



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:36 AM UTC

PDB ID : 8QP8 / pdb_00008qp8
EMDB ID : EMD-18544
Title : Cryo-EM Structure of Pre-B 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 : 2023-09-30
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

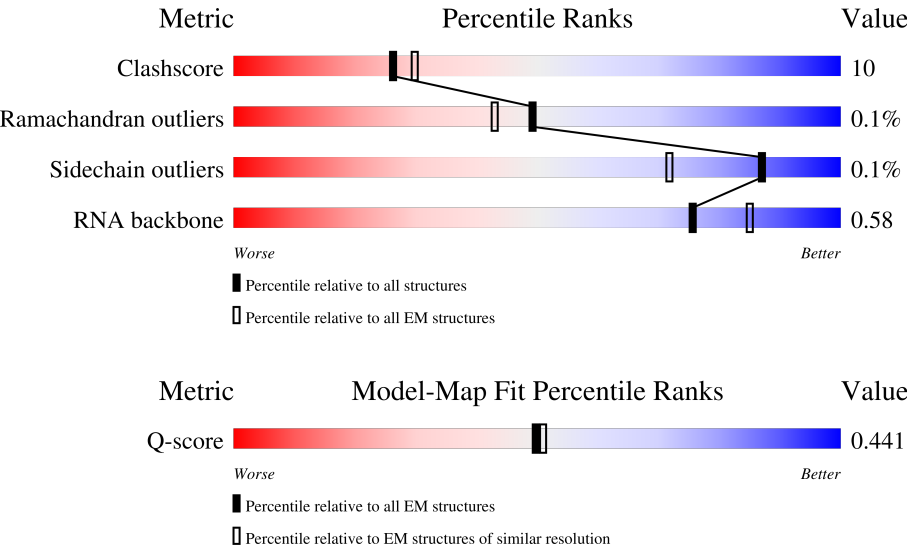
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 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.



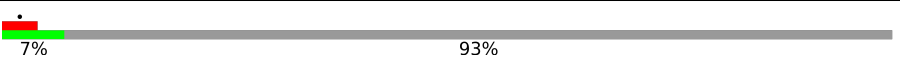
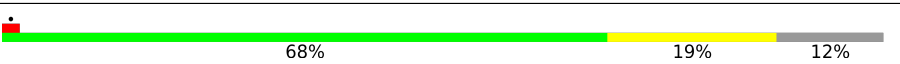
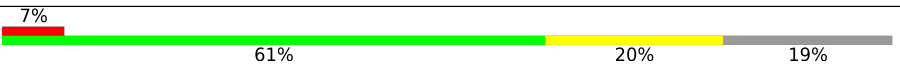
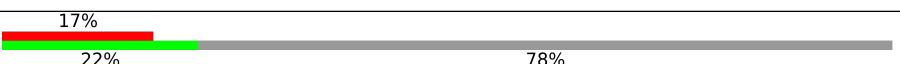
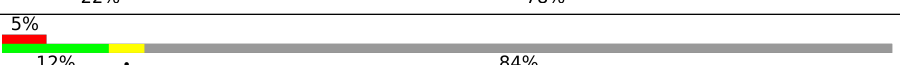
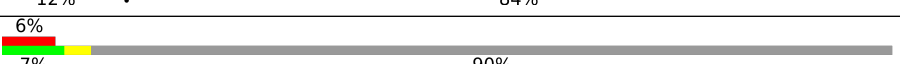
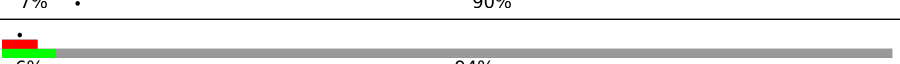
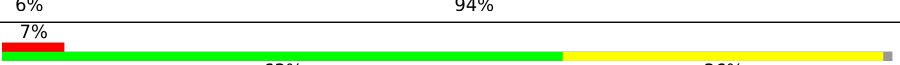
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	7	793	98%
2	G	820	88%
3	6	106	65%

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Mol	Chain	Length	Quality of chain
4	5	117	
5	4	144	
6	S	800	
7	C	972	
8	U	565	
9	A	2335	
10	R	480	
11	N	941	
12	L	499	
13	J	683	
14	D	142	
15	X	155	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 34561 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 Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	7	13	Total	C	N	O	0	0
			107	64	21	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	101	Total	C	N	O	S	0	0
			882	551	169	161	1		

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	37	Total	C	N	O	P	0	0
			795	355	148	255	37		

- Molecule 4 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	71	Total	C	N	O	P	0	0
			1496	672	257	497	70		

- Molecule 5 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	76	Total	C	N	O	P	0	0
			1617	723	286	532	76		

- Molecule 6 is a protein called U4/U6.U5 tri-snRNP-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	S	59	Total	C	N	O	0	0
			294	176	59	59		

- Molecule 7 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	852	Total	C	N	O	S	0	0
			6727	4300	1127	1266	34		

- 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 Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1918	Total	C	N	O	S	0	0
			15169	9735	2684	2686	64		

- Molecule 10 is a protein called RNA-binding protein 42.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	R	106	Total	C	N	O	0	0
			531	319	106	106		

- Molecule 11 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	152	Total	C	N	O	S	0	0
			1221	749	214	252	6		

- Molecule 12 is a protein called U4/U6 small nuclear ribonucleoprotein Prp31.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	50	Total	C	N	O	S	0	0
			390	237	80	71	2		

- Molecule 13 is a protein called U4/U6 small nuclear ribonucleoprotein Prp3.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	J	42	Total	C	N	O	0	0
			216	132	42	42		

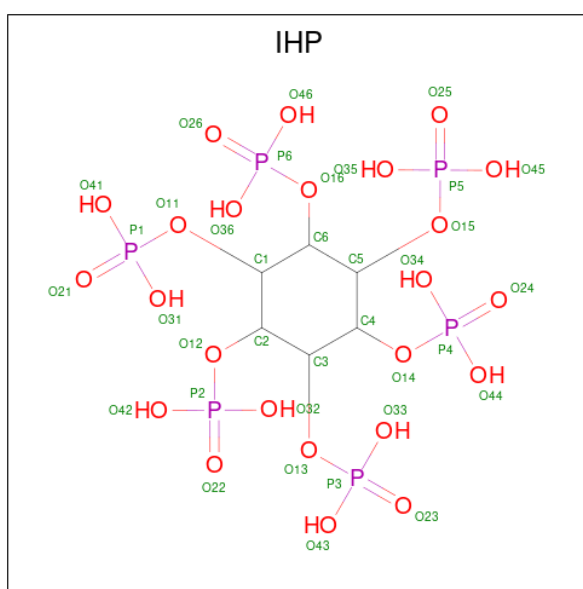
- Molecule 14 is a protein called Thioredoxin-like protein 4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	141	Total	C	N	O	S	0	0
			1169	751	194	214	10		

- Molecule 15 is a protein called U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein.

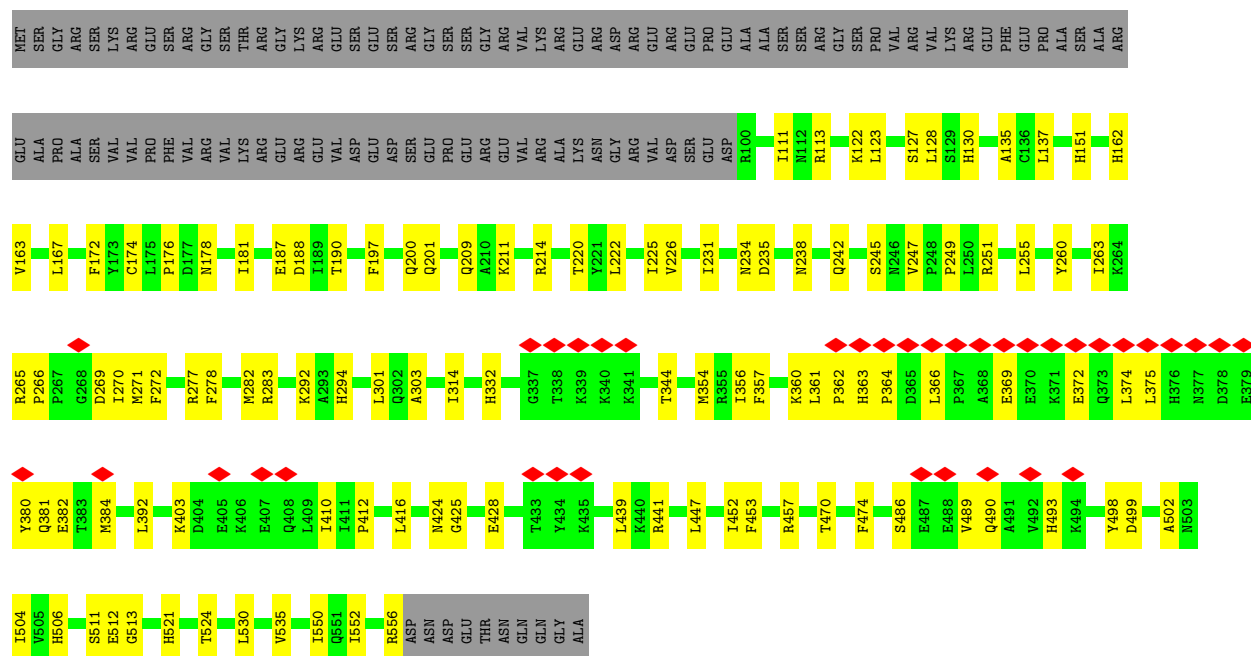
Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	18	Total	C	N	O	S	0	0
			162	102	36	23	1		

- Molecule 16 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).

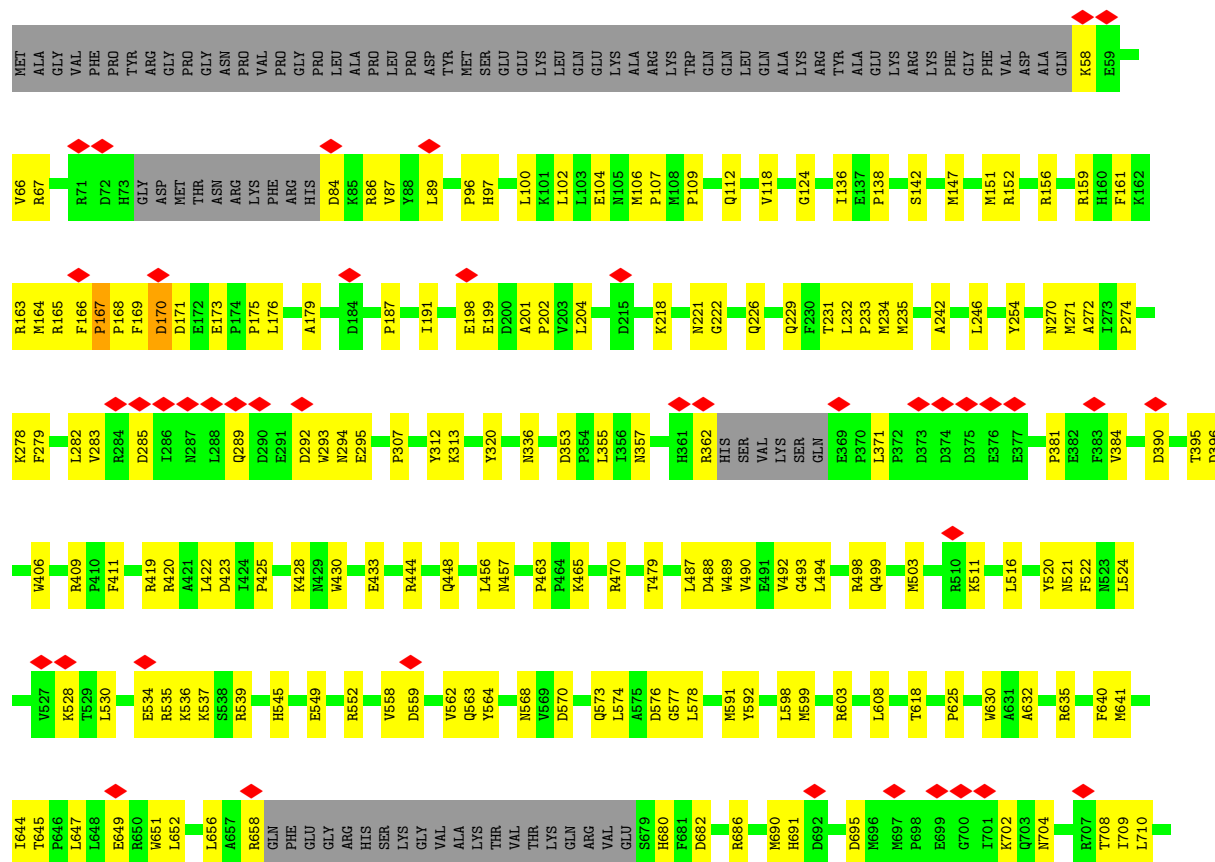


Mol	Chain	Residues	Atoms				AltConf
16	A	1	Total	C	O	P	0
			36	6	24	6	

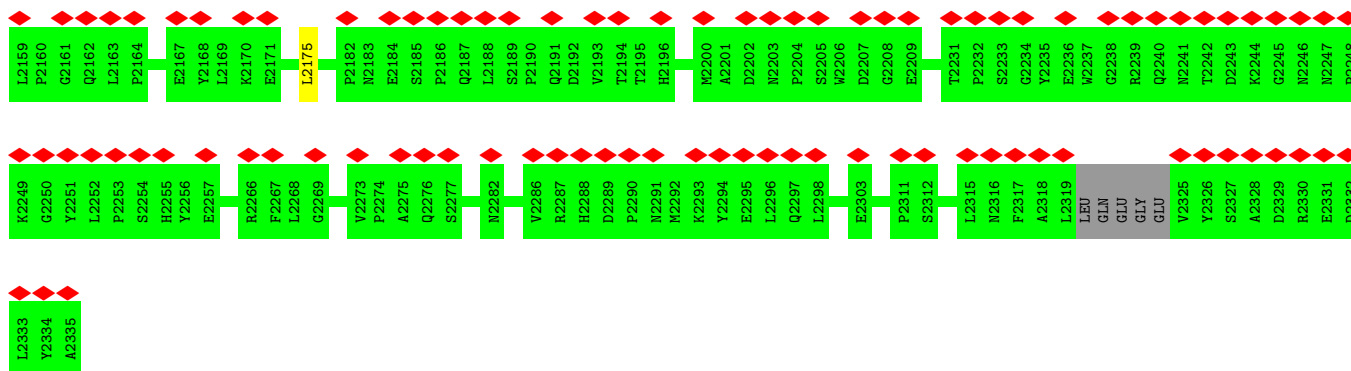




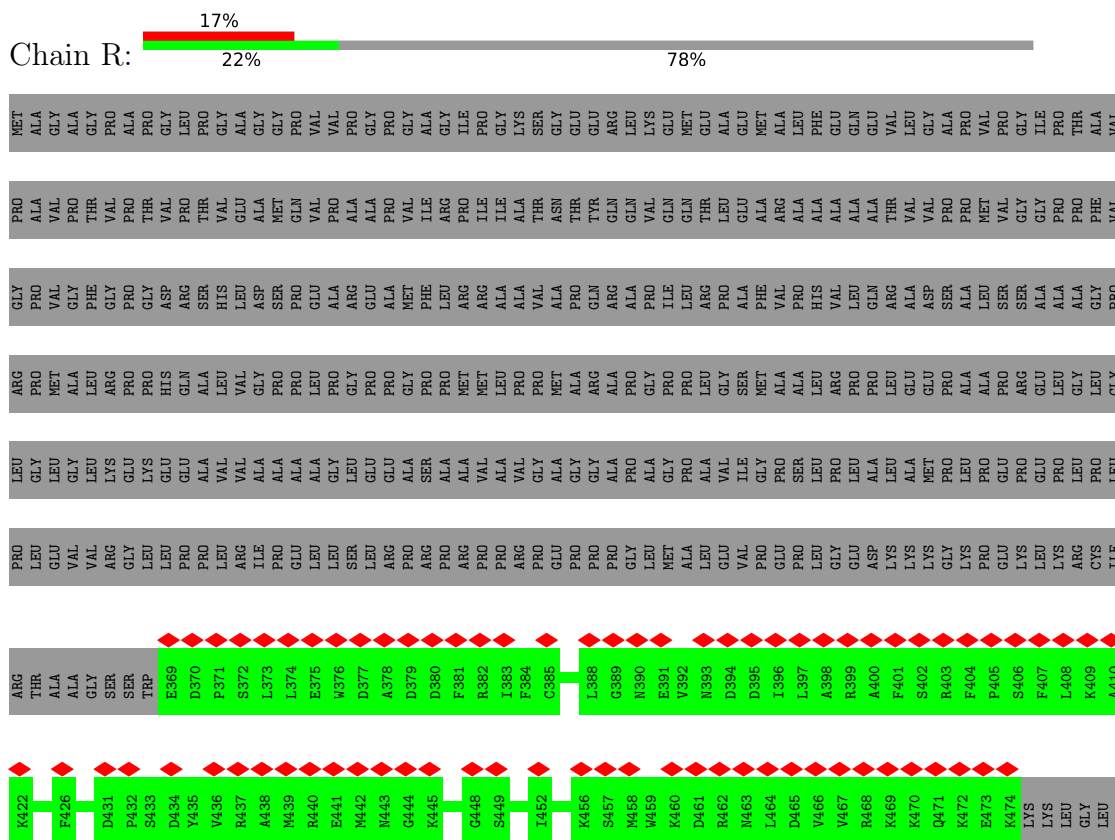
• Molecule 9: Pre-mRNA-processing-splicing factor 8



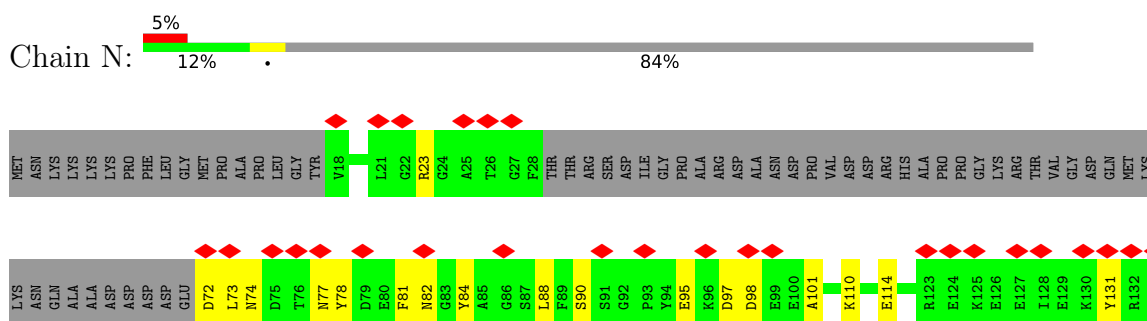


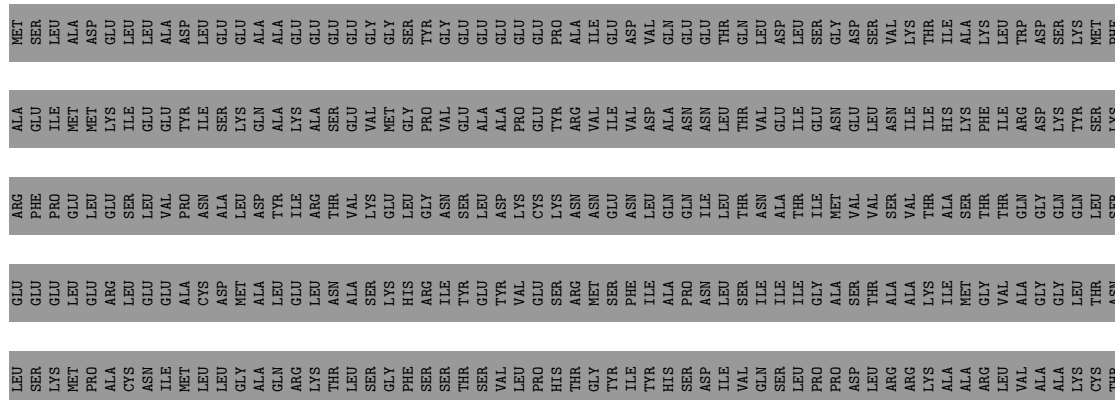


- Molecule 10: RNA-binding protein 42

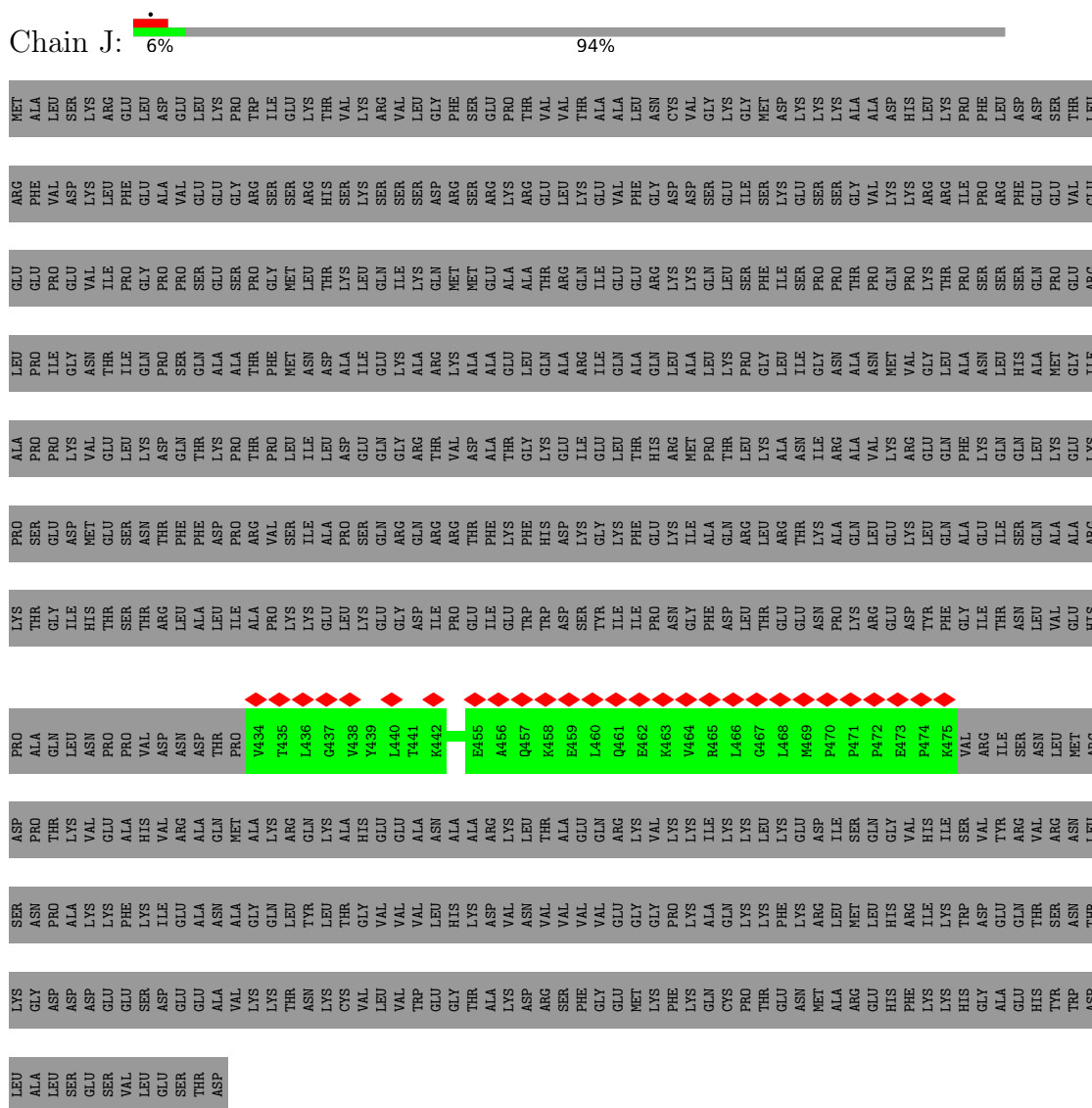


- Molecule 11: Pre-mRNA-processing factor 6



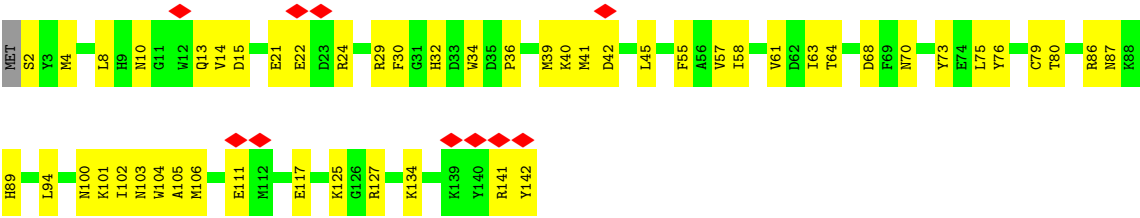


- Molecule 13: U4/U6 small nuclear ribonucleoprotein Prp3

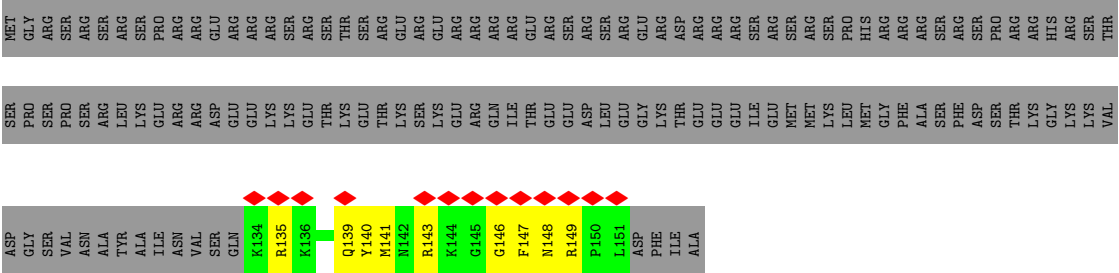


- Molecule 14: Thioredoxin-like protein 4A





• Molecule 15: U4/U6.U5 small nuclear ribonucleoprotein 27 kDa protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	279781	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	0.428	Depositor
Minimum map value	-0.100	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	648.0, 648.0, 648.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	7	0.07	0/106	0.19	0/139
2	G	0.18	0/896	0.35	0/1188
3	6	0.06	0/889	0.15	0/1382
4	5	0.14	0/1669	0.25	0/2594
5	4	0.07	0/1805	0.15	0/2805
6	S	0.07	0/295	0.17	0/410
7	C	0.15	0/6879	0.31	0/9344
8	U	0.14	0/3845	0.31	0/5208
9	A	0.16	0/15576	0.34	2/21190 (0.0%)
10	R	0.10	0/534	0.26	0/745
11	N	0.16	0/1236	0.31	0/1654
12	L	0.23	0/395	0.61	0/523
13	J	0.07	0/219	0.18	0/307
14	D	0.15	0/1198	0.36	0/1620
15	X	0.10	0/165	0.37	0/215
All	All	0.15	0/35707	0.31	2/49324 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1417	PRO	N-CA-C	-6.34	99.42	112.47
9	A	1419	ILE	N-CA-C	-5.89	103.05	111.17

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	7	107	0	110	5	0
2	G	882	0	880	21	0
3	6	795	0	402	14	0
4	5	1496	0	759	18	0
5	4	1617	0	819	23	0
6	S	294	0	138	2	0
7	C	6727	0	6736	116	0
8	U	3749	0	3769	75	0
9	A	15169	0	14419	332	0
10	R	531	0	253	0	0
11	N	1221	0	1175	34	0
12	L	390	0	371	21	0
13	J	216	0	108	0	0
14	D	1169	0	1141	49	0
15	X	162	0	170	15	0
16	A	36	0	6	0	0
All	All	34561	0	31256	644	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 10.

All (644) 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)
9:A:942:PRO:HD2	9:A:1438:VAL:HG22	1.50	0.92
9:A:231:THR:HG22	9:A:233:PRO:HD2	1.52	0.90
9:A:1418:ARG:HB2	9:A:1421:THR:HG23	1.55	0.87
9:A:1616:PRO:HG3	15:X:149:ARG:HH22	1.45	0.82
14:D:101:LYS:HD3	14:D:103:ASN:HD21	1.45	0.80
7:C:478:THR:HA	7:C:494:GLY:HA3	1.66	0.78
9:A:1610:GLN:HB2	9:A:1630:LEU:HB3	1.65	0.78
9:A:170:ASP:HB2	9:A:173:GLU:HB2	1.67	0.75
8:U:361:LEU:HD11	8:U:439:LEU:HG	1.70	0.74
9:A:690:MET:HE1	9:A:709:ILE:HG13	1.68	0.73
9:A:1031:ILE:HG22	9:A:1033:GLY:H	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:71:G:H1	5:4:4:U:H3	1.35	0.73
9:A:536:LYS:HB2	11:N:73:LEU:HD13	1.72	0.72
14:D:75:LEU:HD23	14:D:101:LYS:HZ3	1.54	0.72
15:X:143:ARG:NH1	15:X:146:GLY:O	2.21	0.72
8:U:162:HIS:HD2	8:U:176:PRO:HG2	1.55	0.71
9:A:1418:ARG:HH21	9:A:1464:LEU:HA	1.53	0.71
9:A:1626:CYS:SG	9:A:1627:ALA:N	2.63	0.71
9:A:163:ARG:HG3	9:A:625:PRO:HB2	1.72	0.71
9:A:1640:SER:HA	9:A:1653:ASP:H	1.56	0.71
2:G:282:THR:HG22	2:G:283:SER:H	1.56	0.70
9:A:86:ARG:NH1	9:A:658:ARG:O	2.23	0.70
8:U:260:TYR:OH	8:U:283:ARG:NH2	2.24	0.70
9:A:1589:ILE:HA	9:A:1733:ILE:HD11	1.74	0.70
9:A:1386:TRP:CZ2	9:A:1417:PRO:HB2	2.26	0.69
8:U:375:LEU:O	8:U:381:GLN:NE2	2.25	0.69
9:A:769:LYS:HE2	9:A:773:LYS:HD3	1.75	0.68
3:6:35:A:H61	5:4:74:C:H42	1.39	0.67
9:A:425:PRO:HB2	9:A:428:LYS:HB2	1.76	0.67
9:A:171:ASP:HA	9:A:521:ASN:ND2	2.10	0.67
9:A:1447:VAL:HG12	9:A:1449:LYS:H	1.60	0.66
9:A:1386:TRP:HZ2	9:A:1417:PRO:HB2	1.58	0.66
11:N:137:LYS:HG2	11:N:139:GLN:HG2	1.78	0.66
4:5:20:G:H22	9:A:465:LYS:HA	1.61	0.65
9:A:832:TYR:HB3	9:A:835:ASP:HB3	1.76	0.65
9:A:1365:ILE:HG23	9:A:1474:MET:HE1	1.77	0.65
7:C:711:ARG:HE	7:C:730:ARG:HB3	1.62	0.65
9:A:1636:LYS:HD3	9:A:1656:THR:HG21	1.76	0.65
9:A:1061:MET:HE1	9:A:1088:PHE:HB3	1.78	0.65
12:L:357:ARG:HG3	12:L:358:ARG:H	1.61	0.65
7:C:388:VAL:HG23	7:C:392:LEU:HD22	1.77	0.65
7:C:866:SER:O	9:A:357:ASN:ND2	2.30	0.65
9:A:104:GLU:HB2	9:A:422:LEU:HD11	1.79	0.65
9:A:272:ALA:HB2	9:A:278:LYS:HD3	1.79	0.65
7:C:390:THR:O	7:C:394:ARG:NH2	2.29	0.64
9:A:537:LYS:HG2	11:N:73:LEU:HD11	1.79	0.64
9:A:166:PHE:O	9:A:168:PRO:HD3	1.97	0.64
9:A:1330:MET:HE1	9:A:1369:TYR:H	1.63	0.64
12:L:362:MET:HA	12:L:365:ARG:HD3	1.79	0.64
3:6:56:A:H61	12:L:354:ARG:HD3	1.63	0.64
9:A:164:MET:HE2	9:A:577:GLY:HA3	1.78	0.64
8:U:162:HIS:CD2	8:U:176:PRO:HG2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1532:ARG:HG2	9:A:1568:THR:HG23	1.81	0.63
9:A:168:PRO:HB2	9:A:559:ASP:HB3	1.78	0.63
9:A:976:MET:HG2	9:A:1187:PHE:HB3	1.79	0.63
11:N:154:GLU:HA	11:N:157:TRP:HD1	1.62	0.63
14:D:70:ASN:HA	14:D:75:LEU:HB2	1.80	0.63
9:A:152:ARG:NH2	9:A:618:THR:O	2.31	0.63
9:A:1652:MET:HE1	9:A:1720:PRO:HG3	1.80	0.63
8:U:263:ILE:O	8:U:265:ARG:NH1	2.31	0.63
8:U:360:LYS:HB3	8:U:380:TYR:HA	1.81	0.62
9:A:58:LYS:NZ	9:A:479:THR:O	2.32	0.62
9:A:985:TYR:CG	9:A:1032:ARG:HD3	2.35	0.62
9:A:1613:THR:HB	15:X:148:ASN:HB3	1.81	0.62
8:U:511:SER:OG	8:U:512:GLU:OE1	2.16	0.62
14:D:41:MET:HE1	14:D:79:CYS:HB2	1.82	0.62
8:U:428:GLU:HB3	8:U:439:LEU:HD22	1.81	0.62
7:C:500:THR:HG21	7:C:543:ARG:HH11	1.65	0.62
14:D:75:LEU:HD23	14:D:101:LYS:NZ	2.14	0.62
14:D:32:HIS:CE1	14:D:64:THR:HG23	2.36	0.61
7:C:383:GLN:HG3	7:C:395:THR:HG21	1.82	0.61
9:A:909:TYR:HB2	9:A:1033:GLY:HA3	1.82	0.61
4:5:20:G:N2	9:A:465:LYS:HA	2.15	0.61
8:U:363:HIS:HB3	8:U:366:LEU:HD13	1.83	0.61
14:D:32:HIS:HE1	14:D:64:THR:HG23	1.66	0.61
9:A:67:ARG:HD3	9:A:179:ALA:HB2	1.83	0.60
11:N:131:TYR:OH	11:N:135:ARG:NH1	2.34	0.60
7:C:571:ASN:HB3	7:C:574:ALA:HB2	1.83	0.60
9:A:598:LEU:HD12	9:A:640:PHE:CZ	2.37	0.60
9:A:1434:LYS:O	9:A:1439:ARG:NH2	2.28	0.60
14:D:32:HIS:HB3	14:D:34:TRP:CE2	2.36	0.60
6:S:711:GLU:O	15:X:135:ARG:NH1	2.33	0.60
9:A:118:VAL:HG21	9:A:492:VAL:HG11	1.83	0.59
8:U:111:ILE:HG23	8:U:137:LEU:HB3	1.83	0.59
9:A:202:PRO:HB2	9:A:234:MET:HG2	1.83	0.59
15:X:140:TYR:HE1	15:X:149:ARG:HD2	1.66	0.59
9:A:941:LYS:HB3	9:A:942:PRO:HA	1.85	0.59
7:C:743:ASN:ND2	7:C:784:ILE:O	2.30	0.59
14:D:22:GLU:OE2	14:D:86:ARG:NH1	2.35	0.59
9:A:1416:ILE:C	9:A:1417:PRO:O	2.46	0.59
12:L:357:ARG:O	12:L:360:ARG:HG2	2.03	0.59
7:C:137:HIS:O	7:C:142:LYS:NZ	2.36	0.59
3:6:47:A:H4'	3:6:48:A:O5'	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:804:GLY:H	7:C:808:ILE:HD12	1.67	0.58
7:C:853:ARG:NH2	9:A:312:TYR:OH	2.36	0.58
9:A:1318:THR:HB	9:A:1324:GLY:HA3	1.85	0.58
7:C:135:CYS:HB2	7:C:242:LEU:HD13	1.84	0.58
8:U:384:MET:HE3	8:U:384:MET:HA	1.84	0.58
9:A:1502:PHE:HA	12:L:380:PHE:H	1.68	0.58
9:A:1583:GLN:HE21	9:A:1620:TYR:HE1	1.50	0.58
9:A:142:SER:HA	9:A:242:ALA:HB2	1.86	0.58
14:D:30:PHE:HB3	14:D:63:ILE:HD11	1.84	0.58
7:C:830:PRO:HG2	7:C:877:ALA:HB3	1.84	0.58
9:A:528:LYS:NZ	9:A:534:GLU:OE1	2.37	0.58
14:D:8:LEU:HD22	14:D:13:GLN:HB3	1.85	0.58
8:U:209:GLN:NE2	8:U:211:LYS:O	2.36	0.58
9:A:1382:SER:HA	9:A:1415:GLY:HA2	1.85	0.58
9:A:163:ARG:HG2	9:A:576:ASP:OD2	2.04	0.57
9:A:1072:LEU:HD22	9:A:1087:LEU:HD22	1.87	0.57
9:A:1700:GLY:O	9:A:1717:ASN:N	2.36	0.57
9:A:198:GLU:HG2	9:A:199:GLU:HG2	1.86	0.57
7:C:603:MET:HB2	7:C:651:ILE:HD11	1.86	0.57
9:A:1237:MET:HG2	9:A:1284:LEU:HD13	1.86	0.57
9:A:289:GLN:O	9:A:1139:ARG:NH2	2.28	0.57
9:A:856:LEU:O	9:A:861:ARG:NH2	2.29	0.57
7:C:736:GLY:HA2	7:C:743:ASN:HB2	1.87	0.57
9:A:787:GLU:OE2	9:A:790:ARG:NH2	2.37	0.56
9:A:170:ASP:CB	9:A:173:GLU:HB2	2.32	0.56
12:L:360:ARG:O	12:L:363:LYS:HG3	2.06	0.56
8:U:392:LEU:HD12	8:U:453:PHE:HE1	1.71	0.56
9:A:957:GLN:O	9:A:961:ASN:ND2	2.38	0.56
9:A:558:VAL:O	9:A:562:VAL:HG13	2.06	0.56
14:D:111:GLU:OE2	14:D:134:LYS:NZ	2.38	0.56
9:A:1214:TRP:NE1	9:A:1276:GLU:OE1	2.39	0.56
9:A:1417:PRO:O	9:A:1418:ARG:HD3	2.06	0.56
9:A:1418:ARG:CB	9:A:1421:THR:HG23	2.30	0.56
9:A:1614:ILE:HD11	9:A:1628:ASP:HA	1.88	0.56
14:D:8:LEU:HD13	14:D:14:VAL:HA	1.88	0.56
9:A:1218:ASN:HB3	9:A:1221:THR:HG22	1.89	0.55
9:A:1304:ASN:HB2	9:A:1566:ILE:HG12	1.88	0.55
9:A:1418:ARG:NH2	9:A:1464:LEU:HA	2.20	0.55
9:A:761:ILE:HG12	9:A:767:VAL:HG21	1.89	0.55
9:A:102:LEU:HD21	9:A:493:GLY:HA2	1.88	0.55
9:A:1592:ASP:OD2	9:A:1737:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:466:LEU:HD22	9:A:691:HIS:HB2	1.89	0.55
7:C:346:ASP:HA	7:C:367:ARG:HG2	1.88	0.55
12:L:386:ASP:HB2	12:L:389:GLN:HB2	1.89	0.55
7:C:207:GLY:O	7:C:238:ASN:ND2	2.40	0.55
5:4:64:G:H22	5:4:67:A:H5'	1.72	0.54
7:C:357:THR:HG22	7:C:359:LYS:H	1.72	0.54
9:A:940:ILE:HD11	9:A:1046:LEU:HB2	1.87	0.54
3:6:74:U:H2'	3:6:75:G:H8	1.72	0.54
9:A:1418:ARG:HG2	9:A:1462:GLY:HA3	1.87	0.54
7:C:323:PHE:CD2	7:C:373:ILE:HG12	2.41	0.54
9:A:221:ASN:HD21	9:A:226:GLN:HB2	1.71	0.54
5:4:68:A:O2'	5:4:69:C:OP1	2.23	0.54
11:N:74:ASN:HD21	14:D:63:ILE:HG21	1.72	0.54
8:U:231:ILE:N	8:U:234:ASN:OD1	2.40	0.54
9:A:271:MET:HE1	9:A:313:LYS:HZ1	1.73	0.54
9:A:1291:CYS:O	9:A:1295:ILE:HG12	2.06	0.54
8:U:187:GLU:O	8:U:190:THR:OG1	2.22	0.54
14:D:104:TRP:CH2	14:D:106:MET:HB3	2.43	0.54
9:A:164:MET:CE	9:A:577:GLY:HA3	2.38	0.54
9:A:1236:SER:HA	9:A:1239:ARG:HE	1.72	0.54
12:L:346:PRO:HG2	14:D:117:GLU:HG3	1.90	0.54
14:D:94:LEU:HD11	14:D:102:ILE:HD13	1.88	0.54
7:C:779:LEU:O	7:C:938:ARG:NH1	2.34	0.54
14:D:29:ARG:NH2	14:D:42:ASP:OD2	2.40	0.54
12:L:358:ARG:O	12:L:361:LYS:HG2	2.07	0.54
4:5:56:C:H4'	9:A:100:LEU:HD21	1.89	0.53
9:A:165:ARG:H	9:A:165:ARG:NE	2.06	0.53
9:A:1607:GLU:N	9:A:1632:PHE:O	2.41	0.53
4:5:21:A:H61	4:5:59:G:N2	2.06	0.53
9:A:96:PRO:HB2	9:A:645:THR:HG23	1.89	0.53
11:N:78:TYR:HB2	11:N:84:TYR:CE1	2.44	0.53
8:U:226:VAL:O	8:U:242:GLN:NE2	2.39	0.53
8:U:357:PHE:HB2	8:U:441:ARG:HB2	1.89	0.53
7:C:345:GLY:HA3	9:A:371:LEU:HD21	1.90	0.53
8:U:502:ALA:HB3	8:U:552:ILE:HB	1.90	0.53
9:A:1418:ARG:CG	9:A:1462:GLY:HA3	2.38	0.53
11:N:72:ASP:HB3	11:N:77:ASN:ND2	2.23	0.53
7:C:283:ASP:OD2	9:A:362:ARG:NH2	2.41	0.53
8:U:174:CYS:O	8:U:178:ASN:HA	2.09	0.53
9:A:1615:HIS:CD2	15:X:147:PHE:HB3	2.44	0.53
9:A:944:ASP:HB2	9:A:1436:TRP:NE1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:17:U:OP2	9:A:470:ARG:NH2	2.35	0.53
7:C:559:ILE:HG21	7:C:563:ALA:HB2	1.90	0.53
9:A:530:LEU:HD22	9:A:535:ARG:HD3	1.91	0.53
9:A:1298:ARG:O	9:A:1301:ILE:HG12	2.09	0.53
5:4:57:G:N7	12:L:354:ARG:NE	2.55	0.53
9:A:772:CYS:SG	9:A:1249:MET:HE1	2.49	0.53
9:A:995:ARG:NH2	11:N:252:ASP:OD1	2.41	0.53
4:5:19:A:N3	4:5:21:A:N6	2.57	0.52
7:C:507:VAL:HG11	7:C:565:ILE:HG23	1.90	0.52
14:D:45:LEU:HD22	14:D:58:ILE:HD13	1.90	0.52
7:C:501:ILE:HD11	7:C:527:VAL:HG21	1.90	0.52
8:U:412:PRO:HG2	8:U:470:THR:HA	1.91	0.52
9:A:221:ASN:OD1	9:A:222:GLY:N	2.43	0.52
9:A:1737:ASN:HB3	9:A:1740:LEU:HB2	1.91	0.52
11:N:23:ARG:NH2	14:D:73:TYR:OH	2.42	0.52
7:C:177:ARG:NH2	7:C:638:ASP:OD2	2.39	0.52
9:A:96:PRO:HG2	9:A:649:GLU:HG3	1.92	0.52
9:A:313:LYS:HG2	9:A:320:TYR:HB3	1.91	0.52
9:A:1703:ILE:HG12	9:A:1714:ALA:HB2	1.91	0.52
4:5:23:C:H2'	4:5:58:U:O2	2.10	0.52
8:U:382:GLU:OE2	8:U:441:ARG:NE	2.42	0.52
14:D:102:ILE:O	14:D:104:TRP:HD1	1.93	0.52
8:U:364:PRO:HB2	11:N:147:ARG:HD2	1.91	0.52
9:A:886:LEU:HD11	11:N:273:TYR:CD1	2.45	0.52
3:6:68:C:H2'	3:6:69:A:C8	2.45	0.52
7:C:832:TYR:CD1	7:C:901:PHE:HA	2.45	0.52
8:U:174:CYS:O	8:U:178:ASN:N	2.42	0.52
2:G:242:ASP:OD2	2:G:291:LYS:NZ	2.44	0.51
8:U:263:ILE:HD11	8:U:272:PHE:HE1	1.76	0.51
9:A:1391:LEU:O	9:A:1394:GLN:HG3	2.09	0.51
7:C:863:ILE:HD12	7:C:868:LEU:HB2	1.93	0.51
7:C:205:THR:HB	7:C:215:VAL:HG22	1.93	0.51
2:G:284:ILE:O	2:G:284:ILE:HG13	2.10	0.51
7:C:164:ASP:OD1	7:C:164:ASP:N	2.42	0.51
9:A:66:VAL:HG11	9:A:487:LEU:HD11	1.92	0.51
7:C:388:VAL:HA	7:C:392:LEU:HB2	1.93	0.51
7:C:761:SER:OG	7:C:803:ARG:NH1	2.43	0.51
8:U:416:LEU:HB2	8:U:474:PHE:HB3	1.92	0.51
9:A:89:LEU:HD22	9:A:656:LEU:HD22	1.92	0.51
7:C:310:SER:HA	7:C:316:ILE:O	2.10	0.51
7:C:262:ARG:NH2	9:A:336:ASN:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:604:LEU:HD22	8:U:128:LEU:HD11	1.93	0.51
7:C:140:HIS:CD2	7:C:230:ASP:HB2	2.46	0.51
9:A:1426:ASP:O	9:A:1427:ARG:C	2.54	0.51
11:N:23:ARG:NH1	14:D:87:ASN:OD1	2.42	0.51
9:A:136:ILE:HG22	9:A:138:PRO:HD2	1.93	0.50
2:G:283:SER:HA	9:A:274:PRO:HB3	1.93	0.50
2:G:301:ARG:NH2	9:A:353:ASP:OD2	2.44	0.50
8:U:172:PHE:HB2	8:U:181:ILE:HB	1.93	0.50
9:A:87:VAL:HG22	11:N:101:ALA:HB2	1.93	0.50
9:A:1042:GLN:HA	9:A:1090:ARG:HH22	1.76	0.50
9:A:1418:ARG:HB2	9:A:1421:THR:CG2	2.35	0.50
9:A:1623:ASN:OD1	9:A:1624:SER:N	2.45	0.50
5:4:8:C:H2'	5:4:9:G:C8	2.46	0.50
7:C:343:LEU:HD13	7:C:373:ILE:HD11	1.93	0.50
7:C:510:LEU:HB2	7:C:564:THR:HB	1.94	0.50
9:A:516:LEU:HB3	9:A:524:LEU:HD11	1.93	0.50
9:A:563:GLN:OE1	9:A:568:ASN:ND2	2.25	0.50
9:A:1109:LEU:HG	9:A:1152:ALA:HB1	1.92	0.50
4:5:53:U:OP2	9:A:465:LYS:NZ	2.41	0.50
7:C:747:ASP:HA	7:C:791:ILE:HB	1.93	0.50
9:A:1421:THR:O	9:A:1424:GLN:HG2	2.11	0.50
3:6:55:C:P	12:L:360:ARG:HH22	2.34	0.50
4:5:47:A:O2'	4:5:48:A:O5'	2.28	0.50
8:U:113:ARG:NH1	8:U:188:ASP:OD2	2.45	0.50
11:N:97:ASP:OD1	11:N:97:ASP:N	2.44	0.50
7:C:918:ILE:HD11	7:C:931:ARG:HG3	1.93	0.50
8:U:489:VAL:HG13	8:U:493:HIS:HE1	1.77	0.50
5:4:22:C:H2'	5:4:23:G:H8	1.77	0.50
7:C:134:LEU:HD22	7:C:228:PHE:HE1	1.76	0.50
7:C:461:LEU:O	7:C:465:MET:HG3	2.11	0.50
9:A:218:LYS:O	9:A:229:GLN:NE2	2.44	0.50
9:A:899:MET:HB3	9:A:906:VAL:HB	1.93	0.50
9:A:1485:LEU:HD21	12:L:380:PHE:HZ	1.77	0.50
9:A:1633:ALA:HB2	9:A:1637:TRP:CH2	2.47	0.50
12:L:363:LYS:HD2	12:L:363:LYS:C	2.37	0.50
9:A:839:LEU:HD22	9:A:878:LEU:HG	1.94	0.50
2:G:250:ILE:O	2:G:254:TYR:HD1	1.95	0.49
7:C:678:THR:OG1	7:C:682:LYS:O	2.29	0.49
7:C:707:ILE:HB	7:C:735:PHE:HD2	1.77	0.49
9:A:1230:LEU:O	9:A:1280:ASN:ND2	2.45	0.49
9:A:1296:GLN:CG	9:A:1327:MET:HE1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2129:TYR:HA	9:A:2175:LEU:H	1.76	0.49
7:C:692:LEU:HD23	7:C:788:LYS:HB2	1.94	0.49
9:A:830:LEU:HD23	9:A:830:LEU:H	1.76	0.49
14:D:104:TRP:CZ2	14:D:106:MET:HE3	2.47	0.49
7:C:137:HIS:HB3	7:C:140:HIS:CE1	2.47	0.49
8:U:111:ILE:HD11	8:U:163:VAL:HG21	1.95	0.49
9:A:821:ARG:HH11	9:A:1065:PRO:HG2	1.77	0.49
12:L:357:ARG:HG3	12:L:358:ARG:N	2.26	0.49
7:C:507:VAL:CG1	7:C:565:ILE:HG23	2.42	0.49
9:A:944:ASP:HA	9:A:1437:ARG:HE	1.76	0.49
9:A:850:TYR:OH	9:A:863:GLU:OE1	2.28	0.49
9:A:1587:GLU:HB2	15:X:140:TYR:OH	2.12	0.49
9:A:171:ASP:OD1	9:A:521:ASN:HB2	2.12	0.49
5:4:22:C:H2'	5:4:23:G:C8	2.47	0.49
7:C:388:VAL:HG13	7:C:389:ASP:N	2.28	0.49
11:N:271:LYS:O	11:N:275:THR:HG23	2.13	0.49
7:C:916:ILE:HB	7:C:931:ARG:HG2	1.94	0.49
15:X:140:TYR:CE1	15:X:149:ARG:HD2	2.47	0.49
4:5:45:C:O2	9:A:603:ARG:NH2	2.40	0.49
7:C:241:ARG:HB3	7:C:583:ASN:HD21	1.78	0.49
9:A:1088:PHE:HD1	9:A:1097:ILE:HG12	1.78	0.49
9:A:1701:VAL:HA	9:A:1716:GLY:HA3	1.94	0.49
8:U:174:CYS:O	8:U:178:ASN:CA	2.61	0.49
8:U:278:PHE:CZ	8:U:282:MET:HE1	2.48	0.49
9:A:608:LEU:HD13	9:A:632:ALA:HB1	1.95	0.49
9:A:962:LEU:HB2	9:A:965:VAL:HB	1.95	0.49
9:A:1212:GLY:HA3	9:A:1280:ASN:HB2	1.94	0.49
8:U:247:VAL:HG12	8:U:249:PRO:HD2	1.95	0.48
9:A:1639:VAL:HG21	9:A:1699:THR:OG1	2.13	0.48
9:A:522:PHE:HB2	9:A:552:ARG:HB2	1.95	0.48
7:C:493:PHE:CZ	7:C:549:TRP:HB3	2.48	0.48
7:C:469:ASP:OD1	7:C:469:ASP:N	2.47	0.48
7:C:843:VAL:HG22	7:C:871:ILE:HD11	1.95	0.48
9:A:1088:PHE:CD1	9:A:1097:ILE:HG12	2.48	0.48
9:A:1455:TRP:H	9:A:1455:TRP:CD1	2.30	0.48
1:7:461:ASP:O	1:7:464:SER:OG	2.32	0.48
7:C:434:CYS:O	7:C:438:ILE:HB	2.13	0.48
9:A:1501:LEU:HD23	9:A:1753:LEU:HD21	1.96	0.48
14:D:4:MET:SD	14:D:4:MET:N	2.87	0.48
8:U:260:TYR:HH	8:U:283:ARG:HH21	1.57	0.48
9:A:1719:PHE:CZ	9:A:1722:SER:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:511:LYS:HE2	11:N:88:LEU:HD21	1.94	0.48
7:C:665:THR:HG21	7:C:828:MET:HE3	1.94	0.48
7:C:925:PRO:HD2	7:C:928:HIS:NE2	2.29	0.48
9:A:494:LEU:HD21	9:A:562:VAL:HG11	1.94	0.48
11:N:136:PRO:O	11:N:141:GLN:NE2	2.45	0.48
2:G:247:LEU:HD12	2:G:250:ILE:HD12	1.95	0.48
2:G:249:ALA:HA	2:G:252:GLU:HG2	1.96	0.48
9:A:651:TRP:CD1	11:N:82:ASN:HA	2.48	0.48
5:4:35:G:H2'	5:4:39:A:H61	1.79	0.48
7:C:286:ASN:ND2	7:C:300:LEU:O	2.41	0.48
7:C:354:ARG:NH2	9:A:384:VAL:O	2.30	0.48
9:A:766:THR:O	14:D:141:ARG:NH2	2.46	0.48
9:A:996:LEU:HD13	9:A:1047:VAL:HG21	1.95	0.48
8:U:424:ASN:OD1	8:U:425:GLY:N	2.46	0.47
9:A:109:PRO:HB2	9:A:191:ILE:HD12	1.95	0.47
7:C:130:ARG:NH1	7:C:440:SER:OG	2.46	0.47
8:U:111:ILE:HG12	8:U:163:VAL:HG11	1.95	0.47
8:U:403:LYS:HB3	8:U:410:ILE:HG13	1.96	0.47
9:A:1310:ARG:HE	9:A:1310:ARG:HA	1.79	0.47
8:U:362:PRO:HB3	8:U:374:LEU:HD12	1.96	0.47
9:A:270:ASN:ND2	9:A:285:ASP:OD2	2.44	0.47
9:A:881:ILE:HG23	9:A:918:THR:HG23	1.96	0.47
9:A:1090:ARG:NH1	9:A:1092:ILE:O	2.48	0.47
8:U:447:LEU:HB3	8:U:498:TYR:OH	2.15	0.47
9:A:430:TRP:O	9:A:433:GLU:HG2	2.14	0.47
9:A:545:HIS:O	9:A:549:GLU:HG2	2.14	0.47
14:D:32:HIS:CE1	14:D:63:ILE:HB	2.49	0.47
2:G:282:THR:HG22	9:A:274:PRO:HA	1.95	0.47
9:A:1587:GLU:O	9:A:1591:MET:HG2	2.14	0.47
2:G:330:LEU:O	2:G:334:GLU:HG2	2.15	0.47
7:C:529:ARG:H	7:C:553:GLU:HB3	1.80	0.47
8:U:225:ILE:HG23	8:U:530:LEU:HD11	1.97	0.47
9:A:106:MET:HE2	9:A:578:LEU:HD13	1.97	0.47
9:A:124:GLY:O	9:A:499:GLN:NE2	2.46	0.47
9:A:1416:ILE:O	9:A:1417:PRO:O	2.31	0.47
9:A:1504:GLU:OE2	12:L:377:ARG:NE	2.47	0.47
11:N:73:LEU:HA	11:N:84:TYR:CE1	2.49	0.47
9:A:147:MET:O	9:A:151:MET:HG2	2.13	0.47
14:D:21:GLU:HG3	14:D:57:VAL:HG11	1.97	0.47
9:A:175:PRO:HD3	9:A:520:TYR:CD1	2.49	0.47
9:A:911:VAL:HB	9:A:916:LYS:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:998:ARG:NH1	9:A:1007:ASP:OD1	2.47	0.47
9:A:1591:MET:HE2	9:A:1591:MET:N	2.30	0.47
9:A:1640:SER:OG	9:A:1652:MET:SD	2.73	0.47
14:D:8:LEU:HB2	14:D:61:VAL:HG22	1.96	0.47
2:G:253:ARG:HH11	9:A:313:LYS:HZ3	1.62	0.46
9:A:640:PHE:CZ	9:A:644:ILE:HG21	2.49	0.46
4:5:4:C:N4	4:5:78:U:O2	2.48	0.46
8:U:137:LEU:HB2	8:U:163:VAL:HG13	1.97	0.46
9:A:235:MET:HE1	9:A:411:PHE:HA	1.98	0.46
9:A:390:ASP:OD1	9:A:390:ASP:N	2.46	0.46
9:A:1315:VAL:HG12	9:A:1538:TRP:CE3	2.51	0.46
9:A:1392:LYS:O	9:A:1395:GLU:HG3	2.15	0.46
9:A:271:MET:HE1	9:A:313:LYS:NZ	2.30	0.46
9:A:420:ARG:NH2	9:A:423:ASP:OD1	2.48	0.46
9:A:776:LEU:HD22	9:A:900:ASP:HB2	1.96	0.46
9:A:1049:ASP:OD1	9:A:1090:ARG:HD3	2.15	0.46
9:A:1618:LYS:HD3	9:A:1618:LYS:C	2.40	0.46
14:D:10:ASN:OD1	14:D:13:GLN:NE2	2.48	0.46
7:C:320:LEU:HD21	7:C:344:TRP:HB2	1.97	0.46
7:C:370:VAL:HA	7:C:374:LEU:HB2	1.97	0.46
9:A:1310:ARG:HA	9:A:1310:ARG:NE	2.31	0.46
9:A:1472:THR:O	9:A:1476:GLN:HG2	2.15	0.46
5:4:5:U:H2'	5:4:6:U:C6	2.51	0.46
9:A:279:PHE:HE2	9:A:456:LEU:HG	1.80	0.46
9:A:1536:LEU:HD21	9:A:1576:ILE:HD11	1.98	0.46
1:7:463:GLU:CD	9:A:702:LYS:HD3	2.40	0.46
7:C:935:ILE:HG13	7:C:936:LYS:N	2.30	0.46
9:A:254:TYR:HE2	9:A:433:GLU:HB2	1.81	0.46
9:A:1621:LYS:HE3	9:A:1623:ASN:OD1	2.16	0.46
11:N:74:ASN:HA	14:D:76:TYR:O	2.15	0.46
1:7:463:GLU:CD	1:7:463:GLU:H	2.23	0.46
3:6:71:G:H2'	3:6:72:G:H8	1.80	0.46
8:U:374:LEU:HD22	8:U:380:TYR:HE2	1.80	0.46
9:A:231:THR:H	9:A:234:MET:CE	2.28	0.46
9:A:1018:ASN:ND2	9:A:1019:TYR:O	2.49	0.46
9:A:1616:PRO:HG3	15:X:149:ARG:NH2	2.23	0.46
9:A:231:THR:H	9:A:234:MET:HE3	1.80	0.46
9:A:294:ASN:OD1	9:A:295:GLU:N	2.45	0.46
9:A:1617:ARG:HA	9:A:1620:TYR:CZ	2.50	0.46
15:X:143:ARG:CZ	15:X:149:ARG:HH21	2.28	0.46
7:C:677:GLU:O	7:C:814:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:200:GLN:NE2	8:U:201:GLN:HG3	2.31	0.46
9:A:169:PHE:CZ	9:A:562:VAL:HG23	2.51	0.46
9:A:704:ASN:O	9:A:708:THR:HG23	2.15	0.46
9:A:1307:MET:HE2	9:A:1307:MET:HA	1.98	0.46
7:C:476:CYS:HB3	7:C:565:ILE:HB	1.98	0.46
9:A:107:PRO:HD3	9:A:489:TRP:CE2	2.51	0.46
9:A:796:LYS:HG3	11:N:240:MET:HB3	1.97	0.46
11:N:110:LYS:O	11:N:114:GLU:HG3	2.16	0.46
14:D:2:SER:HB2	14:D:4:MET:SD	2.55	0.46
7:C:208:HIS:HB3	7:C:211:PHE:HD2	1.82	0.45
7:C:711:ARG:HH21	7:C:730:ARG:HB3	1.81	0.45
7:C:888:ARG:HG2	7:C:895:ALA:O	2.16	0.45
14:D:36:PRO:O	14:D:39:MET:HB3	2.15	0.45
2:G:281:ASP:OD2	9:A:444:ARG:NH2	2.35	0.45
5:4:64:G:N2	5:4:67:A:H5'	2.30	0.45
7:C:950:SER:HA	7:C:953:PHE:HD2	1.80	0.45
8:U:301:LEU:HB3	8:U:314:ILE:HG12	1.97	0.45
9:A:1317:TYR:CE1	9:A:1329:SER:HB2	2.51	0.45
12:L:358:ARG:O	12:L:359:TYR:C	2.59	0.45
7:C:946:ASP:OD1	7:C:947:VAL:N	2.49	0.45
9:A:1199:LYS:HD3	9:A:1224:ARG:HE	1.82	0.45
9:A:395:THR:HG22	9:A:396:ASP:N	2.32	0.45
5:4:18:G:C5	12:L:365:ARG:NE	2.85	0.45
7:C:266:GLU:HG2	9:A:406:TRP:CZ2	2.51	0.45
9:A:175:PRO:HG2	9:A:498:ARG:NH1	2.31	0.45
14:D:45:LEU:HD13	14:D:58:ILE:HG21	1.98	0.45
2:G:274:PHE:HZ	9:A:592:TYR:CE1	2.35	0.45
11:N:23:ARG:HD3	14:D:15:ASP:HA	1.98	0.45
8:U:486:SER:O	8:U:490:GLN:HG3	2.17	0.45
3:6:47:A:N7	5:4:66:A:N6	2.65	0.45
7:C:841:ASP:OD1	7:C:842:CYS:N	2.50	0.45
8:U:292:LYS:HD3	8:U:294:HIS:CD2	2.51	0.45
9:A:1544:ARG:HE	9:A:1547:VAL:HG23	1.82	0.45
4:5:26:A:O3'	9:A:635:ARG:NH2	2.50	0.45
2:G:253:ARG:HH11	9:A:313:LYS:NZ	2.15	0.45
7:C:354:ARG:NH2	9:A:381:PRO:O	2.36	0.45
9:A:680:HIS:CE1	14:D:40:LYS:HG2	2.51	0.45
9:A:855:ARG:HA	9:A:855:ARG:HD3	1.81	0.45
9:A:931:ASP:OD2	9:A:1434:LYS:HB3	2.17	0.45
9:A:1418:ARG:C	9:A:1420:ASN:N	2.71	0.45
8:U:530:LEU:HG	8:U:535:VAL:HG22	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:651:TRP:HD1	11:N:82:ASN:HA	1.82	0.44
9:A:1003:HIS:HE1	11:N:265:GLN:HB3	1.82	0.44
9:A:1507:SER:O	9:A:1512:SER:N	2.50	0.44
9:A:1730:MET:HA	9:A:1733:ILE:HG22	1.99	0.44
4:5:64:G:H2'	4:5:65:G:H8	1.82	0.44
7:C:687:MET:HG2	7:C:791:ILE:HA	1.97	0.44
4:5:20:G:C5	9:A:463:PRO:HG2	2.52	0.44
7:C:213:ASP:OD1	7:C:214:GLU:N	2.50	0.44
7:C:692:LEU:HD22	7:C:696:LEU:HD23	1.99	0.44
8:U:504:ILE:HB	8:U:550:ILE:HB	1.99	0.44
9:A:811:THR:HA	9:A:814:VAL:HG22	2.00	0.44
9:A:1641:ARG:HB2	9:A:1651:VAL:HG23	1.98	0.44
5:4:18:G:N7	12:L:365:ARG:HD2	2.33	0.44
7:C:465:MET:HA	7:C:498:SER:OG	2.18	0.44
8:U:499:ASP:OD2	8:U:556:ARG:HD3	2.17	0.44
9:A:107:PRO:HD3	9:A:489:TRP:CD2	2.52	0.44
9:A:695:ASP:HB2	11:N:146:LYS:NZ	2.33	0.44
9:A:1271:MET:SD	9:A:1278:VAL:HG11	2.56	0.44
7:C:834:VAL:HG11	7:C:883:PHE:HE2	1.82	0.44
9:A:1418:ARG:HD3	9:A:1418:ARG:HA	1.80	0.44
15:X:143:ARG:NE	15:X:149:ARG:HH21	2.16	0.44
8:U:270:ILE:HG13	8:U:271:MET:HE2	1.99	0.44
9:A:147:MET:HA	9:A:147:MET:HE2	1.99	0.44
9:A:942:PRO:HD2	9:A:1438:VAL:CG2	2.34	0.44
9:A:1433:ASP:HB3	9:A:1460:HIS:HE1	1.83	0.44
9:A:235:MET:HE3	9:A:235:MET:HB3	1.78	0.44
4:5:28:A:OP2	9:A:457:ASN:ND2	2.36	0.44
8:U:214:ARG:HG2	8:U:220:THR:HG22	1.99	0.44
9:A:97:HIS:ND1	9:A:649:GLU:OE2	2.50	0.44
9:A:490:VAL:HG23	9:A:562:VAL:HG12	2.00	0.44
9:A:803:ALA:O	9:A:807:VAL:HG13	2.18	0.44
9:A:1346:THR:HG22	9:A:1347:ASP:N	2.32	0.44
1:7:461:ASP:OD1	1:7:461:ASP:N	2.48	0.44
4:5:17:U:H2'	4:5:18:C:C6	2.53	0.44
9:A:166:PHE:HB2	9:A:167:PRO:HD3	2.00	0.44
9:A:865:GLY:O	9:A:868:GLU:HG3	2.18	0.44
9:A:1422:LEU:HD22	9:A:1427:ARG:HH21	1.83	0.44
7:C:391:SER:O	7:C:391:SER:OG	2.27	0.43
7:C:516:LEU:HD13	7:C:575:GLN:HG2	2.00	0.43
7:C:619:THR:HA	7:C:628:VAL:O	2.18	0.43
7:C:776:GLU:O	7:C:782:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:127:SER:HB3	8:U:151:HIS:CD2	2.53	0.43
8:U:197:PHE:CE1	8:U:255:LEU:HD22	2.53	0.43
9:A:570:ASP:HB3	9:A:573:GLN:HG3	2.00	0.43
9:A:1633:ALA:HB2	9:A:1637:TRP:CZ2	2.53	0.43
14:D:80:THR:HG21	14:D:101:LYS:HZ3	1.82	0.43
9:A:1248:LEU:HD21	9:A:1295:ILE:HD13	2.00	0.43
14:D:104:TRP:CZ3	14:D:106:MET:HB3	2.53	0.43
7:C:201:ASN:HB3	7:C:549:TRP:CE3	2.53	0.43
9:A:151:MET:HE1	9:A:191:ILE:HD13	2.00	0.43
9:A:1341:ARG:HG2	9:A:1354:ARG:HG2	2.00	0.43
5:4:35:G:H2'	5:4:39:A:N6	2.33	0.43
9:A:201:ALA:HA	9:A:204:LEU:HD23	2.00	0.43
9:A:850:TYR:CE1	9:A:860:GLN:HG2	2.52	0.43
14:D:125:LYS:NZ	14:D:127:ARG:HG3	2.34	0.43
15:X:139:GLN:NE2	15:X:141:MET:O	2.51	0.43
5:4:18:G:C8	12:L:365:ARG:HD2	2.53	0.43
7:C:174:GLU:HG3	7:C:181:ILE:HD12	2.00	0.43
9:A:1555:LEU:HB3	9:A:1558:THR:HB	1.99	0.43
9:A:1607:GLU:H	9:A:1633:ALA:HA	1.83	0.43
7:C:126:SER:HA	7:C:129:ILE:HD12	2.01	0.43
7:C:339:PHE:O	7:C:343:LEU:HG	2.17	0.43
7:C:733:TRP:NE1	7:C:747:ASP:OD1	2.51	0.43
7:C:939:ARG:NH1	7:C:945:GLU:OE1	2.52	0.43
8:U:123:LEU:HB3	8:U:130:HIS:CE1	2.53	0.43
14:D:41:MET:HG3	14:D:105:ALA:HB2	2.01	0.43
2:G:245:LYS:HA	2:G:245:LYS:HD2	1.84	0.43
3:6:58:G:H1'	5:4:55:U:H3	1.82	0.43
3:6:66:C:H2'	3:6:67:G:C8	2.54	0.43
7:C:138:LEU:HD11	7:C:179:VAL:HG22	1.99	0.43
9:A:1304:ASN:OD1	9:A:1305:SER:N	2.51	0.43
9:A:1519:THR:HB	9:A:1522:GLN:HG3	1.99	0.43
9:A:1583:GLN:NE2	9:A:1620:TYR:HE1	2.16	0.43
5:4:12:G:H2'	5:4:13:U:C6	2.53	0.43
5:4:60:A:H2'	5:4:61:A:C8	2.53	0.43
7:C:137:HIS:HB2	7:C:239:THR:HG23	2.00	0.43
7:C:664:GLU:HB3	7:C:820:PHE:CZ	2.54	0.43
8:U:135:ALA:HB2	8:U:167:LEU:HD21	2.00	0.43
9:A:770:THR:HA	9:A:773:LYS:NZ	2.34	0.43
9:A:1132:LYS:HA	9:A:1139:ARG:HD3	2.01	0.43
14:D:102:ILE:HG21	14:D:106:MET:HE1	2.01	0.43
7:C:888:ARG:O	7:C:893:GLY:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:490:VAL:CG2	9:A:562:VAL:HG12	2.49	0.43
9:A:1386:TRP:NE1	9:A:1417:PRO:HD2	2.34	0.43
9:A:1625:SER:OG	9:A:1626:CYS:N	2.51	0.43
9:A:313:LYS:HA	9:A:320:TYR:HB2	2.01	0.43
9:A:1562:MET:HE1	9:A:1570:LYS:HA	2.01	0.43
15:X:143:ARG:HH22	15:X:147:PHE:HA	1.84	0.43
8:U:277:ARG:HH11	8:U:303:ALA:HB2	1.83	0.42
9:A:564:TYR:CG	9:A:574:LEU:HD22	2.53	0.42
9:A:804:GLU:HA	9:A:807:VAL:HG22	2.00	0.42
9:A:1418:ARG:O	9:A:1419:ILE:C	2.59	0.42
9:A:1495:PHE:CD2	9:A:1501:LEU:HD21	2.54	0.42
11:N:253:MET:HE3	11:N:253:MET:HB3	1.89	0.42
8:U:222:LEU:HD22	8:U:521:HIS:CE1	2.54	0.42
9:A:955:TRP:CG	9:A:1189:MET:HE1	2.54	0.42
9:A:1281:THR:HG22	9:A:1284:LEU:H	1.83	0.42
9:A:1597:PHE:HE2	9:A:1631:LEU:HD11	1.83	0.42
12:L:357:ARG:HG3	12:L:358:ARG:HG3	2.00	0.42
14:D:89:HIS:CE1	14:D:100:ASN:HD22	2.37	0.42
7:C:255:VAL:HG23	7:C:300:LEU:HD23	2.00	0.42
8:U:452:ILE:HG12	8:U:552:ILE:HD12	2.00	0.42
9:A:156:ARG:O	9:A:159:ARG:NH1	2.53	0.42
9:A:827:PHE:O	9:A:828:PRO:C	2.62	0.42
9:A:1158:LYS:HE2	9:A:1163:ARG:NH2	2.34	0.42
9:A:1469:ASN:OD1	9:A:1469:ASN:N	2.52	0.42
3:6:61:C:H2'	3:6:62:C:C6	2.54	0.42
8:U:122:LYS:HG2	8:U:167:LEU:HD13	2.01	0.42
8:U:266:PRO:HB2	8:U:269:ASP:HB2	2.01	0.42
9:A:156:ARG:HA	9:A:159:ARG:HH22	1.84	0.42
9:A:574:LEU:O	9:A:578:LEU:HG	2.19	0.42
9:A:1413:ASP:OD1	9:A:1420:ASN:ND2	2.52	0.42
2:G:299:LEU:HD22	9:A:355:LEU:HD22	2.01	0.42
4:5:32:C:H2'	4:5:33:U:C6	2.54	0.42
9:A:84:ASP:OD1	9:A:84:ASP:N	2.52	0.42
9:A:1491:LYS:HD3	9:A:1709:TYR:HD2	1.84	0.42
9:A:1661:TRP:CE2	9:A:1700:GLY:HA3	2.54	0.42
14:D:68:ASP:OD1	14:D:68:ASP:N	2.53	0.42
9:A:1002:ASP:OD1	11:N:267:VAL:HA	2.20	0.42
9:A:1386:TRP:HH2	9:A:1422:LEU:HD21	1.85	0.42
14:D:24:ARG:HG2	14:D:55:PHE:HA	2.02	0.42
14:D:80:THR:HG22	14:D:103:ASN:ND2	2.34	0.42
2:G:305:ALA:HB2	9:A:246:LEU:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:346:ASP:OD1	7:C:367:ARG:NE	2.52	0.42
9:A:232:LEU:HD23	9:A:232:LEU:HA	1.87	0.42
9:A:731:LEU:HD21	9:A:739:ILE:HD12	2.00	0.42
9:A:1045:GLY:HA2	9:A:1048:MET:HE2	2.01	0.42
9:A:1386:TRP:HE1	9:A:1417:PRO:HD2	1.85	0.42
5:4:27:C:H2'	5:4:28:C:C6	2.55	0.42
7:C:158:ARG:HD3	7:C:158:ARG:HA	1.87	0.42
9:A:641:MET:HE2	9:A:641:MET:HB2	1.91	0.42
9:A:1179:SER:O	9:A:1201:ARG:NH1	2.44	0.42
14:D:125:LYS:HZ1	14:D:127:ARG:HG3	1.85	0.42
8:U:457:ARG:NH1	8:U:470:THR:O	2.30	0.42
9:A:686:ARG:NH2	9:A:710:LEU:HD11	2.35	0.42
9:A:947:PRO:HB2	9:A:949:PRO:HD2	2.02	0.42
9:A:1566:ILE:HG22	9:A:1569:LEU:H	1.84	0.42
11:N:23:ARG:HB2	14:D:15:ASP:HB2	2.01	0.42
7:C:666:VAL:HG22	7:C:787:VAL:HG22	2.01	0.42
8:U:369:GLU:O	8:U:372:GLU:HG3	2.20	0.42
9:A:254:TYR:CE2	9:A:433:GLU:HB2	2.55	0.42
9:A:658:ARG:HB2	11:N:90:SER:HA	2.02	0.42
9:A:940:ILE:CD1	9:A:1046:LEU:HB2	2.49	0.42
9:A:1001:VAL:HG22	9:A:1002:ASP:H	1.85	0.42
9:A:1667:ARG:NH2	9:A:1673:SER:OG	2.53	0.42
7:C:134:LEU:HD23	7:C:226:VAL:HB	2.01	0.41
8:U:123:LEU:HD13	8:U:128:LEU:HD13	2.01	0.41
8:U:234:ASN:ND2	8:U:238:ASN:OD1	2.53	0.41
8:U:332:HIS:ND1	8:U:344:THR:OG1	2.43	0.41
9:A:1061:MET:HE1	9:A:1088:PHE:CB	2.47	0.41
7:C:596:ASN:O	7:C:599:GLU:HG2	2.19	0.41
7:C:700:ILE:HD11	7:C:744:ILE:HD11	2.02	0.41
7:C:772:TRP:CZ3	7:C:813:ARG:HD3	2.56	0.41
8:U:506:HIS:NE2	8:U:513:GLY:HA3	2.35	0.41
8:U:521:HIS:ND1	8:U:524:THR:OG1	2.39	0.41
2:G:274:PHE:CD1	9:A:599:MET:HE1	2.56	0.41
2:G:320:TYR:O	2:G:324:MET:HG2	2.20	0.41
8:U:354:MET:HE3	8:U:356:ILE:HG12	2.01	0.41
9:A:750:TRP:HH2	9:A:781:ARG:HB2	1.84	0.41
11:N:95:GLU:N	11:N:98:ASP:OD2	2.48	0.41
3:6:58:G:H1'	5:4:55:U:N3	2.36	0.41
7:C:663:CYS:HB2	7:C:828:MET:HB2	2.03	0.41
7:C:829:GLU:OE2	7:C:854:ARG:NH2	2.37	0.41
7:C:922:GLU:O	7:C:924:GLN:NE2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:161:PHE:HZ	9:A:573:GLN:HA	1.85	0.41
9:A:539:ARG:HB2	11:N:84:TYR:HE2	1.85	0.41
3:6:68:C:H2'	3:6:69:A:H8	1.85	0.41
7:C:863:ILE:HB	7:C:866:SER:HB3	2.02	0.41
9:A:488:ASP:OD1	9:A:489:TRP:N	2.54	0.41
9:A:907:PRO:HG2	9:A:1032:ARG:NH2	2.36	0.41
7:C:716:GLU:O	7:C:720:THR:HG22	2.20	0.41
9:A:1421:THR:C	9:A:1423:PHE:N	2.76	0.41
6:S:712:TYR:HA	15:X:135:ARG:HH12	1.84	0.41
9:A:647:LEU:HD23	11:N:81:PHE:CZ	2.56	0.41
9:A:1110:ILE:HD11	9:A:1149:LEU:HB2	2.02	0.41
9:A:1208:THR:OG1	9:A:1209:HIS:N	2.53	0.41
9:A:1421:THR:C	9:A:1423:PHE:H	2.29	0.41
14:D:39:MET:HE3	14:D:39:MET:HB2	1.88	0.41
2:G:282:THR:H	9:A:448:GLN:HE22	1.69	0.41
7:C:193:THR:HG23	7:C:194:LYS:N	2.36	0.41
9:A:549:GLU:HB2	9:A:591:MET:HE3	2.03	0.41
9:A:1723:LYS:HB3	9:A:1724:PRO:HD3	2.02	0.41
4:5:25:C:C2	9:A:409:ARG:HD2	2.56	0.41
8:U:245:SER:C	8:U:247:VAL:H	2.29	0.41
8:U:251:ARG:O	8:U:255:LEU:HG	2.21	0.41
8:U:425:GLY:O	8:U:441:ARG:NH1	2.52	0.41
9:A:282:LEU:HD23	9:A:283:VAL:HG13	2.02	0.41
9:A:682:ASP:OD1	9:A:682:ASP:N	2.54	0.41
7:C:361:PRO:C	7:C:363:SER:H	2.29	0.41
7:C:412:ILE:HD13	7:C:412:ILE:HA	1.93	0.41
7:C:446:LYS:HB3	7:C:447:PRO:HD3	2.02	0.41
8:U:439:LEU:HD23	8:U:439:LEU:HA	1.89	0.41
9:A:292:ASP:OD1	9:A:1139:ARG:NE	2.53	0.41
9:A:1090:ARG:HG2	9:A:1091:TYR:O	2.21	0.41
9:A:1606:ILE:HG21	9:A:1631:LEU:HD22	2.03	0.41
5:4:18:G:N2	5:4:52:U:O4	2.55	0.40
7:C:227:LEU:HD23	7:C:229:ILE:HD11	2.03	0.40
7:C:686:THR:HB	7:C:793:ASP:HB3	2.03	0.40
9:A:112:GLN:HB3	9:A:187:PRO:HG2	2.03	0.40
9:A:169:PHE:HE2	9:A:176:LEU:HD11	1.85	0.40
9:A:419:ARG:NH2	9:A:423:ASP:O	2.54	0.40
9:A:503:MET:HE1	9:A:652:LEU:HD21	2.02	0.40
9:A:1031:ILE:O	9:A:1032:ARG:HB2	2.21	0.40
9:A:1614:ILE:O	15:X:149:ARG:HG2	2.21	0.40
7:C:589:LYS:HG3	7:C:628:VAL:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:937:PRO:HD2	9:A:940:ILE:CD1	2.52	0.40
7:C:495:ARG:HB3	7:C:549:TRP:CD1	2.56	0.40
7:C:673:LYS:HA	7:C:688:ILE:HG22	2.03	0.40
8:U:235:ASP:OD1	8:U:235:ASP:N	2.53	0.40
9:A:109:PRO:HD3	9:A:630:TRP:CZ2	2.55	0.40
9:A:293:TRP:CD1	9:A:1141:ARG:HB3	2.57	0.40
9:A:521:ASN:HB3	9:A:552:ARG:HH12	1.87	0.40
9:A:733:THR:N	9:A:734:PRO:HD2	2.36	0.40
9:A:1248:LEU:HB3	14:D:142:TYR:CD2	2.57	0.40
9:A:1509:PHE:HE1	9:A:1749:LYS:HG2	1.86	0.40
9:A:521:ASN:HB3	9:A:552:ARG:NH1	2.37	0.40
12:L:357:ARG:HA	12:L:357:ARG:HD2	1.84	0.40
2:G:246:GLU:HG3	9:A:307:PRO:HG3	2.03	0.40
5:4:59:U:H2'	5:4:60:A:C8	2.57	0.40
7:C:614:TYR:HB2	7:C:617:LEU:HB2	2.03	0.40
8:U:188:ASP:OD1	8:U:188:ASP:N	2.53	0.40
9:A:1690:ASP:HB3	9:A:1693:SER:OG	2.20	0.40
14:D:102:ILE:HG22	14:D:104:TRP:CD1	2.57	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	7	11/793 (1%)	11 (100%)	0	0	100	100
2	G	97/820 (12%)	94 (97%)	3 (3%)	0	100	100
6	S	57/800 (7%)	56 (98%)	1 (2%)	0	100	100
7	C	850/972 (87%)	825 (97%)	25 (3%)	0	100	100
8	U	454/565 (80%)	431 (95%)	23 (5%)	0	100	100
9	A	1904/2335 (82%)	1841 (97%)	61 (3%)	2 (0%)	48	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	R	104/480 (22%)	99 (95%)	5 (5%)	0	100	100
11	N	146/941 (16%)	142 (97%)	4 (3%)	0	100	100
12	L	48/499 (10%)	40 (83%)	8 (17%)	0	100	100
13	J	40/683 (6%)	40 (100%)	0	0	100	100
14	D	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
15	X	16/155 (10%)	16 (100%)	0	0	100	100
All	All	3866/9185 (42%)	3731 (96%)	133 (3%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	A	1417	PRO
9	A	167	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7	12/709 (2%)	12 (100%)	0	100	100
2	G	92/721 (13%)	91 (99%)	1 (1%)	65	74
6	S	2/681 (0%)	2 (100%)	0	100	100
7	C	754/866 (87%)	754 (100%)	0	100	100
8	U	418/511 (82%)	418 (100%)	0	100	100
9	A	1520/2108 (72%)	1519 (100%)	1 (0%)	88	87
10	R	4/369 (1%)	4 (100%)	0	100	100
11	N	132/792 (17%)	132 (100%)	0	100	100
12	L	35/424 (8%)	35 (100%)	0	100	100
13	J	4/599 (1%)	4 (100%)	0	100	100
14	D	129/130 (99%)	129 (100%)	0	100	100
15	X	16/144 (11%)	16 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3118/8054 (39%)	3116 (100%)	2 (0%)	87	87

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

Mol	Chain	Res	Type
2	G	248	HIS
9	A	170	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
7	C	366	GLN
7	C	575	GLN
7	C	583	ASN
7	C	807	GLN
8	U	162	HIS
8	U	201	GLN
8	U	246	ASN
8	U	473	ASN
9	A	130	ASN
9	A	325	HIS
9	A	434	HIS
9	A	680	HIS
9	A	752	ASN
9	A	775	ASN
9	A	815	HIS
9	A	1014	ASN
9	A	1169	GLN
9	A	1209	HIS
9	A	1595	GLN
9	A	1727	GLN
11	N	74	ASN
11	N	245	GLN
11	N	278	ASN
14	D	32	HIS
14	D	100	ASN
14	D	103	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	6	36/106 (33%)	3 (8%)	1 (2%)
4	5	69/117 (58%)	19 (27%)	3 (4%)
5	4	74/144 (51%)	12 (16%)	2 (2%)
All	All	179/367 (48%)	34 (18%)	6 (3%)

All (34) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	6	48	A
3	6	49	G
3	6	77	C
4	5	20	G
4	5	21	A
4	5	25	C
4	5	26	A
4	5	28	A
4	5	36	C
4	5	37	G
4	5	38	C
4	5	47	A
4	5	48	A
4	5	58	U
4	5	59	G
4	5	66	A
4	5	67	A
4	5	69	A
4	5	70	A
4	5	71	C
4	5	75	G
4	5	78	U
5	4	2	G
5	4	19	U
5	4	20	A
5	4	25	A
5	4	26	G
5	4	36	U
5	4	37	C
5	4	38	U
5	4	44	A
5	4	45	G
5	4	68	A
5	4	69	C

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	6	47	A
4	5	24	G
4	5	57	G
4	5	58	U
5	4	1	A
5	4	68	A

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	$\# Z > 2$
16	IHP	A	2401	-	36,36,36	0.76	0	60,60,60	1.21	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	IHP	A	2401	-	-	1/30/54/54	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	2401	IHP	C5-C4-C3	3.37	117.82	110.43
16	A	2401	IHP	P5-O15-C5	-2.35	117.16	123.43
16	A	2401	IHP	C6-C5-C4	2.19	115.23	110.43

There are no chirality outliers.

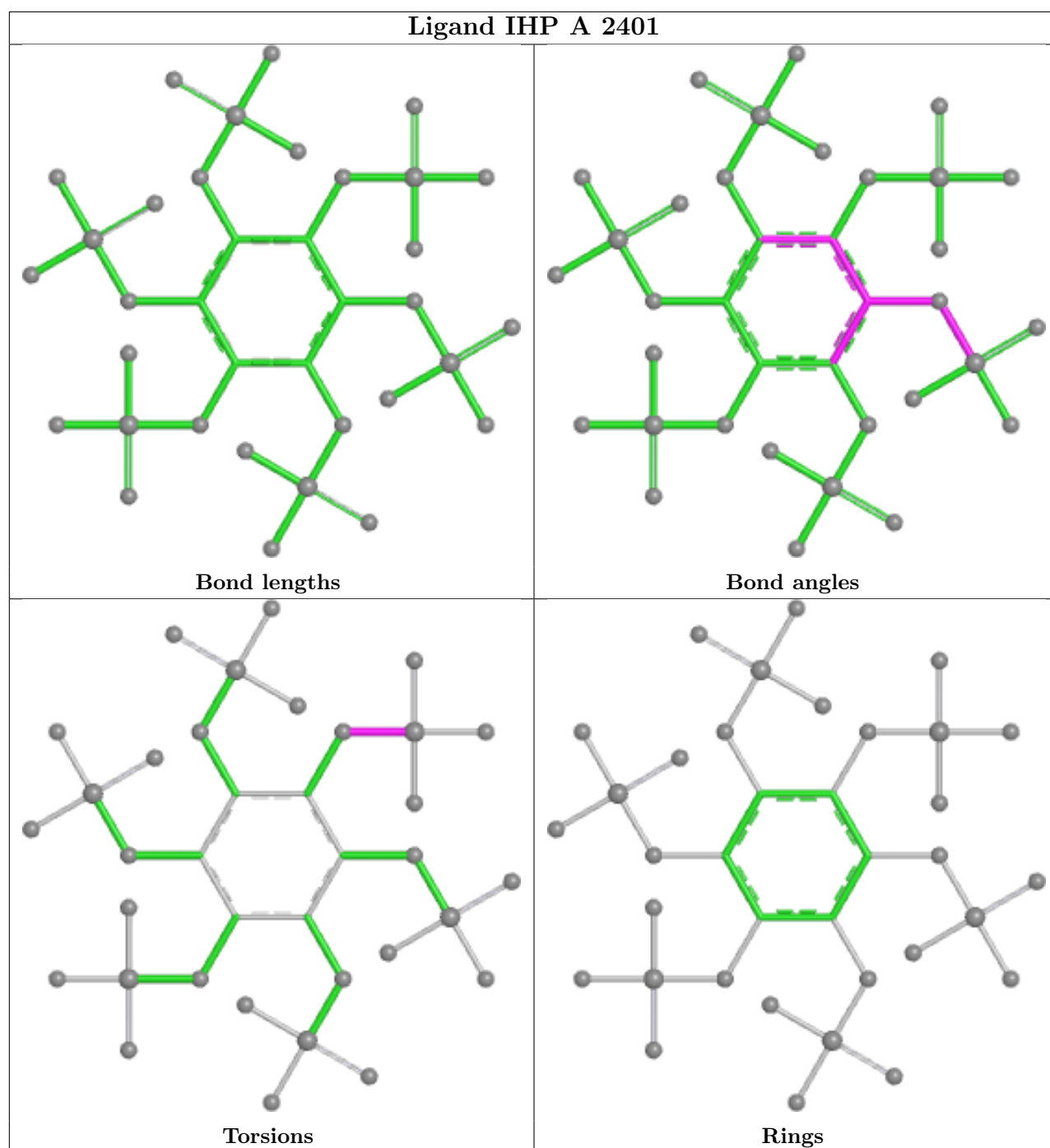
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	2401	IHP	C4-O14-P4-O44

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.

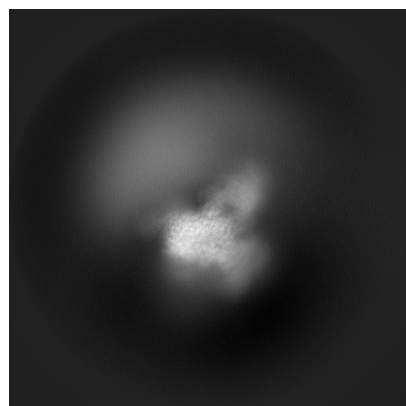
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18544. These allow visual inspection of the internal detail of the map and identification of artifacts.

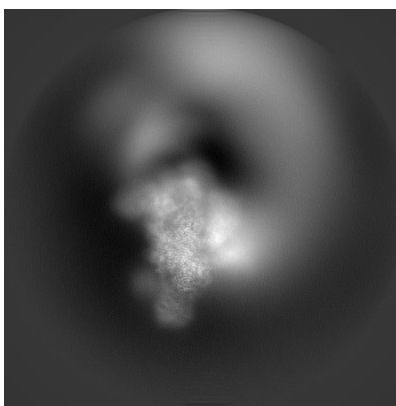
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

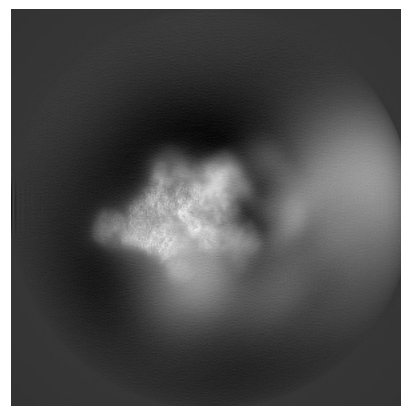
6.1.1 Primary map



X

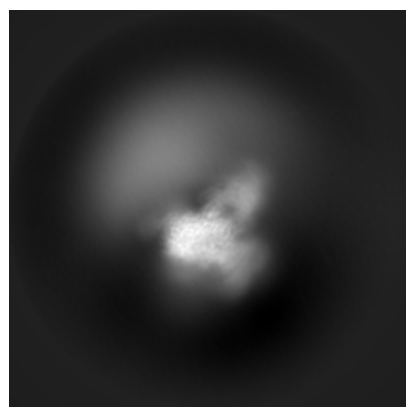


Y

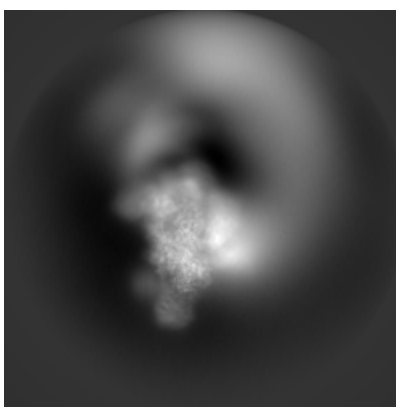


Z

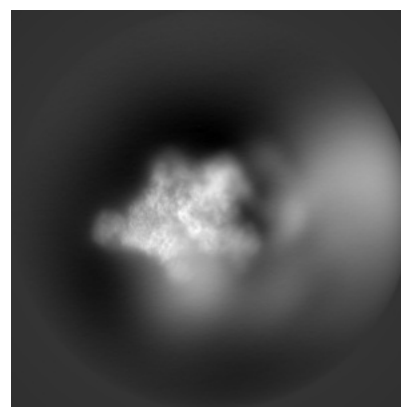
6.1.2 Raw map



X



Y

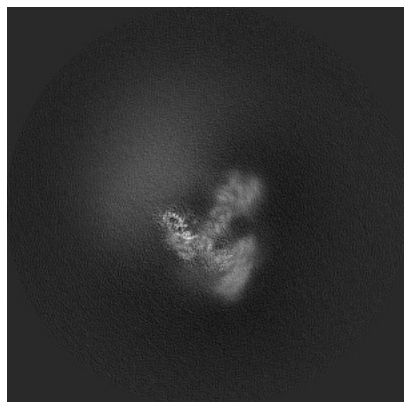


Z

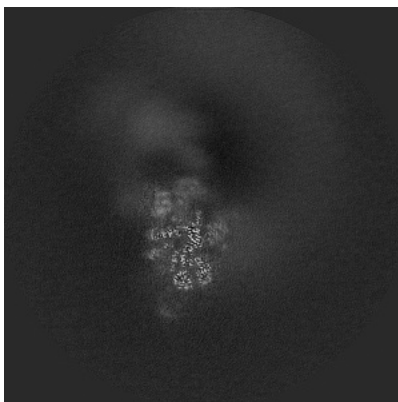
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

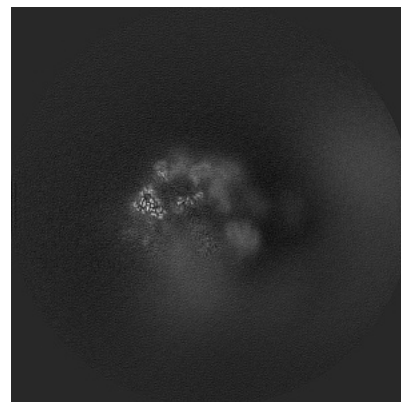
6.2.1 Primary map



X Index: 240

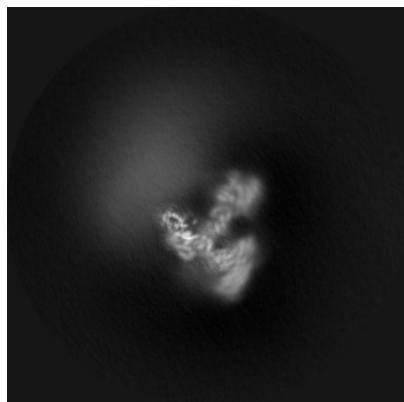


Y Index: 240

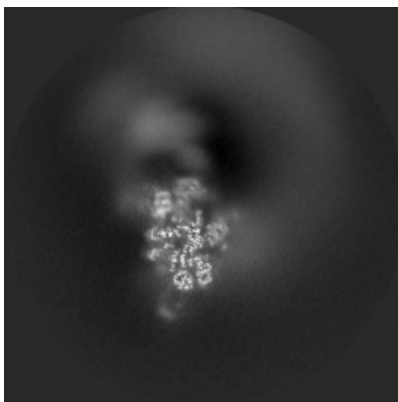


Z Index: 240

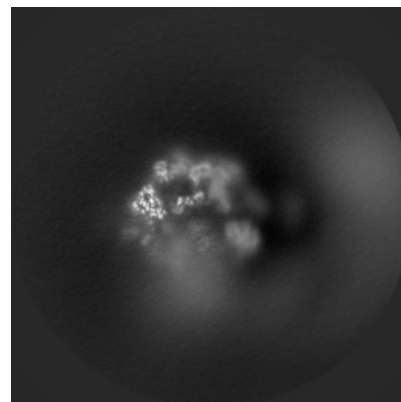
6.2.2 Raw map



X Index: 240



Y Index: 240

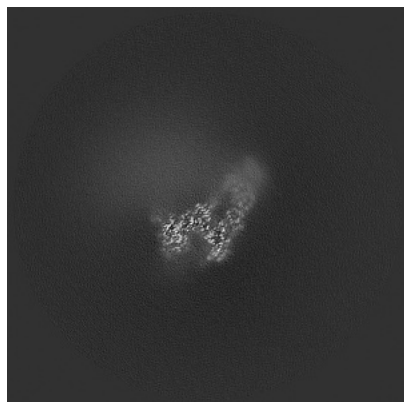


Z Index: 240

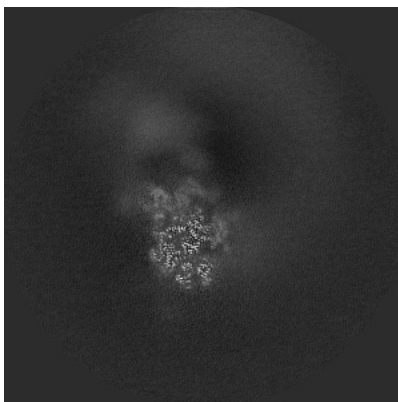
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

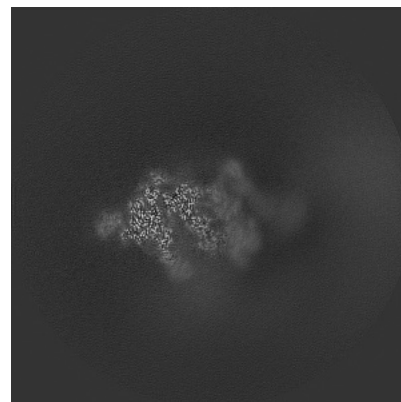
6.3.1 Primary map



X Index: 177

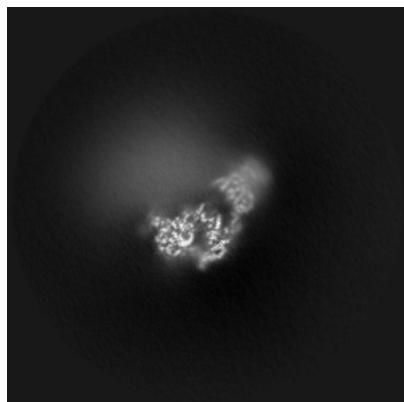


Y Index: 245

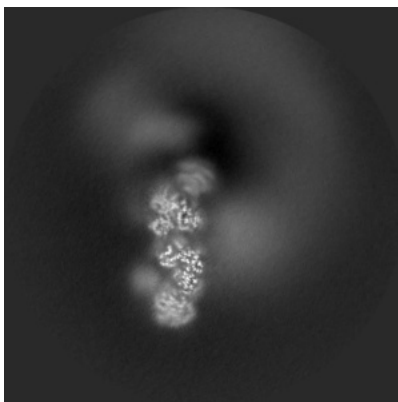


Z Index: 221

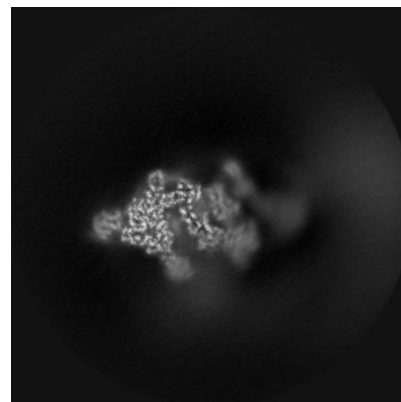
6.3.2 Raw map



X Index: 184



Y Index: 214

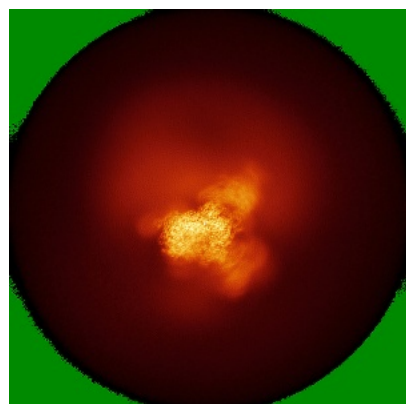


Z Index: 216

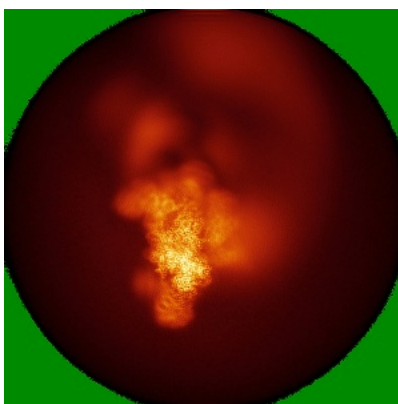
The images above show the largest variance slices of the map in three orthogonal directions.

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

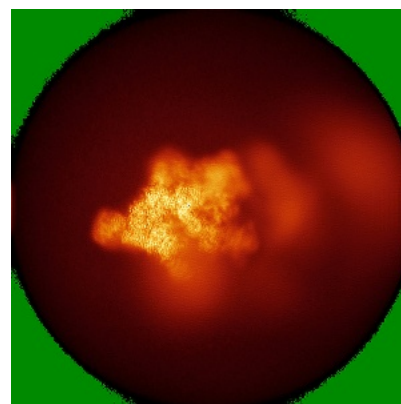
6.4.1 Primary map



X

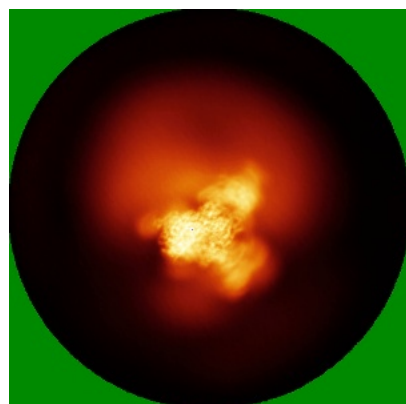


Y

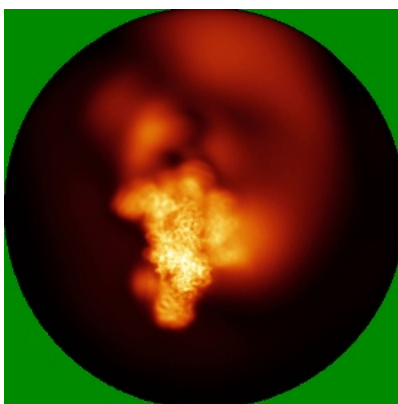


Z

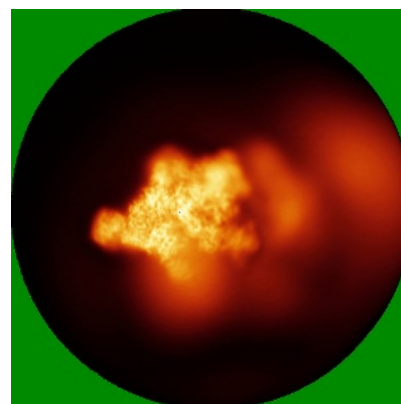
6.4.2 Raw map



X



Y

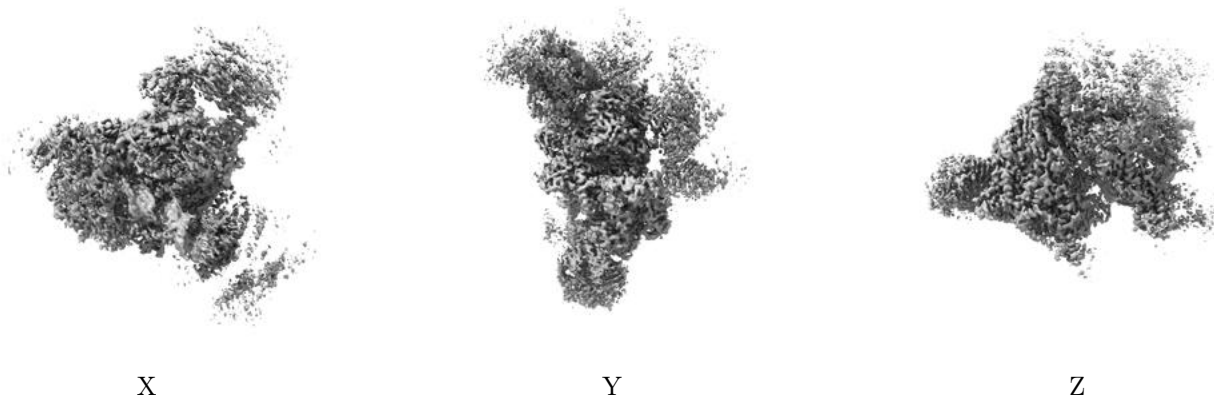


Z

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 0.075. 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.

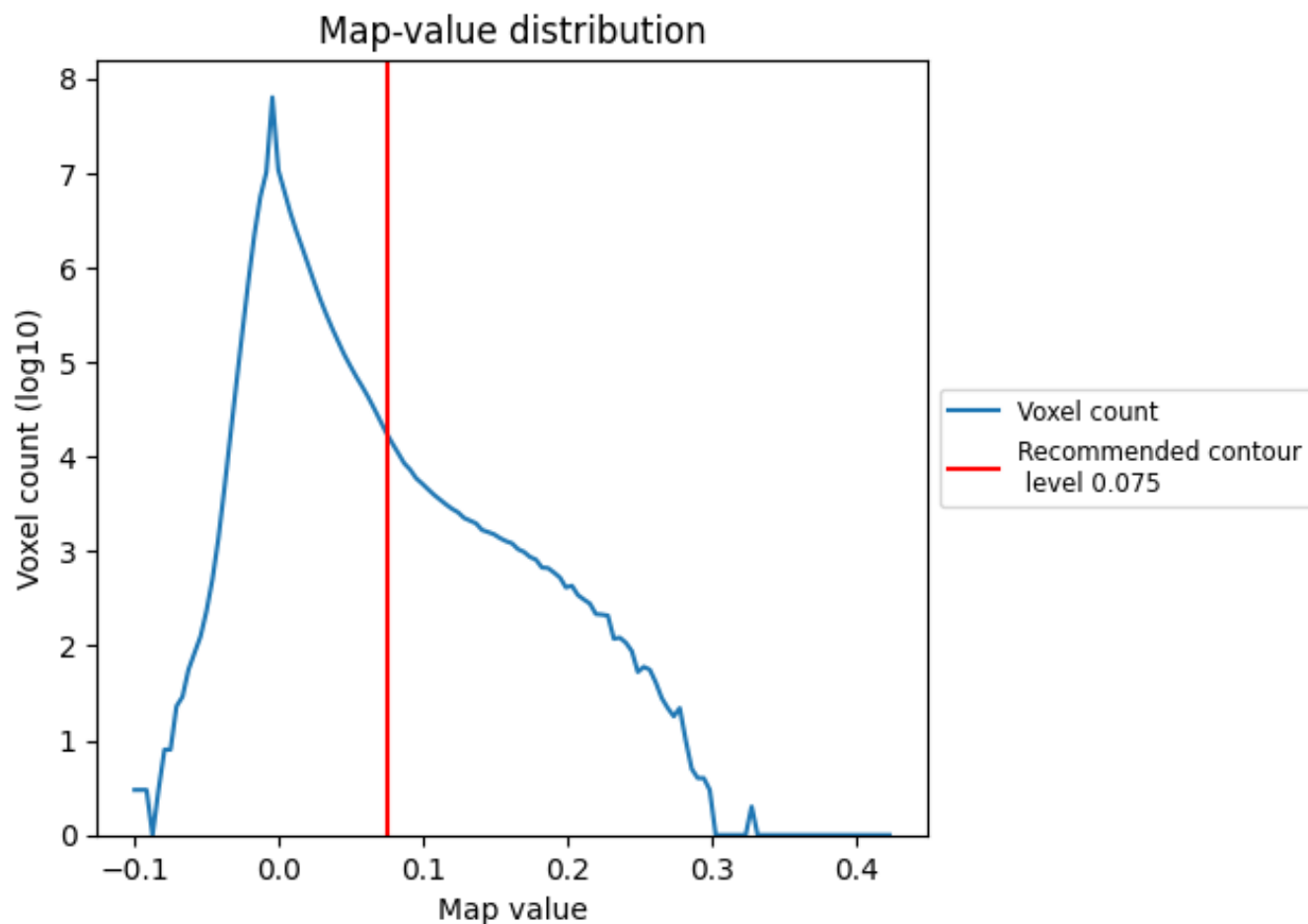
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

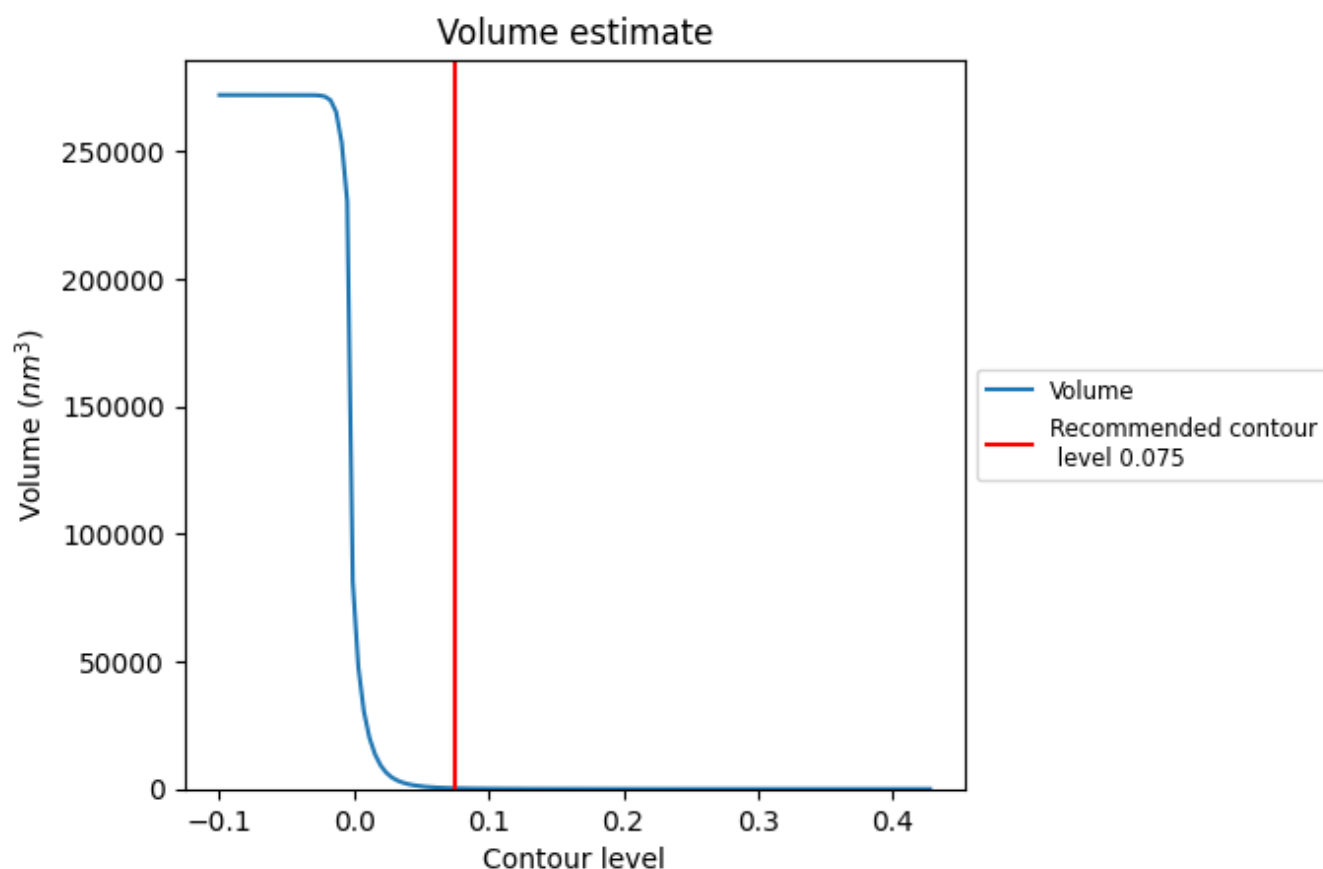
This section contains the results of statistical analysis of the map.

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.

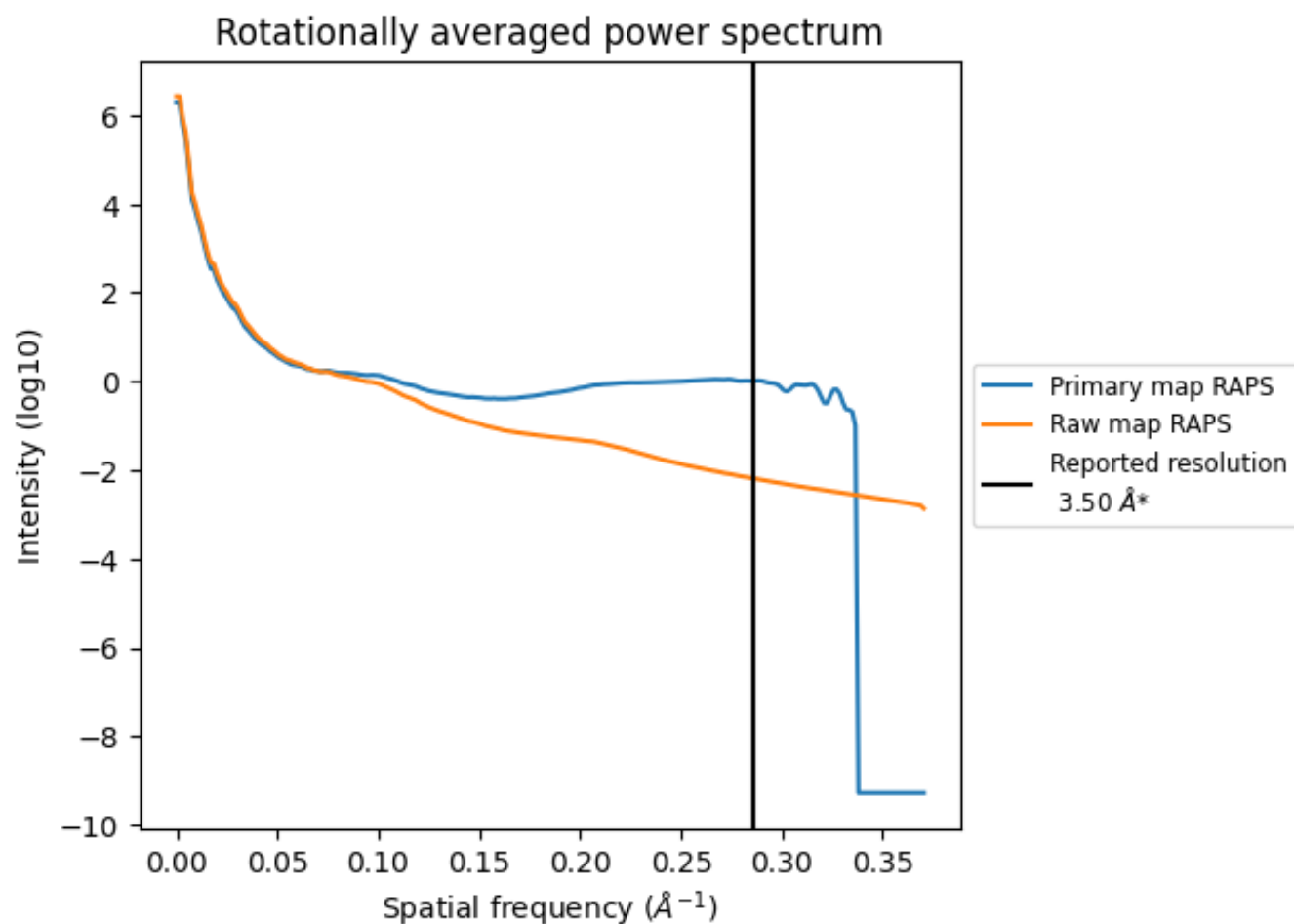
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 280 nm³; this corresponds to an approximate mass of 253 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 ⓘ

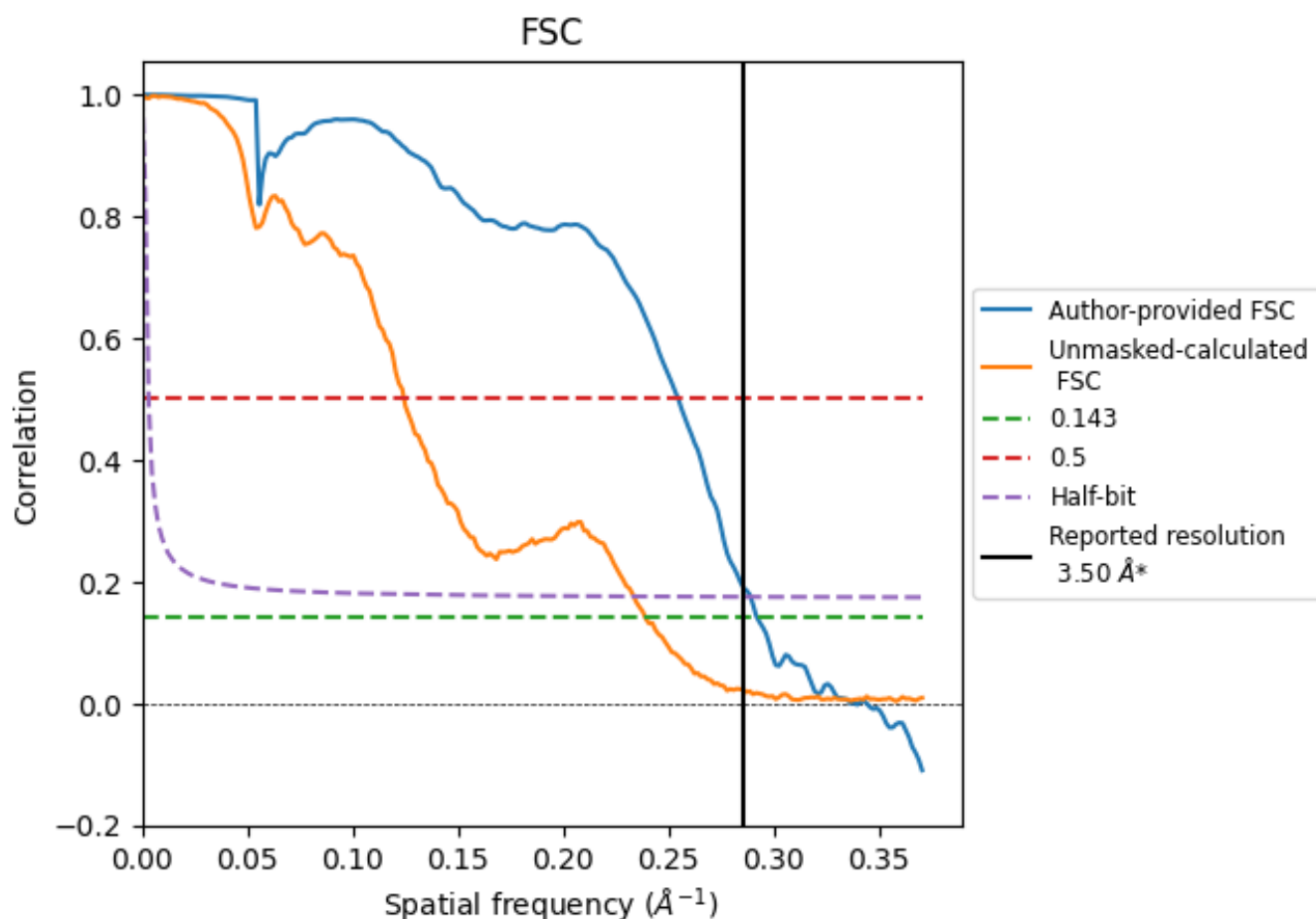


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

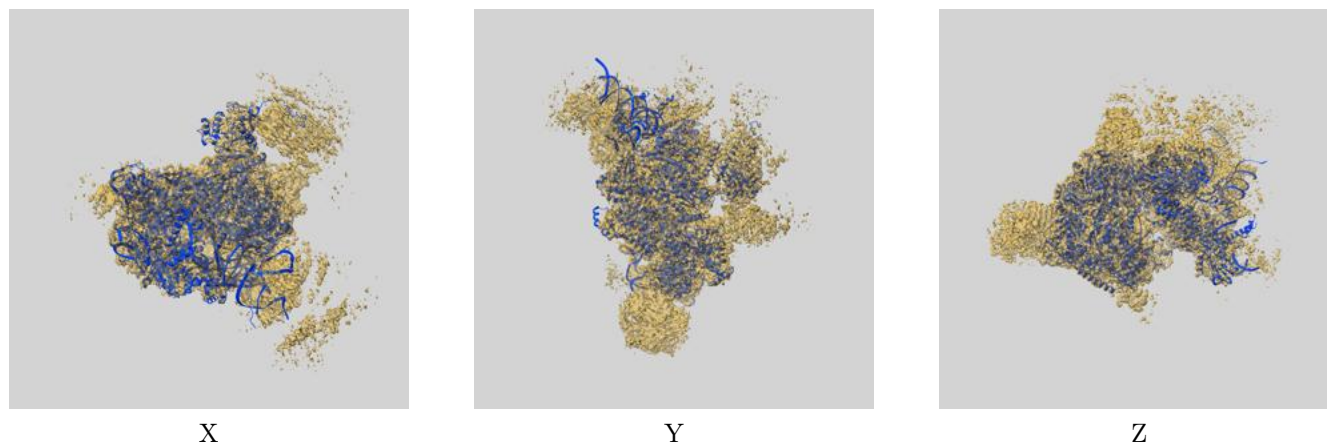
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.43	3.93	3.46
Unmasked-calculated*	4.19	8.05	4.28

*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 4.19 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

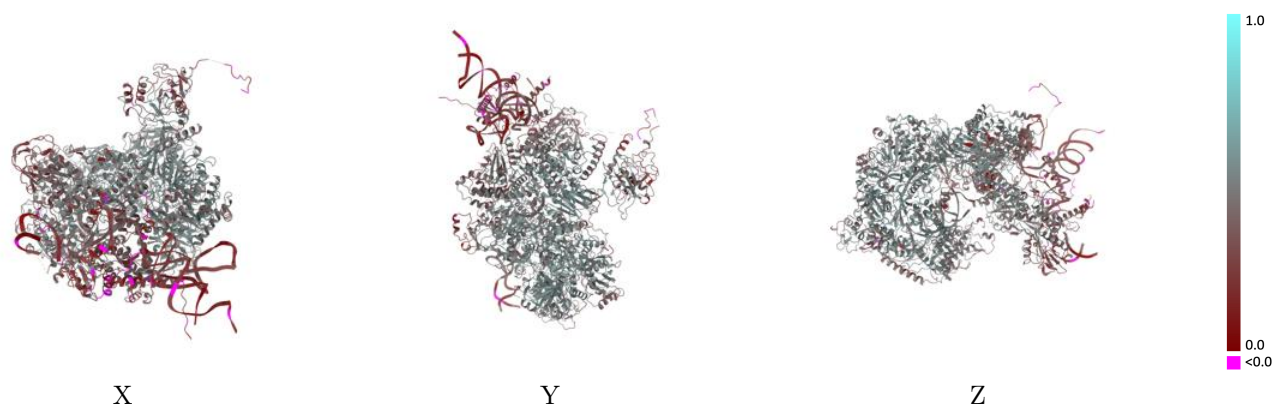
This section contains information regarding the fit between EMDB map EMD-18544 and PDB model 8QP8. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



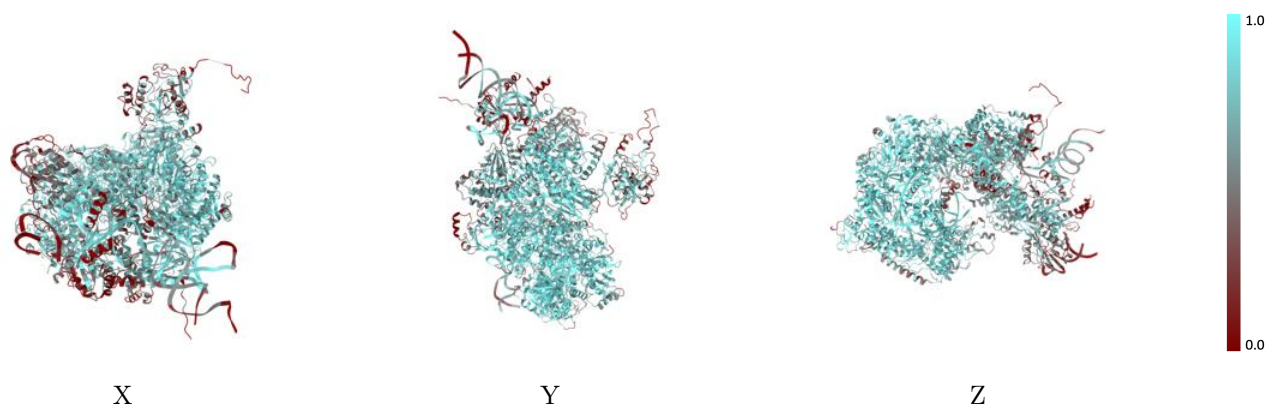
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



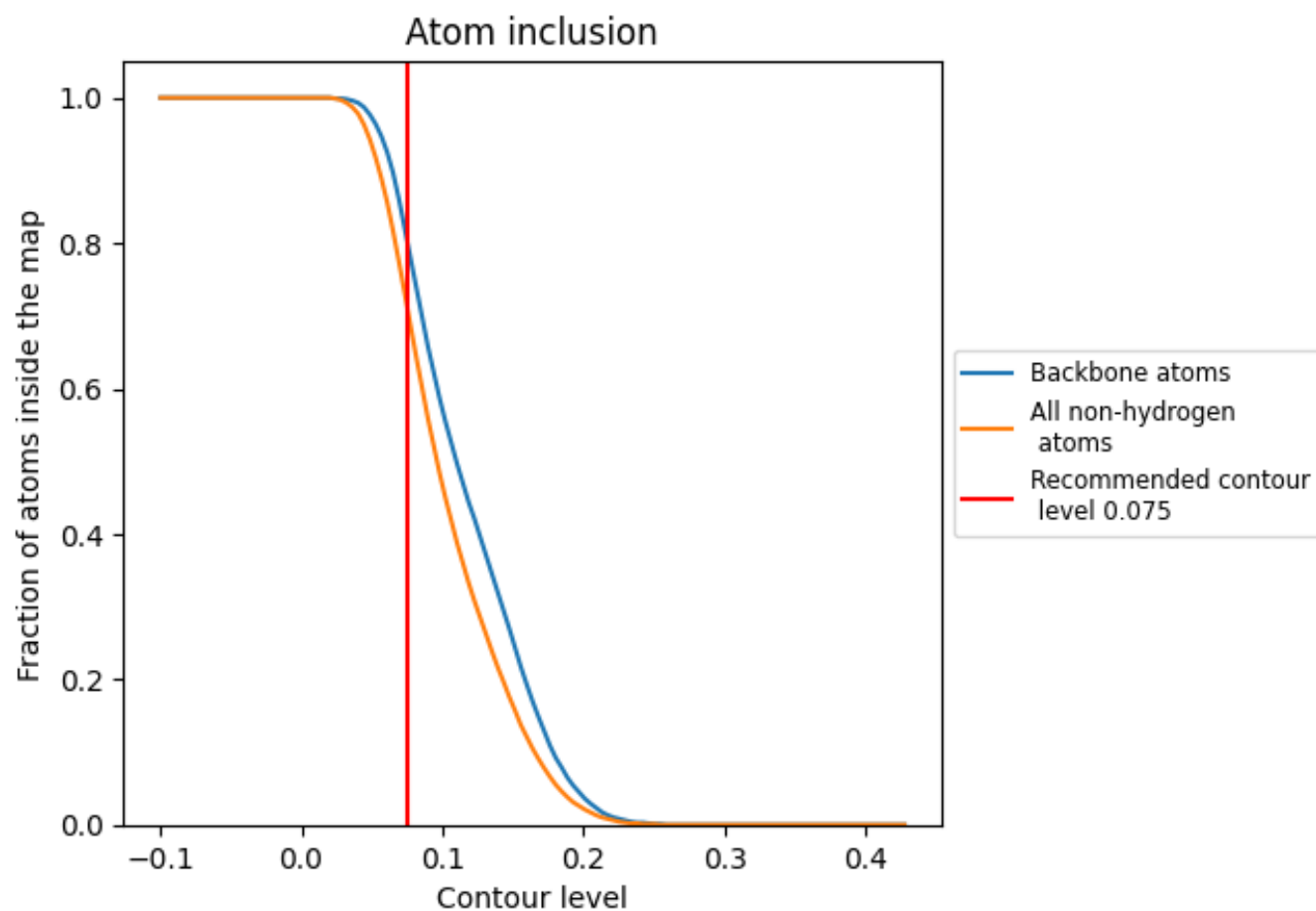
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 71% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7130	 0.4410
4	 0.5660	 0.2230
5	 0.8250	 0.3930
6	 0.4780	 0.1960
7	 0.4470	 0.3750
A	 0.7270	 0.4670
C	 0.8350	 0.5070
D	 0.6510	 0.4210
G	 0.6400	 0.4400
J	 0.3290	 0.1800
L	 0.3450	 0.2820
N	 0.5350	 0.3960
R	 0.2690	 0.2440
S	 0.4490	 0.3650
U	 0.7700	 0.4760
X	 0.2430	 0.2480

