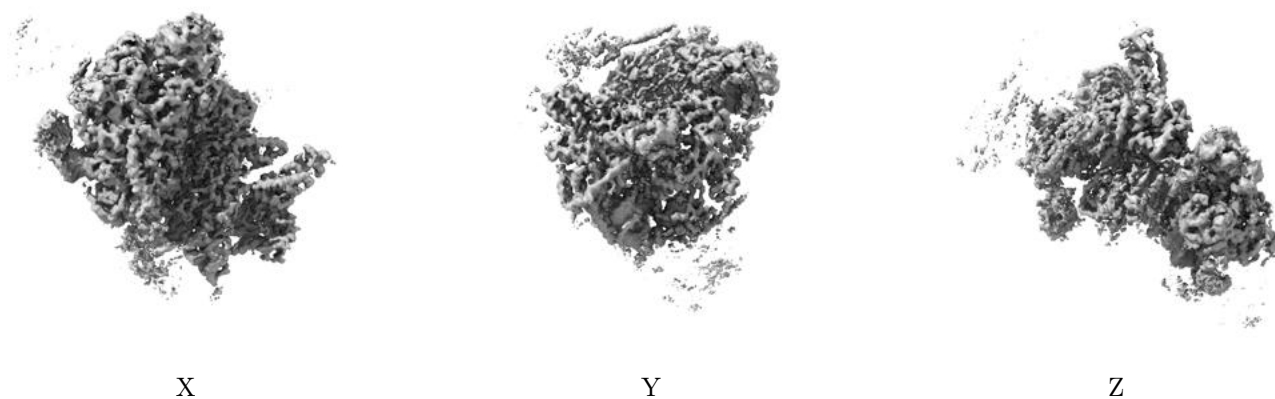
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.031. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

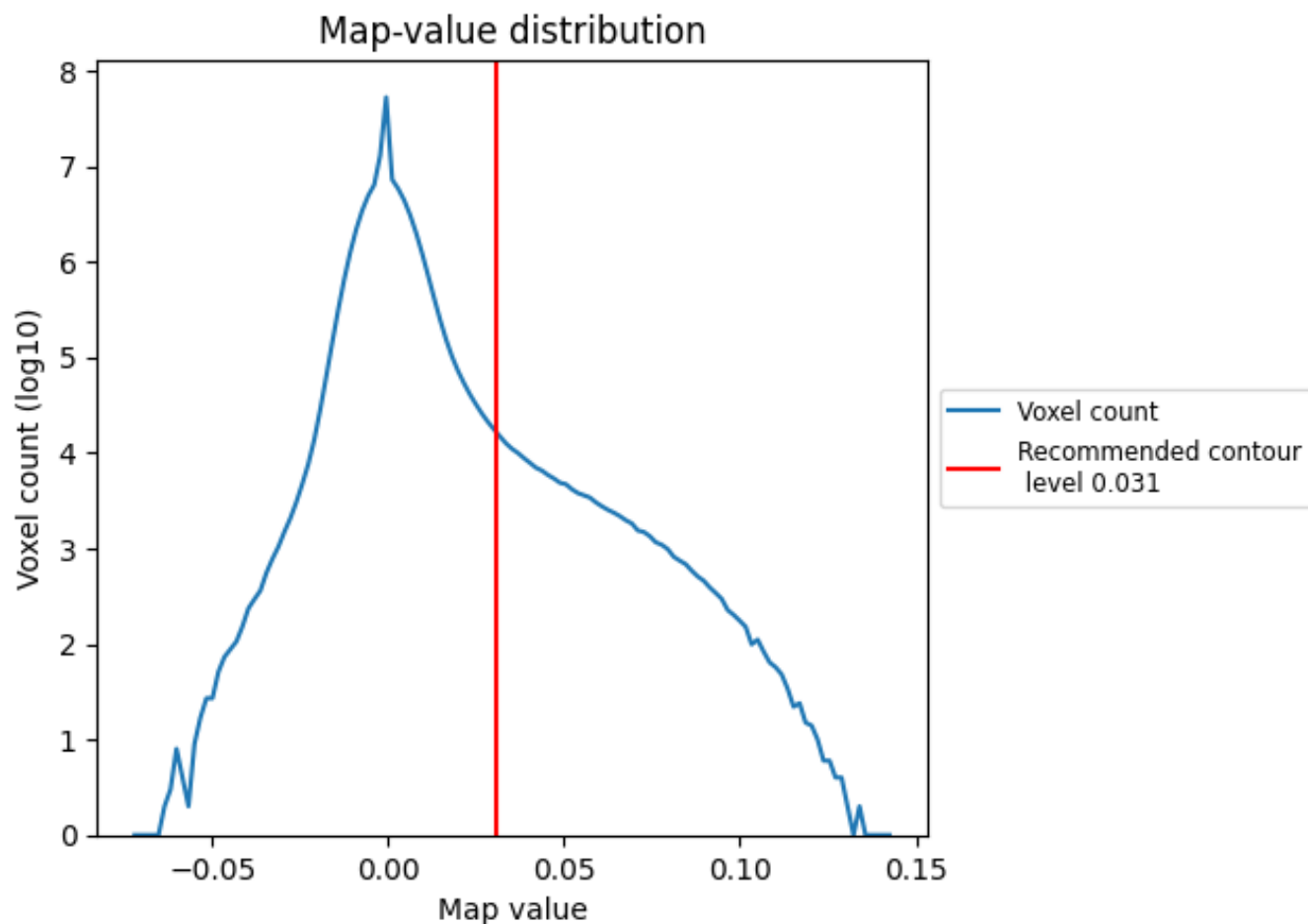
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

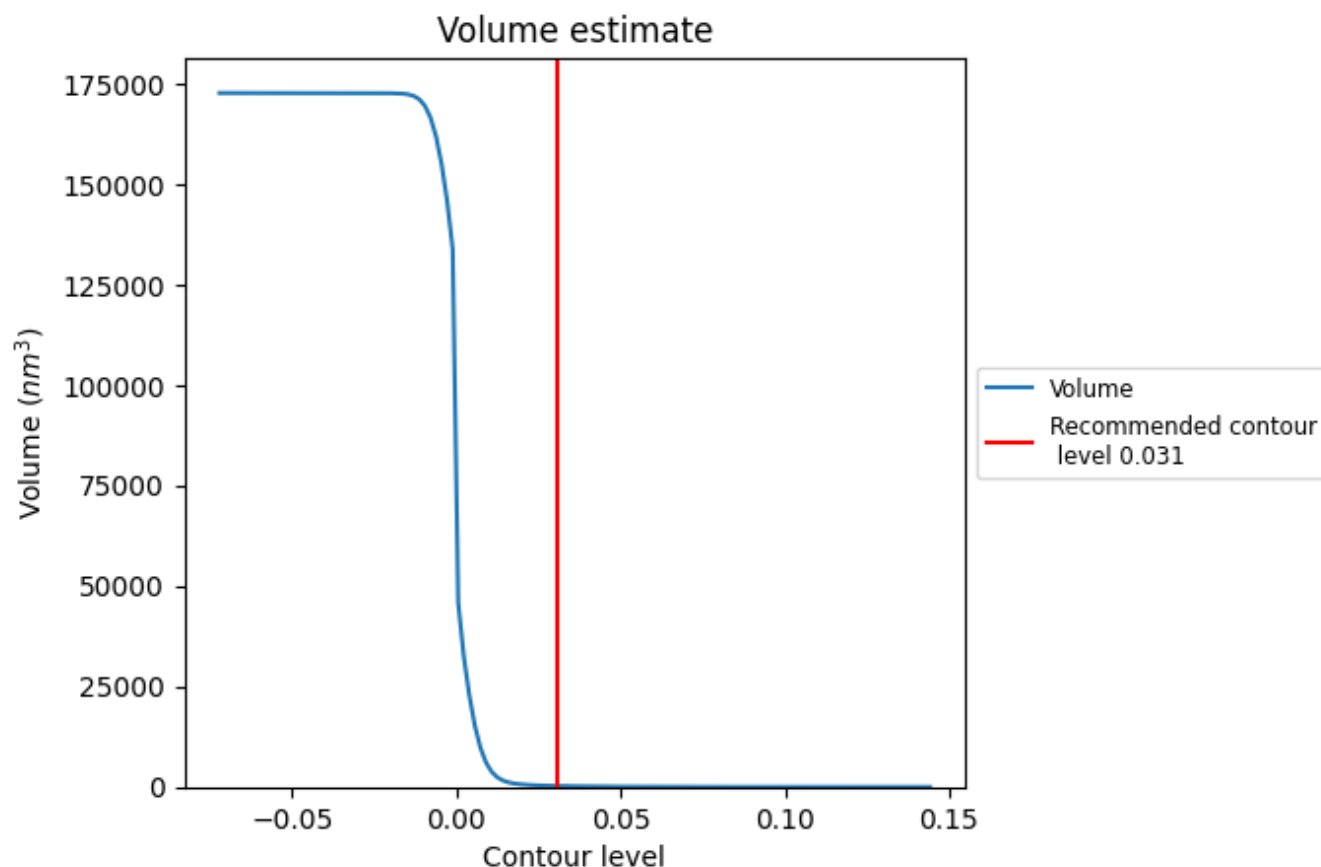
This section contains the results of statistical analysis of the map.

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.

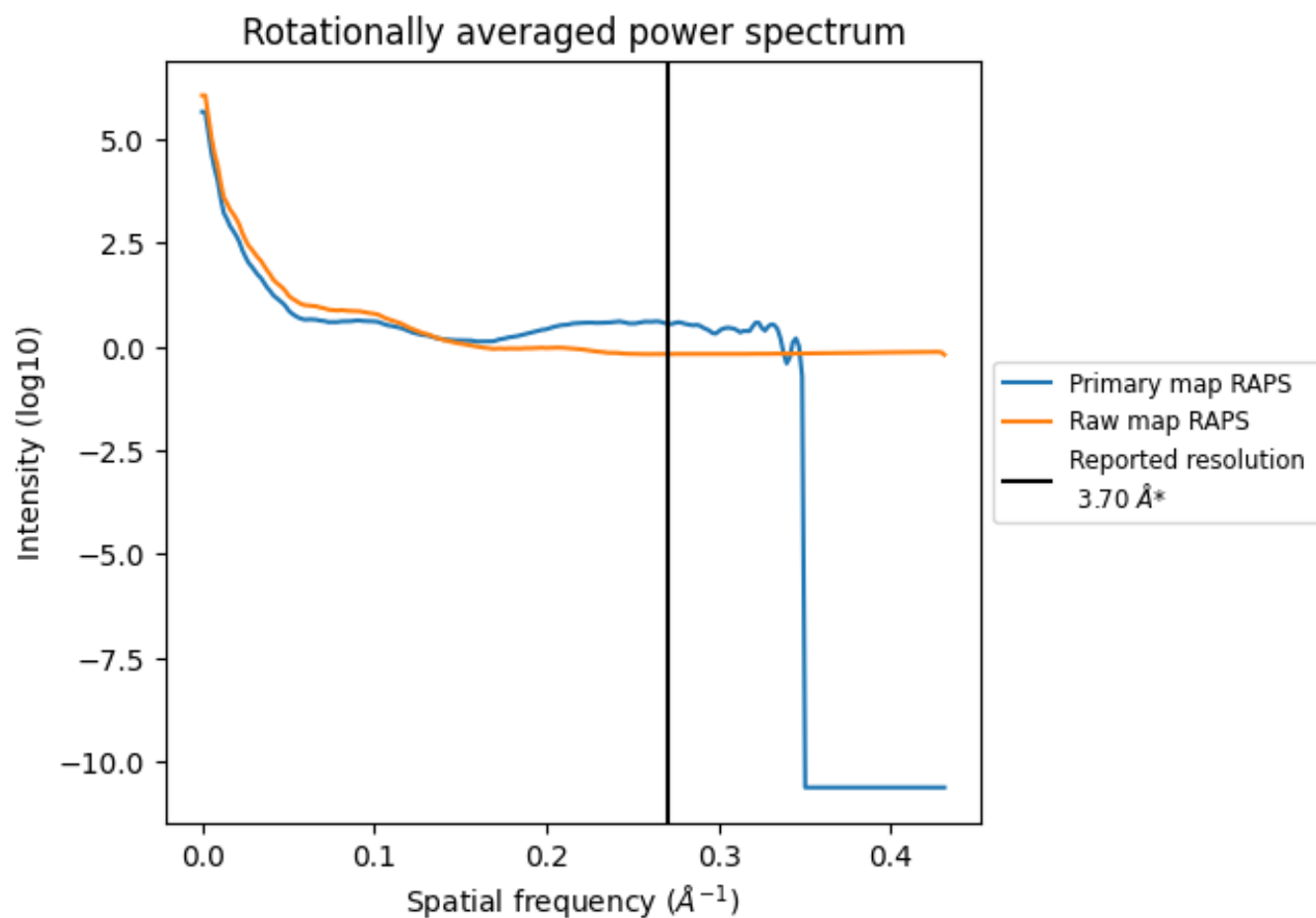
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 238 nm^3 ; this corresponds to an approximate mass of 215 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 ⓘ

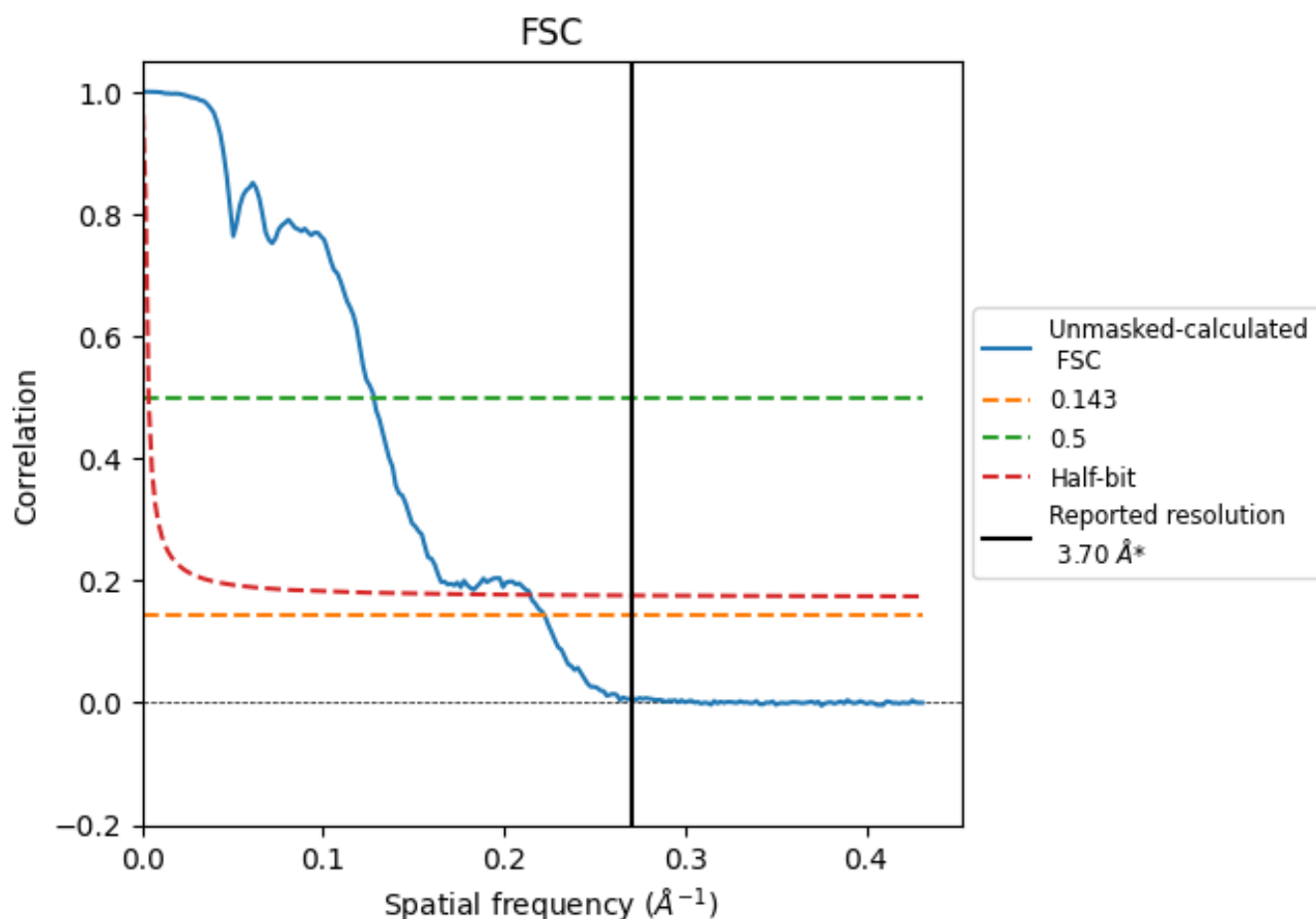


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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](#)

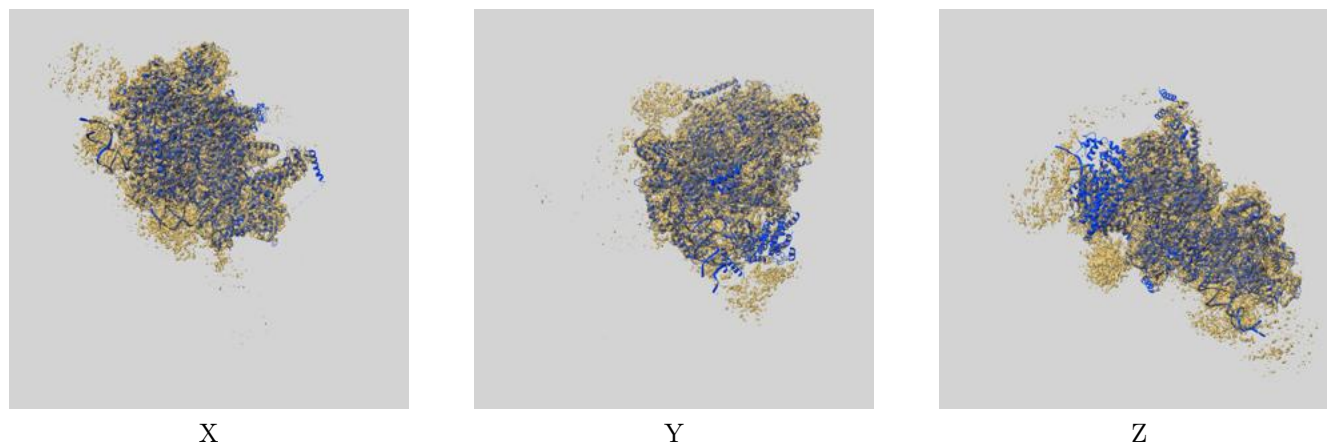
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.50	7.81	4.66

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.50 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

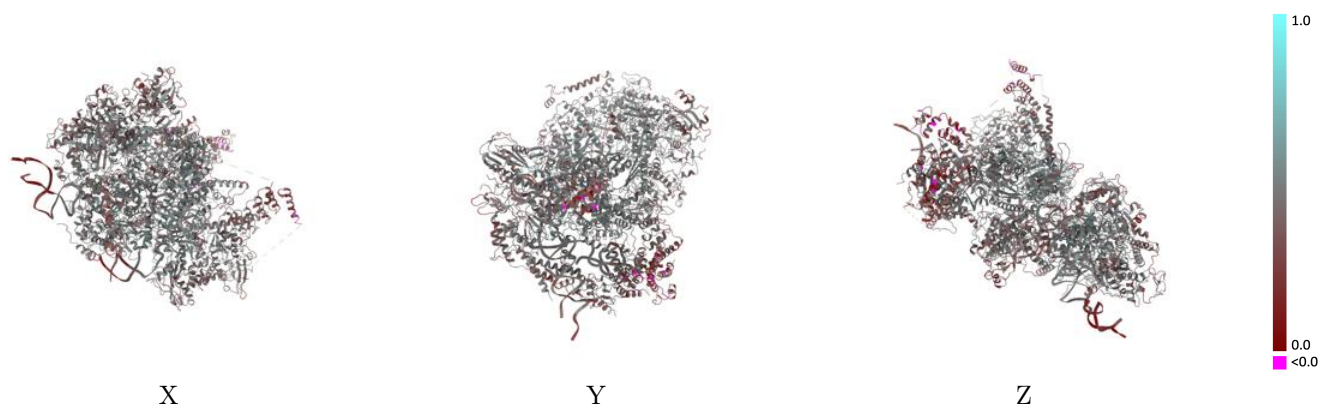
This section contains information regarding the fit between EMDB map EMD-18546 and PDB model 8QPA. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



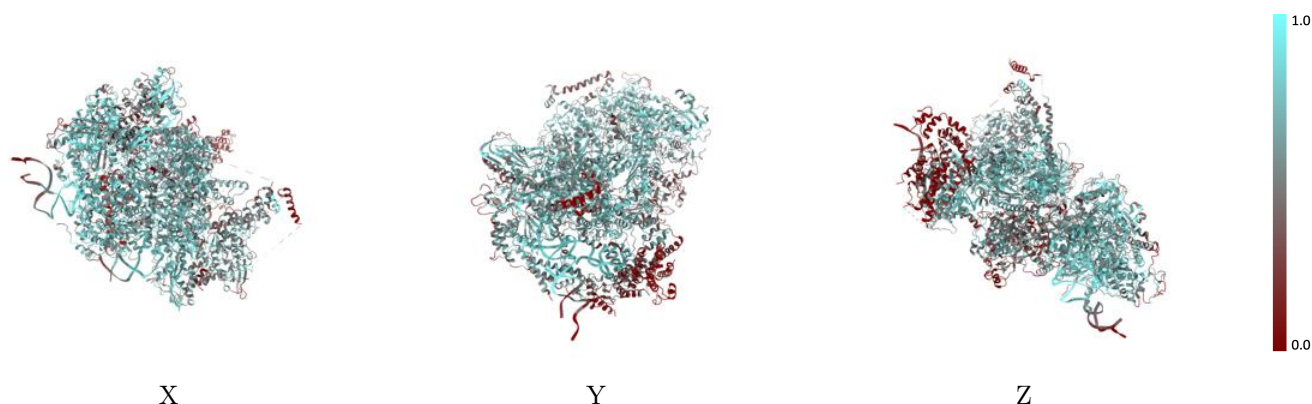
The images above show the 3D surface view of the map at the recommended contour level 0.031 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



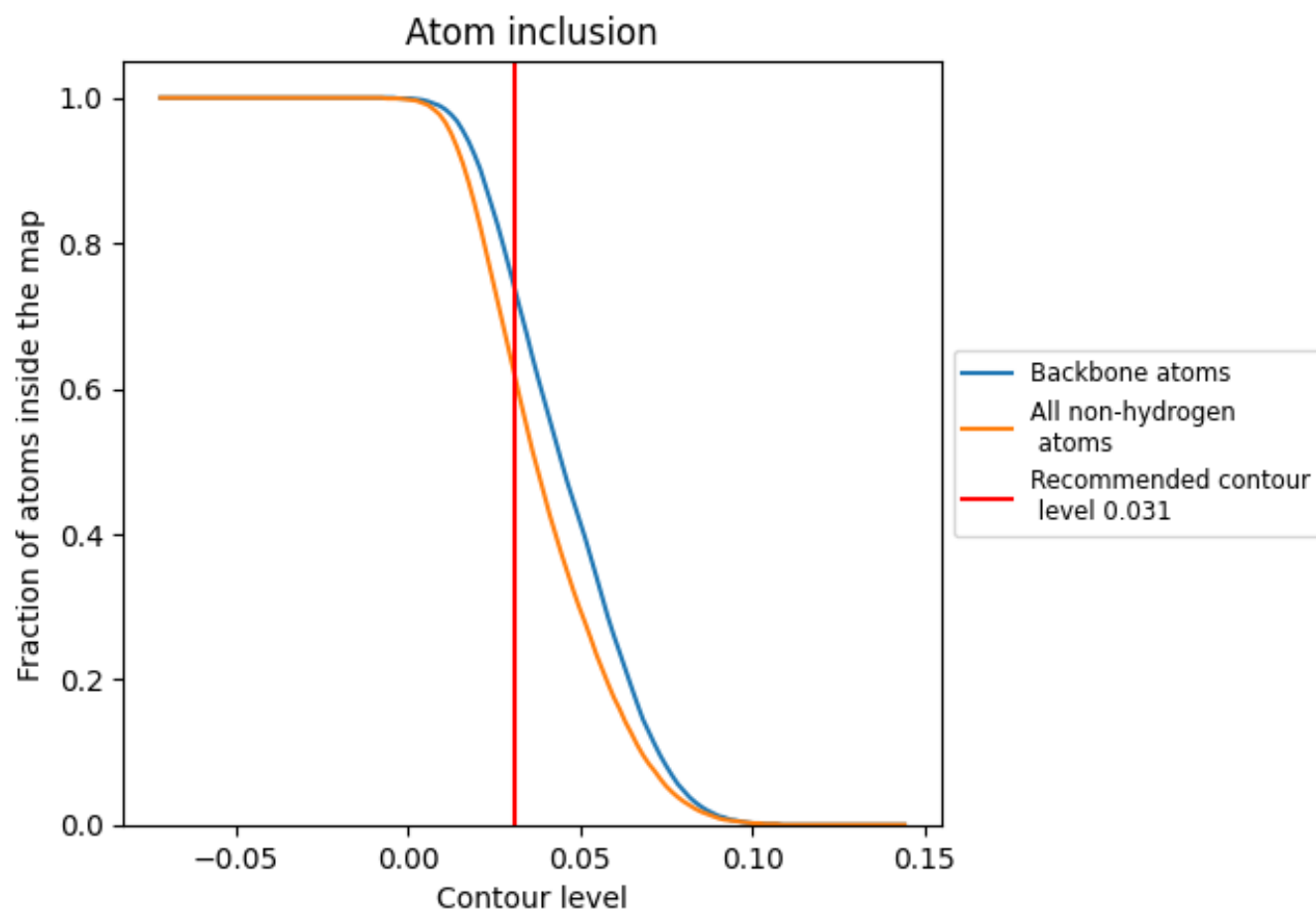
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.031).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 62% 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 (0.031) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6150	0.4390
4	0.8200	0.4640
5	0.7390	0.3960
6	0.6960	0.3970
7	0.5510	0.4130
A	0.6920	0.4740
B	0.4360	0.4480
C	0.7080	0.4540
D	0.7260	0.5050
F	0.5080	0.3480
G	0.4550	0.3950
J	0.6530	0.4490
L	0.5240	0.4130
M	0.3140	0.4010
N	0.4730	0.3870
S	0.3720	0.3700
U	0.3380	0.3960
z	0.6740	0.3540

1.0

0.0

<0.0