



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:10 PM UTC

PDB ID : 8QOZ / pdb_00008qoz
EMDB ID : EMD-18542
Title : Cryo-EM Structure of Pre-B+5'ss+ATPgammaS 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 : 2023-09-29
Resolution : 3.10 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:

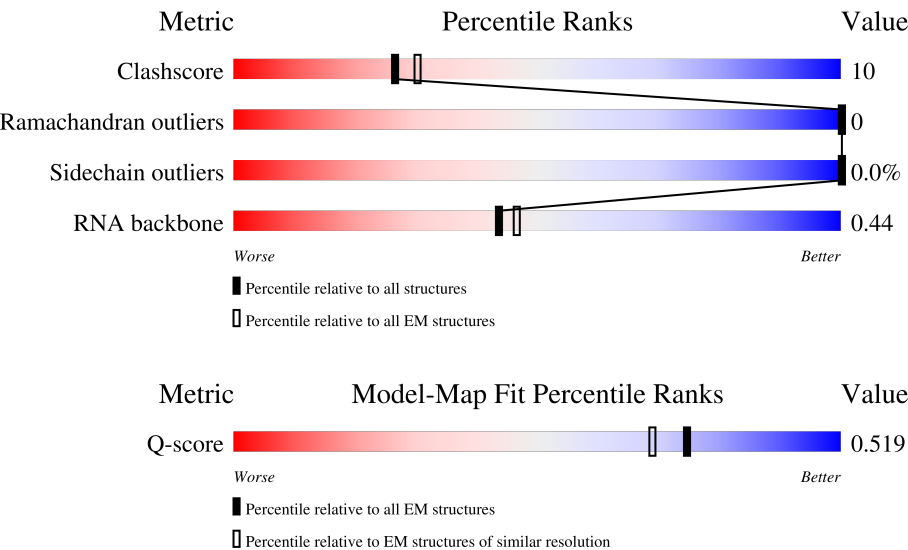
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.10 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.



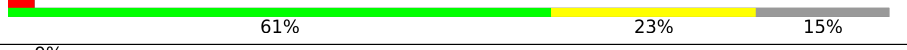
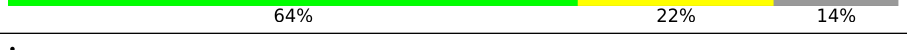
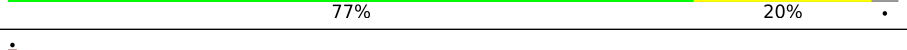
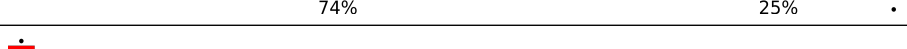
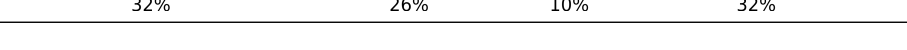
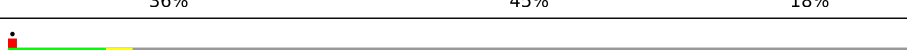
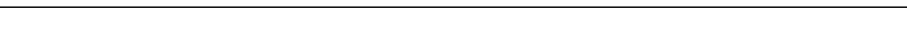
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	160	 11% 86%
2	G	820	 11% 85%
3	J	683	 9% 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	11	
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 44360 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	84	Total	C	N	O	S	0	0
			679	419	138	119	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
			2886	1796	526	552	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
			3502	2191	655	644	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1977	Total	C	N	O	S	0	0
			16419	10577	2865	2907	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
			1164	724	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 RNA oligo.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	z	11	Total	C	N	O	P	0	0
			239	107	46	75	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	7	107	Total	C	N	O	S	0	0
			846	522	152	169	3		

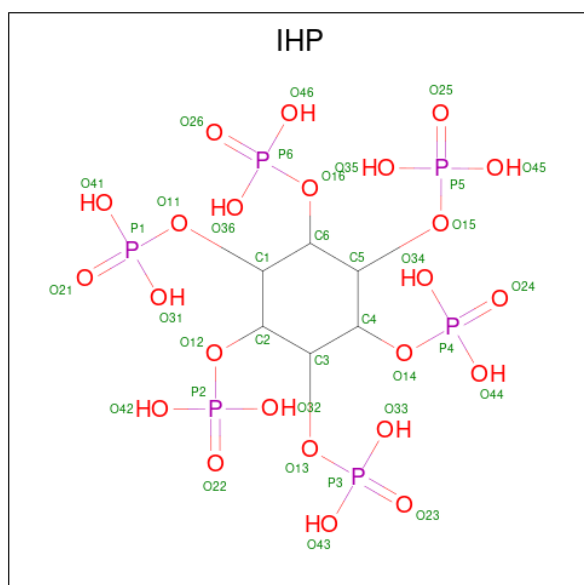
- Molecule 16 is a RNA chain called U4 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	80	Total	C	N	O	P	0	0
			1699	760	297	562	80		

- Molecule 17 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	6	48	Total	C	N	O	P	0	0
			1034	462	196	328	48		

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

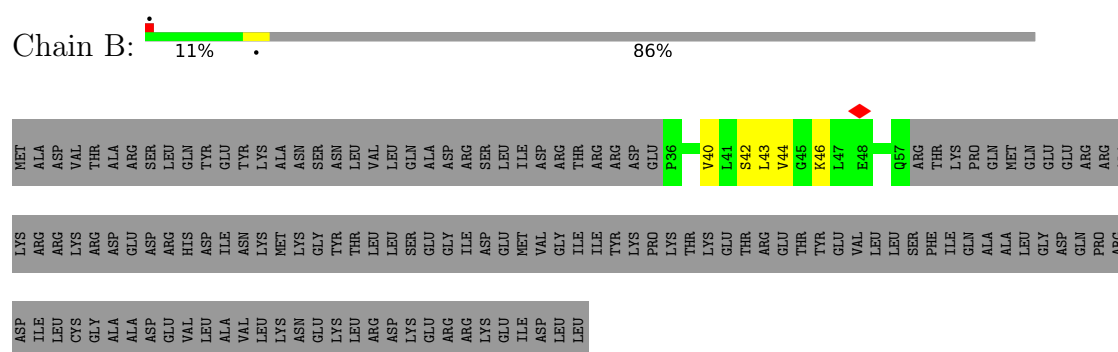


Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			36	6	24	6	

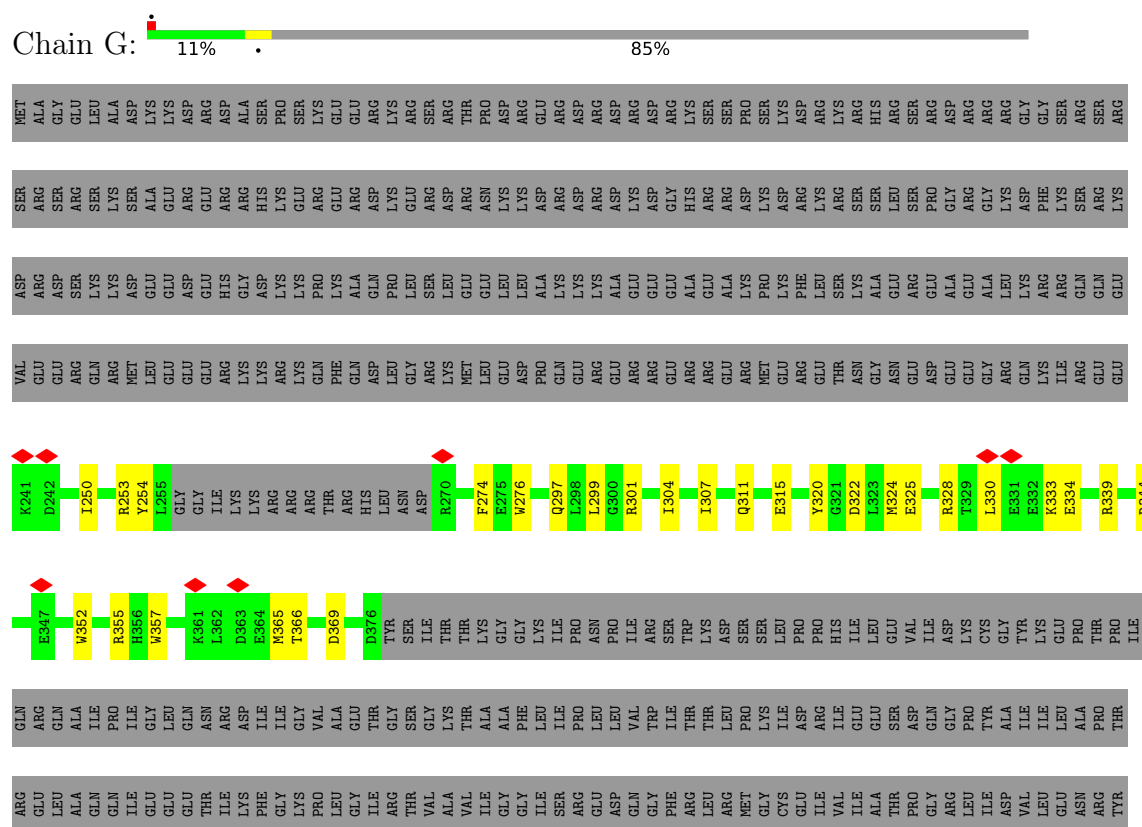
3 Residue-property plots

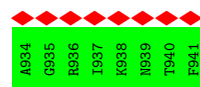
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: U5 small nuclear ribonucleoprotein 200 kDa helicase

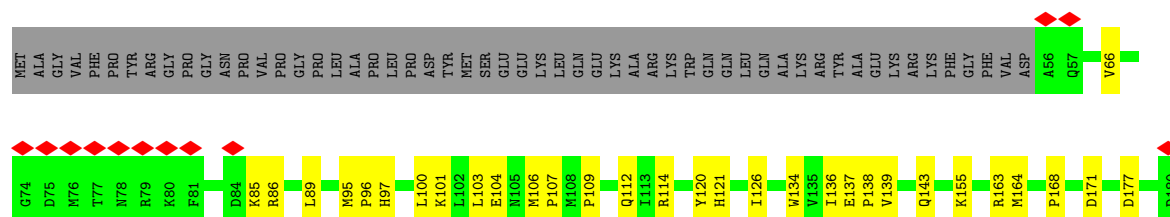


- Molecule 2: Probable ATP-dependent RNA helicase DDX23

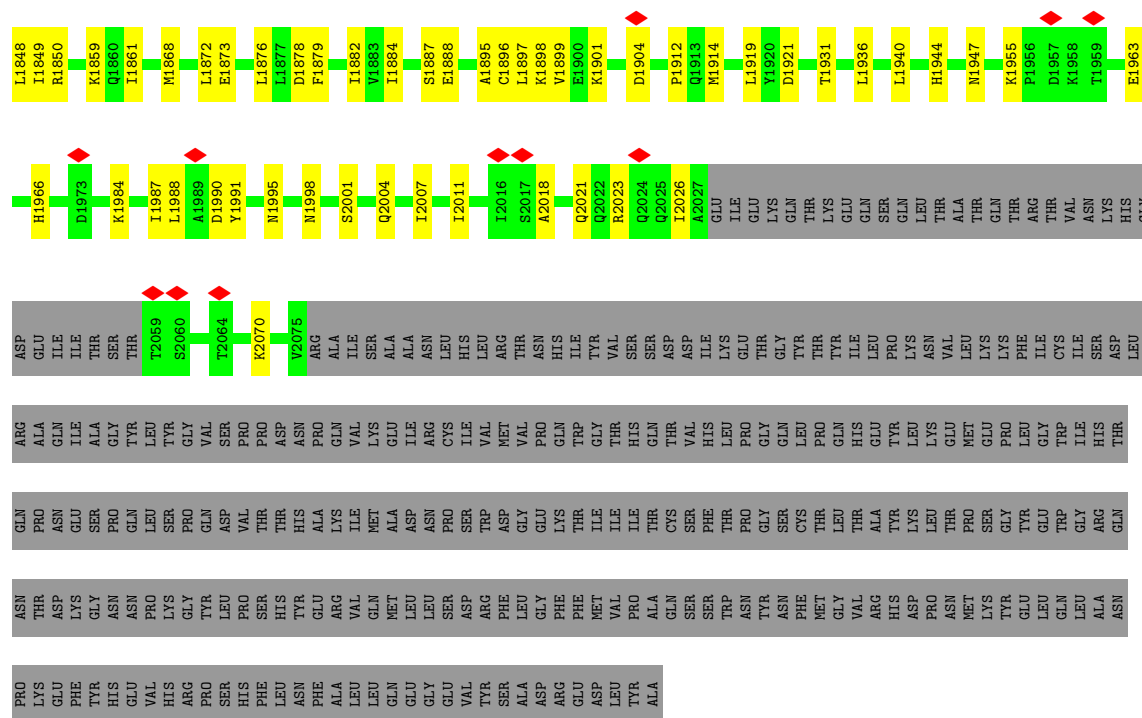




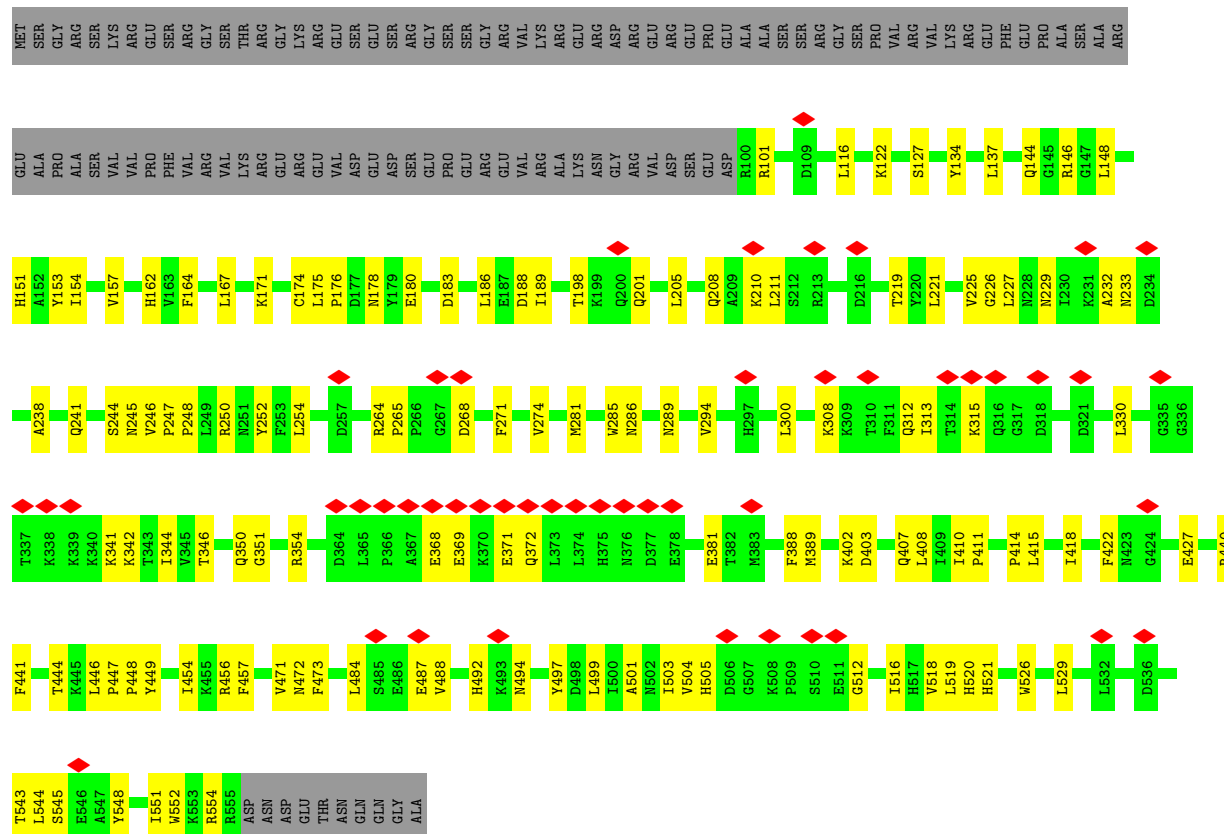
Chain A:



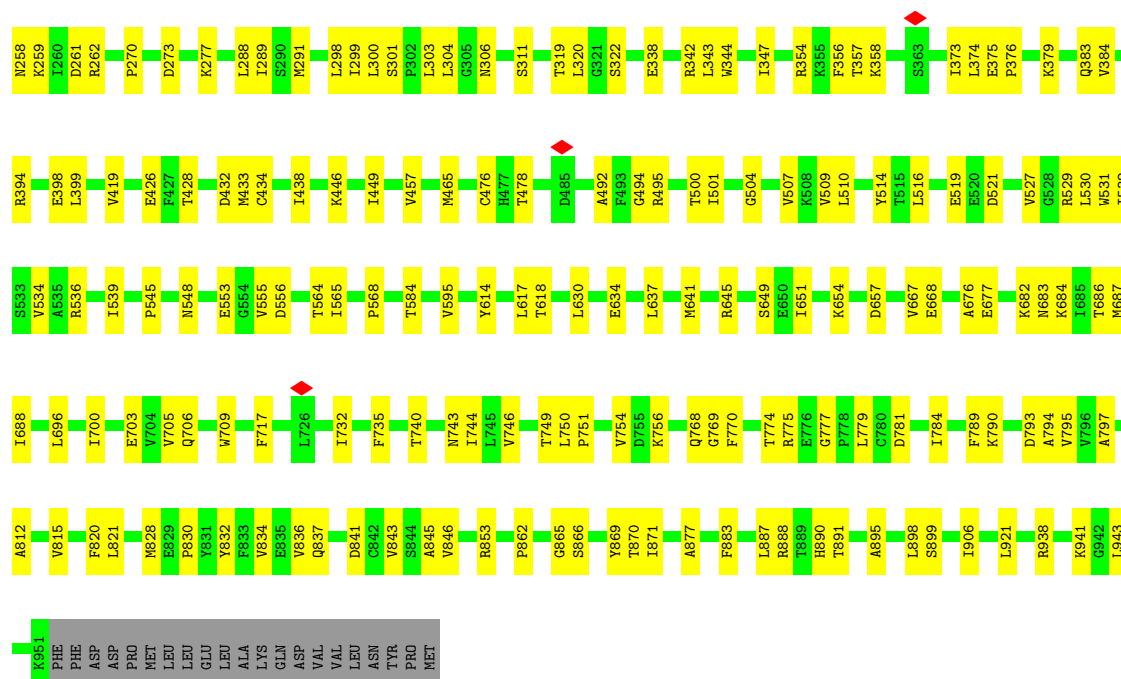




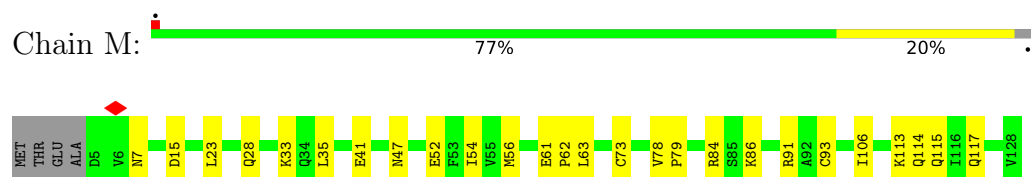
- Molecule 8: Ubiquitin carboxyl-terminal hydrolase 39



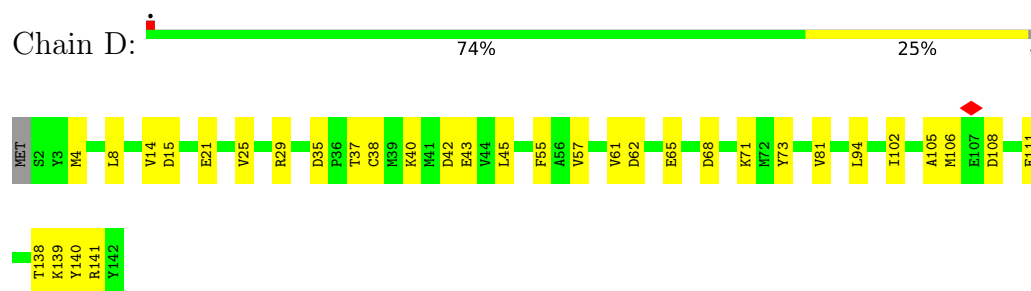
- Molecule 9: U4/U6.U5 tri-snRNP-associated protein 1



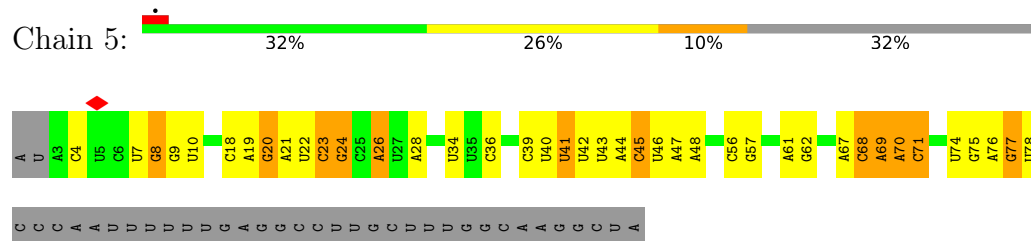
- Molecule 11: NHP2-like protein 1, N-terminally processed



- Molecule 12: Thioredoxin-like protein 4A



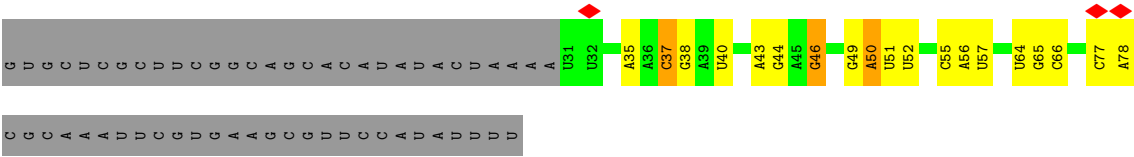
- Molecule 13: U5 snRNA



- Molecule 14: 5'ss RNA oligo

D G A C G A C C U U D G C C A A U A U A U A G U D C G G C C A C C U D G G C A A A U U U D U D U D U G A C A A G U D C C U A A C G C A G A C D G

● Molecule 17: U6 snRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	411185	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	0.224	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.032	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 [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	B	0.10	0/158	0.31	0/209
2	G	0.08	0/1096	0.22	0/1455
3	J	0.11	0/686	0.28	0/914
4	L	0.12	0/2924	0.26	0/3938
5	F	0.09	0/491	0.25	0/657
6	N	0.11	0/3565	0.26	0/4818
7	A	0.12	0/16866	0.28	0/22880
8	U	0.09	0/3845	0.27	0/5208
9	S	0.09	0/1172	0.23	0/1567
10	C	0.12	0/6739	0.29	0/9151
11	M	0.13	0/974	0.32	0/1316
12	D	0.12	0/1199	0.27	0/1620
13	5	0.10	0/1850	0.22	0/2875
14	z	0.11	0/268	0.17	0/416
15	7	0.10	0/858	0.27	0/1152
16	4	0.09	0/1898	0.15	0/2954
17	6	0.10	0/1159	0.22	0/1806
All	All	0.11	0/45748	0.27	0/62936

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	158	0	166	8	0
2	G	1077	0	1066	24	0
3	J	679	0	728	22	0
4	L	2886	0	2885	63	0
5	F	488	0	499	16	0
6	N	3502	0	3379	91	0
7	A	16419	0	16348	402	0
8	U	3749	0	3769	83	0
9	S	1164	0	1173	21	0
10	C	6592	0	6615	144	0
11	M	962	0	1012	20	0
12	D	1170	0	1141	27	0
13	5	1660	0	842	24	0
14	z	239	0	119	4	0
15	7	846	0	837	21	0
16	4	1699	0	858	17	0
17	6	1034	0	521	12	0
18	A	36	0	6	2	0
All	All	44360	0	41964	856	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 (856) 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)
7:A:1809:ILE:HB	7:A:1818:PHE:HB2	1.60	0.83
2:G:253:ARG:HH12	7:A:313:LYS:HZ3	1.29	0.80
7:A:1775:GLN:HB2	7:A:1859:LYS:HE3	1.66	0.76
10:C:846:VAL:HG22	10:C:887:LEU:HD11	1.68	0.76
12:D:138:THR:HG22	12:D:140:TYR:H	1.51	0.76
7:A:781:ARG:HA	7:A:1022:MET:HE1	1.71	0.73
11:M:91:ARG:HH12	15:7:429:MET:HG3	1.54	0.73
7:A:465:LYS:O	13:5:23:C:N4	2.21	0.73
4:L:271:THR:HG22	4:L:276:HIS:CE1	2.24	0.73
2:G:339:ARG:HD3	7:A:344:ASP:HB3	1.72	0.72
12:D:108:ASP:HB3	12:D:111:GLU:HG3	1.71	0.71
7:A:942:PRO:HD2	7:A:1438:VAL:HG22	1.72	0.71
7:A:104:GLU:HB2	7:A:422:LEU:HD11	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1214:TRP:NE1	7:A:1276:GLU:OE1	2.24	0.71
7:A:623:LYS:HB2	18:A:2401:IHP:O46	1.90	0.70
8:U:244:SER:HA	8:U:281:MET:HE2	1.72	0.70
8:U:174:CYS:O	8:U:178:ASN:N	2.25	0.70
8:U:174:CYS:O	8:U:178:ASN:HA	1.92	0.70
10:C:507:VAL:HA	10:C:568:PRO:HD3	1.74	0.69
12:D:139:LYS:H	13:5:41:U:H5'	1.57	0.69
7:A:1411:SER:HA	7:A:1414:ARG:HD2	1.72	0.69
6:N:182:VAL:HG11	7:A:853:LYS:HG3	1.75	0.69
7:A:137:GLU:HG2	7:A:138:PRO:HD3	1.74	0.69
7:A:1146:ASP:OD2	7:A:1182:ASN:ND2	2.25	0.69
7:A:1872:LEU:HB3	7:A:1884:ILE:HD13	1.74	0.68
6:N:873:ASP:H	6:N:878:TRP:HE1	1.41	0.68
7:A:596:TYR:HB2	13:5:45:C:H4'	1.75	0.68
2:G:307:ILE:HG23	7:A:618:THR:HG21	1.75	0.68
6:N:11:MET:HE3	6:N:12:PRO:HD2	1.74	0.68
7:A:909:TYR:HB2	7:A:1033:GLY:HA3	1.76	0.68
7:A:425:PRO:HB2	7:A:428:LYS:HB2	1.76	0.68
13:5:8:G:H22	13:5:71:C:H5''	1.58	0.67
7:A:155:LYS:NZ	7:A:622:GLY:O	2.27	0.67
10:C:504:GLY:N	10:C:527:VAL:O	2.27	0.67
7:A:318:TYR:O	10:C:645:ARG:NH1	2.27	0.67
6:N:362:VAL:HG11	6:N:379:ALA:HB2	1.77	0.66
10:C:476:CYS:HB2	10:C:565:ILE:HB	1.76	0.66
8:U:174:CYS:O	8:U:178:ASN:CA	2.44	0.66
1:B:42:SER:HA	7:A:1289:VAL:HG11	1.76	0.66
6:N:201:ASP:HB2	6:N:204:GLN:HG3	1.76	0.66
7:A:1629:ILE:HB	7:A:1662:ILE:HB	1.76	0.66
7:A:357:ASN:ND2	10:C:866:SER:O	2.28	0.66
10:C:686:THR:HB	10:C:793:ASP:HB3	1.78	0.65
7:A:385:GLU:OE2	10:C:354:ARG:NH1	2.29	0.65
2:G:352:TRP:O	2:G:355:ARG:NH1	2.27	0.65
7:A:975:VAL:HG11	7:A:1153:VAL:HG21	1.79	0.65
6:N:108:LEU:HD21	7:A:476:PHE:HE1	1.61	0.65
8:U:225:VAL:O	8:U:241:GLN:NE2	2.29	0.65
6:N:250:LEU:HD23	7:A:1850:ARG:HE	1.63	0.64
10:C:207:GLY:O	10:C:238:ASN:ND2	2.29	0.64
7:A:510:ARG:NH2	7:A:655:LEU:O	2.28	0.64
3:J:436:LEU:HD11	11:M:23:LEU:HD12	1.80	0.64
7:A:1787:ARG:HG3	7:A:1803:ILE:HG13	1.80	0.64
3:J:444:GLU:OE2	15:7:433:LEU:HD13	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:384:VAL:O	10:C:354:ARG:NH2	2.24	0.64
10:C:843:VAL:HG22	10:C:871:ILE:HD11	1.79	0.64
8:U:402:LYS:HE2	8:U:408:LEU:HG	1.78	0.63
7:A:1507:SER:HB3	7:A:1510:GLU:HB3	1.79	0.63
7:A:828:PRO:HB2	7:A:882:LYS:HE2	1.80	0.63
7:A:1087:LEU:HB2	7:A:1098:PHE:HB3	1.81	0.63
6:N:394:ARG:NH2	9:S:196:TRP:O	2.32	0.63
13:5:8:G:N2	13:5:70:A:O3'	2.31	0.63
13:5:46:U:O4	13:5:47:A:N6	2.32	0.63
7:A:1140:MET:HE3	7:A:1177:VAL:HG12	1.81	0.62
7:A:1596:VAL:HG21	7:A:1729:ALA:HB2	1.80	0.62
8:U:354:ARG:NH2	8:U:487:GLU:OE2	2.33	0.62
6:N:29:THR:HG23	17:6:37:C:H5	1.65	0.62
3:J:518:ARG:NH2	17:6:66:C:O2	2.32	0.62
7:A:312:TYR:OH	10:C:853:ARG:NH2	2.32	0.62
7:A:371:LEU:HD11	10:C:347:ILE:HB	1.82	0.62
6:N:119:ARG:NH2	13:5:18:C:OP2	2.33	0.62
10:C:770:PHE:HE1	10:C:789:PHE:HD2	1.46	0.62
6:N:329:ARG:HE	6:N:354:PRO:HD3	1.65	0.62
7:A:965:VAL:O	7:A:974:ASN:ND2	2.31	0.62
4:L:378:MET:HB2	7:A:1505:LYS:HE2	1.82	0.61
7:A:1762:TYR:CZ	7:A:1888:GLU:HB3	2.35	0.61
7:A:923:ASP:OD2	7:A:1439:ARG:NH1	2.31	0.61
7:A:1590:VAL:HG13	7:A:1629:ILE:HD11	1.81	0.61
10:C:779:LEU:O	10:C:938:ARG:NH1	2.32	0.61
8:U:497:TYR:HB3	8:U:552:TRP:HB3	1.83	0.61
10:C:133:THR:HG21	10:C:219:LEU:HD12	1.83	0.61
7:A:536:LYS:NZ	14:z:-1:G:OP1	2.32	0.61
10:C:384:VAL:HG21	10:C:419:VAL:HG11	1.81	0.61
5:F:101:VAL:HG21	5:F:134:ARG:HG2	1.81	0.61
7:A:929:GLU:OE1	7:A:933:ARG:NH1	2.32	0.61
15:7:415:ILE:HG21	15:7:433:LEU:HD11	1.83	0.61
4:L:271:THR:HG23	4:L:275:TYR:CG	2.35	0.61
7:A:675:GLN:NE2	12:D:105:ALA:O	2.34	0.61
7:A:781:ARG:HD3	7:A:1022:MET:HE2	1.83	0.61
6:N:390:LYS:HA	6:N:413:LEU:HD21	1.83	0.60
10:C:732:ILE:HG23	10:C:744:ILE:HD11	1.83	0.60
7:A:231:THR:H	7:A:234:MET:HE2	1.66	0.60
7:A:1782:ASP:HB3	7:A:1841:THR:HG21	1.82	0.60
7:A:488:ASP:OD2	7:A:565:ARG:NH1	2.30	0.60
15:7:483:ALA:HB3	15:7:486:LYS:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1090:ARG:NH1	7:A:1092:ILE:O	2.35	0.60
8:U:403:ASP:O	8:U:407:GLN:NE2	2.35	0.60
10:C:595:VAL:HG22	10:C:654:LYS:HG3	1.83	0.60
7:A:269:LEU:HD13	7:A:321:ASN:HD21	1.66	0.60
7:A:761:ILE:HD12	7:A:775:ASN:HD22	1.67	0.60
7:A:1919:LEU:HD13	7:A:1936:LEU:HD21	1.83	0.60
8:U:448:PRO:HA	8:U:554:ARG:HD2	1.83	0.60
2:G:344:ARG:O	2:G:344:ARG:NH1	2.35	0.60
4:L:141:GLU:OE1	4:L:154:ASN:ND2	2.35	0.60
7:A:1088:PHE:HD1	7:A:1097:ILE:HG12	1.66	0.60
7:A:1052:VAL:O	7:A:1160:ARG:NH1	2.32	0.59
8:U:246:VAL:HG12	8:U:248:PRO:HD2	1.84	0.59
10:C:749:THR:OG1	10:C:756:LYS:NZ	2.33	0.59
15:7:457:ALA:HB1	15:7:461:ASP:HB3	1.84	0.59
7:A:1834:GLY:HA2	9:S:276:LEU:HD13	1.84	0.59
7:A:1818:PHE:HB3	7:A:1914:MET:HE2	1.84	0.59
8:U:250:ARG:HD3	8:U:285:TRP:CE2	2.36	0.59
6:N:19:PRO:HG3	12:D:68:ASP:HB3	1.83	0.59
8:U:122:LYS:HE3	8:U:167:LEU:HD12	1.85	0.59
4:L:256:ARG:NH2	16:4:39:A:OP1	2.36	0.59
7:A:1279:VAL:HG12	7:A:1369:TYR:HE1	1.67	0.59
7:A:1541:THR:HA	7:A:1544:ARG:HD3	1.83	0.59
7:A:1660:TYR:OH	7:A:1717:ASN:O	2.20	0.59
8:U:154:ILE:HD11	10:C:775:ARG:HH12	1.67	0.59
6:N:252:ASP:OD1	6:N:273:TYR:OH	2.20	0.59
7:A:1386:TRP:HE1	7:A:1417:PRO:HD2	1.67	0.59
7:A:96:PRO:HB2	7:A:645:THR:HG23	1.85	0.59
7:A:1737:ASN:HB3	7:A:1740:LEU:HB2	1.84	0.59
7:A:1354:ARG:NH1	9:S:150:PRO:O	2.36	0.58
7:A:1498:TRP:HA	7:A:1501:LEU:HD22	1.85	0.58
7:A:1551:PHE:O	14:z:1:G:N1	2.34	0.58
10:C:170:ILE:HG22	10:C:536:ARG:HD3	1.85	0.58
10:C:500:THR:HG22	10:C:545:PRO:HA	1.85	0.58
7:A:347:LEU:HD12	7:A:348:PRO:HD2	1.85	0.58
7:A:388:LEU:HD21	10:C:399:LEU:HG	1.86	0.58
10:C:432:ASP:OD1	10:C:433:MET:N	2.36	0.58
10:C:703:GLU:HG2	10:C:740:THR:HG21	1.85	0.58
6:N:298:LEU:HD13	6:N:315:SER:HA	1.84	0.58
7:A:100:LEU:HD21	13:5:56:C:H4'	1.86	0.58
6:N:335:GLY:O	6:N:339:CYS:N	2.37	0.58
7:A:913:PRO:HA	7:A:916:LYS:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:134:TYR:OH	8:U:146:ARG:NH1	2.37	0.58
10:C:338:GLU:O	10:C:342:ARG:NH1	2.37	0.58
4:L:218:ASN:ND2	4:L:306:ASP:OD1	2.35	0.57
6:N:253:MET:HE3	6:N:253:MET:HA	1.86	0.57
10:C:501:ILE:HG12	10:C:530:LEU:HD11	1.85	0.57
7:A:1133:CYS:HB2	7:A:1231:ARG:HE	1.69	0.57
7:A:1314:VAL:O	7:A:1318:THR:OG1	2.22	0.57
10:C:134:LEU:HD13	10:C:202:ILE:HG23	1.84	0.57
10:C:703:GLU:O	10:C:706:GLN:NE2	2.37	0.57
7:A:1589:ILE:HG22	7:A:1664:ILE:HD13	1.86	0.57
7:A:381:PRO:O	10:C:354:ARG:NH2	2.37	0.57
7:A:1576:ILE:HD13	7:A:1747:ILE:HG12	1.86	0.57
7:A:66:VAL:HG11	7:A:487:LEU:HD11	1.87	0.57
10:C:834:VAL:HG11	10:C:883:PHE:HE2	1.70	0.57
3:J:463:LYS:HE3	3:J:469:MET:HG2	1.85	0.57
6:N:203:ARG:NH2	6:N:208:GLY:O	2.33	0.57
10:C:832:TYR:HD2	10:C:899:SER:HB3	1.70	0.57
6:N:20:GLY:HA3	15:7:502:TRP:HE3	1.70	0.57
4:L:88:PRO:HG2	4:L:91:ARG:HG2	1.85	0.57
6:N:122:GLN:NE2	6:N:126:GLU:OE2	2.38	0.57
8:U:494:ASN:O	8:U:554:ARG:NH2	2.33	0.57
3:J:480:ASN:HD21	17:6:55:C:H5''	1.70	0.56
7:A:689:VAL:HG21	7:A:742:TYR:HB2	1.85	0.56
8:U:250:ARG:HA	8:U:281:MET:SD	2.45	0.56
4:L:408:ARG:NH2	7:A:1882:ILE:O	2.26	0.56
5:F:127:ALA:HB1	15:7:439:LEU:HD11	1.86	0.56
11:M:61:GLU:HB2	11:M:62:PRO:HD3	1.87	0.56
15:7:506:SER:HA	15:7:509:MET:HE3	1.87	0.56
7:A:293:TRP:CD1	7:A:1141:ARG:HB3	2.41	0.56
7:A:1357:MET:HB2	9:S:152:THR:HG21	1.85	0.56
7:A:1307:MET:HG3	13:5:40:U:C4	2.41	0.56
6:N:856:LYS:HD3	6:N:859:LYS:HD2	1.87	0.56
10:C:836:VAL:HG21	10:C:846:VAL:HG11	1.87	0.56
7:A:106:MET:HE2	7:A:557:VAL:HG11	1.86	0.56
7:A:494:LEU:HD21	7:A:562:VAL:HG21	1.86	0.56
10:C:301:SER:HB2	10:C:304:LEU:HD12	1.88	0.56
6:N:35:GLY:O	7:A:510:ARG:NH1	2.34	0.56
6:N:268:VAL:HG12	6:N:270:PRO:HD3	1.88	0.56
6:N:325:LEU:O	6:N:329:ARG:NH1	2.35	0.56
15:7:427:GLU:O	15:7:431:ILE:HG12	2.06	0.56
6:N:815:SER:HB2	6:N:846:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:315:ALA:O	10:C:177:ARG:NH2	2.35	0.55
7:A:1639:VAL:HG13	7:A:1717:ASN:HB3	1.86	0.55
8:U:245:ASN:OD1	8:U:521:HIS:NE2	2.39	0.55
4:L:247:CYS:HB2	16:4:41:C:H41	1.72	0.55
7:A:1072:LEU:HD22	7:A:1087:LEU:HD22	1.87	0.55
7:A:1676:ILE:HD13	7:A:1706:ASP:HB2	1.88	0.55
10:C:750:LEU:HD12	10:C:751:PRO:HD2	1.89	0.55
7:A:710:LEU:HD13	12:D:4:MET:HE3	1.87	0.55
4:L:278:ASP:OD1	4:L:279:ILE:N	2.39	0.55
6:N:31:ARG:HG3	6:N:34:ILE:HG22	1.88	0.55
6:N:829:LYS:HE3	11:M:47:ASN:HB3	1.87	0.55
7:A:291:GLU:O	7:A:1136:ARG:NH1	2.40	0.55
7:A:1143:MET:HG3	7:A:1181:ASP:HB3	1.87	0.55
4:L:152:ASN:HB3	4:L:155:LEU:HB2	1.87	0.55
4:L:264:SER:O	4:L:269:PRO:HD3	2.06	0.55
6:N:363:ALA:O	6:N:367:ARG:NH1	2.40	0.55
8:U:341:LYS:HE3	8:U:342:LYS:HE2	1.89	0.55
1:B:42:SER:HB2	7:A:1289:VAL:HG21	1.89	0.55
4:L:421:SER:OG	16:4:20:A:OP1	2.25	0.55
2:G:274:PHE:HB3	7:A:606:LYS:HE3	1.89	0.54
6:N:280:MET:HG3	6:N:317:ARG:HH22	1.72	0.54
6:N:297:LEU:O	6:N:301:VAL:HG23	2.07	0.54
7:A:136:ILE:HG22	7:A:138:PRO:HD2	1.90	0.54
7:A:419:ARG:NH2	7:A:423:ASP:O	2.40	0.54
11:M:15:ASP:HA	11:M:84:ARG:HH22	1.70	0.54
12:D:8:LEU:HB2	12:D:61:VAL:HG22	1.88	0.54
7:A:137:GLU:HG2	7:A:138:PRO:CD	2.36	0.54
10:C:177:ARG:HB3	10:C:179:VAL:HG12	1.87	0.54
7:A:1544:ARG:HD2	7:A:1671:TYR:HB3	1.88	0.54
8:U:208:GLN:NE2	8:U:210:LYS:O	2.40	0.54
10:C:300:LEU:HD23	10:C:306:ASN:HB3	1.89	0.54
4:L:358:ARG:NH2	16:4:18:G:O2'	2.40	0.54
7:A:1330:MET:HE1	7:A:1369:TYR:HB2	1.90	0.54
10:C:299:ILE:O	10:C:306:ASN:ND2	2.40	0.54
8:U:144:GLN:HB3	8:U:151:HIS:HB2	1.88	0.54
7:A:523:ASN:OD1	7:A:552:ARG:NH1	2.40	0.54
10:C:703:GLU:HB3	10:C:706:GLN:HE21	1.73	0.54
4:L:112:LYS:HD2	6:N:855:ARG:HE	1.71	0.54
4:L:408:ARG:NE	7:A:1873:GLU:OE1	2.41	0.54
5:F:108:VAL:HG13	5:F:133:LEU:HD13	1.89	0.54
7:A:2018:ALA:O	7:A:2021:GLN:NE2	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:151:HIS:HA	8:U:154:ILE:HD12	1.90	0.54
7:A:1667:ARG:NH2	7:A:1673:SER:O	2.38	0.54
8:U:198:THR:HG23	8:U:201:GLN:H	1.72	0.54
2:G:366:THR:HG23	2:G:369:ASP:H	1.73	0.54
6:N:252:ASP:HB3	6:N:254:ARG:HH12	1.73	0.54
7:A:984:MET:O	7:A:988:ILE:HG13	2.08	0.54
7:A:1849:ILE:HD11	7:A:1861:ILE:HD11	1.89	0.54
11:M:7:ASN:HD21	11:M:63:LEU:HD22	1.72	0.54
4:L:160:THR:HG22	4:L:163:THR:HG22	1.90	0.54
7:A:712:HIS:HA	7:A:715:GLU:HG2	1.90	0.54
7:A:832:TYR:HB3	7:A:835:ASP:HB3	1.90	0.54
10:C:478:THR:HG21	10:C:492:ALA:HB1	1.89	0.54
7:A:97:HIS:ND1	7:A:649:GLU:OE2	2.41	0.53
10:C:375:GLU:OE2	10:C:379:LYS:NZ	2.34	0.53
7:A:1591:MET:HE1	7:A:1611:LYS:HD2	1.89	0.53
4:L:356:GLY:H	4:L:359:TYR:HB3	1.73	0.53
10:C:261:ASP:OD2	10:C:311:SER:OG	2.22	0.53
4:L:122:PHE:CD2	4:L:125:LEU:HB2	2.43	0.53
4:L:287:LEU:HD21	4:L:331:TRP:HB3	1.91	0.53
7:A:878:LEU:O	7:A:882:LYS:HG2	2.09	0.53
7:A:1064:PRO:HG2	7:A:1067:MET:HB2	1.89	0.53
10:C:203:MET:HG2	10:C:218:GLY:HA3	1.90	0.53
4:L:149:CYS:HA	4:L:152:ASN:ND2	2.24	0.53
4:L:347:LEU:HD12	17:6:50:A:C4	2.44	0.53
6:N:158:LEU:HG	7:A:702:LYS:HD3	1.90	0.53
8:U:265:PRO:HB2	8:U:268:ASP:HB2	1.90	0.53
5:F:89:GLU:OE1	5:F:92:ARG:NH2	2.42	0.53
7:A:103:LEU:O	7:A:634:TRP:NE1	2.24	0.53
7:A:293:TRP:CZ3	7:A:299:ILE:HD13	2.44	0.53
10:C:227:LEU:HD11	10:C:239:THR:HG23	1.91	0.53
10:C:504:GLY:CA	10:C:527:VAL:O	2.56	0.53
7:A:182:ILE:HD11	7:A:562:VAL:HG13	1.91	0.53
7:A:336:ASN:OD1	10:C:837:GLN:NE2	2.32	0.53
8:U:148:LEU:HD11	10:C:768:GLN:HG2	1.91	0.53
7:A:1186:LEU:HD13	7:A:1195:ARG:HB2	1.91	0.53
8:U:312:GLN:HB3	8:U:315:LYS:HG2	1.91	0.53
10:C:244:LYS:O	10:C:248:GLN:HG2	2.09	0.53
2:G:250:ILE:HG12	7:A:307:PRO:HB3	1.92	0.52
3:J:505:ALA:O	3:J:509:LYS:N	2.39	0.52
11:M:113:LYS:CD	11:M:117:GLN:HE22	2.22	0.52
7:A:1088:PHE:CD1	7:A:1097:ILE:HG12	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1536:LEU:HD21	7:A:1576:ILE:HD11	1.91	0.52
7:A:1809:ILE:HG21	7:A:1848:LEU:HD23	1.89	0.52
12:D:62:ASP:HB3	12:D:65:GLU:HB3	1.92	0.52
6:N:814:TRP:HB3	6:N:834:LEU:HD11	1.90	0.52
7:A:109:PRO:HB3	7:A:191:ILE:HD12	1.89	0.52
6:N:178:LYS:O	7:A:861:ARG:NH2	2.32	0.52
7:A:1116:GLU:OE2	7:A:1155:TRP:NE1	2.42	0.52
7:A:1788:VAL:HG12	7:A:1802:PRO:HA	1.91	0.52
4:L:93:ILE:HG13	4:L:215:ILE:HG21	1.91	0.52
6:N:113:ASP:OD2	6:N:120:ARG:NH2	2.42	0.52
7:A:371:LEU:HD21	10:C:347:ILE:HD12	1.92	0.52
7:A:1382:SER:HA	7:A:1415:GLY:HA2	1.91	0.52
6:N:153:THR:HG23	6:N:156:GLU:H	1.75	0.52
8:U:427:GLU:HG3	8:U:440:ARG:HB3	1.92	0.52
10:C:319:THR:HG23	10:C:322:SER:H	1.75	0.52
10:C:556:ASP:OD1	10:C:556:ASP:N	2.41	0.52
6:N:23:ARG:NH2	12:D:73:TYR:OH	2.43	0.52
6:N:119:ARG:NH1	13:5:19:A:OP2	2.42	0.51
11:M:91:ARG:HH22	15:7:429:MET:HE2	1.75	0.51
6:N:810:SER:HB2	6:N:813:LEU:HB2	1.92	0.51
7:A:1806:ALA:HB3	7:A:1897:LEU:HD11	1.91	0.51
7:A:1807:ILE:HB	7:A:1820:LYS:HB3	1.92	0.51
9:S:301:GLU:HA	9:S:304:VAL:HG22	1.93	0.51
1:B:43:LEU:HA	1:B:46:LYS:HB3	1.91	0.51
4:L:412:VAL:HG13	6:N:184:ASP:HB2	1.91	0.51
7:A:1416:ILE:HB	7:A:1417:PRO:HD3	1.92	0.51
7:A:1779:PHE:HE1	7:A:1812:PRO:HG3	1.75	0.51
1:B:44:VAL:HG13	7:A:1282:GLN:HG2	1.93	0.51
7:A:1005:ILE:O	7:A:1009:MET:HG3	2.10	0.51
9:S:258:THR:HA	9:S:350:ARG:HA	1.92	0.51
10:C:743:ASN:HD22	10:C:774:THR:HB	1.74	0.51
1:B:43:LEU:HD21	7:A:1285:LEU:HD12	1.91	0.51
7:A:1421:THR:HA	7:A:1424:GLN:HG3	1.92	0.51
10:C:171:LEU:HD11	10:C:182:LYS:HD2	1.93	0.51
2:G:254:TYR:OH	10:C:657:ASP:OD2	2.27	0.51
7:A:443:VAL:HG12	7:A:610:HIS:HB3	1.93	0.51
7:A:711:GLN:O	7:A:714:SER:OG	2.26	0.51
10:C:320:LEU:HD21	10:C:344:TRP:HB2	1.93	0.51
5:F:124:GLU:HB2	5:F:128:GLU:HB2	1.92	0.51
7:A:888:GLN:O	7:A:889:ARG:NH1	2.40	0.51
7:A:1141:ARG:N	7:A:1182:ASN:OD1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1265:THR:HG22	7:A:1452:PRO:HG3	1.92	0.51
4:L:130:PRO:HG3	4:L:258:THR:HG23	1.93	0.51
7:A:608:LEU:HD13	7:A:632:ALA:HB1	1.93	0.51
7:A:1485:LEU:HD23	7:A:1490:PHE:CD2	2.46	0.51
7:A:1522:GLN:HE21	17:6:49:G:H5'	1.77	0.51
7:A:1608:THR:HG22	7:A:1632:PHE:HB2	1.93	0.51
12:D:35:ASP:HB3	12:D:38:CYS:HB2	1.92	0.51
8:U:238:ALA:HB1	8:U:503:ILE:HD12	1.92	0.50
10:C:532:ILE:HB	10:C:539:ILE:HG13	1.93	0.50
12:D:37:THR:HA	12:D:40:LYS:HE3	1.93	0.50
2:G:250:ILE:HG22	10:C:921:LEU:HD22	1.93	0.50
2:G:304:ILE:HA	7:A:247:THR:HG23	1.93	0.50
7:A:825:ILE:HG12	7:A:929:GLU:HB3	1.93	0.50
7:A:1455:TRP:H	7:A:1455:TRP:CD1	2.29	0.50
15:7:440:GLU:O	15:7:444:ARG:HG2	2.12	0.50
7:A:1318:THR:HB	7:A:1324:GLY:HA3	1.93	0.50
3:J:491:GLN:NE2	7:A:2004:GLN:OE1	2.39	0.50
7:A:143:GLN:NE2	7:A:207:PHE:O	2.42	0.50
2:G:357:TRP:HB3	2:G:369:ASP:OD1	2.12	0.50
8:U:543:THR:HG23	8:U:544:LEU:HD12	1.94	0.50
8:U:226:GLY:HA2	8:U:529:LEU:HD12	1.94	0.50
8:U:350:GLN:HA	8:U:388:PHE:O	2.10	0.50
10:C:187:THR:HG23	10:C:199:LEU:HD11	1.94	0.50
6:N:375:ILE:HG13	6:N:376:TYR:N	2.25	0.50
7:A:1598:ASP:OD2	7:A:2070:LYS:HG2	2.11	0.50
10:C:830:PRO:HG2	10:C:877:ALA:HB3	1.94	0.50
7:A:1504:GLU:HB3	7:A:1752:GLN:HE21	1.77	0.50
8:U:211:LEU:HG	8:U:219:THR:HB	1.94	0.50
7:A:596:TYR:O	7:A:599:MET:HB2	2.12	0.49
7:A:1667:ARG:HD2	7:A:1679:TYR:CE2	2.46	0.49
7:A:1899:VAL:HG12	7:A:1901:LYS:H	1.77	0.49
9:S:157:ASN:HB3	9:S:160:ALA:HB3	1.92	0.49
4:L:121:ARG:NH1	4:L:176:GLY:O	2.45	0.49
5:F:113:ARG:HH22	5:F:119:ILE:HD11	1.77	0.49
6:N:325:LEU:HB3	6:N:329:ARG:HH12	1.77	0.49
7:A:1763:LEU:HB3	7:A:1887:SER:HA	1.93	0.49
7:A:1963:GLU:HG2	7:A:1966:HIS:CE1	2.47	0.49
7:A:1216:LEU:O	7:A:1224:ARG:NH1	2.45	0.49
10:C:182:LYS:HA	10:C:214:GLU:HG2	1.93	0.49
12:D:21:GLU:HG3	12:D:57:VAL:HG11	1.94	0.49
12:D:40:LYS:O	12:D:43:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1214:TRP:HB2	7:A:1228:CYS:HB3	1.94	0.49
7:A:490:VAL:HG21	7:A:565:ARG:HG3	1.93	0.49
7:A:820:ARG:NH1	7:A:1063:GLY:O	2.31	0.49
7:A:1137:ASP:OD1	7:A:1137:ASP:N	2.44	0.49
10:C:509:VAL:HG22	10:C:565:ILE:HG12	1.95	0.49
5:F:115:LEU:HD13	5:F:136:ILE:HG21	1.95	0.49
6:N:267:VAL:HG13	6:N:268:VAL:HG23	1.94	0.49
7:A:1777:ILE:O	7:A:1812:PRO:HD2	2.12	0.49
8:U:286:ASN:ND2	8:U:289:ASN:OD1	2.45	0.49
17:6:64:U:H2'	17:6:65:G:C8	2.48	0.49
2:G:301:ARG:NH2	7:A:353:ASP:OD2	2.46	0.49
6:N:840:ASP:HB3	6:N:843:VAL:HG23	1.95	0.49
7:A:1868:MET:HE2	7:A:1872:LEU:HG	1.95	0.49
10:C:688:ILE:HG22	10:C:790:LYS:HB2	1.94	0.49
3:J:457:GLN:NE2	17:6:57:U:O2'	2.43	0.49
6:N:827:ARG:HA	6:N:831:VAL:HG12	1.94	0.49
7:A:1798:LEU:HD21	9:S:356:THR:HG23	1.95	0.49
10:C:394:ARG:NH2	10:C:398:GLU:OE1	2.45	0.49
15:7:425:MET:O	15:7:429:MET:HG2	2.13	0.49
2:G:357:TRP:HB2	2:G:365:MET:HE1	1.93	0.49
10:C:706:GLN:OE1	10:C:709:TRP:NE1	2.46	0.49
12:D:8:LEU:HD13	12:D:14:VAL:HA	1.94	0.49
3:J:458:LYS:O	3:J:462:GLU:HG2	2.13	0.48
4:L:378:MET:O	7:A:1503:TRP:N	2.37	0.48
7:A:344:ASP:OD1	7:A:344:ASP:N	2.42	0.48
13:5:4:C:O2	13:5:77:G:N2	2.46	0.48
6:N:401:PRO:O	6:N:407:TRP:NE1	2.45	0.48
6:N:928:ASP:HA	6:N:933:VAL:HA	1.95	0.48
7:A:380:LEU:HD12	7:A:384:VAL:HG11	1.94	0.48
7:A:1057:ARG:HG3	7:A:1061:MET:HE3	1.95	0.48
1:B:43:LEU:HD23	1:B:43:LEU:H	1.78	0.48
7:A:320:TYR:OH	10:C:634:GLU:OE2	2.27	0.48
7:A:784:LEU:HD12	7:A:1022:MET:HE3	1.95	0.48
7:A:1560:ILE:HG21	7:A:1573:LEU:HD13	1.95	0.48
7:A:1632:PHE:HE1	7:A:1659:LYS:HE3	1.78	0.48
10:C:239:THR:O	10:C:243:ILE:HG12	2.14	0.48
10:C:845:ALA:HB1	10:C:890:HIS:HD2	1.78	0.48
12:D:117:GLU:OE1	12:D:121:ARG:NE	2.26	0.48
3:J:440:LEU:HG	3:J:445:GLN:HG3	1.94	0.48
7:A:684:GLU:OE2	15:7:473:ARG:NH2	2.46	0.48
7:A:1413:ASP:OD1	7:A:1420:ASN:ND2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:128:LEU:HD21	10:C:196:LYS:HE3	1.95	0.48
10:C:683:ASN:HA	10:C:795:VAL:O	2.14	0.48
5:F:118:PRO:O	5:F:132:ARG:NH2	2.36	0.48
11:M:52:GLU:O	11:M:79:PRO:HD2	2.13	0.48
7:A:762:ARG:HG2	7:A:903:SER:HA	1.95	0.48
7:A:1089:CYS:SG	7:A:1096:HIS:HB2	2.54	0.48
7:A:1275:ARG:HD3	7:A:1375:TRP:CE2	2.48	0.48
10:C:186:VAL:HG13	10:C:534:VAL:HG23	1.96	0.48
4:L:219:LEU:HD12	4:L:303:ALA:HB2	1.95	0.48
6:N:794:ASN:O	6:N:798:THR:HG23	2.14	0.48
7:A:188:LEU:HD11	7:A:567:GLY:HA2	1.95	0.48
10:C:618:THR:HB	10:C:630:LEU:HB2	1.96	0.48
10:C:836:VAL:HG22	10:C:871:ILE:HB	1.96	0.48
7:A:293:TRP:HB3	7:A:1141:ARG:HA	1.96	0.48
7:A:491:GLU:O	7:A:495:GLN:HG3	2.13	0.48
7:A:1197:LEU:HD11	7:A:1202:THR:HB	1.95	0.48
4:L:347:LEU:HD23	4:L:347:LEU:H	1.79	0.47
7:A:375:ASP:HB3	10:C:357:THR:HG22	1.95	0.47
10:C:667:VAL:HG23	10:C:668:GLU:HG3	1.95	0.47
4:L:392:LEU:HD21	7:A:1465:TRP:HH2	1.79	0.47
4:L:422:LYS:NZ	16:4:21:U:OP1	2.42	0.47
7:A:1591:MET:O	7:A:1595:GLN:HG3	2.14	0.47
7:A:1798:LEU:N	9:S:358:ASP:OD1	2.45	0.47
17:6:44:G:O2'	17:6:46:G:OP1	2.27	0.47
4:L:395:SER:OG	7:A:1505:LYS:NZ	2.48	0.47
4:L:431:GLN:HE22	7:A:914:LEU:HD21	1.79	0.47
7:A:1593:LEU:HA	7:A:1596:VAL:HG12	1.95	0.47
10:C:137:HIS:HA	10:C:238:ASN:HB3	1.97	0.47
10:C:637:LEU:O	10:C:641:MET:HG2	2.13	0.47
10:C:705:VAL:HG11	10:C:717:PHE:CD2	2.49	0.47
3:J:475:LYS:HD3	17:6:56:A:H5''	1.96	0.47
3:J:477:ARG:H	3:J:480:ASN:HB3	1.80	0.47
4:L:369:THR:O	4:L:373:LYS:N	2.47	0.47
4:L:419:ARG:HH22	16:4:17:A:H5''	1.78	0.47
7:A:177:ASP:O	7:A:181:ASN:ND2	2.43	0.47
10:C:208:HIS:HB3	10:C:211:PHE:HD2	1.80	0.47
16:4:20:A:H2'	16:4:21:U:C6	2.49	0.47
16:4:75:C:O2	17:6:38:G:N2	2.39	0.47
7:A:850:TYR:HE1	7:A:860:GLN:HG2	1.80	0.47
7:A:1582:TRP:HD1	7:A:1619:SER:HB3	1.79	0.47
6:N:132:ARG:HH12	6:N:135:ARG:HH11	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:519:LEU:HB2	8:U:526:TRP:CE2	2.49	0.47
2:G:330:LEU:O	2:G:334:GLU:HG2	2.15	0.47
6:N:189:LYS:HA	6:N:192:GLN:HG3	1.95	0.47
7:A:552:ARG:NH2	7:A:588:LEU:O	2.47	0.47
7:A:720:TRP:O	7:A:785:LYS:NZ	2.44	0.47
7:A:855:ARG:HH21	7:A:1514:LYS:HG2	1.79	0.47
7:A:1839:TRP:CZ2	9:S:281:VAL:HG11	2.50	0.47
7:A:1991:TYR:O	7:A:1995:ASN:HB2	2.15	0.47
7:A:1998:ASN:O	7:A:2001:SER:OG	2.31	0.47
10:C:649:SER:HB3	10:C:651:ILE:HG12	1.95	0.47
10:C:677:GLU:HG2	10:C:684:LYS:HG3	1.97	0.47
13:5:67:A:C5	13:5:68:C:H2'	2.50	0.47
5:F:82:ARG:HG3	5:F:82:ARG:HH11	1.78	0.47
6:N:205:THR:OG1	6:N:206:GLN:N	2.47	0.47
7:A:1868:MET:O	7:A:1868:MET:HG2	2.14	0.47
12:D:45:LEU:HD21	12:D:112:MET:HE2	1.96	0.47
2:G:299:LEU:HD22	7:A:355:LEU:HD22	1.97	0.47
8:U:183:ASP:HB2	8:U:186:LEU:HD23	1.96	0.47
8:U:415:LEU:HA	8:U:418:ILE:HD12	1.96	0.47
9:S:274:LEU:HD23	9:S:291:ASN:HB2	1.95	0.47
10:C:446:LYS:HE3	10:C:457:VAL:HG21	1.97	0.47
7:A:89:LEU:HB2	7:A:656:LEU:HD12	1.97	0.47
8:U:410:ILE:HD12	8:U:411:PRO:HD2	1.97	0.47
3:J:491:GLN:HB3	7:A:1984:LYS:HD2	1.97	0.46
10:C:769:GLY:HA3	10:C:812:ALA:HB3	1.97	0.46
10:C:845:ALA:HB1	10:C:890:HIS:CD2	2.50	0.46
10:C:853:ARG:HD2	10:C:883:PHE:HD1	1.80	0.46
6:N:157:TRP:CH2	7:A:735:ILE:HD11	2.50	0.46
7:A:1575:GLN:O	7:A:1578:ARG:NH1	2.45	0.46
8:U:369:GLU:O	8:U:372:GLN:HG3	2.15	0.46
9:S:257:LEU:HD11	9:S:289:LEU:HD22	1.97	0.46
9:S:274:LEU:HB3	9:S:289:LEU:HG	1.97	0.46
7:A:1281:THR:HG22	7:A:1284:LEU:H	1.80	0.46
7:A:1598:ASP:O	7:A:1601:LEU:HD22	2.16	0.46
7:A:1821:ILE:O	7:A:1912:PRO:HA	2.15	0.46
8:U:162:HIS:ND1	8:U:176:PRO:HG2	2.31	0.46
4:L:408:ARG:NH1	7:A:1879:PHE:O	2.48	0.46
7:A:828:PRO:HD3	7:A:1005:ILE:HD11	1.97	0.46
7:A:1321:GLU:O	7:A:1503:TRP:NE1	2.42	0.46
12:D:81:VAL:HG11	12:D:112:MET:HE1	1.96	0.46
8:U:164:PHE:CD1	8:U:175:LEU:HD23	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:289:ILE:HG21	10:C:298:LEU:HB3	1.98	0.46
10:C:343:LEU:HD13	10:C:373:ILE:HD11	1.97	0.46
4:L:159:LEU:HB3	4:L:163:THR:HG23	1.98	0.46
4:L:333:GLU:HG2	4:L:334:PRO:HD2	1.97	0.46
7:A:788:GLN:HG2	7:A:1024:HIS:HB3	1.97	0.46
7:A:947:PRO:HD2	7:A:950:LEU:HD23	1.96	0.46
7:A:955:TRP:CG	7:A:1189:MET:HE1	2.51	0.46
10:C:243:ILE:HD11	10:C:288:LEU:HD13	1.96	0.46
7:A:1119:ASP:OD2	7:A:1123:GLU:N	2.48	0.46
7:A:1495:PHE:HE2	7:A:1753:LEU:HG	1.80	0.46
10:C:135:CYS:HB2	10:C:242:LEU:HD13	1.97	0.46
10:C:828:MET:HE3	10:C:906:ILE:HG13	1.98	0.46
6:N:149:LEU:HD11	7:A:738:MET:HE1	1.98	0.46
6:N:873:ASP:N	6:N:878:TRP:HE1	2.13	0.46
7:A:203:VAL:O	7:A:207:PHE:HB2	2.16	0.46
7:A:682:ASP:N	7:A:682:ASP:OD1	2.48	0.46
4:L:253:GLY:HA3	4:L:273:TYR:CE2	2.51	0.46
6:N:138:ILE:HB	15:7:476:ILE:HG23	1.98	0.46
7:A:750:TRP:CZ2	7:A:778:ARG:HG2	2.51	0.46
7:A:836:THR:O	7:A:840:ILE:HG12	2.16	0.46
7:A:1315:VAL:HG12	7:A:1538:TRP:CD2	2.51	0.46
7:A:1830:GLN:HG2	7:A:1836:LEU:HD22	1.97	0.46
10:C:614:TYR:HB2	10:C:617:LEU:HB2	1.98	0.46
15:7:430:ARG:NH1	16:4:25:A:OP2	2.46	0.46
7:A:780:THR:HG22	7:A:898:PHE:CD2	2.51	0.45
7:A:858:GLN:OE1	7:A:861:ARG:NH1	2.46	0.45
7:A:1596:VAL:HG23	9:S:327:GLN:HB3	1.98	0.45
7:A:1641:ARG:HG3	7:A:1642:PRO:HD2	1.97	0.45
10:C:258:ASN:OD1	10:C:259:LYS:N	2.47	0.45
10:C:449:ILE:HD12	10:C:465:MET:HE3	1.98	0.45
13:5:19:A:H4'	13:5:20:G:C8	2.52	0.45
7:A:715:GLU:HG3	7:A:716:ALA:N	2.31	0.45
7:A:1781:ASP:HB3	7:A:1808:PHE:HB2	1.97	0.45
7:A:1808:PHE:CE2	7:A:1896:CYS:HB3	2.51	0.45
11:M:52:GLU:HB3	11:M:106:ILE:HD11	1.98	0.45
6:N:36:PRO:HG2	12:D:71:LYS:HE3	1.99	0.45
6:N:169:LYS:NZ	16:4:50:G:N7	2.50	0.45
7:A:1385:VAL:HG21	7:A:1414:ARG:HD3	1.98	0.45
7:A:1600:GLU:HB3	7:A:1604:LEU:HD13	1.97	0.45
8:U:454:ILE:HD13	8:U:471:VAL:HG11	1.98	0.45
6:N:115:ARG:HG2	7:A:470:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:847:LYS:HG3	7:A:867:ILE:HG21	1.98	0.45
7:A:1378:GLU:OE2	7:A:1418:ARG:NH1	2.37	0.45
7:A:1990:ASP:OD1	7:A:1991:TYR:N	2.49	0.45
13:5:75:G:H2'	13:5:76:A:C8	2.52	0.45
7:A:766:THR:HG22	12:D:141:ARG:HB3	1.99	0.45
7:A:1198:PRO:HA	7:A:1226:ALA:HA	1.98	0.45
8:U:422:PHE:HA	8:U:441:PHE:HB2	1.97	0.45
8:U:446:LEU:HG	8:U:484:LEU:HD21	1.99	0.45
10:C:555:VAL:HG21	10:C:565:ILE:HD11	1.97	0.45
7:A:768:ASP:OD1	7:A:769:LYS:N	2.44	0.45
8:U:381:GLU:OE2	8:U:440:ARG:NE	2.43	0.45
10:C:426:GLU:HB2	10:C:428:THR:HG23	1.98	0.45
4:L:211:ARG:O	4:L:215:ILE:HG12	2.17	0.45
7:A:652:LEU:O	7:A:656:LEU:HD23	2.16	0.45
7:A:1490:PHE:O	7:A:1493:THR:OG1	2.30	0.45
7:A:1522:GLN:NE2	17:6:49:G:H5'	2.31	0.45
7:A:1686:ASP:O	7:A:1690:ASP:HB2	2.17	0.45
7:A:1807:ILE:HD11	7:A:1822:ILE:HD11	1.98	0.45
10:C:696:LEU:O	10:C:700:ILE:HG13	2.17	0.45
15:7:430:ARG:HH22	16:4:25:A:H5'	1.82	0.45
4:L:271:THR:HG23	4:L:275:TYR:CB	2.47	0.45
7:A:1043:TYR:O	7:A:1046:LEU:HB3	2.17	0.45
7:A:1513:MET:SD	7:A:1516:LYS:HD3	2.57	0.45
2:G:328:ARG:HB3	2:G:333:LYS:HG3	1.98	0.45
3:J:444:GLU:OE1	3:J:444:GLU:HA	2.17	0.45
7:A:101:LYS:HA	7:A:101:LYS:HD2	1.74	0.45
8:U:221:LEU:HD22	8:U:520:HIS:HE2	1.81	0.45
10:C:277:LYS:HD3	10:C:865:GLY:HA3	1.99	0.45
6:N:828:THR:OG1	16:4:41:C:OP1	2.33	0.44
7:A:1124:ASN:ND2	7:A:1148:ASN:OD1	2.49	0.44
7:A:2023:ARG:O	7:A:2026:ILE:HG12	2.17	0.44
7:A:902:TYR:OH	7:A:1249:MET:SD	2.59	0.44
7:A:1237:MET:HG2	7:A:1284:LEU:HD13	1.99	0.44
12:D:94:LEU:HD11	12:D:102:ILE:HG12	1.99	0.44
14:z:4:A:H61	17:6:43:A:H2	1.62	0.44
7:A:1057:ARG:NH1	7:A:1060:GLU:OE1	2.40	0.44
10:C:379:LYS:O	10:C:383:GLN:HG2	2.18	0.44
11:M:86:LYS:NZ	16:4:31:U:O4	2.43	0.44
7:A:106:MET:HE1	7:A:582:PHE:CZ	2.53	0.44
7:A:467:GLN:HG3	7:A:469:LYS:H	1.82	0.44
2:G:304:ILE:HD12	2:G:304:ILE:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:148:LYS:O	6:N:151:GLU:HG2	2.18	0.44
6:N:186:PHE:HE2	7:A:850:TYR:HB2	1.82	0.44
7:A:107:PRO:HA	7:A:114:ARG:HD3	2.00	0.44
7:A:676:ARG:HA	12:D:40:LYS:HD3	2.00	0.44
7:A:1592:ASP:OD1	9:S:331:ARG:NH2	2.51	0.44
8:U:250:ARG:O	8:U:254:LEU:HG	2.17	0.44
10:C:756:LYS:HA	10:C:756:LYS:HD3	1.71	0.44
3:J:440:LEU:HA	11:M:91:ARG:HH21	1.82	0.44
7:A:182:ILE:HA	7:A:185:VAL:HG12	2.00	0.44
7:A:550:VAL:O	7:A:554:THR:HG23	2.17	0.44
7:A:641:MET:HA	7:A:644:ILE:HG22	1.99	0.44
10:C:514:TYR:HB2	10:C:521:ASP:HB3	1.99	0.44
5:F:82:ARG:HG3	5:F:82:ARG:NH1	2.32	0.44
7:A:676:ARG:O	7:A:680:HIS:HB2	2.18	0.44
7:A:942:PRO:HB3	7:A:1437:ARG:HD2	2.00	0.44
7:A:1679:TYR:O	7:A:1683:LYS:HG2	2.18	0.44
11:M:41:GLU:CD	16:4:32:G:H1	2.26	0.44
4:L:103:ILE:O	4:L:107:LEU:HB2	2.18	0.44
7:A:163:ARG:HB2	7:A:625:PRO:HB2	1.99	0.44
7:A:779:LEU:HB3	7:A:905:LEU:HD11	1.98	0.44
7:A:1623:ASN:OD1	7:A:1624:SER:N	2.51	0.44
4:L:346:PRO:HG3	12:D:117:GLU:HG2	1.99	0.44
7:A:832:TYR:OH	7:A:929:GLU:OE2	2.33	0.44
7:A:939:TRP:NE1	7:A:1049:ASP:OD2	2.46	0.44
7:A:1565:LYS:HD3	14:z:1:G:H4'	2.00	0.44
7:A:1622:MET:O	7:A:1687:TYR:OH	2.35	0.44
8:U:221:LEU:HD22	8:U:520:HIS:NE2	2.32	0.44
8:U:504:VAL:HG21	8:U:545:SER:HB2	2.00	0.44
10:C:374:LEU:HD23	10:C:374:LEU:HA	1.83	0.44
13:5:47:A:O2'	13:5:48:A:H5''	2.18	0.44
7:A:164:MET:HE1	7:A:574:LEU:HA	2.00	0.43
7:A:536:LYS:HB2	7:A:536:LYS:HE2	1.77	0.43
7:A:999:LEU:HD23	7:A:999:LEU:HA	1.88	0.43
7:A:1404:THR:C	7:A:1406:GLU:H	2.25	0.43
7:A:1433:ASP:HB3	7:A:1460:HIS:CE1	2.52	0.43
8:U:351:GLY:HA3	8:U:447:PRO:HD3	1.99	0.43
10:C:781:ASP:O	10:C:941:LYS:NZ	2.51	0.43
4:L:140:LYS:NZ	4:L:192:ASP:OD1	2.38	0.43
5:F:95:ARG:HG3	5:F:95:ARG:HH11	1.83	0.43
6:N:19:PRO:CG	12:D:68:ASP:HB3	2.48	0.43
7:A:109:PRO:HG3	7:A:630:TRP:HE1	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1590:VAL:HG12	7:A:1591:MET:HE2	2.00	0.43
10:C:504:GLY:HA2	10:C:527:VAL:O	2.19	0.43
10:C:676:ALA:HB3	10:C:815:VAL:HB	1.98	0.43
4:L:275:TYR:HA	4:L:280:VAL:HG11	2.01	0.43
6:N:187:PHE:CD2	7:A:853:LYS:HE2	2.53	0.43
6:N:249:THR:HG22	6:N:281:ILE:HG12	2.01	0.43
7:A:265:THR:HG23	7:A:327:VAL:HG23	2.00	0.43
7:A:299:ILE:HA	7:A:302:ILE:HD12	2.00	0.43
8:U:116:LEU:HD21	8:U:137:LEU:HA	2.00	0.43
10:C:288:LEU:HD23	10:C:291:MET:HE2	2.01	0.43
5:F:112:LEU:HA	5:F:115:LEU:HG	2.01	0.43
6:N:122:GLN:O	6:N:126:GLU:HG2	2.19	0.43
8:U:233:ASN:ND2	8:U:313:ILE:HG23	2.34	0.43
8:U:457:PHE:HZ	8:U:505:HIS:CG	2.36	0.43
10:C:232:ALA:HB3	10:C:262:ARG:HE	1.82	0.43
10:C:781:ASP:HB2	10:C:943:LEU:HD21	2.00	0.43
13:5:7:U:O2	13:5:75:G:N1	2.51	0.43
3:J:468:LEU:C	3:J:469:MET:HE2	2.44	0.43
4:L:244:MET:HE1	4:L:252:LEU:HD21	2.01	0.43
7:A:171:ASP:OD1	7:A:521:ASN:ND2	2.36	0.43
7:A:374:ASP:HB3	10:C:358:LYS:HG3	2.00	0.43
7:A:776:LEU:HD13	7:A:900:ASP:HB2	2.00	0.43
7:A:785:LYS:O	7:A:789:GLU:HG2	2.18	0.43
8:U:154:ILE:CD1	10:C:775:ARG:HH12	2.32	0.43
10:C:205:THR:HB	10:C:215:VAL:HG22	2.01	0.43
10:C:516:LEU:HD23	10:C:516:LEU:HA	1.87	0.43
10:C:732:ILE:HG12	10:C:746:VAL:HG22	1.99	0.43
3:J:500:VAL:O	3:J:504:MET:HG3	2.17	0.43
4:L:321:LYS:O	4:L:325:GLU:HG2	2.18	0.43
6:N:298:LEU:HD12	6:N:318:LEU:HD13	2.00	0.43
7:A:85:LYS:O	7:A:89:LEU:HG	2.17	0.43
7:A:1107:ARG:O	7:A:1111:GLN:HG3	2.18	0.43
7:A:1785:VAL:O	7:A:1805:GLY:HA3	2.18	0.43
8:U:414:PRO:HA	8:U:472:ASN:HB3	1.99	0.43
10:C:529:ARG:HH21	10:C:531:TRP:HH2	1.67	0.43
12:D:106:MET:HE3	12:D:106:MET:HB2	1.93	0.43
3:J:465:ARG:HA	3:J:465:ARG:NE	2.32	0.43
6:N:393:LEU:HD12	6:N:413:LEU:HD13	1.99	0.43
7:A:313:LYS:NZ	7:A:321:ASN:HB3	2.33	0.43
7:A:1562:MET:HE3	7:A:1562:MET:HB3	1.83	0.43
7:A:1706:ASP:O	7:A:1710:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1771:LEU:HD11	7:A:1779:PHE:HZ	1.83	0.43
7:A:1840:LYS:O	7:A:1844:GLU:HG2	2.17	0.43
8:U:127:SER:HB3	8:U:151:HIS:CE1	2.53	0.43
8:U:171:LYS:HD3	8:U:180:GLU:OE2	2.19	0.43
8:U:473:PHE:HE2	8:U:499:LEU:HD22	1.83	0.43
9:S:298:GLU:O	9:S:301:GLU:HG3	2.18	0.43
11:M:54:ILE:HG22	11:M:56:MET:HE2	2.01	0.43
2:G:322:ASP:HA	2:G:325:GLU:HG2	2.00	0.43
6:N:247:ARG:HH12	6:N:318:LEU:N	2.17	0.43
7:A:1174:PHE:CE2	7:A:1176:SER:HB2	2.54	0.43
7:A:1583:GLN:OE1	7:A:1620:TYR:OH	2.26	0.43
7:A:1606:ILE:HG12	7:A:1637:TRP:HZ2	1.82	0.43
7:A:1988:LEU:HD21	7:A:2007:ILE:HG23	2.01	0.43
13:5:68:C:H1'	13:5:69:A:H2'	2.01	0.43
3:J:477:ARG:HG2	3:J:480:ASN:HB2	1.99	0.43
5:F:95:ARG:O	5:F:99:ILE:HG13	2.19	0.43
7:A:961:ASN:ND2	7:A:1219:GLU:HG2	2.34	0.43
7:A:1276:GLU:O	7:A:1279:VAL:HG22	2.18	0.43
8:U:229:ASN:HD21	8:U:232:ALA:HA	1.84	0.43
10:C:241:ARG:HH22	10:C:584:THR:HB	1.84	0.43
4:L:219:LEU:HD21	4:L:231:ILE:HD11	2.01	0.43
7:A:112:GLN:HE21	7:A:190:ALA:H	1.67	0.43
7:A:731:LEU:HD21	7:A:739:ILE:HD12	2.00	0.43
6:N:394:ARG:HB3	9:S:203:TRP:CE2	2.54	0.42
7:A:417:ARG:NH2	13:5:24:G:OP1	2.51	0.42
4:L:146:LEU:HD13	4:L:171:ALA:HB1	2.00	0.42
7:A:168:PRO:HB3	7:A:563:GLN:HG3	2.01	0.42
7:A:449:LYS:HD3	7:A:449:LYS:HA	1.89	0.42
8:U:233:ASN:HD21	8:U:300:LEU:HD13	1.85	0.42
6:N:149:LEU:HD12	7:A:696:MET:HB2	2.00	0.42
6:N:156:GLU:HG2	7:A:732:PRO:HG3	2.01	0.42
6:N:800:MET:HE1	6:N:813:LEU:HD22	2.01	0.42
7:A:227:ARG:HA	7:A:416:GLY:O	2.18	0.42
7:A:547:CYS:HA	7:A:550:VAL:HG12	2.02	0.42
7:A:1112:ARG:HG2	7:A:1155:TRP:HH2	1.84	0.42
7:A:1335:ILE:HD11	7:A:1365:ILE:HG22	2.00	0.42
7:A:1667:ARG:NH1	7:A:1706:ASP:OD2	2.53	0.42
10:C:123:MET:HE2	10:C:548:ASN:CG	2.44	0.42
10:C:743:ASN:ND2	10:C:784:ILE:O	2.44	0.42
7:A:1085:ILE:HG12	7:A:1099:PHE:CE2	2.55	0.42
7:A:1418:ARG:O	7:A:1421:THR:OG1	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:779:LEU:HG	10:C:820:PHE:HE2	1.85	0.42
5:F:115:LEU:HD12	5:F:117:GLU:H	1.83	0.42
7:A:257:LEU:HD22	7:A:314:ILE:HG22	2.00	0.42
7:A:425:PRO:HD3	13:5:26:A:H4'	2.00	0.42
7:A:1149:LEU:HD23	7:A:1177:VAL:HG21	2.01	0.42
7:A:1244:VAL:HG11	7:A:1291:CYS:HB3	2.01	0.42
7:A:1312:PRO:HG3	7:A:1541:THR:CG2	2.49	0.42
7:A:1353:PHE:CD2	9:S:153:ALA:HB2	2.54	0.42
7:A:1921:ASP:HB3	7:A:1966:HIS:CD2	2.54	0.42
10:C:434:CYS:O	10:C:438:ILE:HB	2.18	0.42
11:M:35:LEU:HD21	11:M:93:CYS:SG	2.60	0.42
15:7:473:ARG:HD2	15:7:473:ARG:HA	1.85	0.42
1:B:43:LEU:CD2	7:A:1285:LEU:HD12	2.50	0.42
7:A:1667:ARG:HD2	7:A:1679:TYR:CD2	2.55	0.42
7:A:1895:ALA:HB2	7:A:1944:HIS:HB2	2.02	0.42
8:U:146:ARG:HA	8:U:175:LEU:HD11	2.02	0.42
8:U:444:THR:HG23	8:U:488:VAL:HG11	2.01	0.42
10:C:270:PRO:HD2	10:C:273:ASP:HB2	2.01	0.42
10:C:534:VAL:O	10:C:534:VAL:HG13	2.19	0.42
10:C:836:VAL:O	10:C:870:THR:HA	2.20	0.42
10:C:888:ARG:HG2	10:C:895:ALA:O	2.20	0.42
4:L:95:ASP:O	4:L:99:LEU:HG	2.20	0.42
7:A:1342:TRP:CE2	7:A:1353:PHE:HB2	2.54	0.42
7:A:1354:ARG:HG3	9:S:150:PRO:HB2	2.00	0.42
7:A:1361:GLU:HG2	7:A:1362:ASP:O	2.19	0.42
8:U:492:HIS:HD2	8:U:554:ARG:HH22	1.68	0.42
10:C:862:PRO:HB3	10:C:869:TYR:CZ	2.55	0.42
2:G:297:GLN:HG3	10:C:841:ASP:CG	2.45	0.42
7:A:269:LEU:HD13	7:A:321:ASN:ND2	2.33	0.42
7:A:1631:LEU:HB3	7:A:1637:TRP:CH2	2.54	0.42
7:A:1904:ASP:OD1	7:A:1904:ASP:N	2.52	0.42
4:L:169:VAL:HG13	7:A:810:TYR:CG	2.55	0.42
7:A:121:HIS:HB2	7:A:126:ILE:HG22	2.02	0.42
7:A:913:PRO:HA	7:A:916:LYS:HD3	2.02	0.42
7:A:1861:ILE:HD12	7:A:1876:LEU:HD11	2.02	0.42
8:U:350:GLN:HB2	8:U:389:MET:HE2	2.02	0.42
11:M:33:LYS:HD3	11:M:33:LYS:HA	1.82	0.42
2:G:311:GLN:O	2:G:315:GLU:HG2	2.20	0.42
2:G:324:MET:HE1	7:A:355:LEU:HA	2.02	0.42
4:L:409:GLN:CD	6:N:191:LEU:HD21	2.45	0.42
6:N:289:ASN:C	6:N:289:ASN:HD22	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:813:LEU:HD23	6:N:813:LEU:HA	1.94	0.42
6:N:843:VAL:O	6:N:847:VAL:HG23	2.19	0.42
7:A:86:ARG:NH2	7:A:89:LEU:HD11	2.34	0.42
7:A:1333:VAL:O	7:A:1364:LEU:HD12	2.20	0.42
8:U:227:LEU:HD12	8:U:241:GLN:HG2	2.02	0.42
10:C:347:ILE:HD11	10:C:356:PHE:HB3	2.01	0.42
10:C:898:LEU:HD23	10:C:898:LEU:HA	1.92	0.42
13:5:61:A:H2'	13:5:62:G:C8	2.54	0.42
15:7:447:ARG:HA	15:7:447:ARG:HD3	1.83	0.42
7:A:335:PRO:HG3	10:C:139:HIS:HB3	2.02	0.41
7:A:338:VAL:O	7:A:338:VAL:HG13	2.19	0.41
8:U:501:ALA:HB3	8:U:551:ILE:HB	2.02	0.41
11:M:91:ARG:HA	11:M:91:ARG:HD2	1.72	0.41
13:5:70:A:H4'	13:5:71:C:OP1	2.20	0.41
4:L:186:ARG:O	4:L:189:GLU:HG2	2.20	0.41
6:N:112:MET:O	6:N:115:ARG:HG3	2.21	0.41
7:A:507:LEU:O	7:A:510:ARG:HB2	2.19	0.41
8:U:456:ARG:HG3	8:U:548:TYR:HD1	1.85	0.41
5:F:121:LEU:H	5:F:124:GLU:HG2	1.85	0.41
6:N:200:VAL:HG22	7:A:1403:LEU:HB2	2.01	0.41
7:A:1109:LEU:HG	7:A:1152:ALA:HB1	2.01	0.41
7:A:1730:MET:HE3	7:A:1730:MET:HA	2.02	0.41
8:U:252:TYR:CG	8:U:344:ILE:HG12	2.55	0.41
9:S:260:GLU:HB2	9:S:290:VAL:HG12	2.02	0.41
10:C:637:LEU:HD23	10:C:637:LEU:HA	1.89	0.41
10:C:735:PHE:CE1	10:C:744:ILE:HD13	2.55	0.41
12:D:29:ARG:NH2	12:D:42:ASP:OD2	2.54	0.41
6:N:298:LEU:O	6:N:302:ARG:HG3	2.20	0.41
7:A:784:LEU:O	7:A:788:GLN:HG3	2.20	0.41
7:A:1936:LEU:O	7:A:1940:LEU:HD23	2.20	0.41
7:A:1987:ILE:HG21	7:A:2011:ILE:HD13	2.02	0.41
8:U:101:ARG:H	8:U:101:ARG:HD3	1.85	0.41
8:U:188:ASP:OD1	8:U:189:ILE:N	2.52	0.41
10:C:887:LEU:O	10:C:891:THR:OG1	2.32	0.41
3:J:451:GLN:NE2	15:7:433:LEU:O	2.40	0.41
6:N:178:LYS:N	16:4:19:U:O4	2.52	0.41
6:N:186:PHE:CE2	7:A:850:TYR:HB2	2.56	0.41
6:N:247:ARG:NH2	6:N:288:ILE:HD11	2.35	0.41
7:A:120:TYR:CZ	7:A:483:GLN:HB2	2.55	0.41
7:A:171:ASP:HB3	7:A:519:ASP:OD2	2.20	0.41
7:A:313:LYS:HZ1	7:A:321:ASN:HB3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:959:ILE:HD11	7:A:976:MET:HE1	2.02	0.41
7:A:1640:SER:HB3	7:A:1652:MET:SD	2.60	0.41
8:U:505:HIS:NE2	8:U:512:GLY:HA3	2.36	0.41
10:C:531:TRP:HZ3	10:C:553:GLU:HB2	1.86	0.41
6:N:17:TYR:OH	12:D:15:ASP:OD2	2.29	0.41
7:A:1555:LEU:HB2	7:A:1558:THR:OG1	2.21	0.41
10:C:478:THR:HA	10:C:494:GLY:HA3	2.01	0.41
13:5:74:U:H2'	13:5:75:G:C8	2.56	0.41
2:G:276:TRP:CE2	7:A:449:LYS:HG3	2.56	0.41
4:L:234:VAL:HG11	4:L:273:TYR:HE2	1.86	0.41
4:L:269:PRO:O	4:L:289:ARG:NH2	2.54	0.41
4:L:271:THR:CG2	4:L:275:TYR:CD2	3.03	0.41
4:L:357:ARG:NH1	16:4:17:A:H62	2.19	0.41
4:L:366:LEU:HD13	7:A:1515:TRP:CD1	2.56	0.41
7:A:1288:LEU:HD13	7:A:1330:MET:HG2	2.02	0.41
7:A:1386:TRP:HZ2	7:A:1417:PRO:O	2.04	0.41
7:A:1539:SER:OG	7:A:1540:PRO:HD3	2.19	0.41
7:A:1652:MET:HG2	7:A:1720:PRO:HG3	2.03	0.41
10:C:510:LEU:HD12	10:C:564:THR:HB	2.03	0.41
1:B:40:VAL:HA	7:A:1333:VAL:HG22	2.03	0.41
2:G:320:TYR:O	2:G:324:MET:HG2	2.21	0.41
4:L:144:ASN:HD21	4:L:179:LEU:HB2	1.85	0.41
6:N:319:GLU:HB3	6:N:327:VAL:HG23	2.02	0.41
7:A:472:LEU:C	7:A:474:ARG:H	2.28	0.41
7:A:1310:ARG:NH2	7:A:1338:SER:OG	2.54	0.41
7:A:1536:LEU:HD22	7:A:1572:SER:HB3	2.03	0.41
7:A:1809:ILE:HD12	7:A:1845:VAL:HG22	2.02	0.41
8:U:245:ASN:ND2	8:U:518:VAL:HB	2.36	0.41
8:U:274:VAL:HG23	8:U:330:LEU:HD22	2.02	0.41
10:C:221:ILE:HB	10:C:495:ARG:HB2	2.03	0.41
11:M:73:CYS:HB3	11:M:78:VAL:O	2.21	0.41
3:J:493:PRO:HB2	7:A:1931:THR:HG23	2.02	0.41
4:L:366:LEU:HD22	7:A:1515:TRP:CD1	2.56	0.41
7:A:106:MET:HE1	7:A:582:PHE:CE2	2.56	0.41
7:A:485:THR:OG1	7:A:486:LYS:N	2.54	0.41
7:A:881:ILE:HG23	7:A:918:THR:HG23	2.03	0.41
7:A:1275:ARG:HG2	7:A:1372:ILE:HG21	2.02	0.41
7:A:1376:GLU:O	7:A:1380:ILE:HG12	2.20	0.41
7:A:1441:ASP:O	7:A:1444:GLN:HG2	2.20	0.41
7:A:1515:TRP:CD1	7:A:1515:TRP:O	2.73	0.41
7:A:1808:PHE:CD2	7:A:1817:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1832:ARG:HD3	7:A:1835:GLN:NE2	2.35	0.41
7:A:1841:THR:HG22	7:A:1868:MET:HE1	2.02	0.41
7:A:1898:LYS:HD2	7:A:1947:ASN:ND2	2.36	0.41
8:U:247:PRO:HD2	8:U:449:TYR:CE2	2.55	0.41
8:U:368:GLU:O	8:U:371:GLU:HG3	2.21	0.41
10:C:303:LEU:HD23	10:C:344:TRP:HB3	2.03	0.41
10:C:514:TYR:HE1	10:C:519:GLU:HA	1.86	0.41
10:C:682:LYS:HB3	10:C:797:ALA:HB2	2.03	0.41
12:D:25:VAL:HG12	12:D:55:PHE:O	2.21	0.41
15:7:434:LEU:HD21	15:7:438:TRP:CZ3	2.56	0.41
7:A:1633:ALA:HB2	7:A:1637:TRP:CE3	2.56	0.41
8:U:344:ILE:HD12	8:U:344:ILE:HA	1.92	0.41
10:C:375:GLU:HB3	10:C:376:PRO:HD3	2.03	0.41
10:C:777:GLY:HA2	10:C:784:ILE:HD11	2.03	0.41
13:5:69:A:C2	13:5:70:A:C8	3.09	0.41
4:L:207:TYR:O	4:L:210:SER:OG	2.31	0.40
6:N:148:LYS:HA	6:N:148:LYS:HD2	1.80	0.40
6:N:375:ILE:O	6:N:378:ARG:HB3	2.21	0.40
7:A:95:MET:HA	7:A:126:ILE:HD11	2.03	0.40
7:A:134:TRP:HB3	7:A:418:THR:HG21	2.03	0.40
7:A:1290:LYS:O	7:A:1294:LYS:HG2	2.21	0.40
7:A:1792:LYS:HA	7:A:1798:LEU:HA	2.02	0.40
7:A:1955:LYS:HD2	7:A:1955:LYS:O	2.21	0.40
8:U:205:LEU:HD23	8:U:205:LEU:HA	1.86	0.40
6:N:250:LEU:HD12	7:A:1847:ALA:HB2	2.04	0.40
6:N:844:LEU:HB3	6:N:867:THR:OG1	2.21	0.40
7:A:610:HIS:HE1	18:A:2401:IHP:O23	2.03	0.40
7:A:1215:ASN:C	7:A:1224:ARG:HH12	2.29	0.40
8:U:264:ARG:HD3	8:U:271:PHE:CD2	2.56	0.40
8:U:308:LYS:HD3	8:U:308:LYS:HA	1.92	0.40
3:J:504:MET:HE2	3:J:504:MET:HB3	1.86	0.40
7:A:516:LEU:HA	7:A:516:LEU:HD23	1.88	0.40
7:A:549:GLU:HB3	7:A:591:MET:HB3	2.03	0.40
7:A:1314:VAL:HG23	7:A:1478:LEU:HD22	2.02	0.40
7:A:1606:ILE:HG12	7:A:1637:TRP:CZ2	2.56	0.40
7:A:1807:ILE:CG2	7:A:1841:THR:HG23	2.52	0.40
7:A:1919:LEU:HA	7:A:1919:LEU:HD23	1.88	0.40
8:U:516:ILE:HG23	8:U:529:LEU:HD23	2.03	0.40
10:C:140:HIS:CE1	10:C:230:ASP:H	2.39	0.40
11:M:114:GLN:H	11:M:114:GLN:HG2	1.68	0.40
15:7:415:ILE:HD11	15:7:428:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:6:U:H2'	16:4:7:G:C8	2.56	0.40
7:A:251:ASP:OD1	7:A:251:ASP:N	2.52	0.40
7:A:761:ILE:HG12	7:A:767:VAL:HG21	2.02	0.40
7:A:1307:MET:HA	7:A:1308:PRO:HD3	1.97	0.40
7:A:1308:PRO:HG3	7:A:1548:TYR:CZ	2.56	0.40
8:U:153:TYR:O	8:U:157:VAL:HG22	2.21	0.40
10:C:687:MET:SD	10:C:789:PHE:HB3	2.61	0.40
10:C:754:VAL:HG11	10:C:794:ALA:HB3	2.03	0.40
10:C:821:LEU:HD23	10:C:821:LEU:HA	1.97	0.40
13:5:47:A:O2'	13:5:48:A:H8	2.03	0.40
4:L:366:LEU:HD13	7:A:1515:TRP:HD1	1.85	0.40
4:L:383:ILE:HD13	7:A:1321:GLU:HB2	2.04	0.40
5:F:88:ALA:HA	5:F:91:GLU:OE2	2.22	0.40
6:N:108:LEU:HD21	7:A:476:PHE:CE1	2.49	0.40
6:N:281:ILE:HG21	7:A:1878:ASP:CG	2.46	0.40
7:A:139:VAL:HG11	7:A:212:PRO:HG2	2.04	0.40
7:A:639:PHE:O	7:A:642:ARG:HG2	2.22	0.40
7:A:1607:GLU:HB2	7:A:1634:SER:HA	2.03	0.40
8:U:208:GLN:HE22	8:U:221:LEU:HD23	1.87	0.40
8:U:225:VAL:HG11	8:U:294:VAL:HG23	2.04	0.40
8:U:346:THR:HA	8:U:350:GLN:HB3	2.04	0.40
9:S:165:GLU:O	9:S:169:GLU:HG2	2.21	0.40
11:M:28:GLN:OE1	11:M:115:GLN:NE2	2.51	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	20/160 (12%)	19 (95%)	1 (5%)	0	100	100
2	G	118/820 (14%)	116 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	82/683 (12%)	82 (100%)	0	0	100	100
4	L	372/499 (74%)	362 (97%)	10 (3%)	0	100	100
5	F	59/522 (11%)	59 (100%)	0	0	100	100
6	N	447/941 (48%)	441 (99%)	6 (1%)	0	100	100
7	A	1971/2335 (84%)	1883 (96%)	88 (4%)	0	100	100
8	U	454/565 (80%)	437 (96%)	17 (4%)	0	100	100
9	S	138/800 (17%)	135 (98%)	3 (2%)	0	100	100
10	C	834/972 (86%)	818 (98%)	16 (2%)	0	100	100
11	M	122/128 (95%)	119 (98%)	3 (2%)	0	100	100
12	D	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
15	7	103/793 (13%)	101 (98%)	2 (2%)	0	100	100
All	All	4859/9360 (52%)	4708 (97%)	151 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	17/140 (12%)	17 (100%)	0	100	100
2	G	113/721 (16%)	113 (100%)	0	100	100
3	J	72/599 (12%)	72 (100%)	0	100	100
4	L	303/424 (72%)	302 (100%)	1 (0%)	86	87
5	F	52/442 (12%)	52 (100%)	0	100	100
6	N	341/792 (43%)	341 (100%)	0	100	100
7	A	1788/2108 (85%)	1788 (100%)	0	100	100
8	U	418/511 (82%)	418 (100%)	0	100	100
9	S	120/681 (18%)	120 (100%)	0	100	100
10	C	738/866 (85%)	738 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	M	108/111 (97%)	108 (100%)	0	100	100
12	D	129/130 (99%)	129 (100%)	0	100	100
15	7	91/709 (13%)	91 (100%)	0	100	100
All	All	4290/8234 (52%)	4289 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	267	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	295	GLN
2	G	350	GLN
3	J	480	ASN
4	L	152	ASN
4	L	248	ASN
4	L	374	GLN
4	L	431	GLN
6	N	289	ASN
7	A	73	HIS
7	A	210	HIS
7	A	517	HIS
7	A	542	ASN
7	A	775	ASN
7	A	961	ASN
7	A	1024	HIS
7	A	1117	HIS
7	A	1129	ASN
7	A	1217	GLN
7	A	1238	GLN
7	A	1246	GLN
7	A	1352	HIS
7	A	1424	GLN
7	A	1520	ASN
7	A	1522	GLN
7	A	1575	GLN
7	A	1599	GLN
7	A	1752	GLN

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Mol	Chain	Res	Type
7	A	1784	ASN
7	A	1791	HIS
7	A	1835	GLN
7	A	1966	HIS
7	A	1996	ASN
8	U	275	GLN
8	U	297	HIS
8	U	502	ASN
9	S	293	ASN
10	C	383	GLN
10	C	491	HIS
10	C	575	GLN
10	C	924	GLN
15	7	517	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	5	78/117 (66%)	26 (33%)	3 (3%)
14	z	10/11 (90%)	6 (60%)	0
16	4	79/144 (54%)	23 (29%)	0
17	6	47/106 (44%)	8 (17%)	2 (4%)
All	All	214/378 (56%)	63 (29%)	5 (2%)

All (63) 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	34	U
13	5	36	C
13	5	39	C
13	5	41	U

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Mol	Chain	Res	Type
13	5	42	U
13	5	43	U
13	5	44	A
13	5	45	C
13	5	57	G
13	5	68	C
13	5	69	A
13	5	70	A
13	5	71	C
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	4	A
14	z	6	U
14	z	8	U
16	4	9	G
16	4	11	A
16	4	18	G
16	4	25	A
16	4	26	G
16	4	31	U
16	4	36	U
16	4	39	A
16	4	40	U
16	4	41	C
16	4	44	A
16	4	45	G
16	4	53	U
16	4	55	U
16	4	58	C
16	4	66	A
16	4	68	A
16	4	69	C
16	4	70	U
16	4	71	U
16	4	72	U
16	4	73	U
16	4	74	C
17	6	35	A

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Mol	Chain	Res	Type
17	6	37	C
17	6	40	U
17	6	46	G
17	6	50	A
17	6	52	U
17	6	77	C
17	6	78	A

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
13	5	70	A
13	5	77	G
13	5	78	U
17	6	51	U
17	6	77	C

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	$\# Z > 2$
18	IHP	A	2401	-	36,36,36	0.98	1 (2%)	60,60,60	1.34	5 (8%)

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	-	-	5/30/54/54	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	2401	IHP	P2-O12	2.31	1.63	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	2401	IHP	C5-C6-C1	4.09	119.41	110.43
18	A	2401	IHP	C6-C1-C2	3.88	118.93	110.43
18	A	2401	IHP	C6-C5-C4	3.30	117.66	110.43
18	A	2401	IHP	C4-C3-C2	2.24	115.35	110.43
18	A	2401	IHP	O12-C2-C3	2.00	113.02	108.76

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	2401	IHP	C1-O11-P1-O31
18	A	2401	IHP	C1-O11-P1-O21
18	A	2401	IHP	C2-O12-P2-O22
18	A	2401	IHP	C3-O13-P3-O33
18	A	2401	IHP	C6-O16-P6-O26

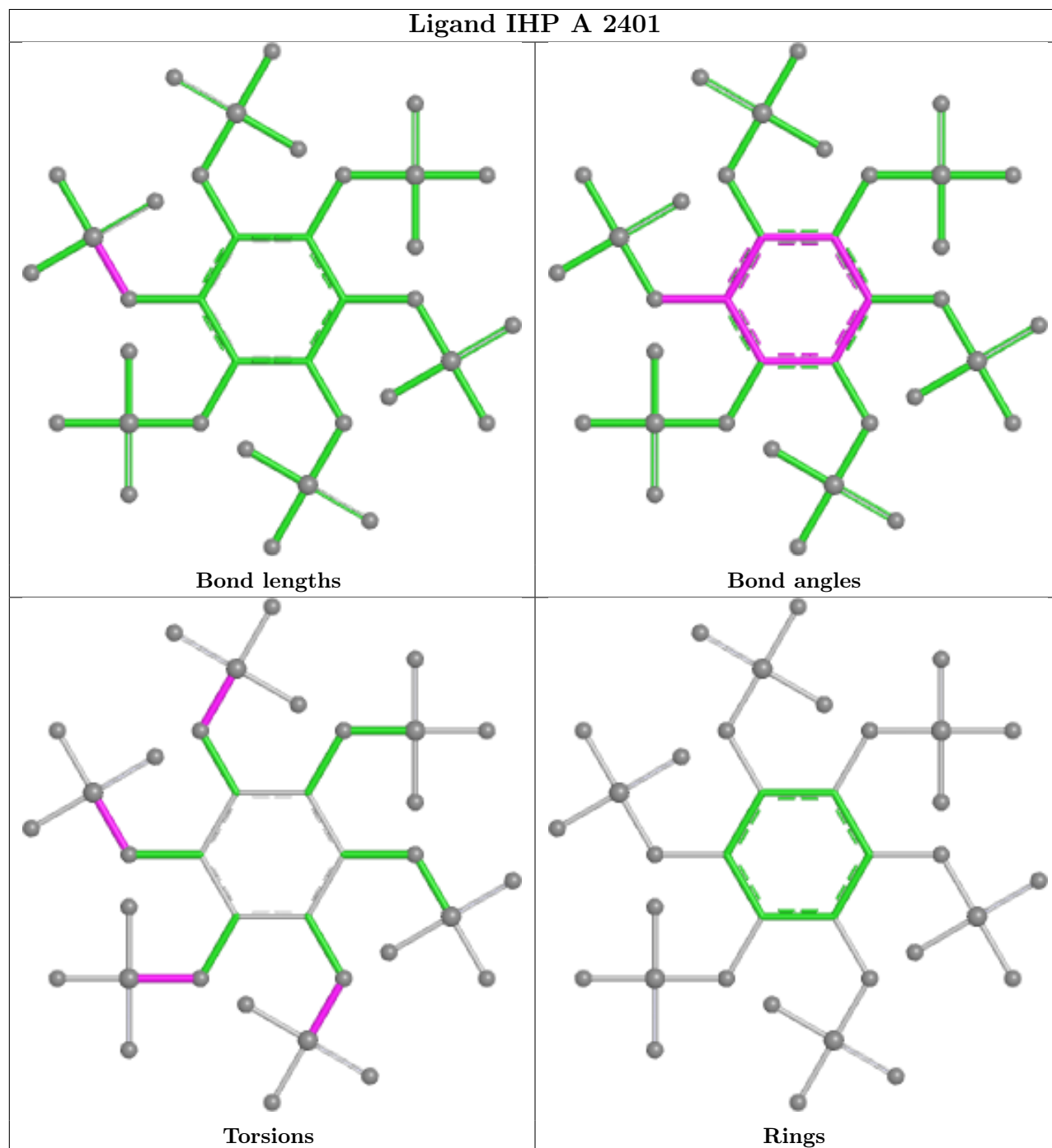
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	2401	IHP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

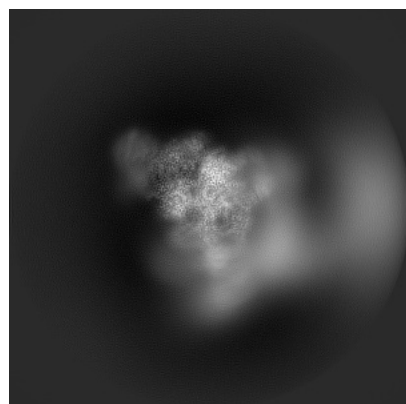
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18542. These allow visual inspection of the internal detail of the map and identification of artifacts.

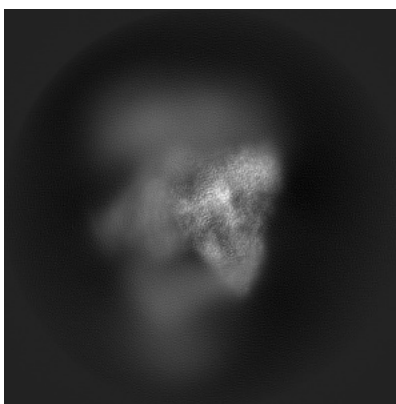
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

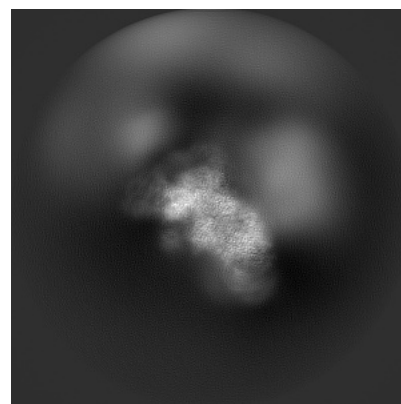
6.1.1 Primary map



X

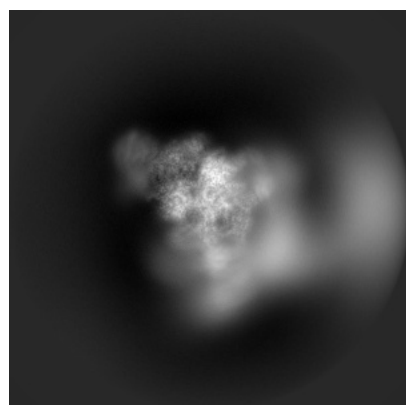


Y

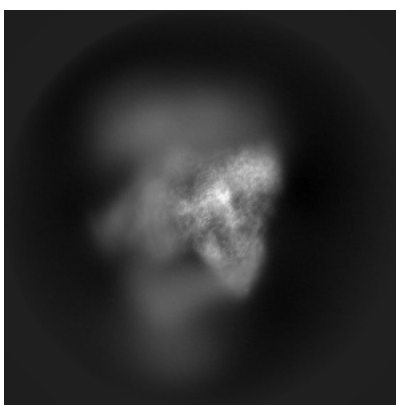


Z

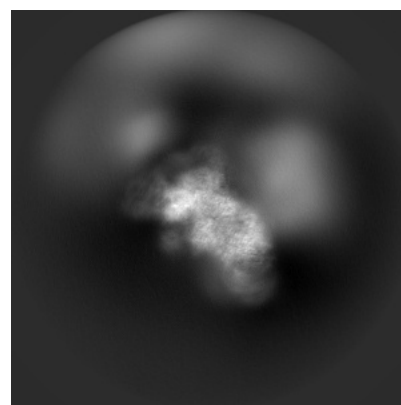
6.1.2 Raw map



X



Y

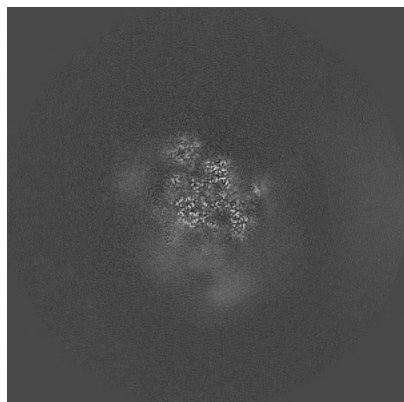


Z

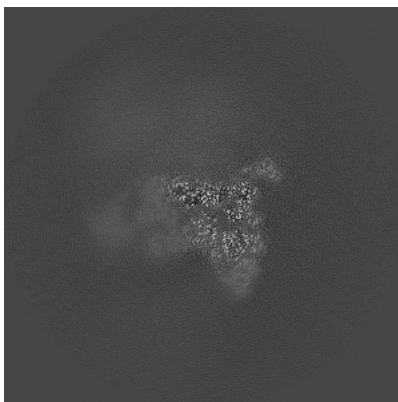
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

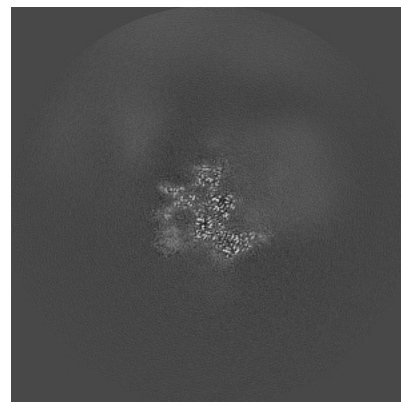
6.2.1 Primary map



X Index: 240

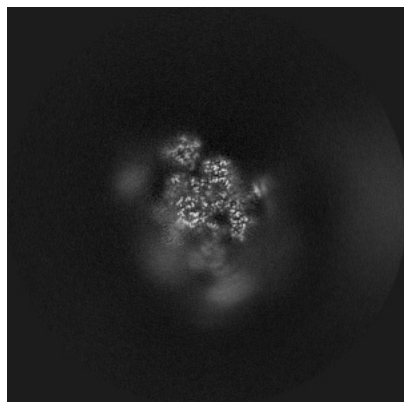


Y Index: 240

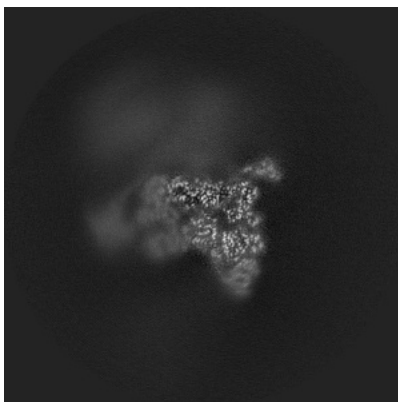


Z Index: 240

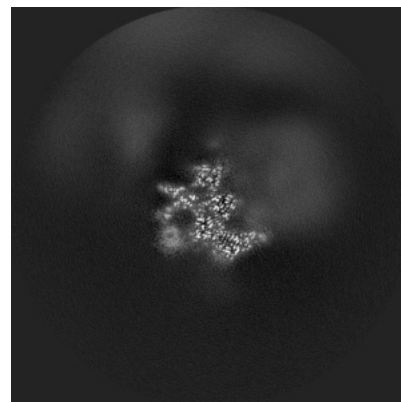
6.2.2 Raw map



X Index: 240



Y Index: 240

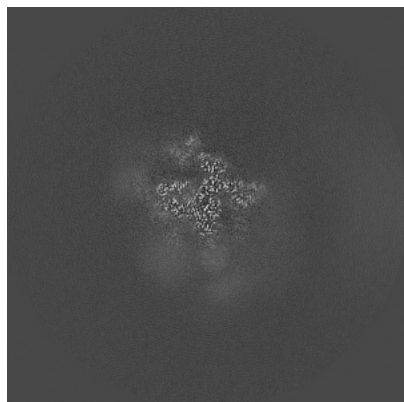


Z Index: 240

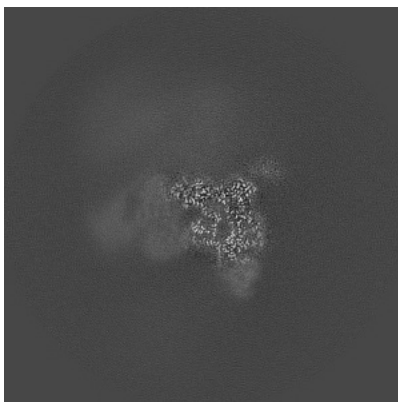
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

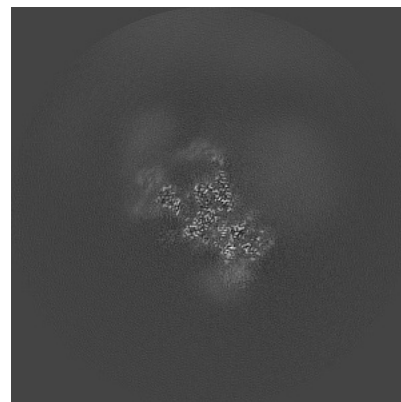
6.3.1 Primary map



X Index: 252

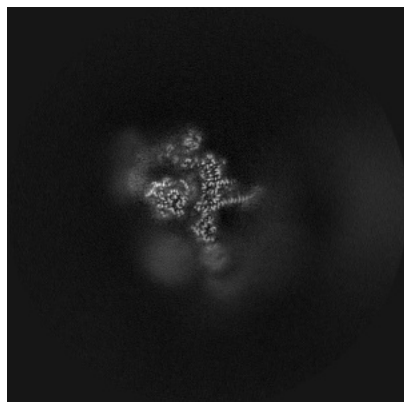


Y Index: 245

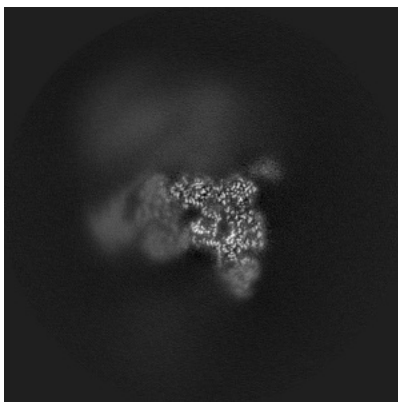


Z Index: 267

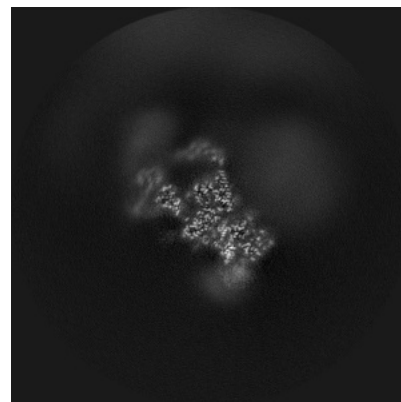
6.3.2 Raw map



X Index: 260



Y Index: 245

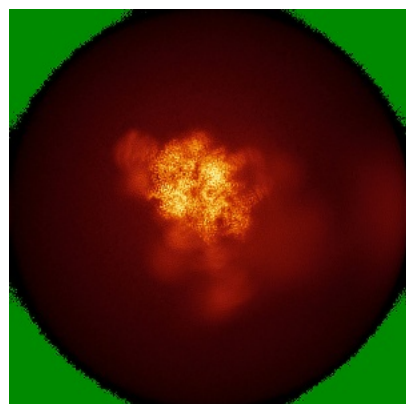


Z Index: 267

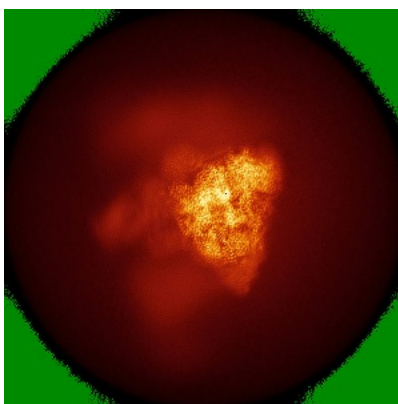
The images above show the largest variance slices of the map in three orthogonal directions.

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

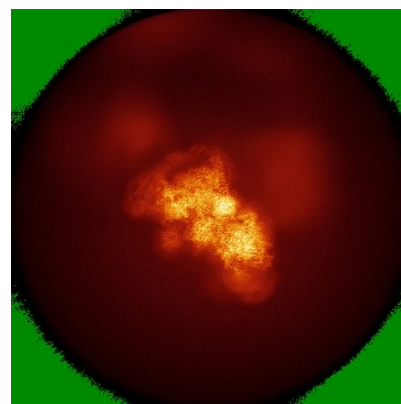
6.4.1 Primary map



X

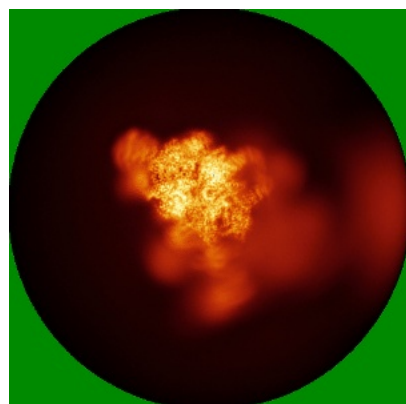


Y

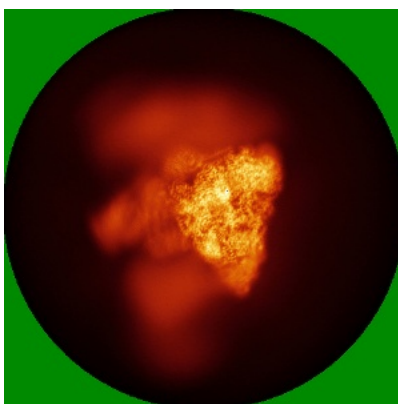


Z

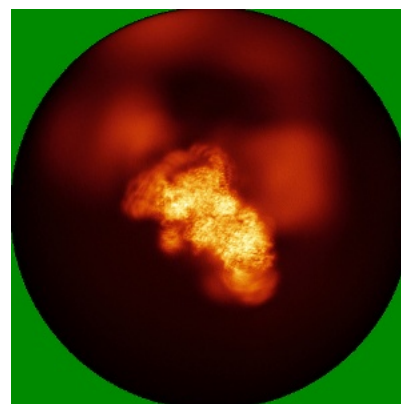
6.4.2 Raw map



X



Y

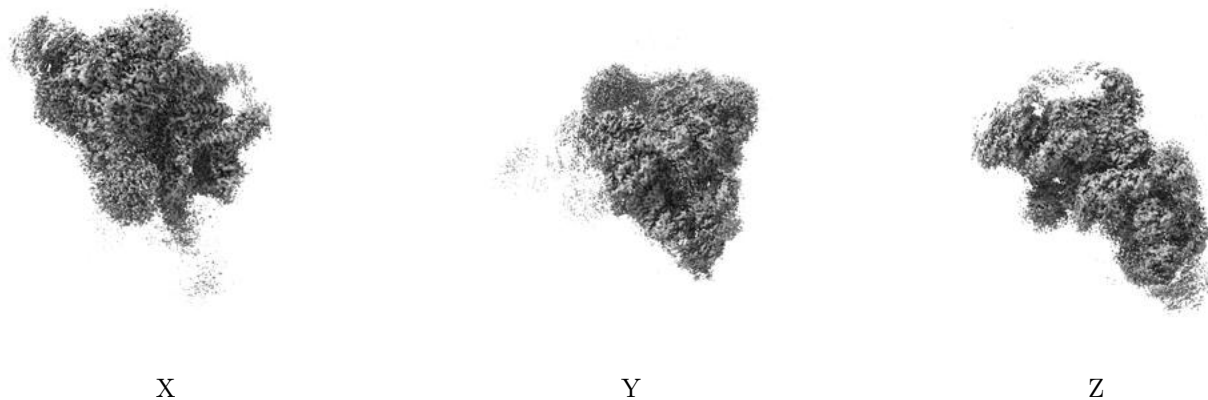


Z

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 0.032. 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.

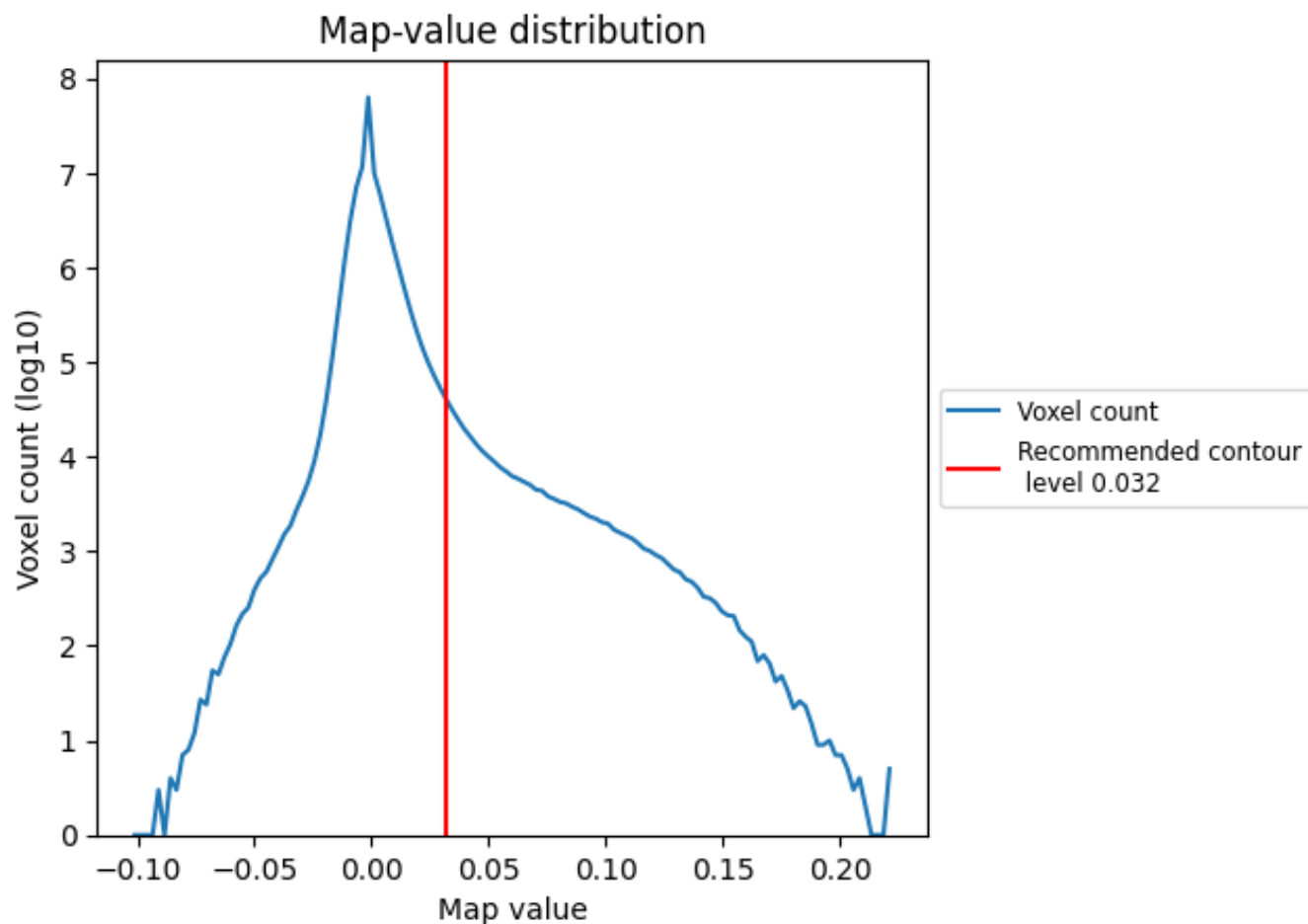
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

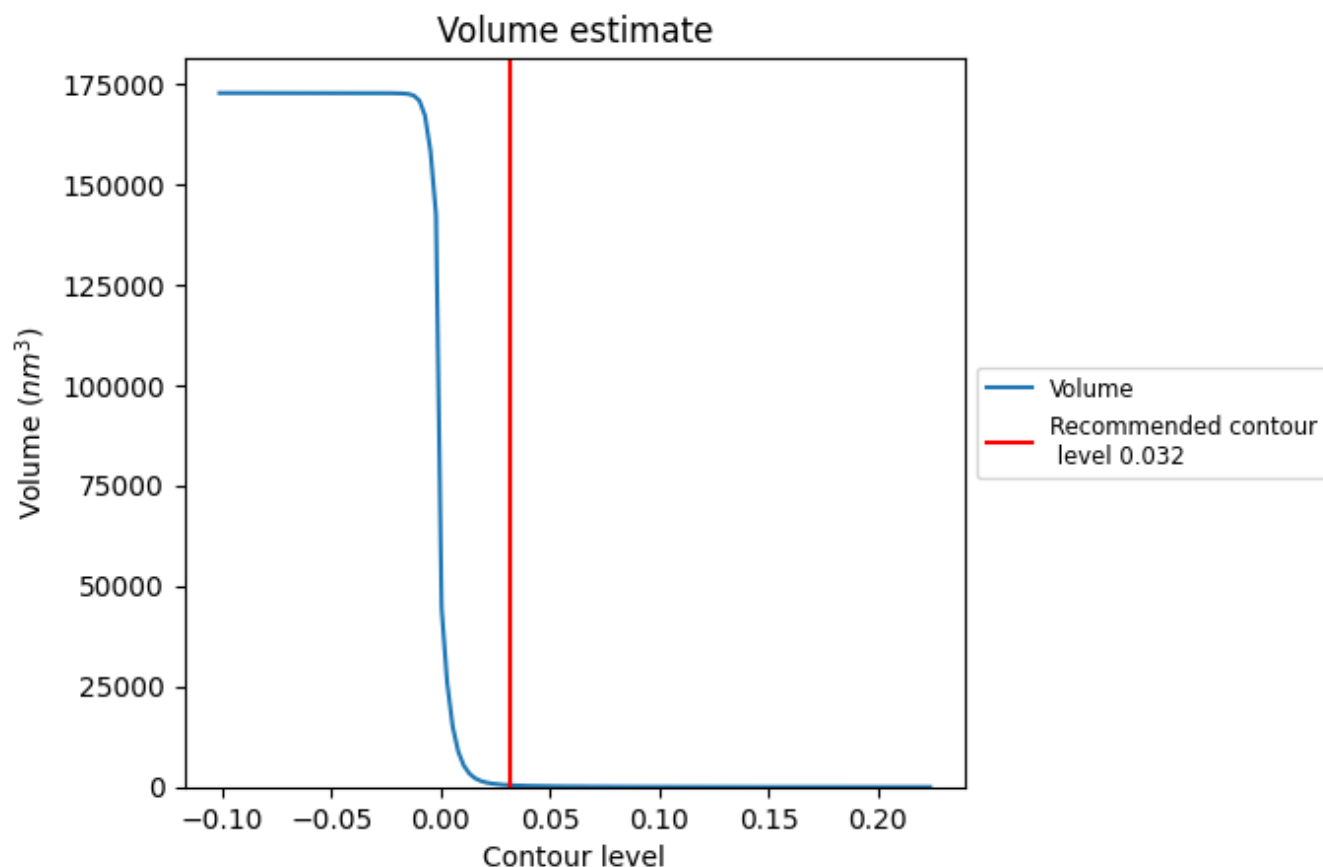
This section contains the results of statistical analysis of the map.

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.

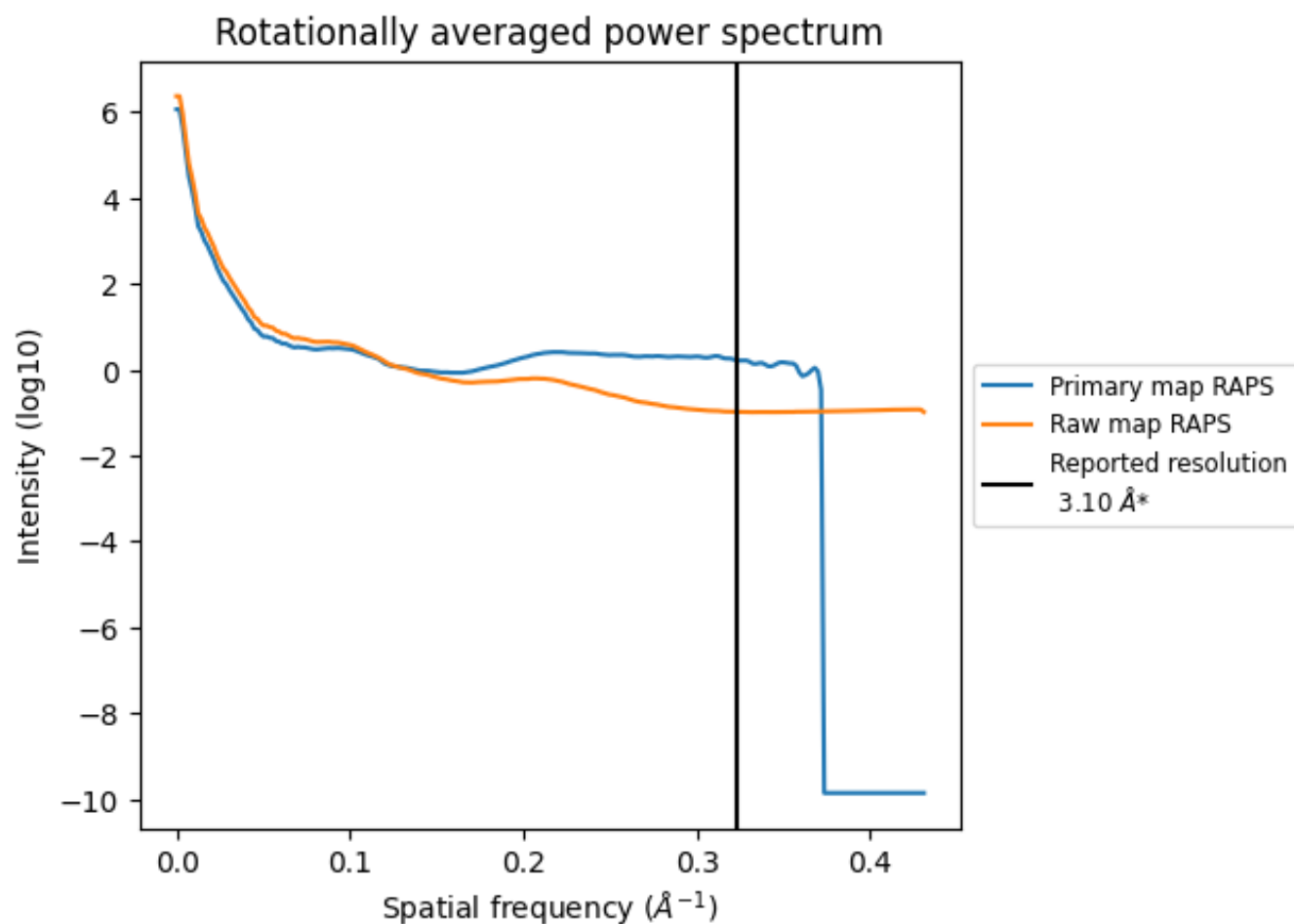
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 424 nm^3 ; this corresponds to an approximate mass of 383 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 ⓘ

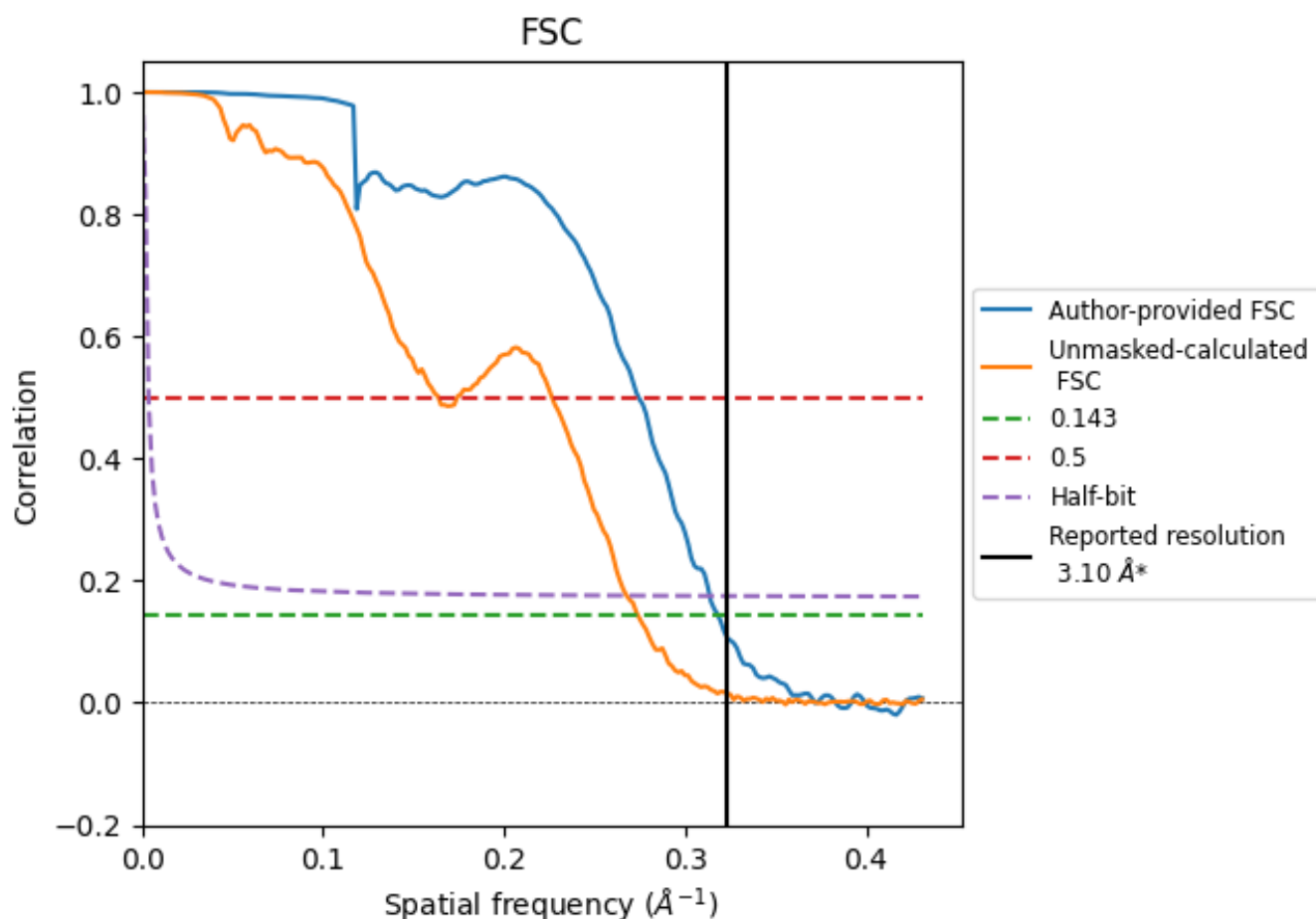


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

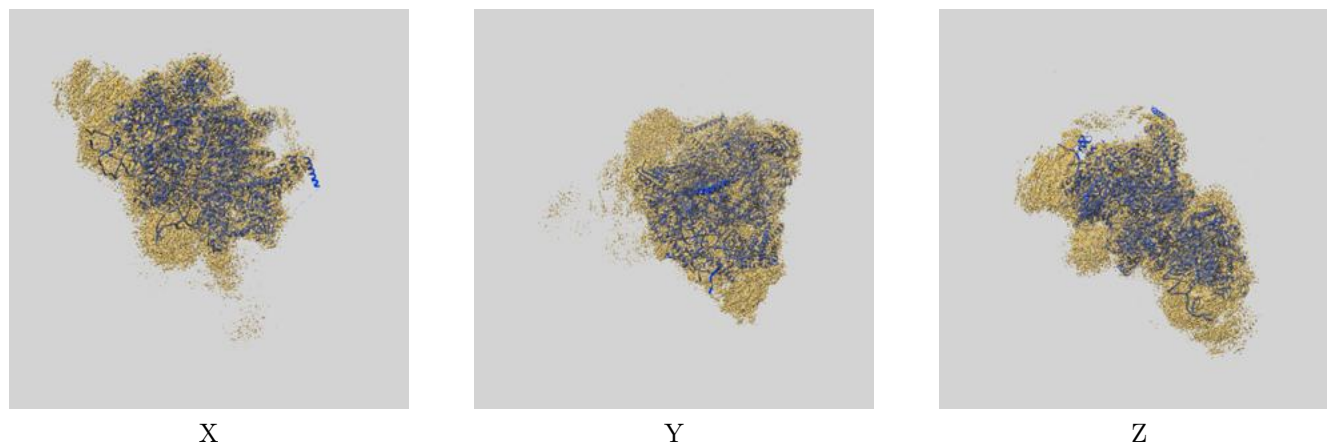
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.14	3.65	3.19
Unmasked-calculated*	3.65	6.11	3.74

*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 3.65 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

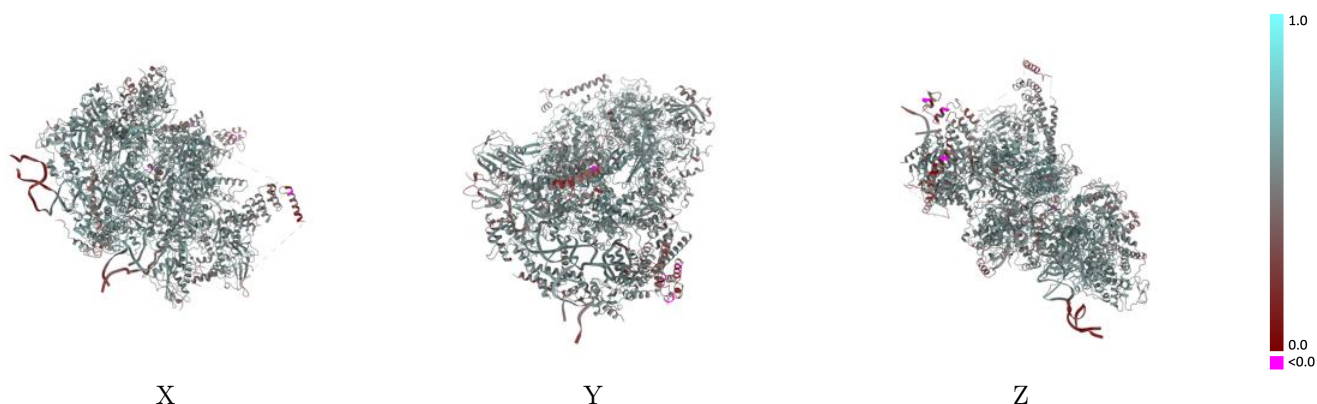
This section contains information regarding the fit between EMDB map EMD-18542 and PDB model 8QOZ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



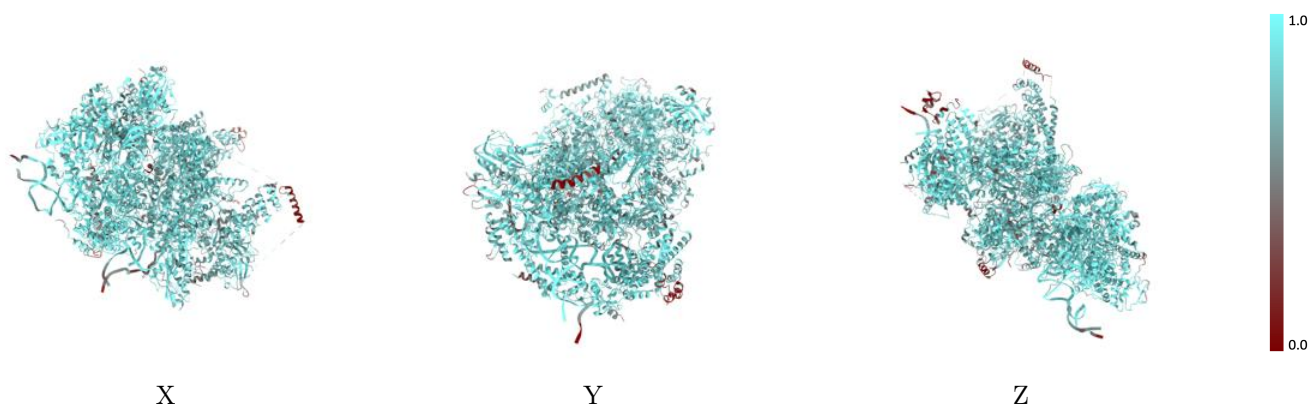
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



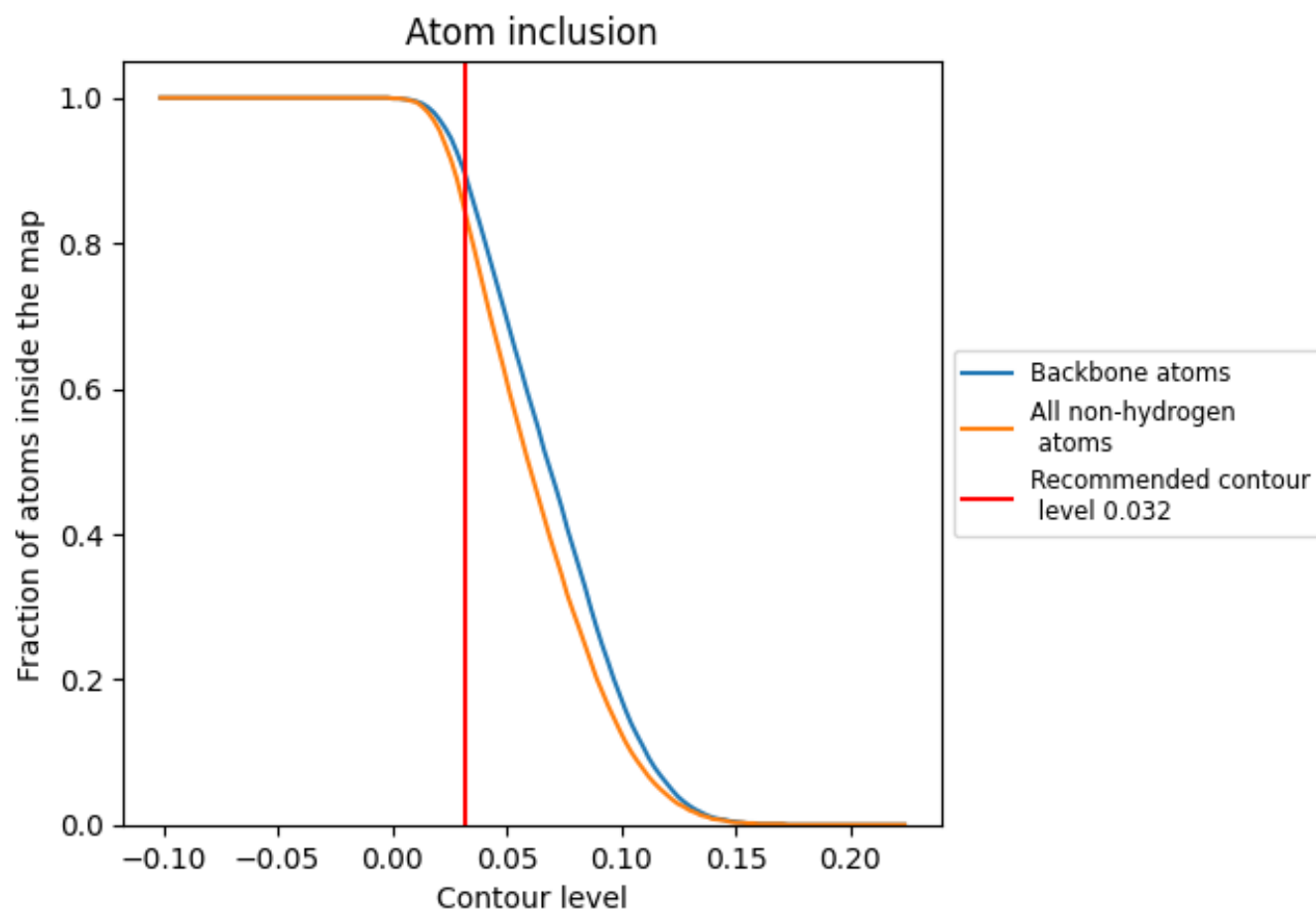
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.5190
4	 0.8380	 0.4980
5	 0.8820	 0.4560
6	 0.8650	 0.5070
7	 0.7720	 0.4840
A	 0.8740	 0.5460
B	 0.7950	 0.4910
C	 0.8970	 0.5390
D	 0.9250	 0.5880
F	 0.7390	 0.4420
G	 0.7680	 0.4890
J	 0.8840	 0.5320
L	 0.8480	 0.5050
M	 0.8720	 0.5180
N	 0.7870	 0.4830
S	 0.5910	 0.4350
U	 0.7170	 0.4800
z	 0.9460	 0.5540

